



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2026 – 05:30 PM JST

PDB ID : 9XAW / pdb_00009xaw
Title : Structure of the SARS-CoV-2 Spike N-terminal domain(NTD) in complex with the BLN8 Fab
Authors : Zhou, J.J.; Gao, G.F.
Deposited on : 2025-10-23
Resolution : 3.13 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
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) : 2.50

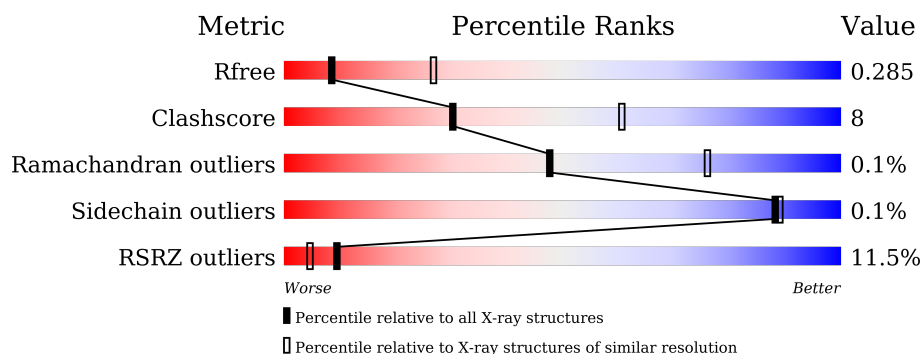
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	A	229	7% 78% 20% .
1	C	229	7% 77% 20% .
1	E	229	7% 81% 16% .
1	G	229	10% 72% 24% .
2	I	298	13% 74% 18% 7%
2	J	298	19% 73% 20% 7%

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Mol	Chain	Length	Quality of chain
2	K	298	
2	L	298	
3	B	212	
3	D	212	
3	F	212	
3	H	212	
4	M	2	
4	O	2	
4	P	2	
5	N	5	
6	Q	5	
7	R	4	
7	T	4	
8	S	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22383 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 BLN8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	C	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	E	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	G	221	Total	C	N	O	S	0	0	0
			1658	1044	283	324	7			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	277	Total	C	N	O	S	0	0	0
			2226	1443	362	413	8			
2	I	276	Total	C	N	O	S	0	0	0
			2212	1434	358	412	8			
2	J	277	Total	C	N	O	S	0	0	0
			2228	1445	361	414	8			
2	L	279	Total	C	N	O	S	0	0	0
			2250	1461	366	415	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	306	HIS	-	expression tag	UNP P0DTC2
K	307	HIS	-	expression tag	UNP P0DTC2
K	308	HIS	-	expression tag	UNP P0DTC2
K	309	HIS	-	expression tag	UNP P0DTC2
K	310	HIS	-	expression tag	UNP P0DTC2
K	311	HIS	-	expression tag	UNP P0DTC2
I	306	HIS	-	expression tag	UNP P0DTC2
I	307	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	308	HIS	-	expression tag	UNP P0DTC2
I	309	HIS	-	expression tag	UNP P0DTC2
I	310	HIS	-	expression tag	UNP P0DTC2
I	311	HIS	-	expression tag	UNP P0DTC2
J	306	HIS	-	expression tag	UNP P0DTC2
J	307	HIS	-	expression tag	UNP P0DTC2
J	308	HIS	-	expression tag	UNP P0DTC2
J	309	HIS	-	expression tag	UNP P0DTC2
J	310	HIS	-	expression tag	UNP P0DTC2
J	311	HIS	-	expression tag	UNP P0DTC2
L	306	HIS	-	expression tag	UNP P0DTC2
L	307	HIS	-	expression tag	UNP P0DTC2
L	308	HIS	-	expression tag	UNP P0DTC2
L	309	HIS	-	expression tag	UNP P0DTC2
L	310	HIS	-	expression tag	UNP P0DTC2
L	311	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called BLN8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	212	Total	C	N	O	S	0	0	0
			1584	988	260	329	7			
3	D	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			
3	F	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			
3	H	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			

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



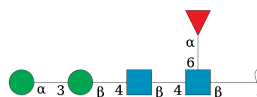
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	O	2	Total	C	N	O	0	0	0
			24	14	1	9			

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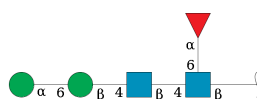
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



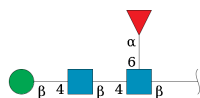
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Q	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



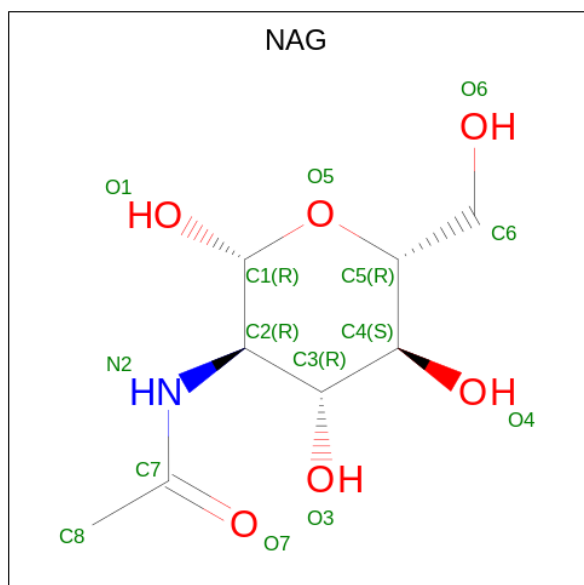
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	R	4	Total	C	N	O	0	0	0
			49	28	2	19			
7	T	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 8 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
8	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

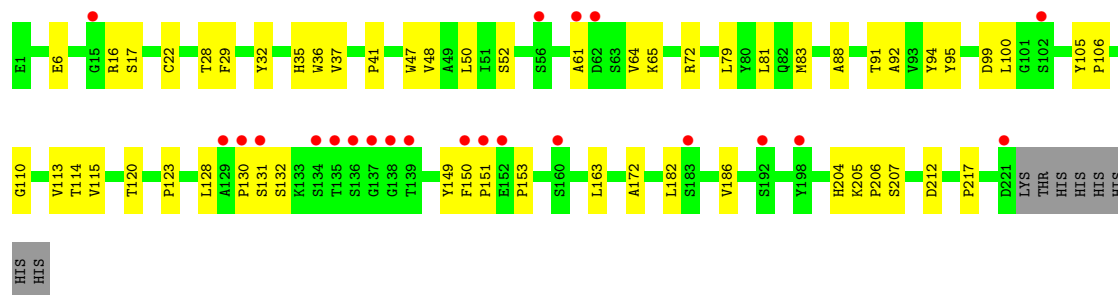


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		

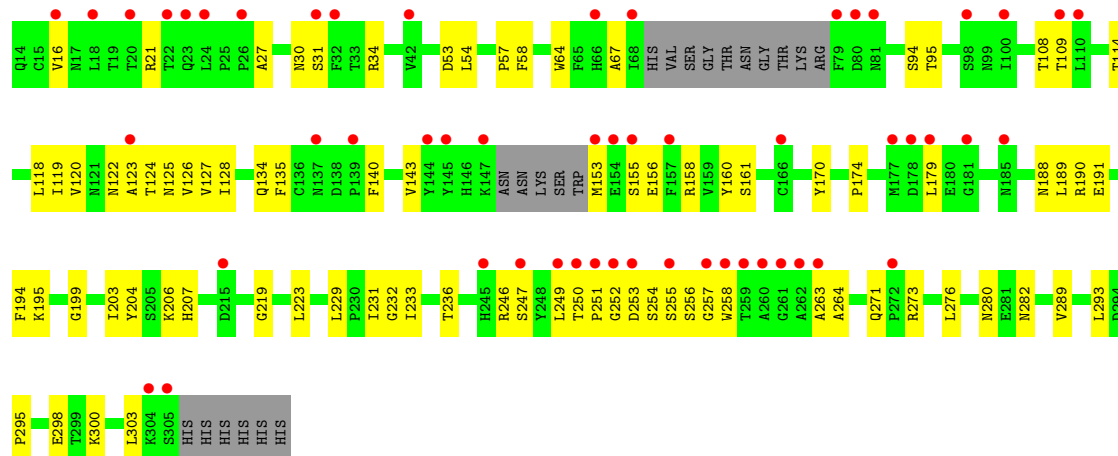
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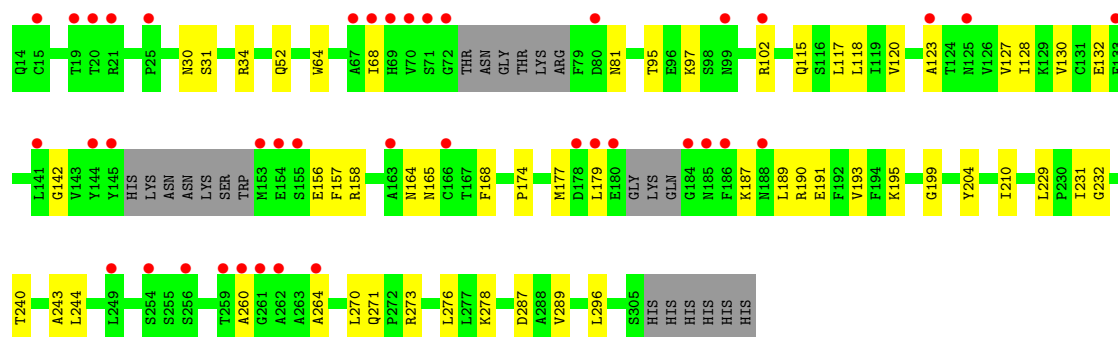
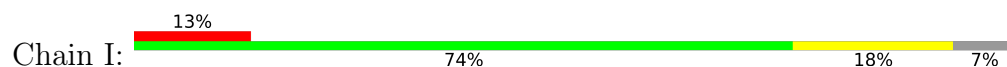
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		



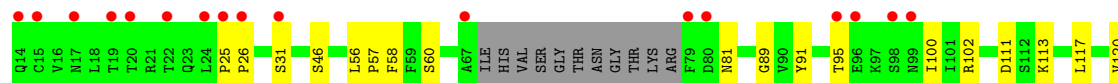
• Molecule 2: Spike protein S1

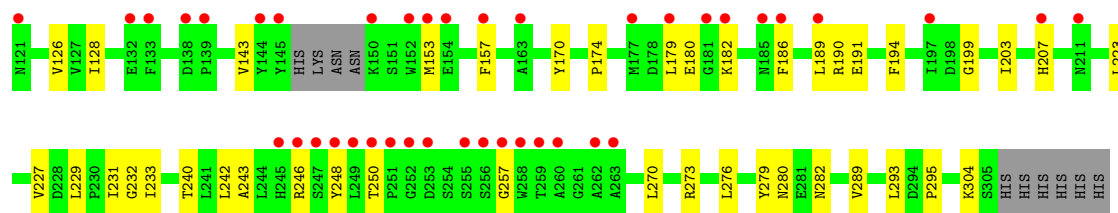


• Molecule 2: Spike protein S1

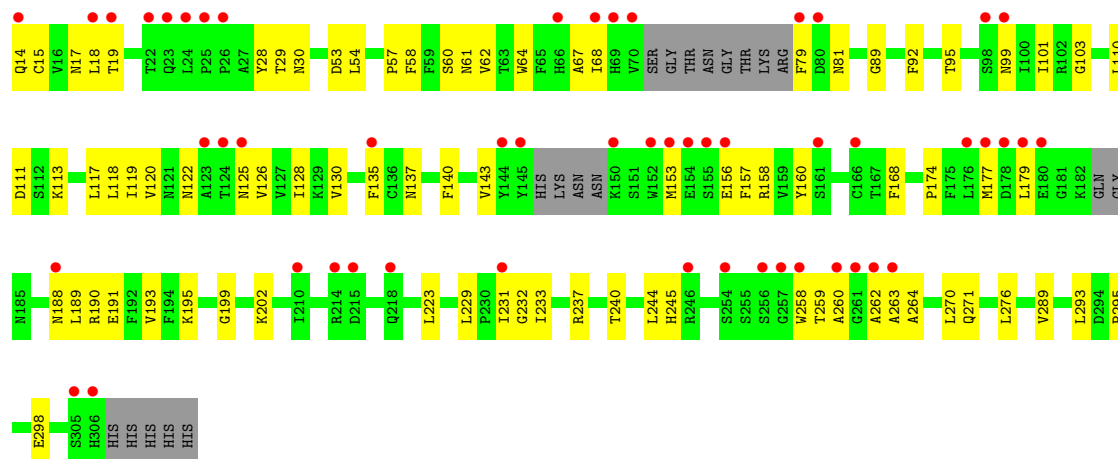


• Molecule 2: Spike protein S1

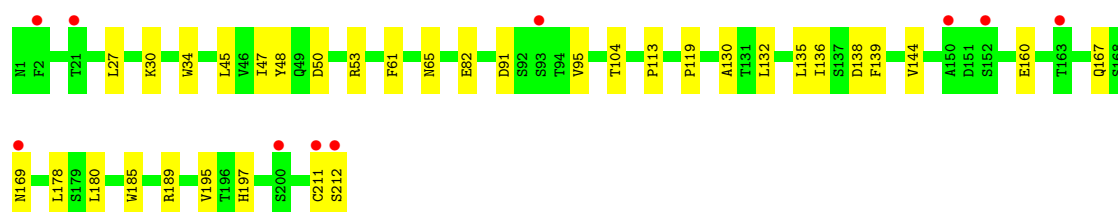
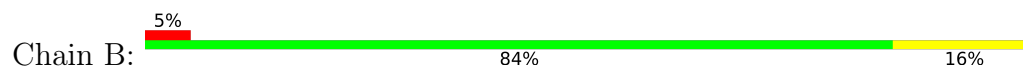




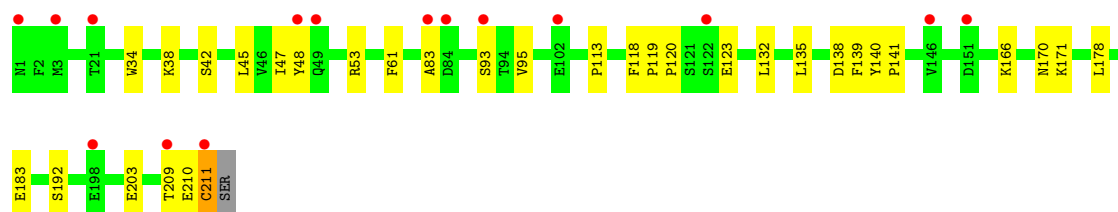
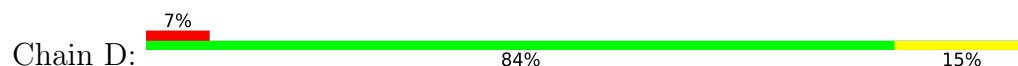
• Molecule 2: Spike protein S1



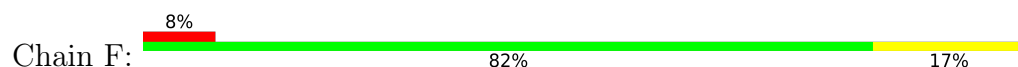
• Molecule 3: BLN8 light chain

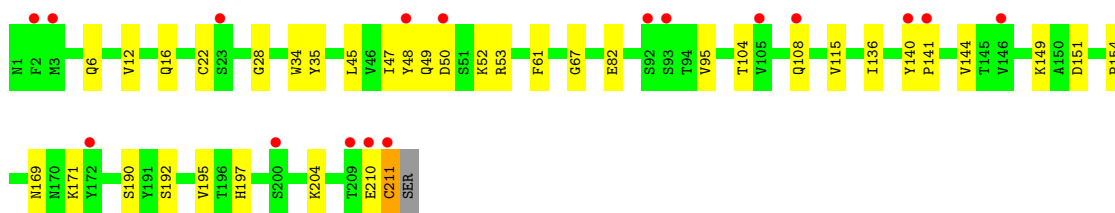


• Molecule 3: BLN8 light chain



• Molecule 3: BLN8 light chain





- Molecule 3: BLN8 light chain



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



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



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



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  25% 75%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.94Å 117.49Å 138.05Å 110.91° 90.27° 96.37°	Depositor
Resolution (Å)	64.40 – 3.13 64.40 – 3.13	Depositor EDS
% Data completeness (in resolution range)	98.4 (64.40-3.13) 98.4 (64.40-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.232 , 0.285 0.232 , 0.285	Depositor DCC
R_{free} test set	3618 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22383	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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, MAN, FUC, NAG

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	0.09	0/1715	0.29	0/2335
1	C	0.10	0/1715	0.31	0/2335
1	E	0.12	0/1715	0.35	0/2335
1	G	0.09	0/1699	0.30	0/2314
2	I	0.15	0/2272	0.33	0/3093
2	J	0.09	0/2290	0.30	0/3117
2	K	0.17	0/2287	0.37	0/3112
2	L	0.11	0/2313	0.34	0/3148
3	B	0.09	0/1623	0.31	0/2216
3	D	0.10	0/1616	0.30	0/2208
3	F	0.10	0/1616	0.34	0/2208
3	H	0.11	0/1616	0.30	0/2208
All	All	0.11	0/22477	0.32	0/30629

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1674	0	1641	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1674	0	1640	32	0
1	E	1674	0	1640	26	0
1	G	1658	0	1620	37	0
2	I	2212	0	2132	37	0
2	J	2228	0	2150	42	0
2	K	2226	0	2154	60	0
2	L	2250	0	2172	56	0
3	B	1584	0	1523	23	0
3	D	1577	0	1517	23	0
3	F	1577	0	1517	25	0
3	H	1577	0	1517	11	0
4	M	24	0	22	0	0
4	O	24	0	22	0	0
4	P	24	0	22	0	0
5	N	60	0	52	0	0
6	Q	60	0	52	0	0
7	R	49	0	43	0	0
7	T	49	0	43	0	0
8	S	28	0	25	0	0
9	I	28	0	26	1	0
9	J	56	0	52	0	0
9	K	28	0	26	0	0
9	L	42	0	39	0	0
All	All	22383	0	21647	370	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 8.

The worst 5 of 370 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)
2:L:189:LEU:HD22	2:L:191:GLU:HG2	1.25	1.10
2:J:189:LEU:HD22	2:J:191:GLU:HG3	1.26	1.06
2:L:189:LEU:HD22	2:L:191:GLU:CG	2.00	0.91
2:J:189:LEU:CD2	2:J:191:GLU:HG3	2.04	0.87
2:L:67:ALA:O	2:L:263:ALA:HB3	1.76	0.85

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	221/229 (96%)	209 (95%)	11 (5%)	1 (0%)	24	54
1	C	221/229 (96%)	214 (97%)	5 (2%)	2 (1%)	14	41
1	E	221/229 (96%)	215 (97%)	6 (3%)	0	100	100
1	G	219/229 (96%)	212 (97%)	6 (3%)	1 (0%)	24	54
2	I	268/298 (90%)	245 (91%)	23 (9%)	0	100	100
2	J	271/298 (91%)	252 (93%)	19 (7%)	0	100	100
2	K	271/298 (91%)	250 (92%)	21 (8%)	0	100	100
2	L	271/298 (91%)	248 (92%)	23 (8%)	0	100	100
3	B	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
3	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
3	F	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
3	H	209/212 (99%)	197 (94%)	12 (6%)	0	100	100
All	All	2800/2956 (95%)	2639 (94%)	157 (6%)	4 (0%)	48	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	C	165	SER
1	G	131	SER
1	C	130	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/193 (97%)	187 (100%)	0	100	100
1	C	187/193 (97%)	187 (100%)	0	100	100
1	E	187/193 (97%)	187 (100%)	0	100	100
1	G	185/193 (96%)	185 (100%)	0	100	100
2	I	248/268 (92%)	248 (100%)	0	100	100
2	J	249/268 (93%)	249 (100%)	0	100	100
2	K	249/268 (93%)	249 (100%)	0	100	100
2	L	252/268 (94%)	252 (100%)	0	100	100
3	B	180/180 (100%)	180 (100%)	0	100	100
3	D	179/180 (99%)	178 (99%)	1 (1%)	78	80
3	F	179/180 (99%)	178 (99%)	1 (1%)	78	80
3	H	179/180 (99%)	178 (99%)	1 (1%)	78	80
All	All	2461/2564 (96%)	2458 (100%)	3 (0%)	88	89

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

Mol	Chain	Res	Type
3	D	211	CYS
3	F	211	CYS
3	H	211	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	128	ASN
2	I	164	ASN
2	L	207	HIS
2	I	115	GLN
2	J	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

26 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
4	NAG	M	1	2,4	14,14,15	0.69	0	17,19,21	1.15	2 (11%)
4	FUC	M	2	4	10,10,11	0.77	0	14,14,16	1.07	1 (7%)
5	NAG	N	1	2,5	14,14,15	0.80	0	17,19,21	1.79	4 (23%)
5	NAG	N	2	5	14,14,15	0.76	0	17,19,21	0.96	2 (11%)
5	BMA	N	3	5	11,11,12	0.81	0	15,15,17	2.36	5 (33%)
5	MAN	N	4	5	11,11,12	0.66	0	15,15,17	1.49	1 (6%)
5	FUC	N	5	5	10,10,11	0.79	0	14,14,16	2.18	3 (21%)
4	NAG	O	1	2,4	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
4	FUC	O	2	4	10,10,11	0.84	0	14,14,16	0.92	0
4	NAG	P	1	2,4	14,14,15	0.72	0	17,19,21	0.90	0
4	FUC	P	2	4	10,10,11	0.83	0	14,14,16	0.94	0
6	NAG	Q	1	2,6	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
6	NAG	Q	2	6	14,14,15	0.75	0	17,19,21	0.97	0
6	BMA	Q	3	6	11,11,12	0.93	0	15,15,17	2.22	4 (26%)
6	MAN	Q	4	6	11,11,12	0.71	0	15,15,17	1.25	1 (6%)
6	FUC	Q	5	6	10,10,11	0.77	0	14,14,16	1.79	5 (35%)
7	NAG	R	1	2,7	14,14,15	0.68	0	17,19,21	1.04	1 (5%)
7	NAG	R	2	7	14,14,15	0.71	0	17,19,21	1.05	2 (11%)
7	BMA	R	3	7	11,11,12	0.88	0	15,15,17	2.08	3 (20%)
7	FUC	R	4	7	10,10,11	0.81	0	14,14,16	2.48	5 (35%)
8	NAG	S	1	2,8	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
8	NAG	S	2	8	14,14,15	0.71	0	17,19,21	0.85	0
7	NAG	T	1	2,7	14,14,15	0.78	0	17,19,21	1.52	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	2	7	14,14,15	0.75	0	17,19,21	0.92	0
7	BMA	T	3	7	11,11,12	0.87	0	15,15,17	2.28	5 (33%)
7	FUC	T	4	7	10,10,11	0.70	0	14,14,16	2.35	6 (42%)

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
4	NAG	M	1	2,4	-	1/6/23/26	0/1/1/1
4	FUC	M	2	4	-	-	0/1/1/1
5	NAG	N	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	2/2/19/22	1/1/1/1
5	FUC	N	5	5	-	-	0/1/1/1
4	NAG	O	1	2,4	-	1/6/23/26	0/1/1/1
4	FUC	O	2	4	-	-	0/1/1/1
4	NAG	P	1	2,4	-	1/6/23/26	0/1/1/1
4	FUC	P	2	4	-	-	0/1/1/1
6	NAG	Q	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	FUC	Q	5	6	-	-	0/1/1/1
7	NAG	R	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	FUC	R	4	7	-	-	0/1/1/1
8	NAG	S	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
7	NAG	T	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	FUC	T	4	7	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	4	FUC	C1-C2-C3	6.76	117.97	109.67
7	T	3	BMA	C1-O5-C5	6.39	120.85	112.19
5	N	3	BMA	C1-O5-C5	6.39	120.84	112.19
5	N	5	FUC	C1-C2-C3	5.96	116.99	109.67
7	R	3	BMA	C1-O5-C5	5.75	119.98	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

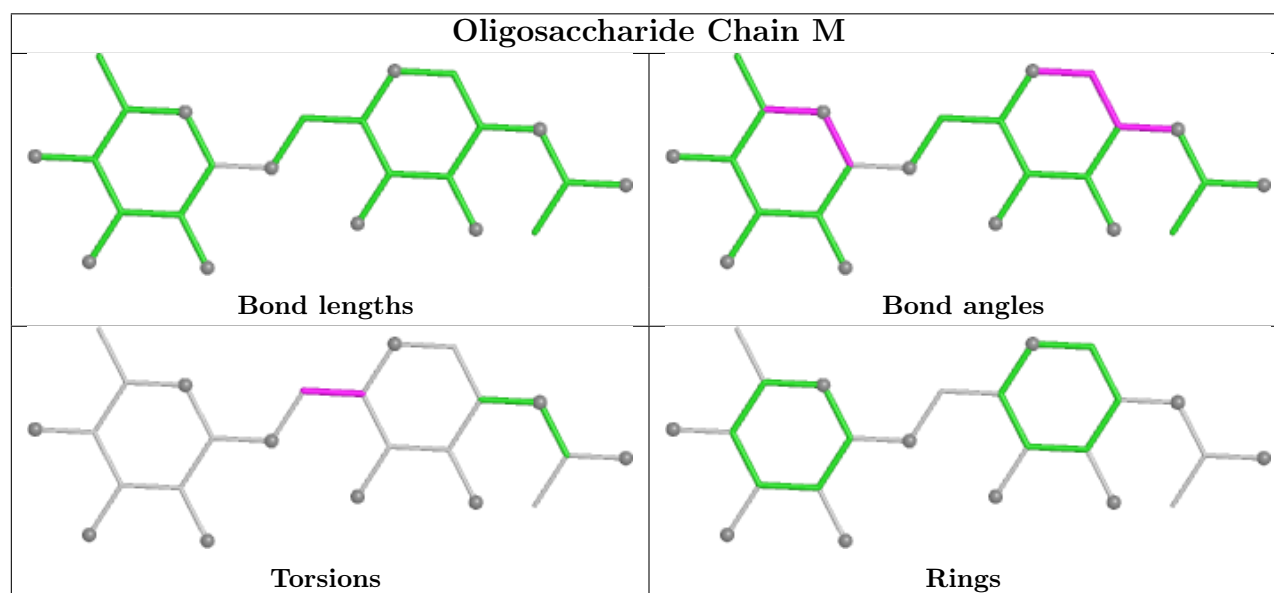
Mol	Chain	Res	Type	Atoms
6	Q	4	MAN	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6

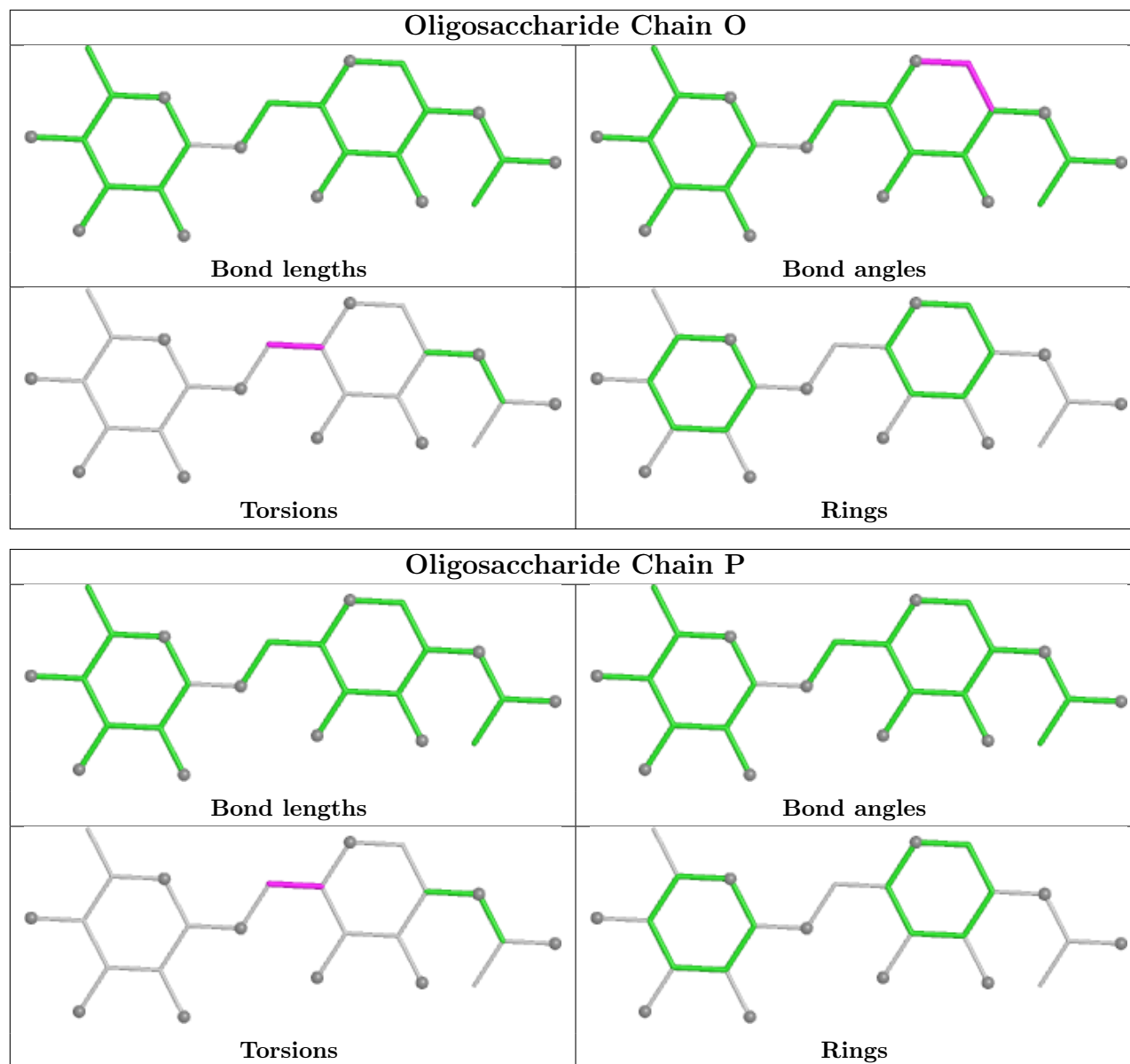
All (1) ring outliers are listed below:

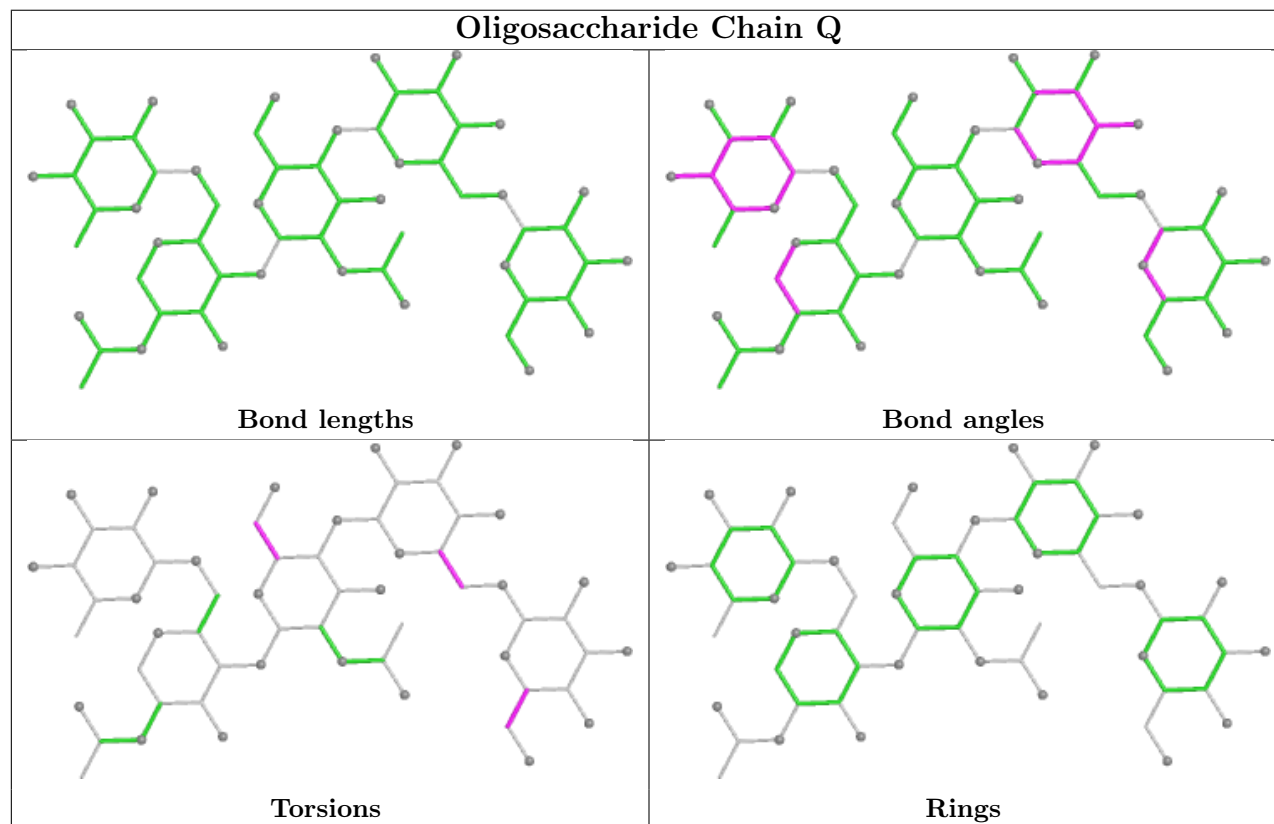
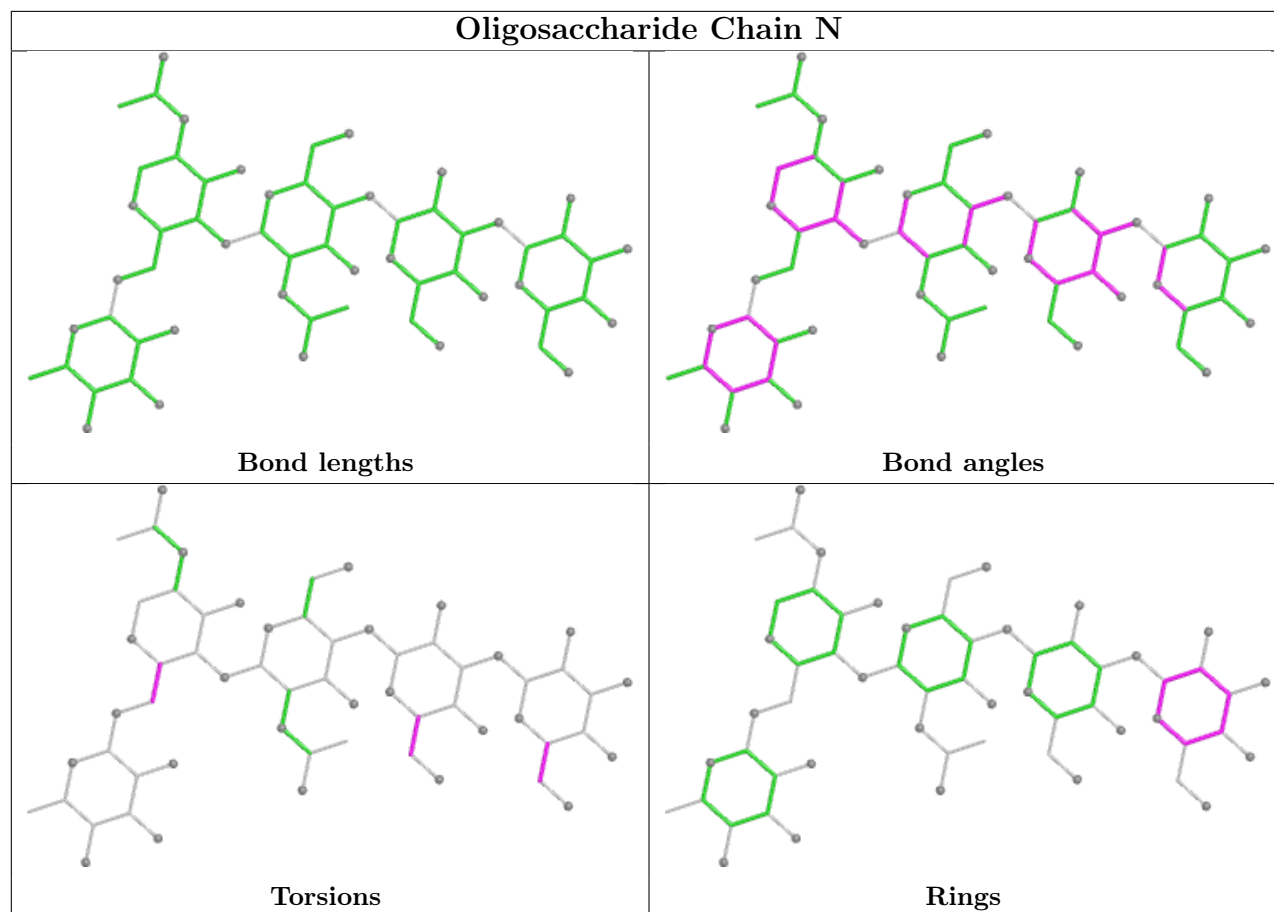
Mol	Chain	Res	Type	Atoms
5	N	4	MAN	C1-C2-C3-C4-C5-O5

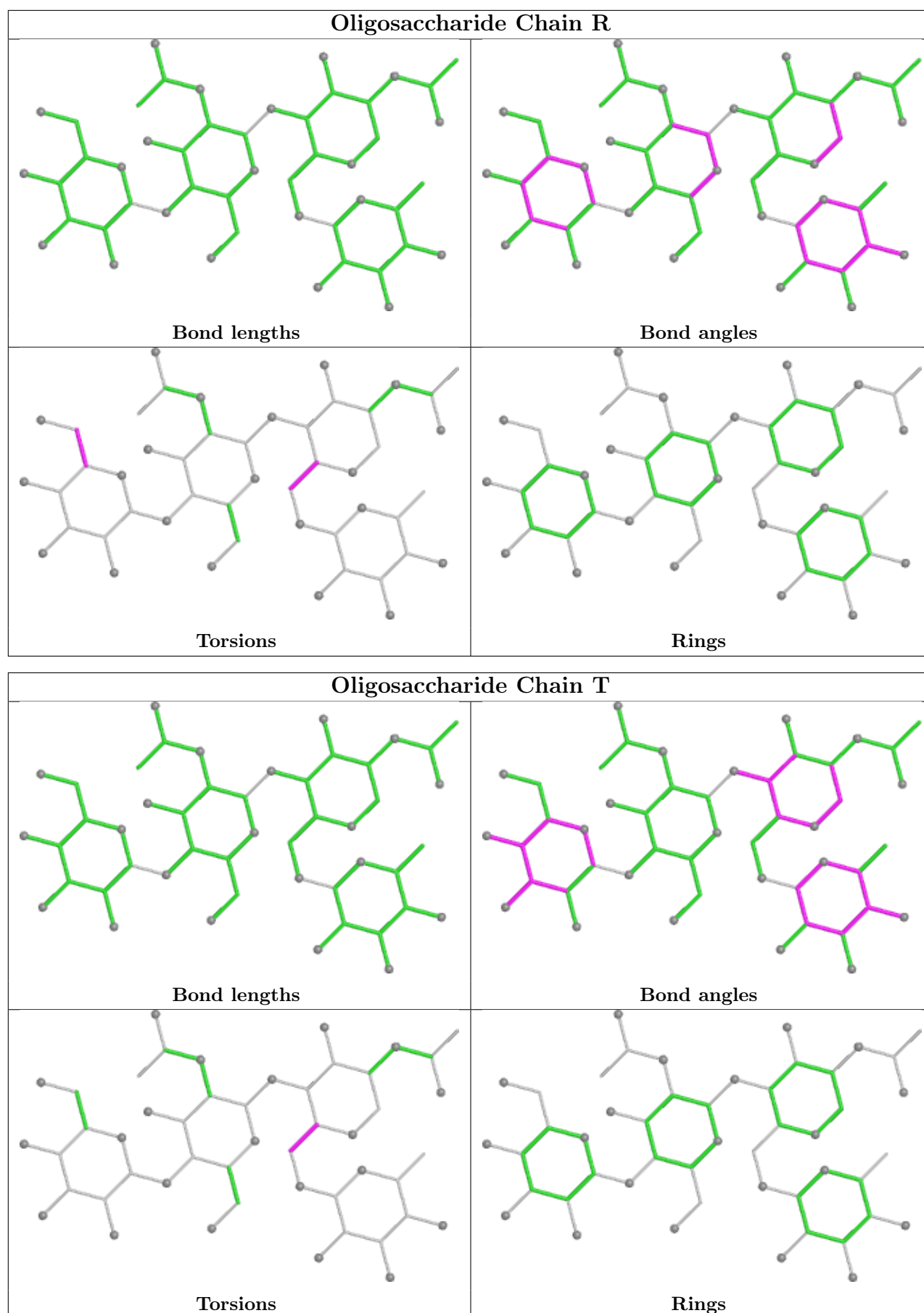
No monomer is involved in short contacts.

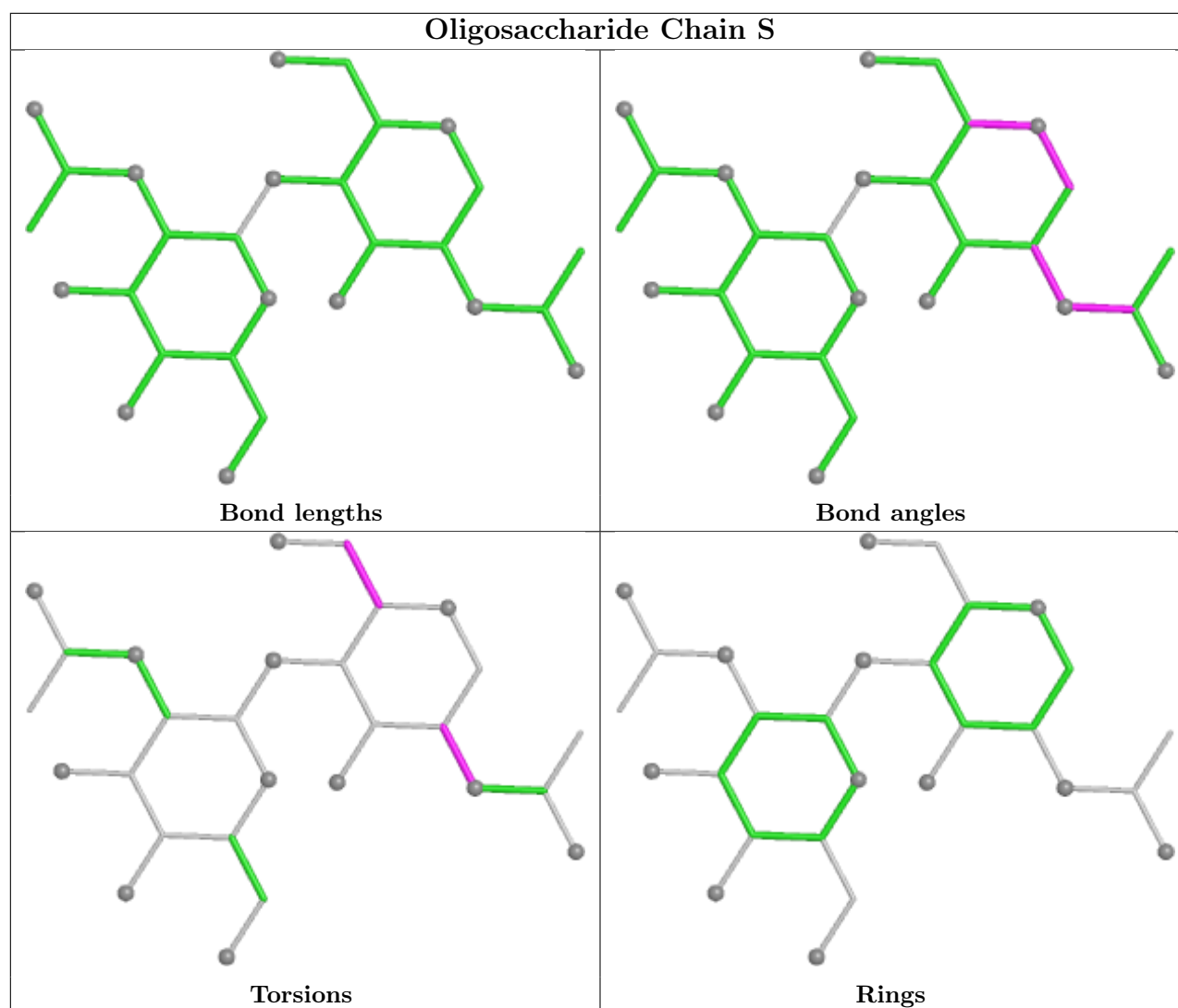
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
9	NAG	J	401	2	14,14,15	0.76	0	17,19,21	0.96	0
9	NAG	J	402	2	14,14,15	0.72	0	17,19,21	0.84	0
9	NAG	L	403	2	14,14,15	0.71	0	17,19,21	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	I	402	2	14,14,15	0.73	0	17,19,21	0.86	0
9	NAG	K	401	2	14,14,15	0.71	0	17,19,21	0.79	0
9	NAG	L	401	2	14,14,15	0.74	0	17,19,21	0.87	0
9	NAG	J	403	2	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
9	NAG	J	404	2	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
9	NAG	K	402	2	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
9	NAG	L	402	2	14,14,15	0.67	0	17,19,21	1.03	1 (5%)
9	NAG	I	401	2	14,14,15	0.72	0	17,19,21	0.87	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
9	NAG	J	401	2	-	2/6/23/26	0/1/1/1
9	NAG	J	402	2	-	0/6/23/26	0/1/1/1
9	NAG	L	403	2	-	1/6/23/26	0/1/1/1
9	NAG	I	402	2	-	0/6/23/26	0/1/1/1
9	NAG	K	401	2	-	0/6/23/26	0/1/1/1
9	NAG	L	401	2	-	0/6/23/26	0/1/1/1
9	NAG	J	403	2	-	0/6/23/26	0/1/1/1
9	NAG	J	404	2	-	2/6/23/26	0/1/1/1
9	NAG	K	402	2	-	2/6/23/26	0/1/1/1
9	NAG	L	402	2	-	3/6/23/26	0/1/1/1
9	NAG	I	401	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	403	NAG	C2-N2-C7	3.11	127.34	122.90
9	L	402	NAG	O5-C1-C2	-2.71	107.01	111.29
9	J	404	NAG	O5-C1-C2	-2.58	107.22	111.29
9	K	402	NAG	C1-O5-C5	2.42	115.47	112.19
9	J	403	NAG	C1-O5-C5	2.31	115.33	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	402	NAG	C4-C5-C6-O6
9	J	401	NAG	O5-C5-C6-O6
9	K	402	NAG	O5-C5-C6-O6
9	J	401	NAG	C4-C5-C6-O6
9	J	404	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	402	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	223/229 (97%)	0.67	16 (7%) 21 11	17, 33, 71, 116	0
1	C	223/229 (97%)	0.71	16 (7%) 21 11	16, 36, 80, 141	0
1	E	223/229 (97%)	0.89	16 (7%) 21 11	17, 40, 83, 123	0
1	G	221/229 (96%)	0.85	22 (9%) 12 6	17, 40, 69, 111	0
2	I	276/298 (92%)	1.00	40 (14%) 6 3	13, 40, 88, 108	0
2	J	277/298 (92%)	1.12	57 (20%) 2 1	12, 41, 104, 117	0
2	K	277/298 (92%)	1.15	54 (19%) 3 1	16, 43, 97, 120	0
2	L	279/298 (93%)	1.14	52 (18%) 3 1	16, 40, 91, 116	0
3	B	212/212 (100%)	0.72	10 (4%) 36 19	17, 40, 61, 122	0
3	D	211/212 (99%)	0.82	15 (7%) 22 11	16, 43, 65, 114	0
3	F	211/212 (99%)	0.92	17 (8%) 18 9	21, 48, 72, 109	0
3	H	211/212 (99%)	0.89	12 (5%) 29 15	23, 46, 67, 112	0
All	All	2844/2956 (96%)	0.92	327 (11%) 9 5	12, 41, 89, 141	0

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	185	ASN	5.1
2	K	262	ALA	5.0
2	K	249	LEU	4.9
2	K	252	GLY	4.8
2	K	251	PRO	4.7

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

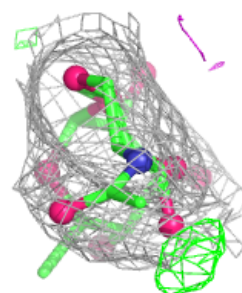
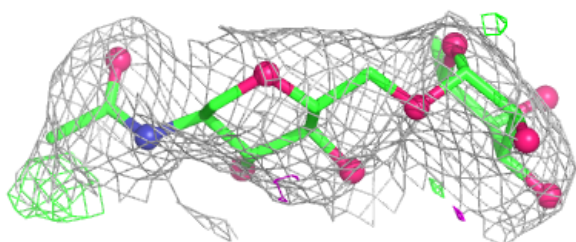
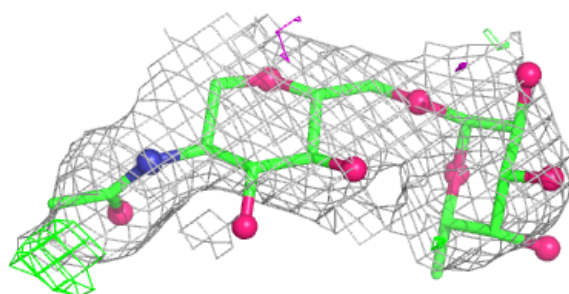
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	Q	3	11/12	0.20	0.22	82,102,114,116	0
4	FUC	P	2	10/11	0.21	0.22	62,85,93,103	0
7	BMA	T	3	11/12	0.22	0.24	69,99,110,119	0
6	MAN	Q	4	11/12	0.44	0.19	68,92,113,119	0
6	NAG	Q	2	14/15	0.46	0.21	57,99,102,103	0
7	BMA	R	3	11/12	0.50	0.19	90,104,125,128	0
5	BMA	N	3	11/12	0.50	0.17	72,112,118,124	0
7	NAG	T	2	14/15	0.56	0.16	44,79,88,96	0
4	FUC	O	2	10/11	0.57	0.23	70,81,91,99	0
8	NAG	S	1	14/15	0.59	0.23	44,73,88,89	0
4	FUC	M	2	10/11	0.61	0.18	52,75,80,87	0
8	NAG	S	2	14/15	0.62	0.16	53,82,92,96	0
7	FUC	R	4	10/11	0.65	0.27	61,83,101,114	0
5	FUC	N	5	10/11	0.68	0.28	75,89,105,105	0
7	FUC	T	4	10/11	0.68	0.23	58,71,90,96	0
7	NAG	R	2	14/15	0.70	0.16	66,97,115,123	0
6	FUC	Q	5	10/11	0.70	0.26	61,90,113,114	0
5	MAN	N	4	11/12	0.72	0.16	69,94,115,118	0
5	NAG	N	2	14/15	0.72	0.17	60,91,105,115	0
4	NAG	P	1	14/15	0.74	0.15	42,57,86,90	0
5	NAG	N	1	14/15	0.77	0.20	66,78,89,97	0
4	NAG	M	1	14/15	0.78	0.14	35,52,77,87	0
4	NAG	O	1	14/15	0.82	0.12	31,50,60,72	0
7	NAG	R	1	14/15	0.82	0.16	63,79,93,93	0
6	NAG	Q	1	14/15	0.83	0.16	57,67,94,97	0
7	NAG	T	1	14/15	0.86	0.14	61,80,86,87	0

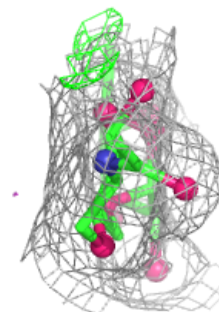
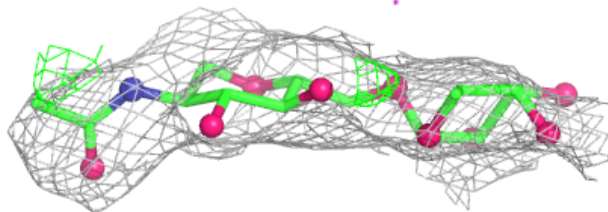
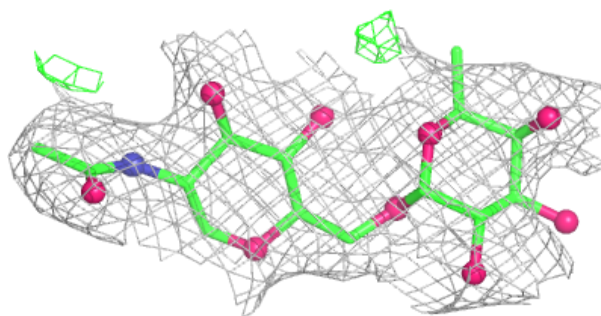
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

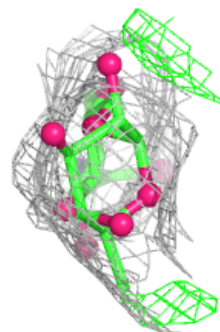
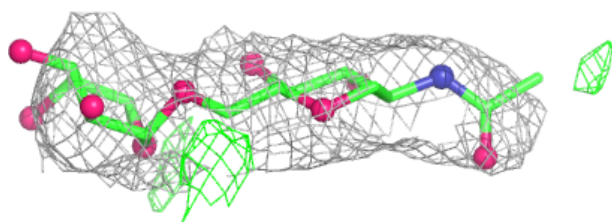
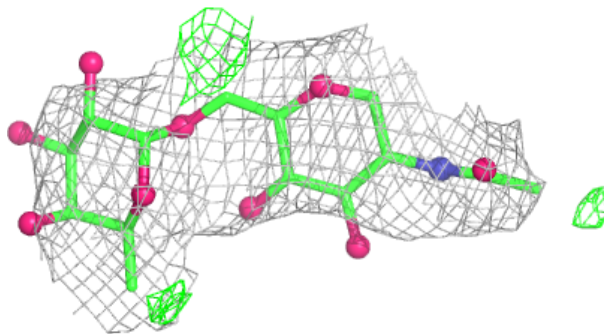
**Electron density around Chain O:**

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



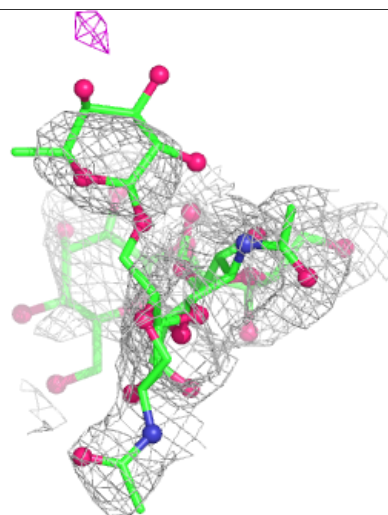
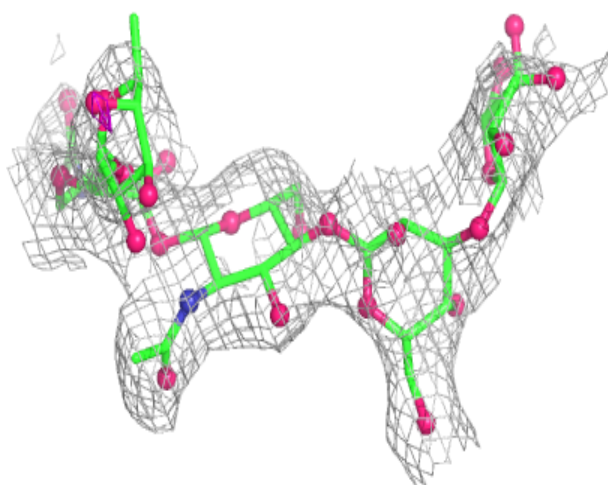
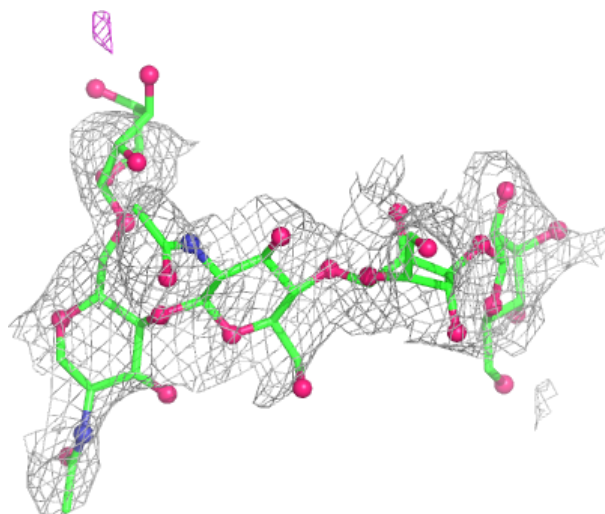
Electron density around Chain P:

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



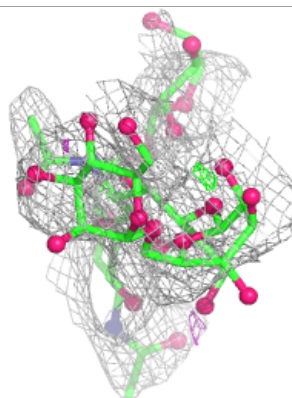
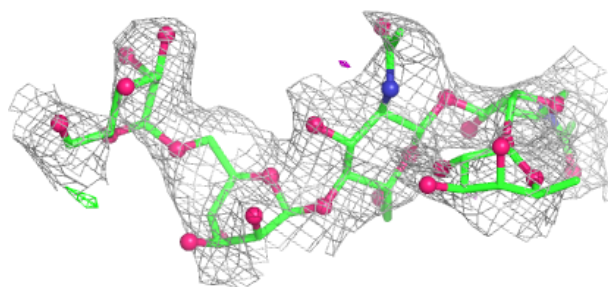
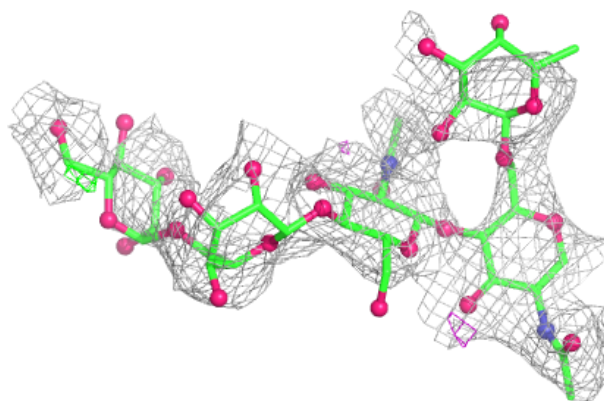
Electron density around Chain N:

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



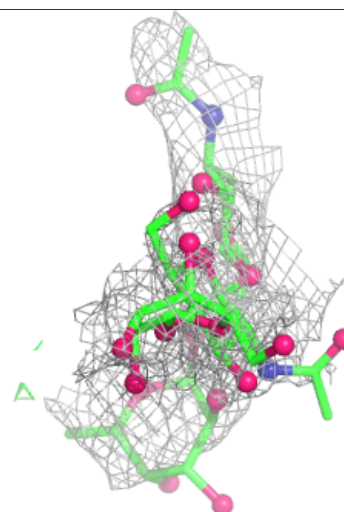
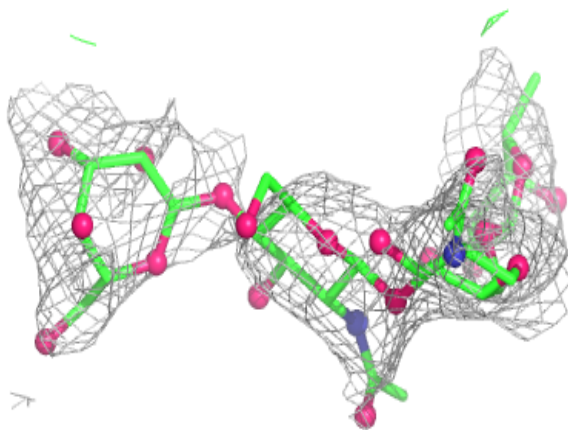
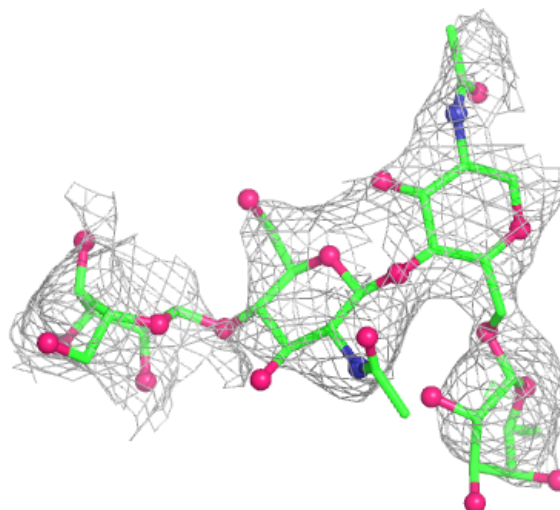
Electron density around Chain Q:

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



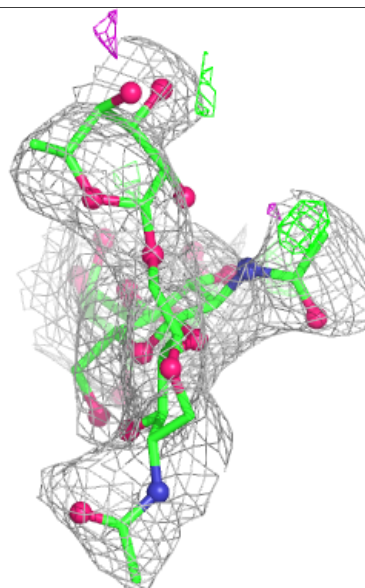
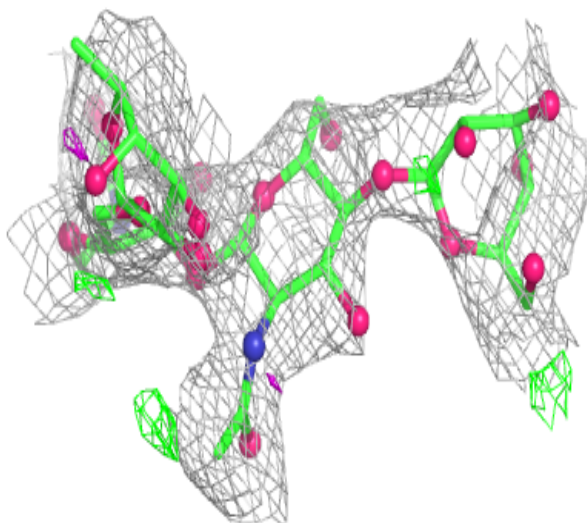
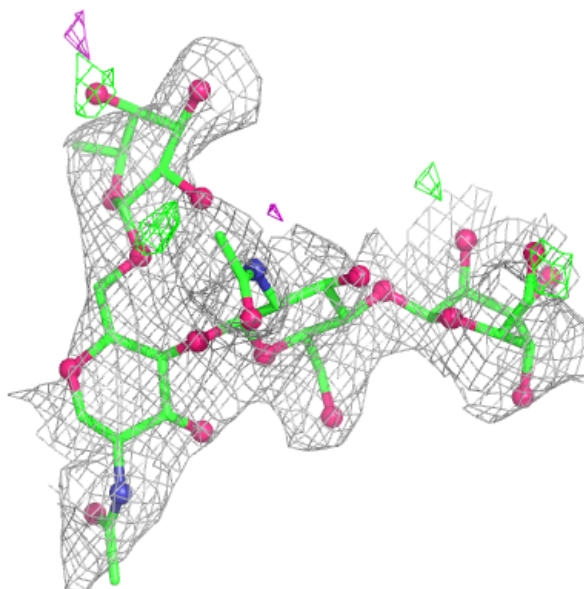
Electron density around Chain R:

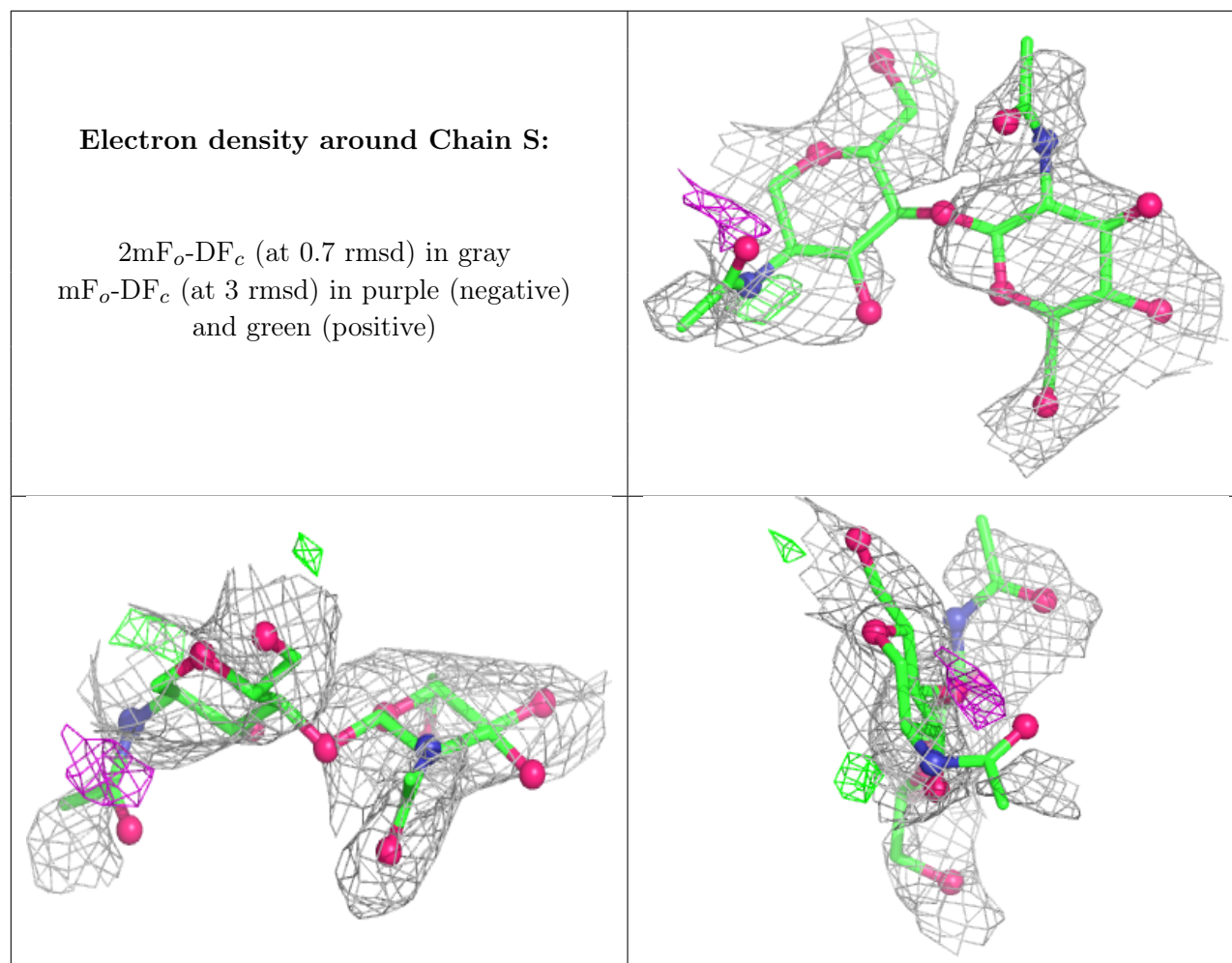
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	L	403	14/15	0.47	0.21	79,90,101,112	0
9	NAG	K	402	14/15	0.60	0.20	51,65,81,88	0
9	NAG	J	401	14/15	0.64	0.16	58,73,80,80	0
9	NAG	I	401	14/15	0.66	0.19	61,82,105,108	0
9	NAG	J	404	14/15	0.66	0.19	69,87,108,110	0
9	NAG	I	402	14/15	0.66	0.19	75,90,103,104	0
9	NAG	J	402	14/15	0.71	0.18	36,67,82,96	0
9	NAG	J	403	14/15	0.75	0.15	48,62,73,74	0
9	NAG	L	401	14/15	0.79	0.14	44,72,89,90	0
9	NAG	K	401	14/15	0.81	0.11	30,43,61,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	L	402	14/15	0.84	0.14	30,48,58,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.