



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:00 AM EDT

PDB ID : 6NSC
Title : Crystal structure of the A/Brisbane/10/2007 (H3N2) influenza virus hemagglutinin G186V/L194P mutant apo form
Authors : Wu, N.C.; Wilson, I.A.
Deposited on : 2019-01-24
Resolution : 2.25 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

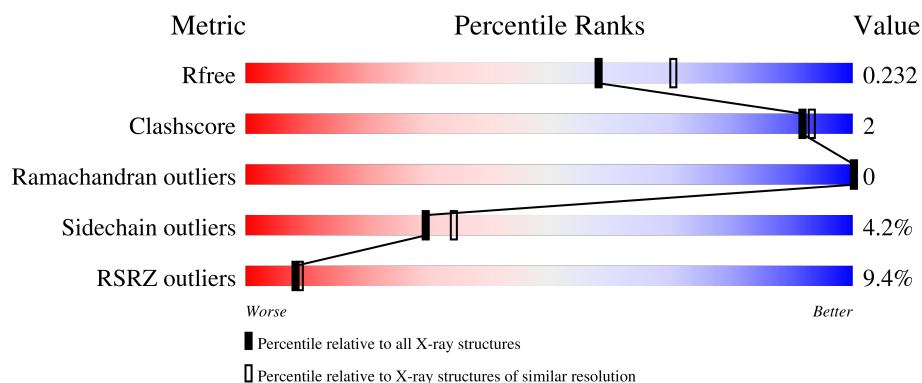
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	321	<div> <div>14%</div> <div>88%</div> <div>10%</div> </div>
2	B	176	<div> <div>%</div> <div>95%</div> </div>
3	C	5	<div> <div>100%</div> </div>
4	D	3	<div> <div>100%</div> </div>
5	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	2	 100%

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	NAG	D	2	-	-	-	X
5	NAG	E	2	-	-	-	X
6	NAG	A	401	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4321 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	3	0
			2489	1561	441	475	12			

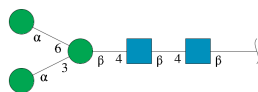
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP A8W893
A	10	GLY	-	expression tag	UNP A8W893
A	186	VAL	GLY	engineered mutation	UNP A8W893
A	194	PRO	LEU	engineered mutation	UNP A8W893

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

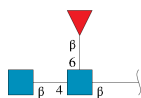
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	3	0
			1409	881	245	277	6			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



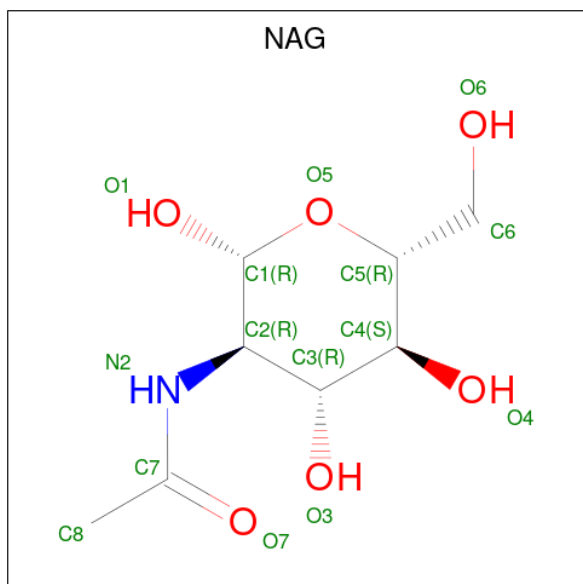
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

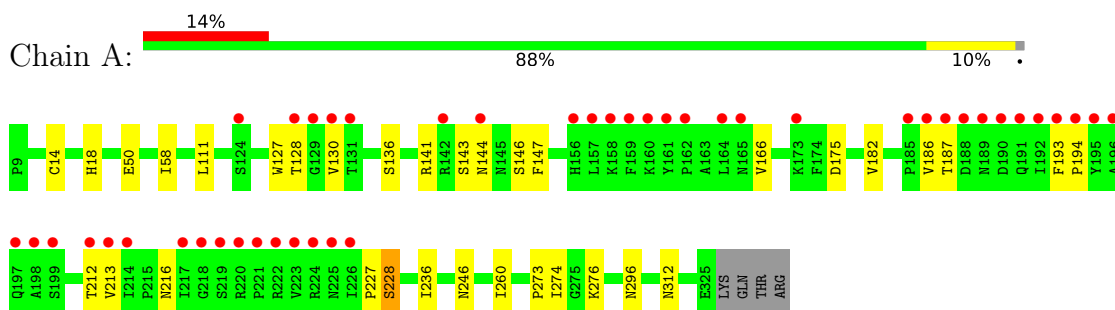
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	121	Total	O	0	0
			121	121		
7	B	119	Total	O	0	0
			119	119		

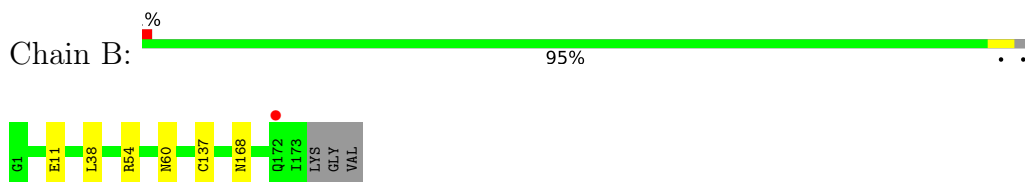
3 Residue-property plots

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.

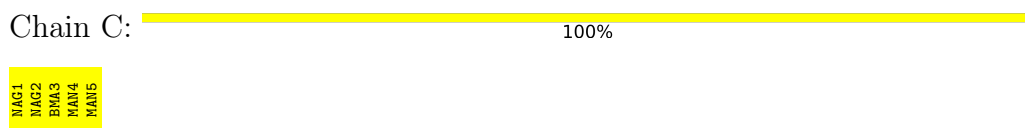
- Molecule 1: Hemagglutinin HA1 chain



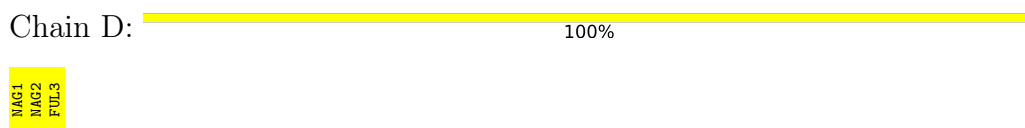
- Molecule 2: Hemagglutinin HA2 chain



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



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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.60Å 100.60Å 384.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.25 43.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.25) 99.8 (43.28-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.198 , 0.228 0.201 , 0.232	Depositor DCC
R_{free} test set	1743 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	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	0.95	EDS
Total number of atoms	4321	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

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

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	0.52	0/2556	0.71	1/3478 (0.0%)
2	B	0.54	0/1442	0.77	2/1937 (0.1%)
All	All	0.53	0/3998	0.73	3/5415 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	B	54	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	312	ASN	CB-CA-C	-5.66	99.07	110.40

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	A	2489	0	2444	13	0
2	B	1409	0	1351	1	0
3	C	61	0	52	0	0
4	D	38	0	34	0	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	28	0	26	0	0
7	A	121	0	0	0	0
7	B	119	0	0	0	0
All	All	4321	0	3957	13	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 2.

All (13) 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:A:141:ARG:NH1	1:A:147:PHE:O	2.26	0.69
1:A:186:VAL:HG11	1:A:227:PRO:HG2	1.78	0.65
1:A:175:ASP:HB2	1:A:260:ILE:HG23	1.84	0.59
1:A:50[A]:GLU:HG2	1:A:273:PRO:HG2	1.95	0.49
1:A:182:VAL:HG21	1:A:213:VAL:CG1	2.43	0.49
1:A:141:ARG:HB3	1:A:146:SER:CB	2.43	0.47
1:A:127:TRP:CZ3	1:A:166:VAL:HG21	2.52	0.44
1:A:193:PHE:HB3	1:A:194:PRO:HD3	1.99	0.44
1:A:58:ILE:HG21	1:A:274:ILE:HD12	1.98	0.43
1:A:182:VAL:HG21	1:A:213:VAL:HG11	2.00	0.43
1:A:186:VAL:HG22	1:A:228:SER:N	2.35	0.41
1:A:14:CYS:HA	2:B:137:CYS:HA	2.04	0.40
1:A:111:LEU:C	1:A:111:LEU:HD12	2.42	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	A	318/321 (99%)	306 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
All	All	492/497 (99%)	470 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/285 (100%)	270 (95%)	14 (5%)	25	27
2	B	149/148 (101%)	145 (97%)	4 (3%)	44	54
All	All	433/433 (100%)	415 (96%)	18 (4%)	30	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	128	THR
1	A	130	VAL
1	A	136	SER
1	A	143	SER
1	A	144	ASN
1	A	187	THR
1	A	212	THR
1	A	216	ASN
1	A	228	SER
1	A	236	ILE
1	A	246	ASN
1	A	276	LYS
1	A	296	ASN
2	B	11	GLU
2	B	38	LEU
2	B	60	ASN
2	B	168	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

12 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	0.49	0	17,19,21	1.26	1 (5%)
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	0.89	1 (5%)
3	BMA	C	3	3	11,11,12	0.38	0	15,15,17	0.90	1 (6%)
3	MAN	C	4	3	11,11,12	0.49	0	15,15,17	1.21	2 (13%)
3	MAN	C	5	3	11,11,12	0.67	0	15,15,17	1.63	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	1.15	1 (5%)
4	FUL	D	3	4	10,10,11	0.42	0	14,14,16	1.01	1 (7%)
5	NAG	E	1	5,1	14,14,15	0.63	0	17,19,21	1.21	1 (5%)
5	NAG	E	2	5	14,14,15	0.69	0	17,19,21	1.58	4 (23%)
5	NAG	F	1	5,1	14,14,15	0.46	0	17,19,21	0.84	0
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.63	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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	FUL	D	3	4	-	-	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	MAN	C1-O5-C5	4.23	117.93	112.19
5	E	1	NAG	C1-O5-C5	4.16	117.82	112.19
3	C	5	MAN	C1-C2-C3	3.92	114.49	109.67
3	C	1	NAG	C1-O5-C5	3.75	117.27	112.19
4	D	2	NAG	C4-C3-C2	3.21	115.72	111.02
3	C	4	MAN	C3-C4-C5	3.03	115.64	110.24
5	E	2	NAG	C1-O5-C5	3.00	116.26	112.19
5	E	2	NAG	O5-C5-C6	2.76	111.53	107.20
5	E	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	C	2	NAG	C1-O5-C5	2.32	115.34	112.19
4	D	3	FUL	O5-C1-C2	-2.26	107.28	110.77
3	C	4	MAN	C1-O5-C5	2.26	115.25	112.19
5	E	2	NAG	O5-C5-C4	-2.16	105.56	110.83
3	C	3	BMA	O5-C5-C6	2.03	110.38	107.20
4	D	1	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6

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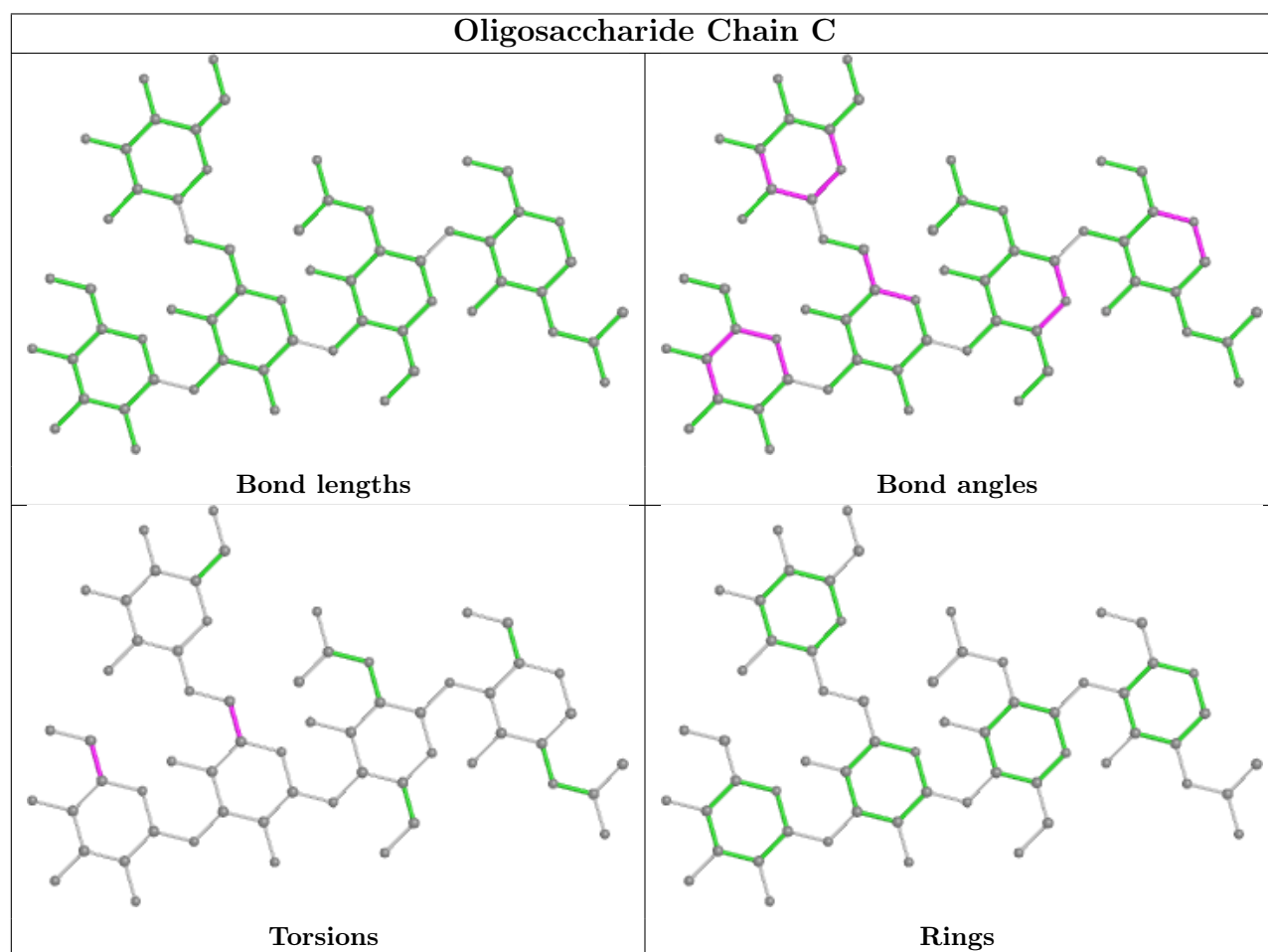
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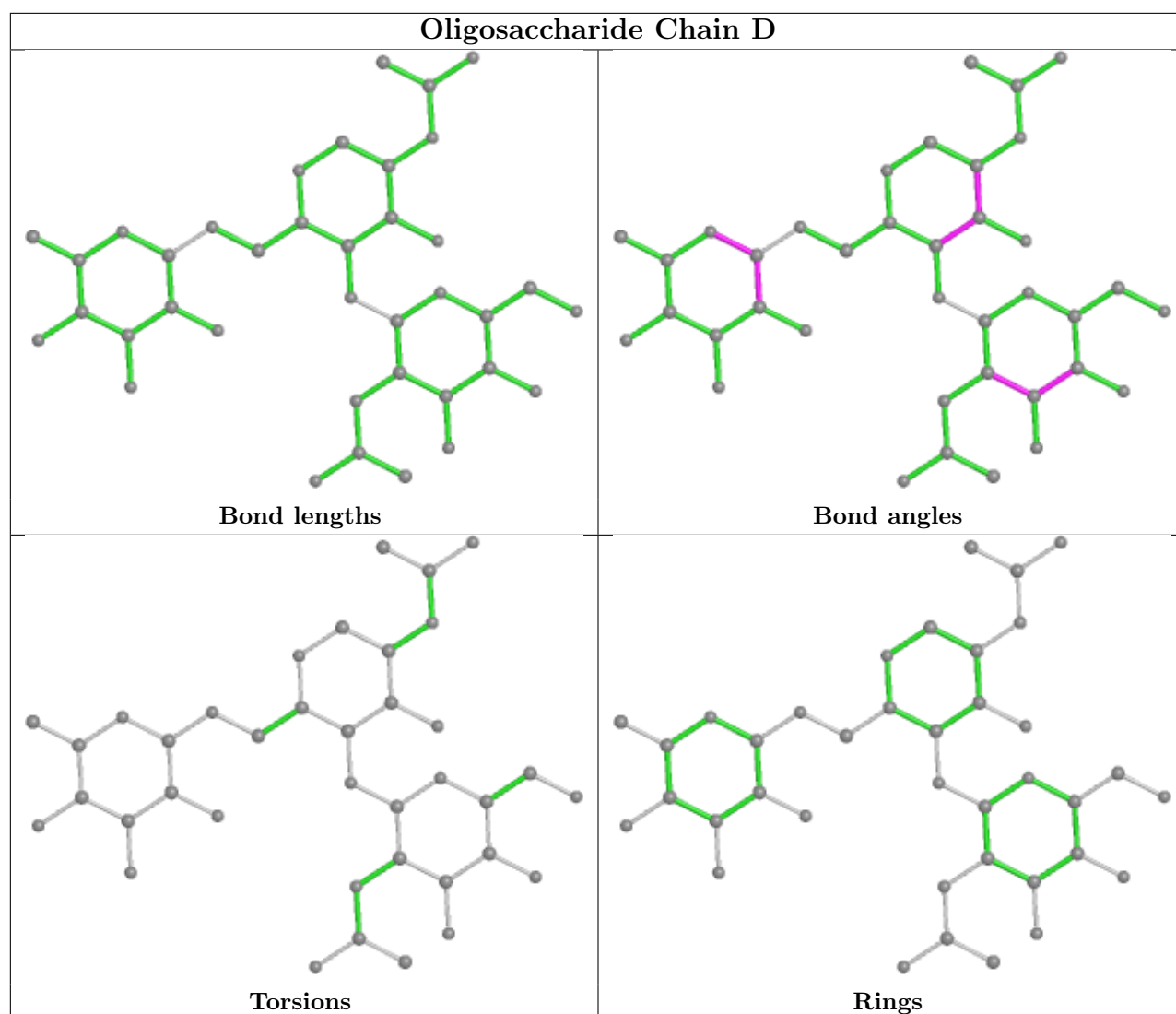
Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6

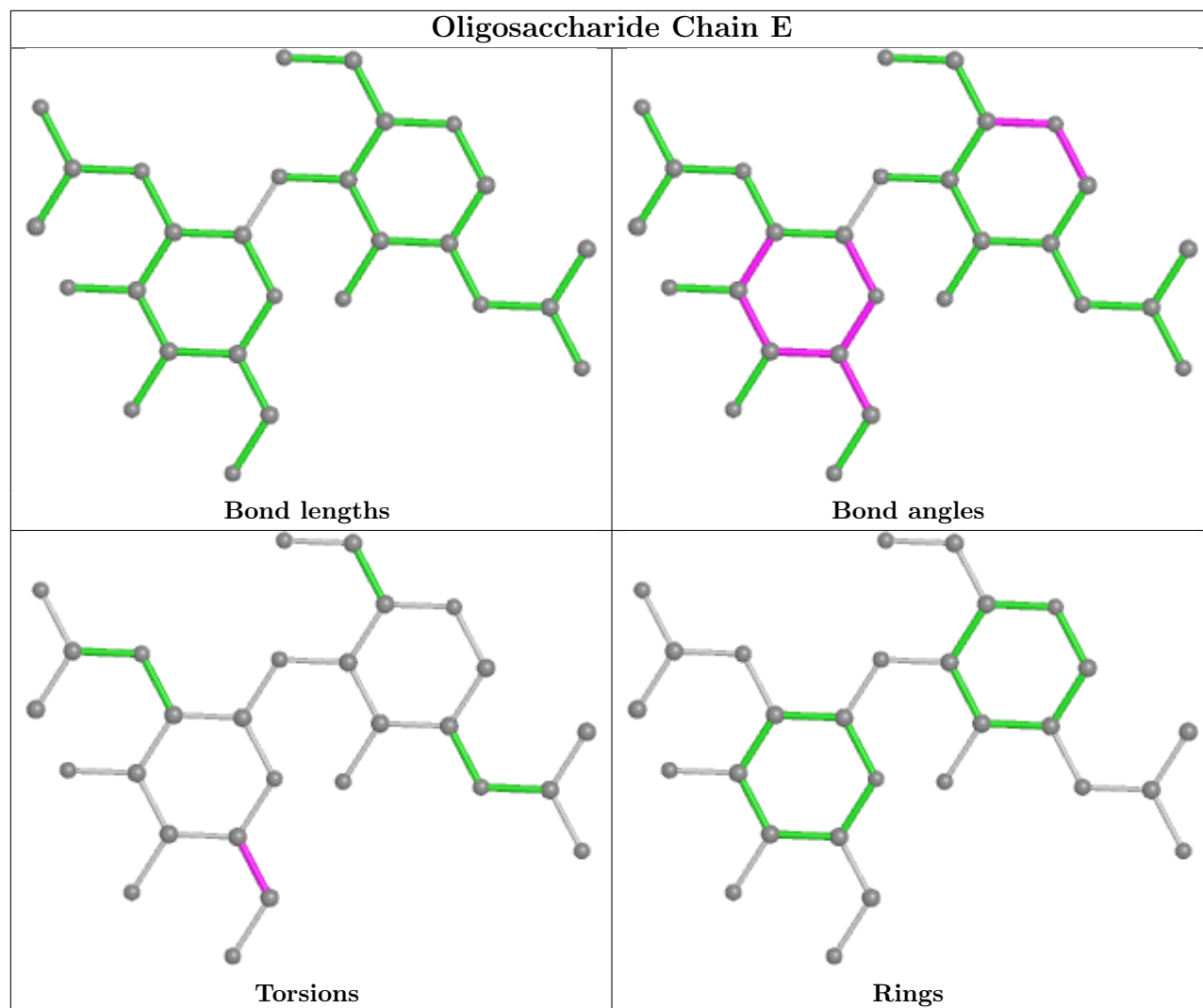
There are no ring outliers.

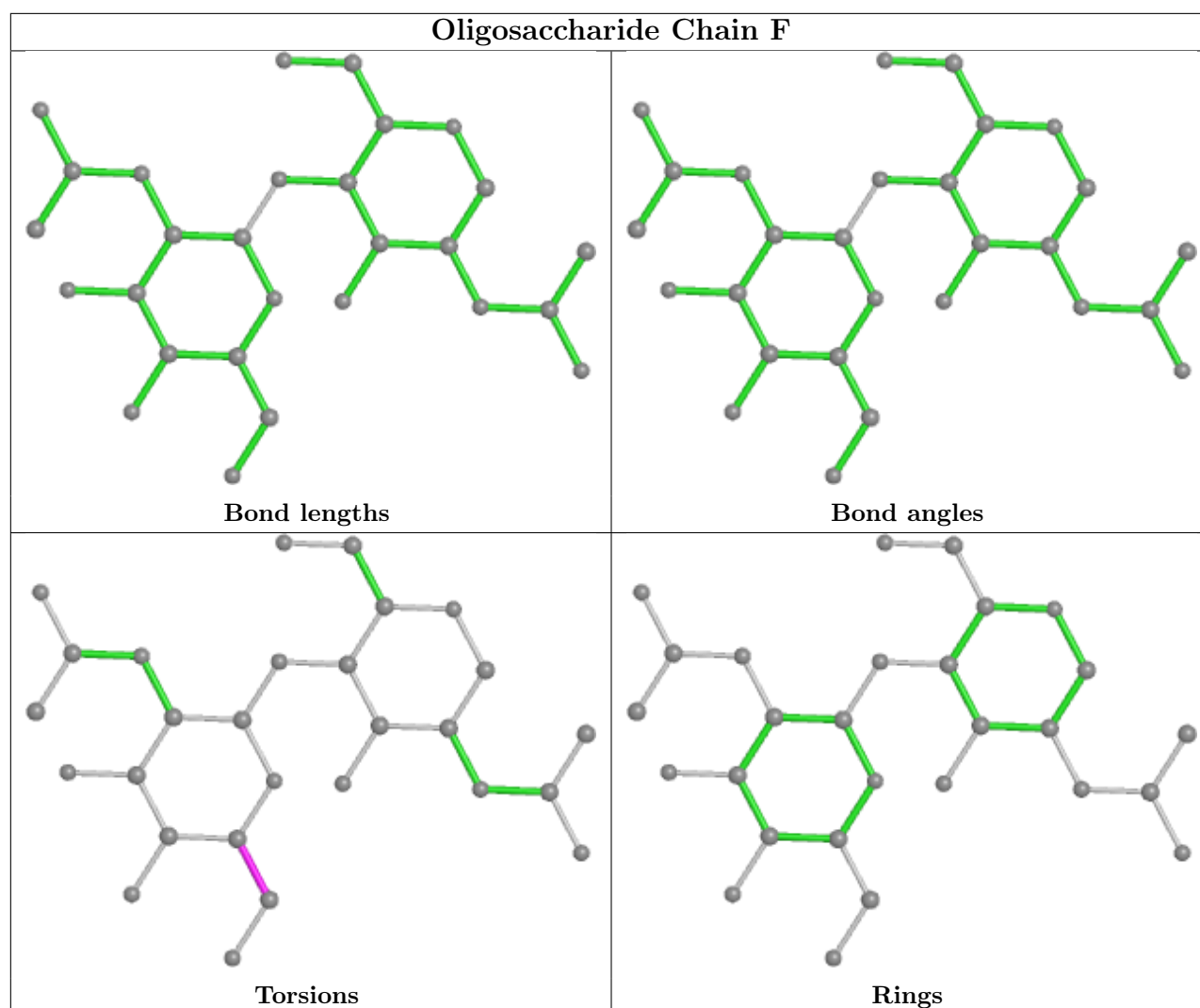
No monomer is involved in short contacts.

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](#)

2 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	$\# Z > 2$
6	NAG	A	401	1	14,14,15	0.64	0	17,19,21	1.53	1 (5%)
6	NAG	A	414	1	14,14,15	0.50	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
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1
6	NAG	A	414	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	NAG	C1-O5-C5	5.20	119.24	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 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	317/321 (98%)	0.90	45 (14%) 2 2	30, 60, 190, 212	0
2	B	173/176 (98%)	-0.32	1 (0%) 89 89	29, 39, 59, 103	0
All	All	490/497 (98%)	0.47	46 (9%) 8 9	29, 47, 153, 212	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ALA	21.0
1	A	193	PHE	17.7
1	A	186	VAL	15.7
1	A	157	LEU	15.6
1	A	195	TYR	14.9
1	A	194	PRO	14.6
1	A	156	HIS	13.5
1	A	189	ASN	11.2
1	A	159	PHE	11.1
1	A	192	ILE	10.3
1	A	188	ASP	10.3
1	A	190	ASP	9.9
1	A	158	LYS	9.5
1	A	191	GLN	8.8
1	A	220	ARG	7.8
1	A	197	GLN	7.7
1	A	219	SER	7.3
1	A	161	TYR	6.6
1	A	218	GLY	6.4
1	A	222	ARG	5.6
1	A	221	PRO	5.6
1	A	187	THR	5.4
1	A	225	ASN	5.2
1	A	198	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	226	ILE	4.9
1	A	129	GLY	4.8
1	A	130	VAL	4.6
1	A	162	PRO	4.5
1	A	199	SER	4.4
1	A	217	ILE	4.0
1	A	223	VAL	3.7
1	A	160	LYS	3.4
1	A	128	THR	3.3
1	A	142	ARG	3.2
1	A	131	THR	3.2
1	A	124	SER	3.1
1	A	173	LYS	2.8
1	A	164	LEU	2.5
1	A	214	ILE	2.4
1	A	212	THR	2.4
1	A	224	ARG	2.4
1	A	165	ASN	2.4
1	A	185	PRO	2.4
2	B	172	GLN	2.3
1	A	144	ASN	2.1
1	A	213	VAL	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.

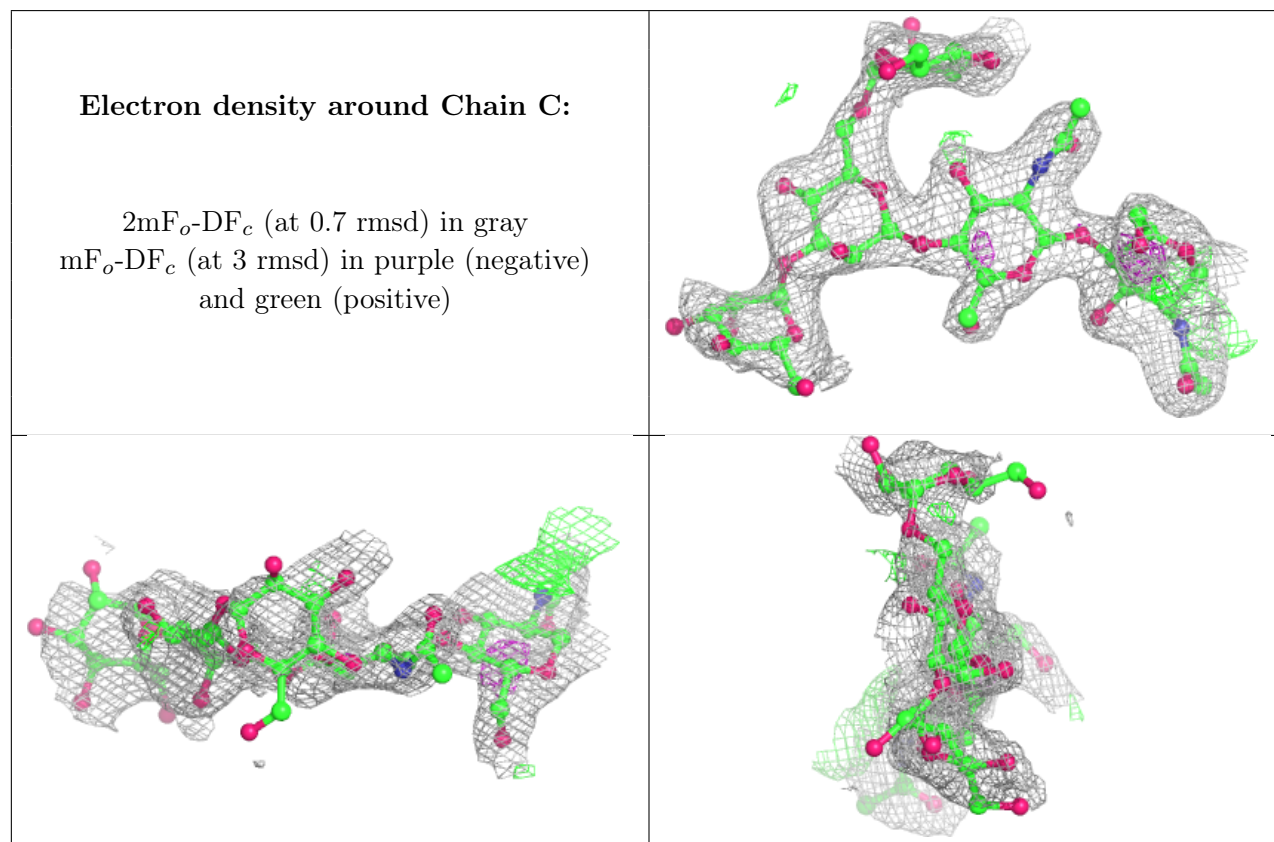
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	1	14/15	0.58	0.37	121,127,132,137	0
3	MAN	C	5	11/12	0.66	0.37	113,119,121,121	0
5	NAG	E	2	14/15	0.70	0.43	138,142,146,147	0
3	BMA	C	3	11/12	0.71	0.19	105,109,116,119	0
4	NAG	D	2	14/15	0.78	0.41	107,115,118,119	0
4	NAG	D	1	14/15	0.79	0.27	78,86,103,105	0

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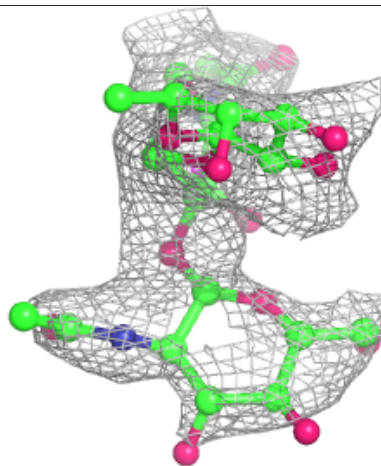
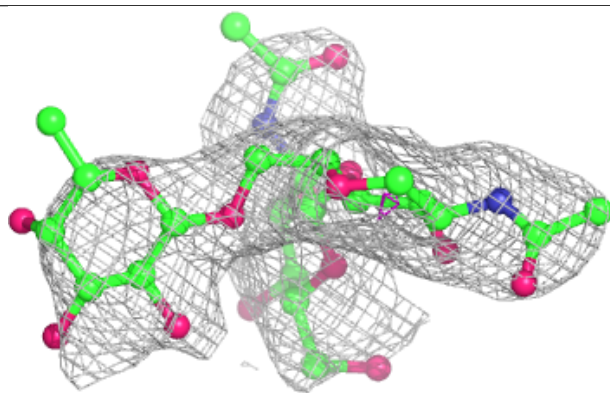
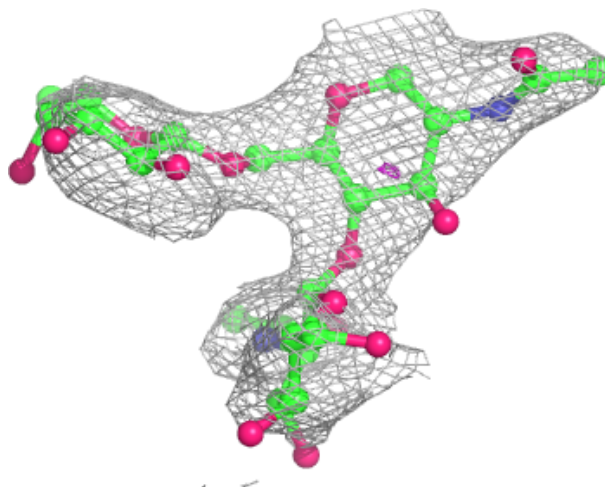
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	C	4	11/12	0.79	0.22	112,117,121,121	0
3	NAG	C	2	14/15	0.80	0.26	75,79,87,96	0
4	FUL	D	3	10/11	0.82	0.44	110,114,117,118	0
3	NAG	C	1	14/15	0.83	0.20	53,58,63,69	0
5	NAG	F	2	14/15	0.83	0.30	84,91,97,97	0
5	NAG	F	1	14/15	0.91	0.17	47,57,62,74	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.



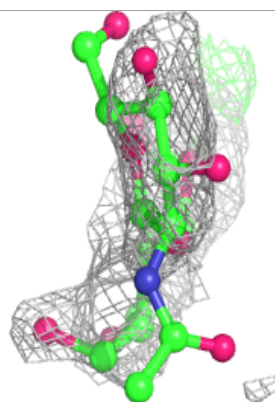
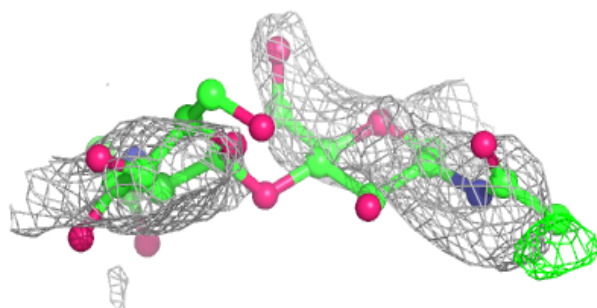
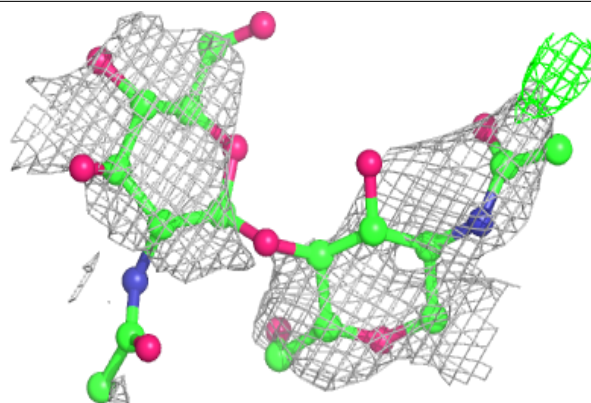
Electron density around Chain D:

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

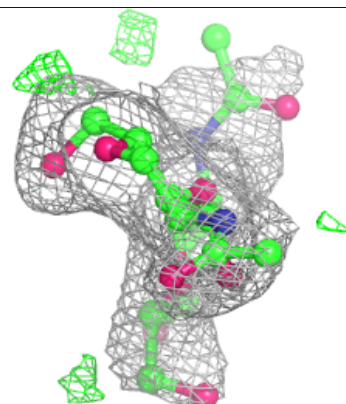
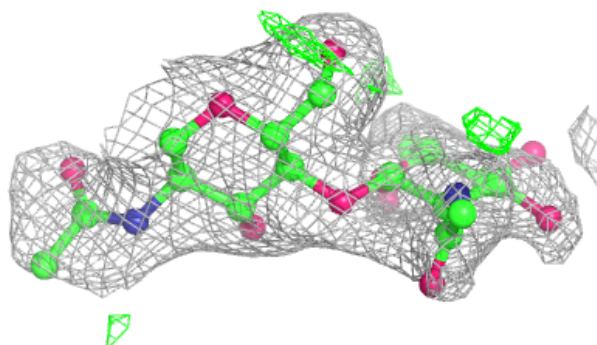
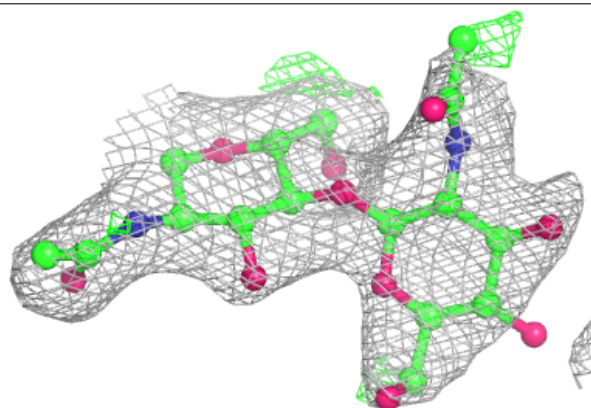


Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
6	NAG	A	401	14/15	0.51	0.45	79,93,94,94	0
6	NAG	A	414	14/15	0.80	0.18	96,106,108,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.