



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2024 – 06:16 PM EDT

PDB ID : 8VQR  
Title : Crystal structure of chimeric SARS-CoV-2 RBD complexed with chimeric raccoon dog ACE2  
Authors : Hsueh, F.-C.; Shi, K.; Aihara, H.; Li, F.  
Deposited on : 2024-01-19  
Resolution : 2.56 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](mailto: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>.

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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

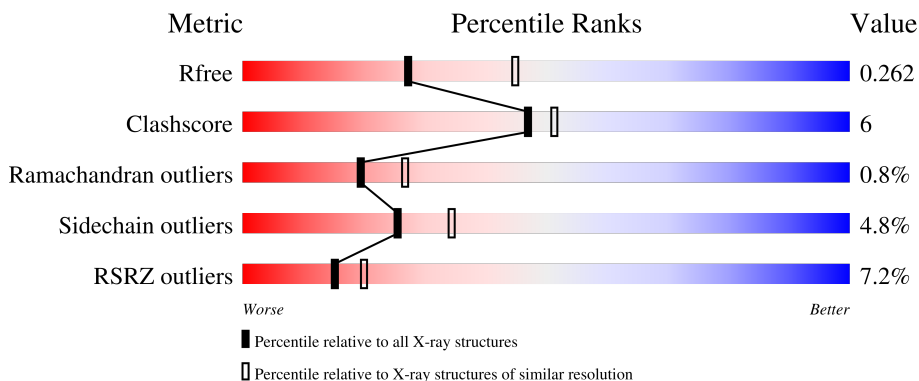
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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  $\geq 3$ , 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	602	 6% 78% 18% ..
1	B	602	 2% 85% 13% ..
2	E	232	 9% 65% 17% • 17%
2	F	232	 17% 65% 16% • 16%
3	C	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	D	5	 60% 40%
5	G	2	 50% 50%
5	I	2	 100%
6	H	4	 75% 25%
7	J	5	 60% 40%
8	K	3	 67% 33%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13126 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 Angiotensin-converting enzyme, Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	594	4860	3108	804	920	28	0	0	0
1	B	595	4866	3111	805	922	28	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
B	616	HIS	-	expression tag	UNP Q9BYF1
B	617	HIS	-	expression tag	UNP Q9BYF1
B	618	HIS	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	193	1524	982	246	287	9	0	0	0
2	F	194	1531	984	248	290	9	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	321	VAL	GLN	engineered mutation	UNP P0DTC2
E	323	SER	THR	engineered mutation	UNP P0DTC2
E	324	GLY	GLU	engineered mutation	UNP P0DTC2
E	325	ASP	SER	engineered mutation	UNP P0DTC2
E	326	VAL	ILE	engineered mutation	UNP P0DTC2
E	346	LYS	ARG	variant	UNP P0DTC2
E	348	PRO	ALA	engineered mutation	UNP P0DTC2
E	354	GLU	ASN	engineered mutation	UNP P0DTC2
E	357	LYS	ARG	engineered mutation	UNP P0DTC2
E	372	THR	ALA	engineered mutation	UNP P0DTC2
E	373	PHE	SER	engineered mutation	UNP P0DTC2
E	384	ALA	PRO	engineered mutation	UNP P0DTC2
E	393	SER	THR	engineered mutation	UNP P0DTC2
E	402	VAL	ILE	engineered mutation	UNP P0DTC2
E	403	LYS	ARG	engineered mutation	UNP P0DTC2
E	406	ASP	GLU	engineered mutation	UNP P0DTC2
E	417	VAL	LYS	engineered mutation	UNP P0DTC2
E	430	MET	THR	engineered mutation	UNP P0DTC2
E	434	LEU	ILE	engineered mutation	UNP P0DTC2
E	438	THR	SER	engineered mutation	UNP P0DTC2
E	439	ARG	ASN	engineered mutation	UNP P0DTC2
E	441	ILE	LEU	engineered mutation	UNP P0DTC2
E	443	ALA	SER	engineered mutation	UNP P0DTC2
E	444	THR	LYS	variant	UNP P0DTC2
E	445	SER	VAL	engineered mutation	UNP P0DTC2
E	446	THR	GLY	engineered mutation	UNP P0DTC2
E	452	LYS	LEU	engineered mutation	UNP P0DTC2
E	519	ASN	HIS	engineered mutation	UNP P0DTC2
E	529	LEU	LYS	engineered mutation	UNP P0DTC2
E	532	ASP	ASN	engineered mutation	UNP P0DTC2
E	534	ILE	VAL	engineered mutation	UNP P0DTC2
E	536	SER	ASN	engineered mutation	UNP P0DTC2
E	537	GLY	-	expression tag	UNP P0DTC2
E	538	GLU	-	expression tag	UNP P0DTC2
E	539	ASN	-	expression tag	UNP P0DTC2
E	540	LEU	-	expression tag	UNP P0DTC2
E	541	TYR	-	expression tag	UNP P0DTC2
E	542	PHE	-	expression tag	UNP P0DTC2
E	543	GLN	-	expression tag	UNP P0DTC2
E	544	GLY	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	548	HIS	-	expression tag	UNP P0DTC2
E	549	HIS	-	expression tag	UNP P0DTC2
E	550	HIS	-	expression tag	UNP P0DTC2
F	321	VAL	GLN	engineered mutation	UNP P0DTC2
F	323	SER	THR	engineered mutation	UNP P0DTC2
F	324	GLY	GLU	engineered mutation	UNP P0DTC2
F	325	ASP	SER	engineered mutation	UNP P0DTC2
F	326	VAL	ILE	engineered mutation	UNP P0DTC2
F	346	LYS	ARG	variant	UNP P0DTC2
F	348	PRO	ALA	engineered mutation	UNP P0DTC2
F	354	GLU	ASN	engineered mutation	UNP P0DTC2
F	357	LYS	ARG	engineered mutation	UNP P0DTC2
F	372	THR	ALA	engineered mutation	UNP P0DTC2
F	373	PHE	SER	engineered mutation	UNP P0DTC2
F	384	ALA	PRO	engineered mutation	UNP P0DTC2
F	393	SER	THR	engineered mutation	UNP P0DTC2
F	402	VAL	ILE	engineered mutation	UNP P0DTC2
F	403	LYS	ARG	engineered mutation	UNP P0DTC2
F	406	ASP	GLU	engineered mutation	UNP P0DTC2
F	417	VAL	LYS	engineered mutation	UNP P0DTC2
F	430	MET	THR	engineered mutation	UNP P0DTC2
F	434	LEU	ILE	engineered mutation	UNP P0DTC2
F	438	THR	SER	engineered mutation	UNP P0DTC2
F	439	ARG	ASN	engineered mutation	UNP P0DTC2
F	441	ILE	LEU	engineered mutation	UNP P0DTC2
F	443	ALA	SER	engineered mutation	UNP P0DTC2
F	444	THR	LYS	variant	UNP P0DTC2
F	445	SER	VAL	engineered mutation	UNP P0DTC2
F	446	THR	GLY	engineered mutation	UNP P0DTC2
F	452	LYS	LEU	engineered mutation	UNP P0DTC2
F	519	ASN	HIS	engineered mutation	UNP P0DTC2
F	529	LEU	LYS	engineered mutation	UNP P0DTC2
F	532	ASP	ASN	engineered mutation	UNP P0DTC2
F	534	ILE	VAL	engineered mutation	UNP P0DTC2
F	536	SER	ASN	engineered mutation	UNP P0DTC2
F	537	GLY	-	expression tag	UNP P0DTC2
F	538	GLU	-	expression tag	UNP P0DTC2
F	539	ASN	-	expression tag	UNP P0DTC2
F	540	LEU	-	expression tag	UNP P0DTC2
F	541	TYR	-	expression tag	UNP P0DTC2
F	542	PHE	-	expression tag	UNP P0DTC2
F	543	GLN	-	expression tag	UNP P0DTC2

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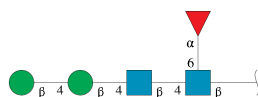
Chain	Residue	Modelled	Actual	Comment	Reference
F	544	GLY	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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.



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

- 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	
			Total	C	N				O
5	G	2	28	16	2	10	0	0	0

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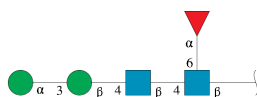
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	2	28	16	2	10	0	0	0

- Molecule 6 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.



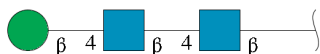
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	H	4	50	28	2	20	0	0	0

- Molecule 7 is an oligosaccharide called 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.



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

- Molecule 8 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			
8	K	3	39	22	2	15	0	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

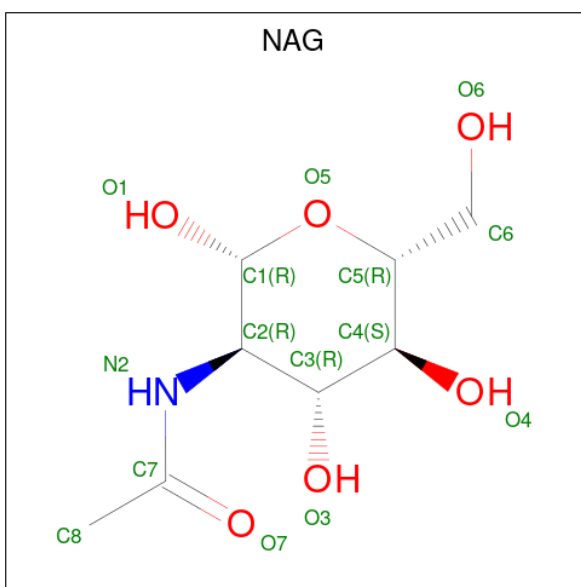


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	B	1	Total	Zn	0	0
			1	1		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

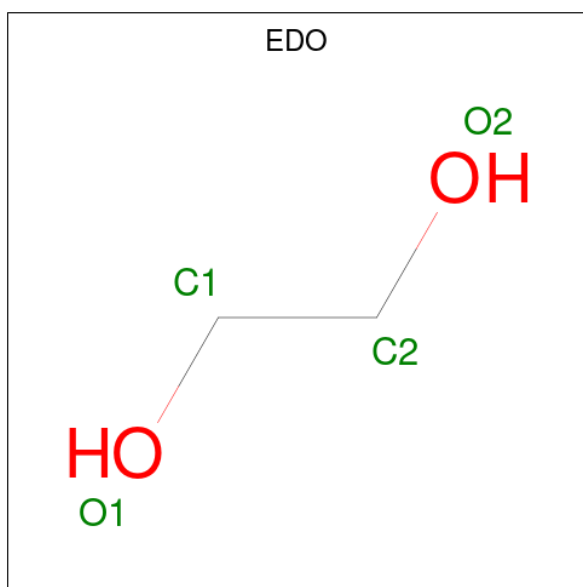
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		
10	B	1	Total	Cl	0	0
			1	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 4 2 2	0	0
12	B	1	Total C O 4 2 2	0	0

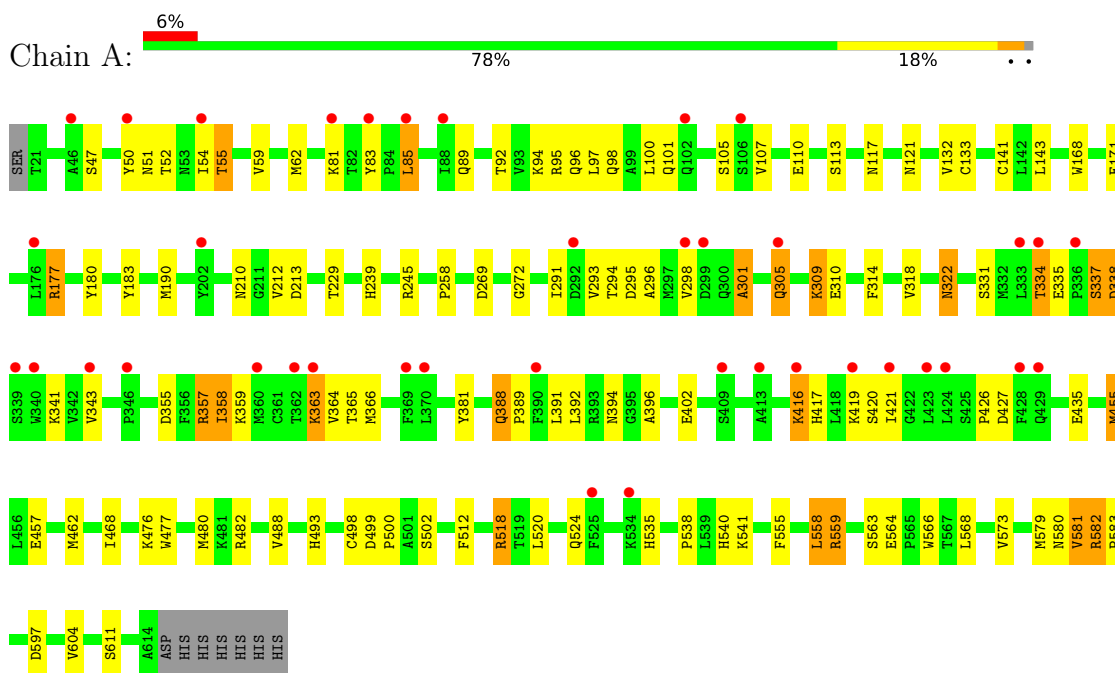
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	8	Total O 8 8	0	0
13	B	6	Total O 6 6	0	0
13	E	1	Total O 1 1	0	0
13	F	1	Total O 1 1	0	0

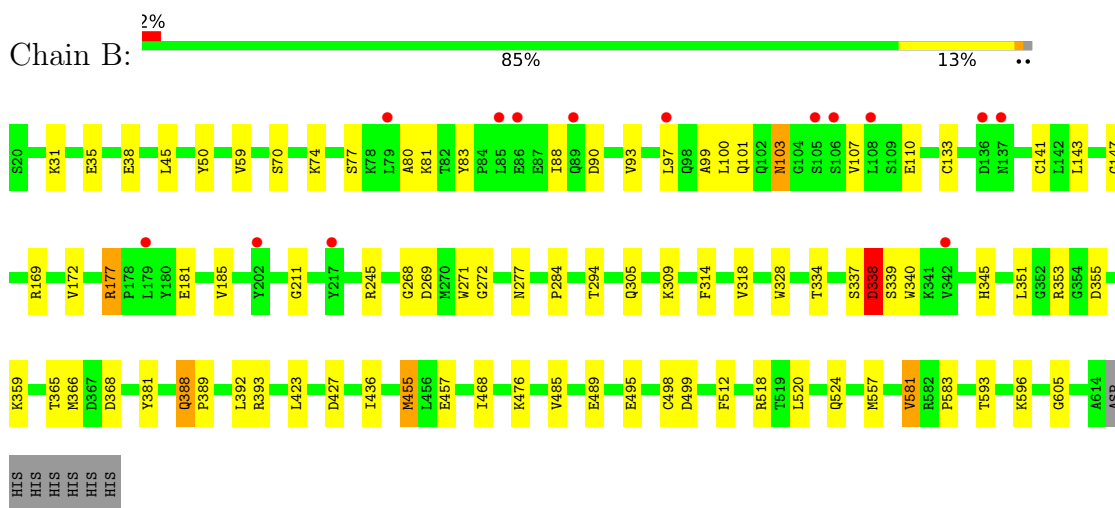
### 3 Residue-property plots i

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: Angiotensin-converting enzyme, Processed angiotensin-converting enzyme 2



- Molecule 1: Angiotensin-converting enzyme, Processed angiotensin-converting enzyme 2



- Molecule 2: Spike protein S1



Chain I:  100%

MAG1  
MAG2

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

Chain H:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 7: 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

Chain J:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
FUC5

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

Chain K:  67% 33%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.96Å 118.11Å 112.23Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	58.41 – 2.56 112.09 – 2.56	Depositor EDS
% Data completeness (in resolution range)	62.8 (58.41-2.56) 59.5 (112.09-2.56)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.214 , 0.264 0.212 , 0.262	Depositor DCC
$R_{free}$ test set	2203 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FUC, NAG, MAN, BMA, ZN, CL, EDO

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	0.24	0/4998	0.45	0/6790
1	B	0.24	0/5004	0.44	0/6798
2	E	0.25	0/1568	0.48	0/2136
2	F	0.26	0/1574	0.48	0/2143
All	All	0.24	0/13144	0.45	0/17867

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	4860	0	4626	68	0
1	B	4866	0	4631	42	0
2	E	1524	0	1437	21	0
2	F	1531	0	1440	27	0
3	C	24	0	22	1	0
4	D	60	0	52	0	0
5	G	28	0	25	1	0
5	I	28	0	25	0	0
6	H	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	60	0	52	0	0
8	K	39	0	34	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	1	0
11	A	14	0	13	0	0
11	B	14	0	13	0	0
12	B	8	0	12	0	0
13	A	8	0	0	0	0
13	B	6	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	13126	0	12425	159	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 6.

The worst 5 of 159 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:98:GLN:HE22	1:A:210:ASN:HD21	1.25	0.81
1:B:338:ASP:N	1:B:338:ASP:OD1	2.22	0.73
1:A:416:LYS:NZ	1:A:541:LYS:O	2.21	0.72
2:F:363:ALA:HB2	2:F:525:CYS:HB3	1.72	0.71
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.74	0.70

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	592/602 (98%)	567 (96%)	21 (4%)	4 (1%)	22	29
1	B	593/602 (98%)	569 (96%)	20 (3%)	4 (1%)	22	29
2	E	191/232 (82%)	171 (90%)	19 (10%)	1 (0%)	29	39
2	F	190/232 (82%)	168 (88%)	19 (10%)	3 (2%)	9	12
All	All	1566/1668 (94%)	1475 (94%)	79 (5%)	12 (1%)	19	27

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	ASP
1	B	147	GLY
1	B	340	TRP
1	A	212	VAL
1	A	337	SER

### 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	527/535 (98%)	496 (94%)	31 (6%)	19	25
1	B	528/535 (99%)	511 (97%)	17 (3%)	39	51
2	E	166/203 (82%)	156 (94%)	10 (6%)	19	24
2	F	167/203 (82%)	158 (95%)	9 (5%)	22	29
All	All	1388/1476 (94%)	1321 (95%)	67 (5%)	25	34

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	523	THR
2	F	357	LYS
2	F	462	LYS
1	A	518	ARG
1	A	455	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
2	F	388	ASN
1	B	194	ASN
2	F	474	GLN
2	E	501	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

23 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	1,3	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
3	FUC	C	2	3	10,10,11	0.71	0	14,14,16	0.97	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	D	2	4	14,14,15	0.52	0	17,19,21	0.66	0
4	BMA	D	3	4	11,11,12	1.46	2 (18%)	15,15,17	1.42	3 (20%)
4	BMA	D	4	4	11,11,12	0.97	0	15,15,17	1.06	1 (6%)
4	FUC	D	5	4	10,10,11	0.70	0	14,14,16	0.84	0
5	NAG	G	1	1,5	14,14,15	0.53	0	17,19,21	0.83	0
5	NAG	G	2	5	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	H	1	1,6	14,14,15	0.38	0	17,19,21	0.44	0
6	NAG	H	2	6	14,14,15	0.35	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	H	3	6	11,11,12	0.70	0	15,15,17	0.87	0
6	MAN	H	4	6	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
5	NAG	I	1	1,5	14,14,15	0.30	0	17,19,21	0.58	0
5	NAG	I	2	5	14,14,15	0.38	0	17,19,21	0.49	0
7	NAG	J	1	1,7	14,14,15	0.31	0	17,19,21	0.54	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.47	0
7	BMA	J	3	7	11,11,12	1.46	2 (18%)	15,15,17	1.13	1 (6%)
7	MAN	J	4	7	11,11,12	0.79	1 (9%)	15,15,17	1.37	2 (13%)
7	FUC	J	5	7	10,10,11	0.74	0	14,14,16	0.83	0
8	NAG	K	1	2,8	14,14,15	0.42	0	17,19,21	1.27	2 (11%)
8	NAG	K	2	8	14,14,15	0.31	0	17,19,21	0.43	0
8	BMA	K	3	8	11,11,12	0.60	0	15,15,17	0.86	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	1,3	-	3/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	1/1/1/1
7	FUC	J	5	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	K	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	3	BMA	C2-C3	3.48	1.57	1.52
4	D	3	BMA	C4-C3	2.86	1.59	1.52
4	D	3	BMA	C2-C3	2.55	1.56	1.52
7	J	3	BMA	O3-C3	2.49	1.48	1.43
7	J	4	MAN	C1-C2	2.08	1.56	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1	NAG	C2-N2-C7	4.33	129.06	122.90
7	J	4	MAN	C1-O5-C5	4.30	118.02	112.19
4	D	3	BMA	C2-C3-C4	3.16	116.36	110.89
6	H	4	MAN	C1-O5-C5	2.72	115.88	112.19
3	C	1	NAG	C1-O5-C5	2.60	115.71	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	D	4	BMA	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

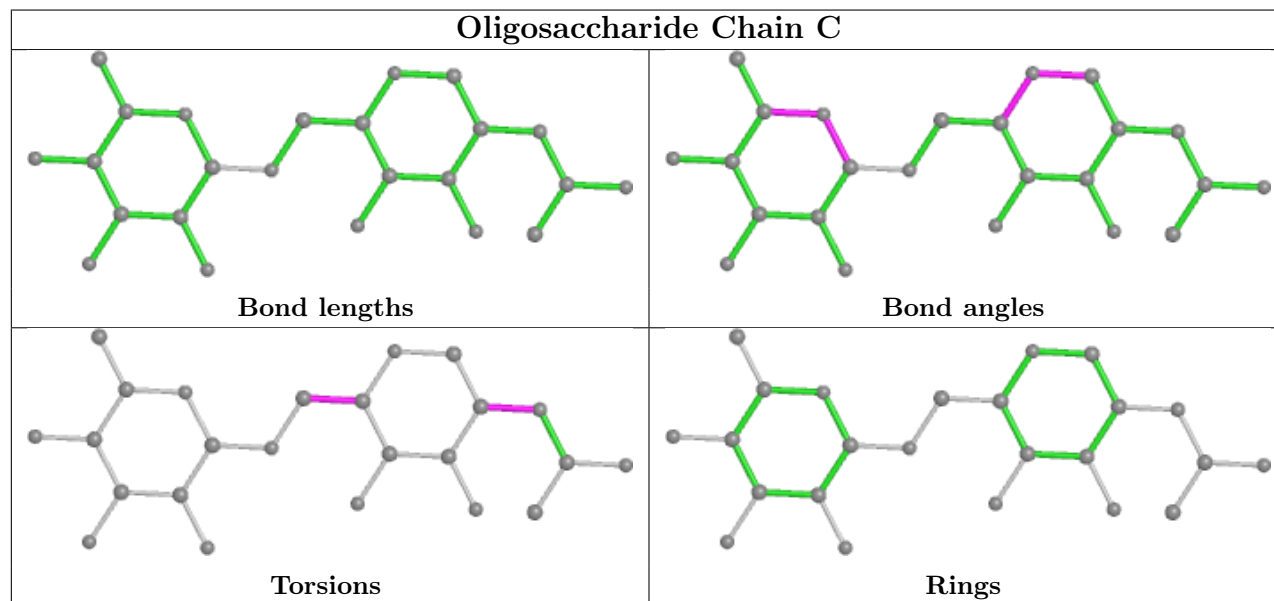
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0

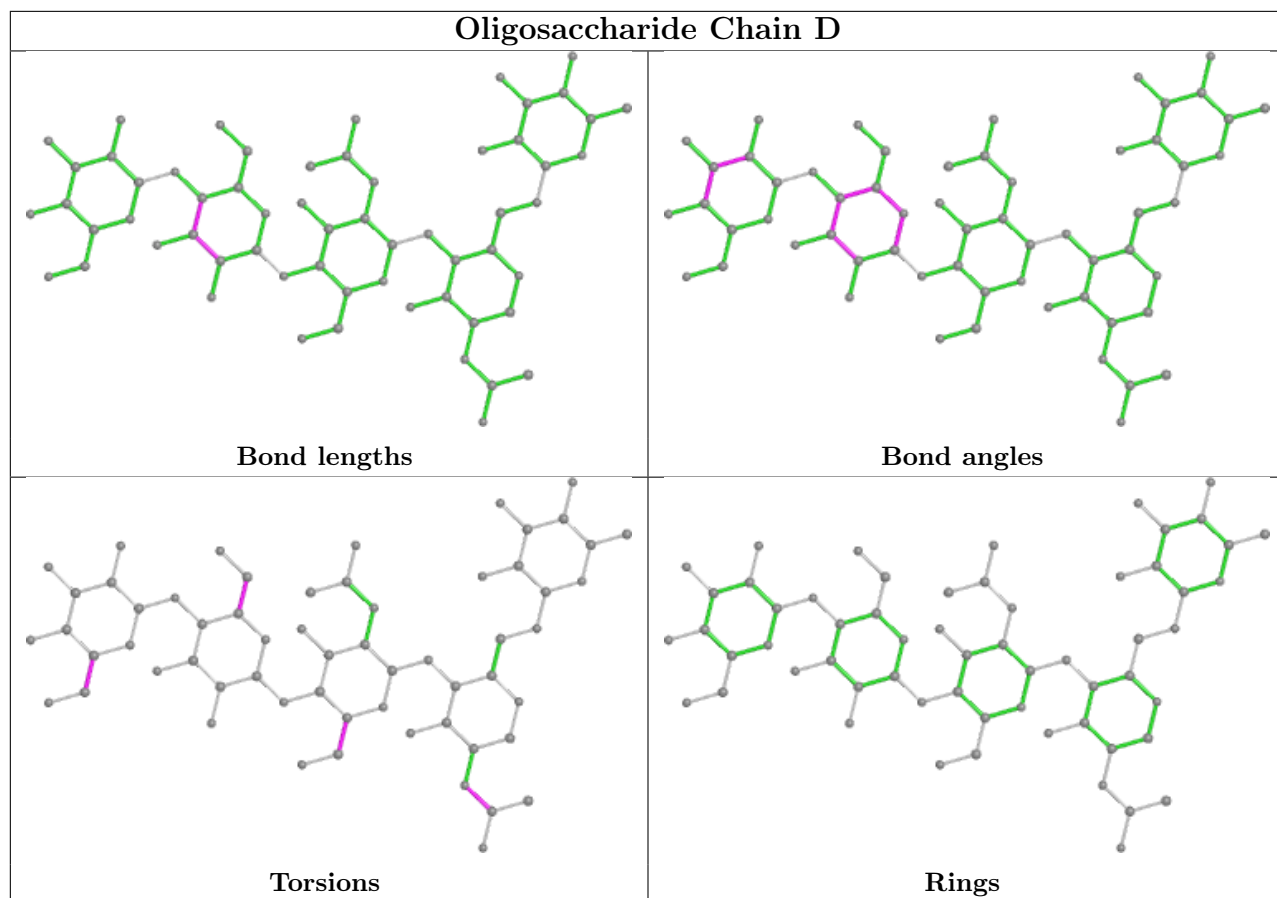
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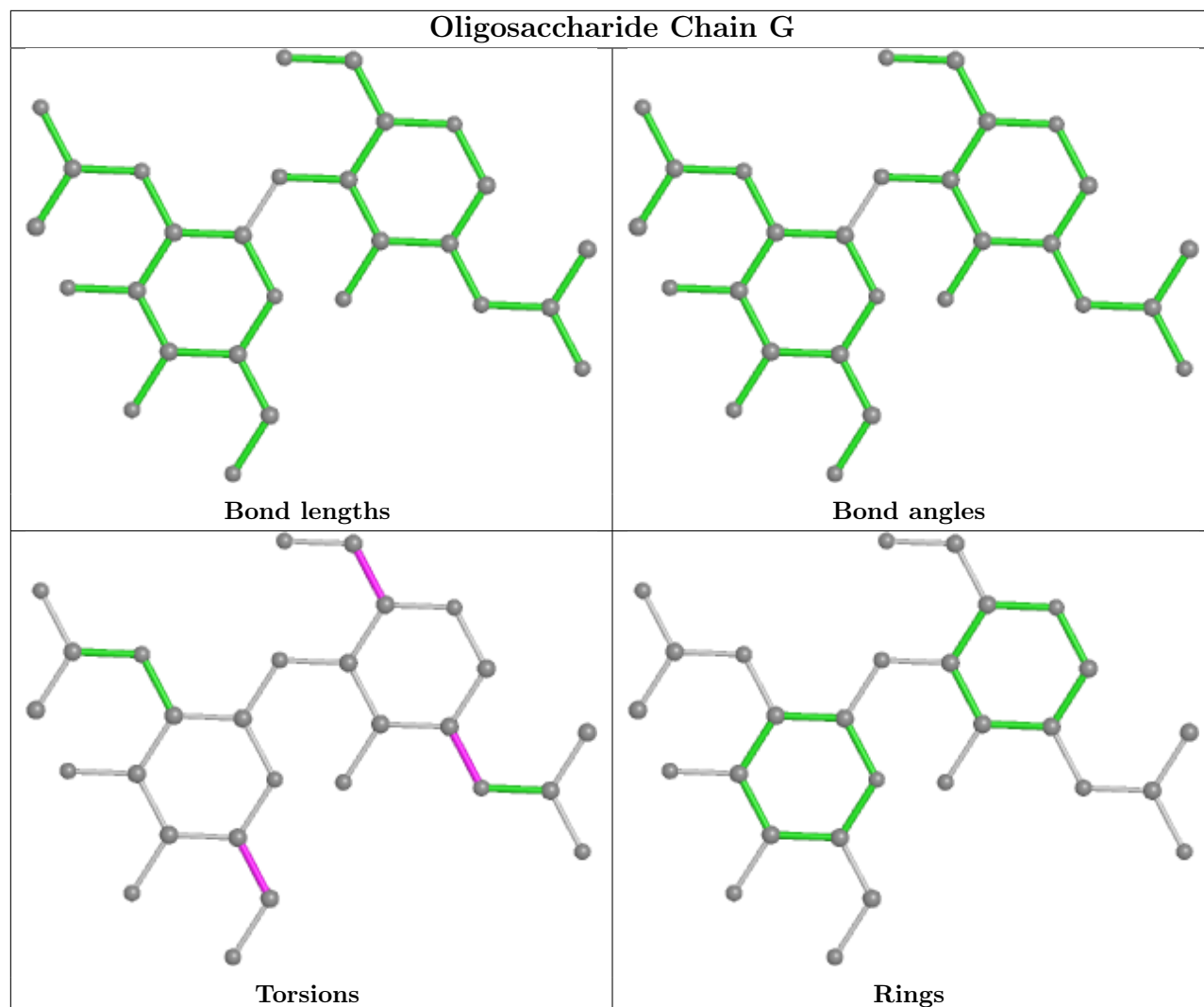
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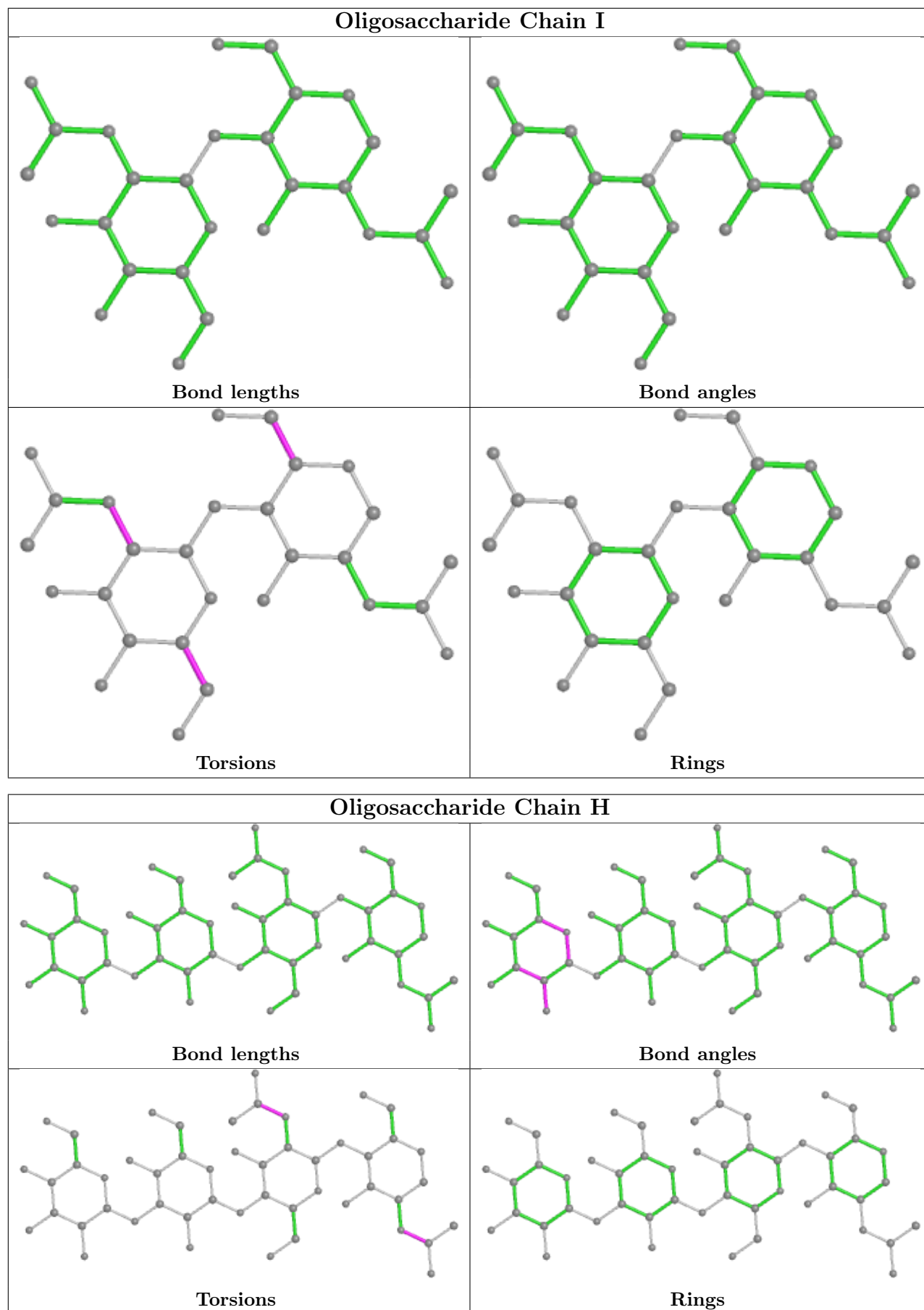
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1	NAG	1	0
5	G	1	NAG	1	0

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

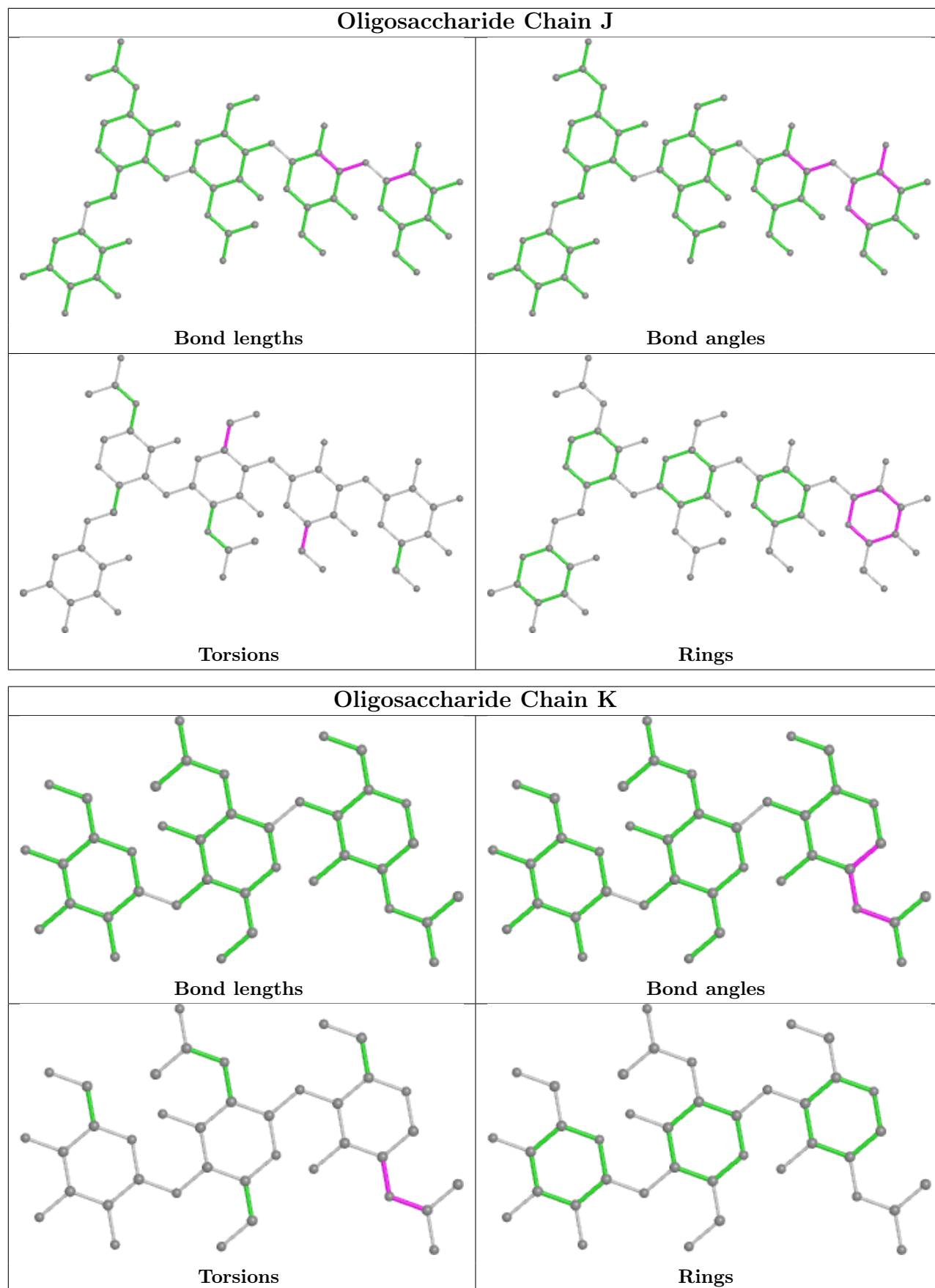












## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	B	705	1	14,14,15	0.26	0	17,19,21	0.46	0
12	EDO	B	703	-	3,3,3	0.45	0	2,2,2	0.34	0
11	NAG	A	703	1	14,14,15	0.25	0	17,19,21	0.44	0
12	EDO	B	704	-	3,3,3	0.45	0	2,2,2	0.34	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
11	NAG	B	705	1	-	4/6/23/26	0/1/1/1
12	EDO	B	703	-	-	0/1/1/1	-
11	NAG	A	703	1	-	2/6/23/26	0/1/1/1
12	EDO	B	704	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	703	NAG	C8-C7-N2-C2
11	A	703	NAG	O7-C7-N2-C2
11	B	705	NAG	C8-C7-N2-C2
11	B	705	NAG	O7-C7-N2-C2
11	B	705	NAG	C4-C5-C6-O6

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/602 (98%)	0.37	39 (6%) 18 23	39, 83, 141, 203	0
1	B	595/602 (98%)	0.19	14 (2%) 59 67	37, 69, 134, 217	0
2	E	193/232 (83%)	0.71	22 (11%) 5 7	45, 77, 167, 277	0
2	F	194/232 (83%)	1.17	39 (20%) 1 1	59, 112, 183, 248	0
All	All	1576/1668 (94%)	0.44	114 (7%) 15 20	37, 80, 155, 277	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	522	ALA	18.8
2	E	521	PRO	18.7
2	F	331	ASN	14.4
2	F	332	ILE	8.4
2	F	522	ALA	8.3

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	I	2	14/15	0.60	0.28	99,114,128,129	0
8	NAG	K	2	14/15	0.67	0.27	115,125,149,149	0

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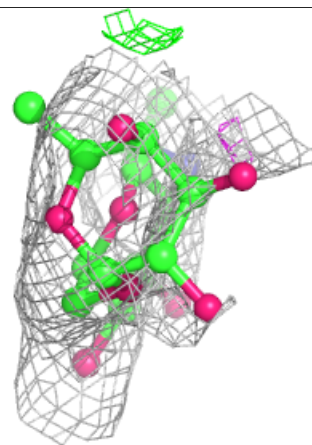
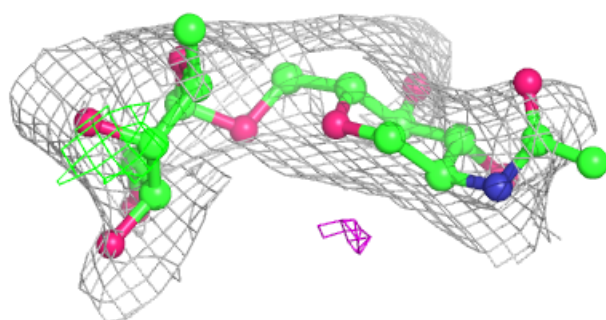
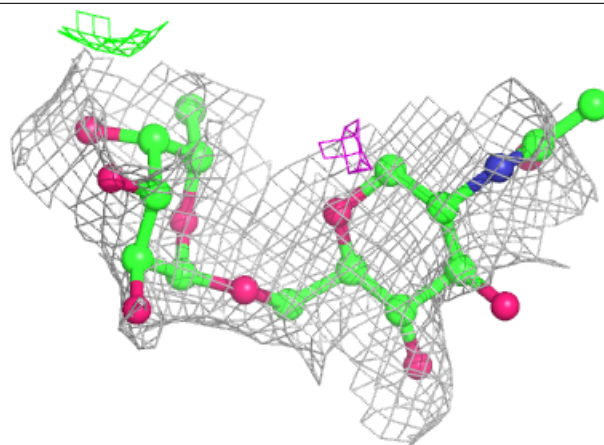
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	C	2	10/11	0.68	0.20	117,141,146,147	0
4	BMA	D	3	11/12	0.68	0.32	114,122,138,138	0
8	BMA	K	3	11/12	0.75	0.17	122,126,144,155	0
3	NAG	C	1	14/15	0.77	0.27	129,138,147,152	0
4	NAG	D	2	14/15	0.80	0.16	88,119,130,134	0
5	NAG	I	1	14/15	0.82	0.15	86,100,116,118	0
6	MAN	H	4	11/12	0.82	0.30	71,100,112,118	0
7	NAG	J	1	14/15	0.83	0.24	101,116,124,129	0
4	BMA	D	4	11/12	0.84	0.21	78,109,117,122	0
5	NAG	G	2	14/15	0.86	0.15	84,118,138,150	0
7	NAG	J	2	14/15	0.86	0.21	80,102,111,115	0
4	NAG	D	1	14/15	0.87	0.19	120,128,136,138	0
4	FUC	D	5	10/11	0.87	0.39	90,102,118,121	0
7	BMA	J	3	11/12	0.88	0.20	84,98,112,114	0
7	FUC	J	5	10/11	0.89	0.23	90,101,114,115	0
5	NAG	G	1	14/15	0.89	0.21	99,116,123,128	0
6	BMA	H	3	11/12	0.89	0.13	69,83,99,101	0
7	MAN	J	4	11/12	0.90	0.13	57,79,93,96	0
8	NAG	K	1	14/15	0.90	0.13	86,115,127,132	0
6	NAG	H	2	14/15	0.95	0.15	49,59,76,93	0
6	NAG	H	1	14/15	0.98	0.13	35,54,73,82	0

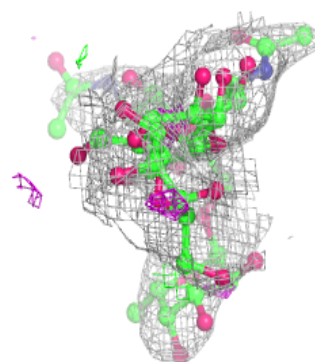
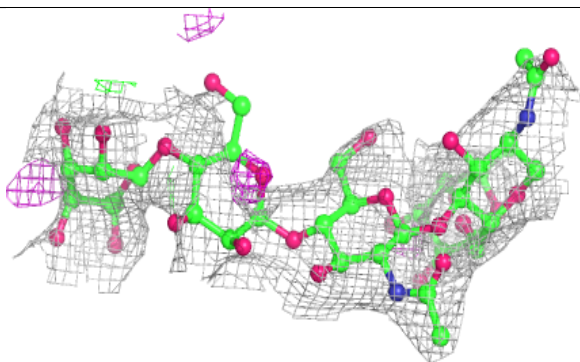
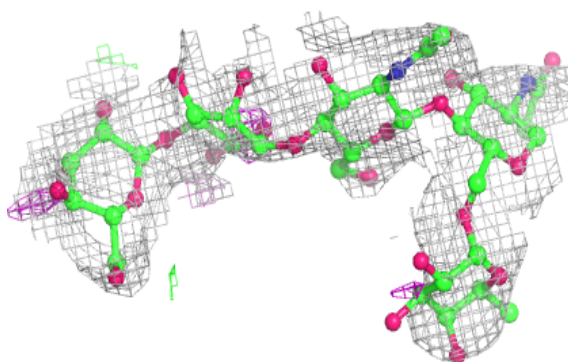
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

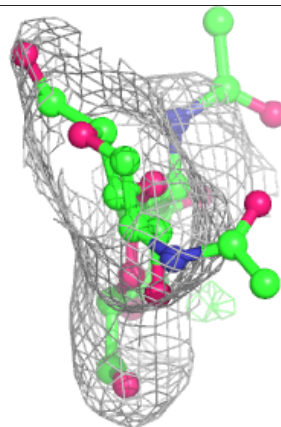
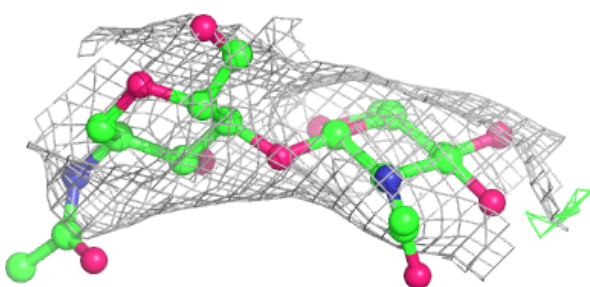
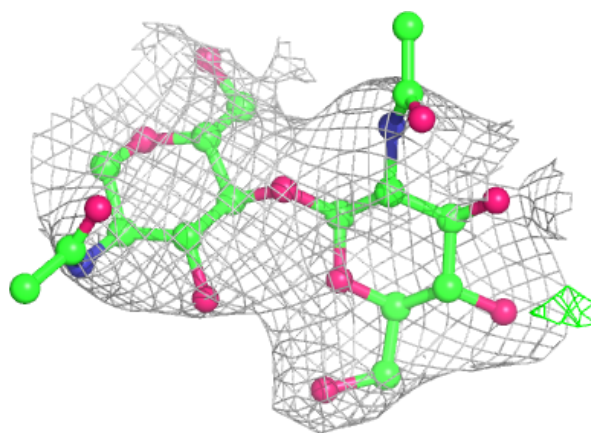
**Electron density around Chain D:**

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

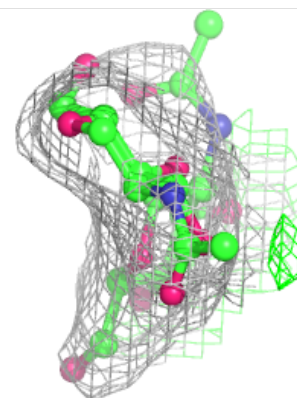
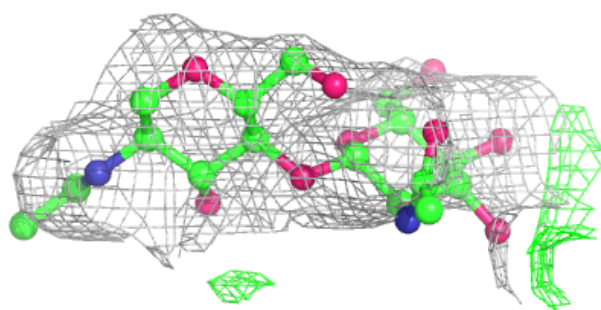
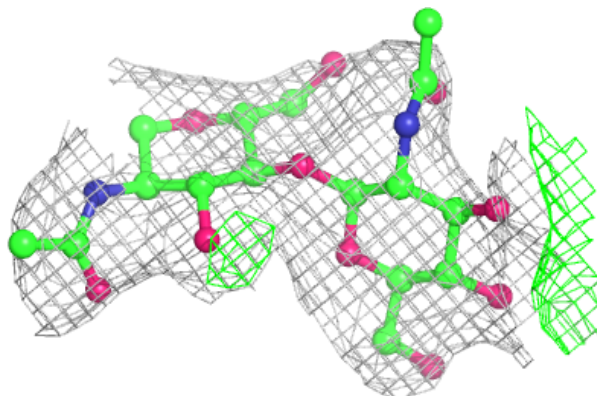


**Electron density around Chain G:**

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

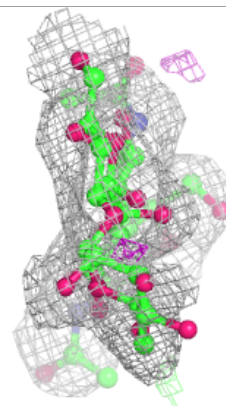
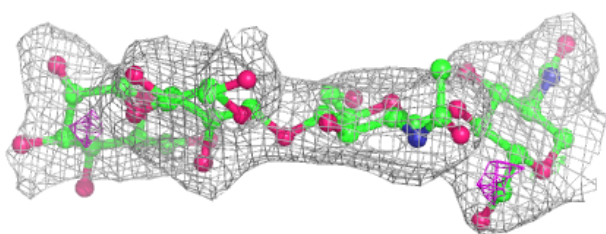
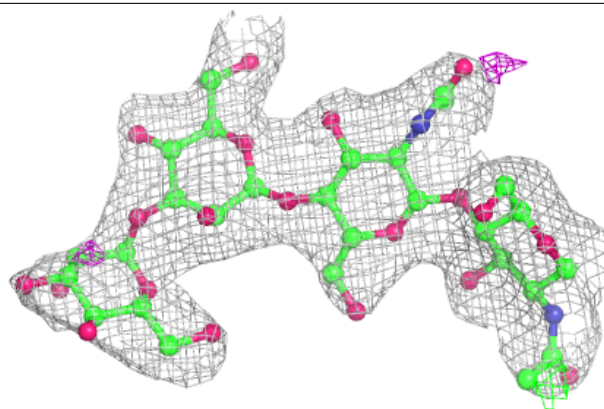
**Electron density around Chain I:**

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

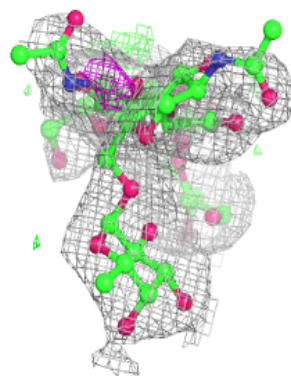
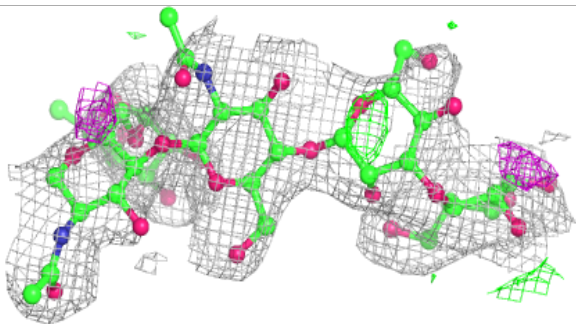
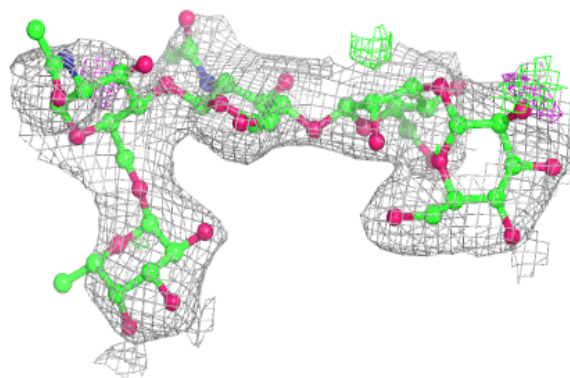


**Electron density around Chain H:**

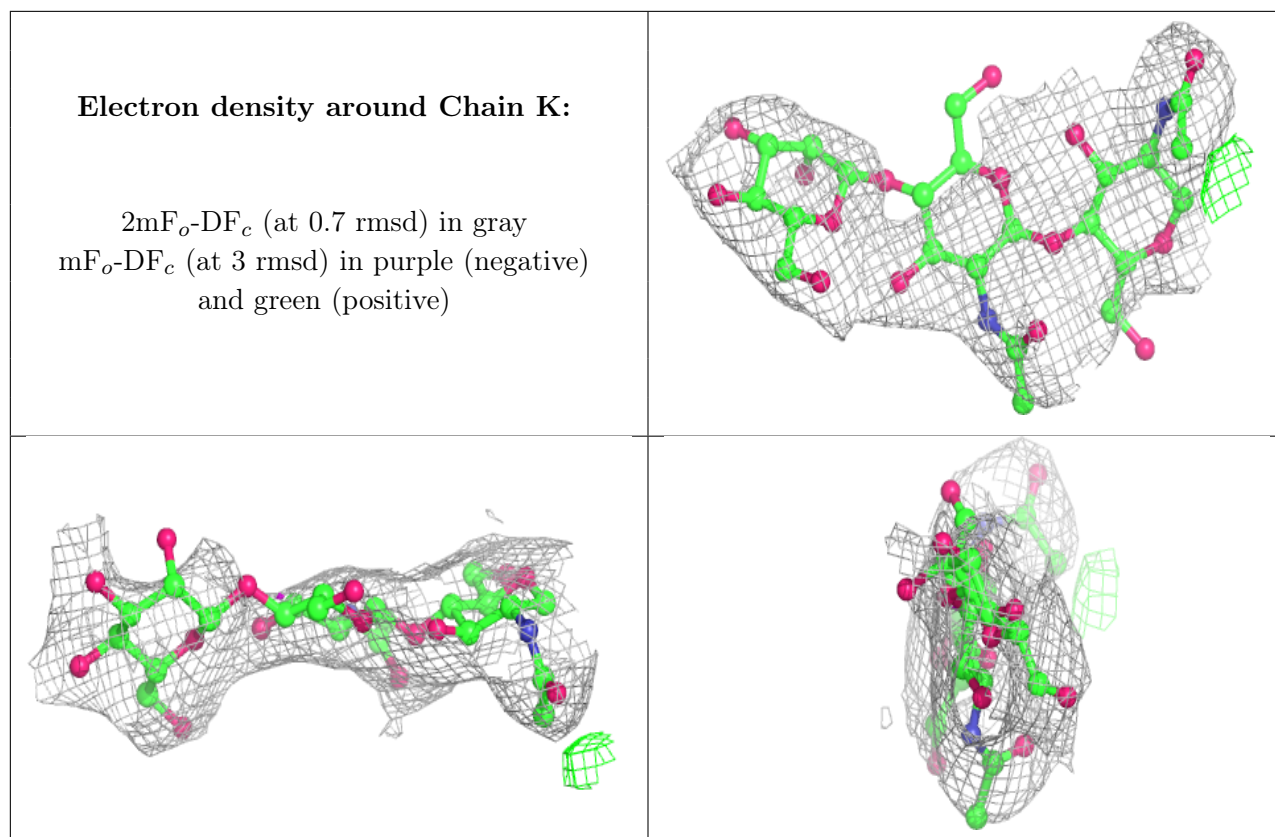
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain J:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	NAG	A	703	14/15	0.74	0.16	98,133,141,147	0
11	NAG	B	705	14/15	0.83	0.26	76,93,105,116	0
12	EDO	B	704	4/4	0.88	0.21	44,52,55,58	0
10	CL	B	702	1/1	0.92	0.09	75,75,75,75	0
12	EDO	B	703	4/4	0.95	0.13	48,53,61,67	0
9	ZN	B	701	1/1	0.95	0.16	85,85,85,85	0
10	CL	A	702	1/1	0.97	0.11	64,64,64,64	0
9	ZN	A	701	1/1	0.97	0.16	85,85,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.