



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:57 PM BST

PDB ID : 5M8Q  
Title : Crystal structure of human tyrosinase related protein 1 mutant (T391V-R374S-Y362F) in complex with kojic acid  
Authors : Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.  
Deposited on : 2016-10-29  
Resolution : 2.85 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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

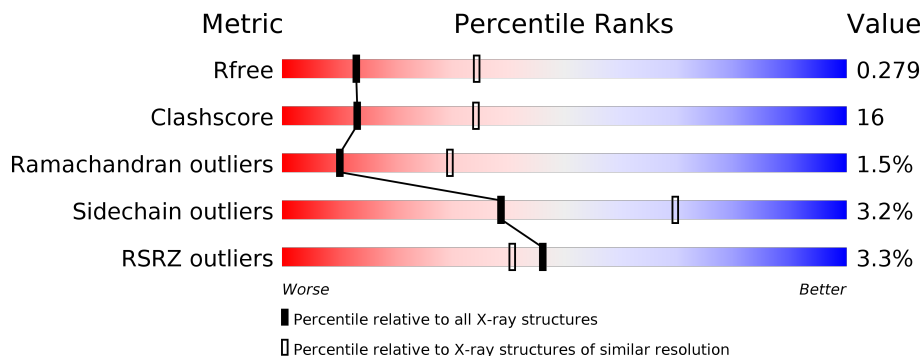
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.



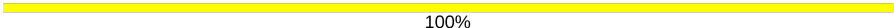

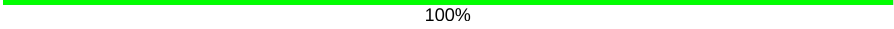

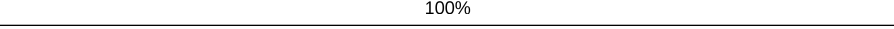
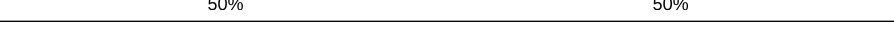
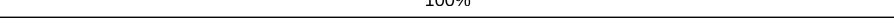
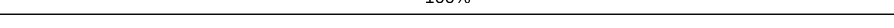

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	446	
1	B	446	
1	C	446	
1	D	446	
2	E	3	
3	F	2	

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	K	2	 50% 50%
3	O	2	 100%
4	G	5	 80% 20%
5	I	2	 100%
5	J	2	 50% 50%
5	M	2	 100%
5	N	2	 100%
6	L	5	 100%

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 14735 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.

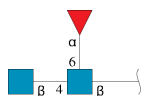
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3554	2231	629	671	23	0	0	0
1	B	446	3554	2231	629	671	23	0	0	0
1	C	446	3554	2231	629	671	23	0	0	0
1	D	446	3554	2231	629	671	23	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

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



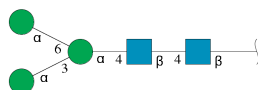
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	38	22	2	14	0	0	0

- Molecule 3 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			
3	F	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	K	2	28	16	2	10	0	0	0
3	O	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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			
4	G	5	61	34	2	25	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



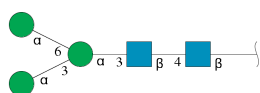
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	2	24	14	1	9	0	0	0

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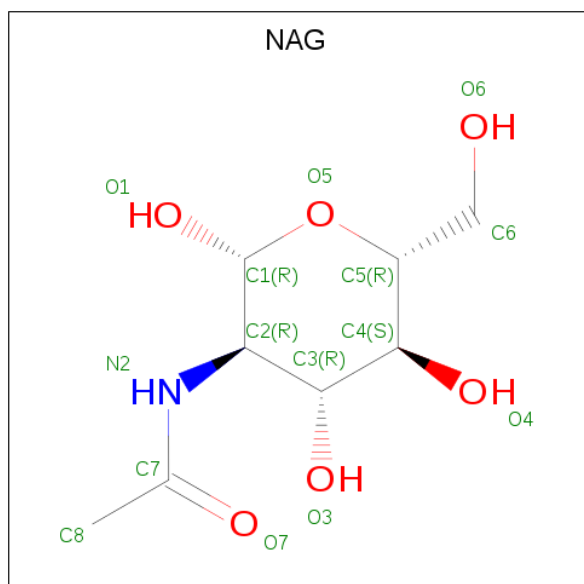
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	2	24	14	1	9	0	0	0
5	M	2	24	14	1	9	0	0	0
5	N	2	24	14	1	9	0	0	0

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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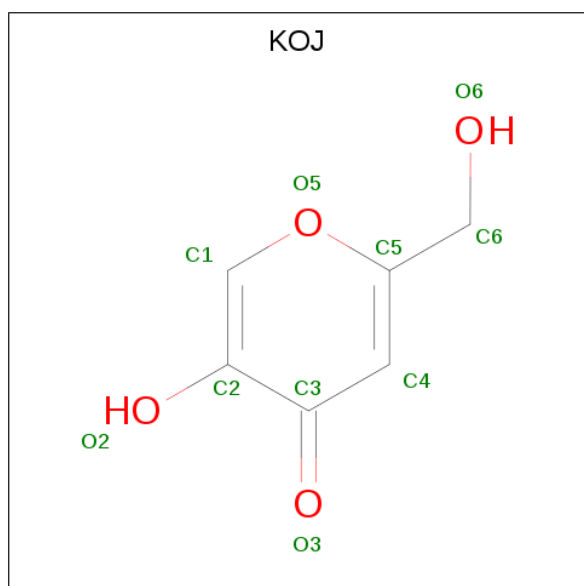
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
	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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Zn	0	0
			2	2		
8	A	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	C	3	Total	Zn	0	0
			3	3		

- Molecule 9 is 5-HYDROXY-2-(HYDROXYMETHYL)-4H-PYRAN-4-ONE (three-letter code: KOJ) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 10 6 4	0	0
9	B	1	Total C O 10 6 4	0	0
9	C	1	Total C O 10 6 4	0	0
9	D	1	Total C O 10 6 4	0	0

- Molecule 10 is water.

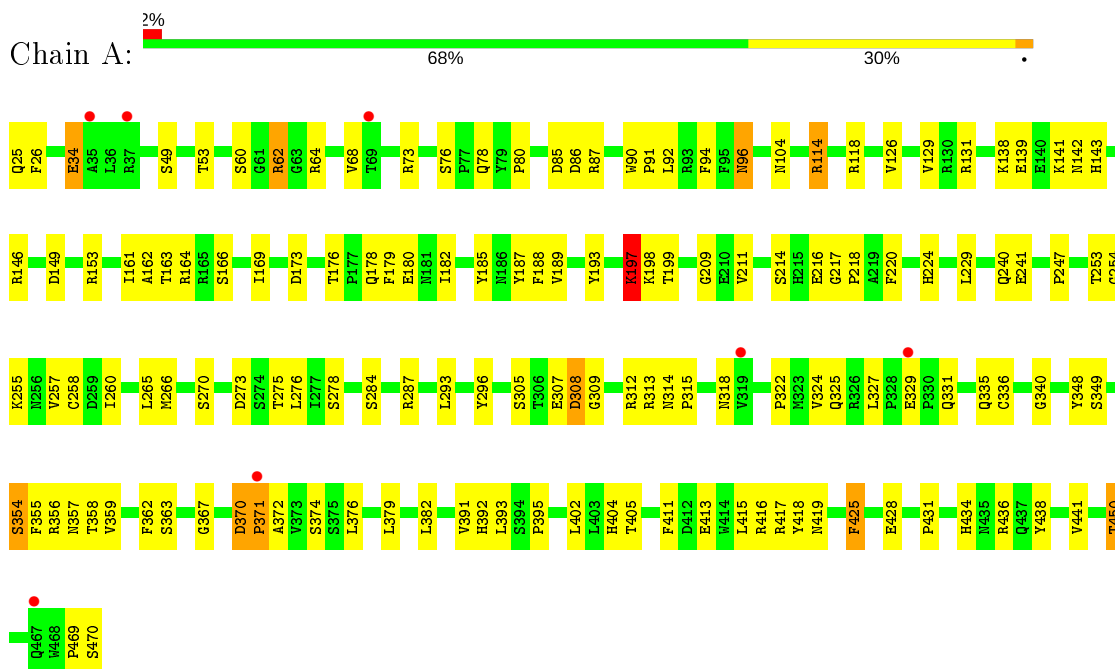
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 1 1	0	0
10	B	1	Total O 1 1	0	0
10	C	1	Total O 1 1	0	0
10	D	1	Total O 1 1	0	0



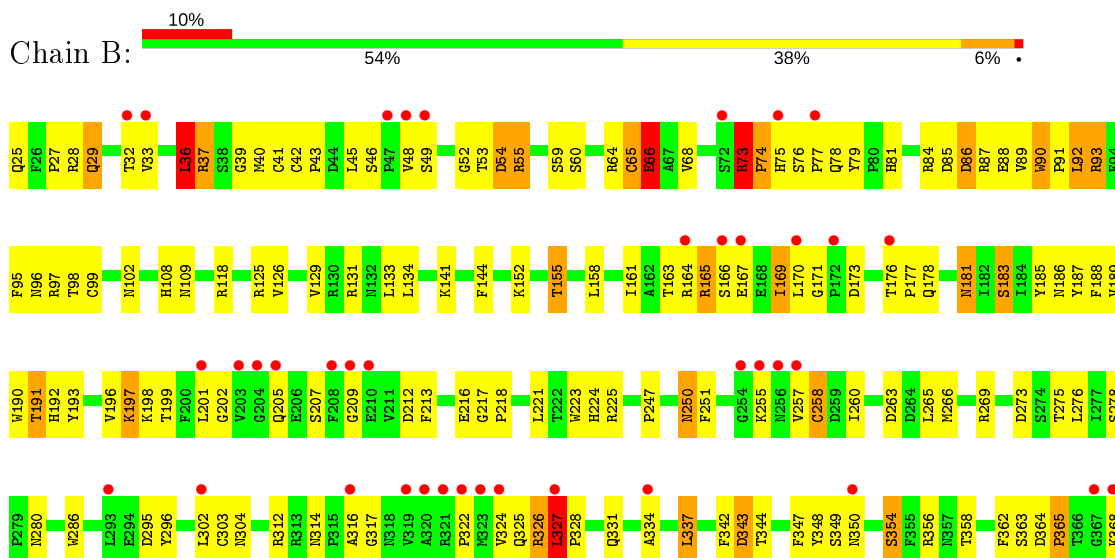
### 3 Residue-property plots [i](#)

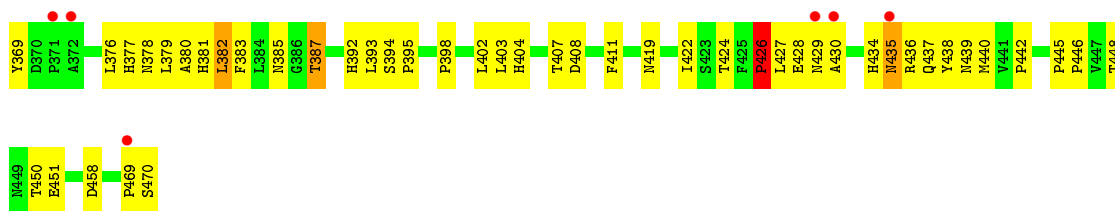
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5,6-dihydroxyindole-2-carboxylic acid oxidase

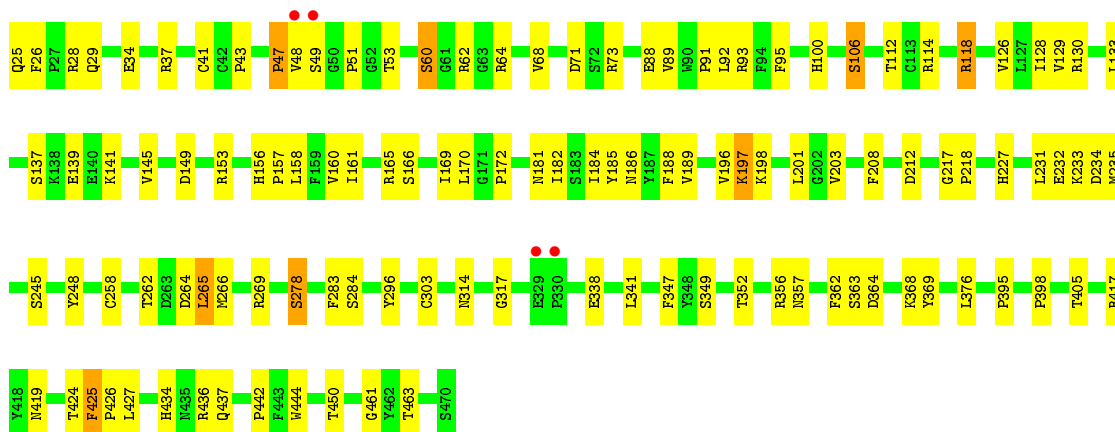
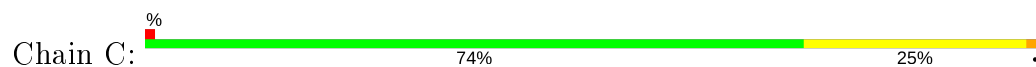


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

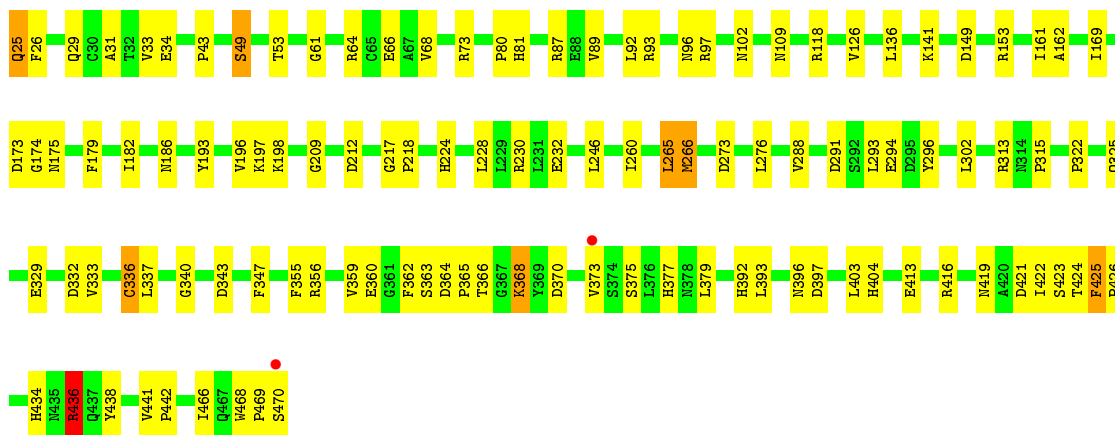




- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



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

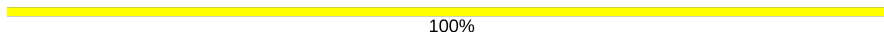


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2

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

Chain K:  50% 50%


MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

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

Chain G:  80% 20%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%


MAG1  
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1  
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%MAG1  
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%MAG1  
FUC2

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

Chain L:  100%MAG1  
MAG2  
MAN3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.64Å 140.43Å 191.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.85 47.87 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.88-2.85) 92.9 (47.87-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.86Å)	Xtrriage
Refinement program	REFMAC, PHENIX	Depositor
R, $R_{free}$	0.208 , 0.275 0.217 , 0.279	Depositor DCC
$R_{free}$ test set	2855 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: MAN, ZN, KOJ, NAG, FUC

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	0.57	5/3661 (0.1%)	0.76	4/4990 (0.1%)
1	B	0.62	5/3661 (0.1%)	0.94	17/4990 (0.3%)
1	C	0.49	0/3661	0.68	2/4990 (0.0%)
1	D	0.49	0/3661	0.65	1/4990 (0.0%)
All	All	0.54	10/14644 (0.1%)	0.76	24/19960 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4
1	C	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	ARG	NE-CZ	-8.60	1.21	1.33
1	B	86	ASP	CB-CG	-7.94	1.35	1.51
1	A	371	PRO	CA-CB	7.03	1.67	1.53
1	B	73	ARG	CZ-NH2	-6.35	1.24	1.33
1	B	66	GLU	CD-OE1	-6.24	1.18	1.25

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	LEU	CB-CG-CD1	-15.77	84.19	111.00
1	B	327	LEU	CA-CB-CG	15.06	149.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	NE-CZ-NH2	14.50	127.55	120.30
1	A	370	ASP	CB-CG-OD1	14.38	131.24	118.30
1	B	73	ARG	NE-CZ-NH2	13.30	126.95	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	426	PRO	Peptide
1	B	435	ASN	Peptide
1	B	65	CYS	Peptide
1	B	99	CYS	Peptide
1	C	48	VAL	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3554	0	3319	107	0
1	B	3554	0	3322	198	0
1	C	3554	0	3321	82	0
1	D	3554	0	3320	80	0
2	E	38	0	34	1	0
3	F	28	0	25	0	0
3	H	28	0	25	1	0
3	K	28	0	25	0	0
3	O	28	0	25	0	0
4	G	61	0	52	1	0
5	I	24	0	22	0	0
5	J	24	0	22	0	0
5	M	24	0	22	1	0
5	N	24	0	22	0	0
6	L	61	0	52	0	0
7	A	14	0	13	0	0
7	B	42	0	39	3	0
7	C	28	0	26	1	0
7	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	3	0	0	0	0
8	D	2	0	0	0	0
9	A	10	0	6	3	0
9	B	10	0	6	3	0
9	C	10	0	6	1	0
9	D	10	0	6	0	0
10	A	1	0	0	2	0
10	B	1	0	0	1	0
10	C	1	0	0	1	0
10	D	1	0	0	0	0
All	All	14735	0	13723	461	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 16.

The worst 5 of 461 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:B:165:ARG:NH2	1:B:167:GLU:OE2	1.62	1.31
1:B:92:LEU:HD11	1:B:96:ASN:HA	1.24	1.20
1:B:327:LEU:HD12	1:B:380:ALA:HA	1.19	1.15
1:B:255:LYS:O	1:B:326:ARG:NH1	1.85	1.09
1:B:350:ASN:HA	1:B:369:TYR:CE2	2.02	0.94

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	444/446 (100%)	402 (90%)	40 (9%)	2 (0%)	29	57
1	B	444/446 (100%)	377 (85%)	51 (12%)	16 (4%)	3	11
1	C	444/446 (100%)	409 (92%)	31 (7%)	4 (1%)	17	43
1	D	444/446 (100%)	403 (91%)	37 (8%)	4 (1%)	17	43
All	All	1776/1784 (100%)	1591 (90%)	159 (9%)	26 (2%)	10	30

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	PRO
1	B	191	THR
1	B	197	LYS
1	B	327	LEU
1	B	427	LEU

### 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	395/395 (100%)	382 (97%)	13 (3%)	38	68
1	B	395/395 (100%)	376 (95%)	19 (5%)	25	55
1	C	395/395 (100%)	386 (98%)	9 (2%)	50	78
1	D	395/395 (100%)	385 (98%)	10 (2%)	47	76
All	All	1580/1580 (100%)	1529 (97%)	51 (3%)	39	69

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	SER
1	B	343	ASP
1	D	363	SER
1	B	258	CYS
1	B	354	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	B	178	GLN
1	B	304	ASN
1	B	378	ASN
1	D	419	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](#)

29 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
2	NAG	E	1	1,2	14,14,15	1.17	2 (14%)	17,19,21	1.27	1 (5%)
2	NAG	E	2	2	14,14,15	0.93	1 (7%)	17,19,21	0.58	0
2	FUC	E	3	2	10,10,11	1.43	0	14,14,16	1.32	2 (14%)
3	NAG	F	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	0.71	0
4	NAG	G	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	G	2	4	14,14,15	0.62	1 (7%)	17,19,21	1.29	2 (11%)
4	MAN	G	3	4	11,11,12	1.18	1 (9%)	15,15,17	1.82	3 (20%)
4	MAN	G	4	4	11,11,12	1.01	1 (9%)	15,15,17	2.00	4 (26%)
4	MAN	G	5	4	11,11,12	1.57	3 (27%)	15,15,17	1.72	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	H	1	1,3	14,14,15	0.56	0	17,19,21	0.60	0
3	NAG	H	2	3	14,14,15	0.77	1 (7%)	17,19,21	0.54	0
5	NAG	I	1	1,5	14,14,15	1.22	3 (21%)	17,19,21	1.22	1 (5%)
5	FUC	I	2	5	10,10,11	1.85	4 (40%)	14,14,16	1.54	3 (21%)
5	NAG	J	1	1,5	14,14,15	0.66	0	17,19,21	0.60	0
5	FUC	J	2	5	10,10,11	1.47	3 (30%)	14,14,16	1.95	2 (14%)
3	NAG	K	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.74	0
3	NAG	K	2	3	14,14,15	0.51	0	17,19,21	0.45	0
6	NAG	L	1	1,6	14,14,15	1.82	2 (14%)	17,19,21	2.39	4 (23%)
6	NAG	L	2	6	14,14,15	1.02	1 (7%)	17,19,21	1.23	2 (11%)
6	MAN	L	3	6	11,11,12	1.29	1 (9%)	15,15,17	1.69	2 (13%)
6	MAN	L	4	6	11,11,12	0.73	0	15,15,17	1.67	3 (20%)
6	MAN	L	5	6	11,11,12	1.25	2 (18%)	15,15,17	1.63	1 (6%)
5	NAG	M	1	1,5	14,14,15	0.56	0	17,19,21	0.75	0
5	FUC	M	2	5	10,10,11	2.42	4 (40%)	14,14,16	2.21	5 (35%)
5	NAG	N	1	1,5	14,14,15	1.91	3 (21%)	17,19,21	1.23	2 (11%)
5	FUC	N	2	5	10,10,11	2.07	3 (30%)	14,14,16	1.63	3 (21%)
3	NAG	O	1	1,3	14,14,15	0.33	0	17,19,21	0.66	0
3	NAG	O	2	3	14,14,15	0.53	0	17,19,21	0.55	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
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	MAN	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	I	2	5	-	-	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	MAN	L	3	6	-	0/2/19/22	1/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	MAN	L	5	6	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	M	2	5	-	-	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	N	2	5	-	-	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1	NAG	O5-C1	5.73	1.52	1.43
5	N	1	NAG	C1-C2	4.86	1.59	1.52
5	M	2	FUC	C2-C3	4.66	1.59	1.52
5	N	1	NAG	O5-C1	-4.55	1.36	1.43
5	N	2	FUC	C1-C2	3.95	1.61	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C1-O5-C5	5.76	120.00	112.19
6	L	1	NAG	O4-C4-C5	5.65	123.33	109.30
5	M	2	FUC	C1-C2-C3	5.49	116.42	109.67
6	L	5	MAN	C1-O5-C5	5.42	119.54	112.19
5	J	2	FUC	O5-C5-C4	5.21	118.86	109.52

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	5	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
6	L	5	MAN	O5-C5-C6-O6

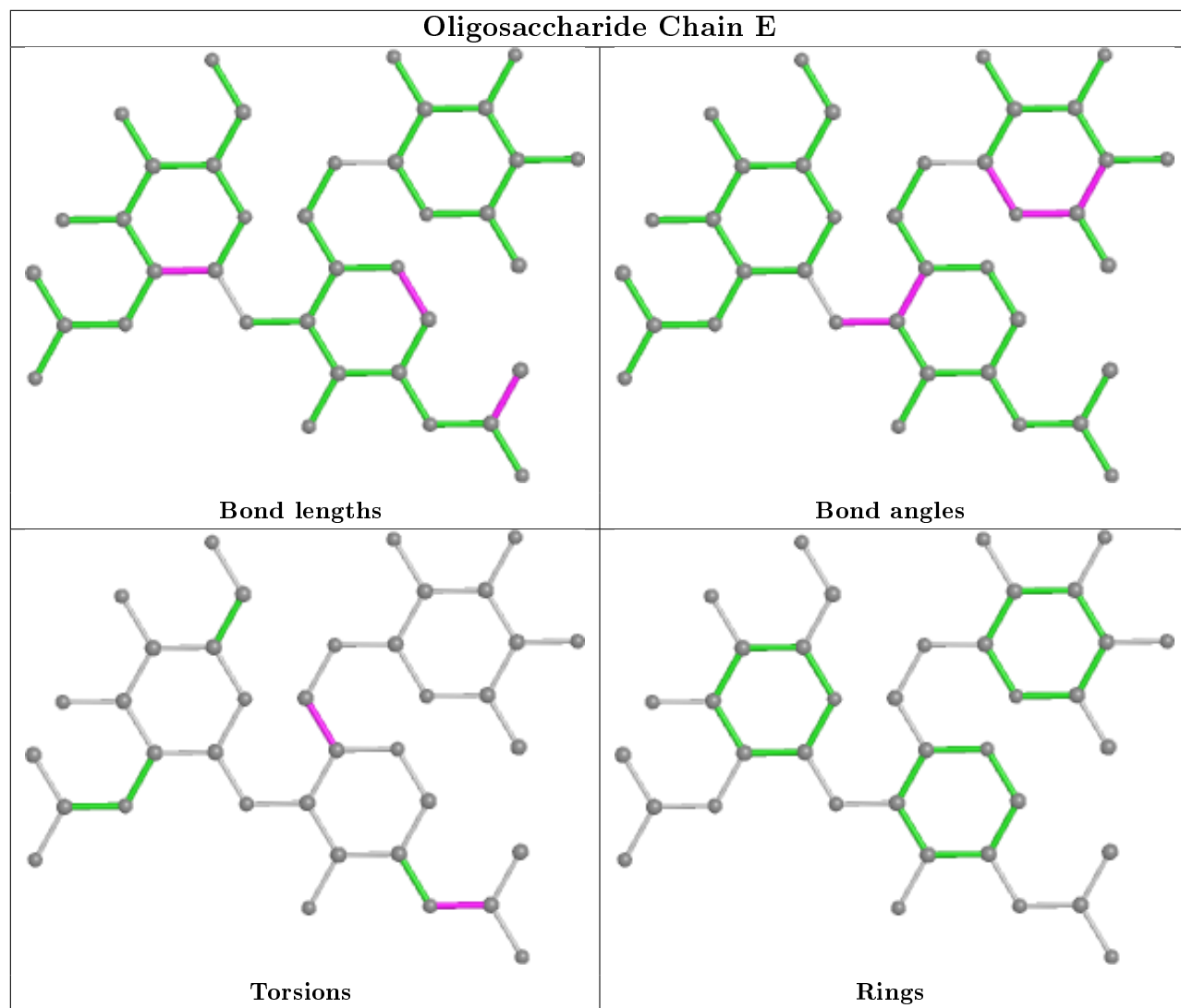
All (1) ring outliers are listed below:

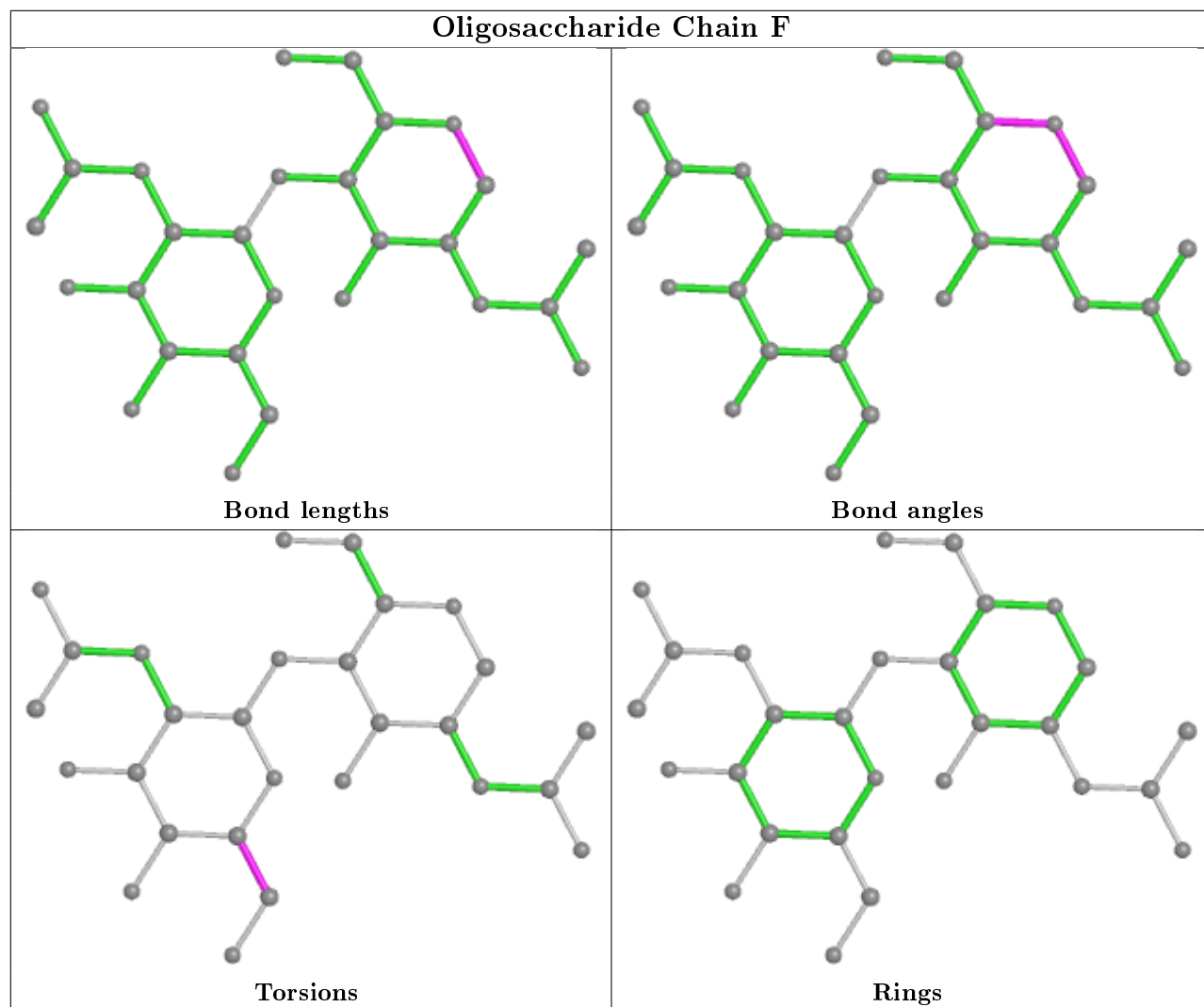
Mol	Chain	Res	Type	Atoms
6	L	3	MAN	C1-C2-C3-C4-C5-O5

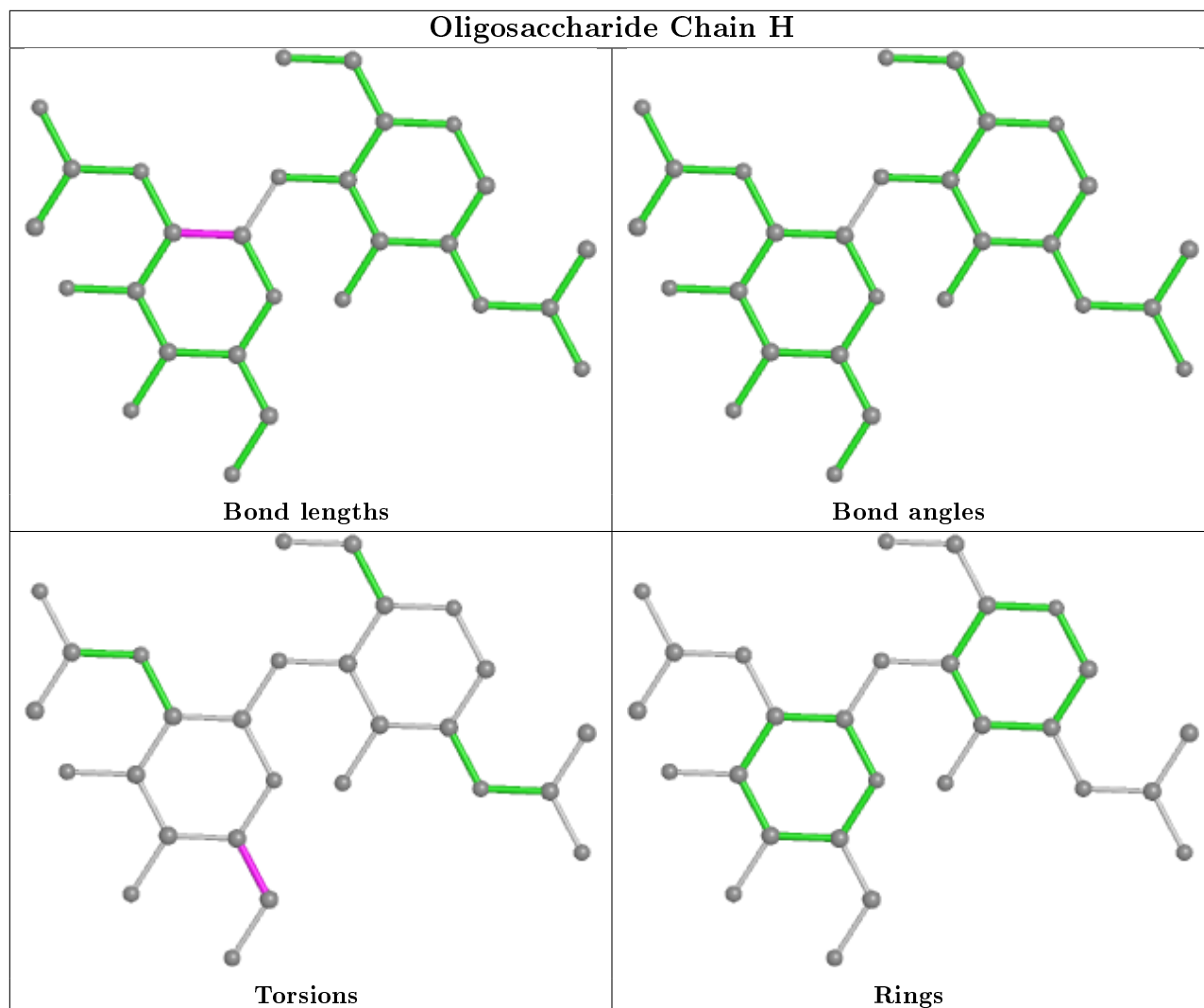
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
2	E	3	FUC	1	0
3	H	1	NAG	1	0
5	M	1	NAG	1	0

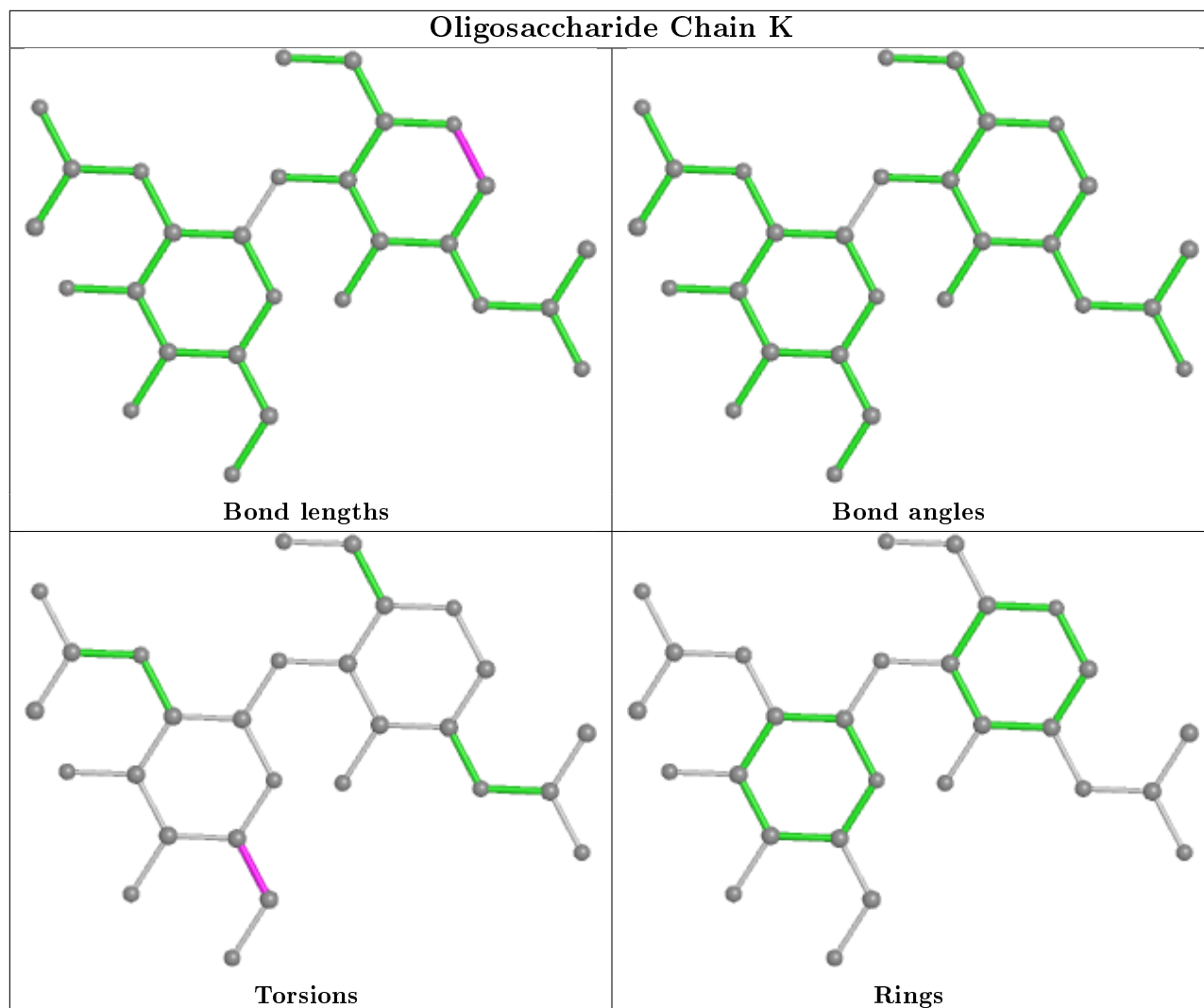
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

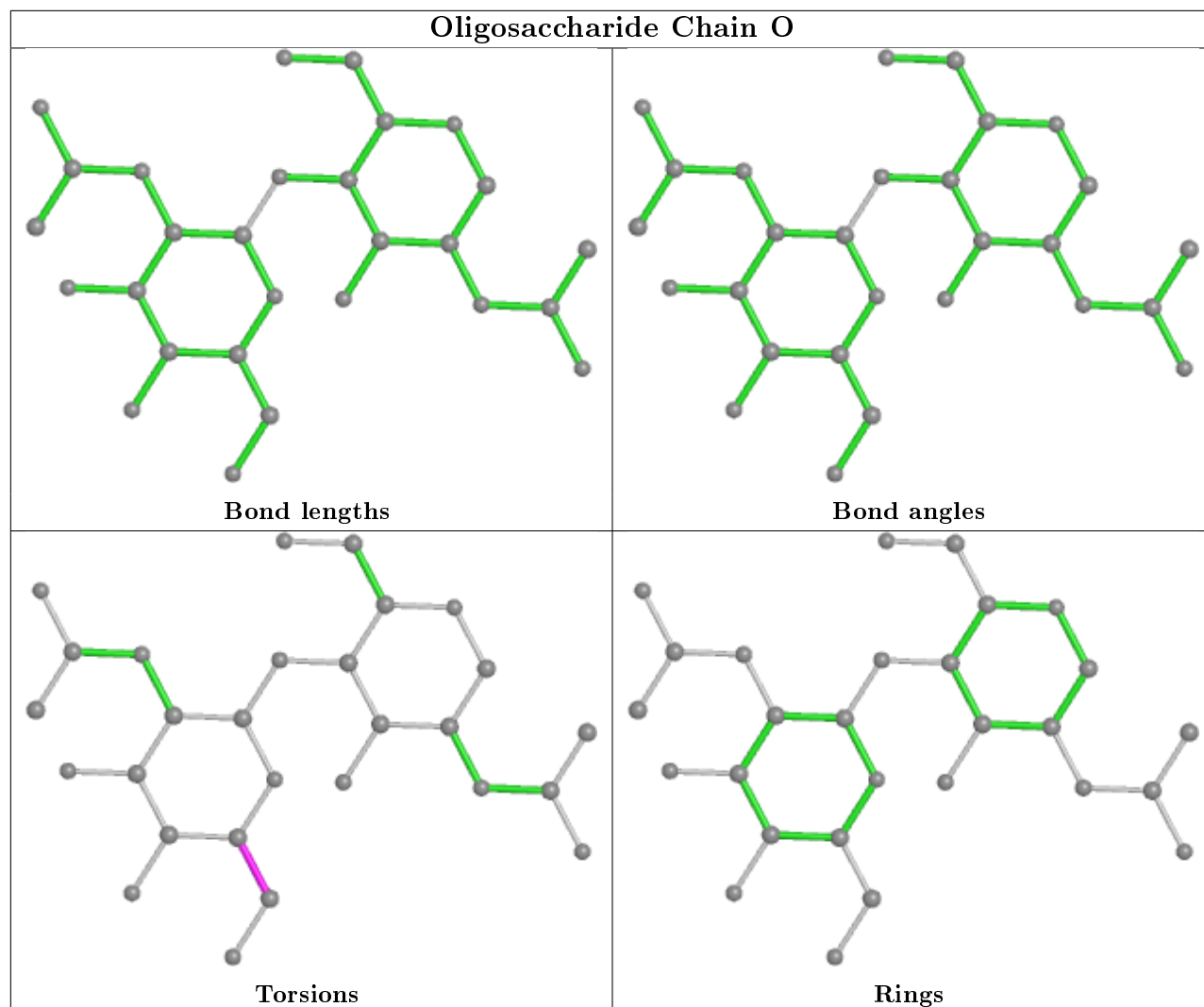


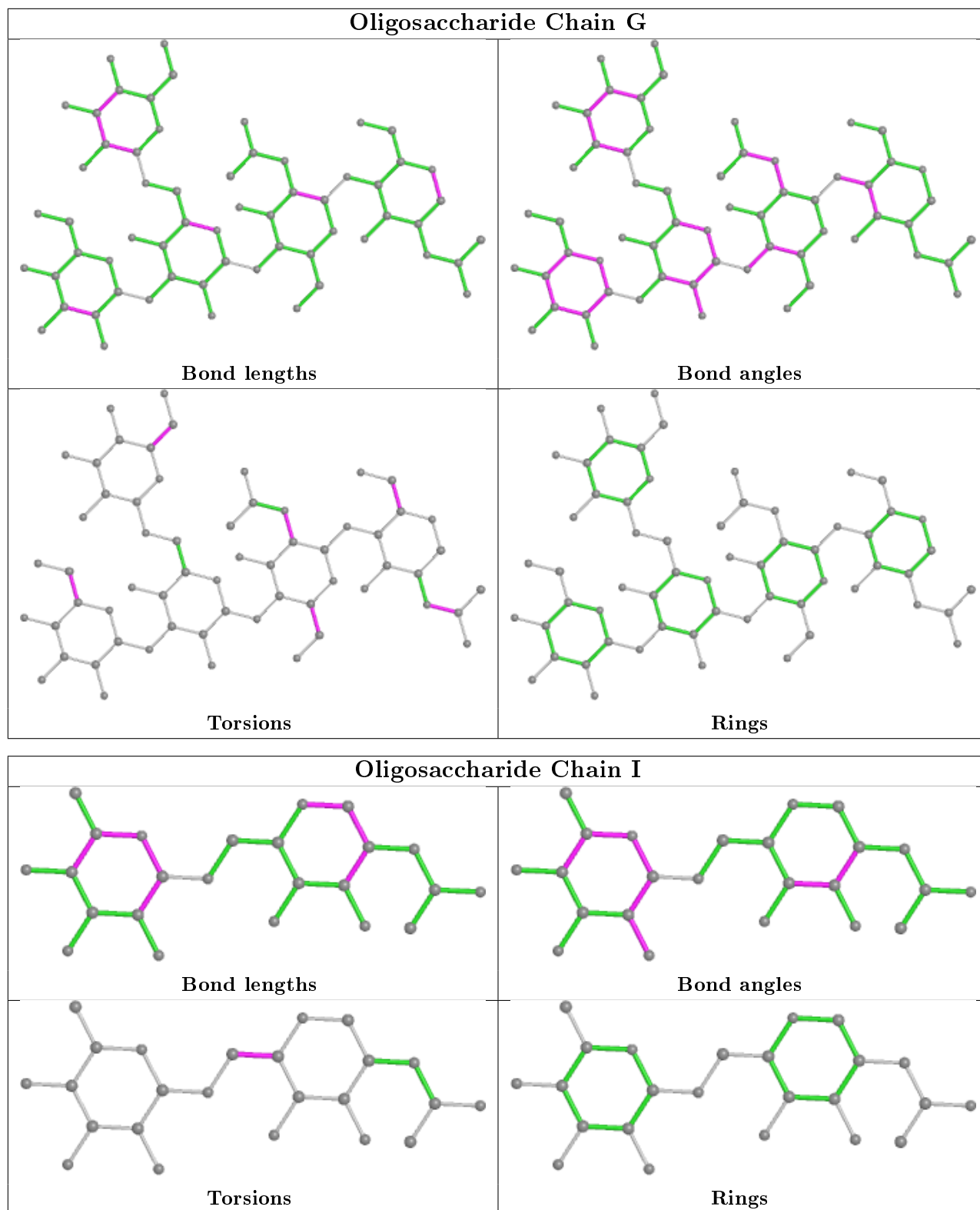


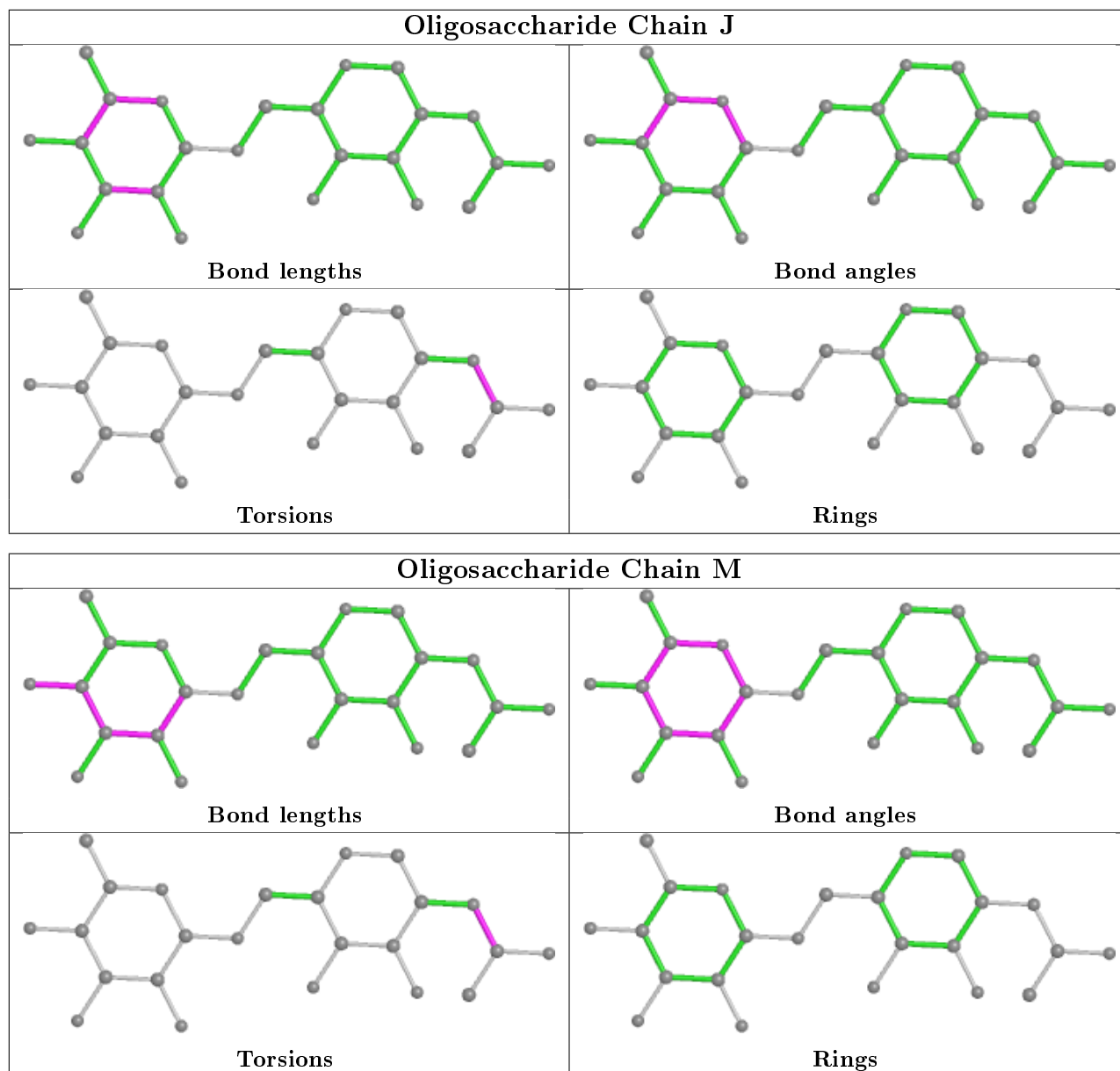


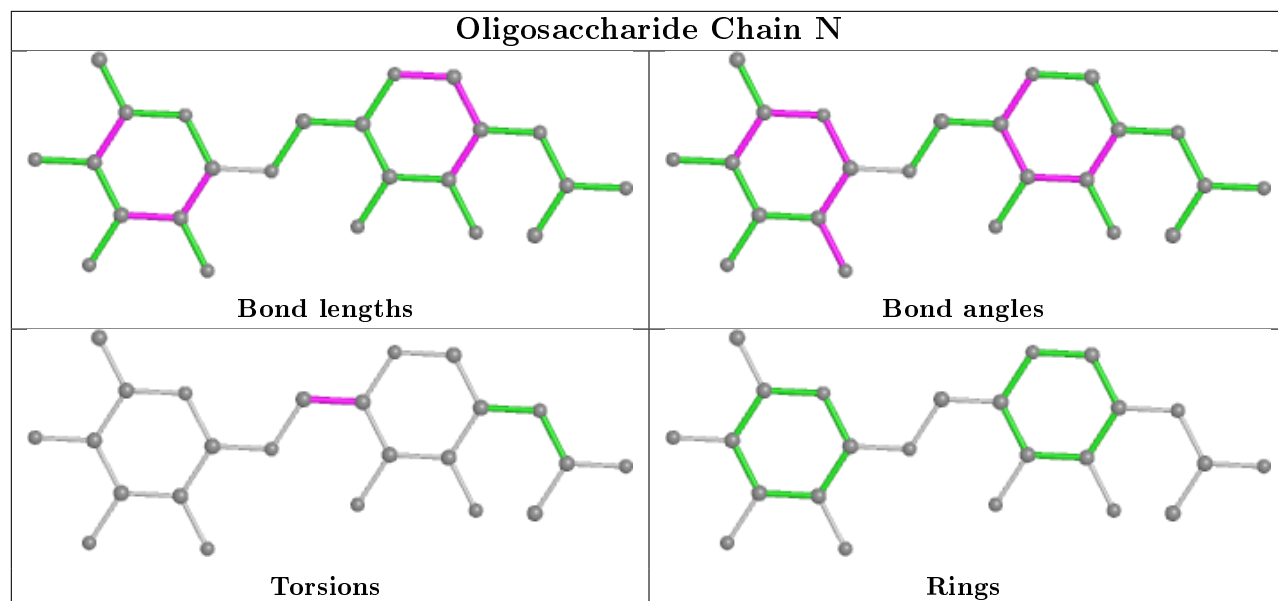


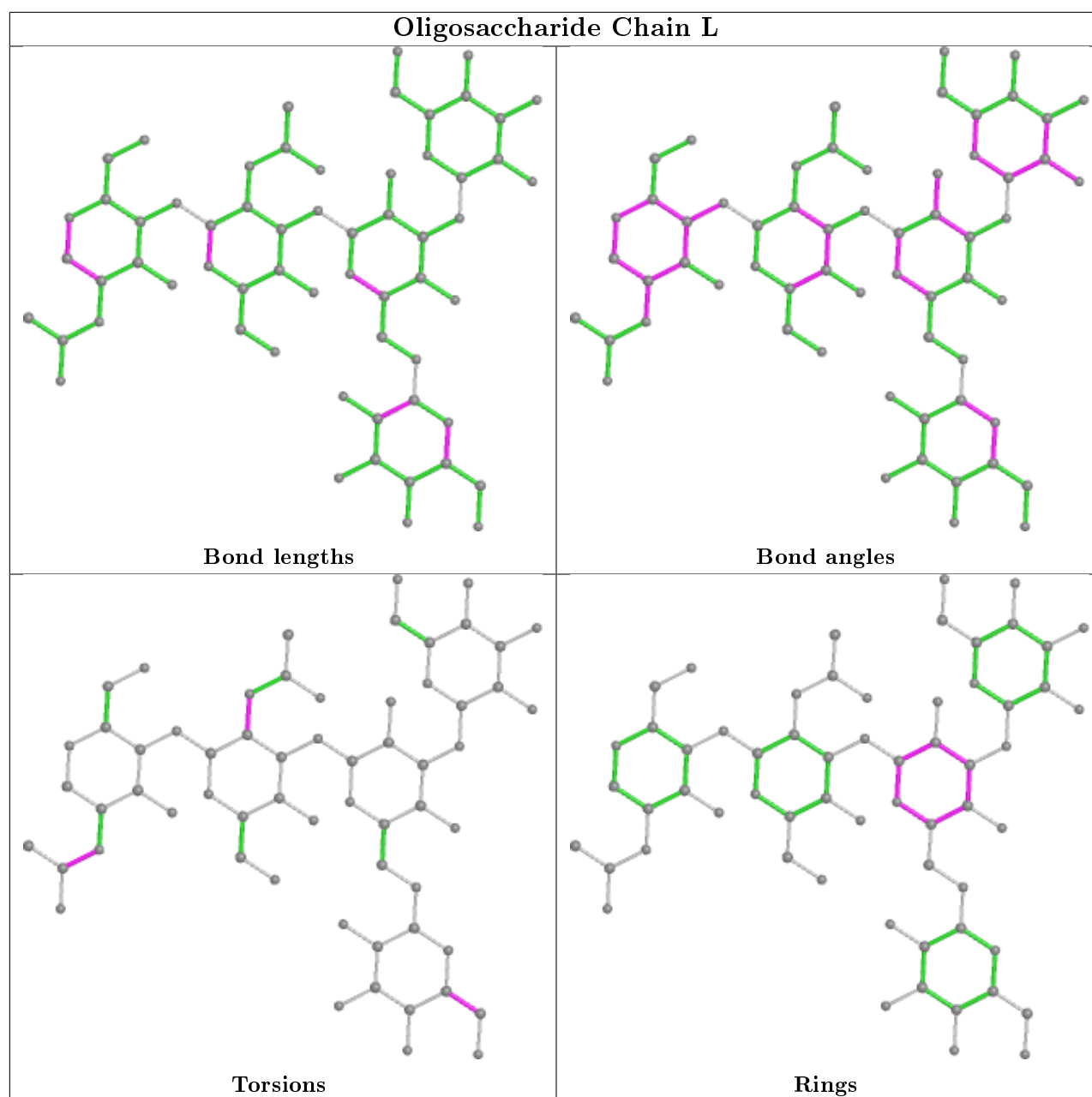












## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	511	1	14,14,15	0.67	1 (7%)	17,19,21	0.72	1 (5%)
7	NAG	D	507	1	14,14,15	1.05	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	C	503	-	14,14,15	1.07	1 (7%)	17,19,21	1.59	3 (17%)
9	KOJ	A	516	-	8,10,10	4.23	6 (75%)	6,13,13	1.26	1 (16%)
9	KOJ	B	508	-	8,10,10	4.08	4 (50%)	6,13,13	0.63	0
7	NAG	A	504	1	14,14,15	1.58	2 (14%)	17,19,21	1.13	3 (17%)
7	NAG	B	501	1	14,14,15	1.88	1 (7%)	17,19,21	2.00	4 (23%)
9	KOJ	D	510	-	8,10,10	4.26	6 (75%)	6,13,13	1.37	1 (16%)
9	KOJ	C	514	-	8,10,10	4.07	5 (62%)	6,13,13	1.36	1 (16%)
7	NAG	B	505	1	14,14,15	0.82	1 (7%)	17,19,21	0.51	0
7	NAG	B	504	-	14,14,15	1.19	1 (7%)	17,19,21	0.62	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
7	NAG	C	511	1	-	2/6/23/26	0/1/1/1
7	NAG	D	507	1	-	2/6/23/26	0/1/1/1
7	NAG	C	503	-	-	0/6/23/26	0/1/1/1
9	KOJ	A	516	-	-	0/1/2/2	0/1/1/1
9	KOJ	B	508	-	-	1/1/2/2	0/1/1/1
7	NAG	A	504	1	-	2/6/23/26	0/1/1/1
7	NAG	B	501	1	-	4/6/23/26	0/1/1/1
9	KOJ	D	510	-	-	1/1/2/2	0/1/1/1
9	KOJ	C	514	-	-	1/1/2/2	0/1/1/1
7	NAG	B	505	1	-	2/6/23/26	0/1/1/1
7	NAG	B	504	-	-	2/6/23/26	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	516	KOJ	O5-C5	9.67	1.48	1.35
9	D	510	KOJ	O5-C5	9.51	1.47	1.35
9	B	508	KOJ	O5-C5	9.12	1.47	1.35
9	C	514	KOJ	O5-C5	8.31	1.46	1.35
7	B	501	NAG	O5-C1	-6.53	1.33	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	NAG	O5-C5-C6	-6.47	97.07	107.20
7	C	503	NAG	C3-C4-C5	3.64	116.73	110.24
7	C	503	NAG	C1-O5-C5	-3.40	107.58	112.19
7	C	503	NAG	C4-C3-C2	3.20	115.70	111.02
7	A	504	NAG	C4-C3-C2	2.81	115.14	111.02

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	511	NAG	O5-C5-C6-O6
7	B	505	NAG	O5-C5-C6-O6
7	B	504	NAG	O5-C5-C6-O6
7	C	511	NAG	C4-C5-C6-O6
7	D	507	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	503	NAG	1	0
9	A	516	KOJ	3	0
9	B	508	KOJ	3	0
7	B	501	NAG	1	0
9	C	514	KOJ	1	0
7	B	504	NAG	2	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, 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	446/446 (100%)	0.10	7 (1%) 72 70	33, 51, 66, 79	0
1	B	446/446 (100%)	0.60	45 (10%) 7 5	42, 71, 95, 108	0
1	C	446/446 (100%)	0.00	4 (0%) 84 84	38, 54, 69, 90	0
1	D	446/446 (100%)	-0.05	2 (0%) 92 92	34, 49, 66, 81	0
All	All	1784/1784 (100%)	0.16	58 (3%) 46 41	33, 54, 87, 108	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ALA	5.4
1	B	164	ARG	5.2
1	B	48	VAL	4.8
1	B	256	ASN	4.8
1	B	327	LEU	4.6

### 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	FUC	I	2	10/11	0.78	0.31	69,83,89,90	0
3	NAG	H	2	14/15	0.82	0.38	77,84,93,93	0

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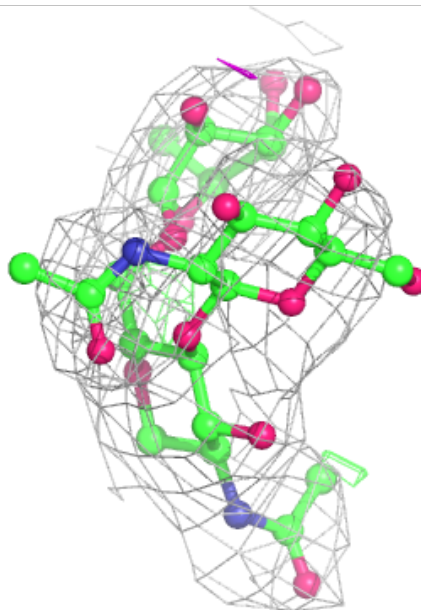
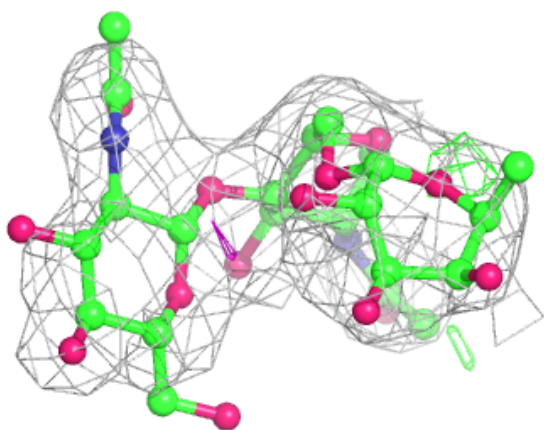
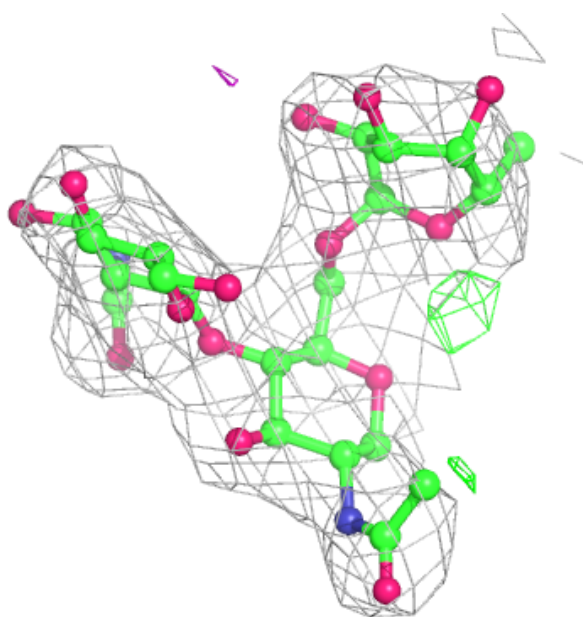
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	K	2	14/15	0.82	0.26	56,63,68,69	0
5	NAG	N	1	14/15	0.84	0.24	53,68,79,79	0
5	FUC	N	2	10/11	0.85	0.35	58,76,83,87	0
5	FUC	M	2	10/11	0.85	0.21	57,63,67,67	0
3	NAG	F	2	14/15	0.86	0.26	57,66,73,78	0
4	MAN	G	5	11/12	0.86	0.25	63,67,75,75	0
4	MAN	G	4	11/12	0.86	0.26	65,71,85,88	0
6	NAG	L	1	14/15	0.88	0.26	43,49,57,58	0
5	NAG	I	1	14/15	0.88	0.20	71,78,86,88	0
2	FUC	E	3	10/11	0.89	0.24	59,61,67,72	0
3	NAG	O	2	14/15	0.89	0.24	64,72,75,76	0
5	NAG	M	1	14/15	0.89	0.19	44,60,69,71	0
2	NAG	E	2	14/15	0.90	0.34	66,78,87,88	0
3	NAG	H	1	14/15	0.90	0.17	55,61,71,75	0
5	FUC	J	2	10/11	0.91	0.21	65,68,72,84	0
6	MAN	L	5	11/12	0.91	0.21	50,58,65,67	0
5	NAG	J	1	14/15	0.92	0.17	54,64,71,72	0
6	MAN	L	4	11/12	0.92	0.20	52,59,63,67	0
4	NAG	G	1	14/15	0.92	0.14	44,49,52,52	0
3	NAG	F	1	14/15	0.92	0.17	56,61,64,65	0
3	NAG	K	1	14/15	0.93	0.18	53,58,65,66	0
3	NAG	O	1	14/15	0.93	0.15	49,56,62,62	0
6	NAG	L	2	14/15	0.93	0.21	33,53,62,68	0
6	MAN	L	3	11/12	0.93	0.16	45,52,58,60	0
2	NAG	E	1	14/15	0.94	0.17	60,70,72,73	0
4	NAG	G	2	14/15	0.95	0.17	45,50,58,70	0
4	MAN	G	3	11/12	0.96	0.16	53,58,67,68	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.

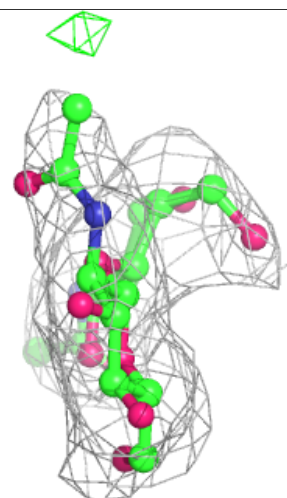
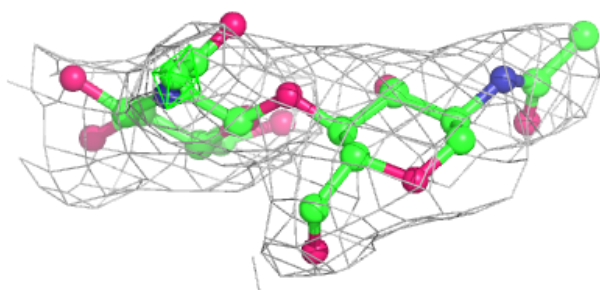
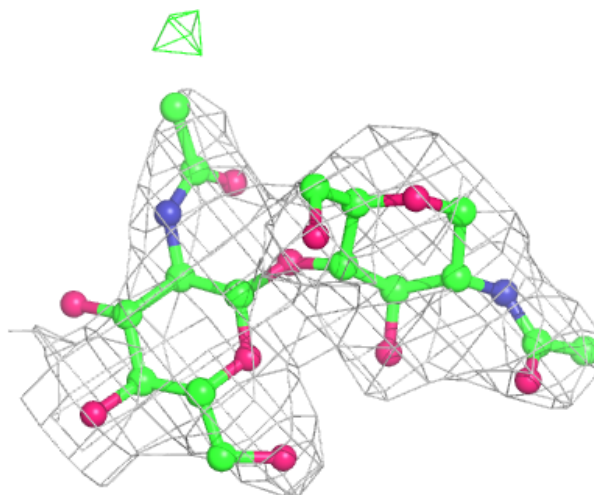
**Electron density around Chain E:**

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



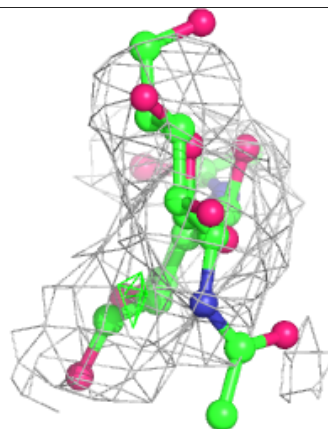
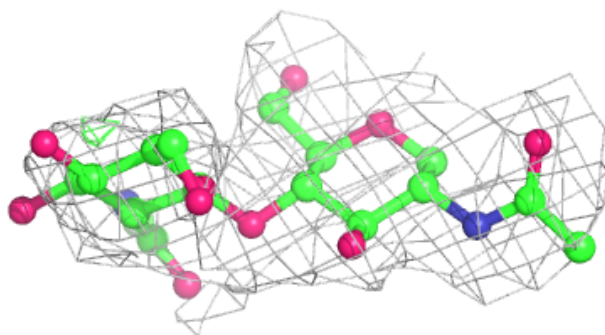
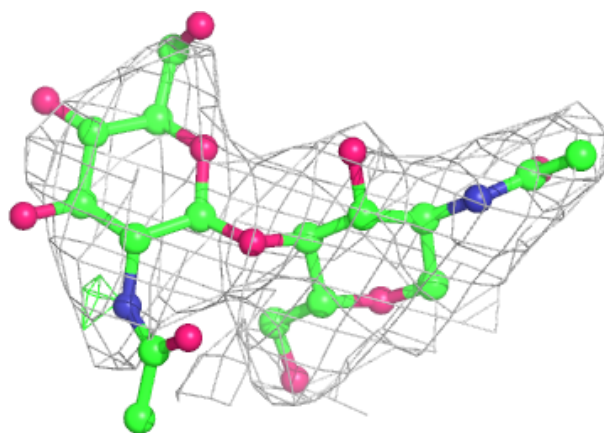
**Electron density around Chain F:**

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

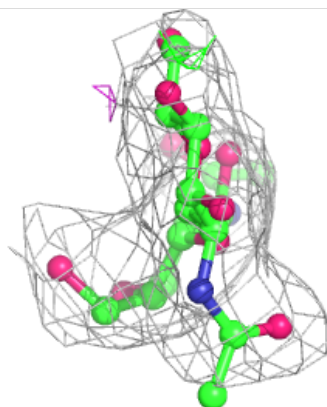
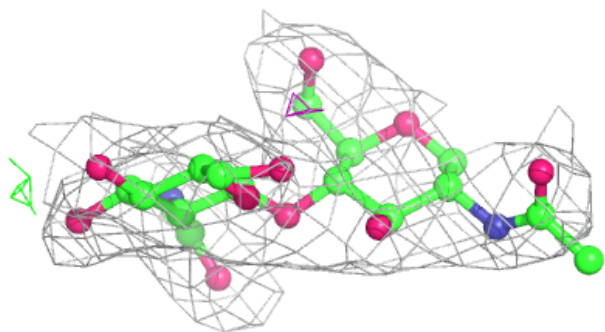
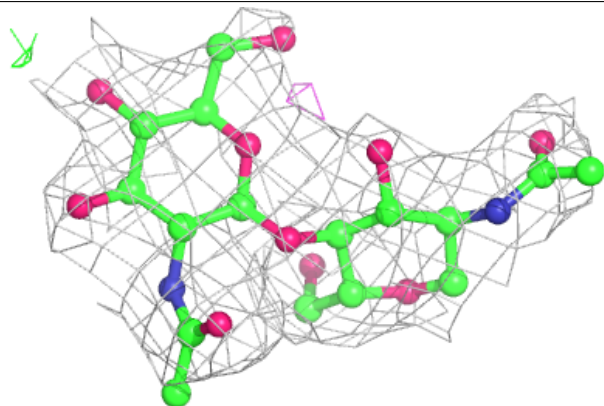


**Electron density around Chain H:**

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

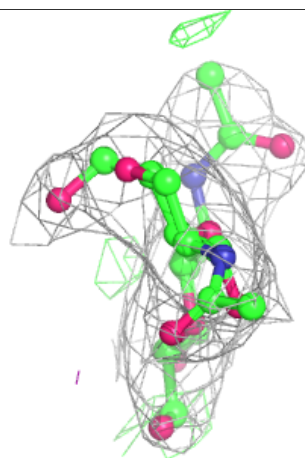
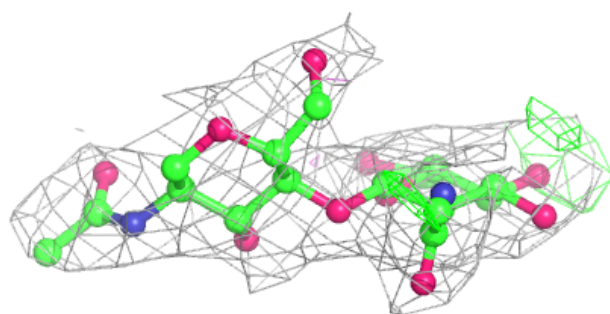
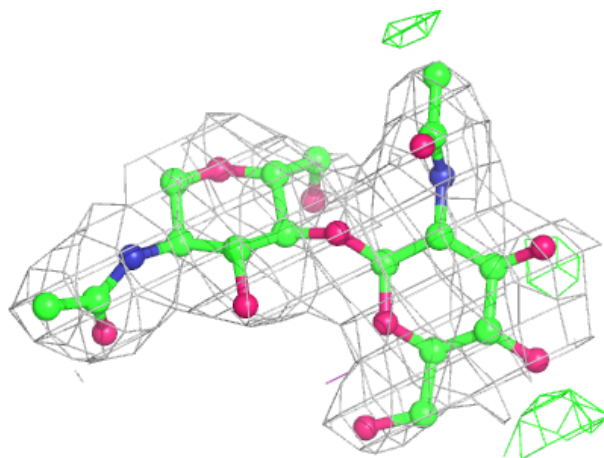
**Electron density around Chain K:**

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



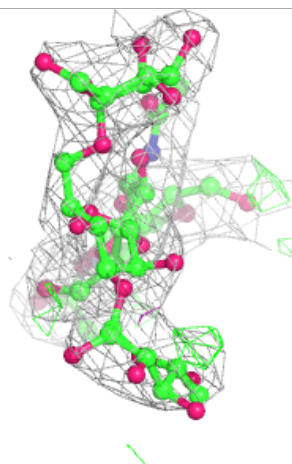
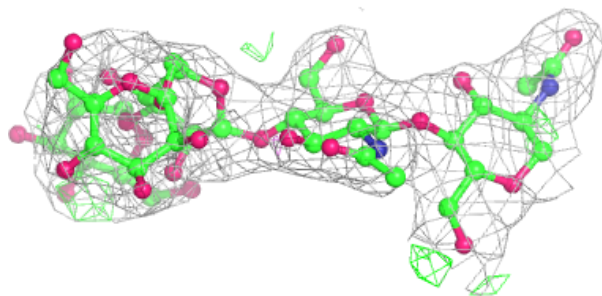
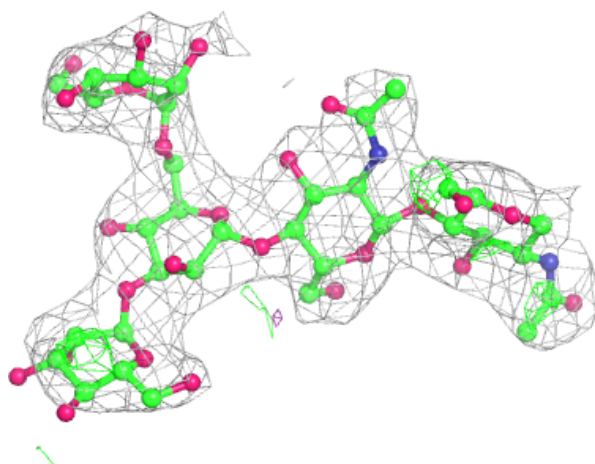
**Electron density around Chain O:**

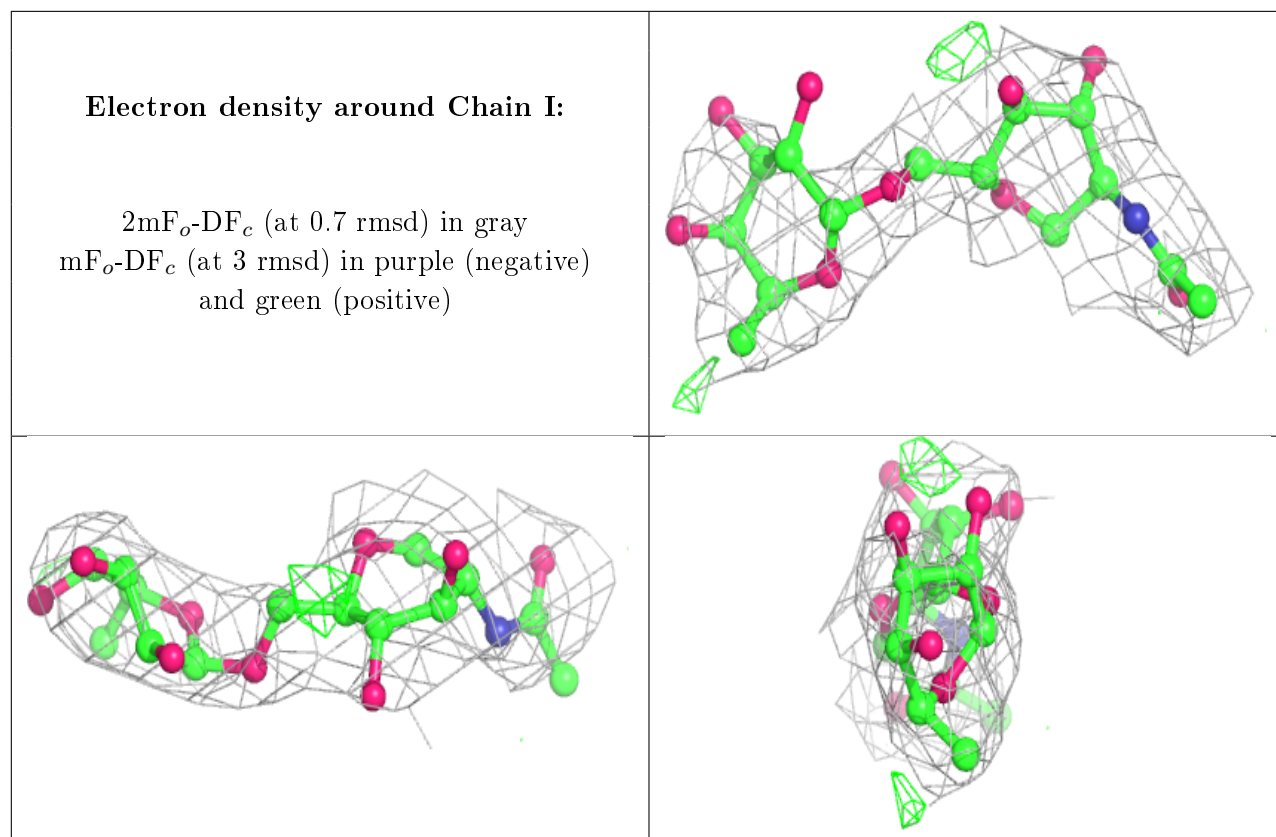
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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

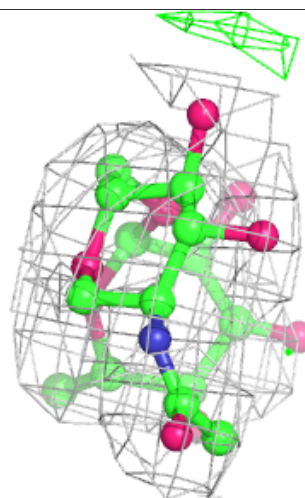
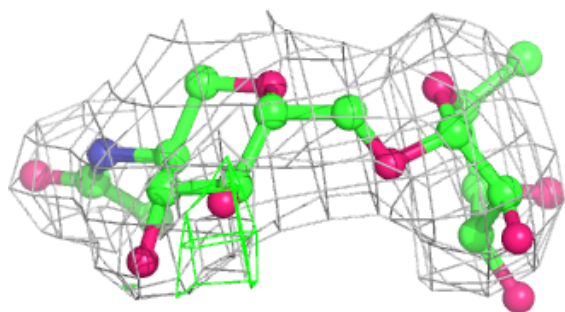
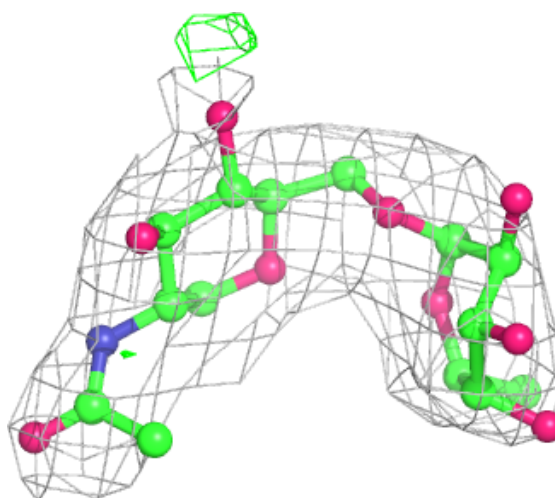






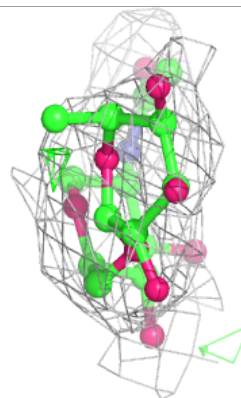
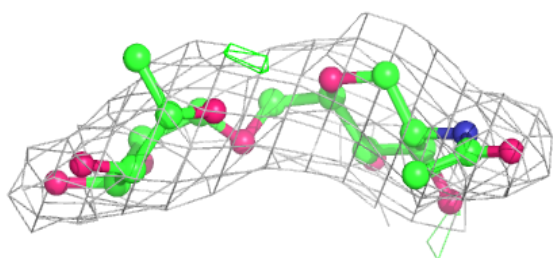
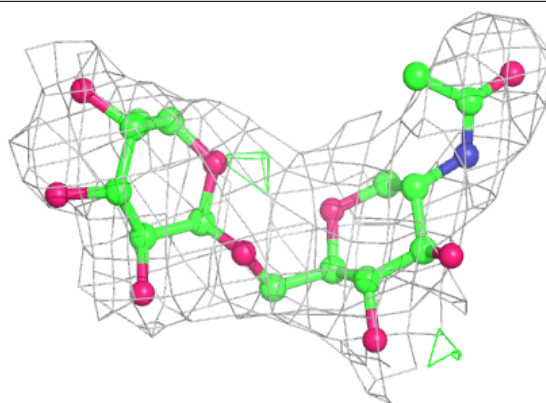
**Electron density around Chain J:**

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

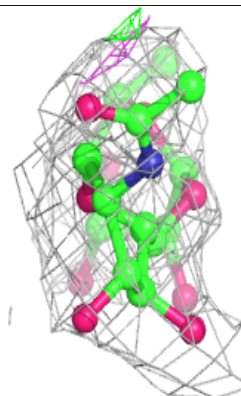
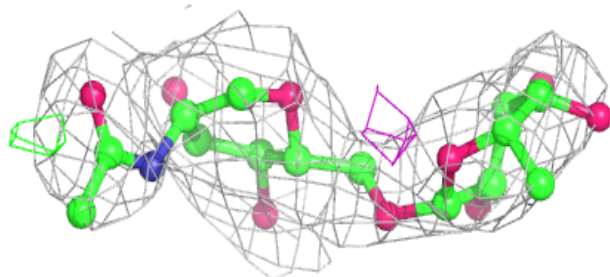
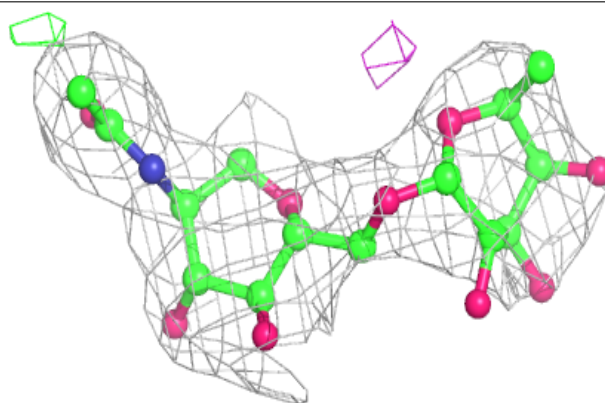


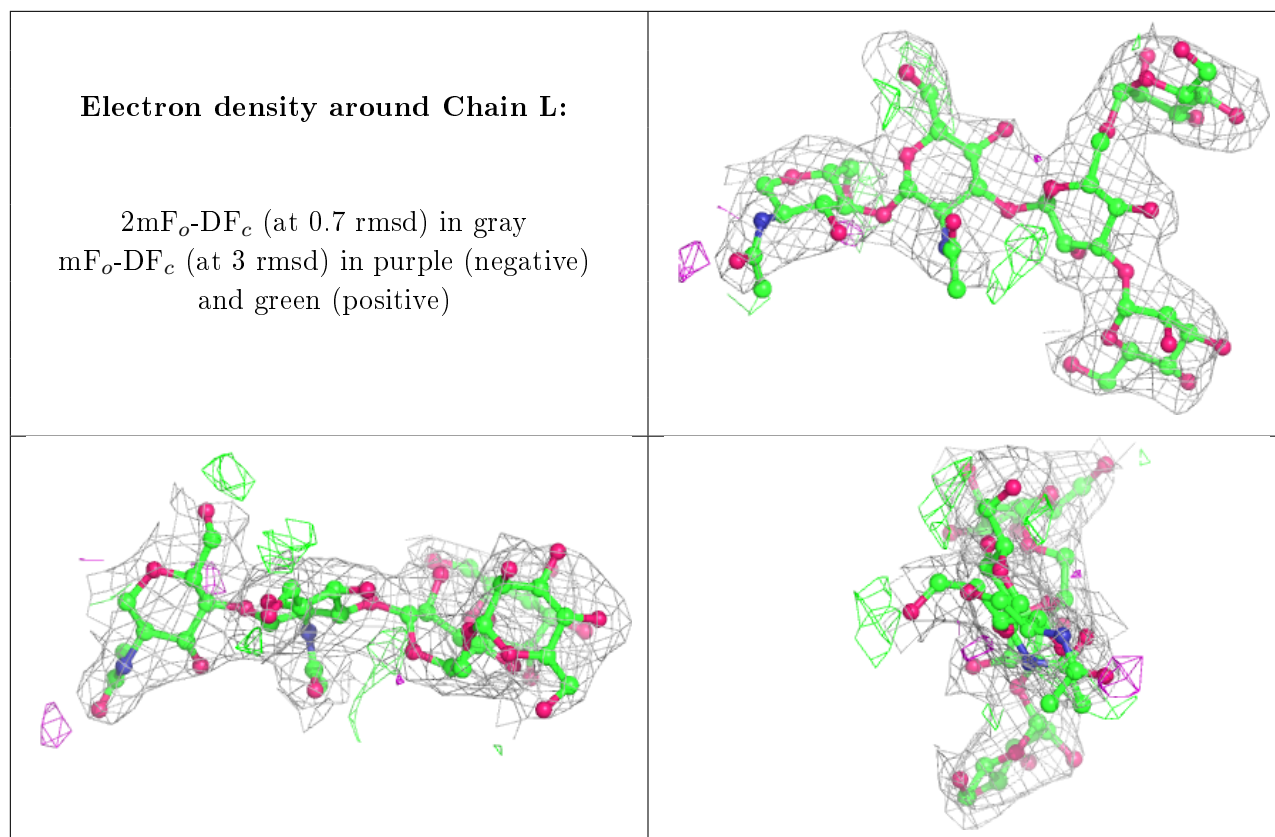
**Electron density around Chain M:**

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

**Electron density around Chain N:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	NAG	C	503	14/15	0.64	0.29	54,71,85,87	0
7	NAG	B	501	14/15	0.66	0.34	68,87,95,95	0
7	NAG	B	505	14/15	0.72	0.31	76,87,93,94	0
7	NAG	A	504	14/15	0.74	0.34	41,67,75,76	0
9	KOJ	D	510	10/10	0.85	0.29	45,50,56,56	0
7	NAG	B	504	14/15	0.88	0.21	59,70,81,82	0
9	KOJ	C	514	10/10	0.89	0.22	50,54,57,59	0
9	KOJ	A	516	10/10	0.90	0.24	50,54,56,62	0
9	KOJ	B	508	10/10	0.90	0.29	74,75,82,83	0
7	NAG	D	507	14/15	0.91	0.21	43,59,64,64	0
7	NAG	C	511	14/15	0.92	0.21	50,57,67,68	0
8	ZN	A	514	1/1	0.97	0.12	40,40,40,40	0
8	ZN	B	506	1/1	0.97	0.14	78,78,78,78	0
8	ZN	B	507	1/1	0.97	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	A	515	1/1	0.98	0.15	51,51,51,51	0
8	ZN	D	509	1/1	0.99	0.14	53,53,53,53	0
8	ZN	C	515	1/1	0.99	0.08	58,58,58,58	0
8	ZN	D	508	1/1	0.99	0.18	39,39,39,39	0
8	ZN	C	513	1/1	0.99	0.14	60,60,60,60	0
8	ZN	C	512	1/1	1.00	0.14	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.