



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2020 – 10:25 AM BST

PDB ID : 6TVD  
Title : Crystal structure of the haemagglutinin from a H10N7 seal influenza virus isolated in Germany in complex with avian receptor analogue, 3'-SLN  
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.  
Deposited on : 2020-01-09  
Resolution : 2.70 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](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 : 2.14.6  
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) : 2.14.6

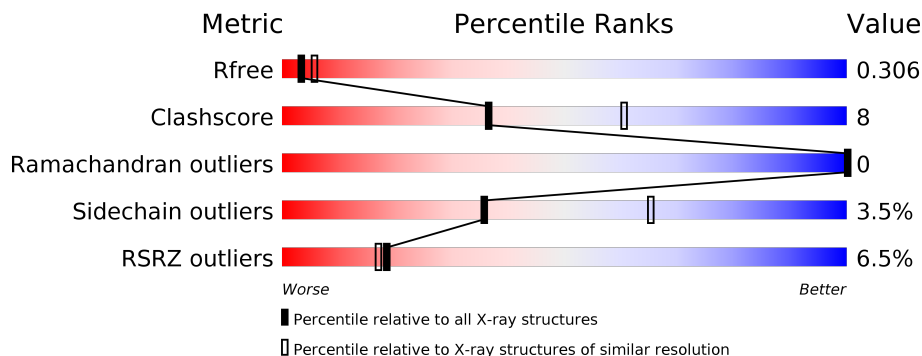
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.










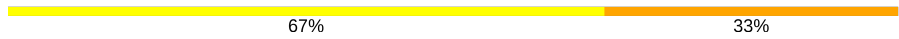
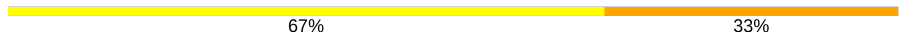

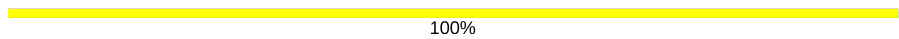


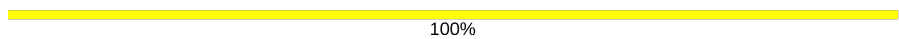
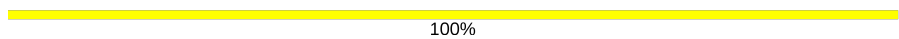
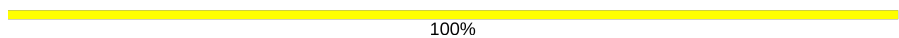
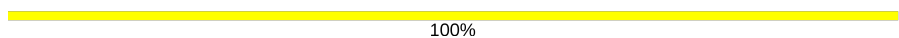
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	325	
1	C	325	
1	E	325	
1	G	325	
1	I	325	
1	K	325	

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Mol	Chain	Length	Quality of chain
2	B	177	 % 79% 19% .
2	D	177	 83% 13% ..
2	F	177	 6% 80% 18% .
2	H	177	 82% 15% .
2	J	177	 5% 84% 12% ..
2	L	177	 % 86% 11% .
3	M	3	 33% 67%
3	N	3	 67% 33%
3	P	3	 67% 33%
3	R	3	 33% 67%
3	V	3	 100%
4	O	2	 50% 50%
4	Q	2	 50% 50%
4	S	2	 100%
4	U	2	 100%
4	W	2	 100%
5	T	2	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23585 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	Total 2446	C 1516	N 444	O 470	S 16	0	0	0
1	C	318	Total 2431	C 1507	N 442	O 466	S 16	0	0	0
1	E	318	Total 2436	C 1510	N 442	O 468	S 16	0	1	0
1	G	316	Total 2418	C 1497	N 439	O 466	S 16	0	0	0
1	I	318	Total 2421	C 1502	N 439	O 464	S 16	0	0	0
1	K	318	Total 2431	C 1507	N 442	O 466	S 16	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	219	GLN	LEU	conflict	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	219	GLN	LEU	conflict	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
E	219	GLN	LEU	conflict	UNP A0A0A7HR51
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
G	219	GLN	LEU	conflict	UNP A0A0A7HR51
I	-1	ASP	-	expression tag	UNP A0A0A7HR51
I	0	PRO	-	expression tag	UNP A0A0A7HR51
I	219	GLN	LEU	conflict	UNP A0A0A7HR51
K	-1	ASP	-	expression tag	UNP A0A0A7HR51
K	0	PRO	-	expression tag	UNP A0A0A7HR51

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Chain	Residue	Modelled	Actual	Comment	Reference
K	219	GLN	LEU	conflict	UNP A0A0A7HR51

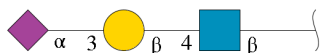
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	H	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	J	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	L	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
H	177	LYS	-	expression tag	UNP A0A0A7HR51
J	177	LYS	-	expression tag	UNP A0A0A7HR51
L	177	LYS	-	expression tag	UNP A0A0A7HR51

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	N	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	P	3	Total	C	N	O	0	0	0
			46	25	2	19			

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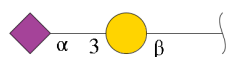
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	V	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 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
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 6 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
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	K	1	Total	Ca	0	0
			1	1		

- Molecule 8 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	14	Total O 14 14	0	0
8	B	1	Total O 1 1	0	0
8	C	35	Total O 35 35	0	0
8	D	7	Total O 7 7	0	0
8	E	18	Total O 18 18	0	0
8	F	10	Total O 10 10	0	0
8	G	3	Total O 3 3	0	0
8	H	2	Total O 2 2	0	0
8	I	2	Total O 2 2	0	0
8	J	1	Total O 1 1	0	0
8	K	50	Total O 50 50	0	0
8	L	12	Total O 12 12	0	0

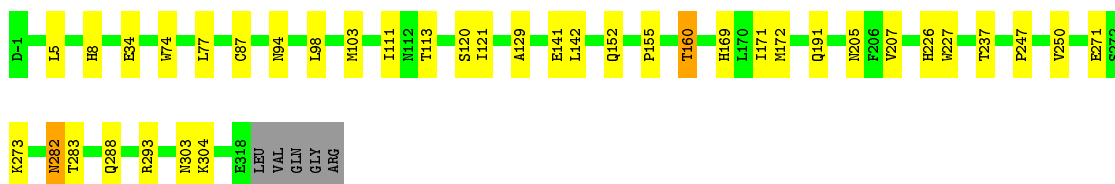


### 3 Residue-property plots [i](#)


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.

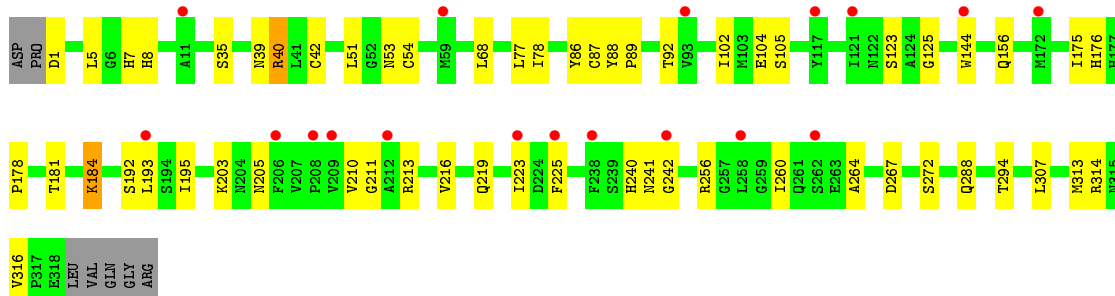
- Molecule 1: Hemagglutinin HA1

Chain A: 




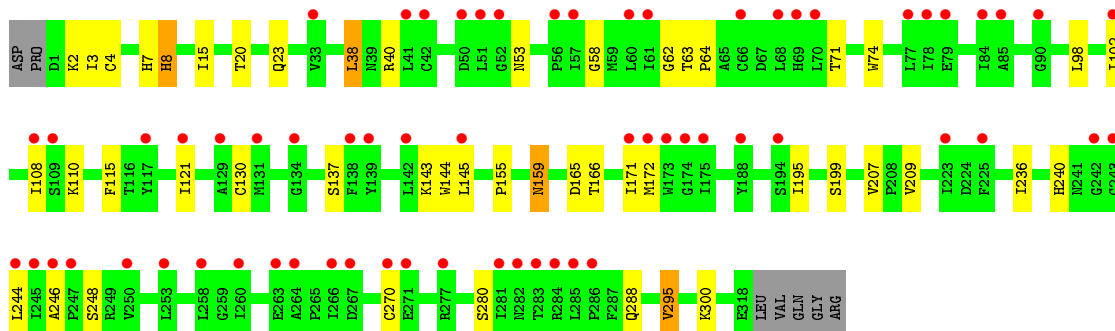
- Molecule 1: Hemagglutinin HA1

Chain C: 

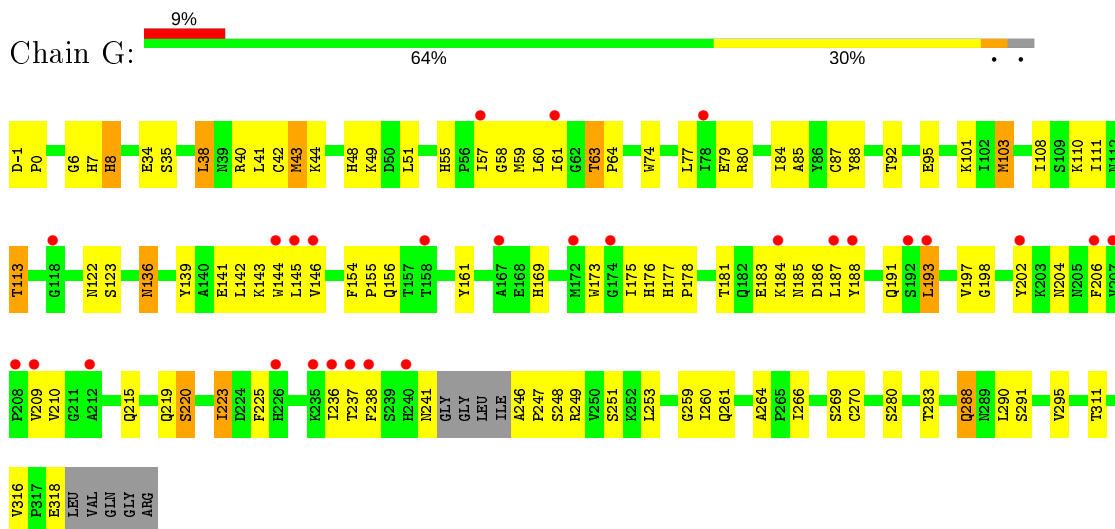


- Molecule 1: Hemagglutinin HA1

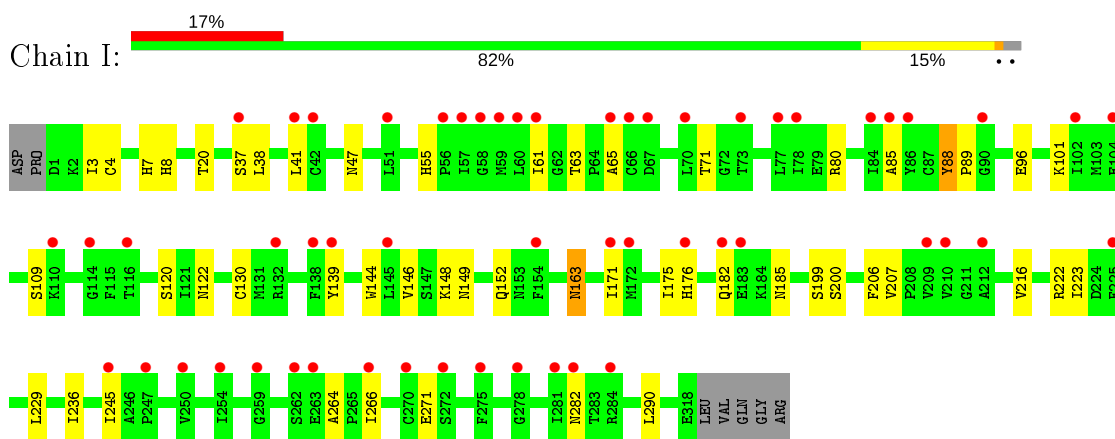
Chain E: 



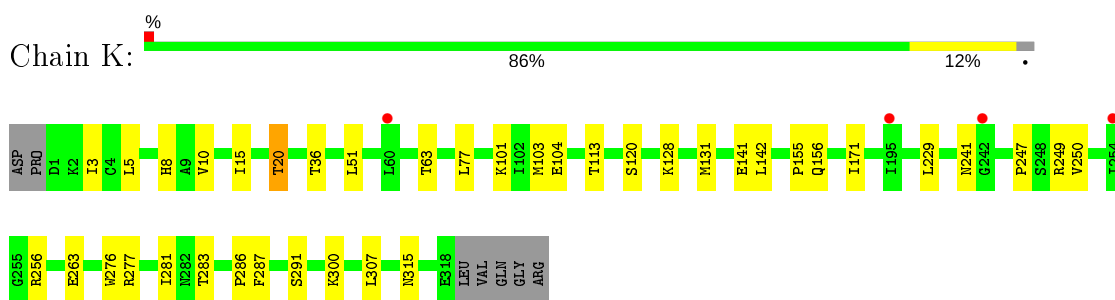
• Molecule 1: Hemagglutinin HA1



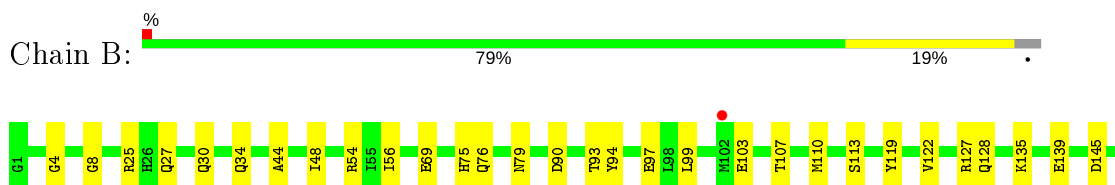
• Molecule 1: Hemagglutinin HA1

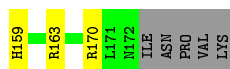


• Molecule 1: Hemagglutinin HA1

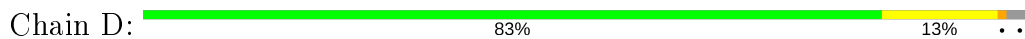


• Molecule 2: Hemagglutinin HA2

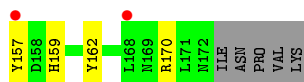
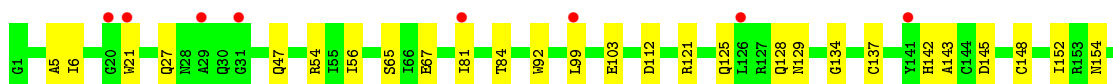
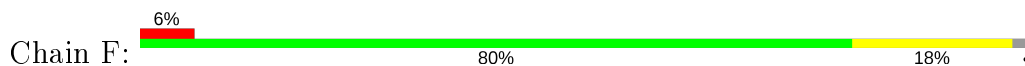




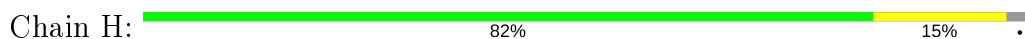
- Molecule 2: Hemagglutinin HA2



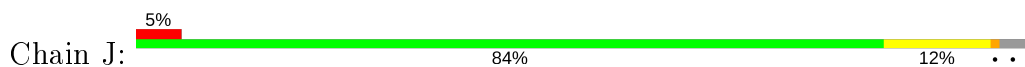
- Molecule 2: Hemagglutinin HA2



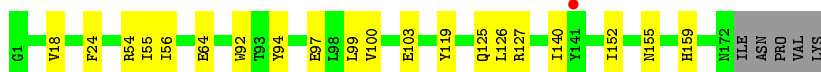
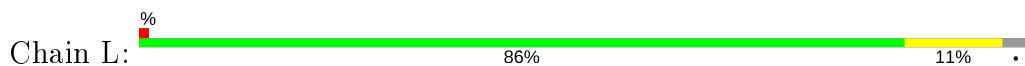
- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



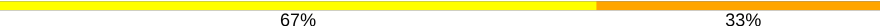
- Molecule 2: Hemagglutinin HA2



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

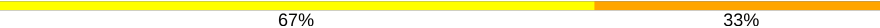


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  67% 33%

NAG1  
GAL2  
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  67% 33%

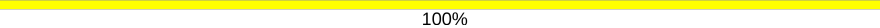
NAG1  
GAL2  
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 67%

NAG1  
GAL2  
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

NAG1  
GAL2  
SIA3

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

Chain O:  50% 50%

NAG1  
NAG2

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

Chain Q:  50% 50%


NAG1  
NAG2

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

Chain S:  100%

MAG1  
MAG2


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

Chain U:  100%MAG1  
MAG2

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

Chain W:  100%MAG1  
MAG2

- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain T:  100%GAL1  
S1A2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.74Å 214.96Å 157.78Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	68.55 – 2.70 65.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (68.55-2.70) 99.0 (65.31-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.243 , 0.313 0.239 , 0.306	Depositor DCC
$R_{free}$ test set	6249 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.0	Xtrriage
Anisotropy	0.502	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3110e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, GAL, NAG, SIA

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	0.66	0/2496	0.79	0/3381
1	C	0.67	0/2480	0.78	0/3358
1	E	0.68	0/2488	0.76	0/3369
1	G	0.66	0/2467	0.79	0/3342
1	I	0.68	0/2470	0.77	0/3346
1	K	0.68	0/2480	0.78	0/3358
2	B	0.66	0/1411	0.77	0/1903
2	D	0.66	0/1411	0.77	0/1903
2	F	0.67	0/1411	0.77	0/1903
2	H	0.65	0/1411	0.76	0/1903
2	J	0.66	0/1411	0.75	0/1903
2	L	0.66	0/1411	0.77	0/1903
All	All	0.67	0/23347	0.77	0/31572

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	2446	0	2404	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2431	0	2393	40	0
1	E	2436	0	2397	34	0
1	G	2418	0	2364	122	0
1	I	2421	0	2378	34	0
1	K	2431	0	2393	28	0
2	B	1386	0	1291	26	0
2	D	1386	0	1291	19	0
2	F	1386	0	1290	26	0
2	H	1386	0	1293	18	0
2	J	1386	0	1291	19	0
2	L	1386	0	1290	21	0
3	M	46	0	40	1	0
3	N	46	0	40	3	0
3	P	46	0	40	1	0
3	R	46	0	40	3	0
3	V	46	0	40	0	0
4	O	28	0	25	0	0
4	Q	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	W	28	0	25	0	0
5	T	32	0	28	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
6	G	14	0	13	1	0
6	I	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	0	0
7	A	1	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
8	A	14	0	0	0	0
8	B	1	0	0	0	0
8	C	35	0	0	0	0
8	D	7	0	0	0	0
8	E	18	0	0	0	0
8	F	10	0	0	1	0
8	G	3	0	0	0	0
8	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	2	0	0	1	0
8	J	1	0	0	0	0
8	K	50	0	0	0	0
8	L	12	0	0	0	0
All	All	23585	0	22545	361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (361) 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:G:111:ILE:HD13	1:G:169:HIS:CE1	1.88	1.08
2:D:30:GLN:HE22	2:D:145:ASP:HA	1.21	1.03
1:G:59:MET:SD	1:G:108:ILE:HD13	2.04	0.98
1:G:43:MET:HG3	1:G:266:ILE:HG23	1.47	0.95
2:D:30:GLN:NE2	2:D:145:ASP:HA	1.81	0.94
1:G:193:LEU:CB	1:G:241:ASN:HD22	1.83	0.92
1:G:193:LEU:HB2	1:G:241:ASN:HB2	1.52	0.88
1:G:43:MET:HG3	1:G:266:ILE:CG2	2.05	0.87
1:G:111:ILE:HD13	1:G:169:HIS:HE1	1.46	0.79
2:D:84:THR:HG21	2:F:84:THR:HG22	1.65	0.78
1:G:122:ASN:OD1	1:G:146:VAL:HG13	1.85	0.77
1:A:303:ASN:H	2:B:93:THR:CG2	1.98	0.76
1:G:123:SER:OG	1:G:143:LYS:HB3	1.86	0.76
1:K:171:ILE:HD12	1:K:250:VAL:HG12	1.68	0.75
1:G:41:LEU:CD1	1:G:264:ALA:HB3	2.17	0.75
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.21	0.73
1:G:183:GLU:O	1:G:187:LEU:HD13	1.86	0.73
1:G:111:ILE:CD1	1:G:169:HIS:CE1	2.70	0.72
1:G:193:LEU:CB	1:G:241:ASN:HB2	2.20	0.72
1:A:205:ASN:HB2	1:G:209:VAL:HG13	1.71	0.72
1:C:144:TRP:HZ3	1:C:223:ILE:HD11	1.55	0.71
1:G:43:MET:CG	1:G:266:ILE:HG23	2.20	0.71
1:K:113:THR:HG21	1:K:247:PRO:O	1.89	0.71
1:G:178:PRO:HG2	1:G:210:VAL:HG22	1.73	0.70
1:C:88:TYR:CD2	1:C:89:PRO:HD2	2.26	0.70
1:E:145:LEU:HD11	1:E:246:ALA:HB2	1.72	0.70
3:R:2:GAL:O2	3:R:3:SIA:H32	1.93	0.69
1:G:193:LEU:HB3	1:G:241:ASN:HD22	1.58	0.69
1:C:88:TYR:CD1	1:C:223:ILE:HD12	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:HIS:CG	1:E:244:LEU:HD23	2.29	0.67
2:L:126:LEU:HD21	2:L:152:ILE:HD12	1.75	0.67
2:F:54:ARG:NH2	2:F:103:GLU:OE1	2.28	0.67
2:B:127:ARG:HD3	2:B:159:HIS:CD2	2.30	0.67
1:G:178:PRO:CG	1:G:210:VAL:HG22	2.24	0.66
1:G:42:CYS:HA	1:G:270:CYS:HB3	1.77	0.66
1:G:191:GLN:HE22	1:G:193:LEU:HD23	1.60	0.66
3:R:3:SIA:O6	3:R:3:SIA:O8	2.09	0.66
1:I:55:HIS:HB3	1:I:85:ALA:HB2	1.76	0.66
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.59	0.66
1:G:177:HIS:HD2	1:G:209:VAL:H	1.44	0.65
1:G:58:GLY:HA2	1:G:61:ILE:HG22	1.76	0.65
2:L:54:ARG:NH2	2:L:103:GLU:OE2	2.20	0.65
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.29	0.65
1:C:178:PRO:O	1:C:210:VAL:HG23	1.96	0.65
2:B:54:ARG:NH2	2:B:103:GLU:OE1	2.26	0.64
1:G:59:MET:SD	1:G:108:ILE:CD1	2.82	0.64
1:G:193:LEU:CA	1:G:241:ASN:HD22	2.08	0.64
1:K:307:LEU:HD22	2:L:100:VAL:HG21	1.80	0.64
2:B:128:GLN:O	2:B:170:ARG:NH1	2.30	0.64
1:E:8:HIS:CD2	2:F:21:TRP:HA	2.32	0.64
1:A:34:GLU:HG3	1:A:283:THR:CB	2.27	0.64
1:G:177:HIS:CD2	1:G:209:VAL:H	2.15	0.63
1:A:113:THR:HG21	1:A:247:PRO:O	1.97	0.63
1:G:88:TYR:CE1	1:G:223:ILE:HD12	2.33	0.63
1:K:156:GLN:OE1	1:K:241:ASN:HB3	1.99	0.63
3:M:1:NAG:O3	3:M:2:GAL:O5	2.18	0.62
1:G:197:VAL:HG12	1:G:238:PHE:HB3	1.82	0.62
1:E:4:CYS:HA	2:F:137:CYS:HA	1.81	0.62
1:A:5:LEU:HD11	2:B:122:VAL:HG21	1.82	0.61
1:G:60:LEU:HD22	1:G:251:SER:CB	2.30	0.61
1:C:40:ARG:NH1	1:C:267:ASP:OD2	2.33	0.61
1:G:145:LEU:HB2	1:G:188:TYR:OH	2.00	0.61
2:J:142:HIS:CD2	2:J:162:TYR:HB2	2.36	0.60
1:C:144:TRP:NE1	3:N:3:SIA:H112	2.16	0.60
1:C:144:TRP:CZ3	1:C:223:ILE:HD11	2.35	0.60
2:J:126:LEU:HD21	2:J:152:ILE:HD12	1.83	0.59
1:G:193:LEU:CB	1:G:241:ASN:ND2	2.61	0.59
1:G:191:GLN:NE2	1:G:193:LEU:HD23	2.17	0.59
1:G:178:PRO:HG2	1:G:210:VAL:HG13	1.85	0.59
1:K:141:GLU:HG3	1:K:249:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:127:ARG:HD3	2:L:159:HIS:CD2	2.37	0.59
1:G:41:LEU:HD11	1:G:264:ALA:HB3	1.84	0.59
1:A:34:GLU:HG3	1:A:283:THR:HB	1.83	0.59
1:A:304:LYS:HE2	2:B:97:GLU:OE1	2.02	0.59
2:B:56:ILE:HG22	2:B:56:ILE:O	2.01	0.58
2:F:154:ASN:HB3	6:F:203:NAG:O5	2.04	0.58
1:G:266:ILE:H	1:G:266:ILE:HD12	1.68	0.58
1:C:88:TYR:HE2	1:C:219:GLN:CG	2.17	0.58
1:K:5:LEU:HD21	2:L:24:PHE:CE2	2.38	0.58
2:B:48:ILE:CD1	2:B:107:THR:HG23	2.33	0.57
1:A:303:ASN:N	2:B:93:THR:CG2	2.68	0.57
1:C:78:ILE:HA	1:C:260:ILE:O	2.05	0.57
2:F:56:ILE:HG22	2:F:56:ILE:O	2.05	0.57
2:D:124:LYS:HD3	2:F:134:GLY:HA2	1.86	0.57
1:G:188:TYR:HB3	1:G:193:LEU:HD21	1.87	0.57
1:C:88:TYR:CE1	1:C:223:ILE:HG13	2.40	0.57
1:E:7:HIS:HA	2:F:21:TRP:O	2.05	0.56
1:G:38:LEU:HD11	1:G:280:SER:HB2	1.87	0.56
2:J:142:HIS:CD2	2:J:162:TYR:CB	2.87	0.56
2:H:144:CYS:HG	2:H:148:CYS:HG	1.53	0.56
1:C:193:LEU:HA	1:C:241:ASN:ND2	2.22	0.55
1:I:163:ASN:HD22	1:I:163:ASN:C	2.10	0.55
1:I:176:HIS:HA	1:I:223:ILE:HG22	1.88	0.55
2:L:56:ILE:HG22	2:L:56:ILE:O	2.05	0.55
1:A:120:SER:HB2	1:A:152:GLN:HE22	1.72	0.55
2:H:50:GLY:HA3	1:I:20:THR:O	2.07	0.55
2:L:18:VAL:O	2:L:18:VAL:HG12	2.08	0.54
1:G:219:GLN:NE2	3:R:3:SIA:O1A	2.40	0.54
1:G:173:TRP:CZ2	1:G:197:VAL:HG11	2.42	0.54
1:K:101:LYS:HE2	1:K:229:LEU:HD21	1.88	0.54
1:G:193:LEU:HA	1:G:241:ASN:HD22	1.72	0.54
2:H:51:LYS:NZ	2:H:103:GLU:OE1	2.35	0.54
1:K:5:LEU:CD1	2:L:119:TYR:HA	2.37	0.54
1:I:63:THR:HG21	1:I:85:ALA:O	2.07	0.54
1:K:128:LYS:O	1:K:131:MET:HG2	2.07	0.54
1:A:121:ILE:HD11	1:A:155:PRO:HG2	1.90	0.54
1:I:266:ILE:HD12	1:I:266:ILE:N	2.23	0.54
1:G:193:LEU:HB2	1:G:241:ASN:CB	2.33	0.53
1:I:182:GLN:O	1:I:185:ASN:OD1	2.25	0.53
1:G:176:HIS:CD2	1:G:223:ILE:CD1	2.92	0.53
1:C:92:THR:HG22	1:C:225:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:ILE:CG2	1:I:139:TYR:CD2	2.92	0.53
1:I:89:PRO:HG3	1:I:216:VAL:HB	1.91	0.53
1:A:77:LEU:HD23	1:A:103:MET:SD	2.49	0.53
1:G:88:TYR:CZ	1:G:223:ILE:HD12	2.44	0.53
1:C:193:LEU:HA	1:C:241:ASN:HD21	1.73	0.53
1:G:103:MET:CG	1:G:259:GLY:HA3	2.39	0.52
1:C:88:TYR:CE2	1:C:219:GLN:CG	2.92	0.52
1:C:89:PRO:HB3	1:C:216:VAL:HB	1.90	0.52
1:I:271:GLU:O	1:I:282:ASN:ND2	2.42	0.52
1:E:3:ILE:HD13	2:F:152:ILE:HG21	1.92	0.52
2:F:143:ALA:N	8:F:303:HOH:O	2.43	0.52
1:E:145:LEU:HD11	1:E:246:ALA:CB	2.38	0.52
1:A:172:MET:HB2	1:A:226:HIS:O	2.09	0.52
1:G:59:MET:CG	1:G:108:ILE:CD1	2.88	0.52
1:G:154:PHE:CD1	1:G:155:PRO:O	2.63	0.52
1:A:160:THR:HG22	1:A:237:THR:HG23	1.92	0.51
2:B:127:ARG:HD3	2:B:159:HIS:NE2	2.24	0.51
1:K:263:GLU:OE1	1:K:277:ARG:NH1	2.43	0.51
1:A:141:GLU:O	1:A:142:LEU:HD23	2.10	0.51
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.93	0.51
2:H:5:ALA:HB3	2:H:112:ASP:OD1	2.10	0.51
1:G:84:ILE:HD12	1:G:84:ILE:N	2.26	0.51
1:C:42:CYS:HB2	1:C:272:SER:HB3	1.93	0.51
1:I:199:SER:OG	1:I:200:SER:N	2.43	0.51
1:G:110:LYS:HD2	1:G:141:GLU:OE1	2.11	0.51
1:G:197:VAL:HG21	1:G:202:TYR:CE1	2.46	0.51
1:C:176:HIS:NE2	3:N:3:SIA:C9	2.74	0.51
1:C:51:LEU:HD21	1:C:77:LEU:HD11	1.93	0.50
2:F:27:GLN:HG3	2:F:27:GLN:O	2.11	0.50
2:L:140:ILE:N	2:L:140:ILE:HD12	2.26	0.50
1:G:49:LYS:CD	1:G:74:TRP:CE3	2.94	0.50
1:K:256:ARG:NH2	2:L:64:GLU:OE2	2.45	0.50
1:G:8:HIS:CE1	2:H:21:TRP:CD1	2.98	0.50
1:G:161:TYR:O	1:G:236:ILE:HG22	2.11	0.50
1:G:144:TRP:CH2	1:G:223:ILE:HD11	2.47	0.50
1:K:15:ILE:HD12	1:K:15:ILE:H	1.77	0.50
1:G:49:LYS:O	1:G:49:LYS:HG2	2.12	0.50
1:E:240:HIS:CD2	1:E:244:LEU:HD23	2.46	0.50
2:H:84:THR:HG21	2:J:84:THR:HG22	1.94	0.50
1:E:240:HIS:CE1	1:E:244:LEU:HD23	2.47	0.49
2:F:128:GLN:O	2:F:170:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLY:O	1:C:144:TRP:HB3	2.12	0.49
1:G:136:ASN:N	1:G:136:ASN:OD1	2.45	0.49
1:K:286:PRO:HG2	1:K:287:PHE:CD2	2.46	0.49
1:G:7:HIS:HB3	2:H:115:MET:CE	2.42	0.49
1:I:149:ASN:O	1:I:152:GLN:HG2	2.12	0.49
1:C:88:TYR:CE2	1:C:219:GLN:HG2	2.46	0.49
1:G:288:GLN:NE2	1:G:291:SER:H	2.11	0.49
1:K:101:LYS:CE	1:K:229:LEU:HD21	2.43	0.49
1:G:103:MET:CA	1:G:103:MET:HE2	2.42	0.49
2:F:142:HIS:CE1	2:F:162:TYR:CD1	3.00	0.49
2:F:99:LEU:HD22	2:L:94:TYR:OH	2.13	0.49
2:F:145:ASP:OD2	2:F:148:CYS:N	2.46	0.48
2:D:142:HIS:CE1	2:D:162:TYR:CD1	3.01	0.48
1:E:15:ILE:HG23	1:E:23:GLN:HA	1.96	0.48
1:I:88:TYR:CD2	1:I:89:PRO:HD2	2.48	0.48
1:G:8:HIS:N	2:H:21:TRP:O	2.45	0.48
1:A:5:LEU:CD1	2:B:119:TYR:HA	2.44	0.48
1:C:181:THR:O	1:C:184:LYS:HB3	2.13	0.48
1:G:143:LYS:O	1:G:246:ALA:HB3	2.13	0.48
1:A:160:THR:HB	1:A:237:THR:OG1	2.14	0.48
1:I:122:ASN:ND2	1:I:146:VAL:HG13	2.29	0.48
2:J:75:HIS:O	2:J:79:ASN:ND2	2.47	0.48
1:G:295:VAL:HA	2:H:63:PHE:O	2.14	0.48
1:G:311:THR:HG21	6:G:404:NAG:H83	1.96	0.48
1:G:49:LYS:HD3	1:G:74:TRP:CE3	2.49	0.48
1:I:37:SER:HB3	1:I:290:LEU:HD22	1.96	0.48
1:C:104:GLU:OE1	1:C:256:ARG:NH2	2.47	0.47
2:H:93:THR:O	2:H:97:GLU:HG3	2.14	0.47
1:I:144:TRP:HA	1:I:245:ILE:HG22	1.94	0.47
1:C:307:LEU:HG	2:D:100:VAL:HG21	1.95	0.47
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.14	0.47
1:C:88:TYR:CE2	1:C:219:GLN:HG3	2.49	0.47
2:D:150:GLU:OE1	2:D:153:ARG:NH2	2.39	0.47
1:G:44:LYS:HG3	1:G:270:CYS:N	2.29	0.47
1:G:57:ILE:HD11	1:G:95:GLU:HG3	1.96	0.47
1:A:271:GLU:O	1:A:282:ASN:ND2	2.33	0.47
1:E:171:ILE:HD13	1:E:236:ILE:HG21	1.95	0.47
1:E:240:HIS:CD2	1:E:244:LEU:HB3	2.48	0.47
1:K:120:SER:OG	1:K:155:PRO:HG3	2.14	0.47
1:K:300:LYS:HG3	2:L:92:TRP:CE2	2.49	0.47
1:I:41:LEU:HD13	1:I:264:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:TRP:CH2	1:E:108:ILE:HG22	2.49	0.47
1:G:177:HIS:HB3	1:G:209:VAL:O	2.15	0.47
2:H:99:LEU:HD22	2:J:94:TYR:OH	2.14	0.47
1:K:3:ILE:HD13	2:L:152:ILE:HG21	1.97	0.47
2:B:56:ILE:CG2	2:B:56:ILE:O	2.62	0.47
1:G:266:ILE:N	1:G:266:ILE:HD12	2.29	0.47
1:I:7:HIS:HB3	2:J:115:MET:CE	2.45	0.47
1:E:300:LYS:HG3	2:F:92:TRP:CE2	2.50	0.47
1:G:43:MET:HE2	1:G:48:HIS:HB3	1.97	0.47
1:K:281:ILE:HG22	1:K:283:THR:HG22	1.97	0.47
1:C:205:ASN:HB2	1:E:209:VAL:CG2	2.44	0.46
1:A:303:ASN:N	2:B:93:THR:HG22	2.30	0.46
1:A:205:ASN:CB	1:G:209:VAL:HG22	2.45	0.46
1:G:55:HIS:CG	1:G:85:ALA:HB2	2.51	0.46
1:E:3:ILE:CD1	2:F:152:ILE:HG21	2.45	0.46
1:G:101:LYS:HG2	1:G:253:LEU:CD1	2.45	0.46
1:G:51:LEU:HD11	1:G:77:LEU:HD11	1.96	0.46
2:L:125:GLN:OE1	2:L:155:ASN:HA	2.15	0.46
1:G:193:LEU:HB2	1:G:241:ASN:HD22	1.76	0.46
1:C:39:ASN:O	1:C:264:ALA:HB1	2.15	0.46
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.15	0.46
1:G:260:ILE:HG22	1:G:261:GLN:N	2.31	0.46
1:A:5:LEU:HD11	2:B:122:VAL:CG2	2.46	0.46
1:C:51:LEU:O	1:C:54:CYS:HB3	2.15	0.46
1:C:68:LEU:N	1:C:68:LEU:HD12	2.31	0.46
1:I:149:ASN:HB2	1:I:152:GLN:CD	2.36	0.46
2:J:26:HIS:CD2	2:J:153:ARG:HH21	2.34	0.46
1:A:293:ARG:NH1	2:B:69:GLU:OE1	2.49	0.45
2:D:142:HIS:CE1	2:D:162:TYR:CG	3.04	0.45
1:G:103:MET:HG2	1:G:259:GLY:HA3	1.97	0.45
1:I:120:SER:O	1:I:148:LYS:HG3	2.16	0.45
1:G:318:GLU:N	1:G:318:GLU:OE1	2.48	0.45
1:E:130:CYS:O	1:E:137:SER:OG	2.24	0.45
1:G:113:THR:HG22	1:G:248:SER:O	2.17	0.45
1:A:74:TRP:CE2	1:A:77:LEU:HD13	2.51	0.45
1:G:223:ILE:CG2	1:G:225:PHE:CZ	3.00	0.45
1:G:142:LEU:HD23	1:G:247:PRO:HA	1.97	0.45
1:G:43:MET:CE	1:G:48:HIS:HB3	2.47	0.45
2:H:110:MET:SD	2:H:110:MET:C	2.95	0.45
1:K:307:LEU:HD22	2:L:100:VAL:CG2	2.46	0.45
1:A:98:LEU:HD21	1:A:172:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ARG:NE	2:B:34:GLN:OE1	2.39	0.45
2:D:50:GLY:HA3	1:E:20:THR:O	2.17	0.45
1:E:240:HIS:ND1	1:E:244:LEU:HD23	2.30	0.45
1:G:176:HIS:HD2	1:G:223:ILE:CD1	2.30	0.45
1:I:175:ILE:HD13	1:I:206:PHE:HB3	1.99	0.45
1:E:295:VAL:HG11	2:F:65:SER:HB2	1.98	0.45
1:G:6:GLY:HA3	2:H:14:TRP:CZ3	2.52	0.45
1:G:79:GLU:HG2	1:G:80:ARG:N	2.31	0.45
1:I:101:LYS:HE2	1:I:229:LEU:HD11	1.98	0.45
1:C:5:LEU:HD22	2:D:119:TYR:HA	1.98	0.44
2:F:129:ASN:ND2	2:F:159:HIS:HA	2.31	0.44
1:G:60:LEU:CD2	1:G:251:SER:CB	2.95	0.44
1:E:144:TRP:CD2	3:P:3:SIA:H112	2.52	0.44
1:A:303:ASN:H	2:B:93:THR:HG21	1.81	0.44
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.99	0.44
1:E:240:HIS:CG	1:E:244:LEU:CD2	3.00	0.44
1:G:178:PRO:HG2	1:G:210:VAL:CG2	2.44	0.44
1:C:211:GLY:O	1:C:213:ARG:NH1	2.50	0.44
1:G:193:LEU:HB2	1:G:241:ASN:ND2	2.31	0.44
1:G:43:MET:CE	1:G:43:MET:HA	2.48	0.44
2:D:75:HIS:HE2	1:K:104:GLU:CD	2.21	0.44
1:G:178:PRO:HG3	1:G:184:LYS:HB2	2.00	0.44
1:G:193:LEU:HA	1:G:241:ASN:ND2	2.32	0.44
1:G:176:HIS:HD2	1:G:223:ILE:HD12	1.82	0.44
1:I:61:ILE:HG21	1:I:139:TYR:CD2	2.52	0.44
2:J:148:CYS:O	2:J:151:SER:OG	2.33	0.44
1:G:154:PHE:CD1	1:G:241:ASN:C	2.91	0.44
1:G:61:ILE:HG13	1:G:139:TYR:CD2	2.52	0.44
2:H:104:ASN:O	2:H:108:ILE:HD13	2.17	0.44
1:I:3:ILE:HD13	2:J:152:ILE:HG21	2.00	0.44
1:C:88:TYR:HE1	1:C:223:ILE:HG13	1.82	0.44
1:C:144:TRP:HZ3	1:C:223:ILE:CD1	2.28	0.43
1:C:195:ILE:HG23	1:C:240:HIS:HB3	1.99	0.43
1:G:176:HIS:CD2	1:G:223:ILE:HD12	2.53	0.43
1:K:15:ILE:HD12	1:K:15:ILE:N	2.33	0.43
1:C:1:ASP:O	2:D:140:ILE:N	2.51	0.43
1:A:205:ASN:HB3	1:G:209:VAL:HG22	2.00	0.43
1:G:49:LYS:HD2	1:G:74:TRP:CE3	2.53	0.43
1:I:96:GLU:HA	1:I:96:GLU:OE2	2.18	0.43
1:E:121:ILE:HD11	1:E:155:PRO:HG2	2.00	0.43
1:C:192:SER:O	1:C:241:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ILE:O	1:E:3:ILE:HG23	2.18	0.43
1:I:88:TYR:HE2	1:I:222:ARG:HA	1.84	0.43
1:G:34:GLU:HB2	1:G:283:THR:HG21	2.01	0.43
1:E:165:ASP:OD1	1:E:166:THR:N	2.48	0.43
1:I:65:ALA:N	8:I:502:HOH:O	2.52	0.43
1:I:80:ARG:NH2	1:I:266:ILE:HD11	2.34	0.43
1:A:87:CYS:HB2	1:A:129:ALA:O	2.19	0.43
1:E:143:LYS:HE2	1:E:248:SER:HB3	2.01	0.43
1:I:122:ASN:HD21	1:I:146:VAL:HG13	1.84	0.43
1:I:7:HIS:HB3	2:J:115:MET:HE2	2.00	0.43
2:L:140:ILE:H	2:L:140:ILE:HD12	1.83	0.43
1:G:223:ILE:HG22	1:G:225:PHE:CZ	2.54	0.42
1:G:44:LYS:HD3	1:G:269:SER:HA	2.01	0.42
1:G:43:MET:HE3	1:G:43:MET:HA	2.01	0.42
1:G:123:SER:HA	1:G:144:TRP:O	2.19	0.42
2:B:110:MET:SD	2:B:110:MET:C	2.98	0.42
2:F:142:HIS:HE2	2:F:157:TYR:HH	1.67	0.42
1:K:307:LEU:HD23	1:K:307:LEU:HA	1.94	0.42
2:D:94:TYR:OH	2:L:99:LEU:HD22	2.19	0.42
1:E:195:ILE:N	1:E:195:ILE:HD12	2.35	0.42
1:E:71:THR:HG22	1:E:110:LYS:HG2	2.02	0.42
2:B:44:ALA:O	2:B:48:ILE:HG12	2.19	0.42
1:G:38:LEU:HD12	1:G:38:LEU:O	2.20	0.42
1:G:55:HIS:HB3	1:G:85:ALA:HA	2.01	0.42
1:A:111:ILE:HD13	1:A:169:HIS:CE1	2.54	0.42
1:A:171:ILE:HG13	1:A:250:VAL:HG12	2.01	0.42
2:L:55:ILE:HD11	2:L:103:GLU:HG3	2.01	0.42
2:L:18:VAL:O	2:L:18:VAL:CG1	2.67	0.42
1:G:185:ASN:OD1	1:G:186:ASP:N	2.53	0.42
1:G:193:LEU:CA	1:G:241:ASN:ND2	2.80	0.42
1:G:-1:ASP:HB3	1:G:0:PRO:HD3	2.02	0.42
2:B:75:HIS:CD2	2:B:79:ASN:HD21	2.38	0.42
1:E:115:PHE:CE2	1:E:159:ASN:HB2	2.54	0.42
1:G:175:ILE:CD1	1:G:206:PHE:HB3	2.50	0.42
1:G:44:LYS:CG	1:G:269:SER:HA	2.50	0.42
1:K:51:LEU:HD21	1:K:77:LEU:HD11	2.02	0.42
1:E:58:GLY:O	1:E:62:GLY:N	2.48	0.41
2:J:102:MET:HG3	2:J:103:GLU:N	2.35	0.41
1:A:205:ASN:HB2	1:G:209:VAL:CG1	2.47	0.41
2:F:67:GLU:CG	2:F:81:ILE:HG21	2.50	0.41
1:G:35:SER:O	1:G:290:LEU:HD21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:ILE:O	2:D:77:ILE:HG12	2.20	0.41
1:E:74:TRP:HH2	1:E:108:ILE:HG22	1.86	0.41
2:F:121:ARG:O	2:F:125:GLN:HB2	2.20	0.41
1:G:77:LEU:HD23	1:G:103:MET:HA	2.03	0.41
2:H:84:THR:HG21	2:J:84:THR:CG2	2.50	0.41
2:J:145:ASP:N	2:J:145:ASP:OD2	2.51	0.41
1:K:300:LYS:HD2	2:L:92:TRP:NE1	2.36	0.41
1:C:7:HIS:HB3	2:D:115:MET:HE1	2.03	0.41
1:G:288:GLN:HG2	1:G:290:LEU:H	1.85	0.41
2:F:47:GLN:HB2	1:K:20:THR:OG1	2.19	0.41
1:K:276:TRP:CE3	1:K:291:SER:HB2	2.55	0.41
1:K:307:LEU:HD11	2:L:97:GLU:HA	2.01	0.41
1:A:94:ASN:HB2	1:A:227:TRP:HE1	1.85	0.41
1:C:195:ILE:HD11	1:C:242:GLY:O	2.21	0.41
1:G:215:GLN:HA	1:G:220:SER:HA	2.02	0.41
1:G:103:MET:HG3	1:G:259:GLY:HA3	2.01	0.41
1:G:57:ILE:CD1	1:G:95:GLU:HG3	2.50	0.41
2:D:2:LEU:HA	2:D:2:LEU:HD23	1.85	0.41
1:G:198:GLY:N	1:G:237:THR:O	2.54	0.41
1:K:141:GLU:O	1:K:142:LEU:HD23	2.19	0.41
1:C:313:MET:HG3	1:C:314:ARG:O	2.21	0.41
1:G:178:PRO:HD2	1:G:210:VAL:HG22	2.03	0.41
1:G:60:LEU:HD22	1:G:251:SER:HB2	2.03	0.41
2:H:127:ARG:HD2	2:H:159:HIS:CD2	2.55	0.41
2:B:139:GLU:OE1	2:J:127:ARG:NH2	2.48	0.41
1:C:176:HIS:NE2	3:N:3:SIA:H91	2.36	0.41
2:F:5:ALA:HB3	2:F:112:ASP:OD1	2.21	0.41
2:B:4:GLY:O	2:B:8:GLY:HA3	2.21	0.41
2:F:129:ASN:HD21	2:F:159:HIS:HA	1.86	0.41
1:I:171:ILE:HD13	1:I:236:ILE:HG21	2.03	0.41
1:E:98:LEU:O	1:E:102:ILE:HD12	2.21	0.41
1:G:178:PRO:CD	1:G:210:VAL:HG22	2.51	0.41
1:C:102:ILE:O	1:C:105:SER:OG	2.26	0.40
1:G:61:ILE:HG13	1:G:139:TYR:HD2	1.86	0.40
1:E:38:LEU:HB2	1:E:280:SER:O	2.22	0.40
1:G:34:GLU:HG2	1:G:283:THR:HB	2.01	0.40
1:G:63:THR:HG23	1:G:64:PRO:HD2	2.04	0.40
1:I:175:ILE:CD1	1:I:206:PHE:CG	3.04	0.40
2:D:90:ASP:HA	2:D:93:THR:HG22	2.02	0.40
1:G:110:LYS:HB3	1:G:249:ARG:HD2	2.03	0.40
1:I:4:CYS:HA	2:J:137:CYS:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:HIS:HA	2:J:21:TRP:O	2.21	0.40
2:D:19:ASP:OD1	2:D:19:ASP:N	2.55	0.40
1:E:63:THR:HG22	1:E:64:PRO:HD2	2.03	0.40
1:G:7:HIS:CE1	2:H:6:ILE:HG23	2.56	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	318/325 (98%)	307 (96%)	11 (4%)	0	100	100
1	C	316/325 (97%)	296 (94%)	20 (6%)	0	100	100
1	E	317/325 (98%)	294 (93%)	23 (7%)	0	100	100
1	G	312/325 (96%)	300 (96%)	12 (4%)	0	100	100
1	I	316/325 (97%)	294 (93%)	22 (7%)	0	100	100
1	K	316/325 (97%)	307 (97%)	9 (3%)	0	100	100
2	B	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
2	D	170/177 (96%)	163 (96%)	7 (4%)	0	100	100
2	F	170/177 (96%)	153 (90%)	17 (10%)	0	100	100
2	H	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
2	J	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	L	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
All	All	2915/3012 (97%)	2770 (95%)	145 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	271/275 (98%)	264 (97%)	7 (3%)	46	75
1	C	269/275 (98%)	255 (95%)	14 (5%)	23	49
1	E	270/275 (98%)	258 (96%)	12 (4%)	28	56
1	G	268/275 (98%)	250 (93%)	18 (7%)	16	37
1	I	267/275 (97%)	258 (97%)	9 (3%)	37	66
1	K	269/275 (98%)	262 (97%)	7 (3%)	46	75
2	B	146/151 (97%)	140 (96%)	6 (4%)	30	59
2	D	146/151 (97%)	141 (97%)	5 (3%)	37	66
2	F	146/151 (97%)	146 (100%)	0	100	100
2	H	146/151 (97%)	142 (97%)	4 (3%)	44	74
2	J	146/151 (97%)	141 (97%)	5 (3%)	37	66
2	L	146/151 (97%)	146 (100%)	0	100	100
All	All	2490/2556 (97%)	2403 (96%)	87 (4%)	36	65

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	160	THR
1	A	191	GLN
1	A	207	VAL
1	A	273	LYS
1	A	282	ASN
1	A	288	GLN
2	B	27	GLN
2	B	76	GLN
2	B	90	ASP
2	B	113	SER
2	B	135	LYS
2	B	163	ARG
1	C	8	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	35	SER
1	C	40	ARG
1	C	53	ASN
1	C	86	TYR
1	C	87	CYS
1	C	123	SER
1	C	156	GLN
1	C	175	ILE
1	C	184	LYS
1	C	203	LYS
1	C	288	GLN
1	C	294	THR
1	C	316	VAL
2	D	30	GLN
2	D	58	LYS
2	D	77	ILE
2	D	113	SER
2	D	155	ASN
1	E	2	LYS
1	E	8	HIS
1	E	38	LEU
1	E	40	ARG
1	E	53	ASN
1	E	159	ASN
1	E	172	MET
1	E	199	SER
1	E	207	VAL
1	E	270	CYS
1	E	288	GLN
1	E	295	VAL
1	G	8	HIS
1	G	38	LEU
1	G	40	ARG
1	G	43	MET
1	G	63	THR
1	G	87	CYS
1	G	92	THR
1	G	103	MET
1	G	113	THR
1	G	136	ASN
1	G	156	GLN
1	G	181	THR

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Mol	Chain	Res	Type
1	G	193	LEU
1	G	204	ASN
1	G	220	SER
1	G	223	ILE
1	G	288	GLN
1	G	316	VAL
2	H	46	ASP
2	H	58	LYS
2	H	76	GLN
2	H	113	SER
1	I	8	HIS
1	I	38	LEU
1	I	47	ASN
1	I	71	THR
1	I	88	TYR
1	I	109	SER
1	I	130	CYS
1	I	163	ASN
1	I	207	VAL
2	J	19	ASP
2	J	30	GLN
2	J	59	THR
2	J	102	MET
2	J	142	HIS
1	K	8	HIS
1	K	10	VAL
1	K	20	THR
1	K	36	THR
1	K	63	THR
1	K	103	MET
1	K	315	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	159	ASN
1	A	185	ASN
2	B	27	GLN
2	B	53	ASN
2	B	75	HIS
2	B	79	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	53	ASN
1	C	177	HIS
1	C	219	GLN
2	D	30	GLN
2	D	95	GLN
1	E	23	GLN
1	E	39	ASN
1	E	47	ASN
1	E	100	GLN
1	E	133	ASN
1	E	149	ASN
1	E	240	HIS
1	E	268	ASN
2	F	30	GLN
2	F	76	GLN
2	F	105	GLN
1	G	8	HIS
1	G	152	GLN
1	G	156	GLN
1	G	177	HIS
1	G	191	GLN
1	G	204	ASN
1	G	205	ASN
1	G	241	ASN
1	G	288	GLN
2	H	76	GLN
1	I	23	GLN
1	I	47	ASN
1	I	100	GLN
1	I	112	ASN
1	I	133	ASN
1	I	163	ASN
1	I	205	ASN
1	I	215	GLN
2	J	26	HIS
2	J	125	GLN
2	J	154	ASN
1	K	152	GLN
1	K	159	ASN
1	K	268	ASN
2	L	79	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](#)

27 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	M	1	3	15,15,15	0.44	0	21,21,21	1.32	2 (9%)
3	GAL	M	2	3	11,11,12	0.27	0	15,15,17	1.36	3 (20%)
3	SIA	M	3	3	17,20,21	0.58	0	21,28,31	1.19	1 (4%)
3	NAG	N	1	3	15,15,15	0.50	0	21,21,21	1.25	2 (9%)
3	GAL	N	2	3	11,11,12	0.34	0	15,15,17	1.61	4 (26%)
3	SIA	N	3	3	17,20,21	0.41	0	21,28,31	1.05	1 (4%)
4	NAG	O	1	2,4,7	14,14,15	0.34	0	17,19,21	1.02	0
4	NAG	O	2	4	14,14,15	0.46	0	17,19,21	1.22	1 (5%)
3	NAG	P	1	3	15,15,15	0.58	0	21,21,21	0.95	1 (4%)
3	GAL	P	2	3	11,11,12	0.45	0	15,15,17	1.57	1 (6%)
3	SIA	P	3	3	17,20,21	0.61	0	21,28,31	1.48	3 (14%)
4	NAG	Q	1	2,4	14,14,15	0.56	0	17,19,21	0.90	0
4	NAG	Q	2	4	14,14,15	0.43	0	17,19,21	1.09	1 (5%)
3	NAG	R	1	3	15,15,15	0.47	0	21,21,21	1.67	5 (23%)
3	GAL	R	2	3	11,11,12	0.45	0	15,15,17	1.26	2 (13%)
3	SIA	R	3	3	17,20,21	0.56	0	21,28,31	1.09	1 (4%)
4	NAG	S	1	2,4,7	14,14,15	0.50	0	17,19,21	1.65	2 (11%)
4	NAG	S	2	4	14,14,15	0.66	0	17,19,21	1.84	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GAL	T	1	5	12,12,12	0.64	0	17,17,17	1.24	3 (17%)
5	SIA	T	2	5	17,20,21	0.53	0	21,28,31	1.18	3 (14%)
4	NAG	U	1	2,4,7	14,14,15	0.39	0	17,19,21	0.97	1 (5%)
4	NAG	U	2	4	14,14,15	0.39	0	17,19,21	1.40	4 (23%)
3	NAG	V	1	3	15,15,15	0.51	0	21,21,21	1.39	3 (14%)
3	GAL	V	2	3	11,11,12	0.34	0	15,15,17	1.25	3 (20%)
3	SIA	V	3	3	17,20,21	0.48	0	21,28,31	1.44	3 (14%)
4	NAG	W	1	2,4	14,14,15	0.29	0	17,19,21	1.07	1 (5%)
4	NAG	W	2	4	14,14,15	0.46	0	17,19,21	1.29	1 (5%)

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	M	1	3	-	1/6/26/26	0/1/1/1
3	GAL	M	2	3	-	2/2/19/22	0/1/1/1
3	SIA	M	3	3	-	5/14/34/38	0/1/1/1
3	NAG	N	1	3	-	2/6/26/26	0/1/1/1
3	GAL	N	2	3	-	1/2/19/22	0/1/1/1
3	SIA	N	3	3	-	1/14/34/38	0/1/1/1
4	NAG	O	1	2,4,7	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
3	NAG	P	1	3	-	0/6/26/26	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	0/14/34/38	0/1/1/1
4	NAG	Q	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3	-	2/6/26/26	0/1/1/1
3	GAL	R	2	3	-	2/2/19/22	0/1/1/1
3	SIA	R	3	3	-	10/14/34/38	0/1/1/1
4	NAG	S	1	2,4,7	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
5	GAL	T	1	5	-	1/2/22/22	0/1/1/1
5	SIA	T	2	5	-	3/14/34/38	0/1/1/1
4	NAG	U	1	2,4,7	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	1	3	-	2/6/26/26	0/1/1/1
3	GAL	V	2	3	-	2/2/19/22	0/1/1/1
3	SIA	V	3	3	-	0/14/34/38	0/1/1/1
4	NAG	W	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	1	NAG	C1-O5-C5	4.96	118.91	112.19
3	P	2	GAL	C1-C2-C3	4.85	115.63	109.67
4	S	2	NAG	C1-O5-C5	4.72	118.59	112.19
3	P	3	SIA	C4-C5-N5	-4.58	101.30	110.38
3	V	1	NAG	C3-C2-N2	-4.05	102.97	110.62
3	M	3	SIA	C4-C5-N5	-4.00	102.46	110.38
4	W	2	NAG	C4-C3-C2	3.69	116.43	111.02
3	N	2	GAL	C1-C2-C3	3.69	114.20	109.67
3	V	3	SIA	C4-C5-N5	-3.61	103.24	110.38
4	S	2	NAG	O5-C5-C6	3.56	112.79	107.20
3	N	2	GAL	C2-C3-C4	3.40	116.79	110.89
3	R	1	NAG	C3-C4-C5	3.40	116.31	110.24
3	N	1	NAG	C1-C2-N2	-3.36	106.83	110.73
5	T	1	GAL	C3-C4-C5	3.20	115.95	110.24
3	R	1	NAG	O5-C5-C4	3.16	115.44	109.69
3	V	3	SIA	C3-C4-C5	-3.14	107.67	111.46
3	M	1	NAG	C1-C2-N2	-3.00	107.25	110.73
3	V	1	NAG	C4-C3-C2	2.99	114.73	110.34
4	W	1	NAG	C1-O5-C5	2.97	116.21	112.19
3	M	2	GAL	O5-C5-C6	2.96	111.84	107.20
3	R	1	NAG	O5-C1-C2	-2.94	106.56	109.52
4	Q	2	NAG	C1-O5-C5	2.91	116.14	112.19
3	N	3	SIA	C4-C5-N5	-2.90	104.64	110.38
4	U	1	NAG	C1-O5-C5	2.90	116.12	112.19
3	R	2	GAL	C1-C2-C3	2.82	113.14	109.67
3	R	3	SIA	C4-C3-C2	2.82	114.87	109.81
3	N	1	NAG	C3-C2-N2	-2.81	105.30	110.62
3	R	1	NAG	C6-C5-C4	-2.81	106.42	113.00
4	U	2	NAG	O5-C5-C6	2.81	111.61	107.20
3	V	3	SIA	C9-C8-C7	-2.79	106.37	112.41
5	T	2	SIA	C4-C3-C2	2.72	114.69	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	SIA	C6-C5-N5	2.70	115.40	110.91
5	T	1	GAL	O5-C1-C2	-2.65	105.55	110.28
3	P	3	SIA	C6-O6-C2	2.60	116.90	111.34
3	M	2	GAL	O3-C3-C2	-2.59	105.03	109.99
3	V	2	GAL	C1-C2-C3	2.55	112.80	109.67
5	T	2	SIA	C6-O6-C2	2.46	116.61	111.34
3	V	1	NAG	C3-C4-C5	2.45	114.62	110.24
3	M	1	NAG	C3-C4-C5	2.43	114.56	110.24
3	V	2	GAL	O3-C3-C2	-2.42	105.35	109.99
3	R	2	GAL	C2-C3-C4	2.37	114.99	110.89
4	S	2	NAG	C1-C2-N2	2.33	114.46	110.49
4	U	2	NAG	O5-C5-C4	-2.32	105.19	110.83
4	S	2	NAG	C4-C3-C2	-2.30	107.65	111.02
5	T	2	SIA	C4-C5-N5	-2.23	105.95	110.38
4	O	2	NAG	C2-N2-C7	2.22	126.06	122.90
3	N	2	GAL	O5-C5-C6	2.17	110.61	107.20
3	M	2	GAL	O5-C1-C2	-2.11	107.52	110.77
5	T	1	GAL	O5-C5-C4	2.09	113.49	109.69
3	R	1	NAG	C1-C2-C3	-2.08	107.71	110.54
4	S	2	NAG	C6-C5-C4	-2.08	108.14	113.00
3	P	1	NAG	C1-C2-N2	-2.07	108.33	110.73
4	U	2	NAG	C3-C4-C5	-2.04	106.60	110.24
3	V	2	GAL	O5-C5-C6	2.04	110.39	107.20
3	N	2	GAL	O3-C3-C2	-2.03	106.11	109.99
4	U	2	NAG	O5-C1-C2	2.02	114.47	111.29
4	S	1	NAG	O7-C7-N2	2.01	125.65	121.95

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1	NAG	C1-C2-N2-C7
3	R	3	SIA	C5-C6-C7-C8
3	R	3	SIA	C5-C6-C7-O7
3	R	3	SIA	O6-C6-C7-C8
3	R	3	SIA	O6-C6-C7-O7
3	R	3	SIA	C6-C7-C8-O8
3	R	3	SIA	O7-C7-C8-O8
3	M	3	SIA	O6-C6-C7-C8
3	M	3	SIA	O6-C6-C7-O7
5	T	2	SIA	O6-C6-C7-O7
4	S	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	R	2	GAL	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
3	R	2	GAL	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	R	3	SIA	O7-C7-C8-C9
4	W	2	NAG	C4-C5-C6-O6
3	R	3	SIA	C6-C7-C8-C9
3	V	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	V	2	GAL	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	N	2	GAL	O5-C5-C6-O6
3	V	2	GAL	O5-C5-C6-O6
3	R	3	SIA	C6-C5-N5-C10
4	Q	2	NAG	O5-C5-C6-O6
3	M	2	GAL	C4-C5-C6-O6
3	M	2	GAL	O5-C5-C6-O6
3	M	3	SIA	O8-C8-C9-O9
4	W	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
5	T	1	GAL	O5-C5-C6-O6
3	M	3	SIA	C5-C6-C7-C8
3	M	3	SIA	C5-C6-C7-O7
5	T	2	SIA	C5-C6-C7-O7
5	T	2	SIA	O6-C6-C7-C8
3	M	1	NAG	C4-C5-C6-O6
3	R	3	SIA	C4-C5-N5-C10
3	R	1	NAG	C3-C2-N2-C7
4	O	2	NAG	C3-C2-N2-C7
3	N	3	SIA	C4-C5-N5-C10

There are no ring outliers.

6 monomers are involved in 8 short contacts:

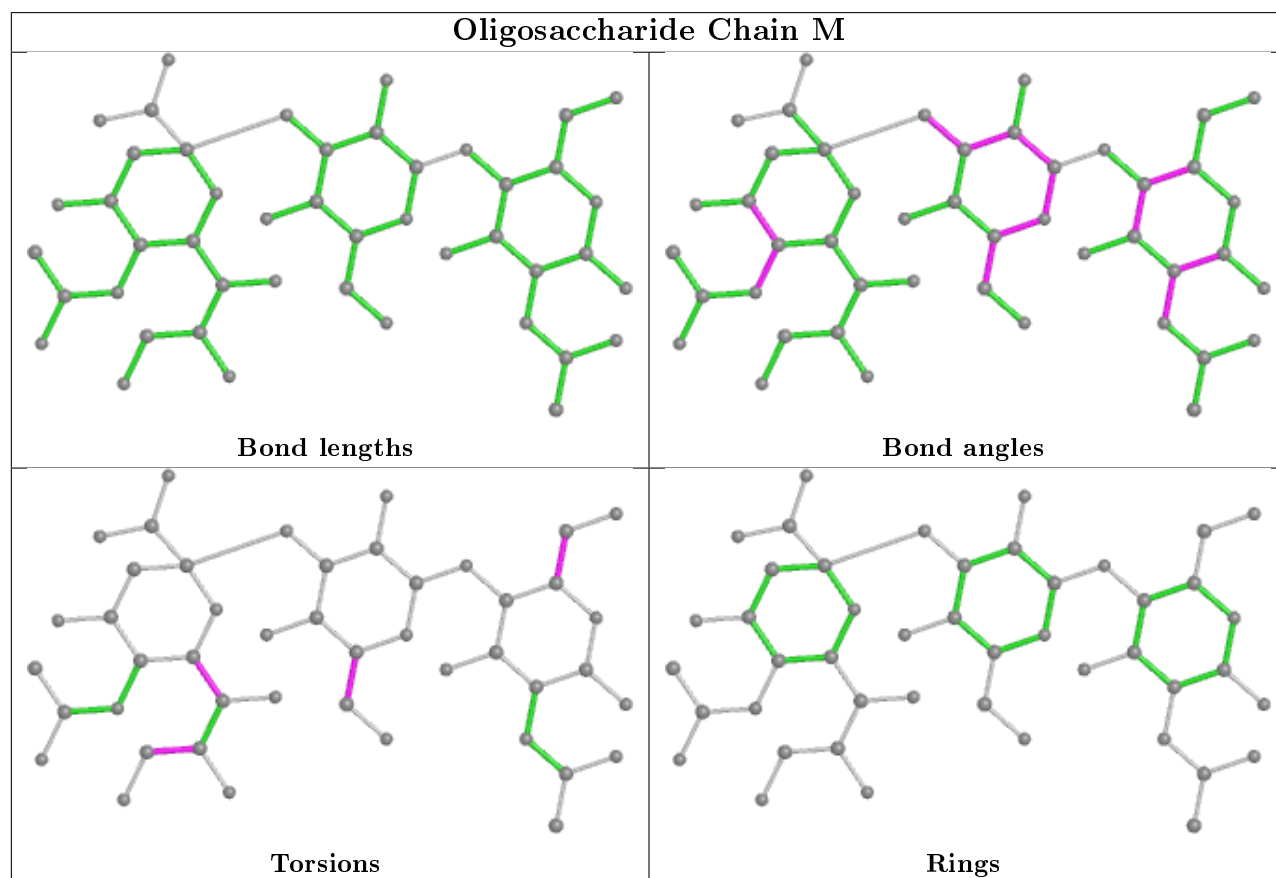
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	3	SIA	1	0
3	R	2	GAL	1	0
3	N	3	SIA	3	0

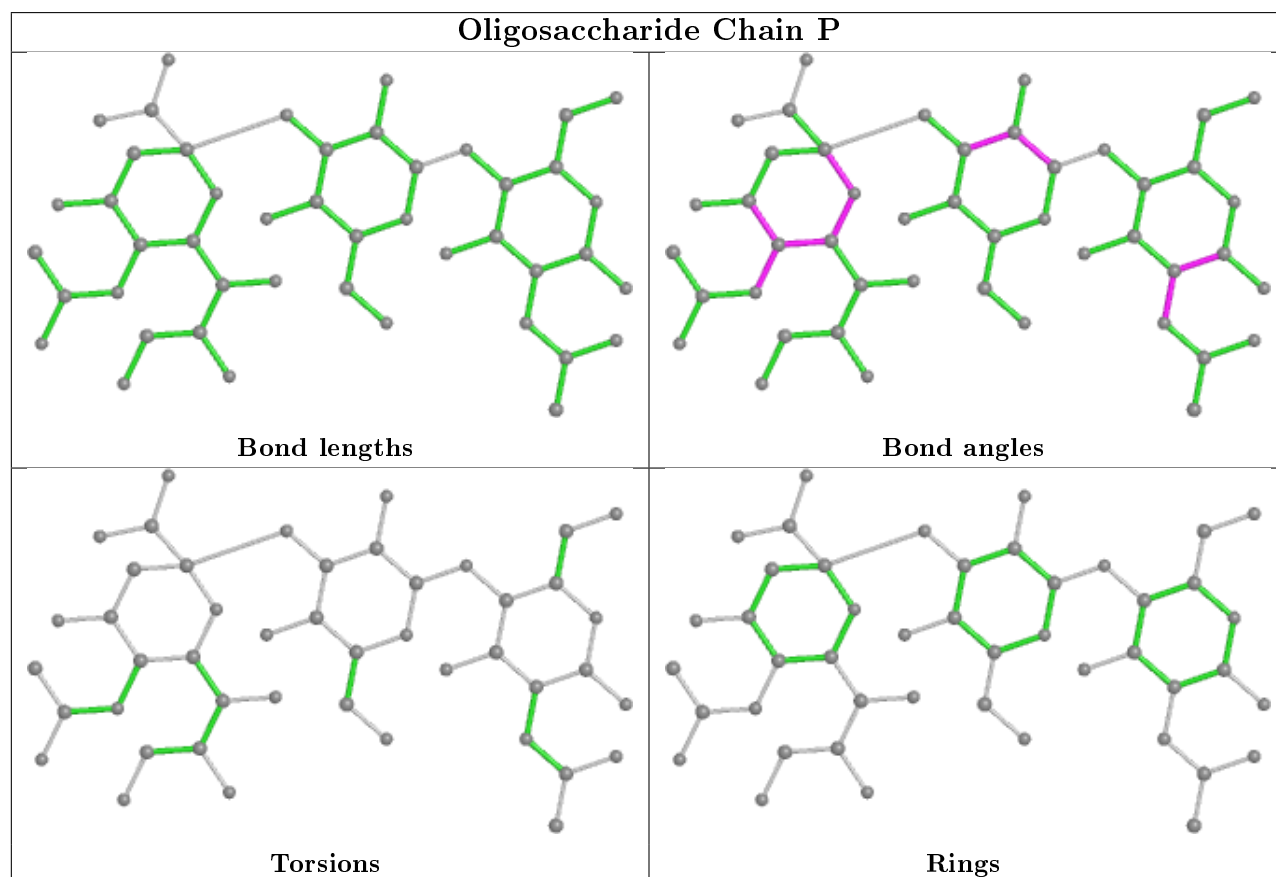
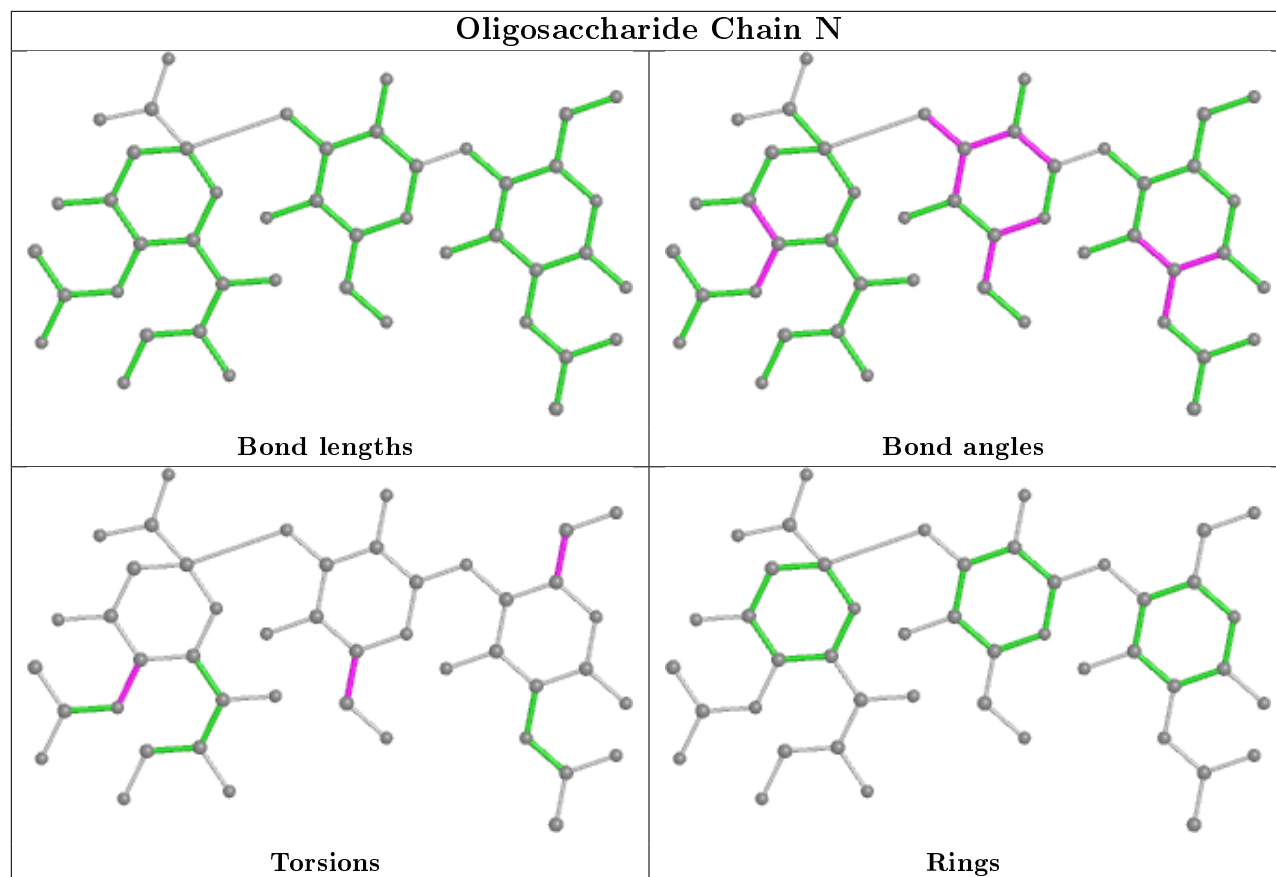
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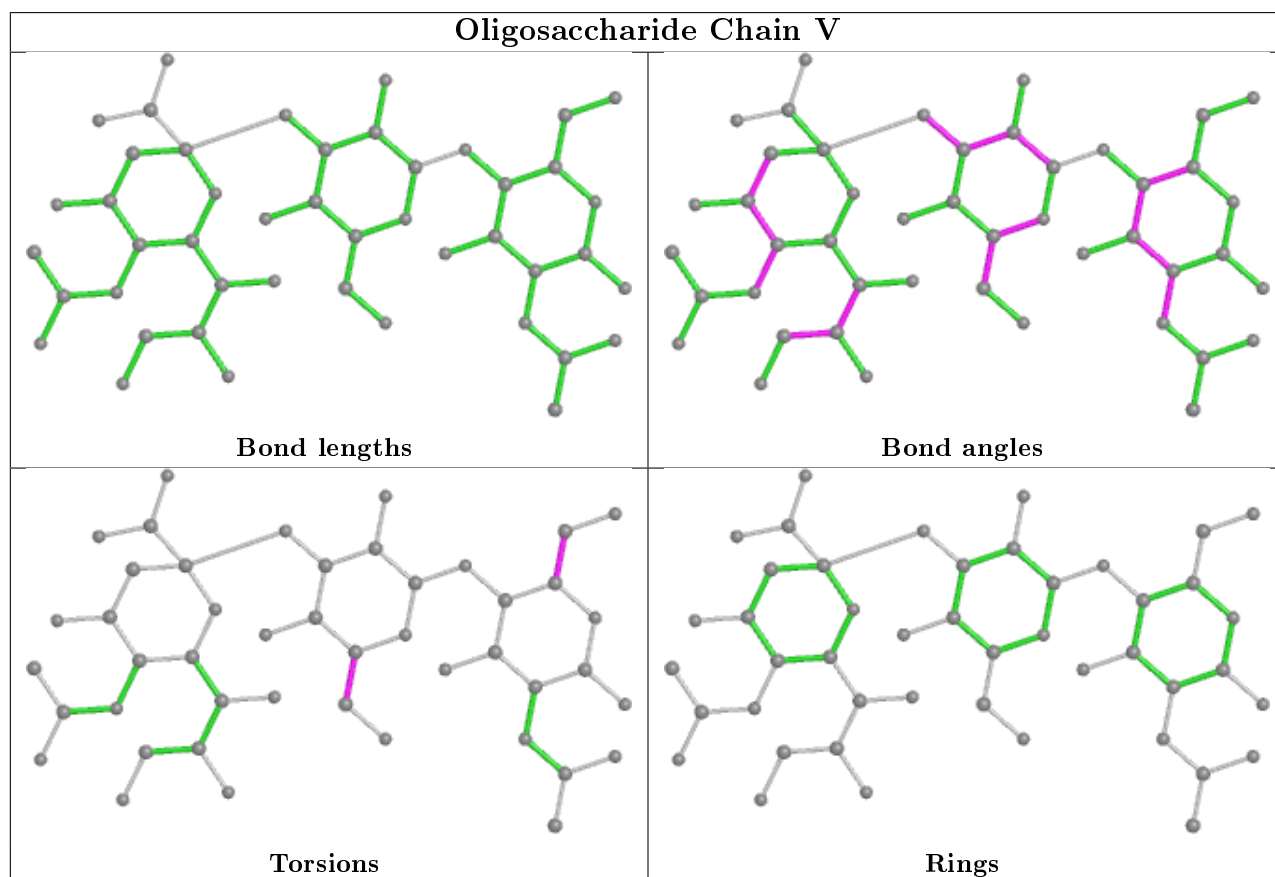
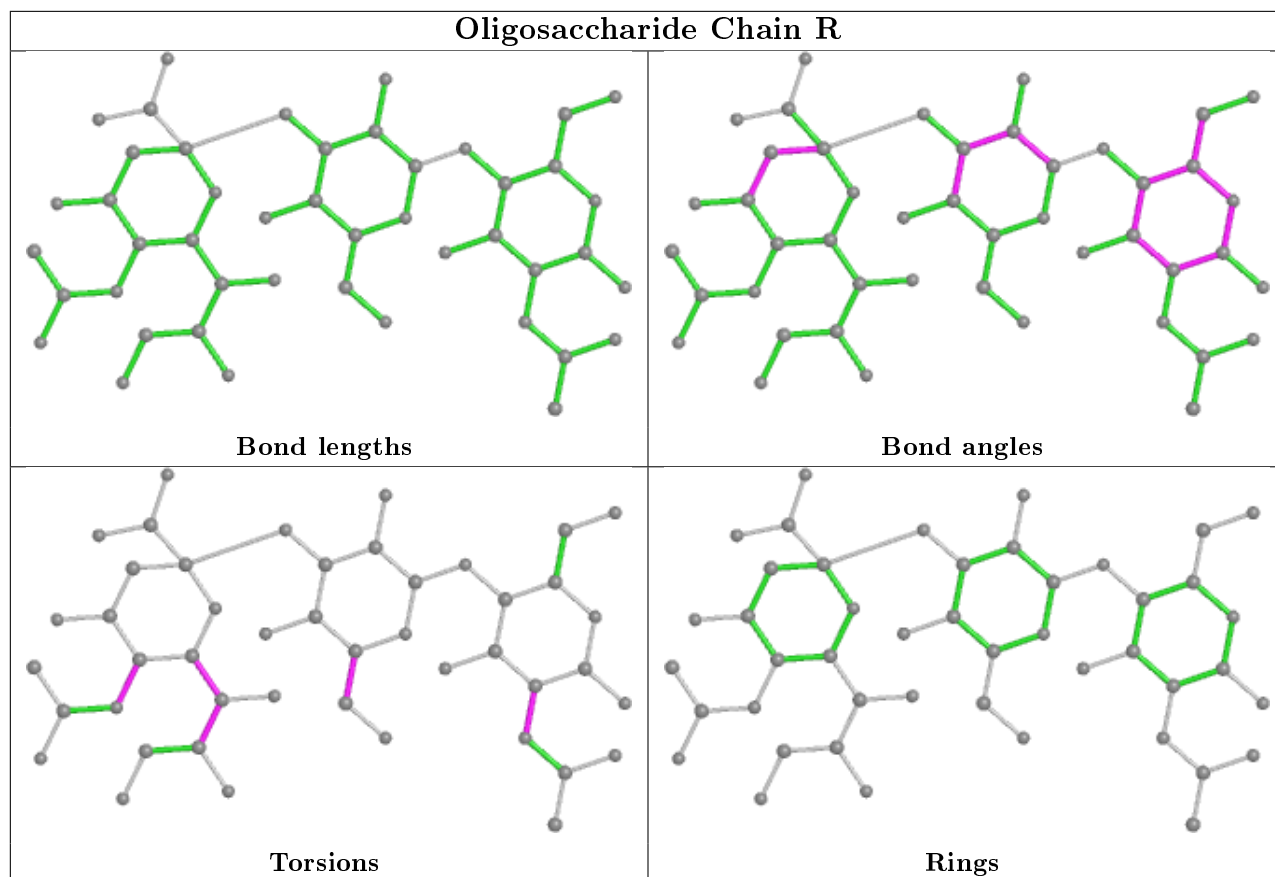
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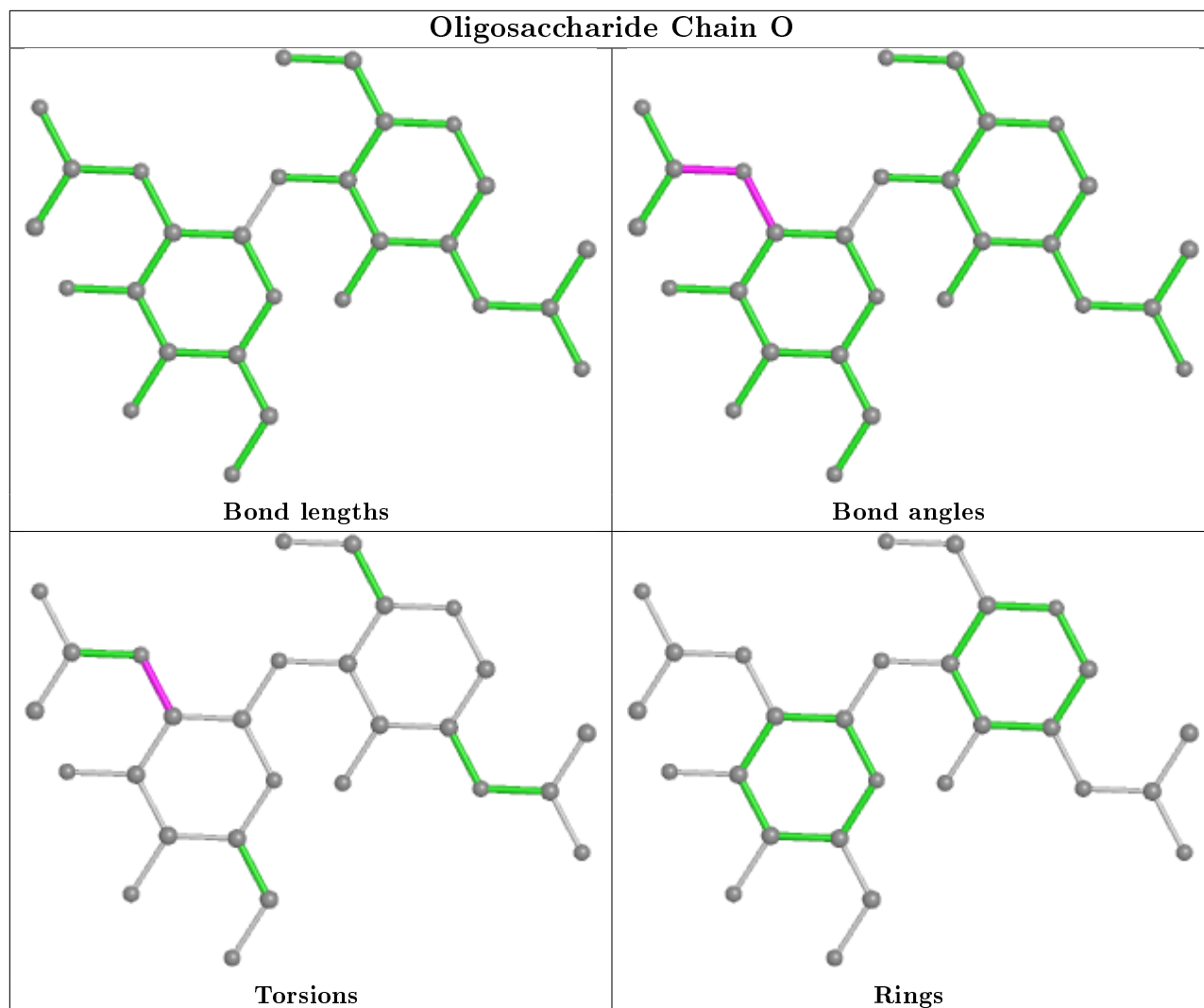
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	3	SIA	3	0
3	M	1	NAG	1	0
3	M	2	GAL	1	0

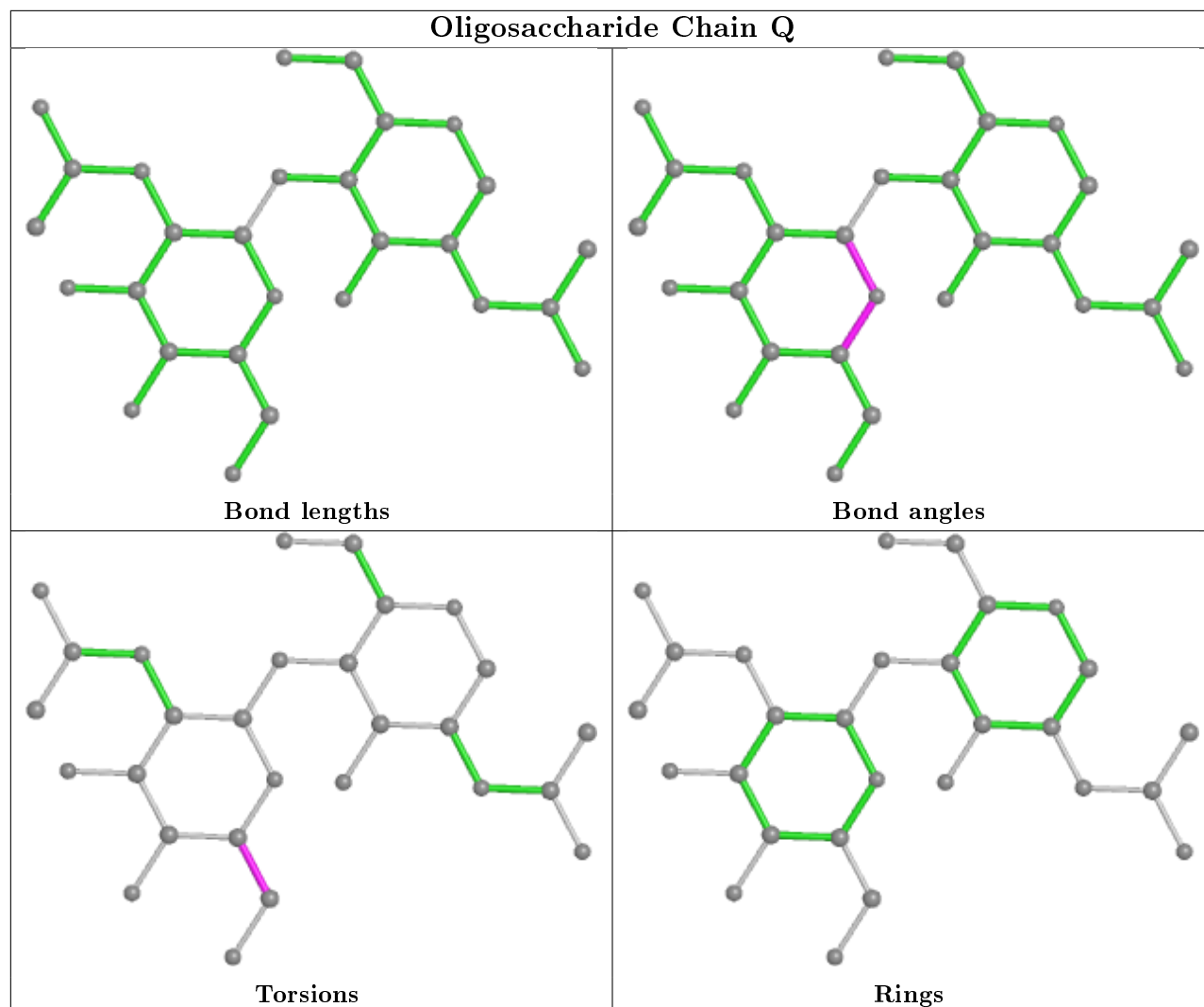
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



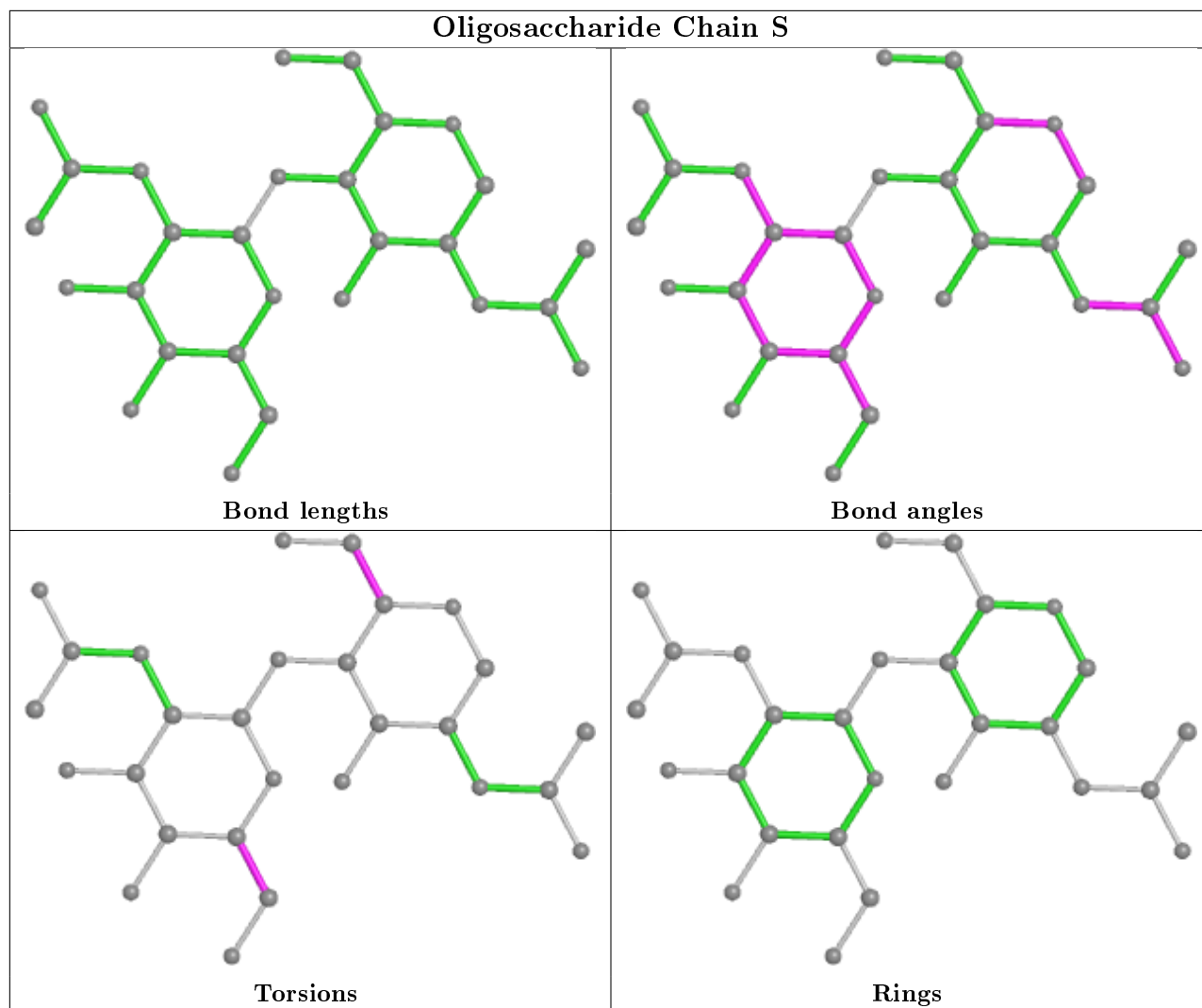


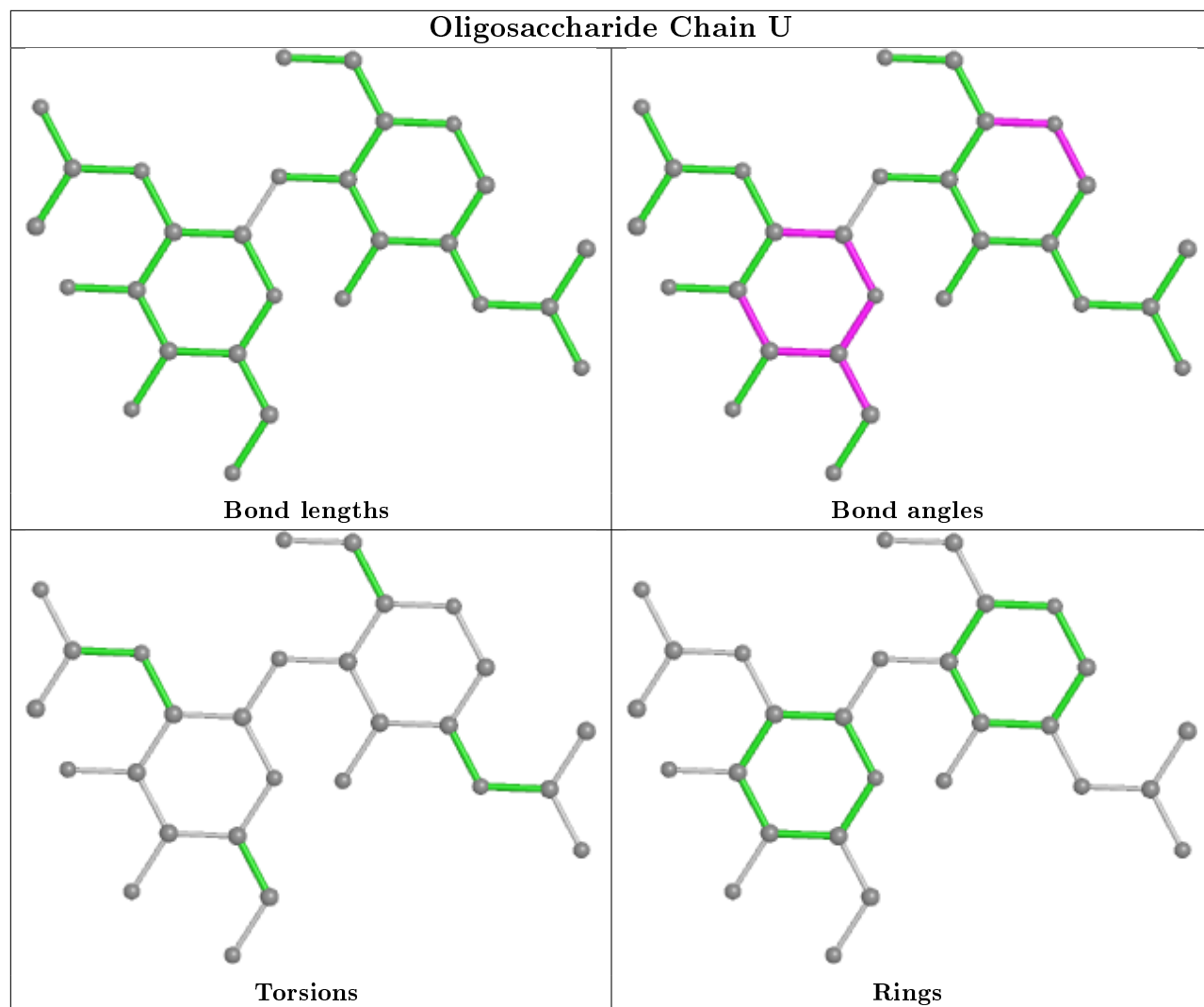


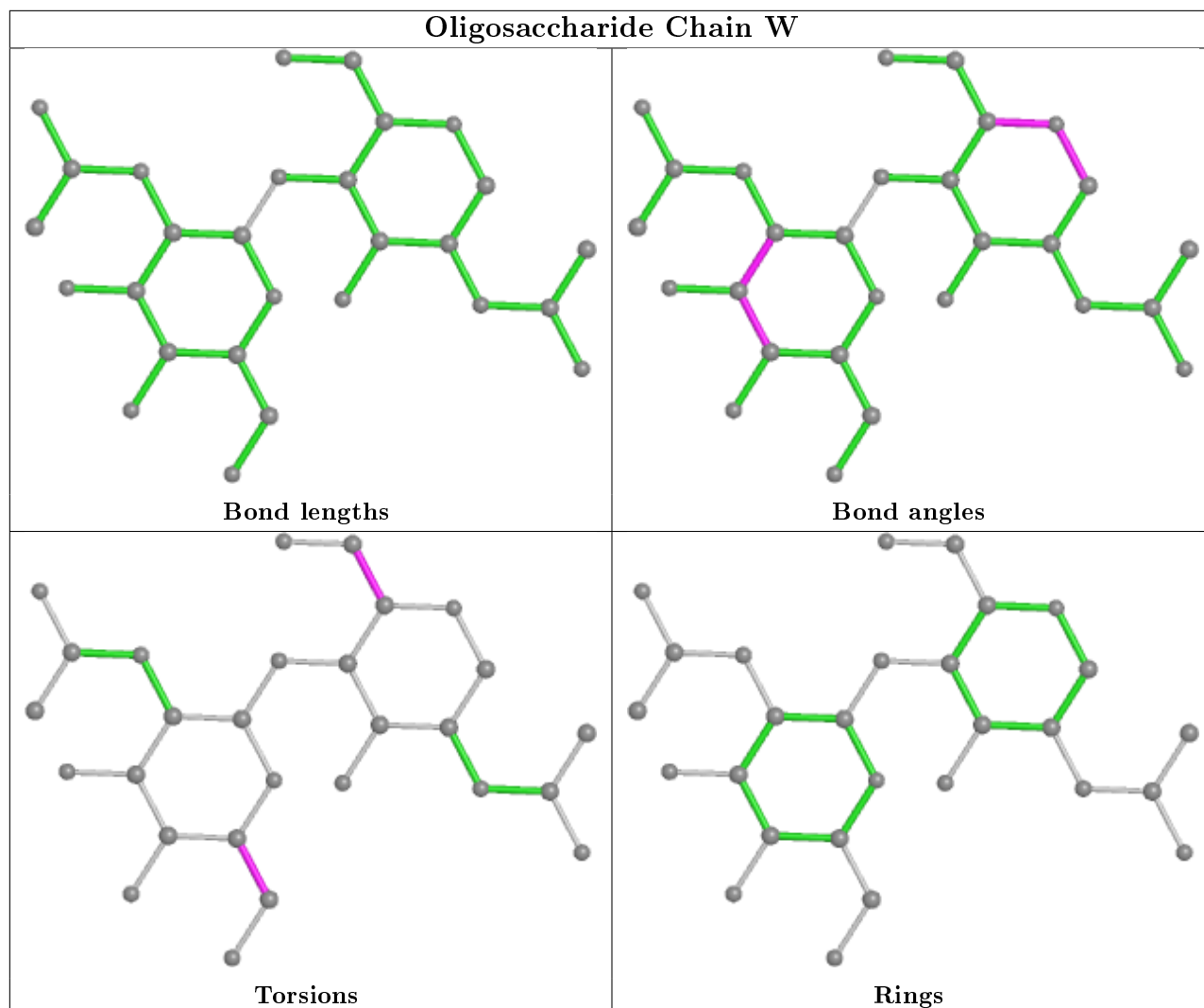


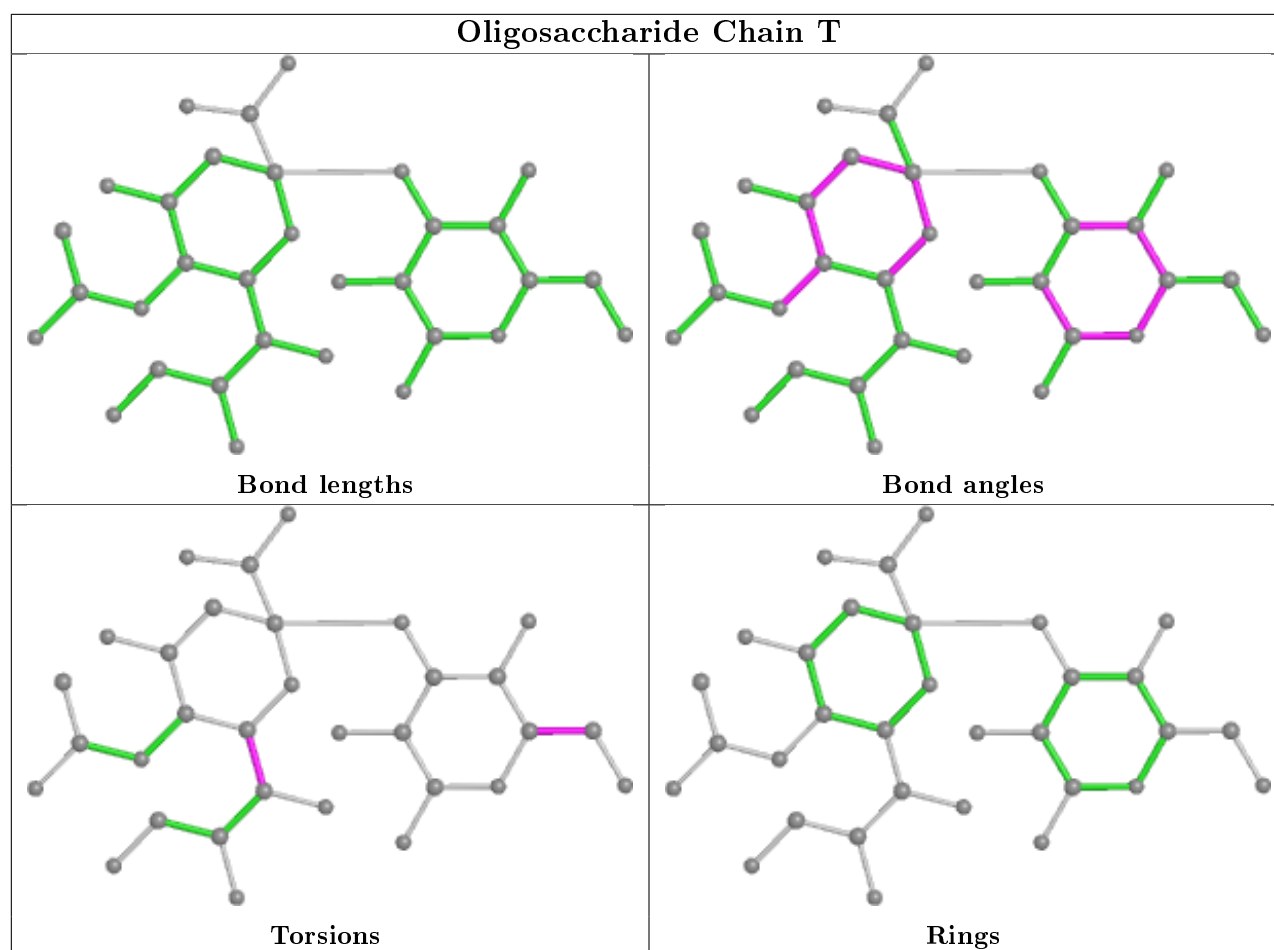












## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
6	NAG	E	401	1	14,14,15	0.33	0	17,19,21	1.34	3 (17%)
6	NAG	K	401	1	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
6	NAG	F	203	2	14,14,15	0.68	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	A	404	1	14,14,15	0.59	0	17,19,21	1.47	3 (17%)
6	NAG	G	404	1	14,14,15	0.46	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	L	203	2	14,14,15	0.44	0	17,19,21	1.12	2 (11%)
6	NAG	I	403	1	14,14,15	0.43	0	17,19,21	1.13	1 (5%)
6	NAG	B	201	2	14,14,15	0.44	0	17,19,21	1.29	3 (17%)
6	NAG	C	401	1	14,14,15	0.46	0	17,19,21	0.80	1 (5%)

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	E	401	1	-	3/6/23/26	0/1/1/1
6	NAG	K	401	1	-	2/6/23/26	0/1/1/1
6	NAG	F	203	2	-	1/6/23/26	0/1/1/1
6	NAG	A	404	1	-	4/6/23/26	0/1/1/1
6	NAG	G	404	1	-	3/6/23/26	0/1/1/1
6	NAG	L	203	2	-	2/6/23/26	0/1/1/1
6	NAG	I	403	1	-	4/6/23/26	0/1/1/1
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
6	NAG	C	401	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	203	NAG	C1-C2	2.06	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	404	NAG	C1-C2-N2	2.93	115.50	110.49
6	B	201	NAG	C4-C3-C2	2.85	115.20	111.02
6	K	401	NAG	C4-C3-C2	-2.80	106.92	111.02
6	I	403	NAG	O5-C5-C6	2.73	111.49	107.20
6	F	203	NAG	C1-O5-C5	2.72	115.88	112.19
6	E	401	NAG	C1-O5-C5	2.65	115.78	112.19
6	B	201	NAG	O5-C1-C2	-2.57	107.22	111.29
6	E	401	NAG	O5-C1-C2	-2.47	107.38	111.29
6	E	401	NAG	C2-N2-C7	2.44	126.38	122.90
6	A	404	NAG	C4-C3-C2	-2.40	107.50	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	401	NAG	C1-O5-C5	2.35	115.37	112.19
6	L	203	NAG	O5-C5-C6	2.34	110.87	107.20
6	B	201	NAG	C1-O5-C5	2.32	115.34	112.19
6	G	404	NAG	C1-O5-C5	2.29	115.30	112.19
6	F	203	NAG	C1-C2-N2	2.24	114.31	110.49
6	A	404	NAG	C8-C7-N2	2.13	119.71	116.10
6	L	203	NAG	O5-C1-C2	2.10	114.61	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	404	NAG	C3-C2-N2-C7
6	K	401	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
6	I	403	NAG	O5-C5-C6-O6
6	A	404	NAG	O5-C5-C6-O6
6	B	201	NAG	C4-C5-C6-O6
6	K	401	NAG	O5-C5-C6-O6
6	I	403	NAG	C4-C5-C6-O6
6	A	404	NAG	C4-C5-C6-O6
6	A	404	NAG	C8-C7-N2-C2
6	A	404	NAG	O7-C7-N2-C2
6	I	403	NAG	C8-C7-N2-C2
6	I	403	NAG	O7-C7-N2-C2
6	G	404	NAG	O5-C5-C6-O6
6	G	404	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	E	401	NAG	C4-C5-C6-O6
6	E	401	NAG	O5-C5-C6-O6
6	L	203	NAG	C4-C5-C6-O6
6	E	401	NAG	C3-C2-N2-C7
6	L	203	NAG	O5-C5-C6-O6
6	F	203	NAG	C4-C5-C6-O6
6	C	401	NAG	C3-C2-N2-C7
6	C	401	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	203	NAG	1	0
6	G	404	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	320/325 (98%)	-0.05	0 <a href="#">100</a> <a href="#">100</a>	56, 84, 113, 134	0
1	C	318/325 (97%)	0.43	18 (5%) <a href="#">23</a> <a href="#">22</a>	58, 114, 163, 186	0
1	E	318/325 (97%)	0.87	64 (20%) <a href="#">1</a> <a href="#">0</a>	79, 126, 159, 189	0
1	G	316/325 (97%)	0.57	28 (8%) <a href="#">9</a> <a href="#">7</a>	59, 120, 169, 193	0
1	I	318/325 (97%)	0.78	55 (17%) <a href="#">1</a> <a href="#">1</a>	77, 130, 182, 219	0
1	K	318/325 (97%)	0.01	4 (1%) <a href="#">77</a> <a href="#">78</a>	61, 89, 114, 136	0
2	B	172/177 (97%)	0.09	1 (0%) <a href="#">89</a> <a href="#">91</a>	60, 87, 114, 125	0
2	D	172/177 (97%)	0.16	0 <a href="#">100</a> <a href="#">100</a>	48, 88, 118, 142	0
2	F	172/177 (97%)	0.45	10 (5%) <a href="#">23</a> <a href="#">22</a>	67, 106, 141, 150	0
2	H	172/177 (97%)	0.15	0 <a href="#">100</a> <a href="#">100</a>	51, 86, 111, 126	0
2	J	172/177 (97%)	0.37	9 (5%) <a href="#">27</a> <a href="#">25</a>	64, 102, 131, 141	0
2	L	172/177 (97%)	0.12	1 (0%) <a href="#">89</a> <a href="#">91</a>	61, 89, 117, 140	0
All	All	2940/3012 (97%)	0.36	190 (6%) <a href="#">18</a> <a href="#">17</a>	48, 101, 156, 219	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	LEU	8.4
1	E	243	GLY	7.2
1	I	210	VAL	6.9
1	I	41	LEU	6.6
1	I	86	TYR	6.3
1	C	238	PHE	6.1
1	G	212	ALA	5.9
1	G	188	TYR	5.9
1	G	144	TRP	5.9
1	E	171	ILE	5.8
1	E	41	LEU	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	244	LEU	5.7
1	C	117	TYR	5.7
1	I	90	GLY	5.6
1	E	61	ILE	5.2
1	E	250	VAL	5.0
1	E	84	ILE	4.9
1	I	102	ILE	4.7
1	I	57	ILE	4.7
1	E	284	ARG	4.6
1	I	60	LEU	4.6
1	I	145	LEU	4.6
1	E	281	ILE	4.5
1	G	236	ILE	4.5
1	G	167	ALA	4.5
1	I	59	MET	4.5
1	G	192	SER	4.5
1	I	225	PHE	4.4
1	E	134	GLY	4.4
1	G	226	HIS	4.4
1	G	146	VAL	4.3
1	E	145	LEU	4.3
1	E	258	LEU	4.2
1	I	172	MET	4.2
1	E	246	ALA	4.2
1	E	138	PHE	4.2
1	I	77	LEU	4.1
1	G	172	MET	4.1
1	I	266	ILE	4.0
1	I	70	LEU	4.0
1	I	85	ALA	3.9
1	E	57	ILE	3.9
1	I	171	ILE	3.9
1	E	139	TYR	3.9
1	C	193	LEU	3.8
2	J	20	GLY	3.8
1	I	212	ALA	3.8
2	F	141	TYR	3.7
1	I	114	GLY	3.7
1	E	245	ILE	3.7
1	I	259	GLY	3.7
1	C	172	MET	3.7
1	E	78	ILE	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	176	HIS	3.6
1	I	275	PHE	3.6
1	G	174	GLY	3.6
1	E	283	THR	3.5
1	E	77	LEU	3.5
2	F	157	TYR	3.4
1	G	209	VAL	3.4
1	E	42	CYS	3.4
1	E	286	PRO	3.4
1	E	253	LEU	3.4
1	G	207	VAL	3.4
1	E	108	ILE	3.4
1	I	78	ILE	3.3
1	I	37	SER	3.3
1	E	175	ILE	3.3
1	E	285	LEU	3.2
1	E	70	LEU	3.2
1	E	270	CYS	3.2
1	I	250	VAL	3.2
1	E	85	ALA	3.2
1	C	209	VAL	3.2
1	E	266	ILE	3.2
1	E	33	VAL	3.1
1	E	174	GLY	3.1
1	E	66	CYS	3.1
1	E	109	SER	3.1
1	G	61	ILE	3.1
2	F	168	LEU	3.0
1	I	284	ARG	3.0
1	E	260	ILE	3.0
1	G	184	LYS	3.0
1	E	173	TRP	3.0
1	E	142	LEU	3.0
1	C	206	PHE	3.0
2	F	29	ALA	3.0
1	I	132	ARG	3.0
1	E	267	ASP	2.9
1	E	271	GLU	2.9
1	E	282	ASN	2.9
1	E	52	GLY	2.9
1	G	206	PHE	2.9
1	E	90	GLY	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	225	PHE	2.9
1	E	121	ILE	2.9
1	G	238	PHE	2.9
1	I	65	ALA	2.8
1	I	116	THR	2.8
1	C	208	PRO	2.8
1	C	225	PHE	2.7
1	G	193	LEU	2.7
2	F	20	GLY	2.7
1	I	282	ASN	2.7
1	C	258	LEU	2.7
1	C	242	GLY	2.7
1	I	245	ILE	2.7
1	E	69	HIS	2.6
1	I	51	LEU	2.6
2	J	19	ASP	2.6
1	E	242	GLY	2.6
1	E	194	SER	2.6
1	C	121	ILE	2.6
1	G	57	ILE	2.6
1	E	129	ALA	2.6
1	G	145	LEU	2.6
1	E	60	LEU	2.6
1	I	138	PHE	2.6
1	E	102	ILE	2.5
1	E	51	LEU	2.5
1	I	209	VAL	2.5
1	I	84	ILE	2.5
2	J	55	ILE	2.5
1	I	272	SER	2.5
1	I	270	CYS	2.5
1	I	73	THR	2.5
1	E	68	LEU	2.5
1	C	144	TRP	2.5
1	E	117	TYR	2.4
2	J	18	VAL	2.4
1	G	118	GLY	2.4
1	I	56	PRO	2.4
1	I	262	SER	2.4
1	I	110	LYS	2.4
2	L	141	TYR	2.3
1	K	195	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	254	ILE	2.3
2	F	126	LEU	2.3
1	I	58	GLY	2.3
2	F	81	ILE	2.3
1	I	154	PHE	2.3
1	E	172	MET	2.3
1	G	235	LYS	2.3
1	C	223	ILE	2.3
1	I	104	GLU	2.3
2	J	56	ILE	2.3
2	F	31	GLY	2.3
1	E	264	ALA	2.3
2	J	152	ILE	2.3
1	I	183	GLU	2.2
1	G	158	THR	2.2
1	C	93	VAL	2.2
1	E	56	PRO	2.2
1	I	182	GLN	2.2
1	E	263	GLU	2.2
1	I	254	ILE	2.2
1	K	60	LEU	2.2
1	I	67	ASP	2.2
1	G	78	ILE	2.2
1	I	281	ILE	2.2
2	F	21	TRP	2.2
1	E	131	MET	2.2
1	I	139	TYR	2.2
1	G	208	PRO	2.2
1	I	66	CYS	2.1
1	C	262	SER	2.1
1	I	263	GLU	2.1
1	I	247	PRO	2.1
1	E	79	GLU	2.1
1	I	278	GLY	2.1
2	F	99	LEU	2.1
1	I	42	CYS	2.1
1	C	59	MET	2.1
1	E	188	TYR	2.1
2	J	77	ILE	2.1
2	J	138	PHE	2.1
1	E	50	ASP	2.1
1	E	223	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	102	MET	2.1
1	E	277	ARG	2.1
1	I	61	ILE	2.0
1	C	212	ALA	2.0
1	G	240	HIS	2.0
1	G	202	TYR	2.0
1	G	237	THR	2.0
1	E	247	PRO	2.0
2	J	121	ARG	2.0
1	C	11	ALA	2.0
1	K	242	GLY	2.0

## 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.

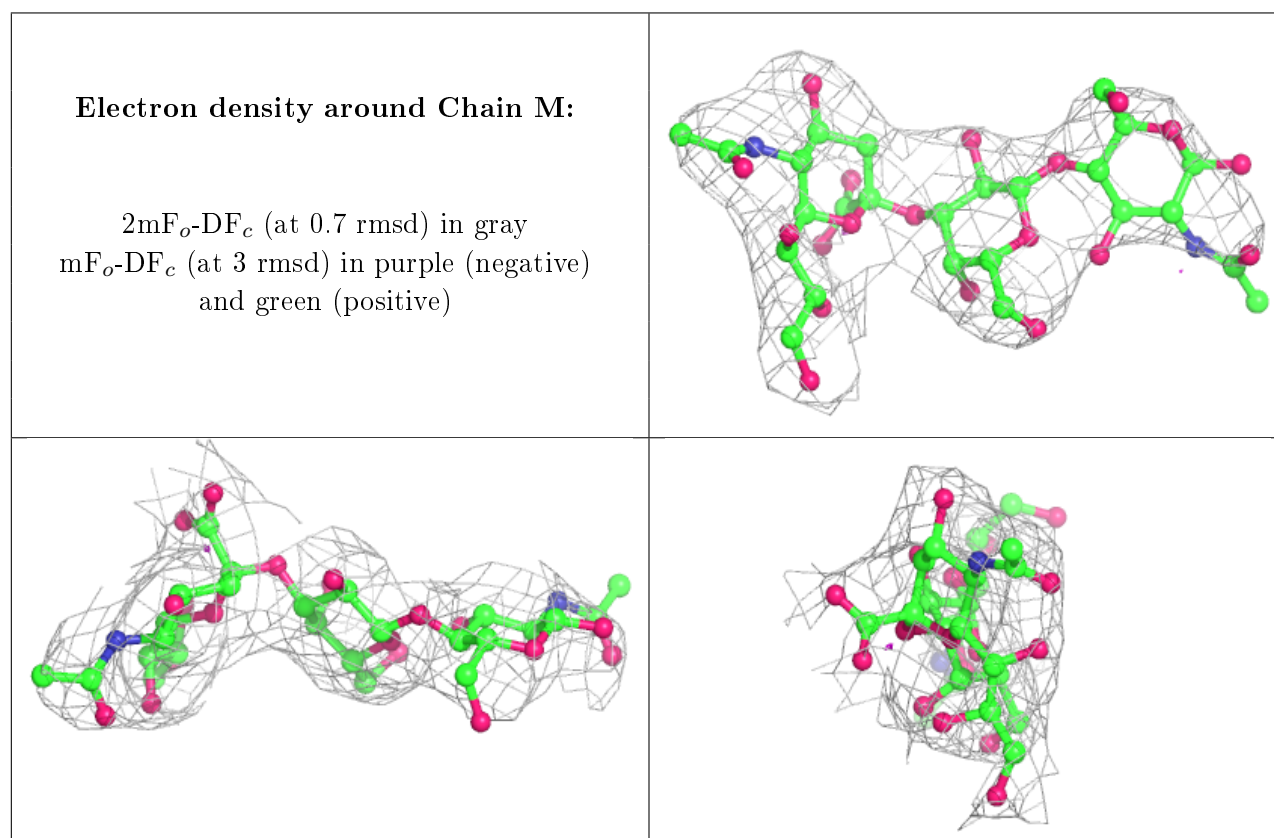
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	N	1	15/15	0.76	0.23	117,154,163,166	0
4	NAG	Q	2	14/15	0.76	0.21	142,160,173,174	0
4	NAG	Q	1	14/15	0.81	0.15	124,139,152,158	0
3	NAG	P	1	15/15	0.86	0.24	133,160,170,171	0
4	NAG	O	2	14/15	0.87	0.17	121,132,139,146	0
3	GAL	R	2	11/12	0.87	0.10	148,164,176,180	0
3	NAG	R	1	15/15	0.87	0.12	129,151,159,161	0
5	GAL	T	1	12/12	0.88	0.13	144,160,164,167	0
4	NAG	W	2	14/15	0.89	0.14	99,134,137,140	0
3	SIA	R	3	20/21	0.89	0.14	118,142,175,175	0
4	NAG	S	2	14/15	0.89	0.13	118,130,141,145	0
4	NAG	U	2	14/15	0.89	0.19	125,154,169,180	0
5	SIA	T	2	20/21	0.90	0.14	115,141,157,158	0
3	NAG	M	1	15/15	0.90	0.33	143,155,163,164	0
3	NAG	V	1	15/15	0.90	0.22	119,142,153,168	0
4	NAG	U	1	14/15	0.91	0.15	107,133,141,145	0
3	GAL	P	2	11/12	0.91	0.13	132,149,157,160	0

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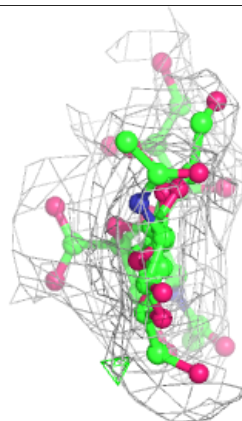
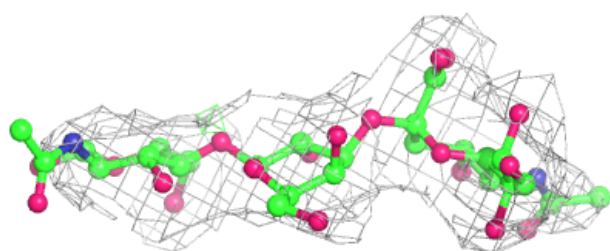
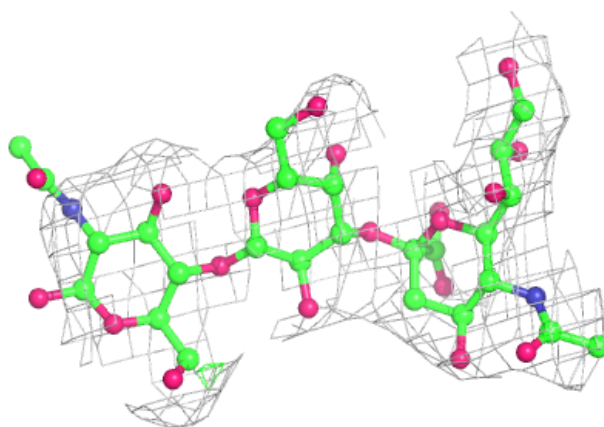
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	N	2	11/12	0.92	0.11	129,140,157,157	0
4	NAG	W	1	14/15	0.94	0.13	123,134,139,140	0
3	SIA	N	3	20/21	0.94	0.12	118,133,144,145	0
4	NAG	O	1	14/15	0.94	0.14	90,96,106,117	0
3	SIA	P	3	20/21	0.95	0.12	106,125,143,156	0
3	GAL	V	2	11/12	0.95	0.09	100,123,129,133	0
3	SIA	V	3	20/21	0.95	0.15	66,79,117,125	0
4	NAG	S	1	14/15	0.95	0.13	82,90,97,105	0
3	GAL	M	2	11/12	0.96	0.09	108,117,121,125	0
3	SIA	M	3	20/21	0.97	0.14	75,85,108,121	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.

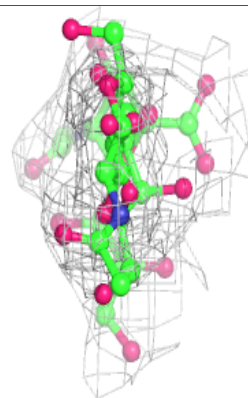
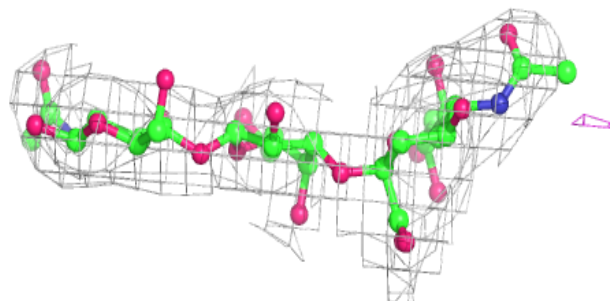
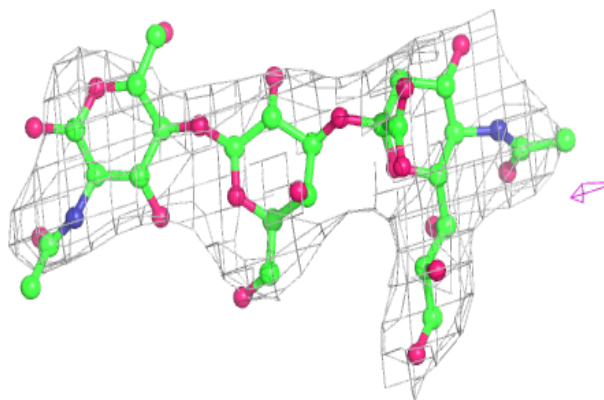


**Electron density around Chain N:**

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

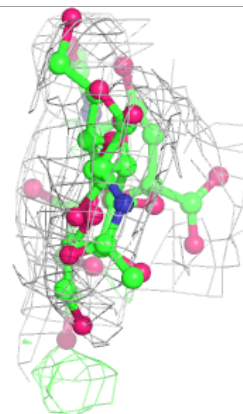
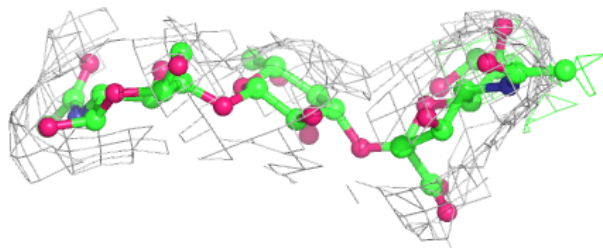
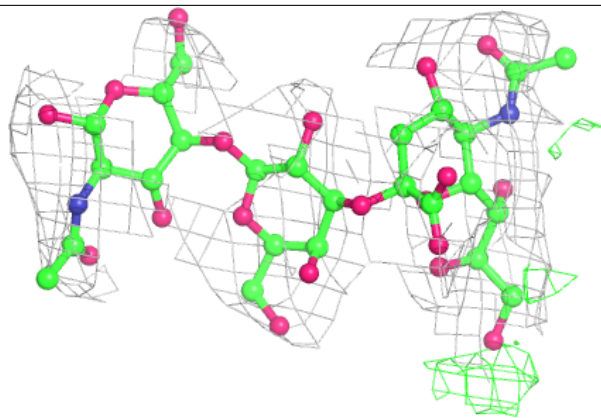
**Electron density around Chain P:**

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

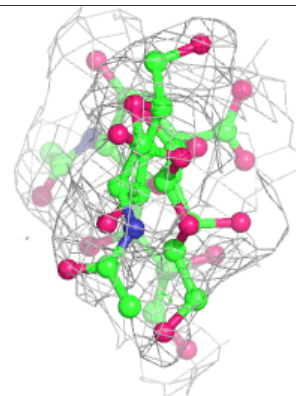
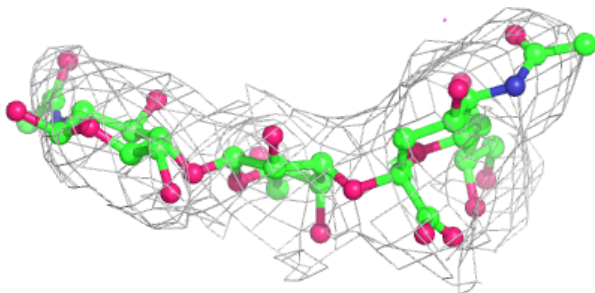
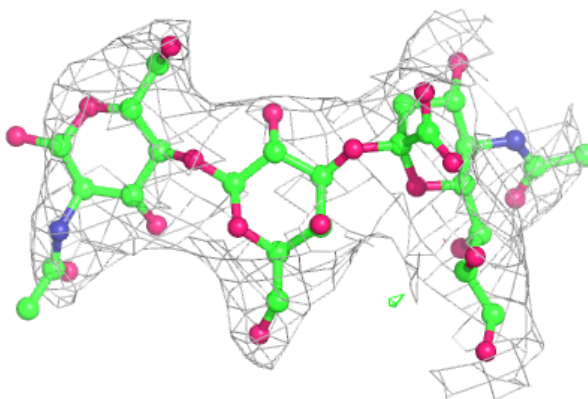


**Electron density around Chain R:**

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

**Electron density around Chain V:**

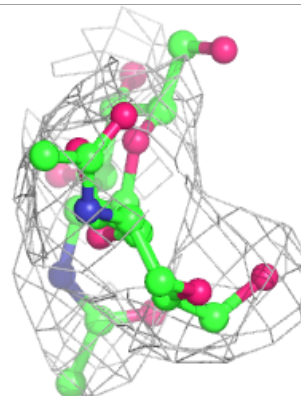
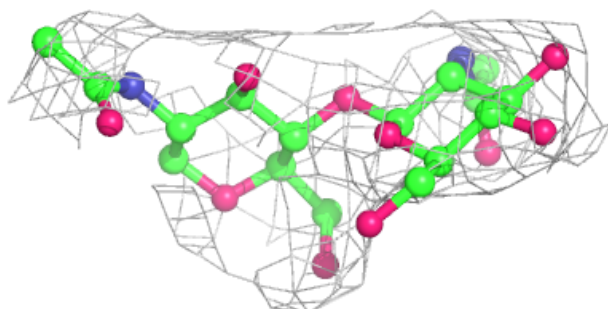
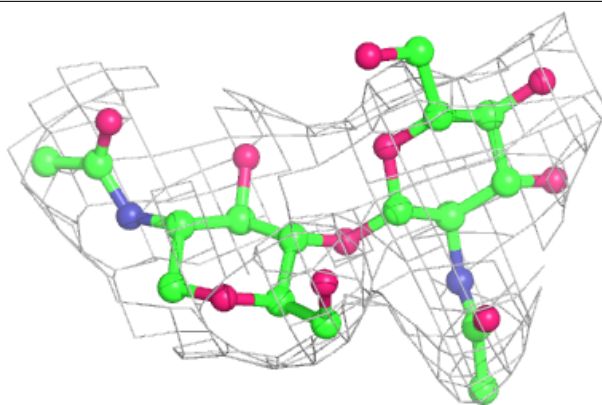
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



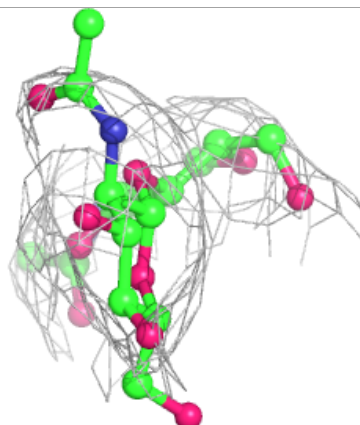
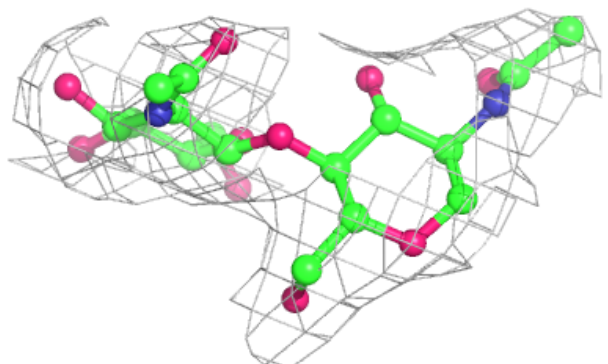
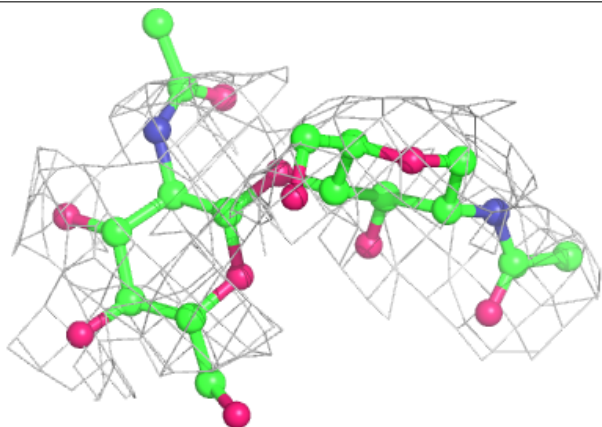


**Electron density around Chain O:**

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

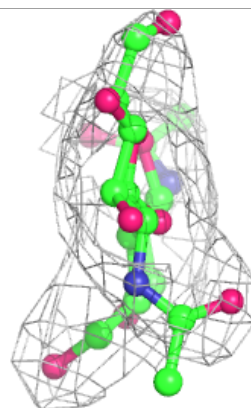
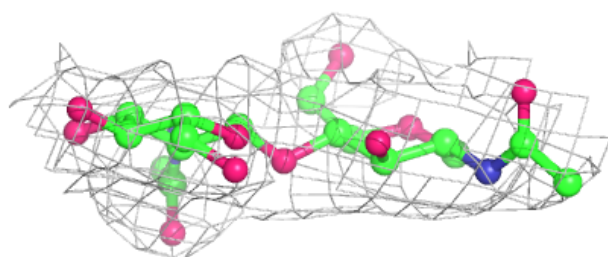
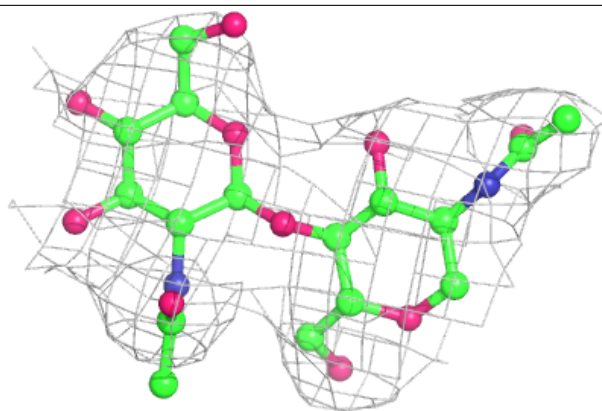
**Electron density around Chain Q:**

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

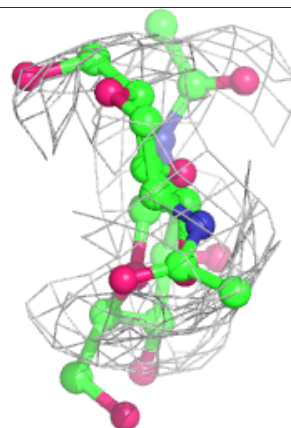
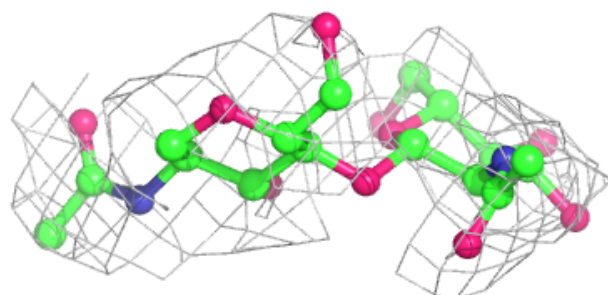
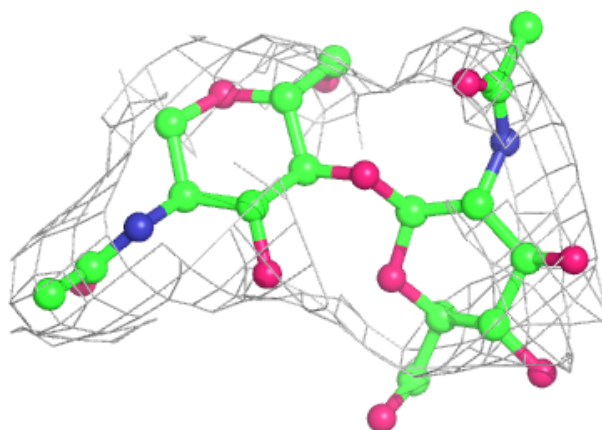


**Electron density around Chain S:**

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

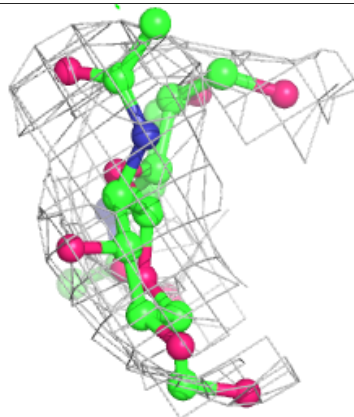
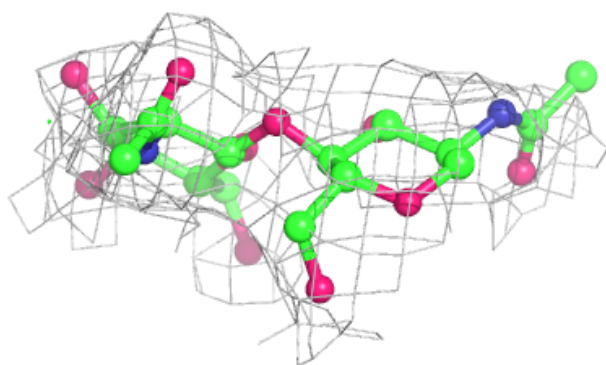
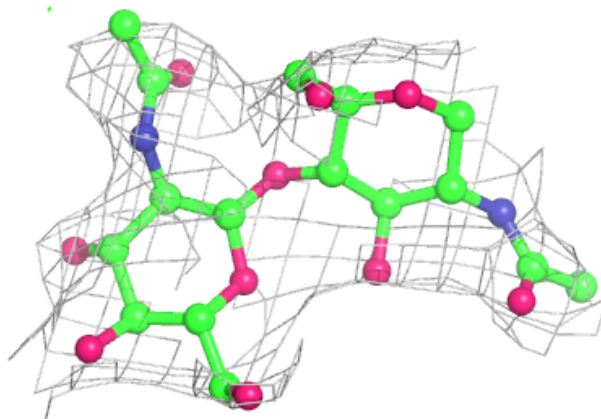
**Electron density around Chain U:**

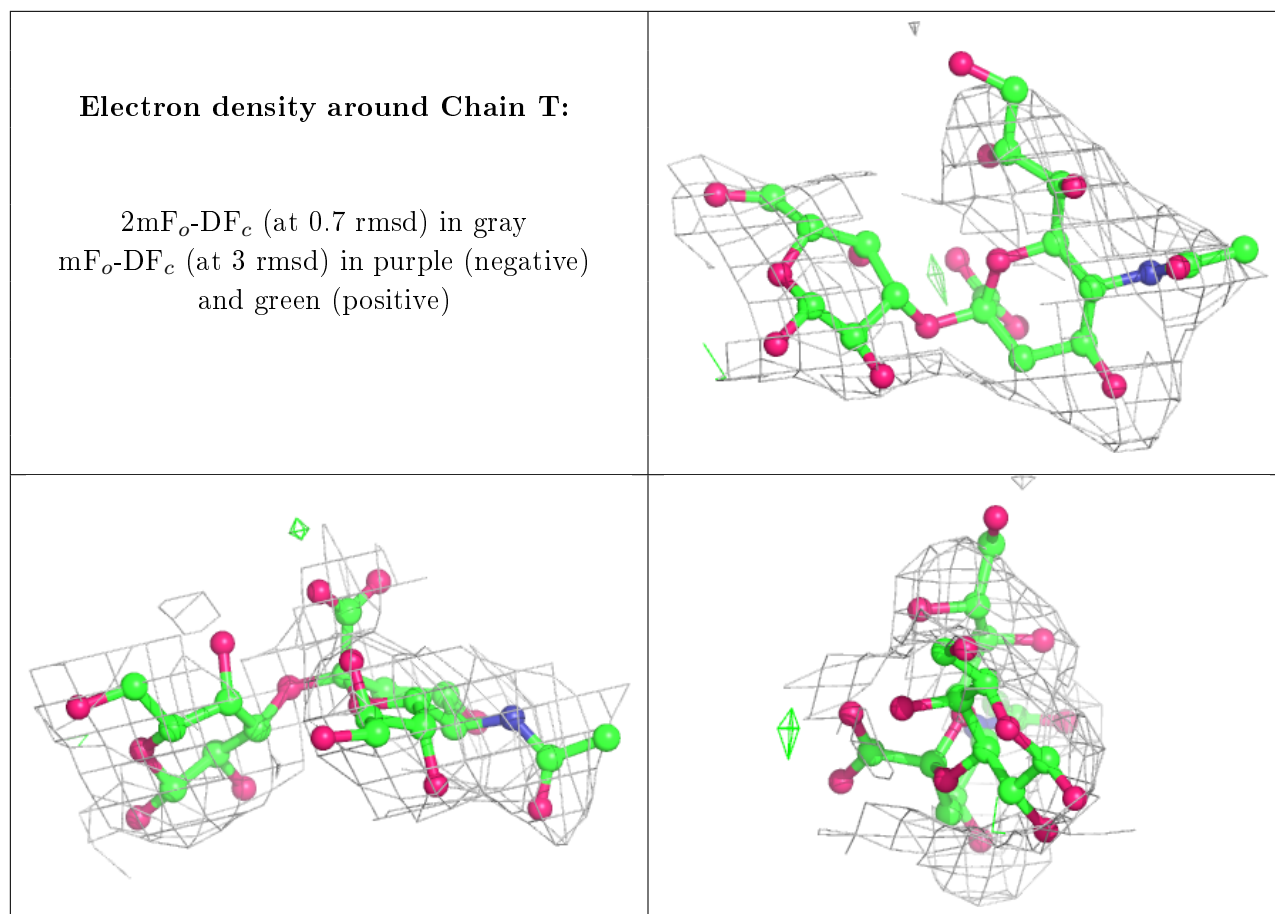
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain W:**

$2mF_o-DF_c$  (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
6	NAG	F	203	14/15	0.67	0.19	129,166,175,178	0
6	NAG	L	203	14/15	0.81	0.23	153,171,186,189	0
6	NAG	A	404	14/15	0.84	0.22	113,138,150,153	0
6	NAG	K	401	14/15	0.86	0.17	115,127,142,145	0
6	NAG	I	403	14/15	0.88	0.20	138,163,171,174	0
6	NAG	E	401	14/15	0.90	0.25	127,155,167,181	0
6	NAG	G	404	14/15	0.92	0.12	117,130,144,147	0
6	NAG	C	401	14/15	0.92	0.14	105,125,132,143	0
6	NAG	B	201	14/15	0.93	0.16	97,109,121,122	0
7	CA	H	203	1/1	0.93	0.17	113,113,113,113	0
7	CA	A	405	1/1	0.94	0.17	76,76,76,76	0
7	CA	K	405	1/1	0.96	0.19	77,77,77,77	0

## 6.5 Other polymers

There are no such residues in this entry.