



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2020 – 01:11 AM EST

PDB ID : 6WIX  
Title : Crystal Structure of HIV-1 MI369 RnS-DS.SOSIP Prefusion Env Trimer in Complex with Human Antibodies 3H109L and 35O22 at 3.5 Angstrom  
Authors : Lai, Y.-T.; Olia, A.; Kwong, P.D.  
Deposited on : 2020-04-10  
Resolution : 2.67 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 : 2.14.6  
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

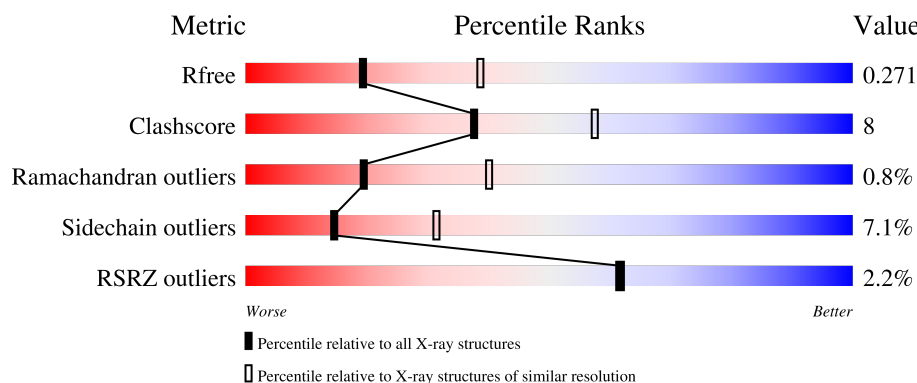
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	B	153	<div> <div>9%</div> <div>61% 16% • 22%</div> </div>
2	D	134	<div> <div>9%</div> <div>69% 22% • •</div> </div>
3	E	114	<div> <div>4%</div> <div>68% 23% • 8%</div> </div>
4	G	498	<div> <div>•</div> <div>65% 19% • 15%</div> </div>
5	H	244	<div> <div>2%</div> <div>72% 18% • 7%</div> </div>

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Mol	Chain	Length	Quality of chain
6	L	217	
7	A	6	
8	C	2	
8	F	2	
8	J	2	
8	M	2	
8	P	2	
9	I	3	
9	O	3	
10	K	10	
11	N	3	

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9952 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	120	Total	C	N	O	S	0	0	0
			967	623	162	177	5			

- Molecule 2 is a protein called 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 3 is a protein called 35O22 scFv light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	105	Total	C	N	O	S	0	0	0
			805	506	133	160	6			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	425	Total	C	N	O	S	0	0	0
			3363	2118	601	616	28			

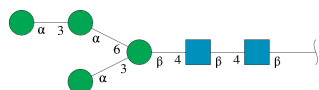
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1715	1093	278	338	6			

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



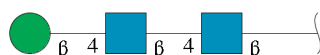
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



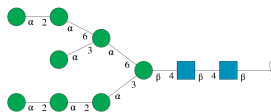
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



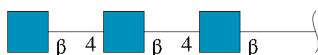
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



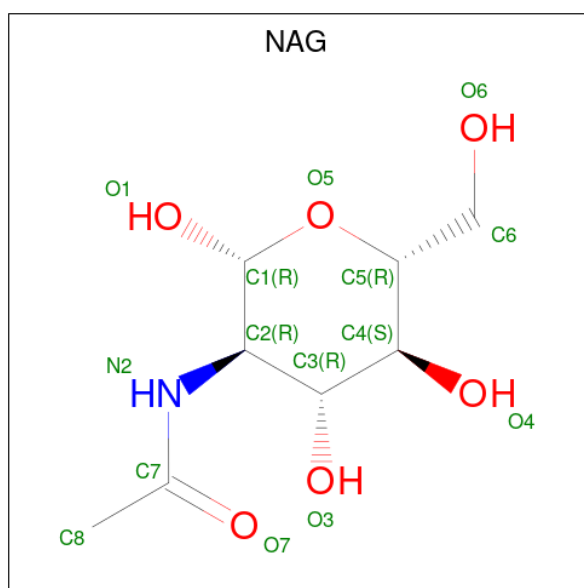
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
11	N	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 12 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>).

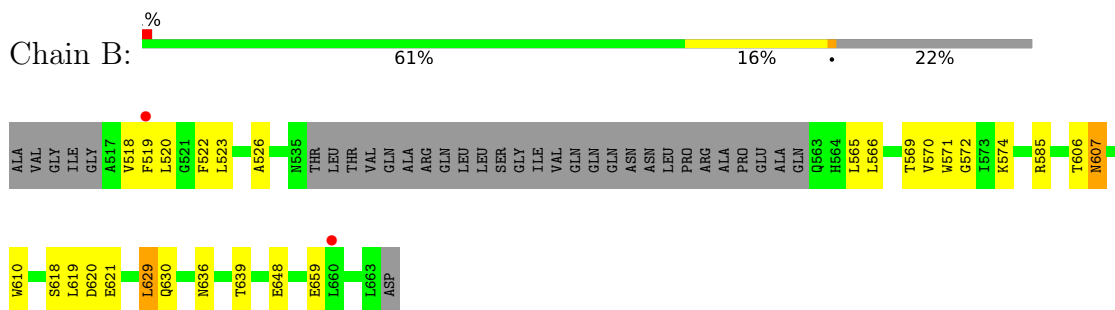


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		

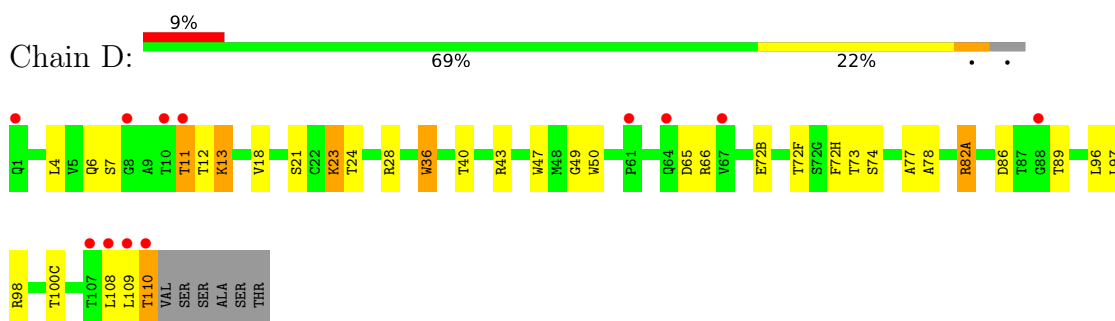
### 3 Residue-property plots [i](#)

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.

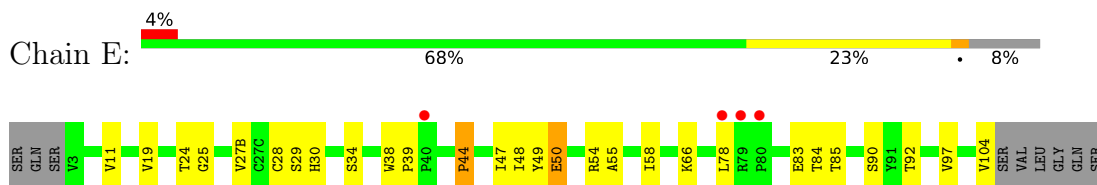
- Molecule 1: Envelope glycoprotein gp41



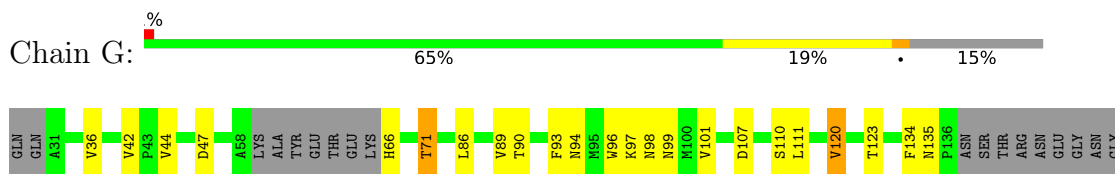
- Molecule 2: 35O22 scFv heavy chain



- Molecule 3: 35O22 scFv light chain

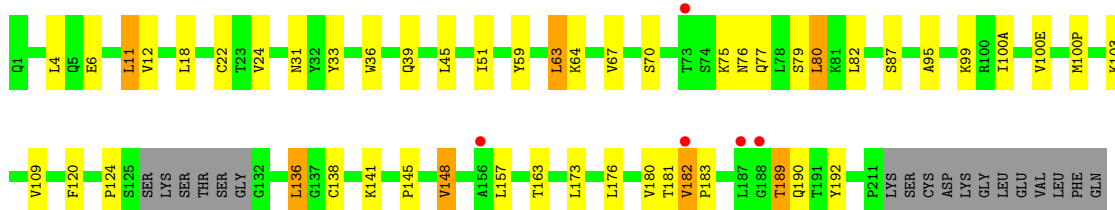


- Molecule 4: Envelope glycoprotein gp120

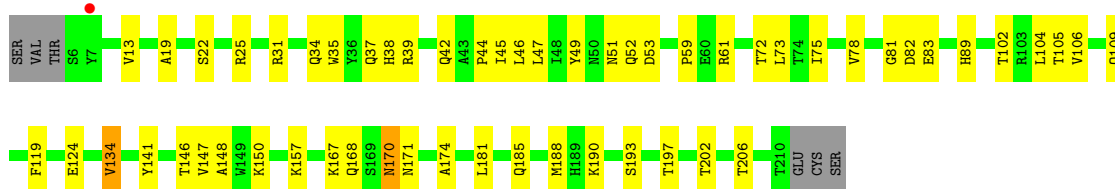




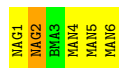
- Molecule 5: 3H109L Fab heavy chain



- Molecule 6: 3H109L Fab light chain



- Molecule 7:  $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose



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





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

Chain F:  50% 50%



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

Chain J:  100%



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

Chain M:  100%



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

Chain P:  100%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 10:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain K:  10% 80% 10%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 11: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain N:  67% 33%

MAG1  
MAG2  
MAG3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.86Å 131.86Å 316.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.39 – 2.67 42.39 – 2.67	Depositor EDS
% Data completeness (in resolution range)	39.4 (42.39-2.67) 39.4 (42.39-2.67)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.225 , 0.270 0.226 , 0.271	Depositor DCC
$R_{free}$ test set	1724 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.072 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	9952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: BMA, NAG, MAN

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	B	0.37	0/987	0.45	0/1340
2	D	0.23	0/1021	0.45	0/1390
3	E	0.24	0/829	0.45	0/1133
4	G	0.24	0/3434	0.44	0/4658
5	H	0.25	0/1758	0.46	0/2397
6	L	0.24	0/1647	0.44	0/2247
All	All	0.26	0/9676	0.45	0/13165

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	B	967	0	954	13	0
2	D	994	0	953	19	0
3	E	805	0	752	12	0
4	G	3363	0	3308	55	0
5	H	1715	0	1687	25	0
6	L	1604	0	1553	30	0
7	A	72	0	61	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	28	0	25	0	0
8	F	28	0	25	0	0
8	J	28	0	25	0	0
8	M	28	0	25	0	0
8	P	28	0	25	0	0
9	I	39	0	34	2	0
9	O	39	0	34	0	0
10	K	116	0	97	2	0
11	N	42	0	37	1	0
12	G	56	0	52	0	0
All	All	9952	0	9647	150	0

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

The worst 5 of 150 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)
6:L:37:GLN:HE21	6:L:45:ILE:HD11	1.53	0.74
6:L:61:ARG:NH1	6:L:82:ASP:OD2	2.23	0.71
4:G:270:VAL:HG23	4:G:348:GLN:HG3	1.72	0.69
4:G:270:VAL:HG12	4:G:288:LEU:HA	1.76	0.68
4:G:360:ILE:HG23	4:G:394:THR:HG22	1.76	0.68

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	B	116/153 (76%)	108 (93%)	6 (5%)	2 (2%)	<b>9</b> <b>20</b>
2	D	126/134 (94%)	113 (90%)	12 (10%)	1 (1%)	<b>19</b> <b>40</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	103/114 (90%)	81 (79%)	19 (18%)	3 (3%)	4	9
4	G	411/498 (82%)	377 (92%)	31 (8%)	3 (1%)	22	44
5	H	222/244 (91%)	198 (89%)	24 (11%)	0	100	100
6	L	209/217 (96%)	195 (93%)	14 (7%)	0	100	100
All	All	1187/1360 (87%)	1072 (90%)	106 (9%)	9 (1%)	19	40

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	VAL
1	B	565	LEU
3	E	29	SER
3	E	50	GLU
4	G	269	GLU

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	104/130 (80%)	92 (88%)	12 (12%)	5	11
2	D	107/112 (96%)	97 (91%)	10 (9%)	9	19
3	E	92/100 (92%)	85 (92%)	7 (8%)	13	28
4	G	382/445 (86%)	360 (94%)	22 (6%)	20	41
5	H	196/212 (92%)	181 (92%)	15 (8%)	13	27
6	L	175/181 (97%)	166 (95%)	9 (5%)	24	46
All	All	1056/1180 (90%)	981 (93%)	75 (7%)	14	31

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	123	THR
4	G	344	GLN

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Mol	Chain	Res	Type
6	L	147	VAL
4	G	134	PHE
4	G	270	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	L	168	GLN
6	L	170	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

35 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	$\# Z  > 2$
7	NAG	A	1	4,7	14,14,15	0.35	0	17,19,21	0.45	0
7	NAG	A	2	7	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
7	BMA	A	3	7	11,11,12	0.83	0	15,15,17	0.77	0
7	MAN	A	4	7	11,11,12	1.10	1 (9%)	15,15,17	1.66	3 (20%)
7	MAN	A	5	7	11,11,12	1.65	2 (18%)	15,15,17	2.20	4 (26%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.25	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.28	0	17,19,21	0.42	0
8	NAG	C	2	8	14,14,15	0.25	0	17,19,21	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	F	1	8,4	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
8	NAG	F	2	8	14,14,15	0.33	0	17,19,21	0.41	0
9	NAG	I	1	9,4	14,14,15	0.27	0	17,19,21	0.56	0
9	NAG	I	2	9	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
9	BMA	I	3	9	11,11,12	0.91	0	15,15,17	0.90	0
8	NAG	J	1	8,4	14,14,15	0.30	0	17,19,21	0.43	0
8	NAG	J	2	8	14,14,15	0.23	0	17,19,21	0.49	0
10	NAG	K	1	10,4	14,14,15	0.51	0	17,19,21	1.32	1 (5%)
10	MAN	K	10	10	11,11,12	1.07	1 (9%)	15,15,17	1.30	2 (13%)
10	NAG	K	2	10	14,14,15	0.32	0	17,19,21	0.43	0
10	BMA	K	3	10	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
10	MAN	K	4	10	11,11,12	0.89	1 (9%)	15,15,17	1.59	3 (20%)
10	MAN	K	5	10	11,11,12	0.51	0	15,15,17	1.01	2 (13%)
10	MAN	K	6	10	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
10	MAN	K	7	10	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
10	MAN	K	8	10	11,11,12	0.66	0	15,15,17	1.14	1 (6%)
10	MAN	K	9	10	11,11,12	0.81	1 (9%)	15,15,17	1.47	2 (13%)
8	NAG	M	1	8,4	14,14,15	0.42	0	17,19,21	0.51	0
8	NAG	M	2	8	14,14,15	0.34	0	17,19,21	0.53	0
11	NAG	N	1	11,4	14,14,15	0.41	0	17,19,21	0.73	0
11	NAG	N	2	11	14,14,15	0.37	0	17,19,21	0.55	0
11	NAG	N	3	11	14,14,15	0.35	0	17,19,21	0.53	0
9	NAG	O	1	9,4	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	O	2	9	14,14,15	0.30	0	17,19,21	0.47	0
9	BMA	O	3	9	11,11,12	0.61	0	15,15,17	0.72	0
8	NAG	P	1	8,4	14,14,15	0.23	0	17,19,21	0.54	0
8	NAG	P	2	8	14,14,15	0.25	0	17,19,21	0.41	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	A	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	5/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
9	NAG	I	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	4/6/23/26	0/1/1/1
10	MAN	K	10	10	-	0/2/19/22	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	2/2/19/22	0/1/1/1
10	MAN	K	6	10	-	0/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1
10	MAN	K	8	10	-	2/2/19/22	0/1/1/1
10	MAN	K	9	10	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8,4	-	1/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
11	NAG	N	1	11,4	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	1/6/23/26	0/1/1/1
11	NAG	N	3	11	-	2/6/23/26	0/1/1/1
9	NAG	O	1	9,4	-	4/6/23/26	0/1/1/1
9	NAG	O	2	9	-	1/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
8	NAG	P	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5	MAN	C1-C2	4.27	1.62	1.52
7	A	5	MAN	O5-C1	3.05	1.48	1.43
10	K	10	MAN	C1-C2	2.92	1.58	1.52
7	A	4	MAN	C1-C2	2.87	1.58	1.52
10	K	4	MAN	C1-C2	2.38	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5	MAN	C1-O5-C5	6.68	121.24	112.19
10	K	9	MAN	C1-O5-C5	4.62	118.45	112.19
10	K	1	NAG	C2-N2-C7	4.41	129.18	122.90
7	A	2	NAG	C2-N2-C7	4.31	129.03	122.90
10	K	4	MAN	C1-O5-C5	4.22	117.90	112.19

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

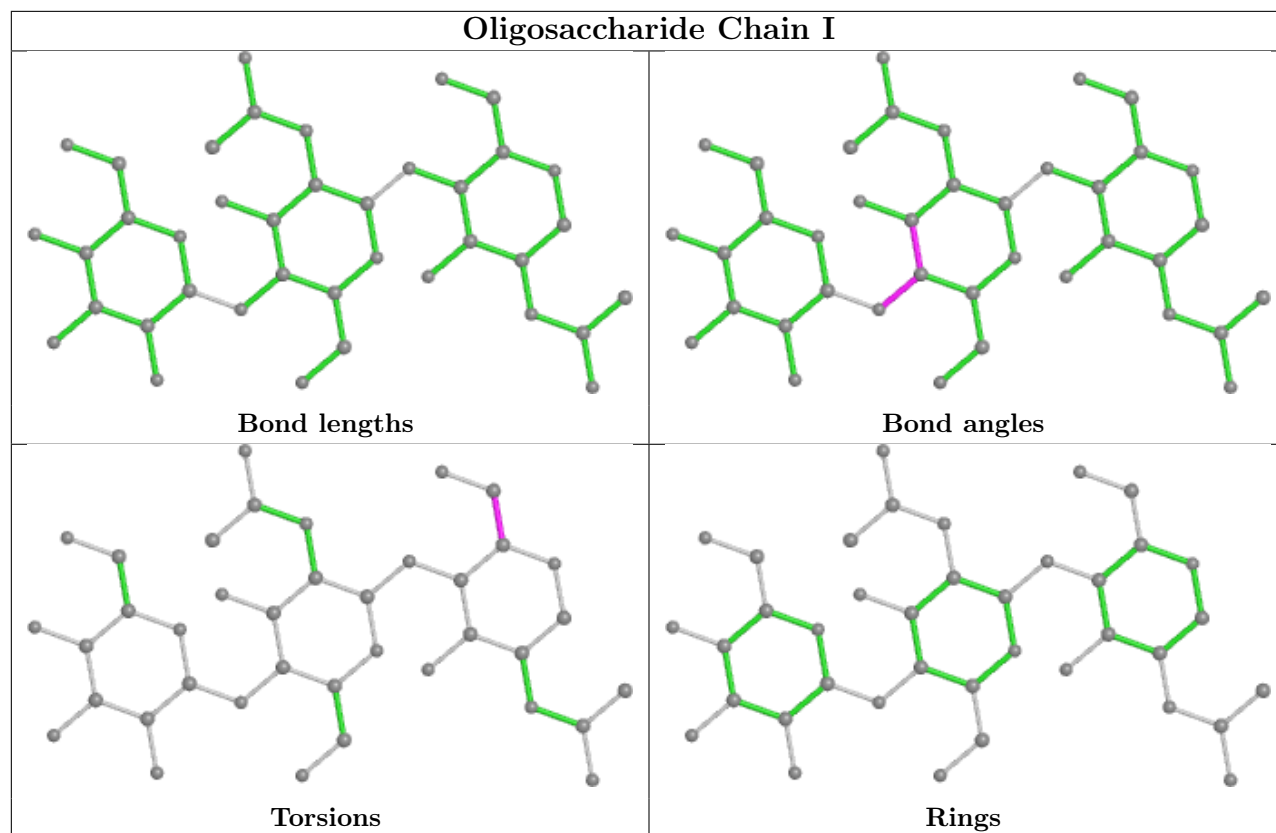
Mol	Chain	Res	Type	Atoms
7	A	3	BMA	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
10	K	5	MAN	O5-C5-C6-O6

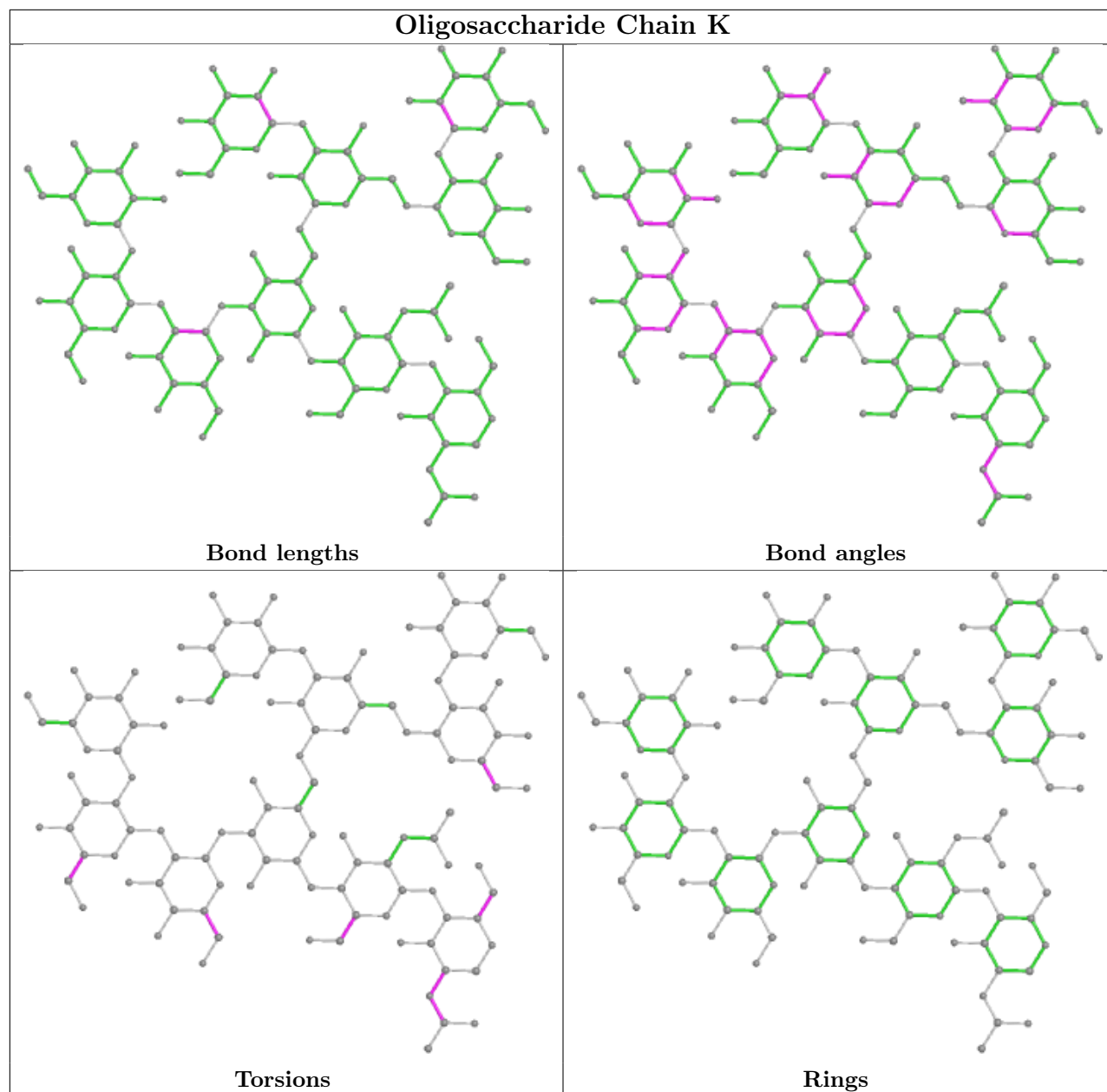
There are no ring outliers.

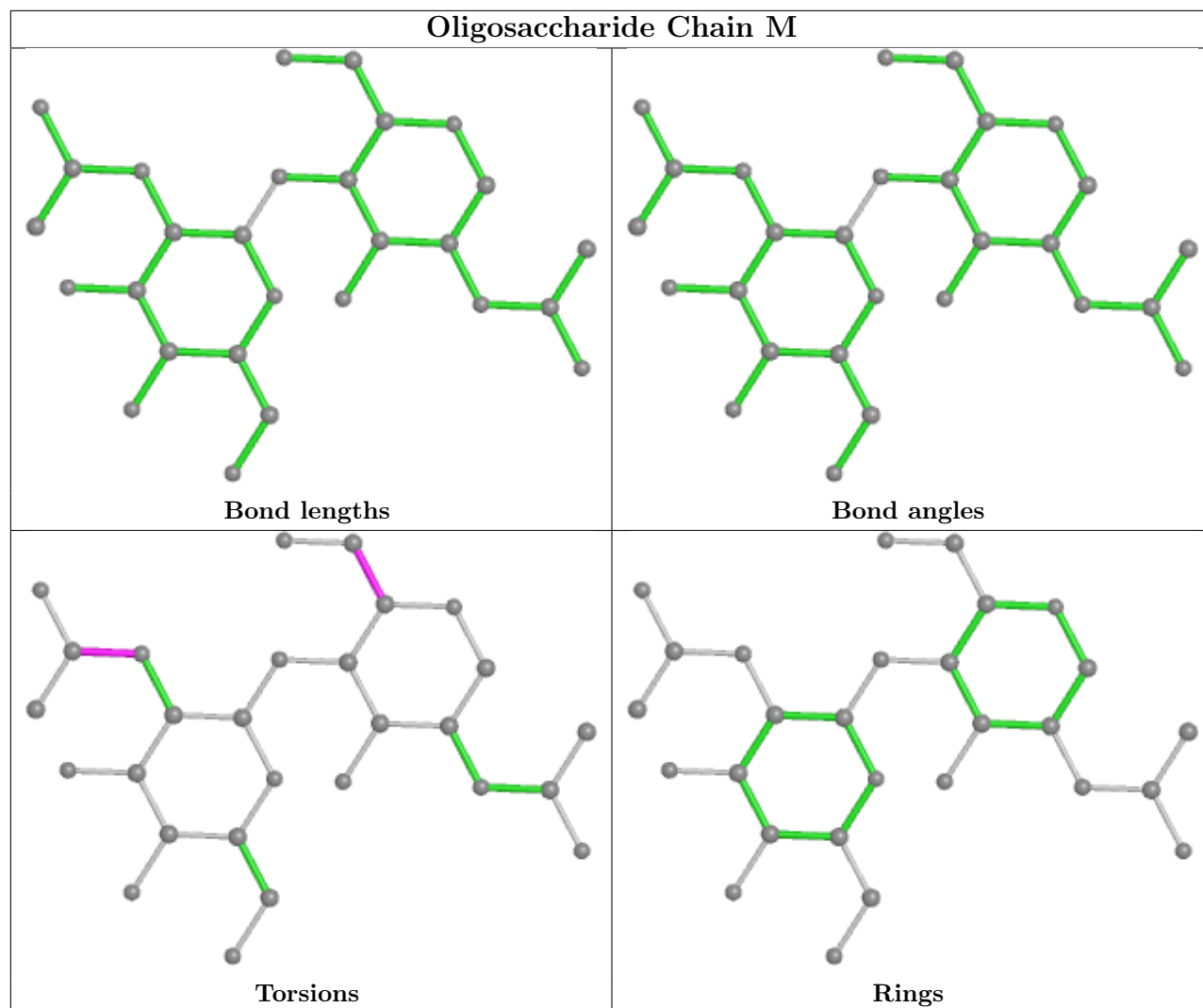
6 monomers are involved in 7 short contacts:

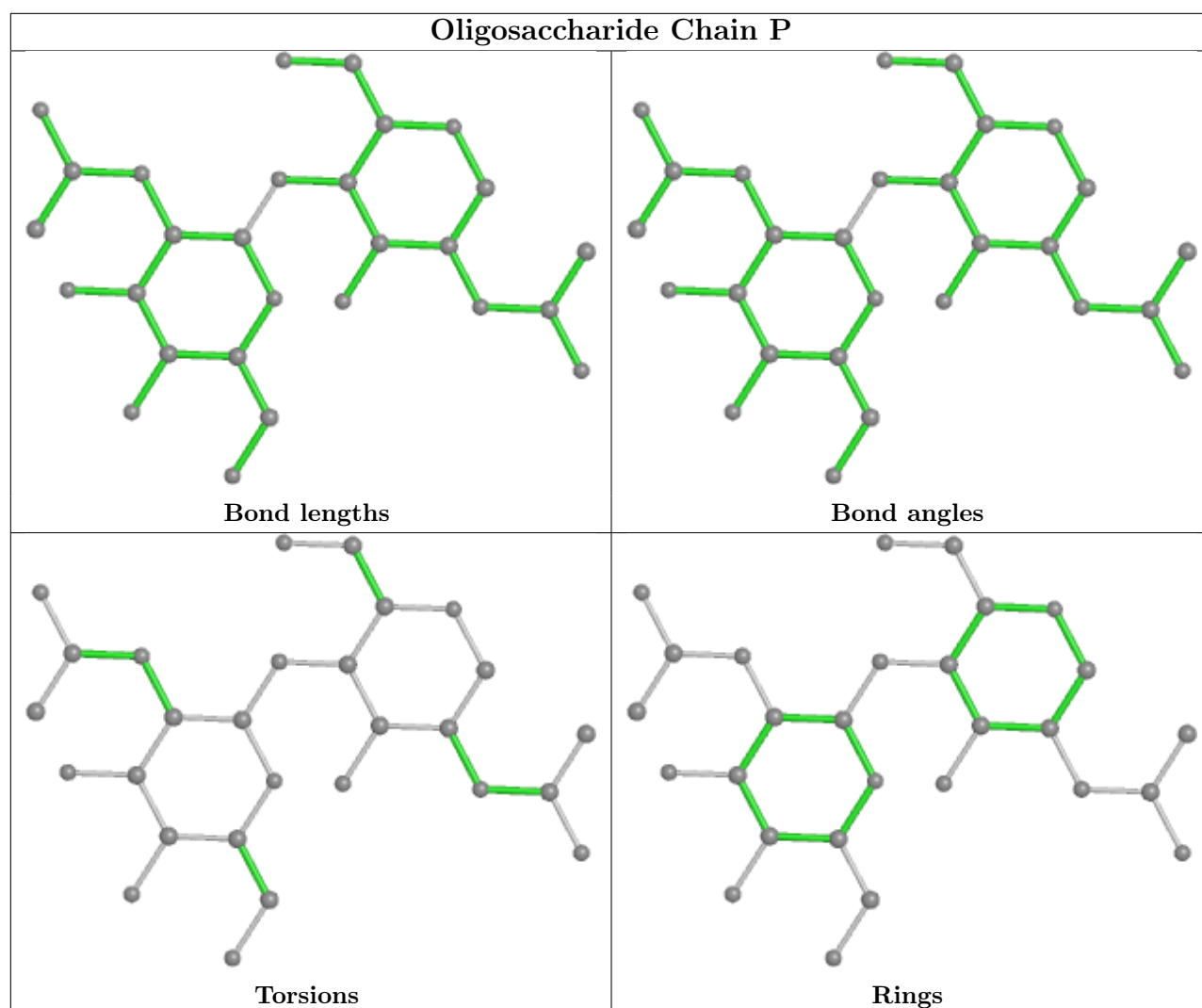
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	1	NAG	1	0
9	I	1	NAG	2	0
9	I	2	NAG	2	0
7	A	2	NAG	3	0
10	K	1	NAG	2	0
7	A	1	NAG	1	0

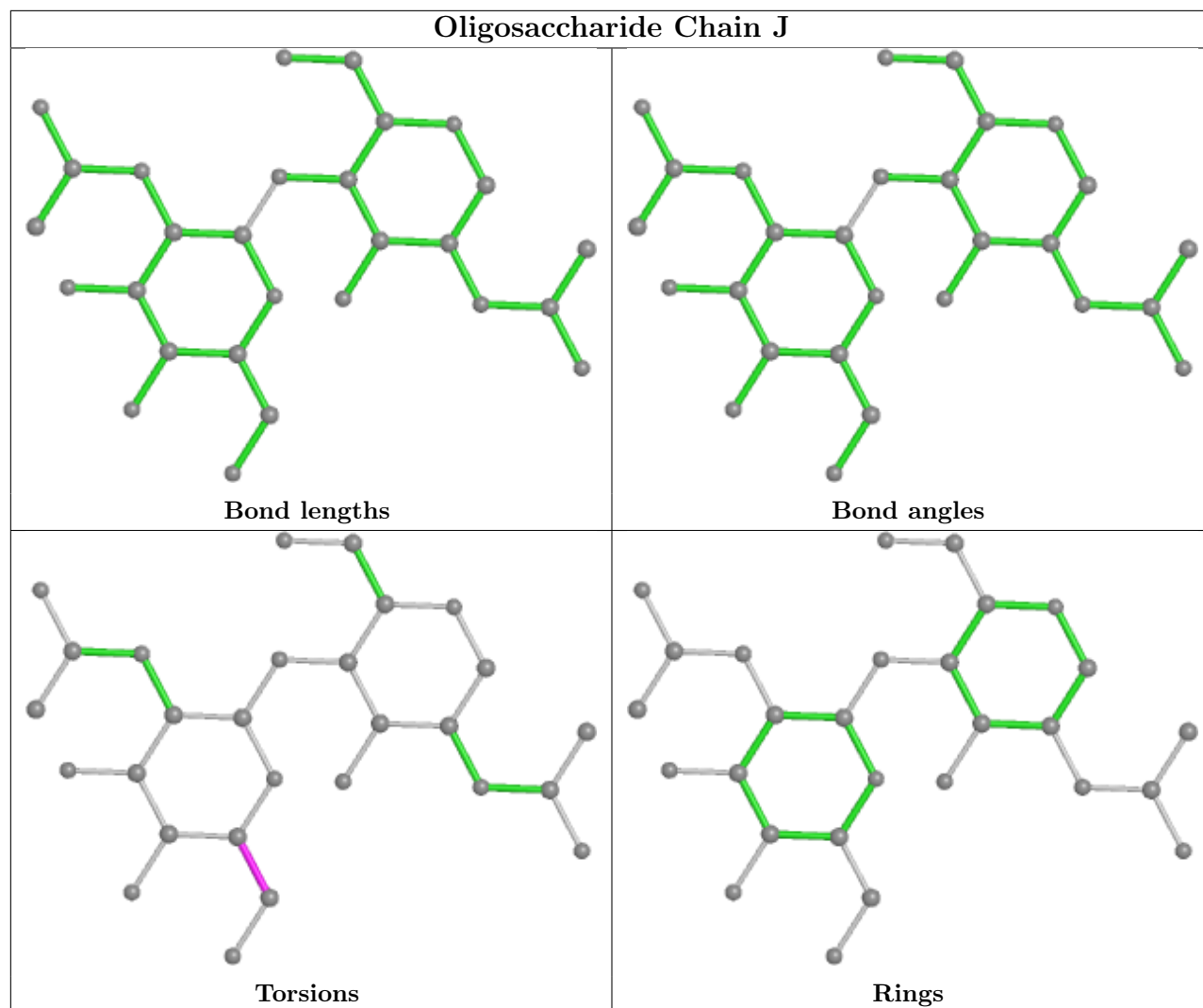
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



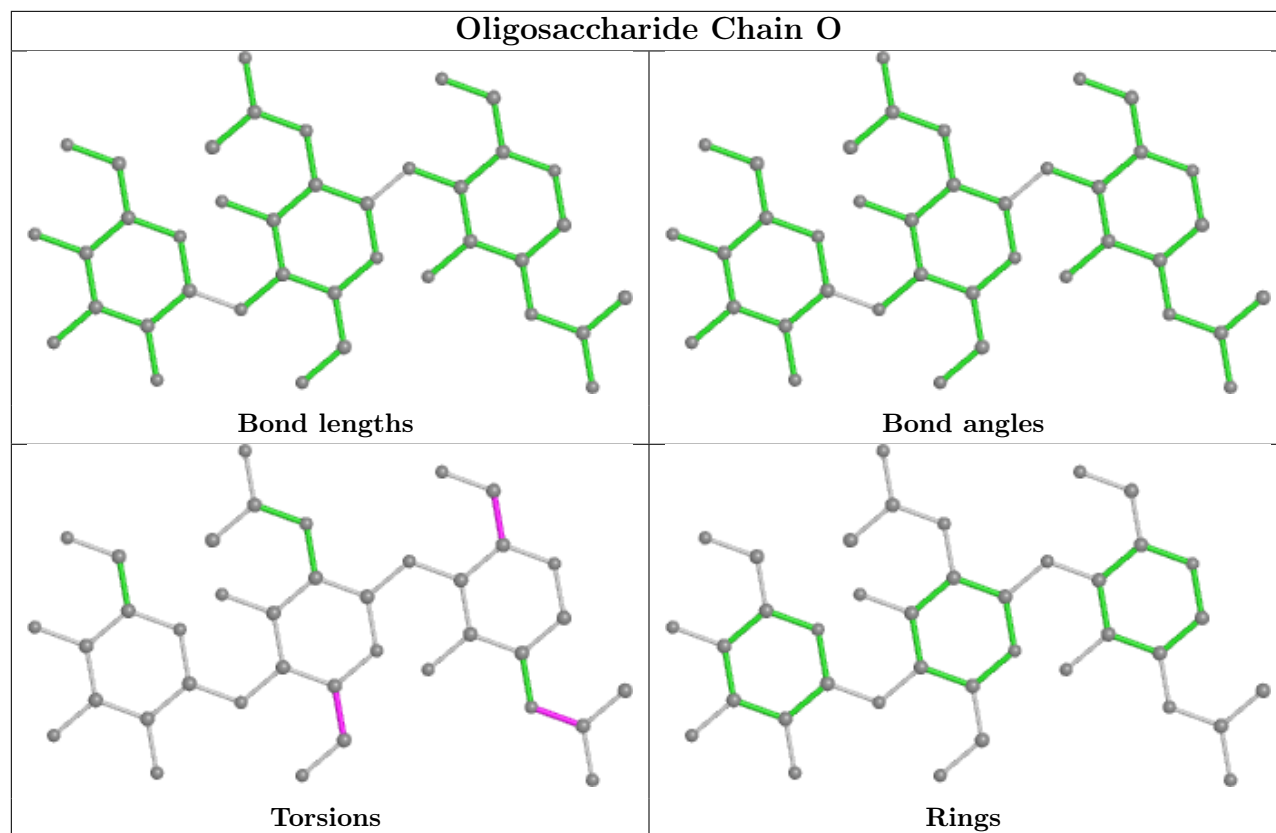


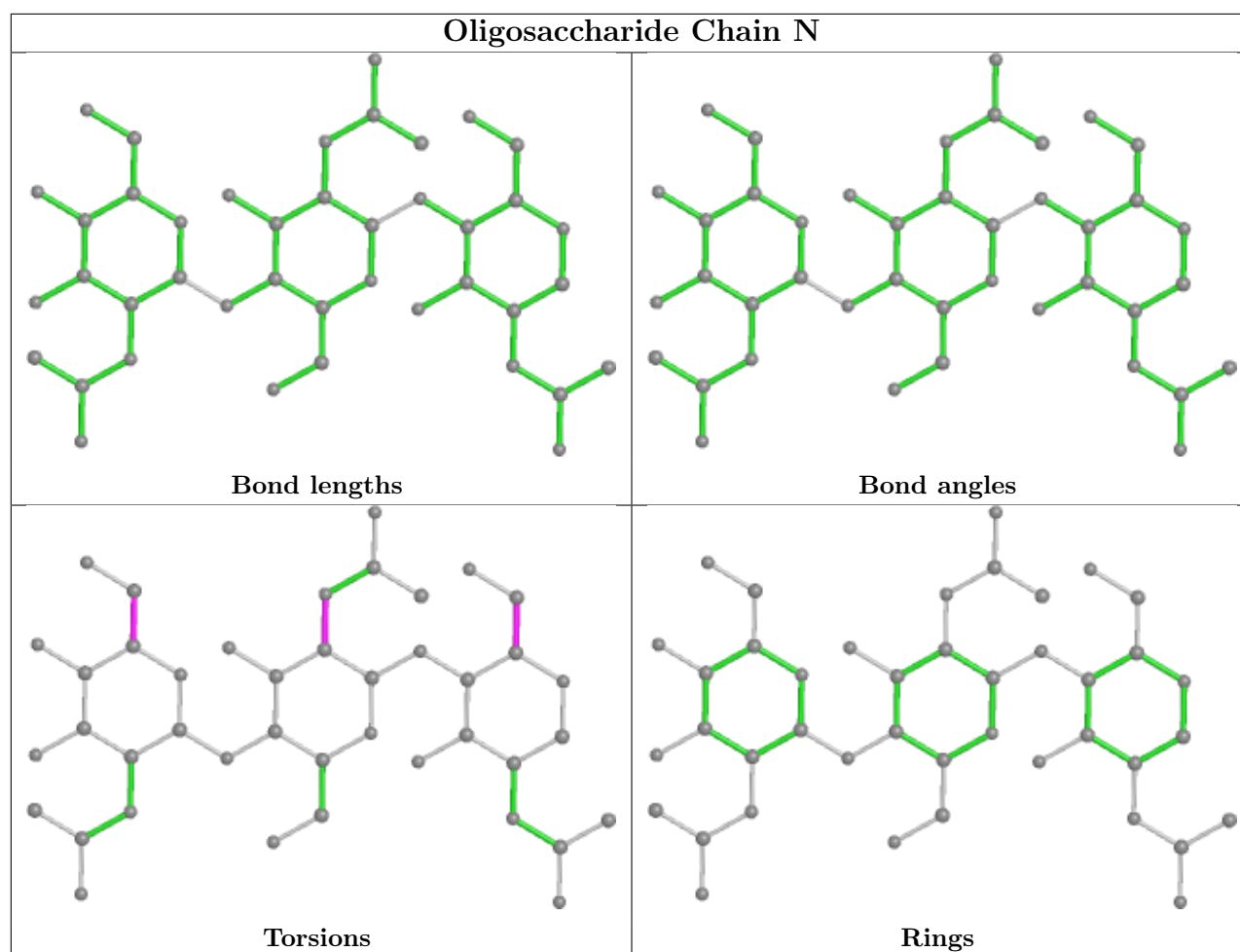












## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	NAG	G	602	4	14,14,15	0.34	0	17,19,21	0.54	0
12	NAG	G	601	4	14,14,15	0.31	0	17,19,21	0.43	0
12	NAG	G	604	4	14,14,15	0.27	0	17,19,21	0.49	0
12	NAG	G	603	4	14,14,15	0.23	0	17,19,21	0.44	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
12	NAG	G	602	4	-	2/6/23/26	0/1/1/1
12	NAG	G	601	4	-	2/6/23/26	0/1/1/1
12	NAG	G	604	4	-	0/6/23/26	0/1/1/1
12	NAG	G	603	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	O5-C5-C6-O6
12	G	603	NAG	O5-C5-C6-O6
12	G	602	NAG	C8-C7-N2-C2
12	G	602	NAG	O7-C7-N2-C2
12	G	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	120/153 (78%)	-0.57	2 (1%) 70 71	11, 36, 74, 84	0
2	D	128/134 (95%)	0.18	12 (9%) 8 6	28, 72, 108, 124	0
3	E	105/114 (92%)	-0.11	4 (3%) 40 38	31, 60, 105, 116	0
4	G	425/498 (85%)	-0.65	3 (0%) 87 88	11, 30, 74, 115	0
5	H	226/244 (92%)	-0.27	5 (2%) 62 61	23, 54, 90, 108	0
6	L	211/217 (97%)	-0.68	1 (0%) 91 92	13, 36, 64, 115	0
All	All	1215/1360 (89%)	-0.44	27 (2%) 62 61	11, 42, 93, 124	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	79	ARG	3.7
2	D	109	LEU	3.6
6	L	7	TYR	3.4
1	B	519	PHE	3.4
2	D	1	GLN	3.3

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

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

### 6.3 Carbohydrates [i](#)

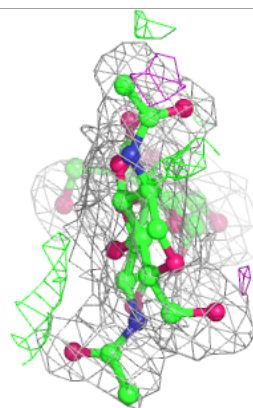
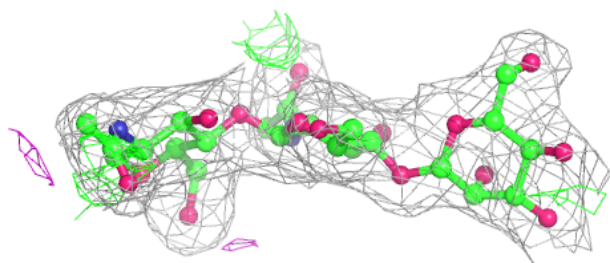
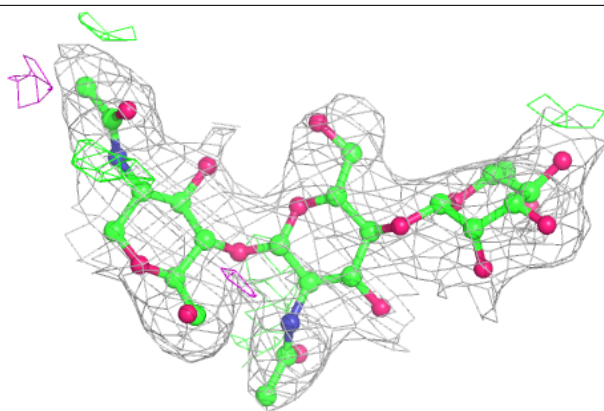
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	M	2	14/15	0.78	0.31	93,103,115,115	0
8	NAG	J	2	14/15	0.82	0.36	77,107,117,120	0
9	BMA	O	3	11/12	0.83	0.17	83,103,123,132	0
8	NAG	P	2	14/15	0.83	0.35	78,104,121,132	0
8	NAG	F	2	14/15	0.86	0.33	49,100,112,114	0
7	MAN	A	4	11/12	0.87	0.16	55,78,98,104	0
9	BMA	I	3	11/12	0.87	0.23	66,88,99,103	0
11	NAG	N	3	14/15	0.89	0.26	68,82,95,99	0
8	NAG	F	1	14/15	0.89	0.25	49,93,105,114	0
7	MAN	A	5	11/12	0.90	0.18	79,94,110,110	0
10	MAN	K	10	11/12	0.90	0.18	67,89,106,107	0
10	MAN	K	9	11/12	0.91	0.21	48,83,97,112	0
8	NAG	C	2	14/15	0.91	0.22	68,107,123,129	0
11	NAG	N	2	14/15	0.93	0.14	40,54,77,88	0
9	NAG	I	2	14/15	0.93	0.14	52,66,84,88	0
8	NAG	M	1	14/15	0.94	0.14	50,63,70,84	0
8	NAG	J	1	14/15	0.94	0.16	36,52,70,70	0
10	MAN	K	8	11/12	0.94	0.14	56,68,81,82	0
10	MAN	K	6	11/12	0.94	0.16	35,54,65,77	0
9	NAG	O	1	14/15	0.96	0.09	41,49,62,66	0
9	NAG	O	2	14/15	0.96	0.14	53,81,95,97	0
7	MAN	A	6	11/12	0.96	0.10	31,40,47,50	0
10	NAG	K	2	14/15	0.96	0.12	29,54,68,69	0
10	MAN	K	7	11/12	0.96	0.09	58,71,87,87	0
8	NAG	P	1	14/15	0.96	0.13	50,67,82,91	0
7	BMA	A	3	11/12	0.96	0.10	33,45,57,59	0
11	NAG	N	1	14/15	0.96	0.12	31,44,56,74	0
7	NAG	A	1	14/15	0.96	0.13	21,30,41,45	0
7	NAG	A	2	14/15	0.97	0.12	29,35,47,48	0
10	NAG	K	1	14/15	0.97	0.10	20,41,52,55	0
9	NAG	I	1	14/15	0.97	0.10	10,28,52,55	0
10	BMA	K	3	11/12	0.97	0.10	30,43,58,77	0
8	NAG	C	1	14/15	0.98	0.16	31,49,83,88	0
10	MAN	K	5	11/12	0.99	0.11	30,38,43,44	0
10	MAN	K	4	11/12	0.99	0.10	18,27,34,44	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.

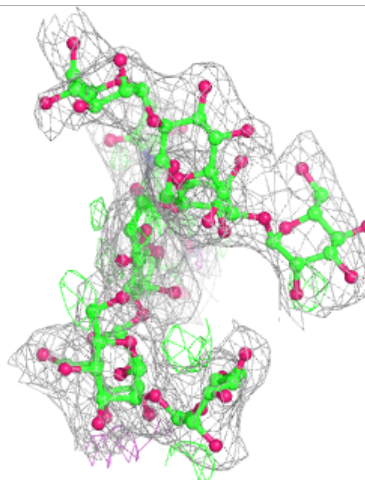
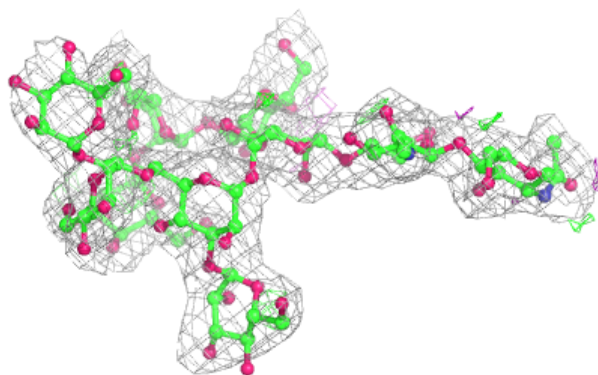
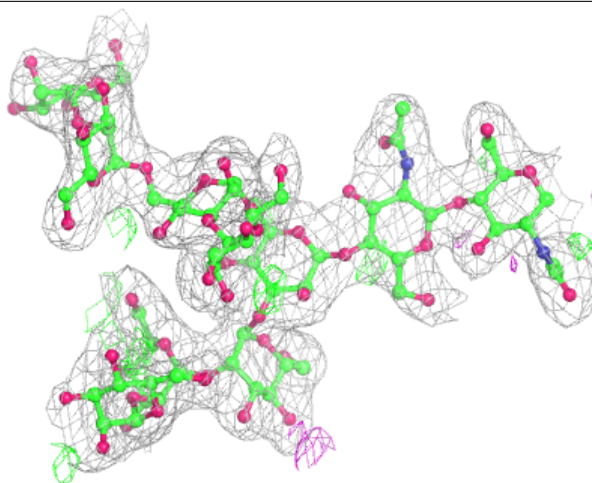
**Electron density around Chain I:**

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



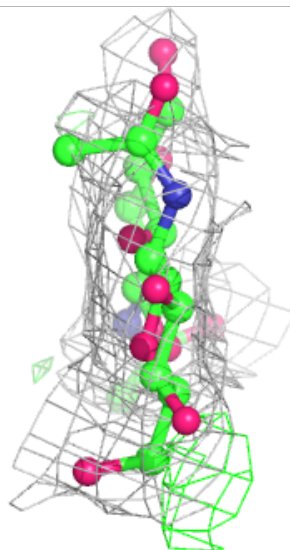
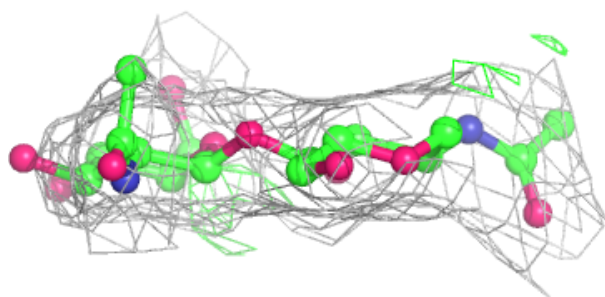
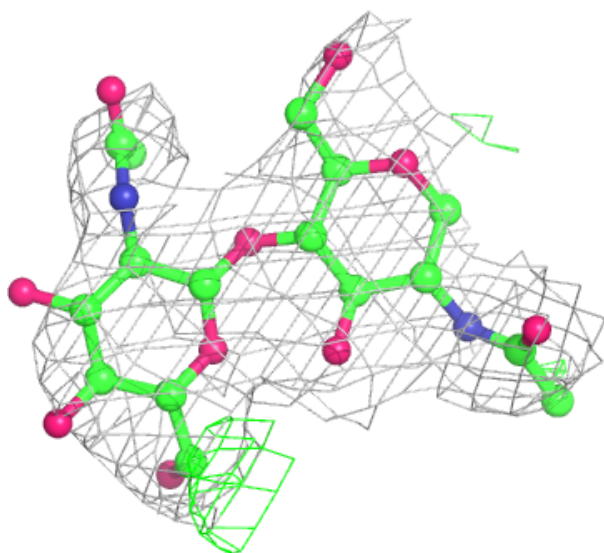
**Electron density around Chain K:**

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



**Electron density around Chain M:**

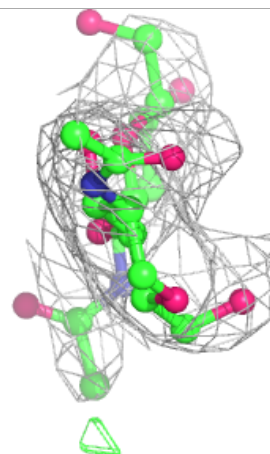
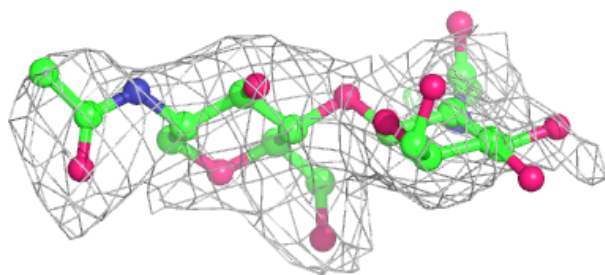
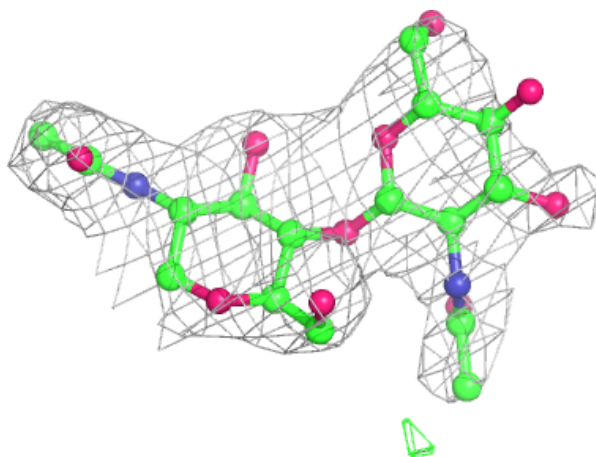
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





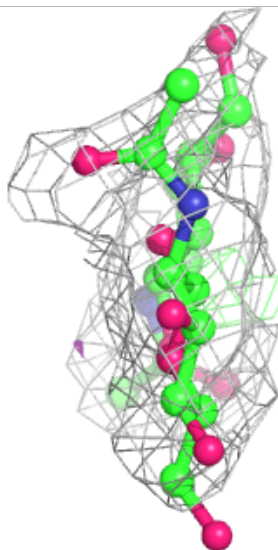
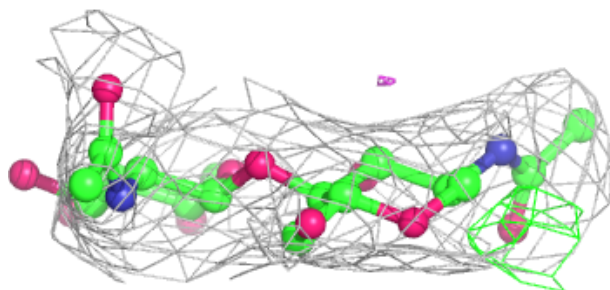
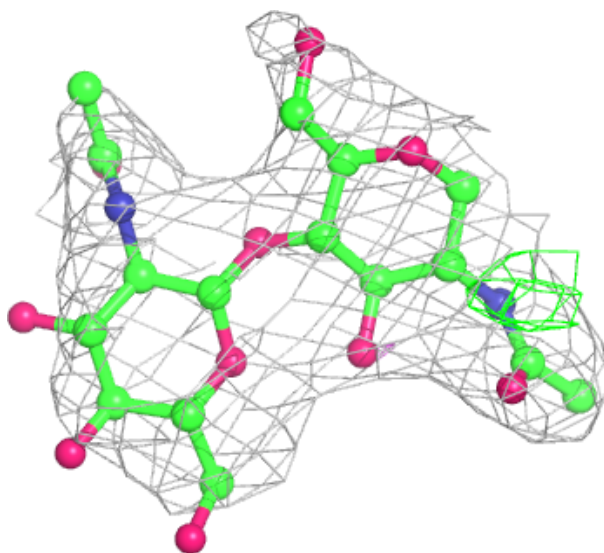
**Electron density around Chain P:**

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



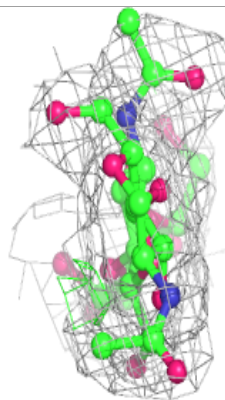
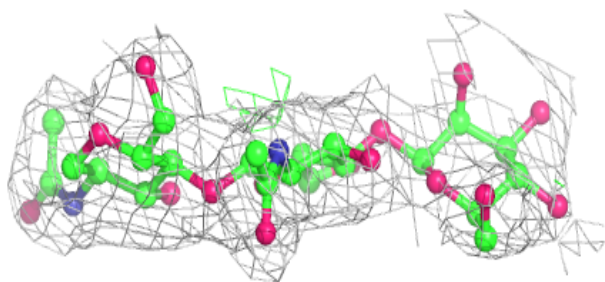
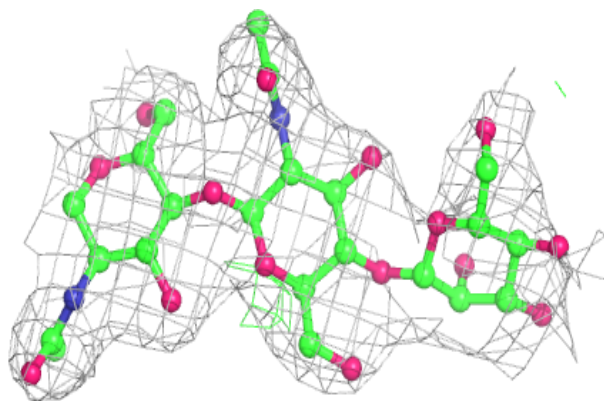
**Electron density around Chain J:**

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

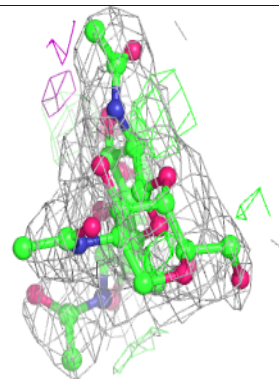
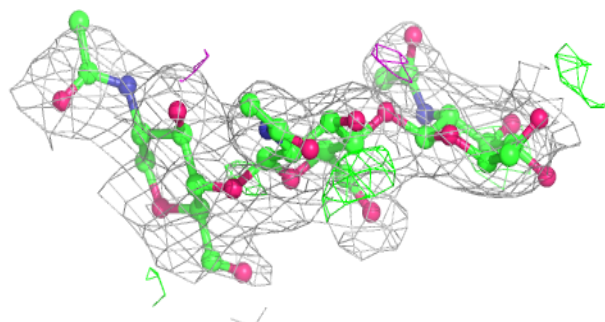
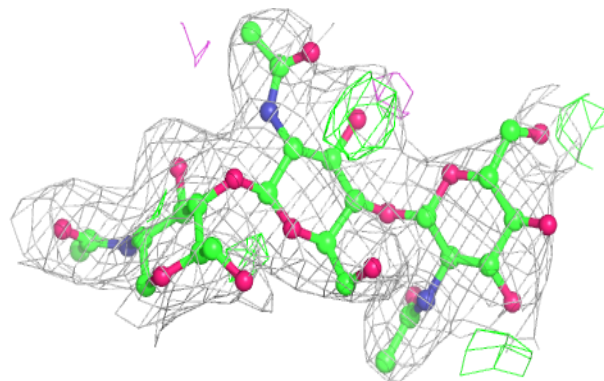


**Electron density around Chain O:**

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

**Electron density around Chain 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( $\text{\AA}^2$ )	Q<0.9
12	NAG	G	604	14/15	0.90	0.29	52,88,114,119	0
12	NAG	G	603	14/15	0.93	0.15	53,75,109,110	0
12	NAG	G	602	14/15	0.94	0.16	26,66,86,88	0
12	NAG	G	601	14/15	0.96	0.10	39,50,65,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.