



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:13 PM UTC

PDB ID : 5K9K / pdb_00005k9k
Title : Crystal structure of multidonor HV6-1-class broadly neutralizing Influenza A antibody 56.a.09 in complex with Hemagglutinin Hong Kong 1968.
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-05-31
Resolution : 2.97 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

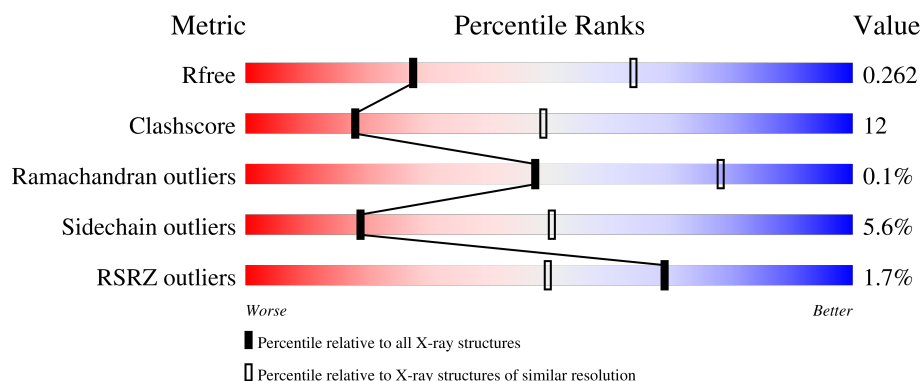
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	% 78% 19% ..
1	H	229	79% 17% ..
2	B	215	% 77% 20% .
2	L	215	% 78% 20% .
3	F	503	3% 72% 22% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	503	
4	C	5	
4	J	5	
4	K	5	
4	P	5	
5	D	3	
5	N	3	
6	E	2	
7	G	5	
8	M	6	
9	O	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	E	1	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 15108 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 56.a.09 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1710	1082	288	333	7			
1	H	224	Total	C	N	O	S	0	0	0
			1695	1073	285	330	7			

- Molecule 2 is a protein called 56.a.09 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1652	1032	279	336	5			
2	L	215	Total	C	N	O	S	0	0	0
			1652	1032	279	336	5			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	490	Total	C	N	O	S	0	1	0
			3876	2416	681	760	19			
3	F	497	Total	C	N	O	S	0	1	0
			3923	2447	691	766	19			

There are 2 discrepancies between the modelled and reference sequences:

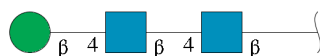
Chain	Residue	Modelled	Actual	Comment	Reference
I	218	GLU	GLY	conflict	UNP Q91MA7
F	218	GLU	GLY	conflict	UNP Q91MA7

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



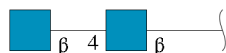
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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.



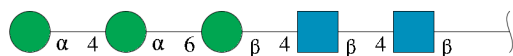
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



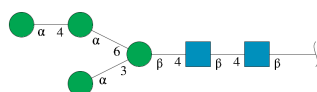
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-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.



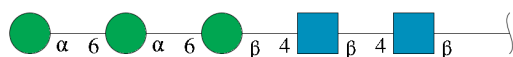
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-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.



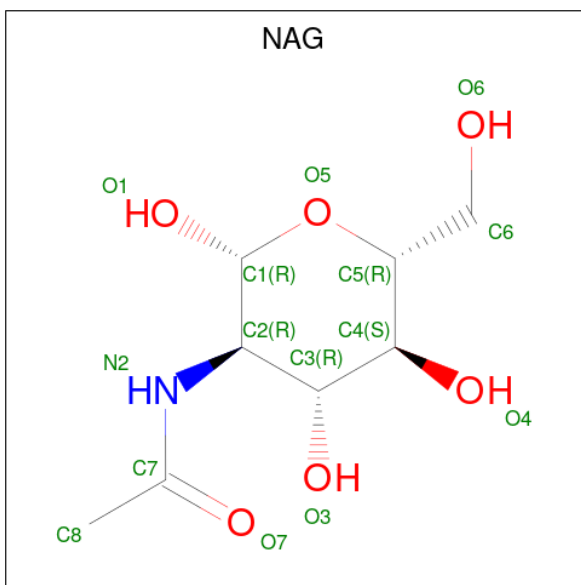
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.

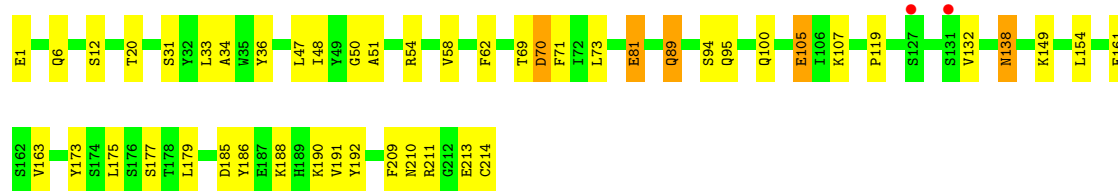


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

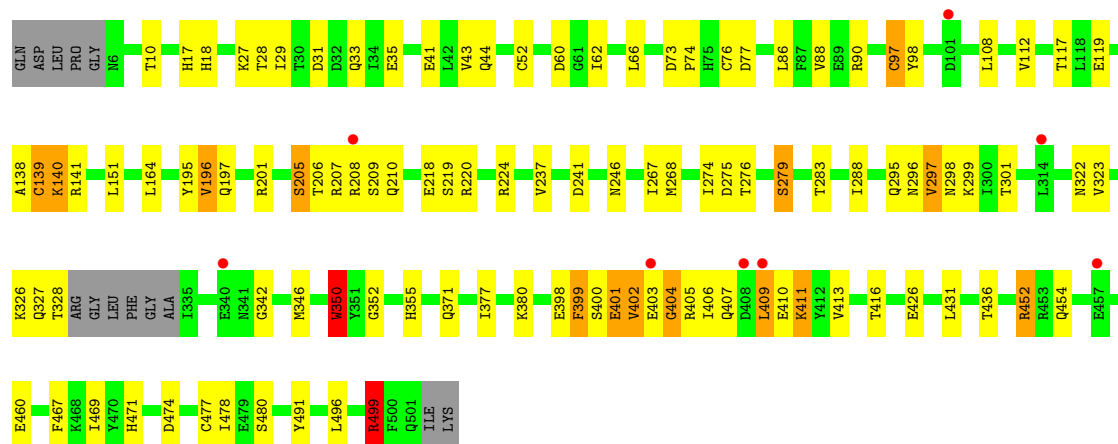
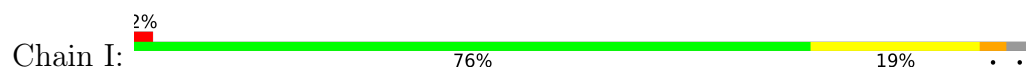
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



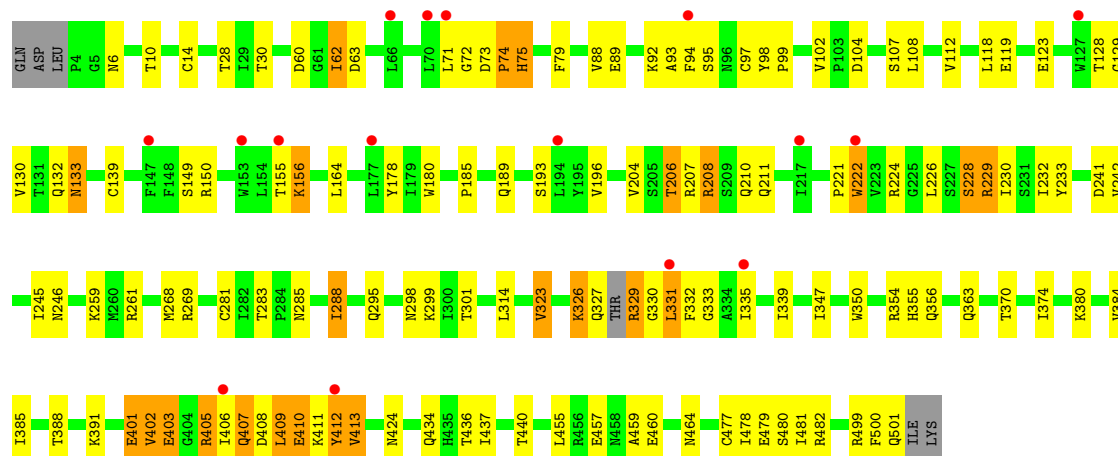
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	N	O	0	0
			14	8	1	5		
10	I	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		



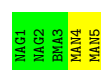
• Molecule 3: Hemagglutinin



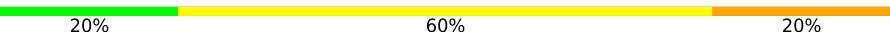
• Molecule 3: Hemagglutinin

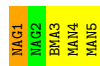


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain J: 

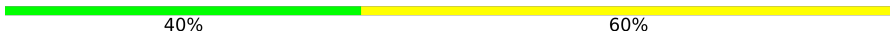


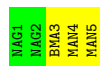
- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K: 

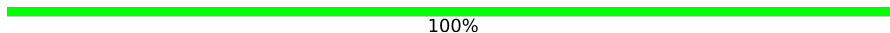


- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain P: 

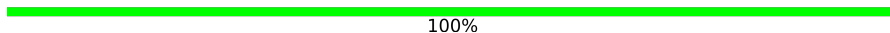


- Molecule 5: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D: 



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

Chain N: 



- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain E: 



- Molecule 7: alpha-D-mannopyranose-(1-4)-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 G:  20% 80%

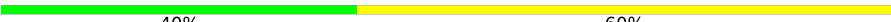


- Molecule 8: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 33% 17%



- Molecule 9: alpha-D-mannopyranose-(1-6)-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 O:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.90Å 136.56Å 311.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 2.97 46.01 – 2.97	Depositor EDS
% Data completeness (in resolution range)	75.0 (46.01-2.97) 71.6 (46.01-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.225 , 0.265 0.229 , 0.262	Depositor DCC
R_{free} test set	2058 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15108	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	A	0.39	0/1750	0.52	1/2386 (0.0%)
1	H	0.38	0/1735	0.54	1/2367 (0.0%)
2	B	0.44	0/1687	0.47	0/2288
2	L	0.44	0/1687	0.46	1/2288 (0.0%)
3	F	0.39	1/4009 (0.0%)	0.58	7/5436 (0.1%)
3	I	0.44	2/3960 (0.1%)	0.60	12/5372 (0.2%)
All	All	0.41	3/14828 (0.0%)	0.55	22/20137 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	350[A]	TRP	CA-C	7.18	1.62	1.52
3	I	350[B]	TRP	CA-C	7.18	1.62	1.52
3	F	74	PRO	N-CD	5.02	1.54	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	404	GLY	N-CA-C	-10.56	99.70	112.48
1	A	148	GLU	C-N-CD	-9.57	99.55	120.60
1	H	32	ASN	N-CA-C	-8.19	99.49	110.55
3	I	140	LYS	N-CA-C	-7.47	98.39	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	138	ASN	N-CA-C	6.44	120.44	111.74

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	350[A]	TRP	Mainchain
3	I	350[B]	TRP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1710	0	1709	36	0
1	H	1695	0	1691	38	0
2	B	1652	0	1599	50	0
2	L	1652	0	1599	30	0
3	F	3923	0	3776	135	0
3	I	3876	0	3729	85	0
4	C	61	0	52	0	0
4	J	61	0	52	3	0
4	K	61	0	52	0	0
4	P	61	0	52	0	0
5	D	39	0	34	0	0
5	N	39	0	34	0	0
6	E	28	0	25	0	0
7	G	61	0	52	0	0
8	M	72	0	61	1	0
9	O	61	0	52	0	0
10	F	28	0	26	0	0
10	I	28	0	26	0	0
All	All	15108	0	14621	362	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 12.

The worst 5 of 362 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)
3:F:402:VAL:CG1	3:F:409:LEU:HD11	1.52	1.39
3:F:402:VAL:CG1	3:F:409:LEU:CD1	2.06	1.31
3:F:402:VAL:HG13	3:F:409:LEU:CD1	1.64	1.24
3:F:156:LYS:HE2	3:F:193:SER:O	1.40	1.21
2:B:27:GLN:OE1	4:J:1:NAG:H81	1.43	1.17

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	222/229 (97%)	210 (95%)	11 (5%)	1 (0%)	24	58
1	H	220/229 (96%)	207 (94%)	13 (6%)	0	100	100
2	B	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	L	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
3	F	494/503 (98%)	470 (95%)	24 (5%)	0	100	100
3	I	487/503 (97%)	467 (96%)	20 (4%)	0	100	100
All	All	1849/1894 (98%)	1769 (96%)	79 (4%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO

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	198/200 (99%)	191 (96%)	7 (4%)	32	63
1	H	196/200 (98%)	186 (95%)	10 (5%)	21	53
2	B	185/185 (100%)	173 (94%)	12 (6%)	15	45
2	L	185/185 (100%)	175 (95%)	10 (5%)	20	51
3	F	435/440 (99%)	409 (94%)	26 (6%)	17	48
3	I	432/440 (98%)	406 (94%)	26 (6%)	17	48
All	All	1631/1650 (99%)	1540 (94%)	91 (6%)	19	50

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	47	LEU
3	F	206	THR
2	L	81	GLU
3	F	62	ILE
3	F	222	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
2	L	147	GLN
2	L	95	GLN
3	F	44	GLN
2	B	155	GLN

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 ⓘ

44 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	$\# Z > 2$
4	NAG	C	1	3,4	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	C	2	4	14,14,15	0.24	0	17,19,21	0.81	0
4	BMA	C	3	4	11,11,12	0.52	0	15,15,17	0.76	0
4	MAN	C	4	4	11,11,12	0.58	0	15,15,17	0.96	2 (13%)
4	MAN	C	5	4	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
5	NAG	D	1	3,5	14,14,15	0.36	0	17,19,21	0.58	0
5	NAG	D	2	5	14,14,15	0.28	0	17,19,21	0.48	0
5	BMA	D	3	5	11,11,12	0.55	0	15,15,17	0.75	0
6	NAG	E	1	3,6	14,14,15	0.48	0	17,19,21	1.84	3 (17%)
6	NAG	E	2	6	14,14,15	0.29	0	17,19,21	0.50	0
7	NAG	G	1	3,7	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	G	2	7	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
7	BMA	G	3	7	11,11,12	0.66	0	15,15,17	1.08	1 (6%)
7	MAN	G	4	7	11,11,12	0.76	0	15,15,17	0.93	2 (13%)
7	MAN	G	5	7	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
4	NAG	J	1	3,4	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	0.57	0
4	BMA	J	3	4	11,11,12	1.67	2 (18%)	15,15,17	1.39	2 (13%)
4	MAN	J	4	4	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
4	MAN	J	5	4	11,11,12	0.75	0	15,15,17	1.12	2 (13%)
4	NAG	K	1	3,4	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	K	2	4	14,14,15	0.27	0	17,19,21	0.54	0
4	BMA	K	3	4	11,11,12	0.71	0	15,15,17	0.85	0
4	MAN	K	4	4	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
4	MAN	K	5	4	11,11,12	0.82	1 (9%)	15,15,17	1.29	2 (13%)
8	NAG	M	1	8,3	14,14,15	0.35	0	17,19,21	0.67	0
8	NAG	M	2	8	14,14,15	0.21	0	17,19,21	0.76	0
8	BMA	M	3	8	11,11,12	0.59	0	15,15,17	0.84	0
8	MAN	M	4	8	11,11,12	0.76	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	M	5	8	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
8	MAN	M	6	8	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
5	NAG	N	1	3,5	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	N	2	5	14,14,15	0.31	0	17,19,21	0.40	0
5	BMA	N	3	5	11,11,12	0.63	0	15,15,17	0.66	0
9	NAG	O	1	9,3	14,14,15	0.99	1 (7%)	17,19,21	0.83	0
9	NAG	O	2	9	14,14,15	0.22	0	17,19,21	0.57	0
9	BMA	O	3	9	11,11,12	0.56	0	15,15,17	0.72	0
9	MAN	O	4	9	11,11,12	0.68	0	15,15,17	0.90	2 (13%)
9	MAN	O	5	9	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
4	NAG	P	1	3,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	P	2	4	14,14,15	0.36	0	17,19,21	0.69	0
4	BMA	P	3	4	11,11,12	0.87	0	15,15,17	1.43	1 (6%)
4	MAN	P	4	4	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
4	MAN	P	5	4	11,11,12	0.92	0	15,15,17	0.89	2 (13%)

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
4	NAG	C	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	1/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1
6	NAG	E	1	3,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	1/6/23/26	0/1/1/1
7	NAG	G	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	1/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	BMA	C1-C2	4.05	1.61	1.52
9	O	1	NAG	O5-C1	-3.45	1.37	1.43
4	J	3	BMA	C2-C3	3.27	1.57	1.52
4	K	5	MAN	C1-C2	2.32	1.57	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1	NAG	C1-O5-C5	6.15	120.42	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	3	BMA	C1-O5-C5	4.51	118.23	112.19
4	K	5	MAN	C1-O5-C5	3.76	117.22	112.19
4	J	3	BMA	C1-C2-C3	3.40	114.60	109.64
4	J	5	MAN	C1-O5-C5	3.27	116.57	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	1	NAG	C1

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	3	BMA	O5-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	D	1	NAG	C4-C5-C6-O6

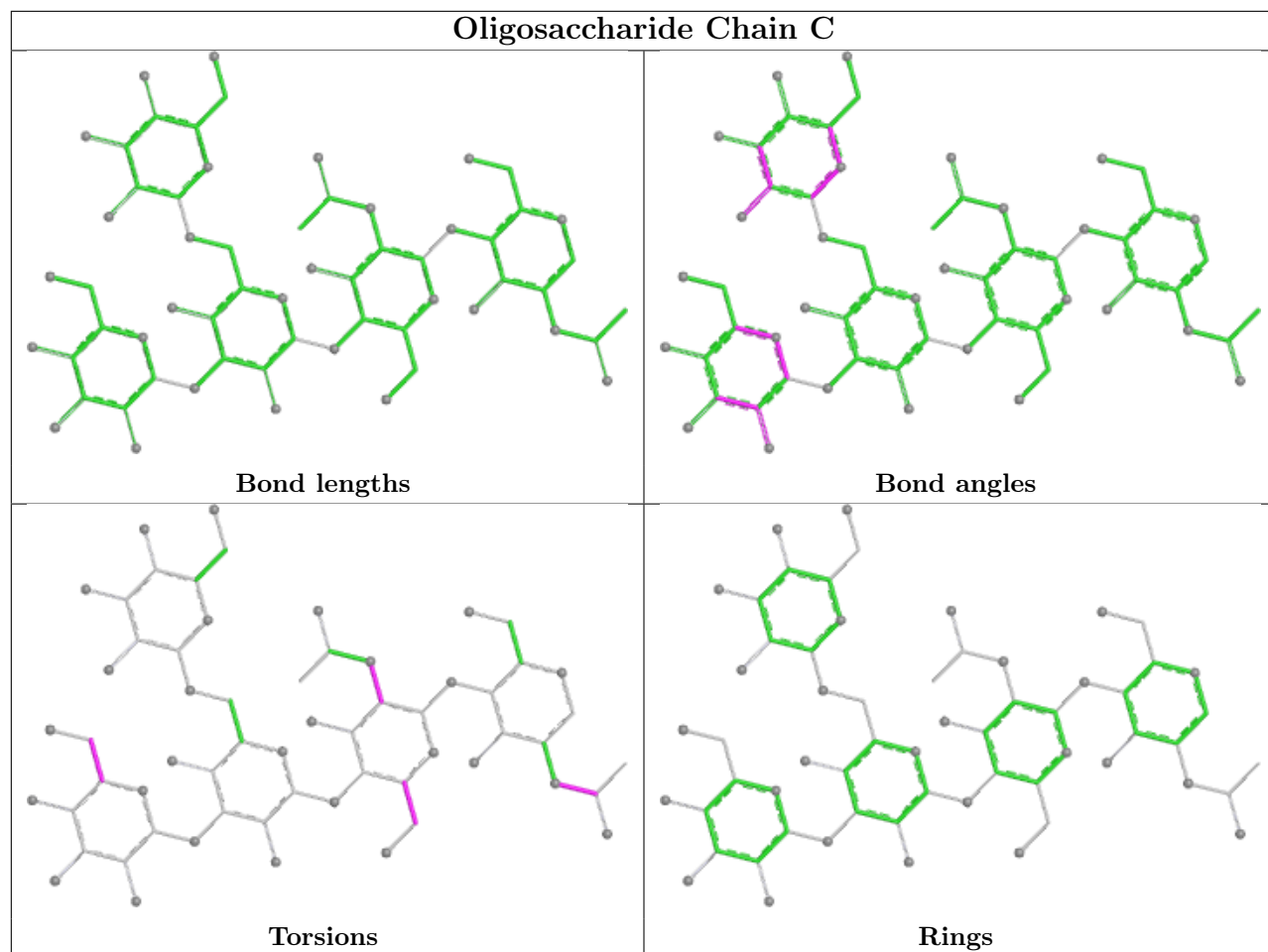
All (4) ring outliers are listed below:

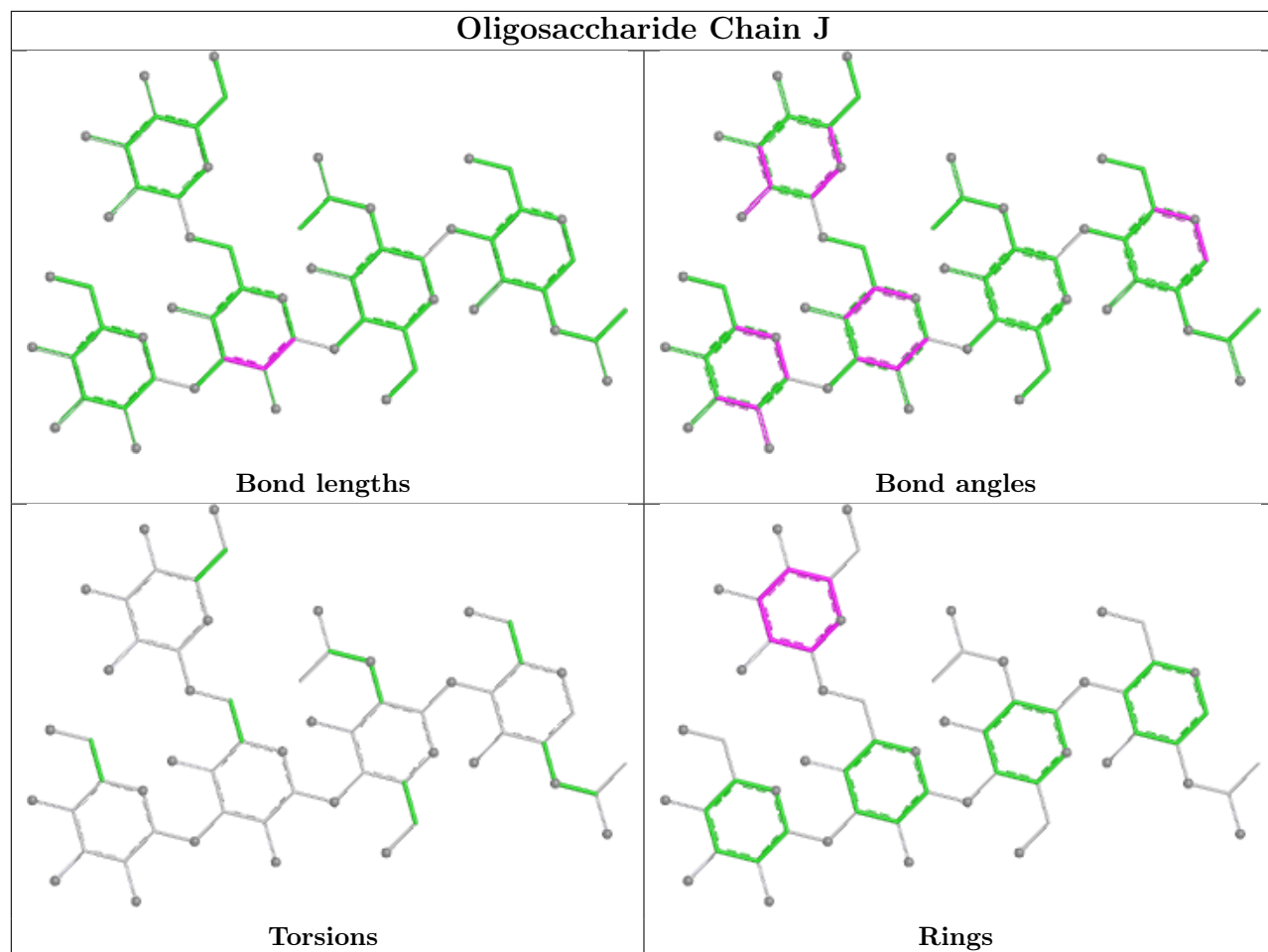
Mol	Chain	Res	Type	Atoms
4	P	3	BMA	C1-C2-C3-C4-C5-O5
4	P	5	MAN	C1-C2-C3-C4-C5-O5
7	G	5	MAN	C1-C2-C3-C4-C5-O5
4	J	5	MAN	C1-C2-C3-C4-C5-O5

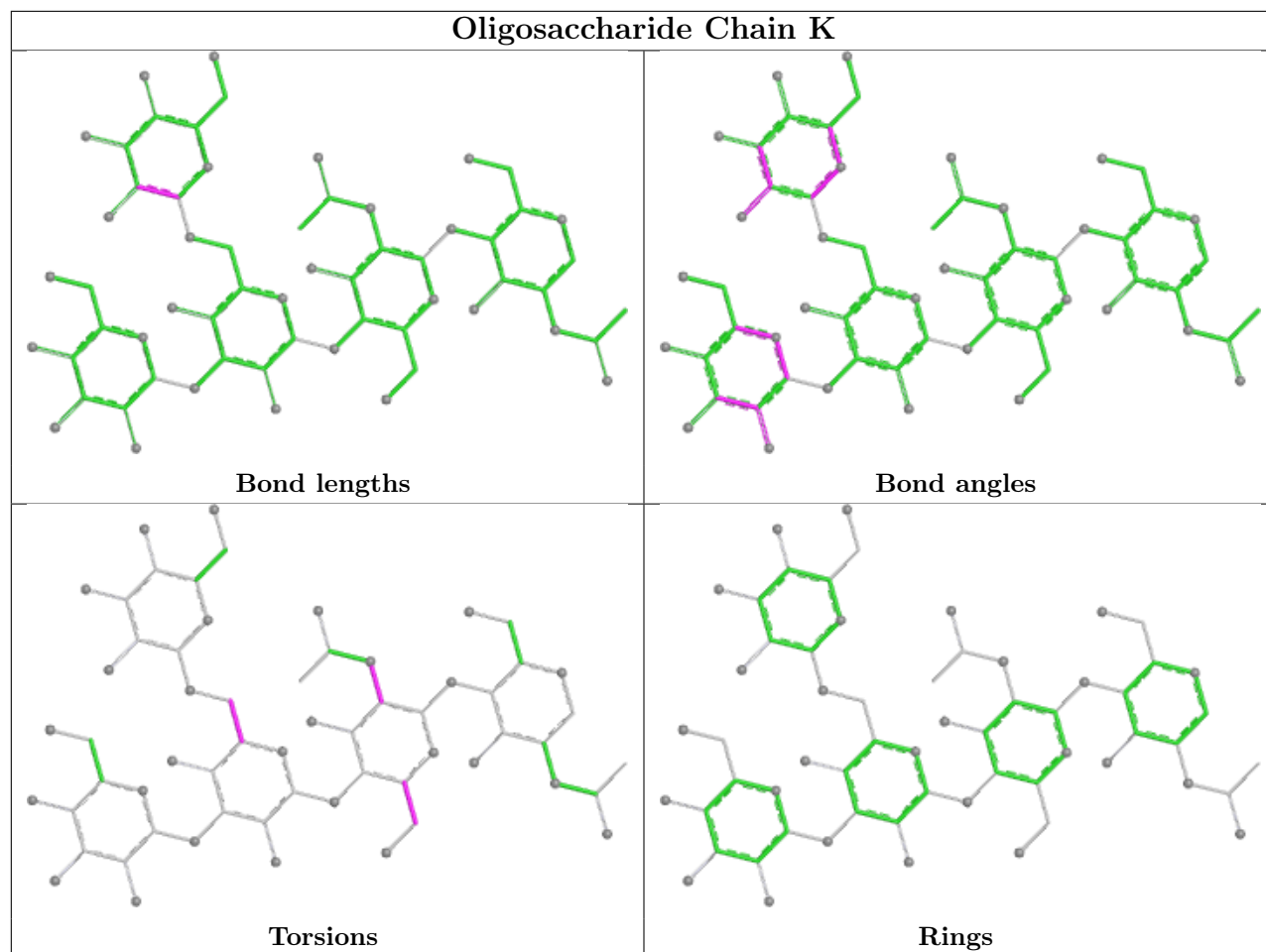
2 monomers are involved in 4 short contacts:

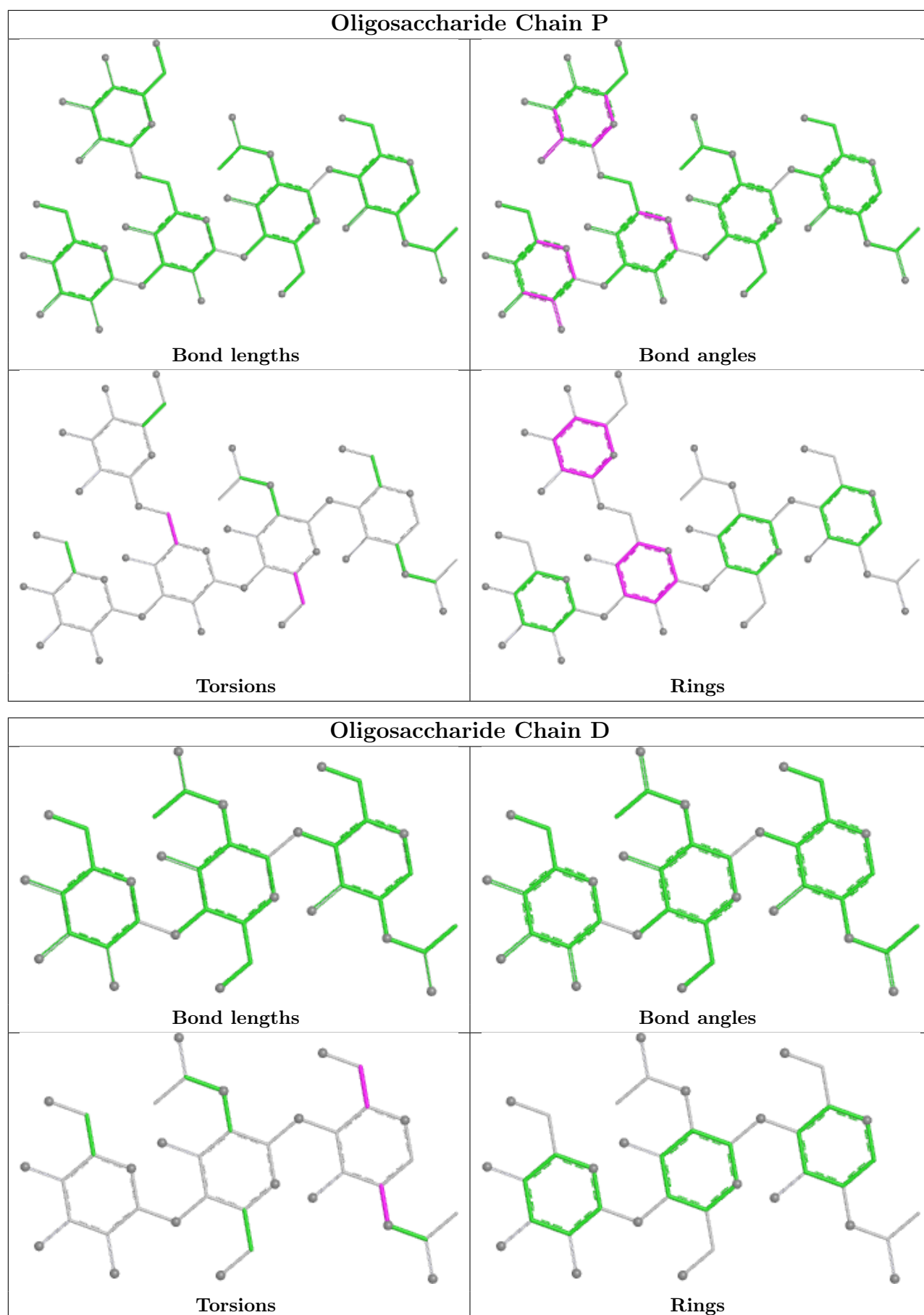
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	6	MAN	1	0
4	J	1	NAG	3	0

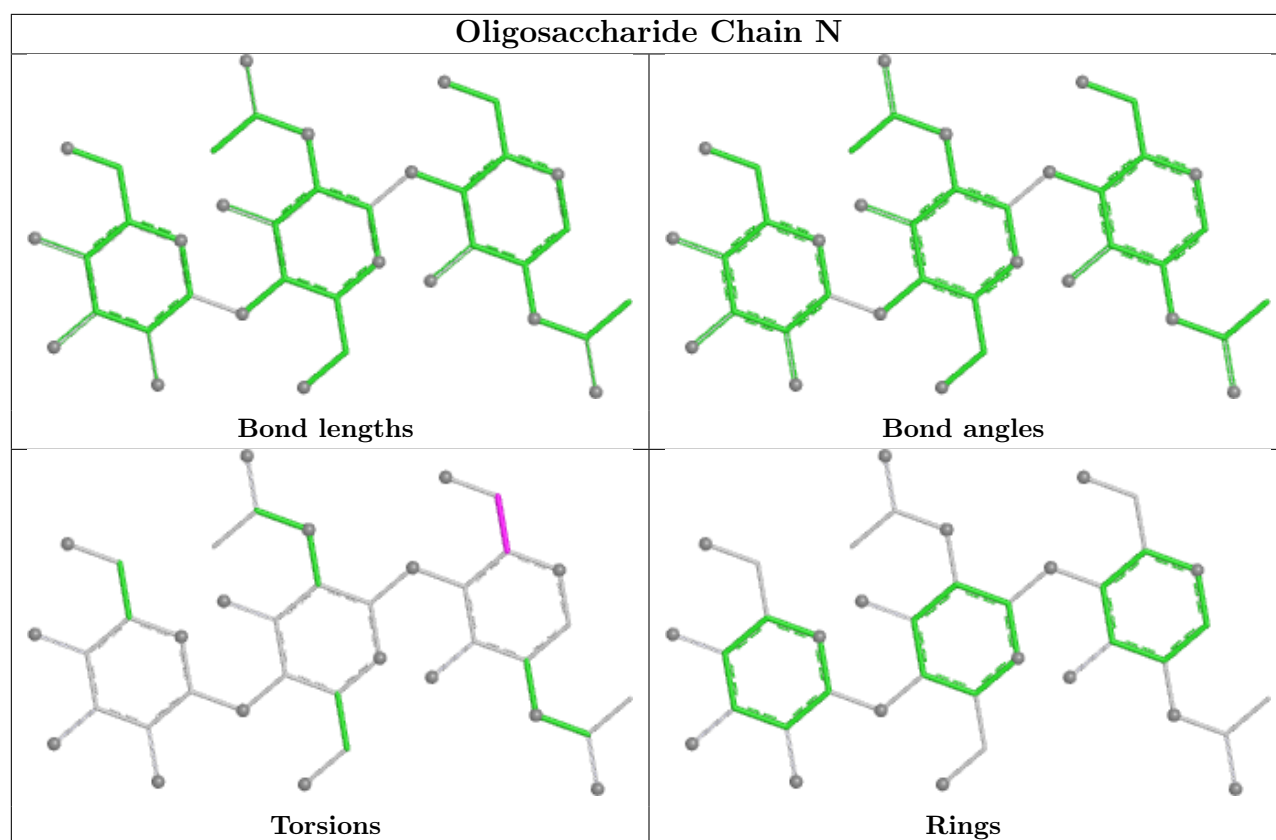
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

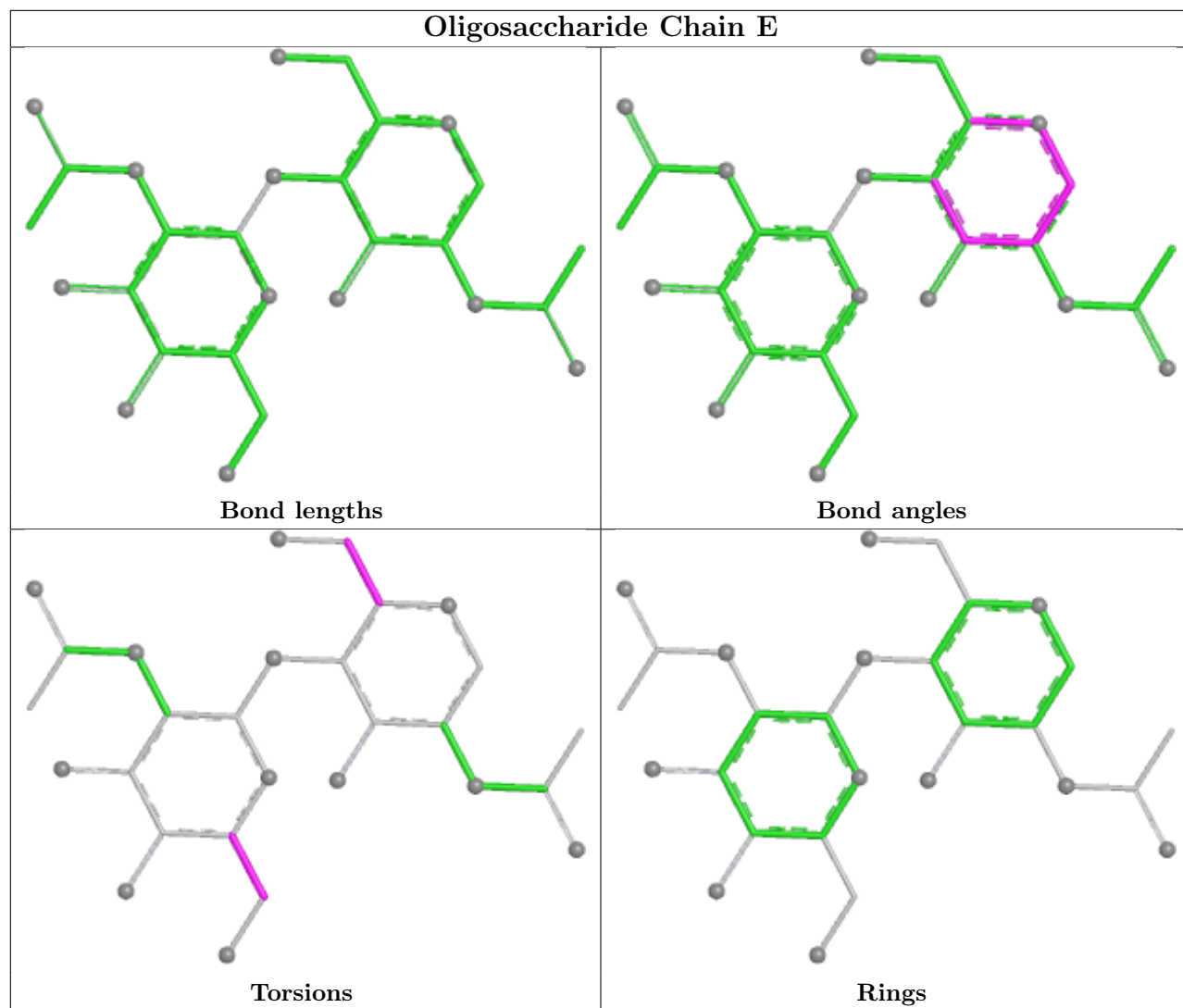


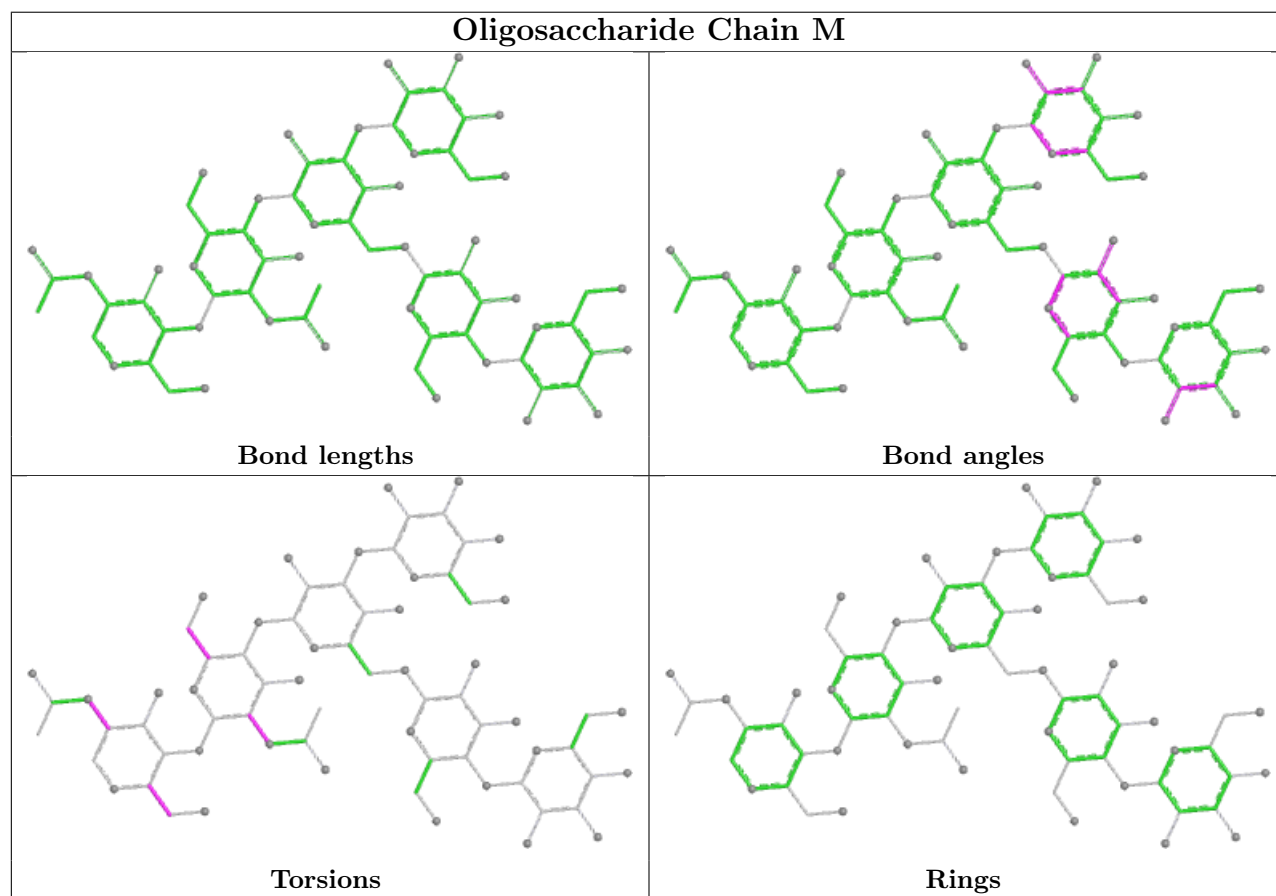
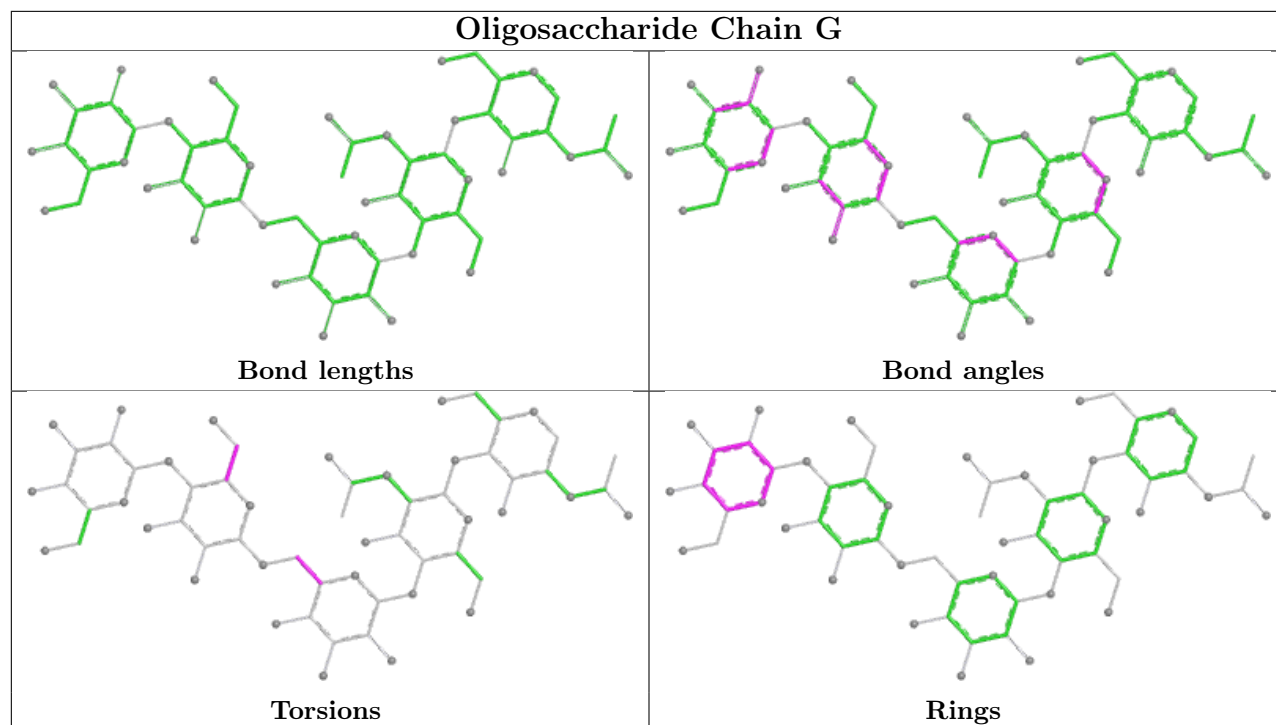


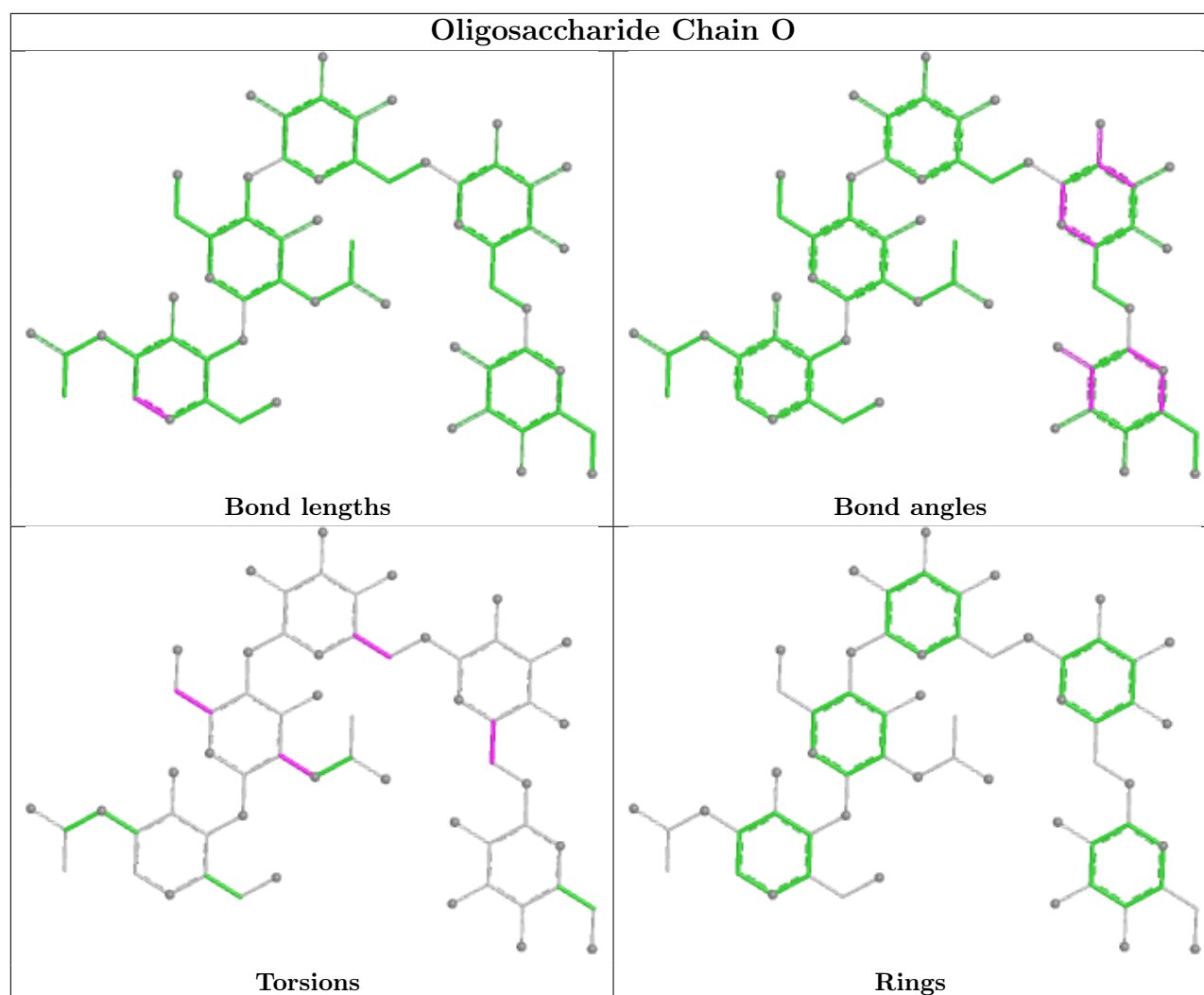












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	NAG	F	601	3	14,14,15	0.19	0	17,19,21	0.42	0
10	NAG	I	601	-	14,14,15	0.21	0	17,19,21	0.42	0
10	NAG	F	621	3	14,14,15	0.28	0	17,19,21	0.43	0
10	NAG	I	602	3	14,14,15	0.25	0	17,19,21	0.47	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
10	NAG	F	601	3	-	1/6/23/26	0/1/1/1
10	NAG	I	601	-	-	0/6/23/26	0/1/1/1
10	NAG	F	621	3	-	1/6/23/26	0/1/1/1
10	NAG	I	602	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	621	NAG	O5-C5-C6-O6
10	F	601	NAG	O5-C5-C6-O6
10	I	602	NAG	O5-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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/229 (98%)	0.09	2 (0%) 81 65	37, 62, 98, 162	1 (0%)
1	H	224/229 (97%)	0.03	1 (0%) 88 79	24, 64, 94, 155	0
2	B	215/215 (100%)	0.04	2 (0%) 81 65	45, 67, 96, 149	1 (0%)
2	L	215/215 (100%)	0.13	2 (0%) 81 65	37, 61, 100, 162	1 (0%)
3	F	497/503 (98%)	0.43	16 (3%) 50 33	32, 84, 137, 182	3 (0%)
3	I	490/503 (97%)	0.26	8 (1%) 70 51	33, 70, 117, 168	4 (0%)
All	All	1867/1894 (98%)	0.22	31 (1%) 69 50	24, 69, 122, 182	10 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	331	LEU	4.0
3	I	101	ASP	4.0
3	I	457	GLU	3.7
1	A	92	CYS	3.5
3	F	66	LEU	3.4

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	29,35,60,70	0
4	NAG	C	2	14/15	-	-	32,41,56,56	0
4	BMA	C	3	11/12	-	-	63,70,79,89	0
4	MAN	C	4	11/12	-	-	77,80,86,92	0
4	MAN	C	5	11/12	-	-	82,102,117,121	0
5	BMA	N	3	11/12	0.10	0.13	168,171,173,173	0
5	NAG	N	1	14/15	0.13	0.18	109,135,142,144	0
5	NAG	N	2	14/15	0.19	0.18	131,148,158,165	0
4	MAN	K	4	11/12	0.29	0.11	171,189,191,193	0
8	MAN	M	4	11/12	0.34	0.15	114,121,126,127	0
9	MAN	O	5	11/12	0.39	0.11	150,154,156,161	0
4	MAN	P	4	11/12	0.42	0.11	140,143,146,148	0
4	BMA	K	3	11/12	0.43	0.10	194,195,199,199	0
4	MAN	J	4	11/12	0.44	0.11	149,153,156,164	0
4	MAN	K	5	11/12	0.46	0.11	187,191,196,197	0
9	MAN	O	4	11/12	0.49	0.11	150,158,162,163	0
9	BMA	O	3	11/12	0.52	0.09	128,131,151,154	0
8	MAN	M	5	11/12	0.54	0.18	127,130,136,137	0
4	MAN	P	5	11/12	0.54	0.10	105,126,133,133	0
7	MAN	G	5	11/12	0.57	0.12	159,168,173,177	0
5	NAG	D	1	14/15	-	-	87,99,121,129	0
5	NAG	D	2	14/15	-	-	121,147,156,161	0
5	BMA	D	3	11/12	-	-	134,151,164,164	0
4	MAN	J	5	11/12	0.57	0.14	117,124,127,130	0
4	BMA	J	3	11/12	0.58	0.11	129,146,152,155	0
4	BMA	P	3	11/12	0.61	0.09	128,134,137,139	0
6	NAG	E	1	14/15	-	-	103,136,165,170	0
6	NAG	E	2	14/15	-	-	127,145,172,173	0
4	NAG	K	2	14/15	0.63	0.13	185,188,196,197	0
4	NAG	P	2	14/15	0.63	0.12	86,96,108,118	0
8	MAN	M	6	11/12	0.64	0.14	96,101,115,118	0
9	NAG	O	2	14/15	0.69	0.12	73,107,115,121	0
7	MAN	G	4	11/12	0.74	0.09	140,153,157,163	0
4	NAG	K	1	14/15	0.80	0.11	124,150,158,173	0
4	NAG	J	1	14/15	0.80	0.10	68,85,104,107	0
8	BMA	M	3	11/12	0.80	0.08	59,75,97,106	0
9	NAG	O	1	14/15	0.80	0.11	63,81,93,96	0
8	NAG	M	2	14/15	0.84	0.10	32,51,58,72	0
4	NAG	J	2	14/15	0.84	0.08	108,115,138,139	0
7	BMA	G	3	11/12	0.86	0.07	127,131,145,151	0
4	NAG	P	1	14/15	0.89	0.08	60,71,93,97	0
7	NAG	G	2	14/15	0.90	0.08	81,100,113,121	0
7	NAG	G	1	14/15	0.91	0.09	59,83,90,100	0

Continued on next page...

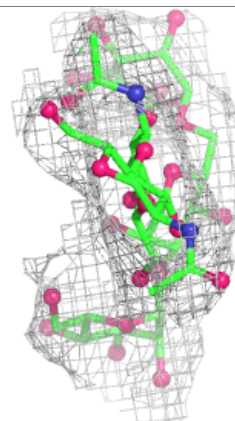
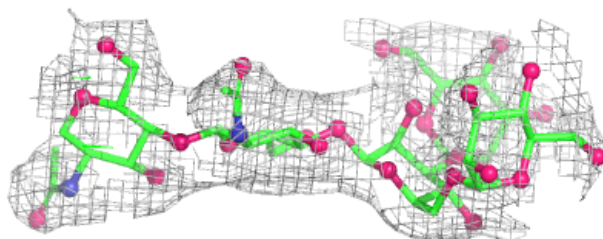
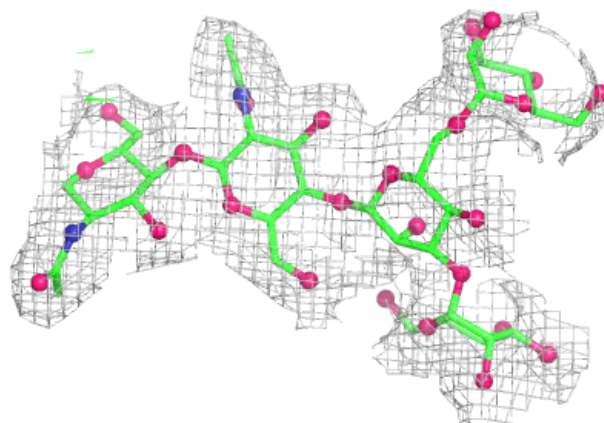
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	M	1	14/15	0.91	0.08	26,38,57,61	0

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

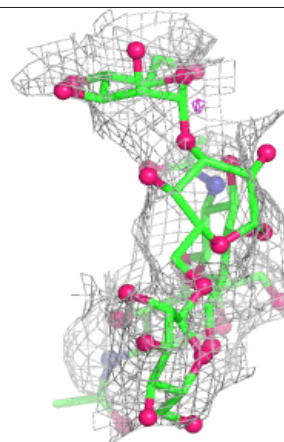
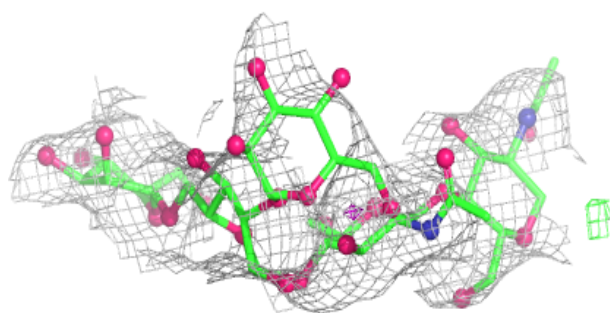
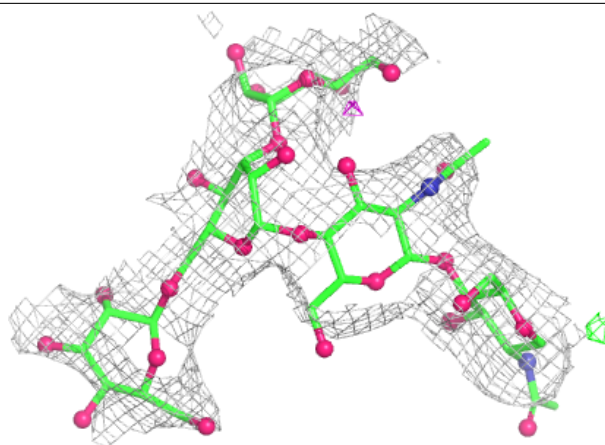
Electron density around Chain C:

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



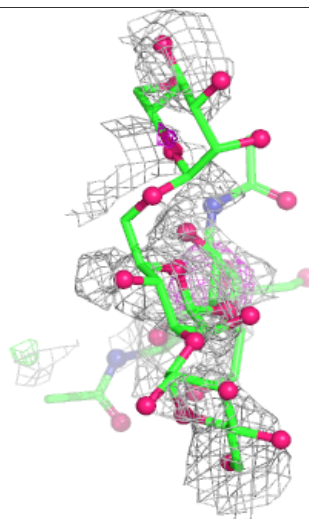
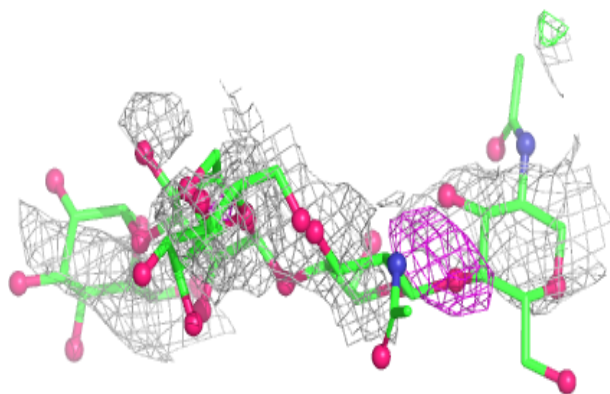
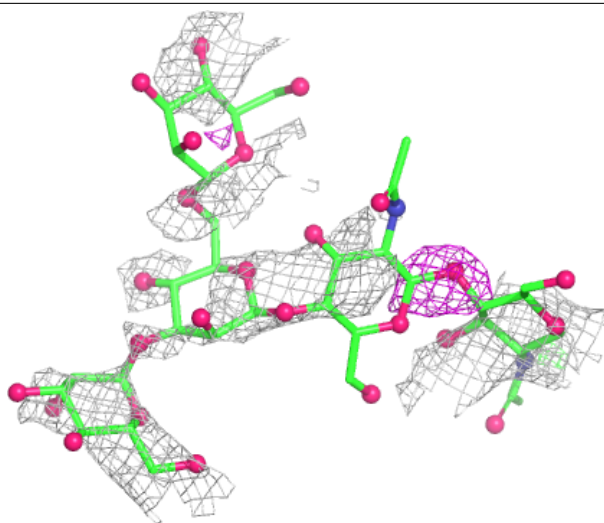
Electron density around Chain J:

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



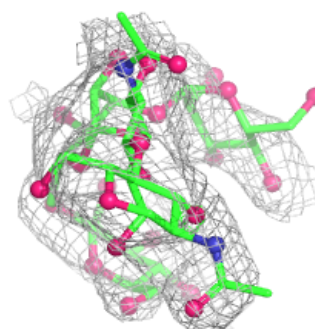
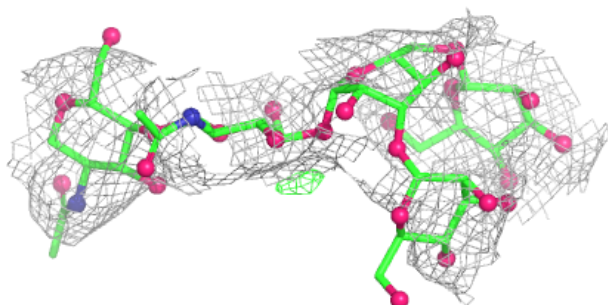
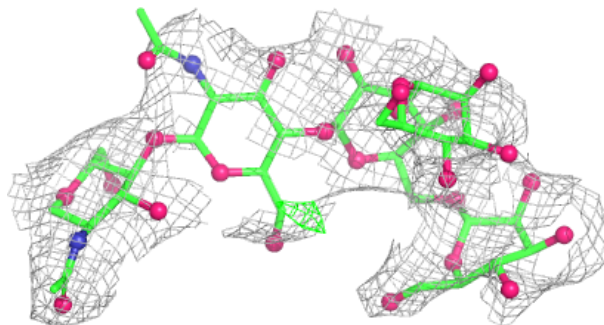
Electron density around Chain K:

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

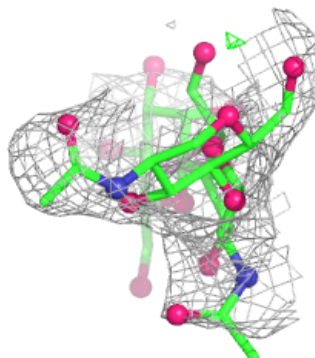
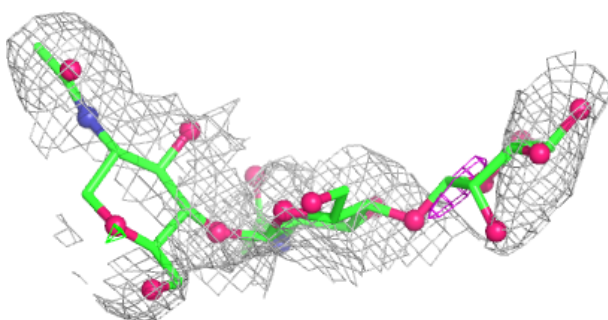
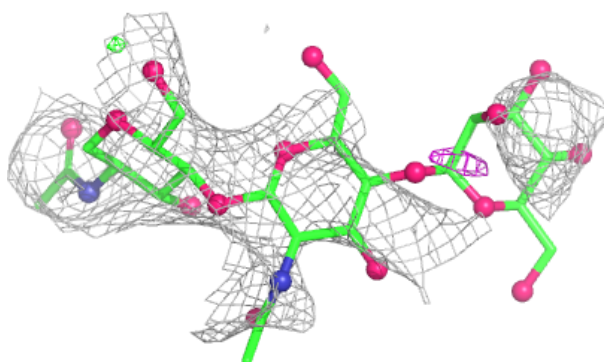


Electron density around Chain P:

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

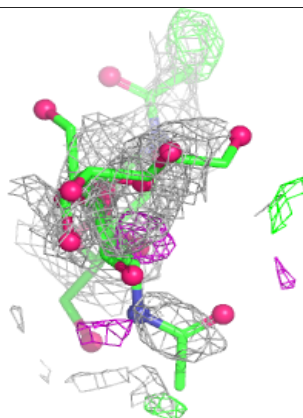
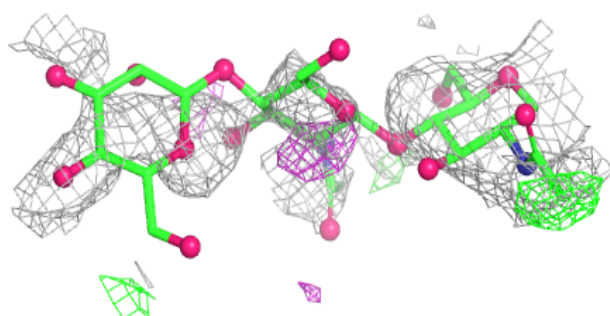
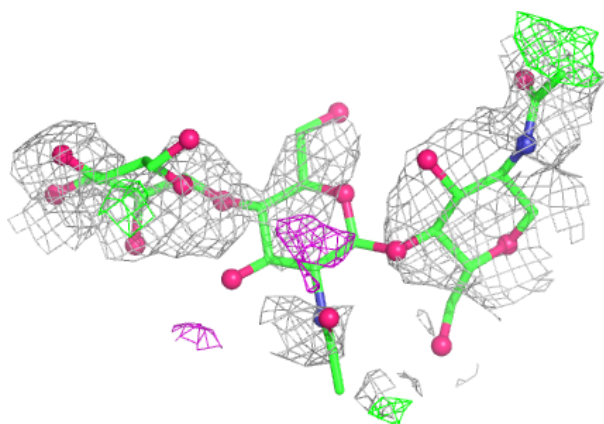
**Electron density around Chain D:**

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



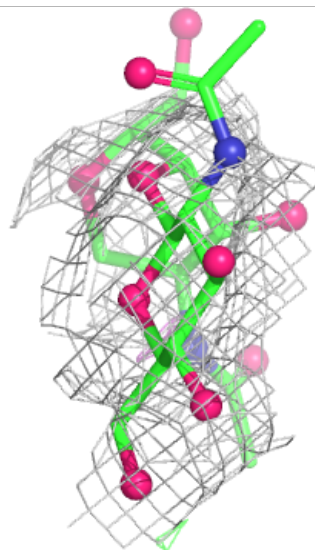
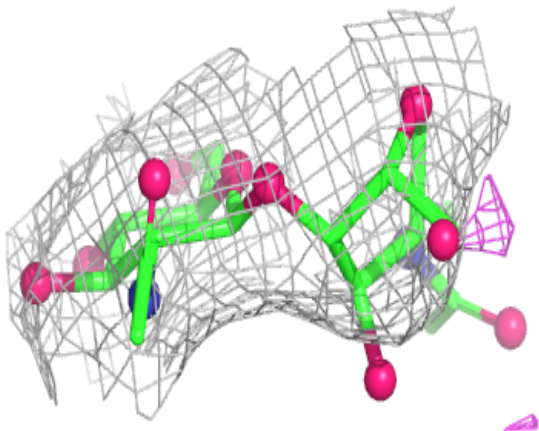
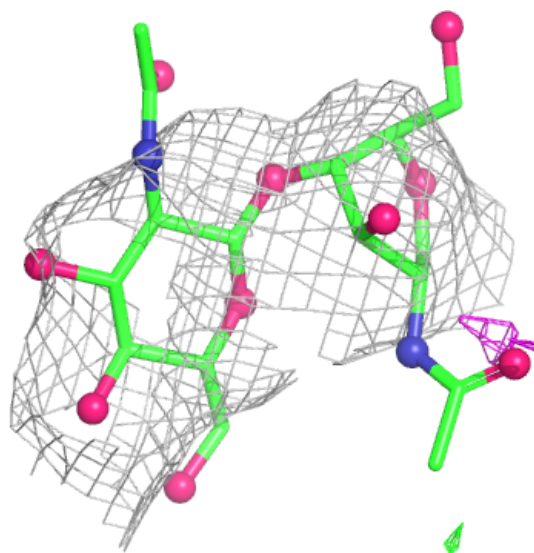
Electron density around Chain N:

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



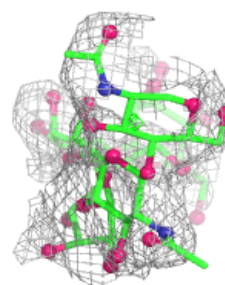
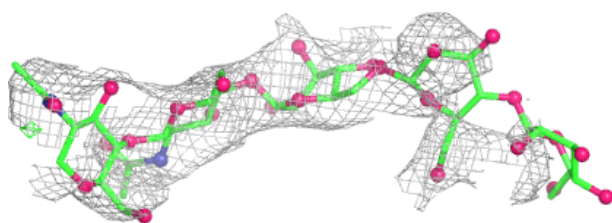
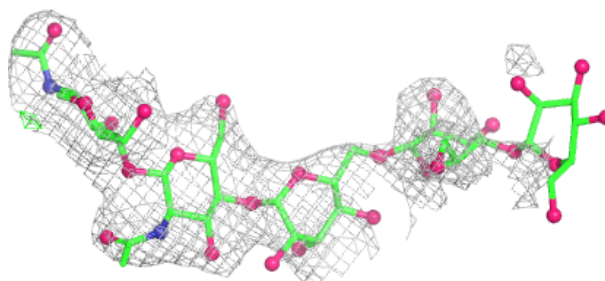
Electron density around Chain E:

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

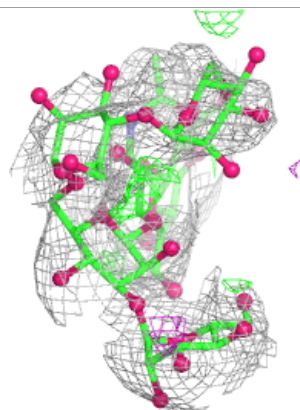
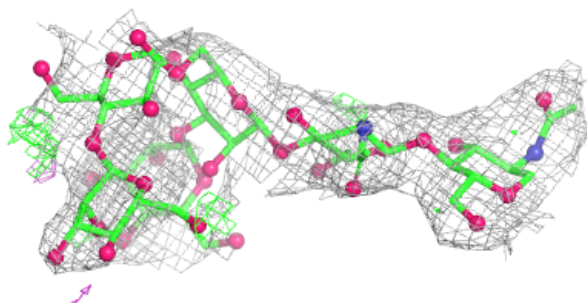
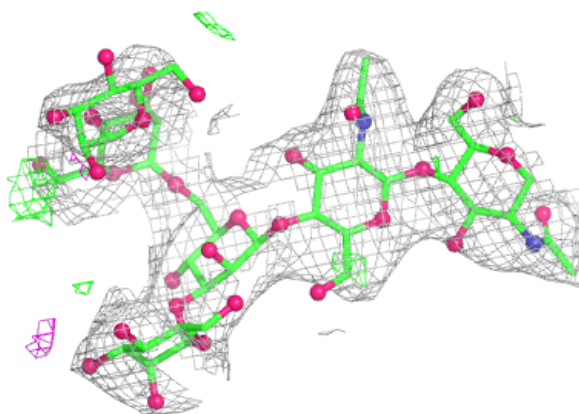


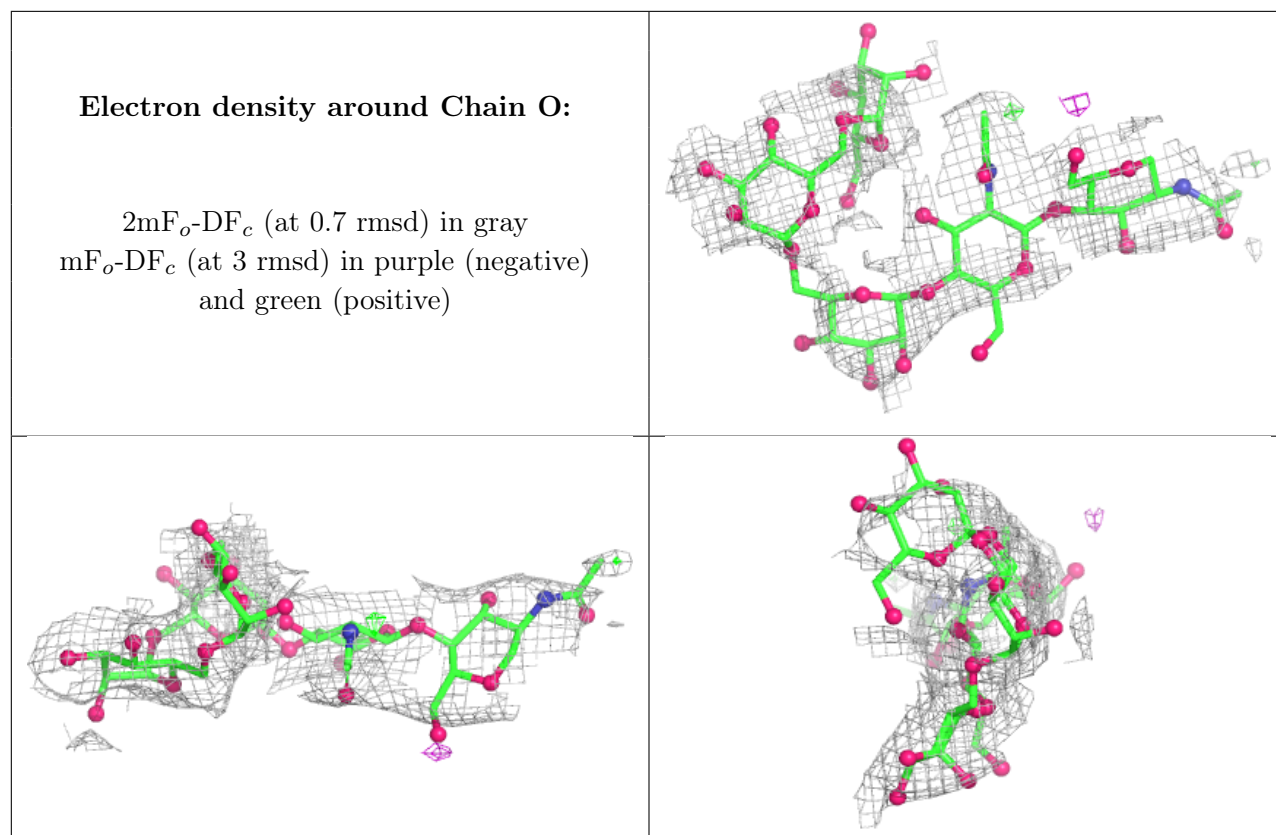
Electron density around Chain G:

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

**Electron density around Chain M:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	I	601	14/15	0.07	0.14	128,134,148,150	0
10	NAG	F	601	14/15	0.14	0.15	127,140,147,149	0
10	NAG	I	602	14/15	0.23	0.16	118,133,151,151	0
10	NAG	F	621	14/15	0.62	0.12	96,110,124,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.