



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 5JIF / pdb_00005jif
Title : Crystal structure of mouse hepatitis virus strain DVIM Hemagglutinin-Esterase
Authors : Zeng, Q.H.; Bakkers, M.J.G.; Feitsma, L.J.; de Groot, R.J.; Huizinga, E.G.
Deposited on : 2016-04-22
Resolution : 2.00 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

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

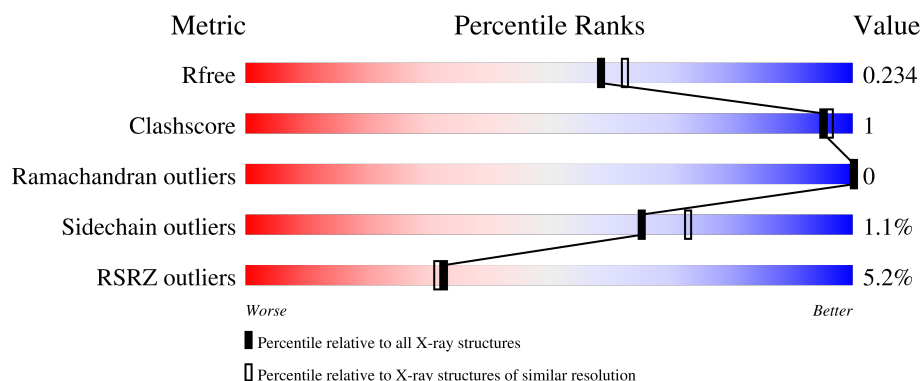
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



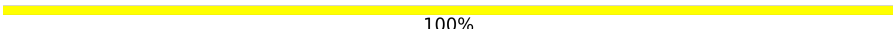
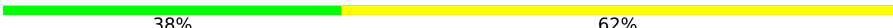
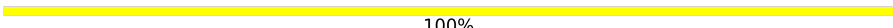
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	381	4% 92% 5%
1	B	381	5% 89% 7%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	 50%50%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 50%50%
3	F	8	 38%62%
4	G	5	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6394 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-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2889	1843	474	554	18			
1	B	355	Total	C	N	O	S	0	0	0
			2819	1797	465	539	18			

There are 18 discrepancies between the modelled and reference sequences:

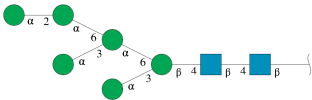
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LEU	-	expression tag	UNP O92367
A	23	ALA	-	expression tag	UNP O92367
A	396	SER	-	expression tag	UNP O92367
A	397	ASP	-	expression tag	UNP O92367
A	398	PRO	-	expression tag	UNP O92367
A	399	LEU	-	expression tag	UNP O92367
A	400	VAL	-	expression tag	UNP O92367
A	401	PRO	-	expression tag	UNP O92367
A	402	ARG	-	expression tag	UNP O92367
B	22	LEU	-	expression tag	UNP O92367
B	23	ALA	-	expression tag	UNP O92367
B	396	SER	-	expression tag	UNP O92367
B	397	ASP	-	expression tag	UNP O92367
B	398	PRO	-	expression tag	UNP O92367
B	399	LEU	-	expression tag	UNP O92367
B	400	VAL	-	expression tag	UNP O92367
B	401	PRO	-	expression tag	UNP O92367
B	402	ARG	-	expression tag	UNP O92367

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



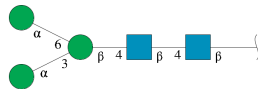
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
3	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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.

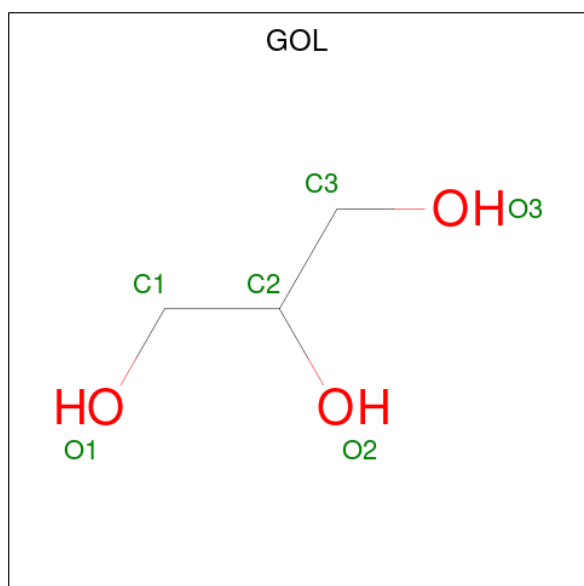


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

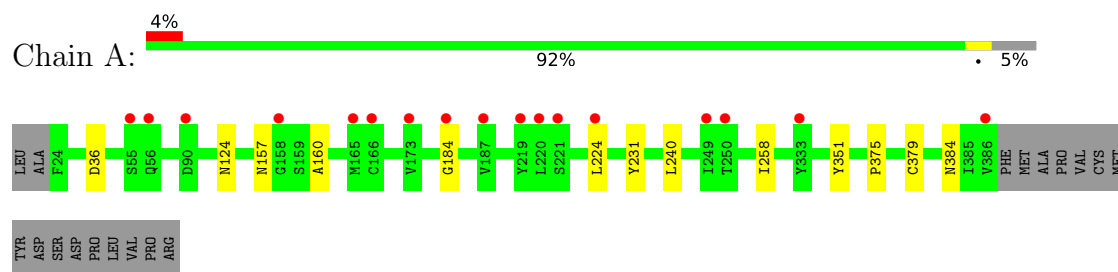
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	127	Total	O	0	0
			127	127		
8	B	96	Total	O	0	0
			96	96		

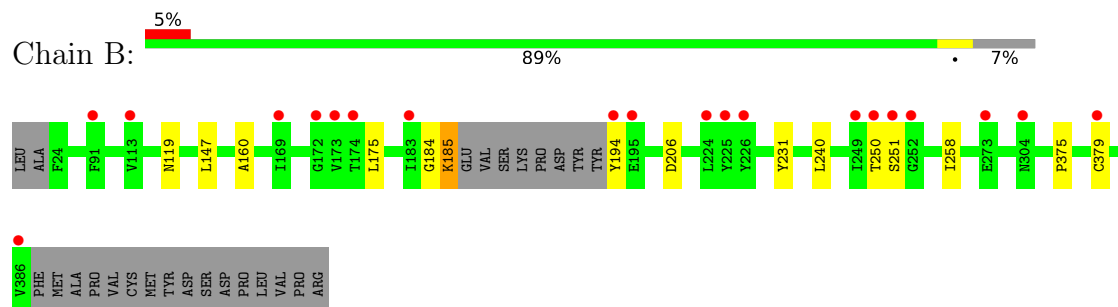
3 Residue-property plots [i](#)

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.

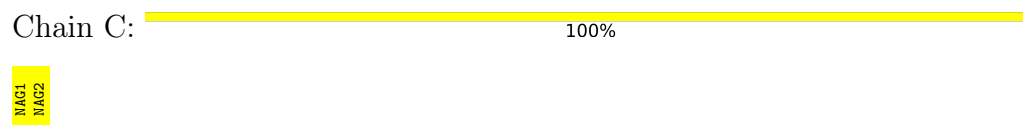
- Molecule 1: Hemagglutinin-esterase



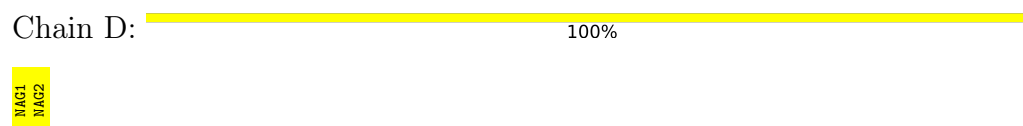
- Molecule 1: Hemagglutinin-esterase



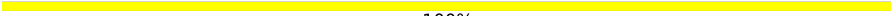
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain E:  100%

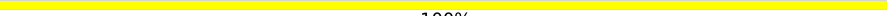
MAG1
MAG2

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

Chain H:  50% 50%

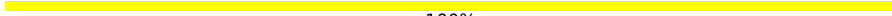
MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

Chain F:  38% 62%



- 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 G:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.52Å 88.82Å 122.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 2.00 39.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.73-2.00) 97.0 (39.73-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.226 0.215 , 0.234	Depositor DCC
R_{free} test set	3263 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6394	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GOL, NAG, NA, 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	0.72	0/2971	0.81	0/4047
1	B	0.67	0/2897	0.78	0/3944
All	All	0.70	0/5868	0.79	0/7991

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	2889	0	2696	7	0
1	B	2819	0	2634	7	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	F	94	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	61	0	52	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	12	0	16	0	0
7	A	42	0	39	3	0
7	B	28	0	26	0	0
8	A	127	0	0	0	0
8	B	96	0	0	1	0
All	All	6394	0	5742	14	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 1.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ALA:HB1	1:B:184:GLY:O	1.99	0.62
1:B:375:PRO:HB2	1:B:379:CYS:SG	2.46	0.55
1:A:375:PRO:HB2	1:A:379:CYS:SG	2.48	0.53
1:A:36:ASP:OD2	7:A:823:NAG:H3	2.09	0.52
1:B:250:THR:O	1:B:251:SER:C	2.53	0.51
1:B:231:TYR:HB3	1:B:240:LEU:HD11	1.96	0.47
1:A:160:ALA:HB1	1:A:184:GLY:O	2.15	0.47
1:A:231:TYR:HB3	1:A:240:LEU:HD11	1.96	0.46
1:A:157:ASN:OD1	7:A:807:NAG:H83	2.16	0.45
1:A:224:LEU:HD22	1:A:224:LEU:N	2.34	0.42
1:A:351:TYR:HA	7:A:823:NAG:H82	2.01	0.42
1:B:206:ASP:OD1	8:B:901:HOH:O	2.21	0.41
1:B:185:LYS:HA	1:B:194:TYR:CD1	2.56	0.41
1:B:147:LEU:C	1:B:147:LEU:HD23	2.46	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	361/381 (95%)	351 (97%)	10 (3%)	0	100	100
1	B	351/381 (92%)	337 (96%)	14 (4%)	0	100	100
All	All	712/762 (93%)	688 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	320/336 (95%)	317 (99%)	3 (1%)	70	78
1	B	312/336 (93%)	308 (99%)	4 (1%)	61	68
All	All	632/672 (94%)	625 (99%)	7 (1%)	65	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	258	ILE
1	A	384	ASN
1	B	119	ASN
1	B	175	LEU
1	B	185	LYS
1	B	258	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	218	GLN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	358	GLN
1	B	119	ASN
1	B	136	GLN
1	B	143	HIS
1	B	330	ASN
1	B	358	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues 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	G	1	1,4	14,14,15	0.93	0	17,19,21	1.06	1 (5%)
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	1.24	2 (11%)
7	NAG	A	823	1	14,14,15	0.56	0	17,19,21	1.51	2 (11%)
2	NAG	I	2	2	14,14,15	0.60	0	17,19,21	1.37	2 (11%)
2	NAG	C	1	2,1	14,14,15	0.60	0	17,19,21	1.34	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.47	0	17,19,21	1.05	2 (11%)
3	MAN	F	8	3	11,11,12	0.98	1 (9%)	15,15,17	1.12	1 (6%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	1.52	1 (5%)
7	NAG	B	802	1	14,14,15	0.94	1 (7%)	17,19,21	1.54	5 (29%)
4	MAN	G	5	4	11,11,12	0.96	1 (9%)	15,15,17	1.97	3 (20%)
2	NAG	J	1	2,1	14,14,15	0.55	0	17,19,21	1.21	3 (17%)
2	NAG	H	1	2,1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
3	MAN	F	5	3	11,11,12	0.56	0	15,15,17	1.75	3 (20%)
7	NAG	A	807	1	14,14,15	0.53	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	6	3	11,11,12	0.57	0	15,15,17	0.65	0
7	NAG	A	824	1	14,14,15	0.53	0	17,19,21	1.76	5 (29%)
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	1.37	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.75	0	17,19,21	1.19	0
2	NAG	J	2	2	14,14,15	0.79	0	17,19,21	1.47	3 (17%)
4	NAG	G	2	4	14,14,15	0.63	0	17,19,21	1.73	4 (23%)
2	NAG	L	2	2	14,14,15	0.44	0	17,19,21	1.27	1 (5%)
4	MAN	G	4	4	11,11,12	0.63	0	15,15,17	1.28	3 (20%)
7	NAG	B	807	1	14,14,15	0.56	0	17,19,21	1.74	6 (35%)
2	NAG	L	1	2,1	14,14,15	0.63	0	17,19,21	0.93	0
2	NAG	K	2	2	14,14,15	0.51	0	17,19,21	1.69	6 (35%)
2	NAG	E	1	2,1	14,14,15	0.66	0	17,19,21	1.24	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.62	0	17,19,21	1.13	2 (11%)
2	NAG	K	1	2,1	14,14,15	0.58	0	17,19,21	1.33	1 (5%)
3	MAN	F	7	3	11,11,12	0.78	0	15,15,17	1.30	3 (20%)
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.55	1 (5%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.04	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
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
7	NAG	A	823	1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
7	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	807	1	-	0/6/23/26	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
7	NAG	A	824	1	-	2/6/23/26	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
7	NAG	B	807	1	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	802	NAG	O5-C1	-2.92	1.38	1.43
4	G	5	MAN	C2-C3	2.47	1.56	1.52
3	F	8	MAN	C2-C3	2.09	1.55	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	MAN	C1-C2-C3	5.98	118.35	109.64
2	C	2	NAG	C1-O5-C5	4.92	118.78	112.19
7	A	823	NAG	C1-O5-C5	4.75	118.55	112.19
3	F	4	MAN	C1-O5-C5	4.64	118.41	112.19
3	F	5	MAN	C1-O5-C5	4.46	118.17	112.19
4	G	2	NAG	C1-O5-C5	-4.25	106.48	112.19
3	F	2	NAG	C1-O5-C5	-4.07	106.73	112.19
7	A	824	NAG	C1-C2-N2	3.98	116.71	110.43
2	K	2	NAG	C1-O5-C5	3.40	116.74	112.19
4	G	2	NAG	O5-C1-C2	-3.35	106.10	111.29
7	B	807	NAG	C1-C2-N2	3.26	115.56	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	4	MAN	C1-O5-C5	3.21	116.49	112.19
7	B	807	NAG	O5-C5-C6	3.17	113.82	107.66
2	J	2	NAG	C2-N2-C7	3.01	126.93	122.90
2	D	1	NAG	C3-C4-C5	-2.98	104.84	110.23
2	K	2	NAG	C2-N2-C7	2.96	126.87	122.90
3	F	5	MAN	C6-C5-C4	-2.94	105.79	113.02
7	B	807	NAG	O7-C7-C8	-2.93	116.83	122.05
2	E	2	NAG	C4-C3-C2	2.89	115.25	111.02
2	D	2	NAG	C1-O5-C5	2.85	116.01	112.19
2	E	2	NAG	O5-C1-C2	-2.79	106.98	111.29
3	F	7	MAN	C2-C3-C4	-2.71	106.10	110.86
7	A	824	NAG	C3-C4-C5	-2.70	105.33	110.23
4	G	2	NAG	C4-C3-C2	2.68	114.95	111.02
2	E	1	NAG	C1-O5-C5	2.63	115.71	112.19
3	F	8	MAN	C2-C3-C4	2.63	115.49	110.86
2	I	2	NAG	C2-N2-C7	-2.63	119.38	122.90
3	F	5	MAN	O5-C5-C4	2.61	117.18	110.83
2	K	1	NAG	O5-C1-C2	-2.60	107.27	111.29
7	A	824	NAG	O5-C5-C6	2.58	112.69	107.66
2	I	2	NAG	O5-C1-C2	-2.55	107.35	111.29
7	B	807	NAG	C6-C5-C4	-2.52	106.82	113.02
7	B	802	NAG	C1-C2-N2	-2.51	106.48	110.43
2	C	1	NAG	C3-C4-C5	-2.51	105.69	110.23
2	L	2	NAG	O7-C7-C8	-2.50	117.60	122.05
2	J	1	NAG	C3-C4-C5	-2.50	105.69	110.23
2	J	2	NAG	O7-C7-N2	2.44	126.28	121.98
2	J	2	NAG	C1-C2-N2	-2.41	106.63	110.43
7	A	823	NAG	C4-C3-C2	-2.40	107.50	111.02
2	I	1	NAG	C1-O5-C5	2.36	115.36	112.19
2	J	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	K	2	NAG	C3-C4-C5	-2.34	105.98	110.23
4	G	4	MAN	O2-C2-C3	2.34	115.00	110.15
2	I	1	NAG	O3-C3-C2	-2.29	104.64	109.40
7	A	807	NAG	O3-C3-C2	-2.29	104.65	109.40
2	C	1	NAG	O7-C7-C8	-2.22	118.10	122.05
7	B	807	NAG	O5-C1-C2	-2.22	107.86	111.29
7	B	802	NAG	O5-C5-C6	-2.22	103.35	107.66
3	F	7	MAN	O5-C5-C6	2.21	111.96	107.66
2	H	1	NAG	O5-C1-C2	2.20	114.69	111.29
3	F	7	MAN	O4-C4-C3	-2.18	105.23	110.38
7	B	802	NAG	O6-C6-C5	-2.18	103.90	111.33
7	A	824	NAG	O3-C3-C2	-2.17	104.90	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	2.15	125.78	122.90
2	D	2	NAG	C3-C4-C5	-2.15	106.34	110.23
7	A	807	NAG	O4-C4-C5	2.15	114.62	109.32
2	K	2	NAG	O4-C4-C5	2.15	114.61	109.32
4	G	2	NAG	C3-C4-C5	2.15	114.12	110.23
2	J	1	NAG	C4-C3-C2	-2.14	107.89	111.02
2	K	2	NAG	O7-C7-C8	-2.12	118.28	122.05
7	B	802	NAG	O3-C3-C4	2.10	115.33	110.38
7	A	824	NAG	O7-C7-C8	-2.09	118.33	122.05
2	K	2	NAG	O5-C1-C2	2.08	114.52	111.29
2	D	1	NAG	O5-C1-C2	-2.08	108.07	111.29
4	G	1	NAG	C4-C3-C2	-2.07	107.98	111.02
2	E	1	NAG	C4-C3-C2	2.06	114.03	111.02
7	B	807	NAG	C8-C7-N2	2.04	119.51	116.12
7	B	802	NAG	C3-C4-C5	-2.04	106.53	110.23
4	G	5	MAN	C3-C4-C5	-2.04	106.54	110.23
4	G	5	MAN	O6-C6-C5	-2.02	104.44	111.33
4	G	4	MAN	O3-C3-C2	2.01	114.16	110.05

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	7	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
7	A	824	NAG	O5-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
7	B	807	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
7	A	824	NAG	C4-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6
7	A	823	NAG	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
7	B	807	NAG	C4-C5-C6-O6
7	A	823	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	823	NAG	2	0
7	A	807	NAG	1	0

5.5 Carbohydrates [i](#)

29 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.60	0	17,19,21	1.34	3 (17%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	1.52	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.62	0	17,19,21	1.13	2 (11%)
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	1.24	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.66	0	17,19,21	1.24	2 (11%)
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.75	0	17,19,21	1.19	0
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.55	1 (5%)
3	BMA	F	3	3	11,11,12	0.48	0	15,15,17	0.88	0
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	1.37	1 (6%)
3	MAN	F	5	3	11,11,12	0.56	0	15,15,17	1.75	3 (20%)
3	MAN	F	6	3	11,11,12	0.57	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	7	3	11,11,12	0.78	0	15,15,17	1.30	3 (20%)
3	MAN	F	8	3	11,11,12	0.98	1 (9%)	15,15,17	1.12	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.93	0	17,19,21	1.06	1 (5%)
4	NAG	G	2	4	14,14,15	0.63	0	17,19,21	1.73	4 (23%)
4	BMA	G	3	4	11,11,12	0.72	0	15,15,17	1.04	1 (6%)
4	MAN	G	4	4	11,11,12	0.63	0	15,15,17	1.28	3 (20%)
4	MAN	G	5	4	11,11,12	0.96	1 (9%)	15,15,17	1.97	3 (20%)
2	NAG	H	1	2,1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.04	0
2	NAG	I	1	2,1	14,14,15	0.47	0	17,19,21	1.05	2 (11%)
2	NAG	I	2	2	14,14,15	0.60	0	17,19,21	1.37	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.55	0	17,19,21	1.21	3 (17%)
2	NAG	J	2	2	14,14,15	0.79	0	17,19,21	1.47	3 (17%)
2	NAG	K	1	2,1	14,14,15	0.58	0	17,19,21	1.33	1 (5%)
2	NAG	K	2	2	14,14,15	0.51	0	17,19,21	1.69	6 (35%)
2	NAG	L	1	2,1	14,14,15	0.63	0	17,19,21	0.93	0
2	NAG	L	2	2	14,14,15	0.44	0	17,19,21	1.27	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	MAN	C2-C3	2.47	1.56	1.52
3	F	8	MAN	C2-C3	2.09	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	MAN	C1-C2-C3	5.98	118.35	109.64
2	C	2	NAG	C1-O5-C5	4.92	118.78	112.19
3	F	4	MAN	C1-O5-C5	4.64	118.41	112.19
3	F	5	MAN	C1-O5-C5	4.46	118.17	112.19
4	G	2	NAG	C1-O5-C5	-4.25	106.48	112.19
3	F	2	NAG	C1-O5-C5	-4.07	106.73	112.19
2	K	2	NAG	C1-O5-C5	3.40	116.74	112.19
4	G	2	NAG	O5-C1-C2	-3.35	106.10	111.29
4	G	4	MAN	C1-O5-C5	3.21	116.49	112.19
4	G	3	BMA	O5-C5-C6	3.07	113.64	107.66
2	J	2	NAG	C2-N2-C7	3.01	126.93	122.90
2	D	1	NAG	C3-C4-C5	-2.98	104.84	110.23
2	K	2	NAG	C2-N2-C7	2.96	126.87	122.90
3	F	5	MAN	C6-C5-C4	-2.94	105.79	113.02
2	E	2	NAG	C4-C3-C2	2.89	115.25	111.02
2	D	2	NAG	C1-O5-C5	2.85	116.01	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	O5-C1-C2	-2.79	106.98	111.29
3	F	7	MAN	C2-C3-C4	-2.71	106.10	110.86
4	G	2	NAG	C4-C3-C2	2.68	114.95	111.02
2	E	1	NAG	C1-O5-C5	2.63	115.71	112.19
3	F	8	MAN	C2-C3-C4	2.63	115.49	110.86
2	I	2	NAG	C2-N2-C7	-2.63	119.38	122.90
3	F	5	MAN	O5-C5-C4	2.61	117.18	110.83
2	K	1	NAG	O5-C1-C2	-2.60	107.27	111.29
2	I	2	NAG	O5-C1-C2	-2.55	107.35	111.29
2	C	1	NAG	C3-C4-C5	-2.51	105.69	110.23
2	L	2	NAG	O7-C7-C8	-2.50	117.60	122.05
2	J	1	NAG	C3-C4-C5	-2.50	105.69	110.23
2	J	2	NAG	O7-C7-N2	2.44	126.28	121.98
2	J	2	NAG	C1-C2-N2	-2.41	106.63	110.43
2	I	1	NAG	C1-O5-C5	2.36	115.36	112.19
2	J	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	K	2	NAG	C3-C4-C5	-2.34	105.98	110.23
4	G	4	MAN	O2-C2-C3	2.34	115.00	110.15
2	I	1	NAG	O3-C3-C2	-2.29	104.64	109.40
2	C	1	NAG	O7-C7-C8	-2.22	118.10	122.05
3	F	7	MAN	O5-C5-C6	2.21	111.96	107.66
2	H	1	NAG	O5-C1-C2	2.20	114.69	111.29
3	F	7	MAN	O4-C4-C3	-2.18	105.23	110.38
2	C	1	NAG	C2-N2-C7	2.15	125.78	122.90
2	D	2	NAG	C3-C4-C5	-2.15	106.34	110.23
2	K	2	NAG	O4-C4-C5	2.15	114.61	109.32
4	G	2	NAG	C3-C4-C5	2.15	114.12	110.23
2	J	1	NAG	C4-C3-C2	-2.14	107.89	111.02
2	K	2	NAG	O7-C7-C8	-2.12	118.28	122.05
2	K	2	NAG	O5-C1-C2	2.08	114.52	111.29
2	D	1	NAG	O5-C1-C2	-2.08	108.07	111.29
4	G	1	NAG	C4-C3-C2	-2.07	107.98	111.02
2	E	1	NAG	C4-C3-C2	2.06	114.03	111.02
4	G	5	MAN	C3-C4-C5	-2.04	106.54	110.23
4	G	5	MAN	O6-C6-C5	-2.02	104.44	111.33
4	G	4	MAN	O3-C3-C2	2.01	114.16	110.05

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	7	MAN	O5-C5-C6-O6

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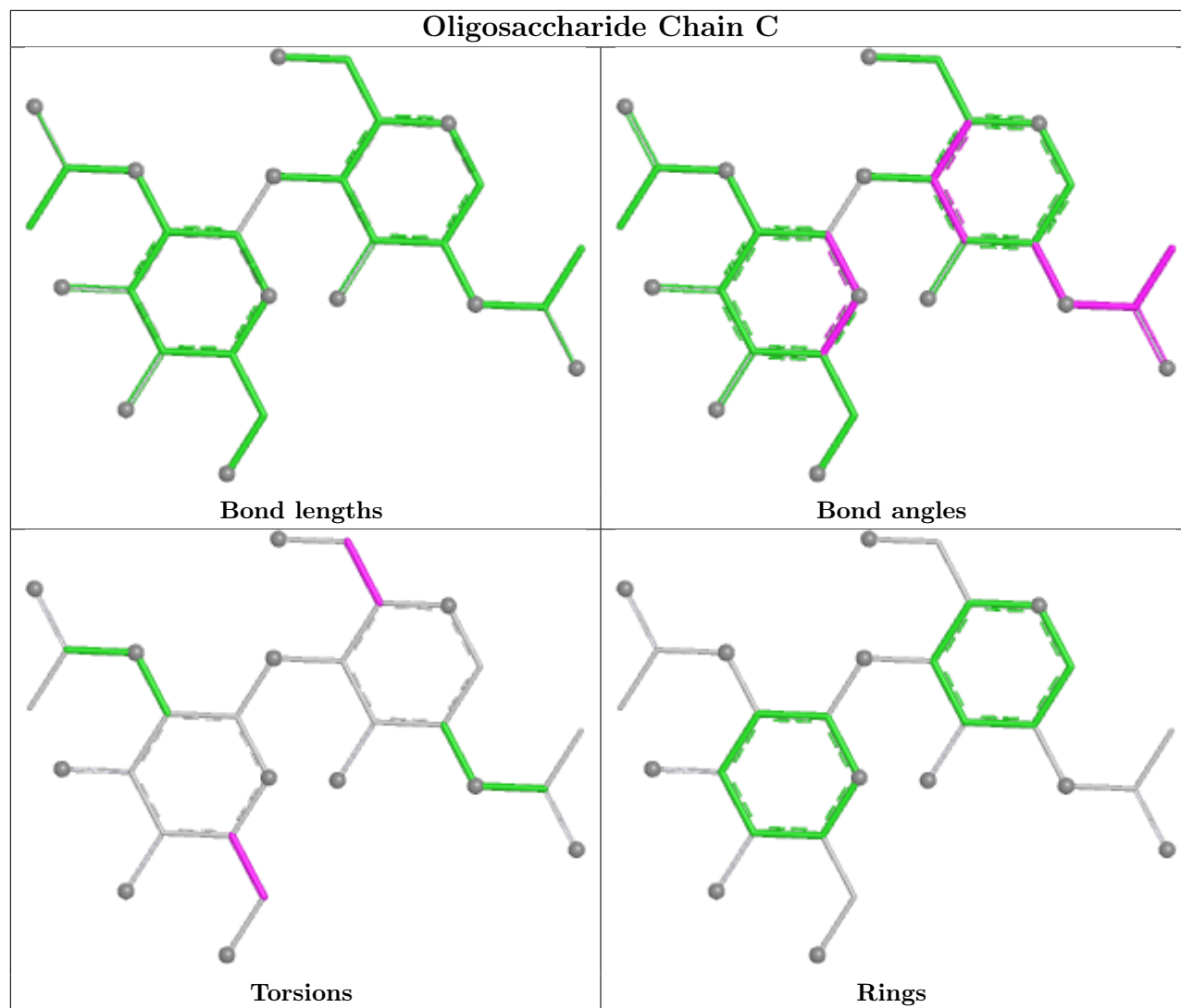
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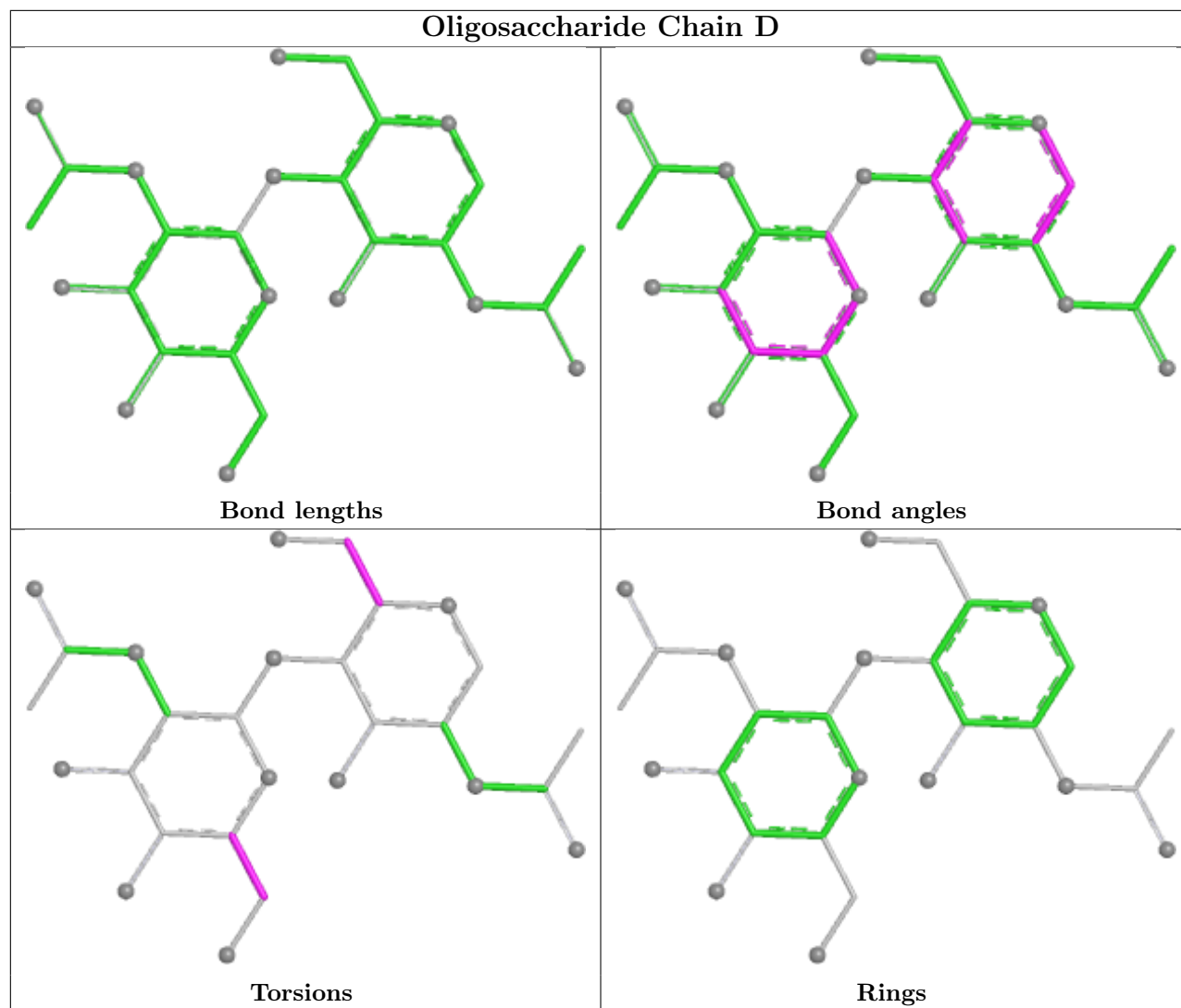
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

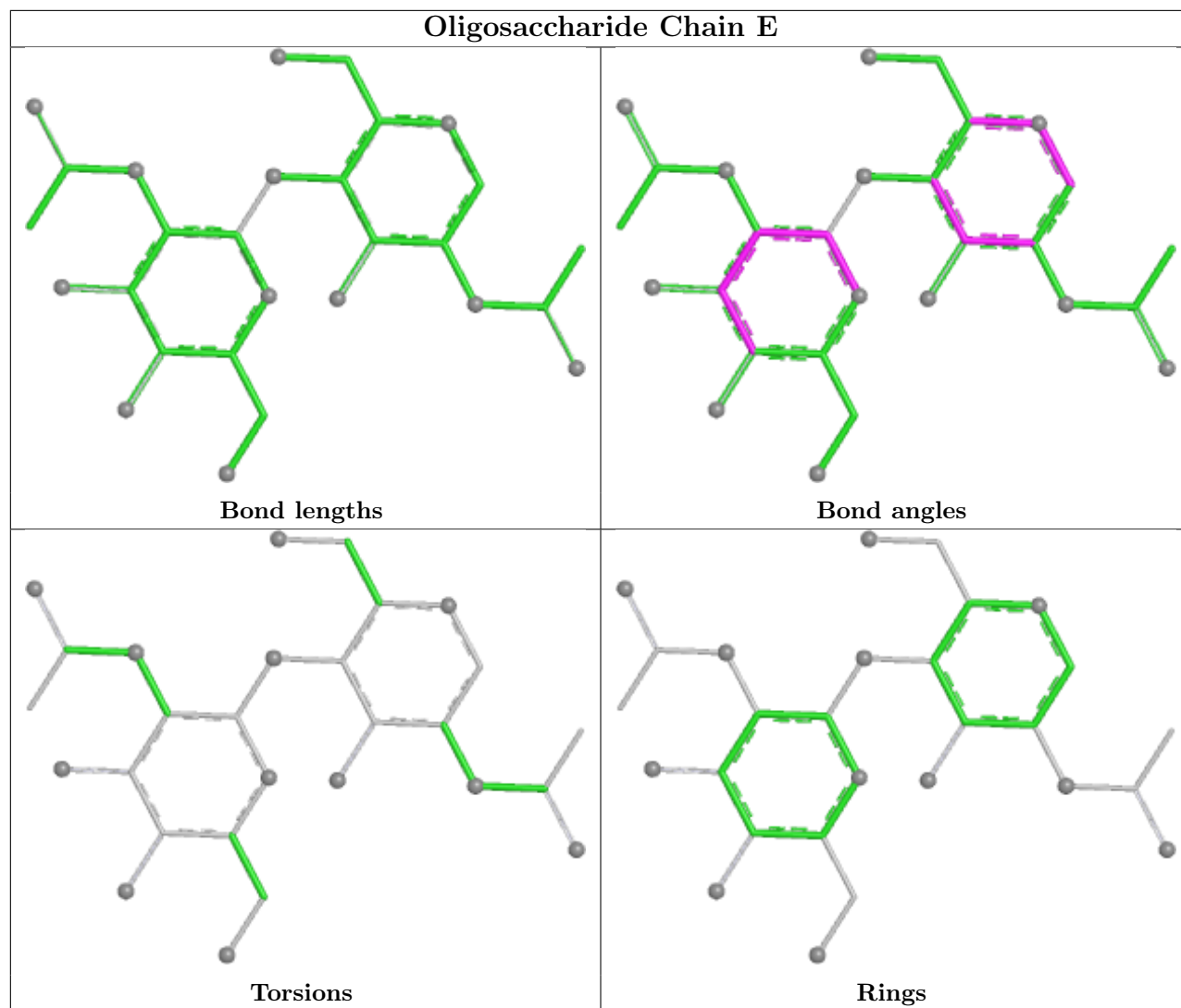
There are no ring outliers.

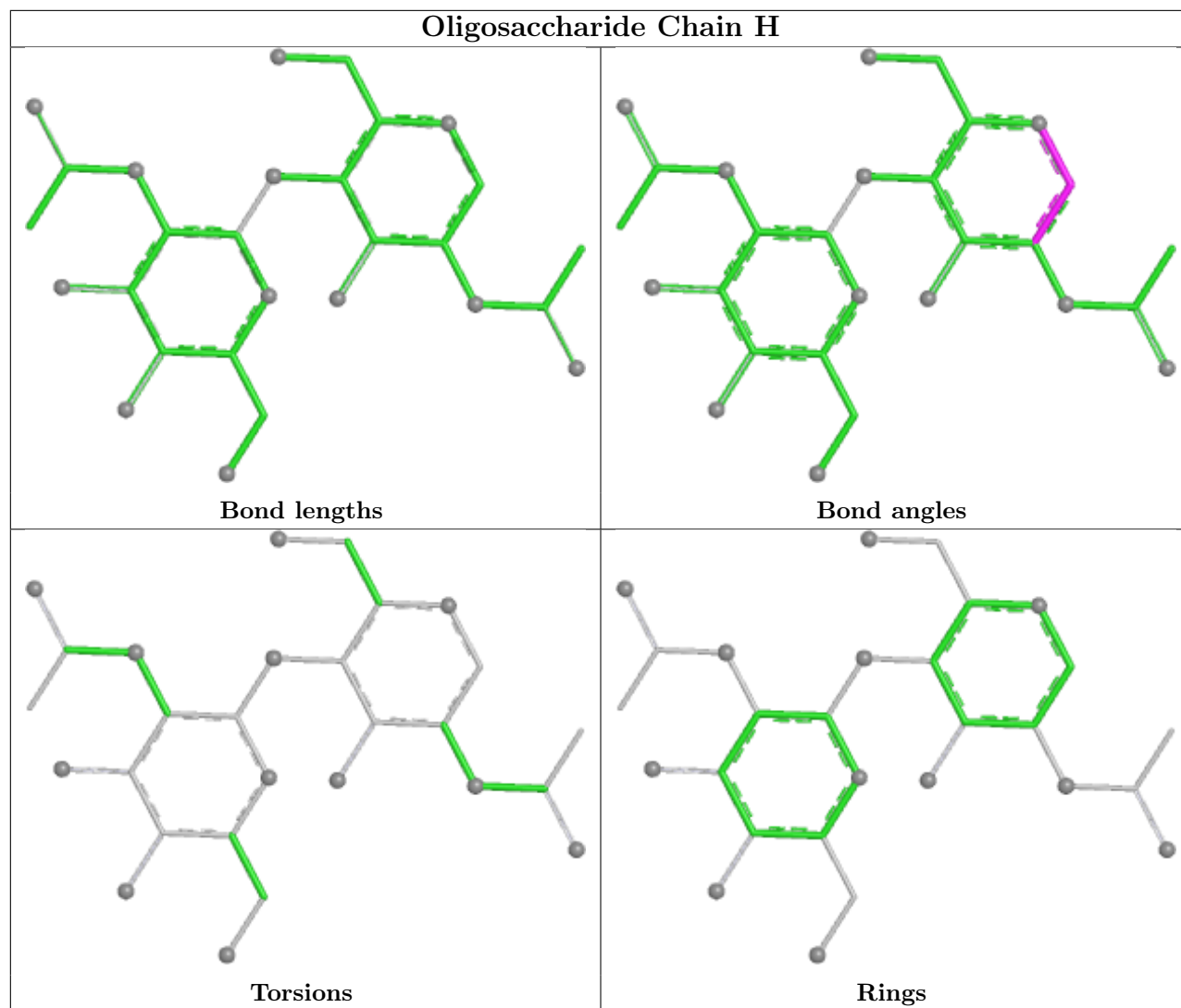
No monomer is involved in short contacts.

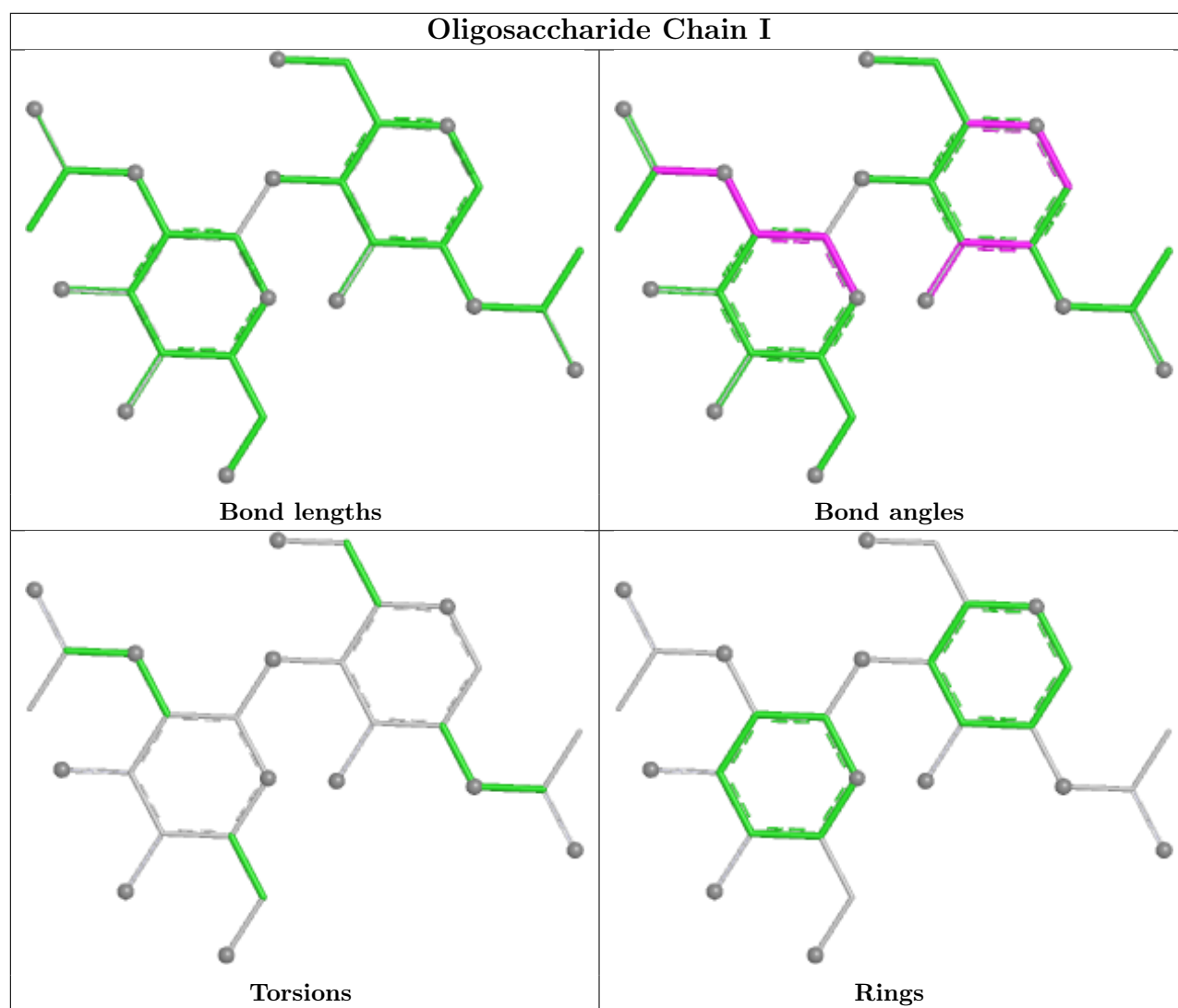
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

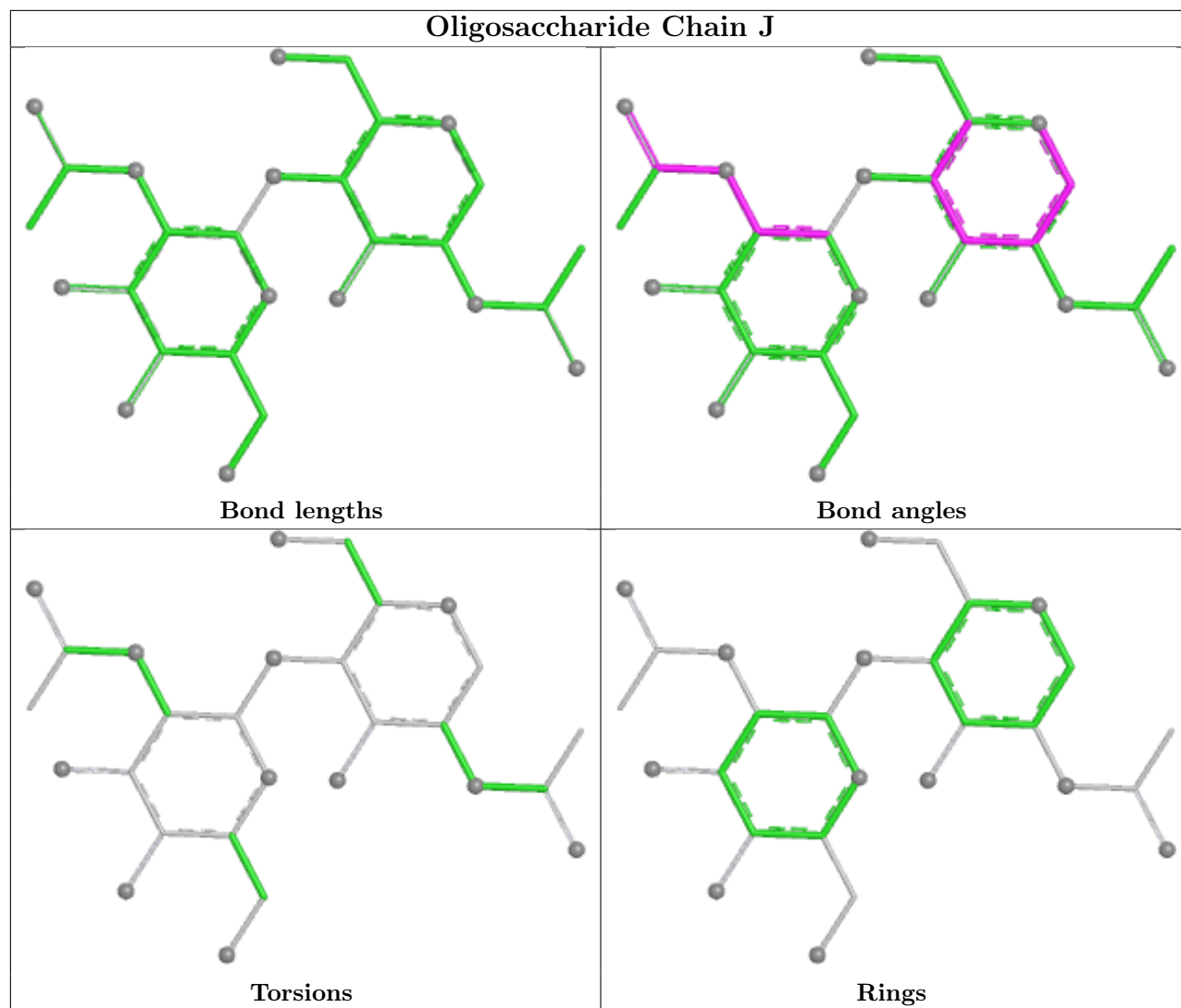


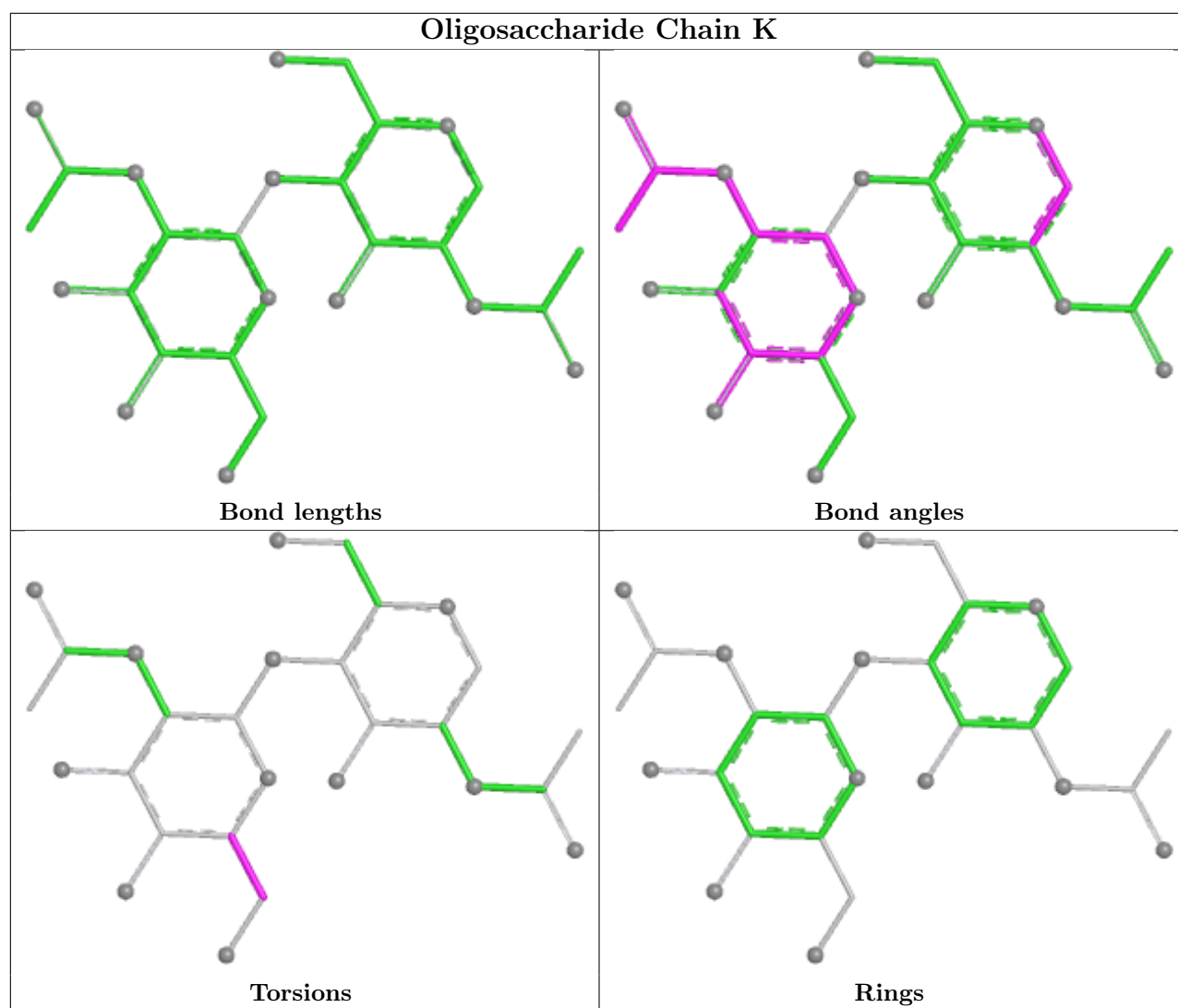


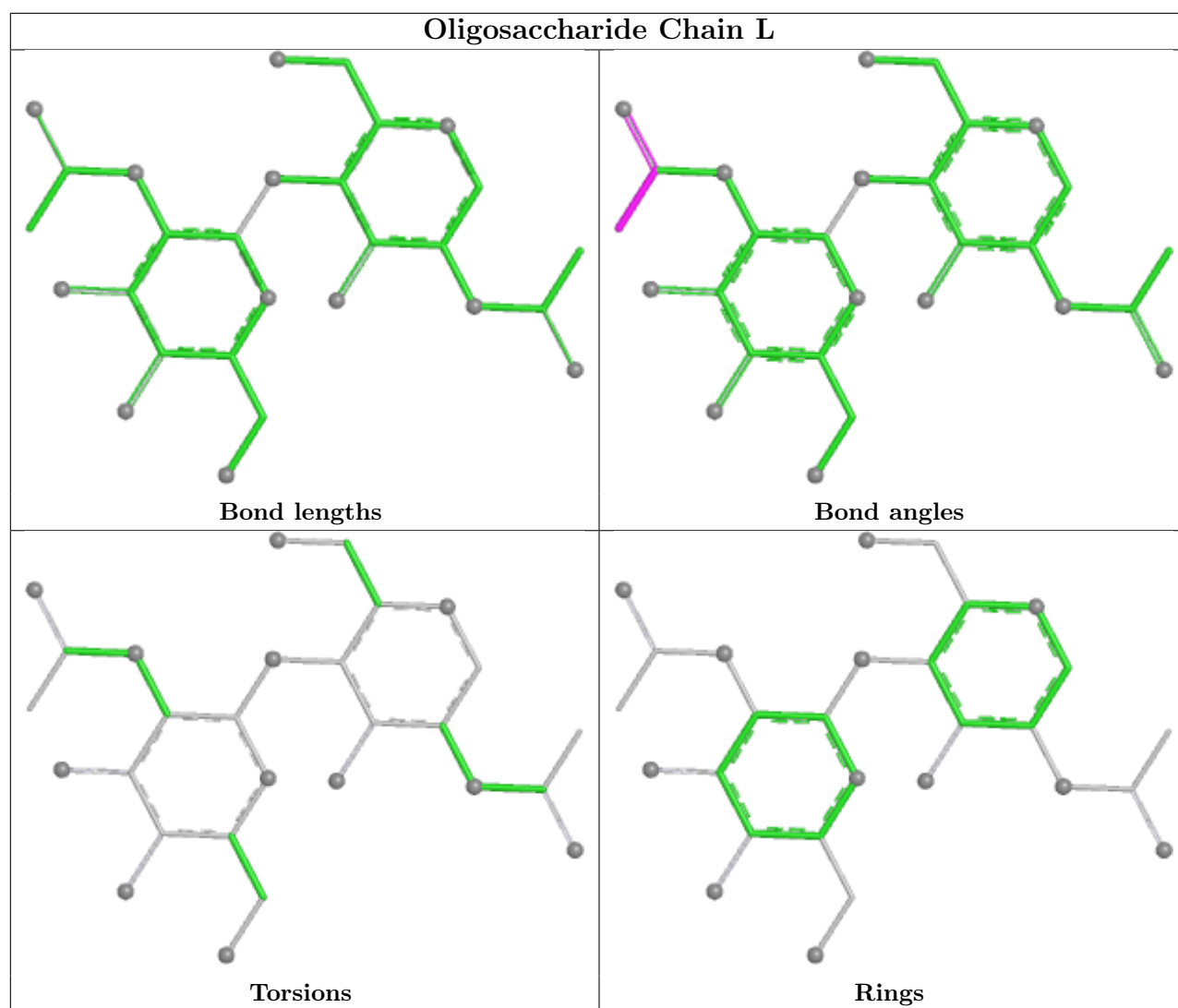


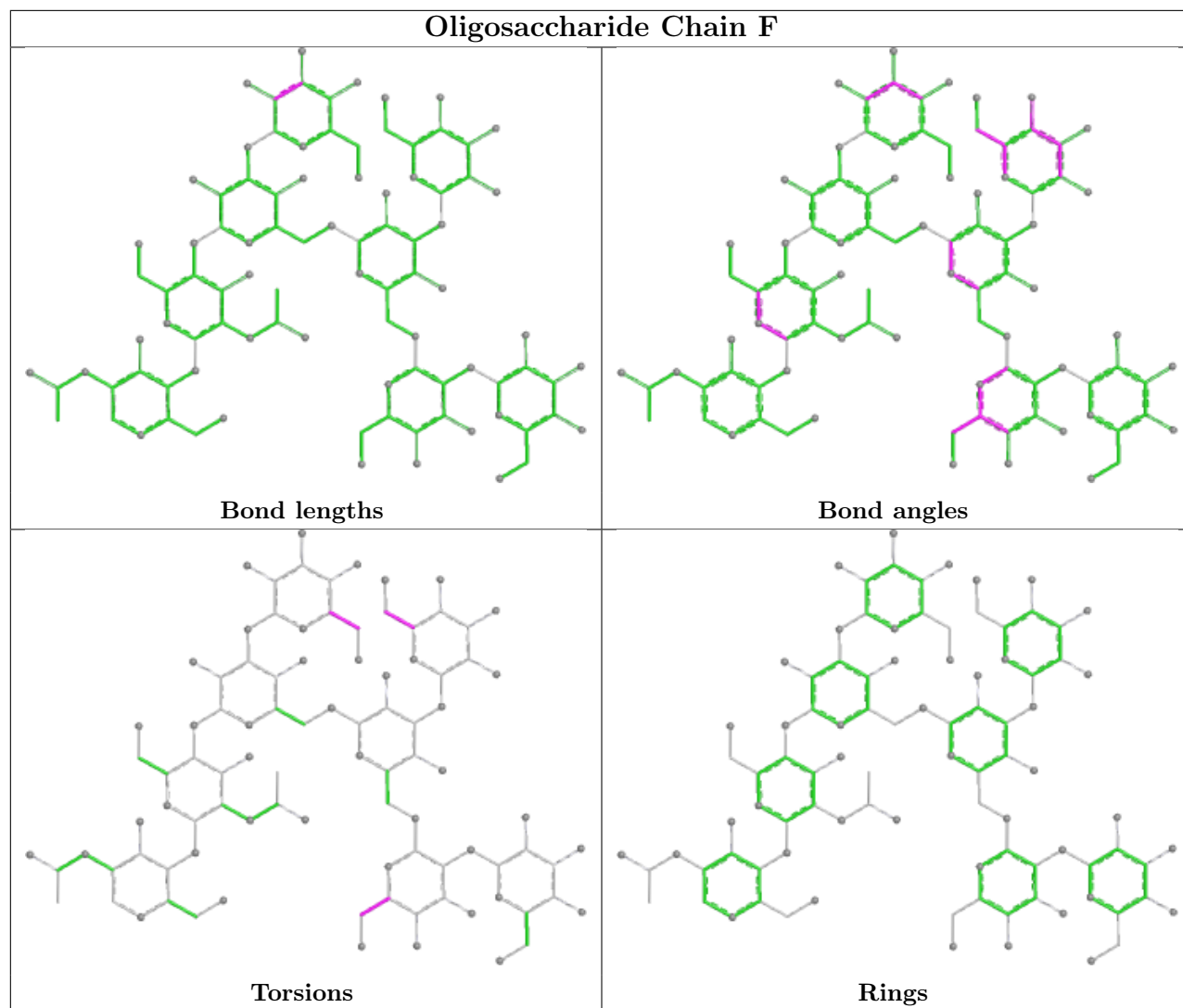


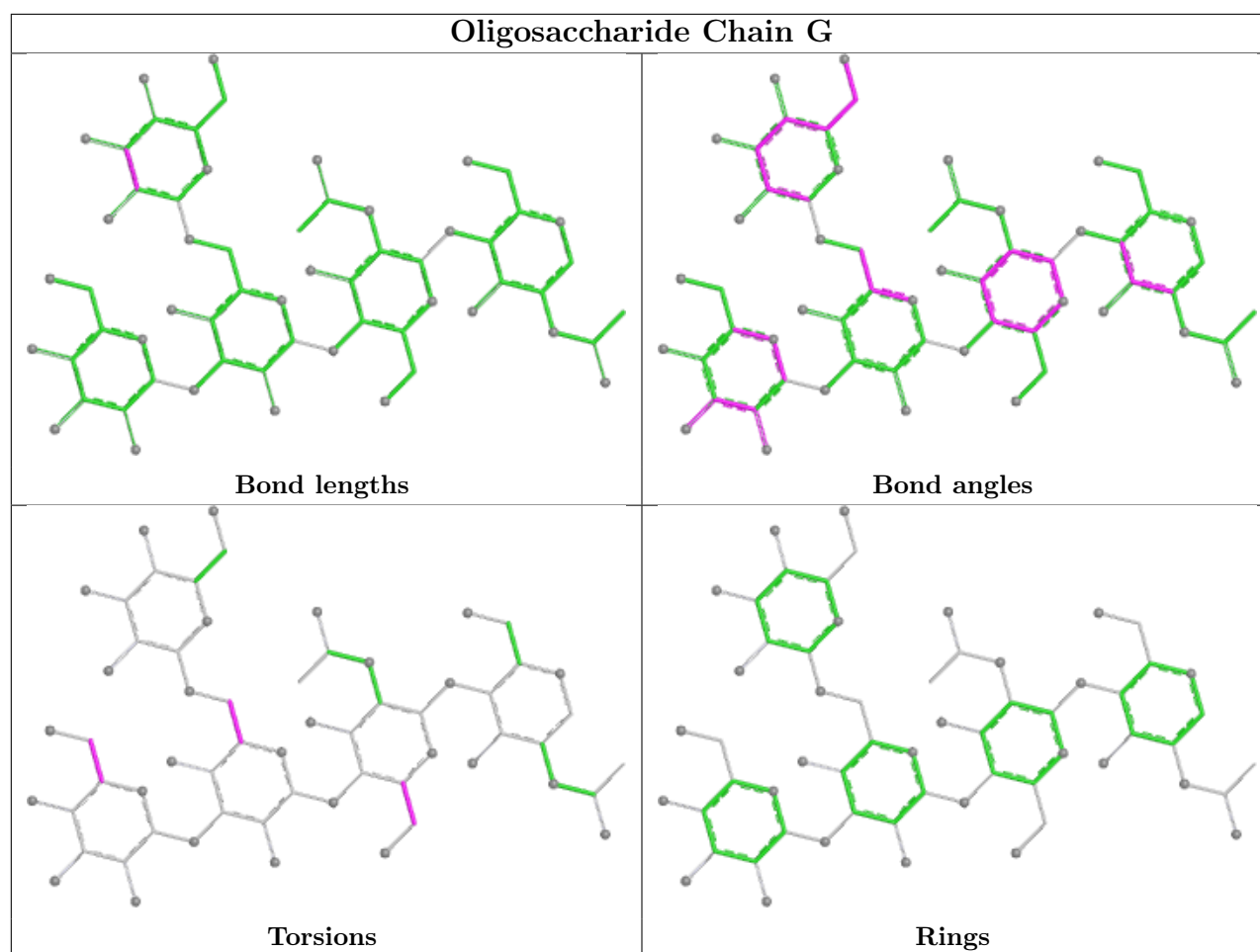












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	823	1	14,14,15	0.56	0	17,19,21	1.51	2 (11%)
7	NAG	A	807	1	14,14,15	0.53	0	17,19,21	1.15	2 (11%)
7	NAG	B	802	1	14,14,15	0.94	1 (7%)	17,19,21	1.54	5 (29%)
7	NAG	B	807	1	14,14,15	0.56	0	17,19,21	1.74	6 (35%)
6	GOL	A	802	-	5,5,5	0.26	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	824	1	14,14,15	0.53	0	17,19,21	1.76	5 (29%)
6	GOL	A	825	-	5,5,5	0.67	0	5,5,5	0.81	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	823	1	-	2/6/23/26	0/1/1/1
7	NAG	A	807	1	-	0/6/23/26	0/1/1/1
7	NAG	B	802	1	-	0/6/23/26	0/1/1/1
7	NAG	B	807	1	-	2/6/23/26	0/1/1/1
6	GOL	A	802	-	-	2/4/4/4	-
7	NAG	A	824	1	-	2/6/23/26	0/1/1/1
6	GOL	A	825	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	802	NAG	O5-C1	-2.92	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	823	NAG	C1-O5-C5	4.75	118.55	112.19
7	A	824	NAG	C1-C2-N2	3.98	116.71	110.43
7	B	807	NAG	C1-C2-N2	3.26	115.56	110.43
7	B	807	NAG	O5-C5-C6	3.17	113.82	107.66
7	B	807	NAG	O7-C7-C8	-2.93	116.83	122.05
7	A	824	NAG	C3-C4-C5	-2.70	105.33	110.23
7	A	824	NAG	O5-C5-C6	2.58	112.69	107.66
7	B	807	NAG	C6-C5-C4	-2.52	106.82	113.02
7	B	802	NAG	C1-C2-N2	-2.51	106.48	110.43
7	A	823	NAG	C4-C3-C2	-2.40	107.50	111.02
7	A	807	NAG	O3-C3-C2	-2.29	104.65	109.40
7	B	807	NAG	O5-C1-C2	-2.22	107.86	111.29
7	B	802	NAG	O5-C5-C6	-2.22	103.35	107.66
7	B	802	NAG	O6-C6-C5	-2.18	103.90	111.33
7	A	824	NAG	O3-C3-C2	-2.17	104.90	109.40
7	A	807	NAG	O4-C4-C5	2.15	114.62	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	802	NAG	O3-C3-C4	2.10	115.33	110.38
7	A	824	NAG	O7-C7-C8	-2.09	118.33	122.05
7	B	807	NAG	C8-C7-N2	2.04	119.51	116.12
7	B	802	NAG	C3-C4-C5	-2.04	106.53	110.23

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	802	GOL	O1-C1-C2-C3
6	A	825	GOL	C1-C2-C3-O3
7	A	824	NAG	O5-C5-C6-O6
7	B	807	NAG	O5-C5-C6-O6
7	A	824	NAG	C4-C5-C6-O6
7	A	823	NAG	O5-C5-C6-O6
6	A	802	GOL	O1-C1-C2-O2
7	B	807	NAG	C4-C5-C6-O6
6	A	825	GOL	O2-C2-C3-O3
7	A	823	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	823	NAG	2	0
7	A	807	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

6.1 Protein, DNA and RNA chains

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	363/381 (95%)	0.31	17 (4%) 36 35	34, 46, 76, 97	0
1	B	355/381 (93%)	0.50	20 (5%) 30 29	39, 50, 83, 113	0
All	All	718/762 (94%)	0.40	37 (5%) 33 31	34, 48, 79, 113	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	ILE	4.4
1	B	195	GLU	3.9
1	B	251	SER	3.6
1	B	386	VAL	3.4
1	B	91	PHE	3.4
1	A	386	VAL	3.3
1	A	249	ILE	3.3
1	A	333	TYR	3.2
1	B	194	TYR	3.0
1	A	187	VAL	3.0
1	A	221	SER	3.0
1	A	165	MET	2.9
1	B	250	THR	2.9
1	A	55	SER	2.8
1	A	224	LEU	2.7
1	B	273	GLU	2.6
1	A	250	THR	2.5
1	B	173	VAL	2.5
1	A	56	GLN	2.5
1	A	158	GLY	2.5
1	A	184	GLY	2.5
1	B	225	TYR	2.4
1	B	169	ILE	2.4
1	A	173	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	183	ILE	2.4
1	A	90	ASP	2.3
1	A	219	TYR	2.3
1	B	379	CYS	2.3
1	B	174	THR	2.3
1	B	172	GLY	2.3
1	B	226	TYR	2.3
1	B	252	GLY	2.2
1	A	166	CYS	2.2
1	A	220	LEU	2.2
1	B	113	VAL	2.1
1	B	304	ASN	2.1
1	B	224	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
4	MAN	G	5	11/12	0.53	0.16	79,94,100,100	0
2	NAG	H	2	14/15	0.65	0.12	77,89,94,95	0
4	MAN	G	4	11/12	0.66	0.17	91,102,105,105	0
2	NAG	D	2	14/15	0.67	0.14	65,75,83,83	0
3	MAN	F	8	11/12	0.75	0.12	51,63,67,71	0
2	NAG	C	2	14/15	0.75	0.12	60,74,83,86	0
2	NAG	E	2	14/15	0.76	0.14	60,75,86,87	0
2	NAG	K	2	14/15	0.76	0.13	71,77,81,82	0
2	NAG	J	2	14/15	0.77	0.13	62,67,74,74	0
4	NAG	G	2	14/15	0.78	0.14	58,64,81,84	0
7	NAG	B	807	14/15	0.80	0.12	48,53,64,66	0
7	NAG	A	807	14/15	0.81	0.11	54,64,70,73	0
7	NAG	B	802	14/15	0.81	0.12	54,60,66,67	0
3	MAN	F	7	11/12	0.82	0.10	59,64,72,73	0
2	NAG	H	1	14/15	0.83	0.10	60,69,74,84	0
2	NAG	I	2	14/15	0.84	0.10	61,62,68,73	0
2	NAG	L	2	14/15	0.84	0.11	70,80,92,100	0
7	NAG	A	824	14/15	0.85	0.11	47,55,66,71	0
3	MAN	F	5	11/12	0.85	0.12	53,60,71,76	0
7	NAG	A	823	14/15	0.85	0.11	57,76,84,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	K	1	14/15	0.87	0.12	54,65,76,76	0
3	NAG	F	1	14/15	0.89	0.10	41,44,54,54	0
2	NAG	D	1	14/15	0.89	0.10	48,54,63,65	0
3	NAG	F	2	14/15	0.90	0.08	46,51,56,57	0
2	NAG	C	1	14/15	0.91	0.09	43,49,60,64	0
3	MAN	F	6	11/12	0.92	0.08	45,48,51,52	0
2	NAG	L	1	14/15	0.92	0.10	50,58,65,69	0
2	NAG	J	1	14/15	0.92	0.07	46,48,53,53	0
4	NAG	G	1	14/15	0.93	0.07	40,42,47,49	0
3	MAN	F	4	11/12	0.94	0.06	50,55,58,60	0
2	NAG	E	1	14/15	0.95	0.07	39,48,51,57	0
2	NAG	I	1	14/15	0.95	0.07	46,49,54,60	0

6.3 Carbohydrates

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.

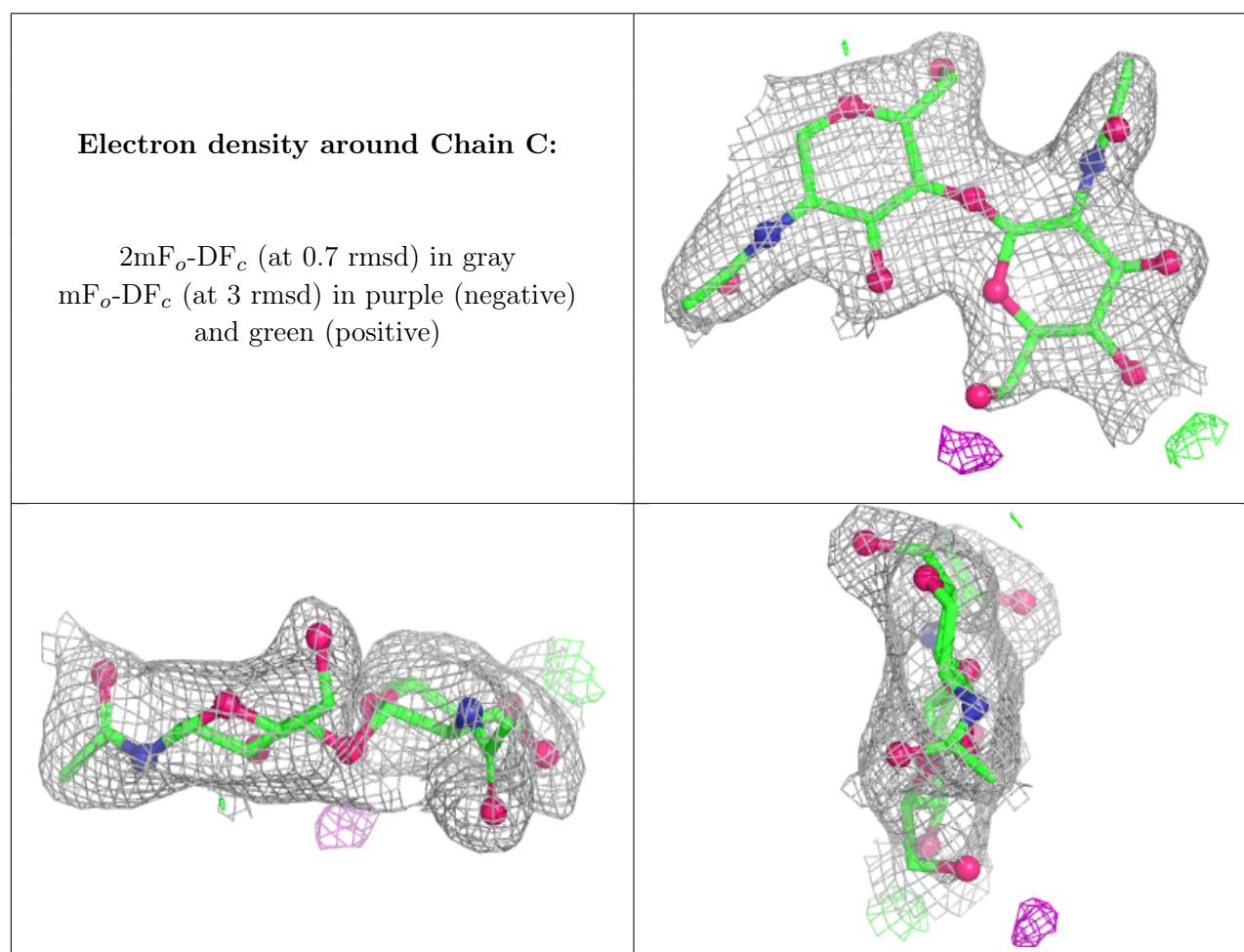
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	G	5	11/12	0.53	0.16	79,94,100,100	0
4	BMA	G	3	11/12	0.63	0.18	90,94,99,100	0
2	NAG	H	2	14/15	0.65	0.12	77,89,94,95	0
4	MAN	G	4	11/12	0.66	0.17	91,102,105,105	0
2	NAG	D	2	14/15	0.67	0.14	65,75,83,83	0
3	MAN	F	8	11/12	0.75	0.12	51,63,67,71	0
2	NAG	C	2	14/15	0.75	0.12	60,74,83,86	0
2	NAG	E	2	14/15	0.76	0.14	60,75,86,87	0
2	NAG	K	2	14/15	0.76	0.13	71,77,81,82	0
2	NAG	J	2	14/15	0.77	0.13	62,67,74,74	0
4	NAG	G	2	14/15	0.78	0.14	58,64,81,84	0
3	MAN	F	7	11/12	0.82	0.10	59,64,72,73	0
2	NAG	H	1	14/15	0.83	0.10	60,69,74,84	0
2	NAG	I	2	14/15	0.84	0.10	61,62,68,73	0
2	NAG	L	2	14/15	0.84	0.11	70,80,92,100	0
3	MAN	F	5	11/12	0.85	0.12	53,60,71,76	0
2	NAG	K	1	14/15	0.87	0.12	54,65,76,76	0
3	NAG	F	1	14/15	0.89	0.10	41,44,54,54	0
2	NAG	D	1	14/15	0.89	0.10	48,54,63,65	0
3	NAG	F	2	14/15	0.90	0.08	46,51,56,57	0
2	NAG	C	1	14/15	0.91	0.09	43,49,60,64	0

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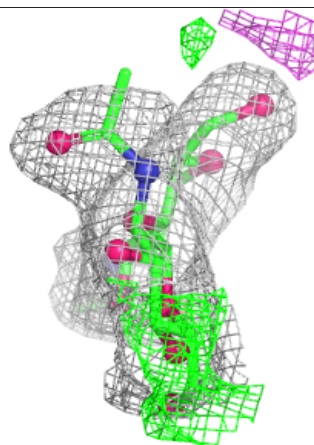
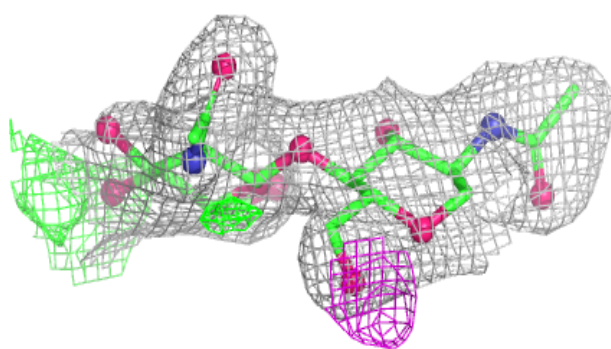
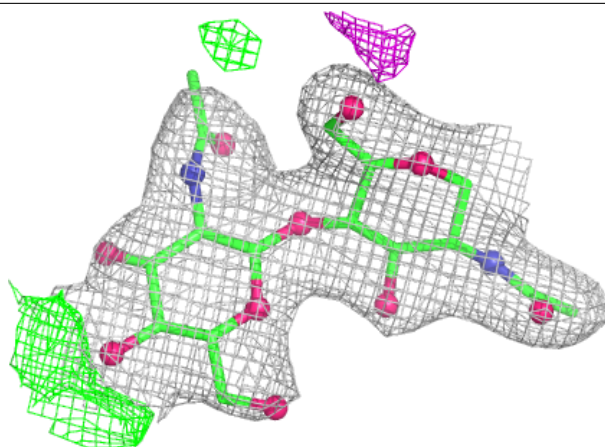
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	L	1	14/15	0.92	0.10	50,58,65,69	0
3	MAN	F	6	11/12	0.92	0.08	45,48,51,52	0
2	NAG	J	1	14/15	0.92	0.07	46,48,53,53	0
3	BMA	F	3	11/12	0.92	0.07	54,58,60,66	0
4	NAG	G	1	14/15	0.93	0.07	40,42,47,49	0
3	MAN	F	4	11/12	0.94	0.06	50,55,58,60	0
2	NAG	E	1	14/15	0.95	0.07	39,48,51,57	0
2	NAG	I	1	14/15	0.95	0.07	46,49,54,60	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.



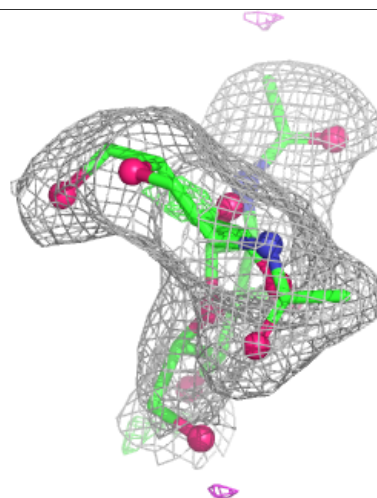
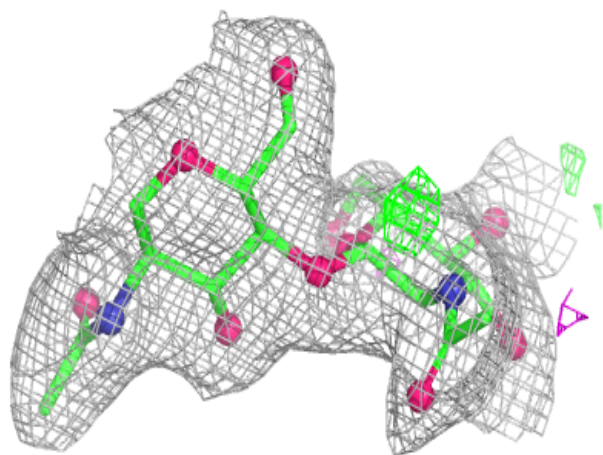
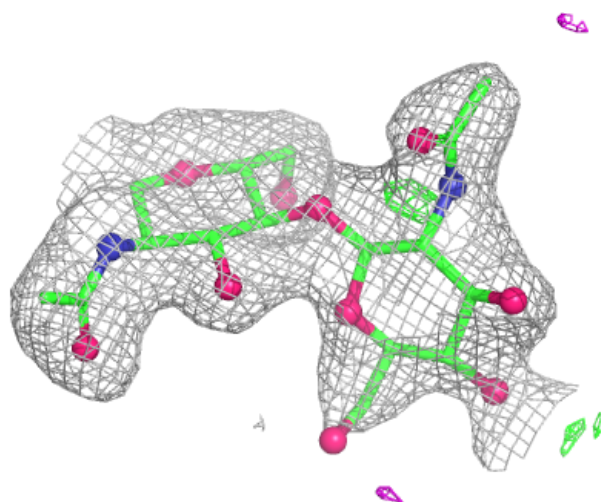
Electron density around Chain D:

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



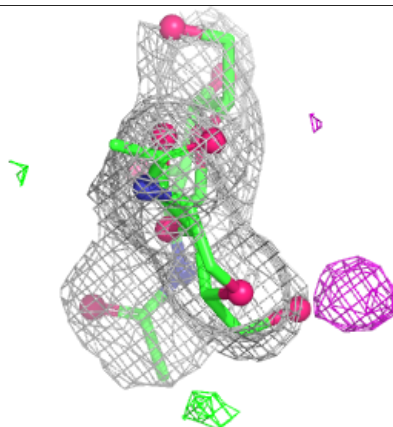
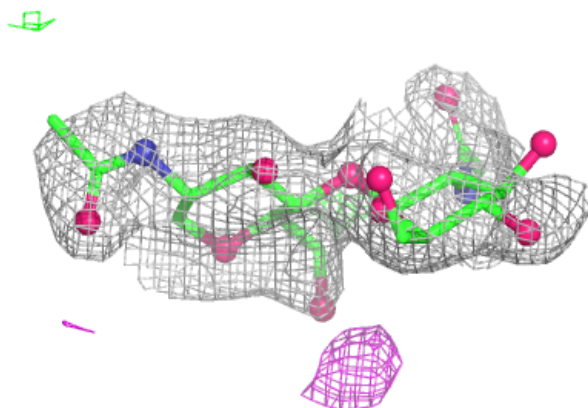
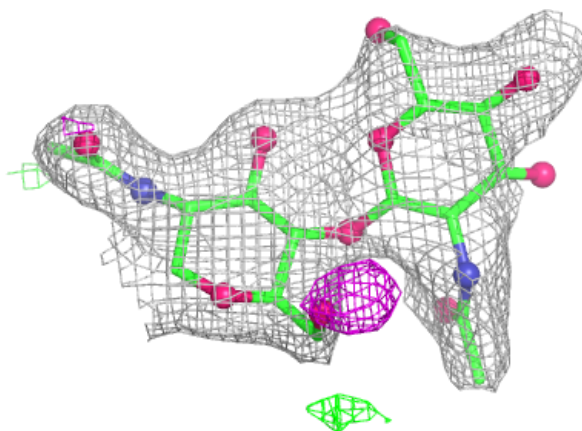
Electron density around Chain E:

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

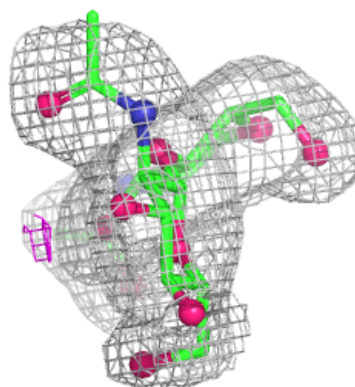
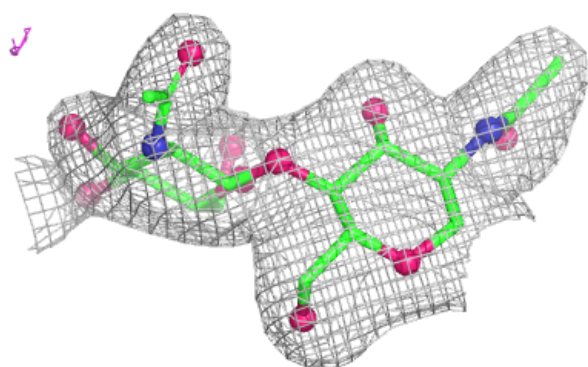
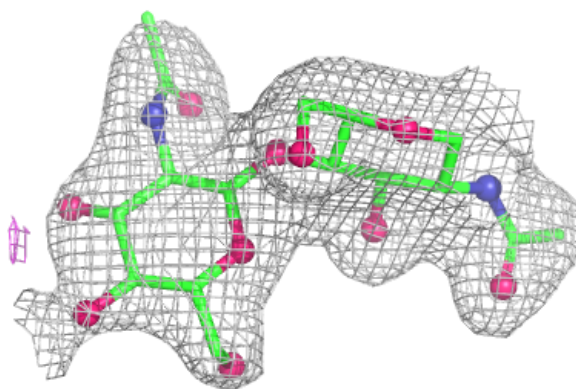


Electron density around Chain H:

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

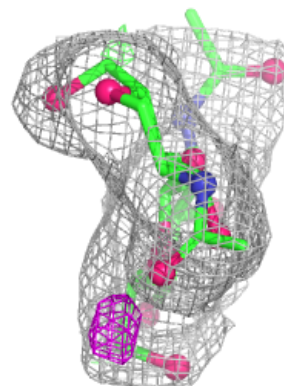
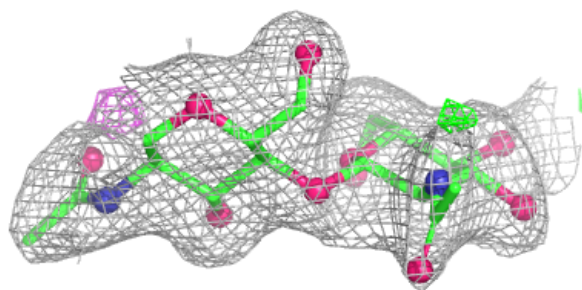
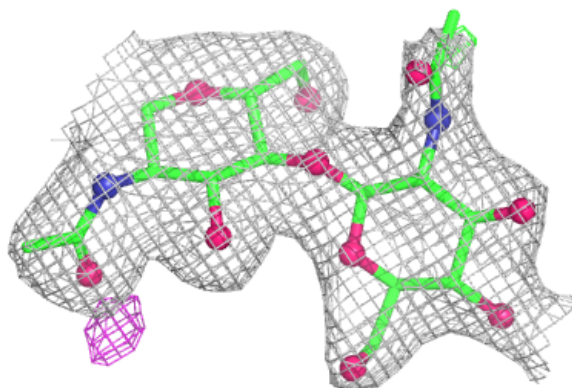
**Electron density around Chain I:**

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



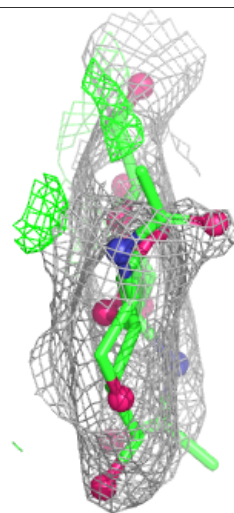
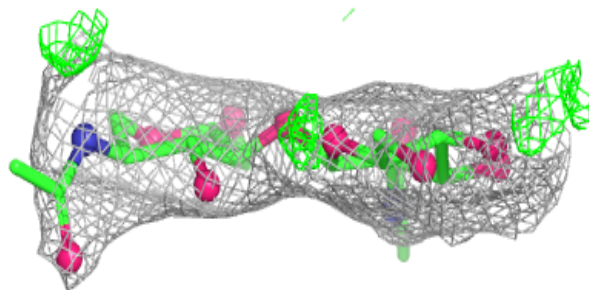
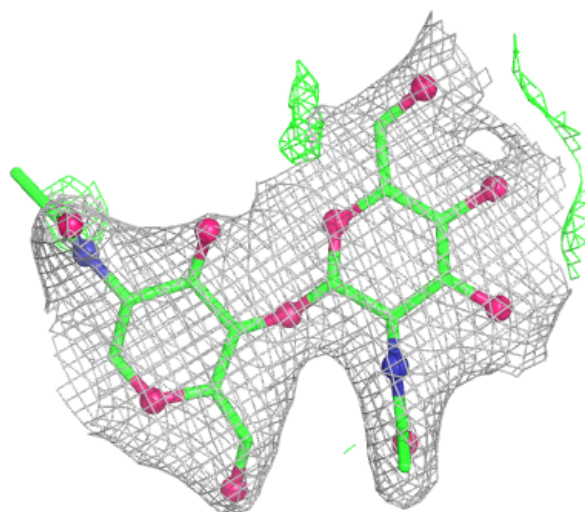
Electron density around Chain J:

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



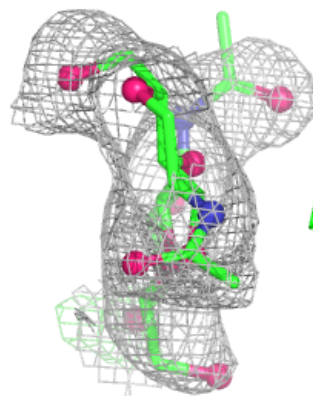
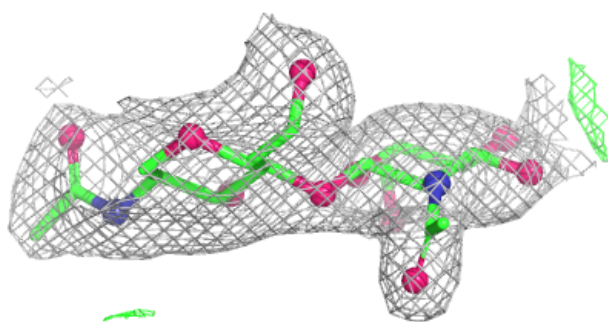
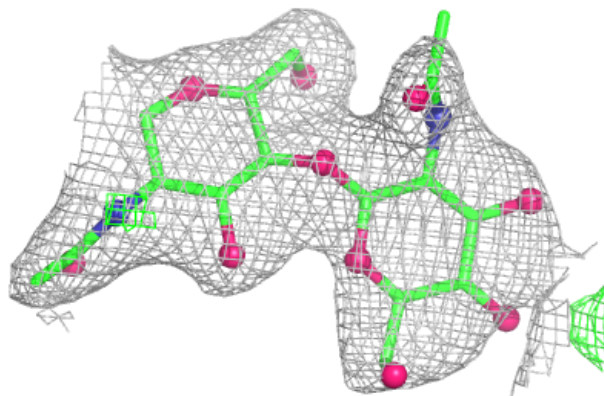
Electron density around Chain K:

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



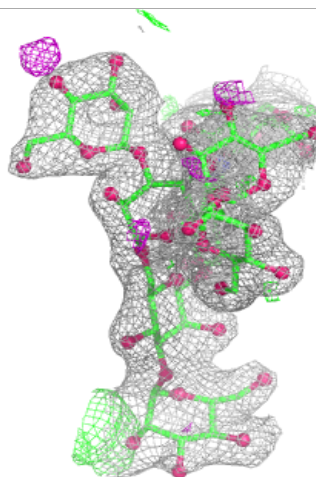
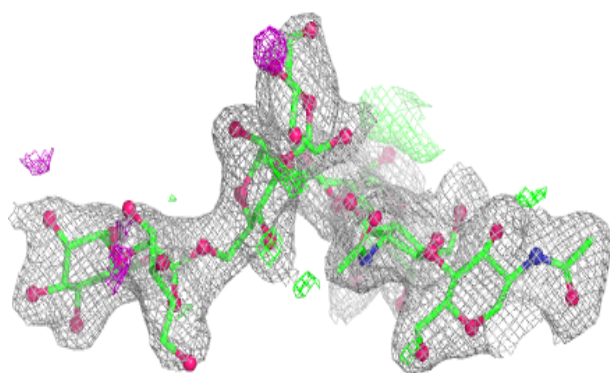
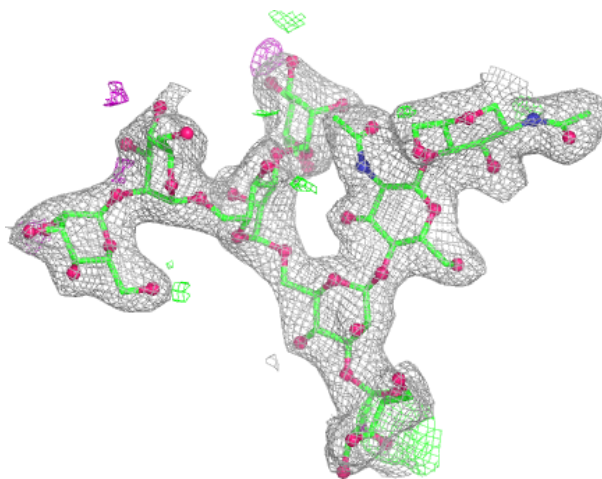
Electron density around Chain L:

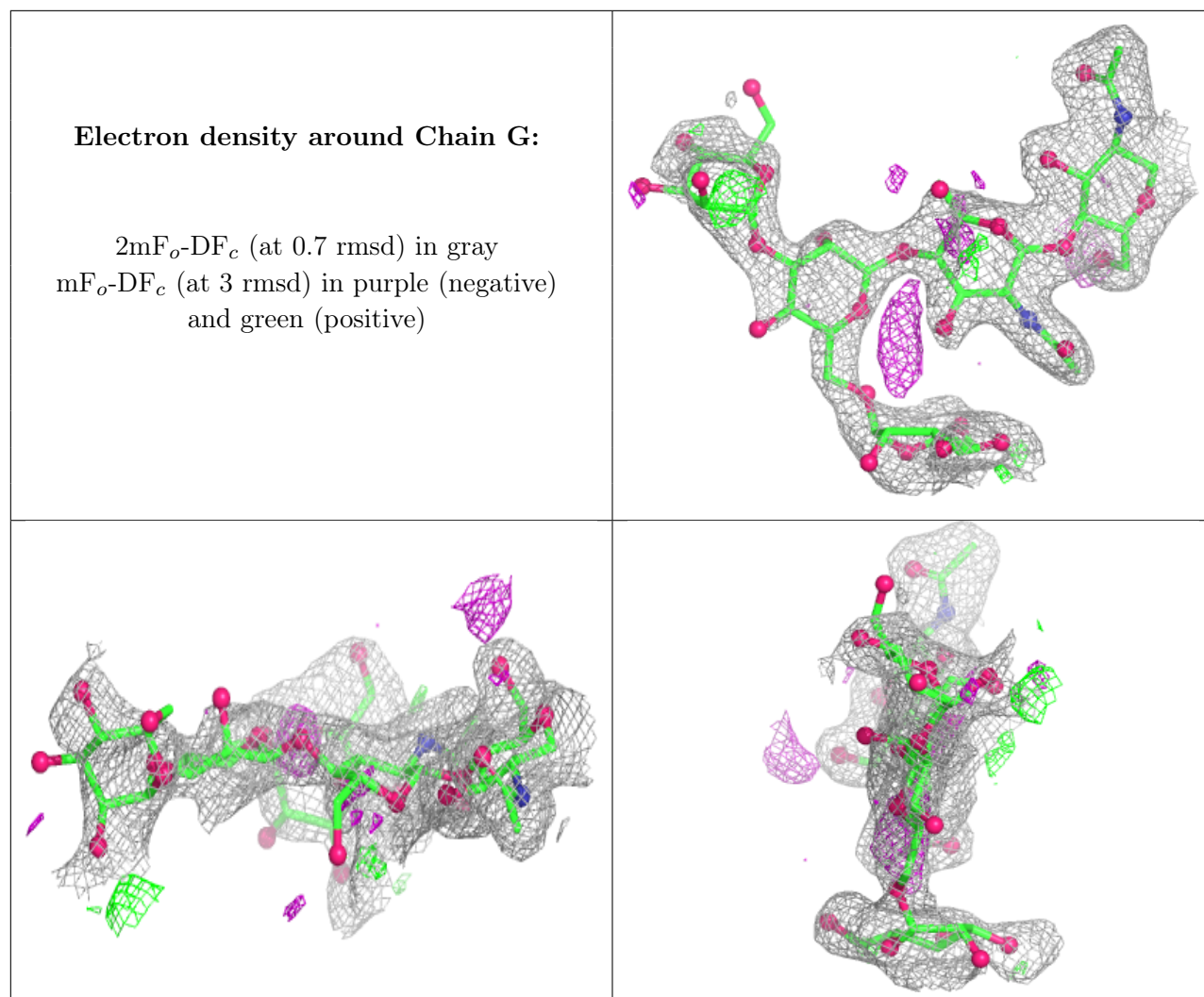
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands ⓘ

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
6	GOL	A	825	6/6	0.73	0.21	72,77,79,80	0
7	NAG	B	807	14/15	0.80	0.12	48,53,64,66	0
7	NAG	B	802	14/15	0.81	0.12	54,60,66,67	0
7	NAG	A	807	14/15	0.81	0.11	54,64,70,73	0
7	NAG	A	823	14/15	0.85	0.11	57,76,84,87	0
7	NAG	A	824	14/15	0.85	0.11	47,55,66,71	0
6	GOL	A	802	6/6	0.87	0.14	77,77,81,81	0
5	NA	B	801	1/1	0.95	0.10	50,50,50,50	0
5	NA	A	801	1/1	0.99	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.