



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:57 PM EDT

PDB ID : 7DMU / pdb_00007dmu
Title : Structure of SARS-CoV-2 spike receptor-binding domain complexed with high affinity ACE2 mutant 3N39
Authors : Arimori, T.; Takagi, J.
Deposited on : 2020-12-07
Resolution : 3.20 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

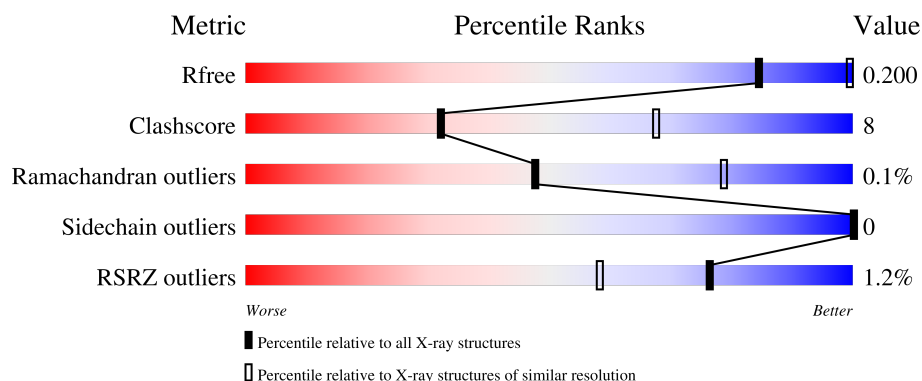
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



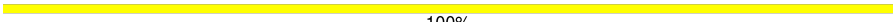
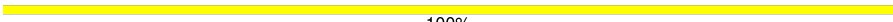
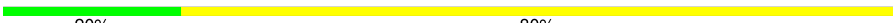
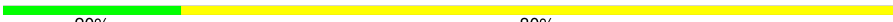
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	606	80% 18% .
1	C	606	81% 17% .
2	B	218	2% 74% 16% 10%
2	D	218	72% 17% 11%
3	E	5	20% 80%

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	G	2	 50%50%
4	K	2	 100%
4	M	2	 50%50%
5	H	5	 20%80%
5	J	5	 20%80%
5	L	5	 20%80%
6	I	3	 33%67%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13306 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4876	3122	806	919	29			
1	C	598	Total	C	N	O	S	0	0	0
			4885	3127	808	921	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ALA	engineered mutation	UNP Q9BYF1
A	26	GLU	LYS	engineered mutation	UNP Q9BYF1
A	31	ASN	LYS	engineered mutation	UNP Q9BYF1
A	35	LYS	GLU	engineered mutation	UNP Q9BYF1
A	64	ILE	ASN	engineered mutation	UNP Q9BYF1
A	79	PHE	LEU	engineered mutation	UNP Q9BYF1
A	90	HIS	ASN	engineered mutation	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
C	25	VAL	ALA	engineered mutation	UNP Q9BYF1
C	26	GLU	LYS	engineered mutation	UNP Q9BYF1
C	31	ASN	LYS	engineered mutation	UNP Q9BYF1
C	35	LYS	GLU	engineered mutation	UNP Q9BYF1
C	64	ILE	ASN	engineered mutation	UNP Q9BYF1
C	79	PHE	LEU	engineered mutation	UNP Q9BYF1
C	90	HIS	ASN	engineered mutation	UNP Q9BYF1
C	616	SER	-	expression tag	UNP Q9BYF1
C	617	SER	-	expression tag	UNP Q9BYF1
C	618	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	619	HIS	-	expression tag	UNP Q9BYF1
C	620	HIS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1551	995	258	290	8			
2	D	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 10 discrepancies between the modelled and reference sequences:

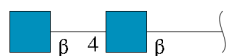
Chain	Residue	Modelled	Actual	Comment	Reference
B	532	GLY	-	expression tag	UNP P0DTC2
B	533	THR	-	expression tag	UNP P0DTC2
B	534	LEU	-	expression tag	UNP P0DTC2
B	535	LEU	-	expression tag	UNP P0DTC2
B	536	GLY	-	expression tag	UNP P0DTC2
D	532	GLY	-	expression tag	UNP P0DTC2
D	533	THR	-	expression tag	UNP P0DTC2
D	534	LEU	-	expression tag	UNP P0DTC2
D	535	LEU	-	expression tag	UNP P0DTC2
D	536	GLY	-	expression tag	UNP P0DTC2

- Molecule 3 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.



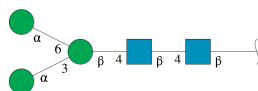
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



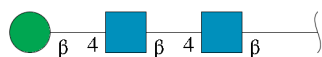
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		
8	C	1	Total	Zn	0	0
			1	1		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

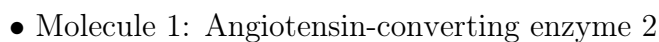


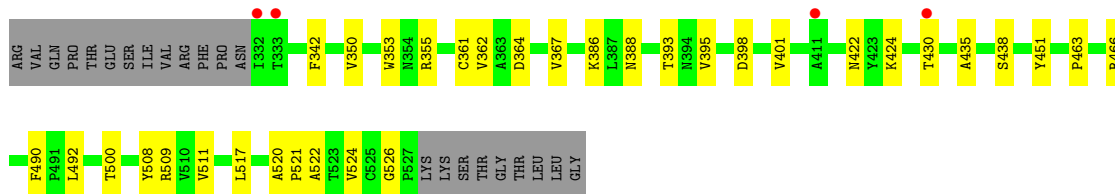
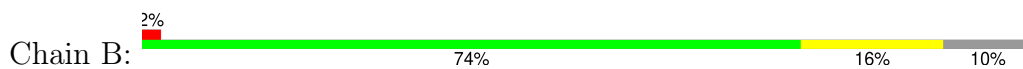
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

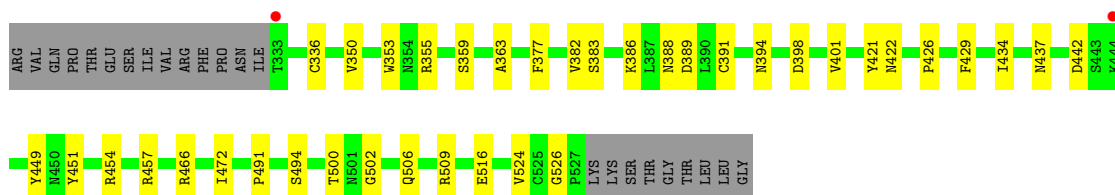
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	C	1	Total	O	0	0
			1	1		

- Molecule 1: Angiotensin-converting enzyme 2

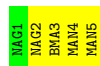




- Molecule 2: Spike protein S1



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



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



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



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

Chain M:  50% 50%

NAG1
NAG2

- Molecule 5: 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 H:  20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 5: 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 J:  20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 5: 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 L:  20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain I:  33% 67%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	227.80Å 227.80Å 147.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 3.20 47.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.91-3.20) 99.9 (47.91-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.179 , 0.198 0.183 , 0.200	Depositor DCC
R_{free} test set	6193 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	133.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 111.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13306	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: ZN, MAN, NAG, SO4, BMA

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	0.31	0/5015	0.52	0/6815
1	C	0.32	0/5024	0.52	1/6827 (0.0%)
2	B	0.31	0/1595	0.53	0/2172
2	D	0.30	0/1587	0.51	0/2161
All	All	0.31	0/13221	0.52	1/17975 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ARG	NE-CZ-NH2	5.05	123.74	119.20

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	4876	0	4639	75	0
1	C	4885	0	4647	76	0
2	B	1551	0	1470	26	0
2	D	1543	0	1459	28	0
3	E	61	0	52	0	0
4	F	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	28	0	25	1	0
4	K	28	0	25	1	0
4	M	28	0	25	1	0
5	H	61	0	52	0	0
5	J	61	0	52	2	0
5	L	61	0	52	0	0
6	I	39	0	34	0	0
7	A	14	0	13	0	0
7	C	28	0	26	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	5	0	0	0	0
9	C	5	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
All	All	13306	0	12596	206	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 206 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:A:323:MET:HE1	1:A:379:ILE:HG21	1.50	0.93
1:C:355:ASP:OD2	1:C:357:ARG:NH1	2.19	0.73
2:D:353:TRP:O	2:D:466:ARG:NH1	2.24	0.71
1:C:109:SER:HB3	1:C:112:LYS:HD2	1.74	0.70
1:A:411:SER:HB3	1:A:543:ASP:HA	1.72	0.69

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	595/606 (98%)	574 (96%)	21 (4%)	0	100	100
1	C	596/606 (98%)	577 (97%)	18 (3%)	1 (0%)	43	73
2	B	194/218 (89%)	185 (95%)	9 (5%)	0	100	100
2	D	193/218 (88%)	184 (95%)	9 (5%)	0	100	100
All	All	1578/1648 (96%)	1520 (96%)	57 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	339	VAL

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	528/537 (98%)	528 (100%)	0	100	100
1	C	529/537 (98%)	529 (100%)	0	100	100
2	B	169/189 (89%)	169 (100%)	0	100	100
2	D	168/189 (89%)	168 (100%)	0	100	100
All	All	1394/1452 (96%)	1394 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	360	ASN
2	D	506	GLN
1	A	195	HIS
1	C	58	ASN
1	C	134	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 ⓘ

31 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,1	14,14,15	0.59	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.68	0
3	BMA	E	3	3	11,11,12	0.78	0	15,15,17	0.98	1 (6%)
3	MAN	E	4	3	11,11,12	1.34	1 (9%)	15,15,17	1.60	3 (20%)
3	MAN	E	5	3	11,11,12	0.87	0	15,15,17	1.43	3 (20%)
4	NAG	F	1	4,1	14,14,15	0.54	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	0.83	0
4	NAG	G	1	4,1	14,14,15	0.40	0	17,19,21	0.46	0
4	NAG	G	2	4	14,14,15	0.65	0	17,19,21	1.41	2 (11%)
5	NAG	H	1	5,1	14,14,15	0.45	0	17,19,21	0.75	1 (5%)
5	NAG	H	2	5	14,14,15	0.34	0	17,19,21	0.64	0
5	BMA	H	3	5	11,11,12	1.78	2 (18%)	15,15,17	1.41	3 (20%)
5	MAN	H	4	5	11,11,12	1.52	2 (18%)	15,15,17	1.59	1 (6%)
5	MAN	H	5	5	11,11,12	1.84	3 (27%)	15,15,17	1.92	3 (20%)
6	NAG	I	1	2,6	14,14,15	0.32	0	17,19,21	0.72	1 (5%)
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.51	0
6	BMA	I	3	6	11,11,12	1.18	1 (9%)	15,15,17	1.29	1 (6%)
5	NAG	J	1	5,1	14,14,15	0.55	0	17,19,21	0.74	0
5	NAG	J	2	5	14,14,15	0.52	0	17,19,21	0.59	0
5	BMA	J	3	5	11,11,12	0.93	0	15,15,17	1.62	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	J	4	5	11,11,12	1.57	3 (27%)	15,15,17	1.96	4 (26%)
5	MAN	J	5	5	11,11,12	1.43	2 (18%)	15,15,17	1.43	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	K	2	4	14,14,15	0.39	0	17,19,21	0.43	0
5	NAG	L	1	5,1	14,14,15	0.26	0	17,19,21	0.62	1 (5%)
5	NAG	L	2	5	14,14,15	0.66	1 (7%)	17,19,21	0.63	0
5	BMA	L	3	5	11,11,12	0.74	0	15,15,17	0.92	0
5	MAN	L	4	5	11,11,12	1.25	2 (18%)	15,15,17	1.17	1 (6%)
5	MAN	L	5	5	11,11,12	1.21	1 (9%)	15,15,17	0.83	1 (6%)
4	NAG	M	1	2,4	14,14,15	0.28	0	17,19,21	0.90	1 (5%)
4	NAG	M	2	4	14,14,15	0.67	1 (7%)	17,19,21	1.30	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	4.50	1.63	1.52
5	H	5	MAN	C4-C5	4.07	1.61	1.53
3	E	2	NAG	O5-C1	-3.25	1.38	1.43
5	H	5	MAN	O5-C1	-3.18	1.38	1.43
5	J	5	MAN	C2-C3	3.12	1.57	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4	MAN	C1-O5-C5	6.23	120.54	112.19
5	H	5	MAN	C1-C2-C3	-5.77	101.25	109.64
5	H	4	MAN	C1-O5-C5	5.16	119.11	112.19
4	G	2	NAG	C2-N2-C7	4.80	129.33	122.90
4	M	2	NAG	C2-N2-C7	4.65	129.13	122.90

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

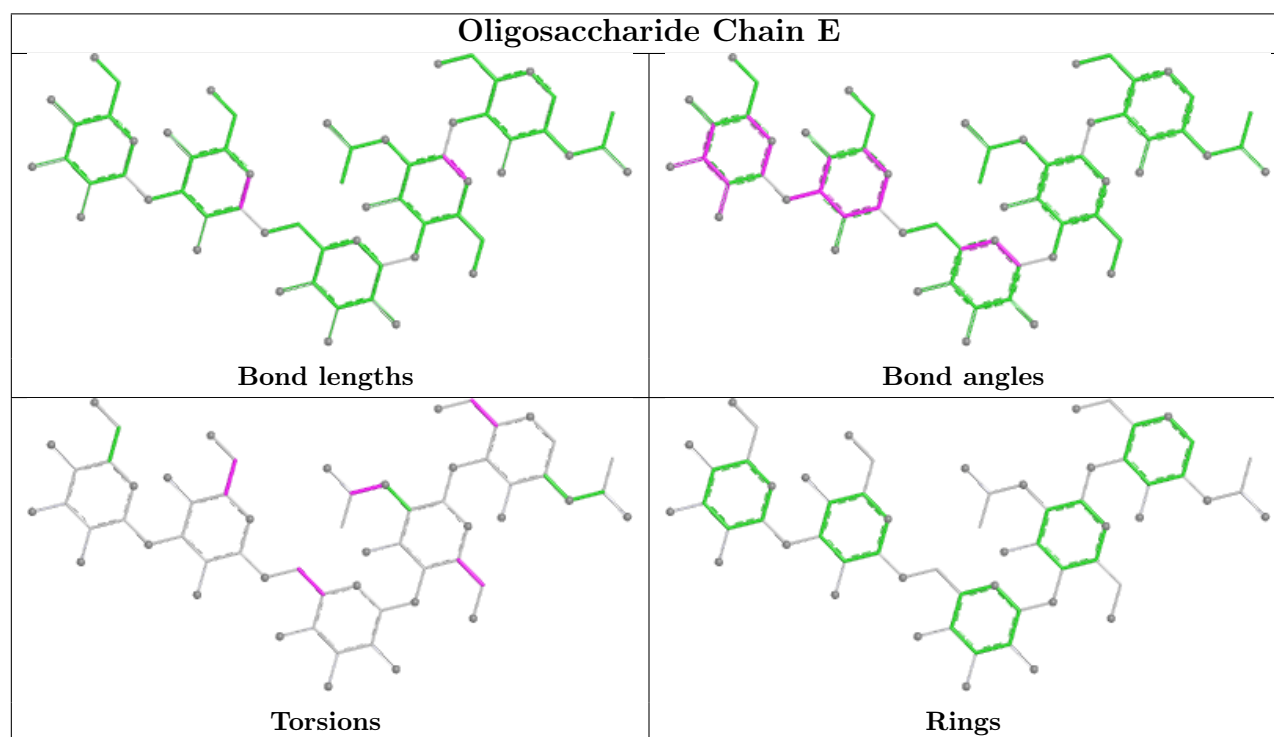
All (2) ring outliers are listed below:

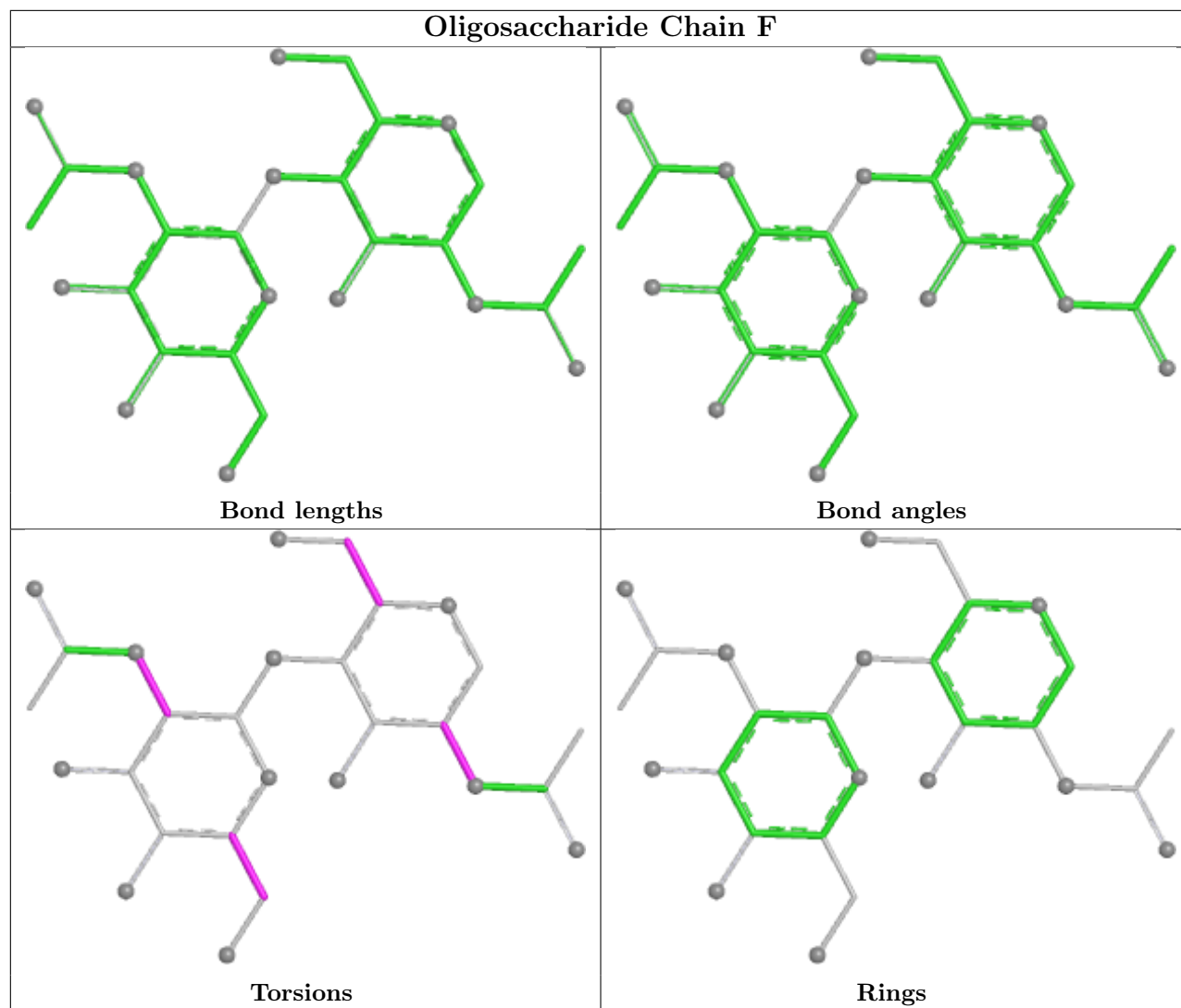
Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C1-C2-C3-C4-C5-O5
5	L	4	MAN	C1-C2-C3-C4-C5-O5

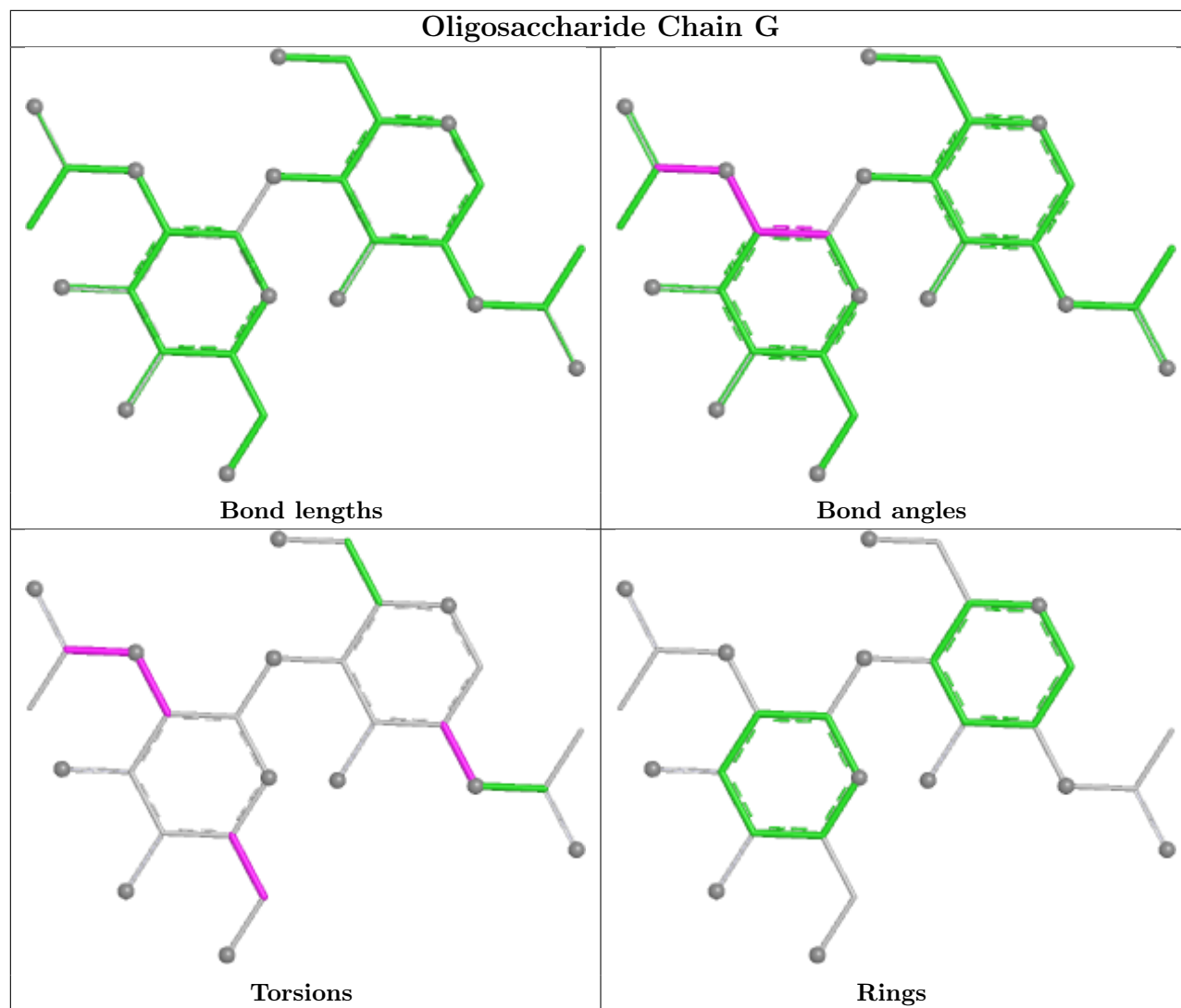
7 monomers are involved in 7 short contacts:

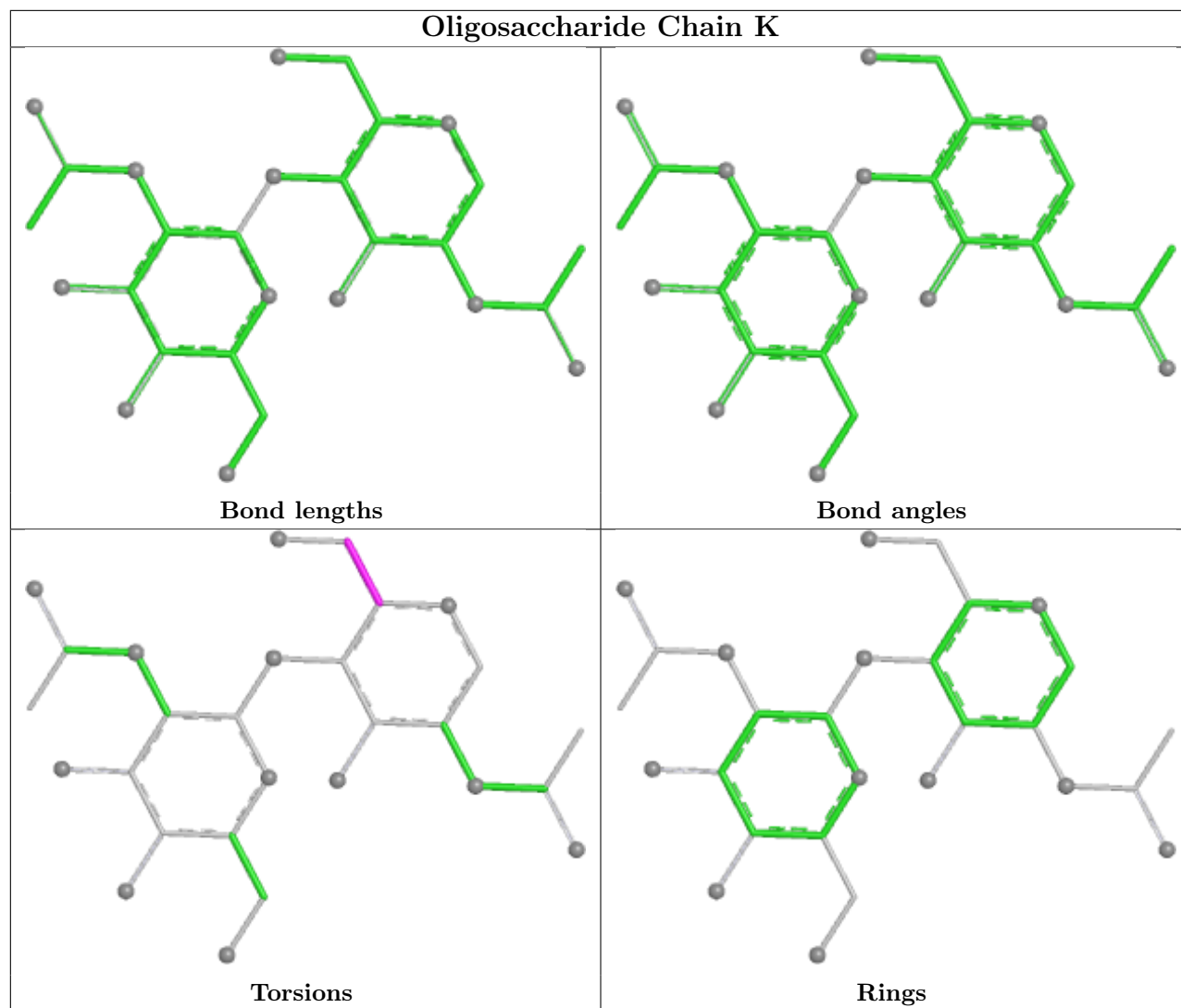
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	K	2	NAG	1	0
4	M	2	NAG	1	0
5	J	1	NAG	2	0
4	K	1	NAG	1	0
4	F	1	NAG	1	0
4	G	2	NAG	1	0

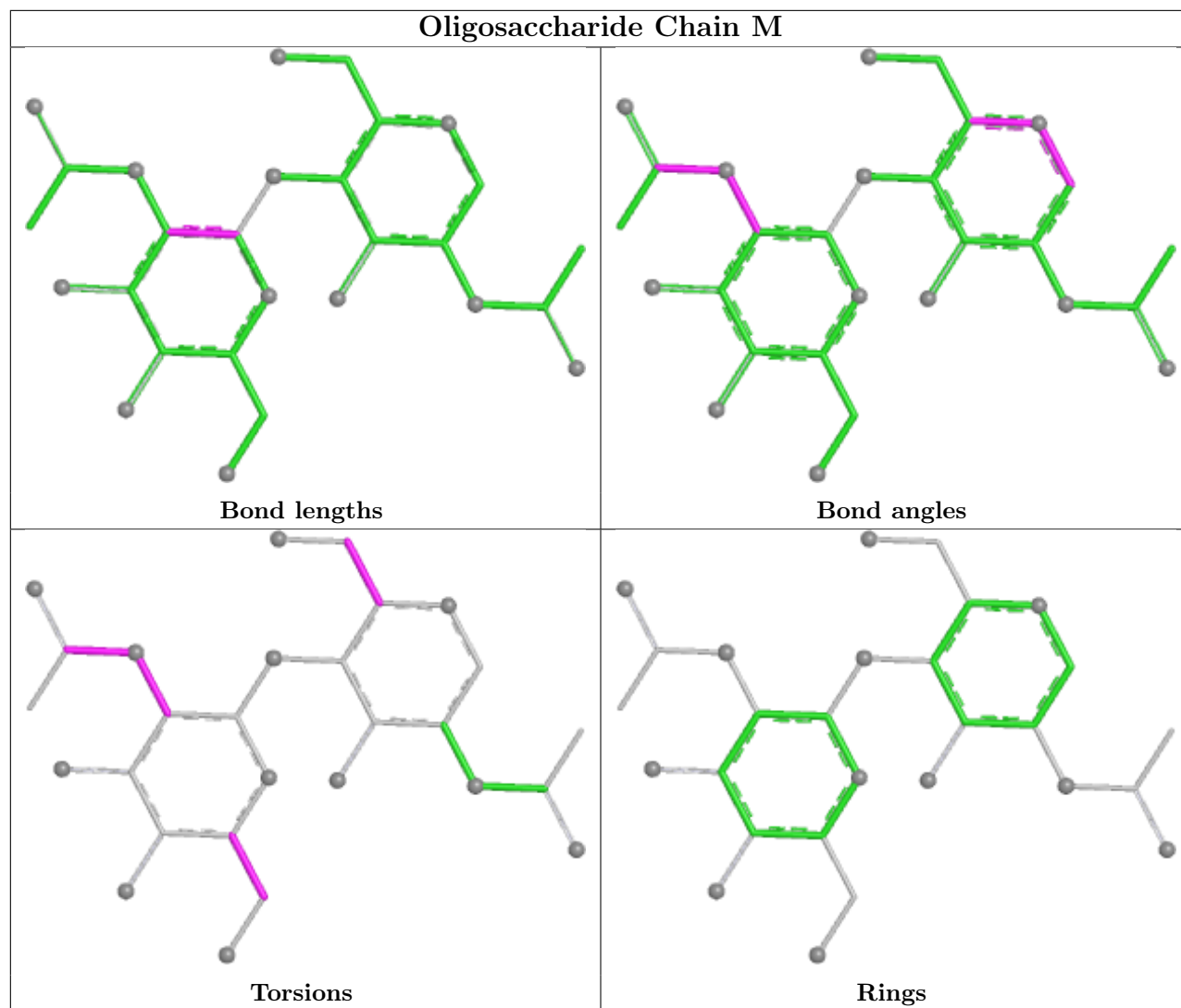
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

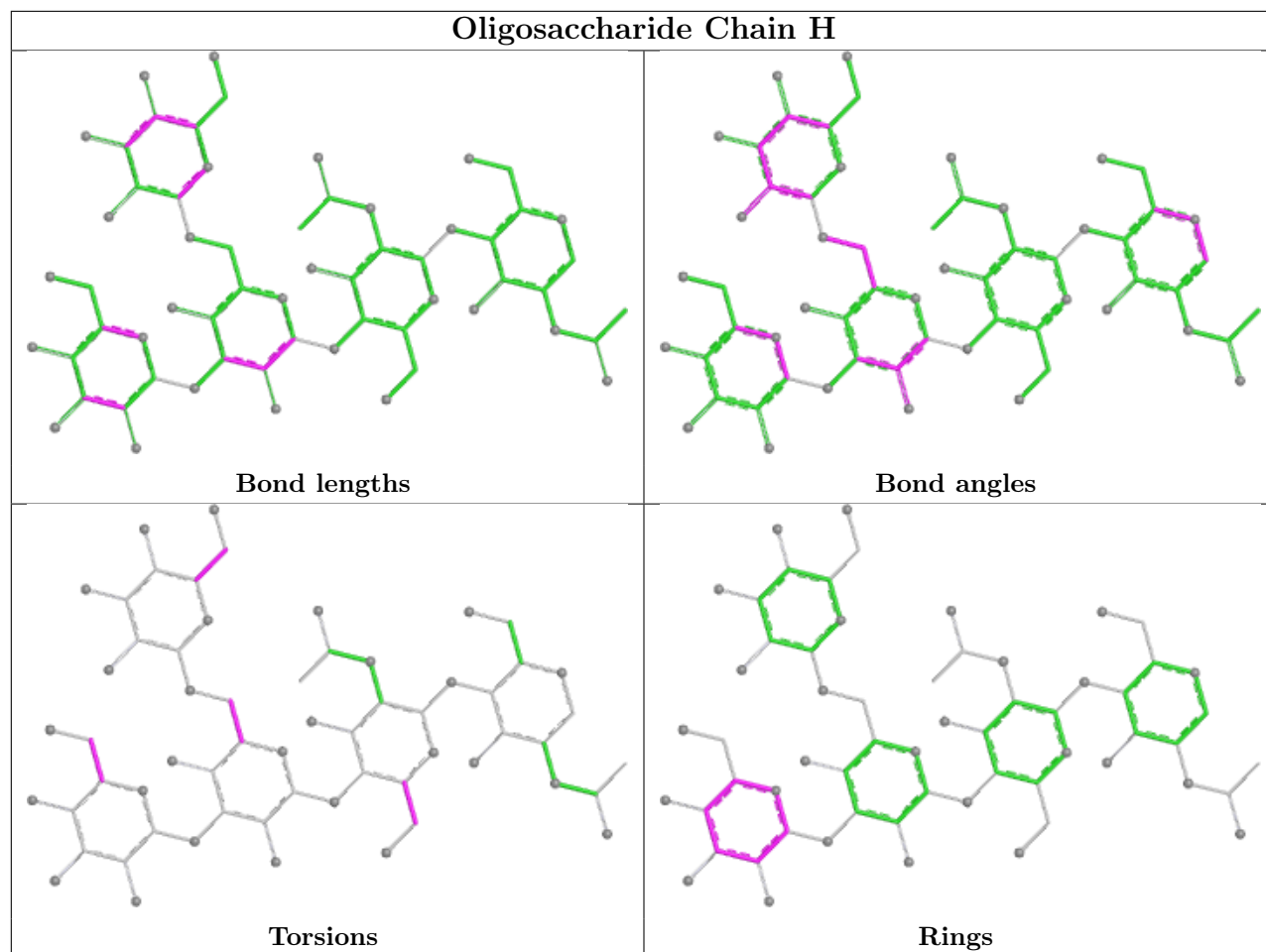


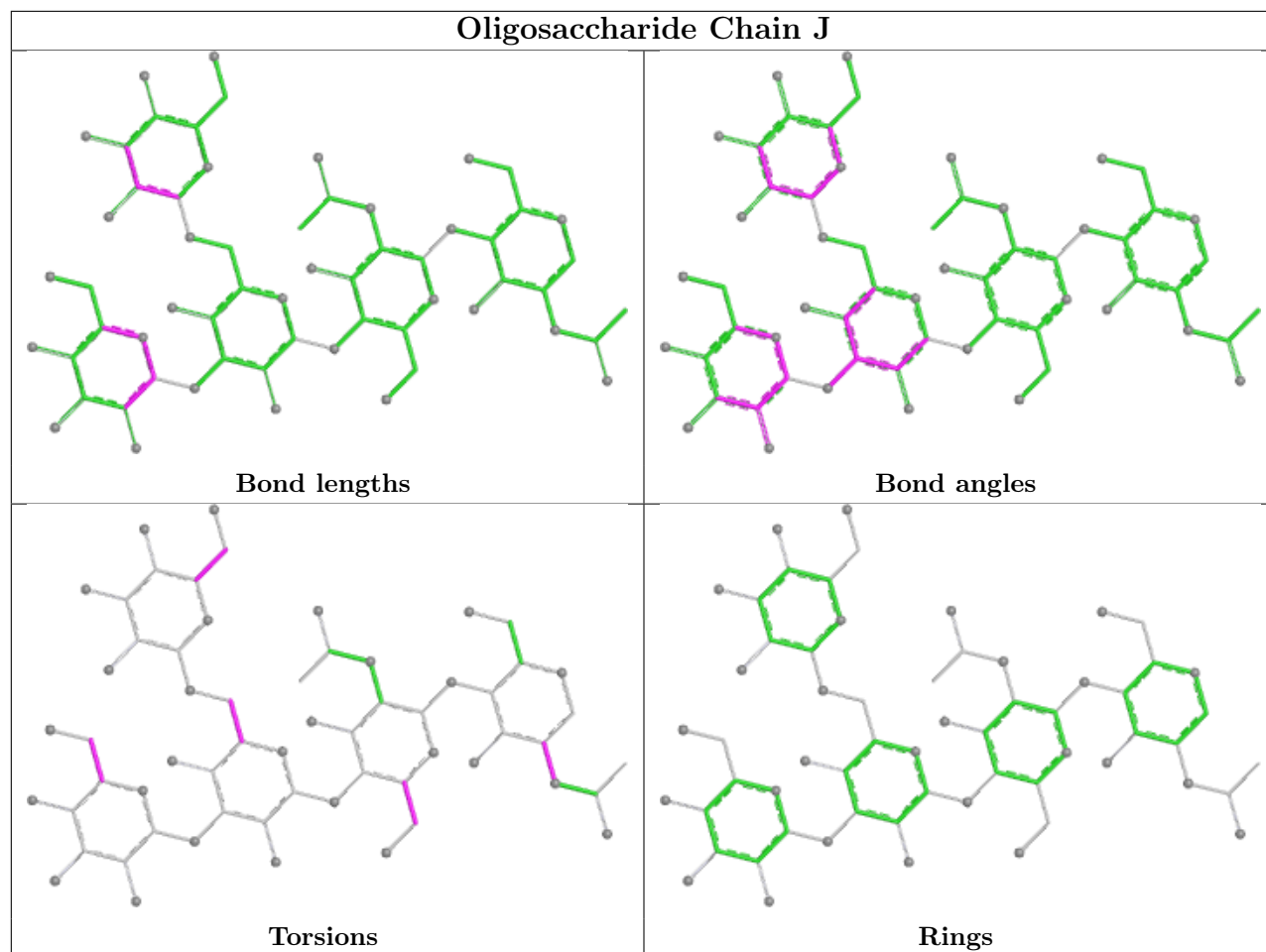


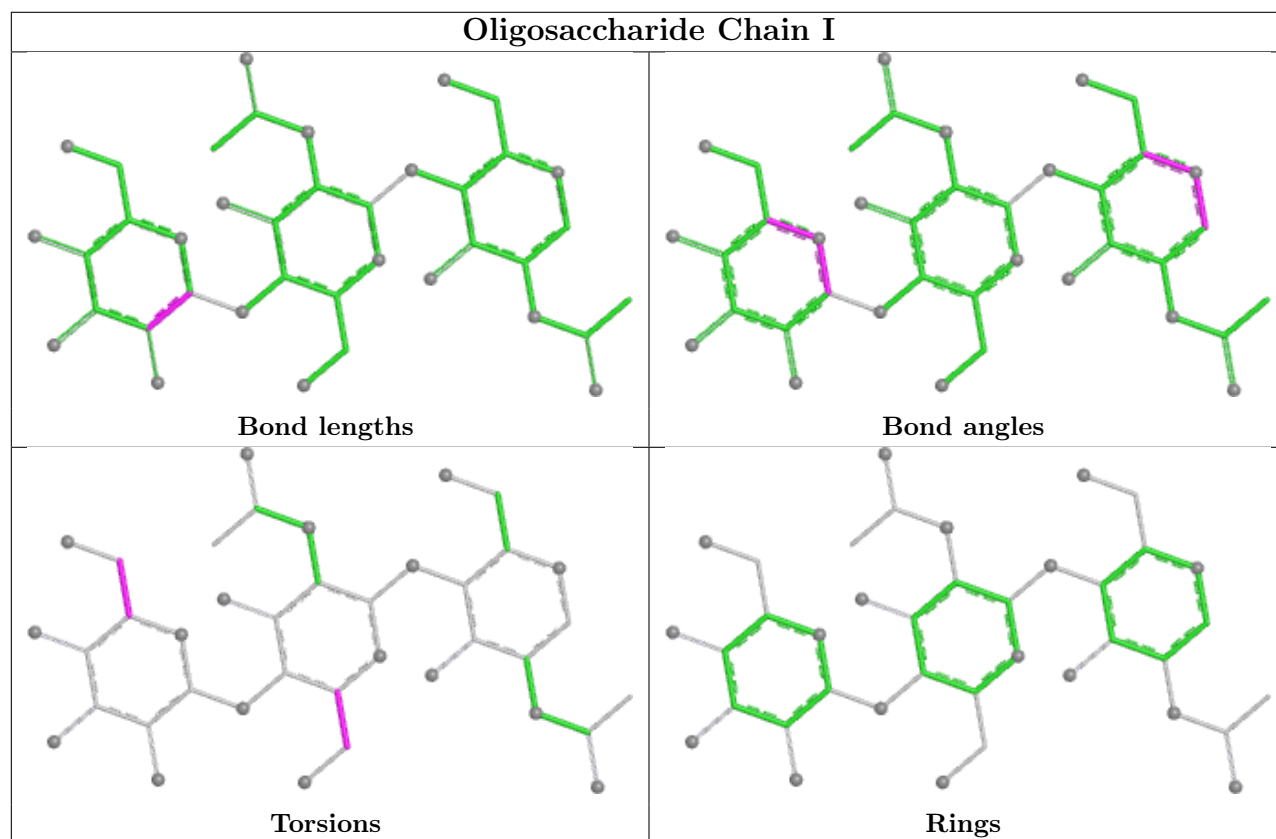
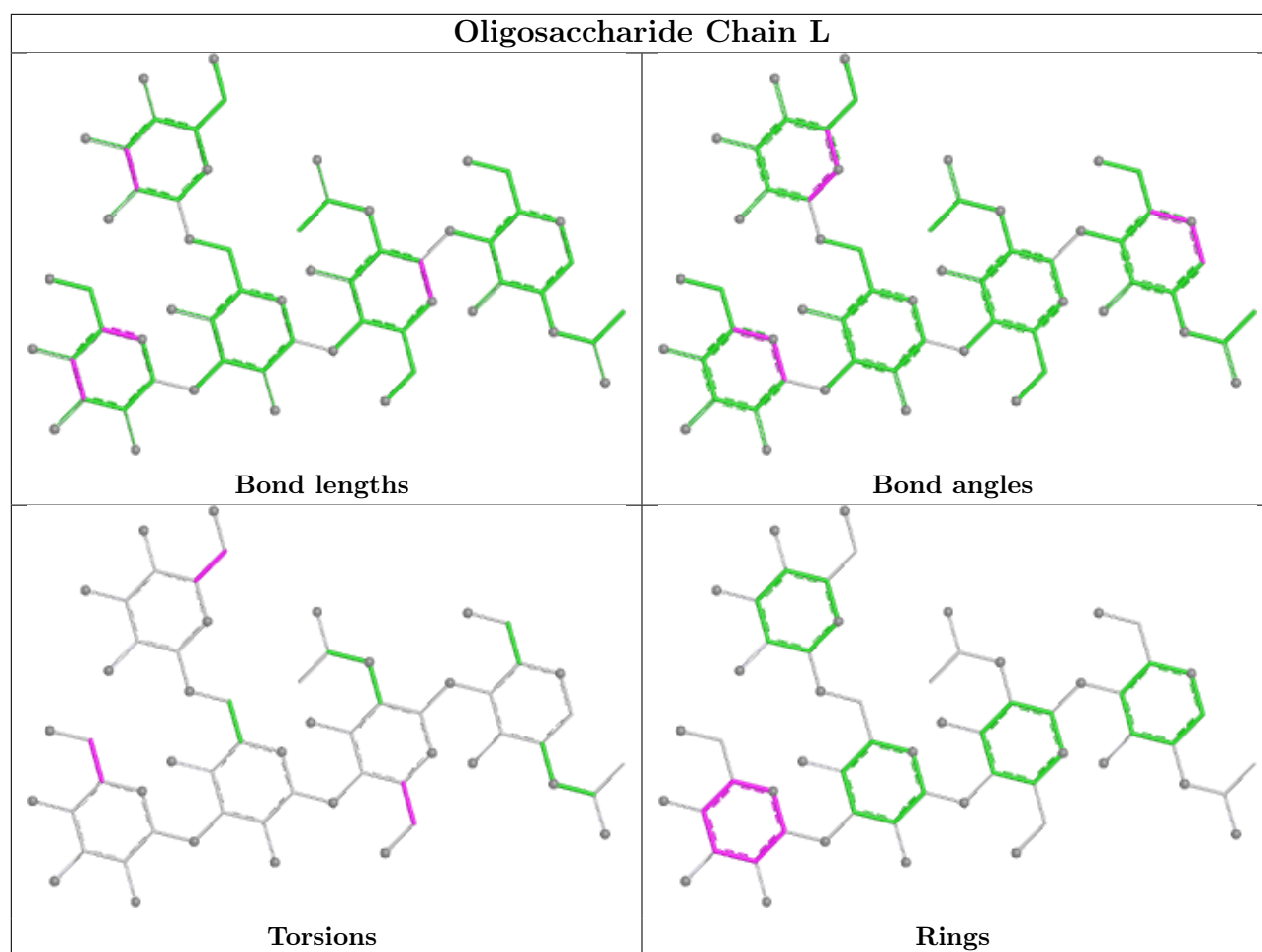












5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	1001	1	14,14,15	1.54	1 (7%)	17,19,21	1.26	2 (11%)
9	SO4	C	804	-	4,4,4	0.21	0	6,6,6	0.24	0
7	NAG	C	802	1	14,14,15	0.39	0	17,19,21	0.51	0
9	SO4	A	1003	-	4,4,4	0.26	0	6,6,6	0.32	0
7	NAG	C	801	1	14,14,15	1.09	2 (14%)	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	801	1	-	2/6/23/26	0/1/1/1
7	NAG	C	802	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	NAG	C1-C2	5.00	1.59	1.52
7	C	801	NAG	C1-C2	3.21	1.56	1.52
7	C	801	NAG	O5-C1	2.27	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	NAG	C4-C3-C2	3.71	116.45	111.02
7	A	1001	NAG	O5-C5-C4	-2.61	104.48	110.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	802	NAG	O5-C5-C6-O6
7	A	1001	NAG	C8-C7-N2-C2
7	A	1001	NAG	O7-C7-N2-C2
7	C	802	NAG	C4-C5-C6-O6
7	A	1001	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	597/606 (98%)	-0.49	8 (1%) 75 55	96, 126, 165, 201	0
1	C	598/606 (98%)	-0.49	5 (0%) 82 67	99, 126, 166, 207	0
2	B	196/218 (89%)	-0.11	4 (2%) 65 45	110, 139, 182, 222	0
2	D	195/218 (89%)	-0.25	2 (1%) 79 63	105, 138, 179, 225	0
All	All	1586/1648 (96%)	-0.41	19 (1%) 76 58	96, 129, 171, 225	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	332	ILE	6.2
1	C	577	LYS	3.7
1	C	614	ALA	3.6
2	B	430	THR	3.4
1	A	470	LYS	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(Å ²)	Q<0.9
4	NAG	K	2	14/15	0.12	0.14	149,225,241,244	0
3	BMA	E	3	11/12	0.35	0.13	225,248,263,264	0

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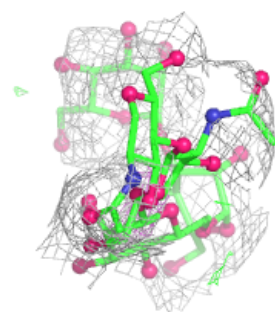
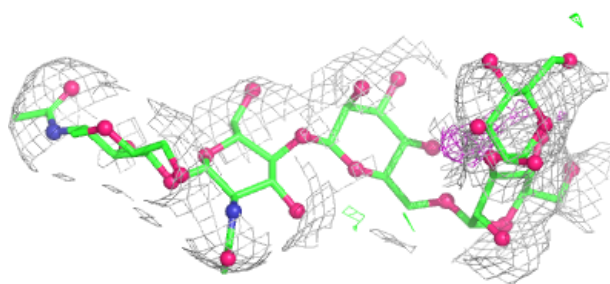
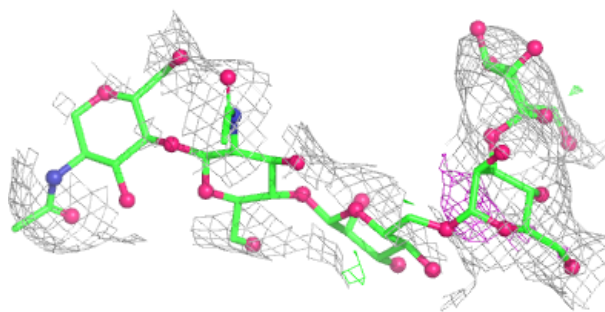
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	2	14/15	0.45	0.13	174,210,226,232	0
5	MAN	J	5	11/12	0.46	0.10	183,236,248,254	0
5	MAN	H	5	11/12	0.48	0.13	201,268,279,288	0
5	MAN	L	4	11/12	0.48	0.12	183,224,246,247	0
4	NAG	G	2	14/15	0.51	0.11	165,222,234,235	0
6	BMA	I	3	11/12	0.51	0.18	194,233,257,261	0
5	MAN	L	5	11/12	0.55	0.11	221,240,261,263	0
5	MAN	H	4	11/12	0.55	0.11	174,241,256,259	0
5	MAN	J	4	11/12	0.63	0.09	177,246,273,283	0
6	NAG	I	2	14/15	0.71	0.13	181,211,243,269	0
4	NAG	F	2	14/15	0.72	0.12	164,228,249,252	0
5	BMA	J	3	11/12	0.73	0.08	209,267,286,301	0
3	MAN	E	4	11/12	0.75	0.12	233,268,291,297	0
3	NAG	E	2	14/15	0.75	0.11	171,194,234,258	0
3	MAN	E	5	11/12	0.82	0.17	182,228,279,298	0
5	BMA	H	3	11/12	0.82	0.07	223,253,260,262	0
5	NAG	J	2	14/15	0.82	0.11	158,202,235,257	0
5	NAG	L	2	14/15	0.82	0.10	172,203,223,241	0
5	BMA	L	3	11/12	0.83	0.08	234,238,246,248	0
5	NAG	H	2	14/15	0.88	0.09	175,200,230,253	0
4	NAG	M	1	14/15	0.88	0.11	132,157,199,203	0
5	NAG	H	1	14/15	0.89	0.10	149,177,186,199	0
6	NAG	I	1	14/15	0.89	0.13	128,163,201,211	0
5	NAG	J	1	14/15	0.89	0.11	143,152,172,193	0
4	NAG	G	1	14/15	0.89	0.12	164,184,216,217	0
5	NAG	L	1	14/15	0.91	0.11	149,174,186,197	0
4	NAG	K	1	14/15	0.91	0.11	143,168,198,216	0
4	NAG	F	1	14/15	0.93	0.10	164,173,215,239	0
3	NAG	E	1	14/15	0.96	0.07	143,148,160,183	0

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

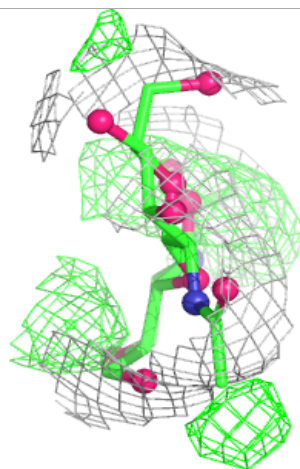
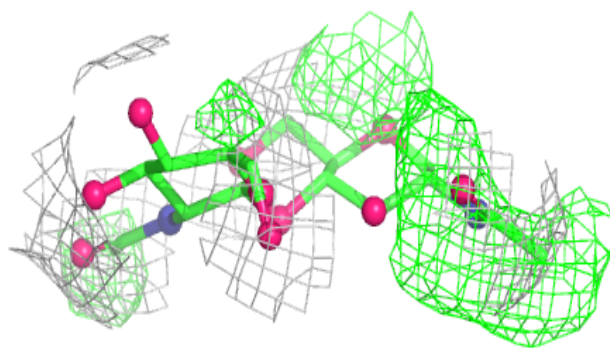
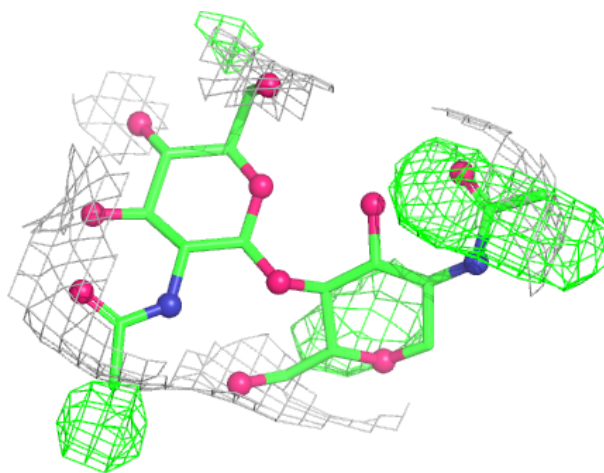
Electron density around Chain E:

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



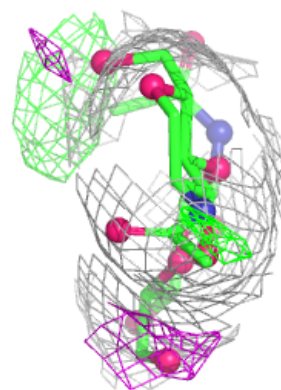
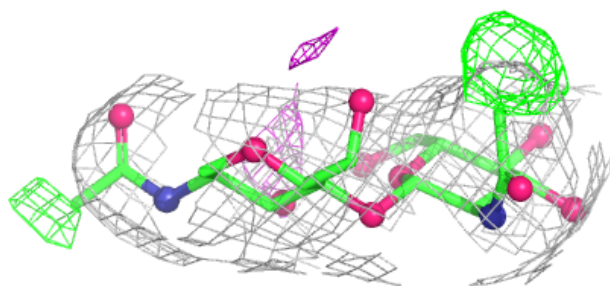
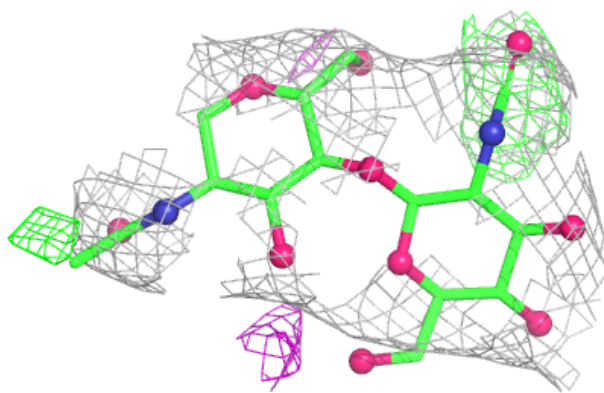
Electron density around Chain F:

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and green (positive)



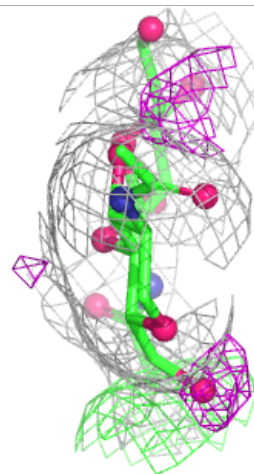
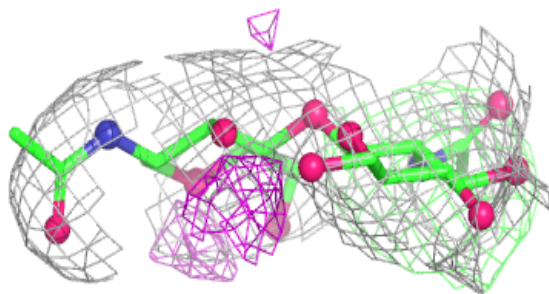
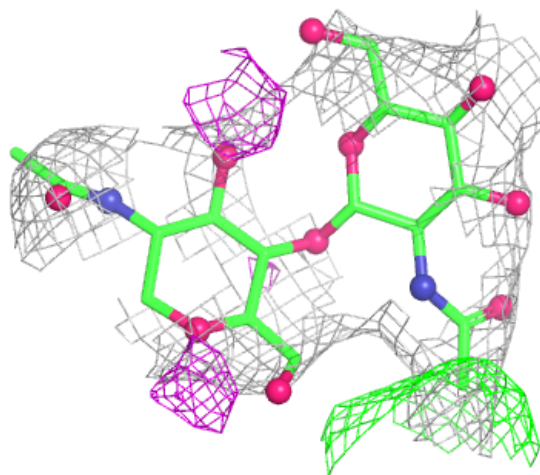
Electron density around Chain G:

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and green (positive)



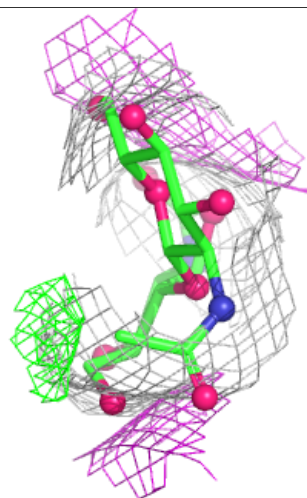
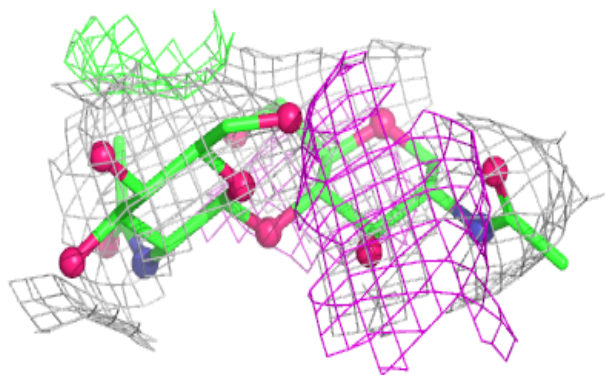
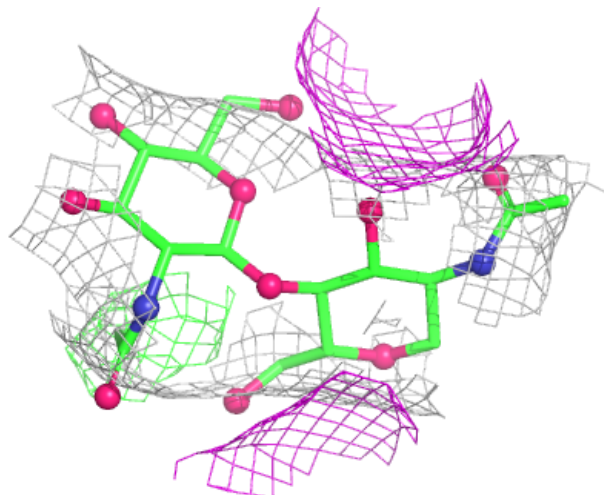
Electron density around Chain K:

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and green (positive)



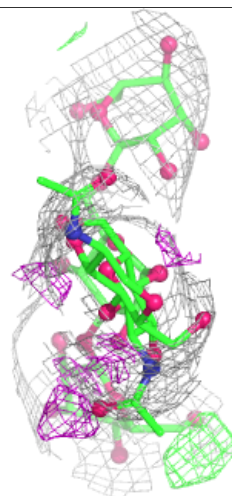
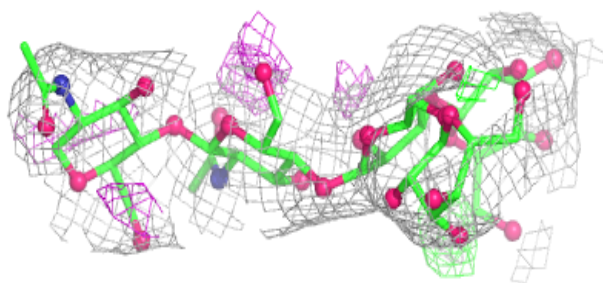
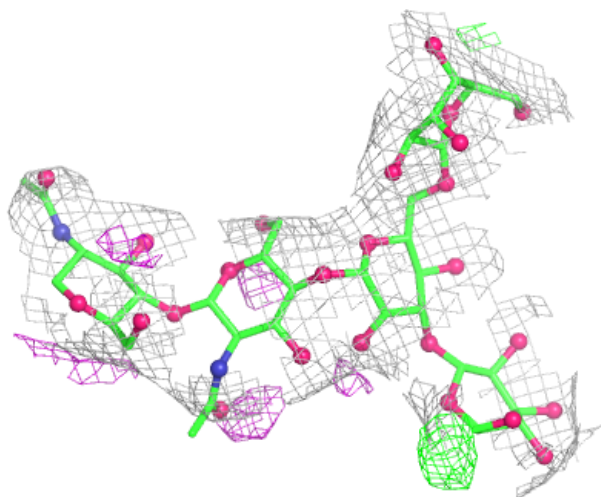
Electron density around Chain M:

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



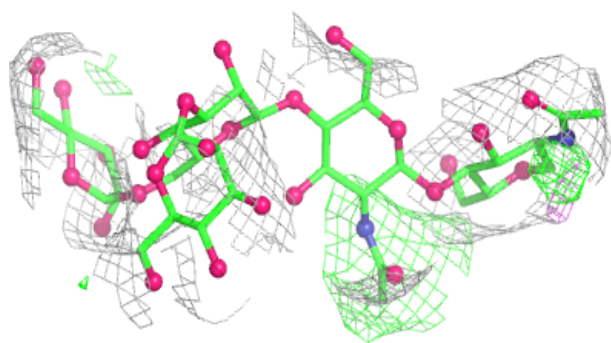
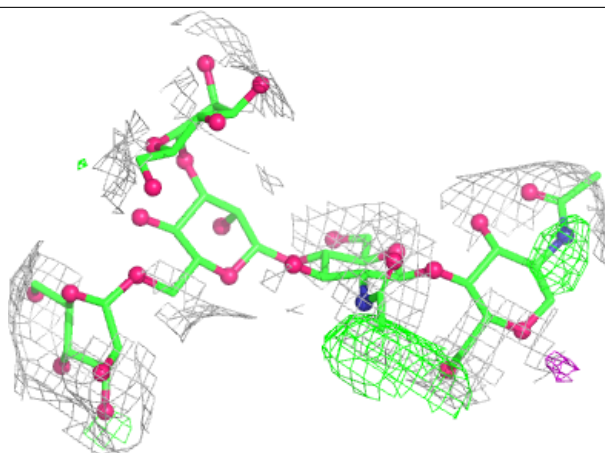
Electron density around Chain H:

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



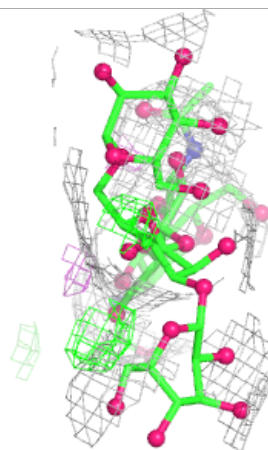
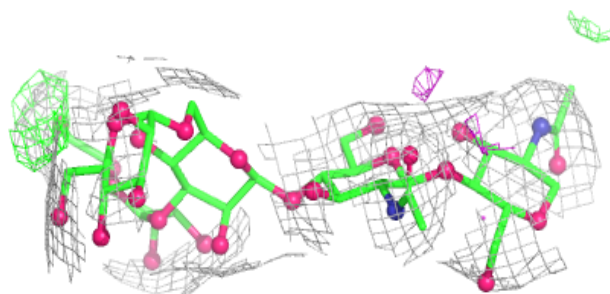
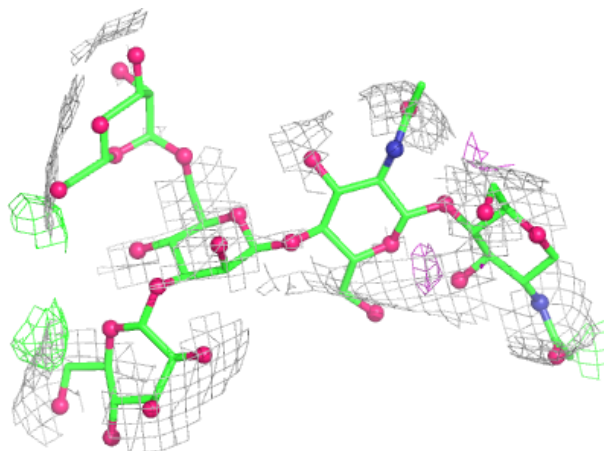
Electron density around Chain J:

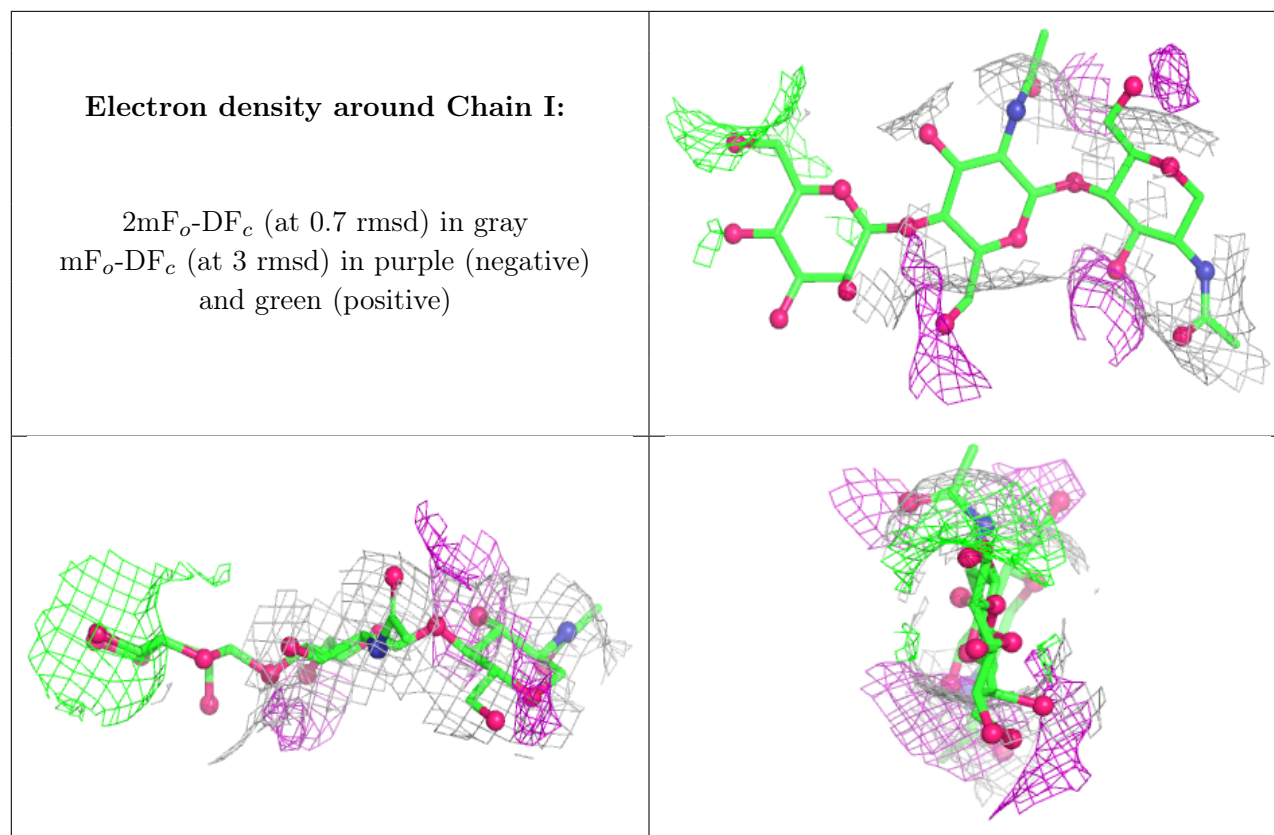
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	NAG	A	1001	14/15	0.70	0.10	160,192,215,218	0
7	NAG	C	802	14/15	0.72	0.12	170,194,215,224	0
7	NAG	C	801	14/15	0.91	0.08	123,159,193,202	0
9	SO4	A	1003	5/5	0.97	0.08	121,132,142,150	0
9	SO4	C	804	5/5	0.97	0.10	125,136,157,157	0
8	ZN	A	1002	1/1	1.00	0.03	144,144,144,144	0
8	ZN	C	803	1/1	1.00	0.04	167,167,167,167	0

6.5 Other polymers [i](#)

There are no such residues in this entry.