



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 2A0Z / pdb_00002a0z
Title : The molecular structure of toll-like receptor 3 ligand binding domain
Authors : Bell, J.K.; Botos, I.; Hall, P.R.; Askins, J.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on : 2005-06-17
Resolution : 2.40 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

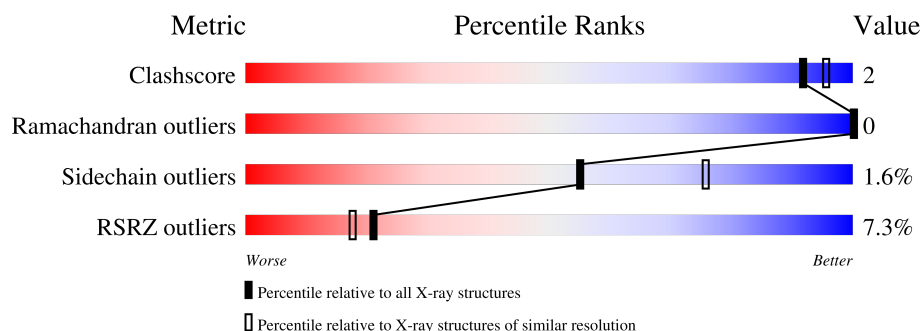
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



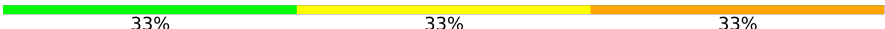
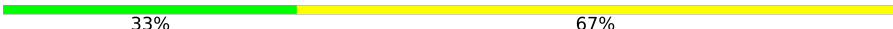
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	705	7% 88% 7% 5%
2	B	2	50% 50%
2	C	2	50% 50%
2	D	2	50% 50%
2	F	2	50% 50%
2	G	2	100%

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Mol	Chain	Length	Quality of chain
3	E	3	 67%33%
4	H	3	 33%33%33%
4	J	3	 33%67%
5	I	5	 100%
6	K	2	 50%50%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6183 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	6	0
			5420	3459	919	1023	19			

There are 23 discrepancies between the modelled and reference sequences:

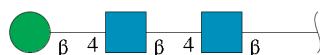
Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLU	-	SEE REMARK 999	UNP O15455
A	705	ASN	-	SEE REMARK 999	UNP O15455
A	706	LEU	-	SEE REMARK 999	UNP O15455
A	707	TYR	-	SEE REMARK 999	UNP O15455
A	708	PHE	-	SEE REMARK 999	UNP O15455
A	709	GLN	-	SEE REMARK 999	UNP O15455
A	710	GLY	-	SEE REMARK 999	UNP O15455
A	711	ASP	-	SEE REMARK 999	UNP O15455
A	712	TYR	-	SEE REMARK 999	UNP O15455
A	713	LYS	-	SEE REMARK 999	UNP O15455
A	714	ASP	-	SEE REMARK 999	UNP O15455
A	715	ASP	-	SEE REMARK 999	UNP O15455
A	716	ASP	-	SEE REMARK 999	UNP O15455
A	717	ASP	-	SEE REMARK 999	UNP O15455
A	718	LYS	-	SEE REMARK 999	UNP O15455
A	719	GLY	-	expression tag	UNP O15455
A	720	SER	-	expression tag	UNP O15455
A	721	HIS	-	expression tag	UNP O15455
A	722	HIS	-	expression tag	UNP O15455
A	723	HIS	-	expression tag	UNP O15455
A	724	HIS	-	expression tag	UNP O15455
A	725	HIS	-	expression tag	UNP O15455
A	726	HIS	-	expression tag	UNP O15455

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



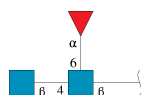
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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.



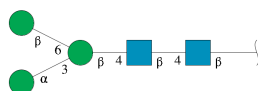
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			37	22	2	13			
4	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-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.



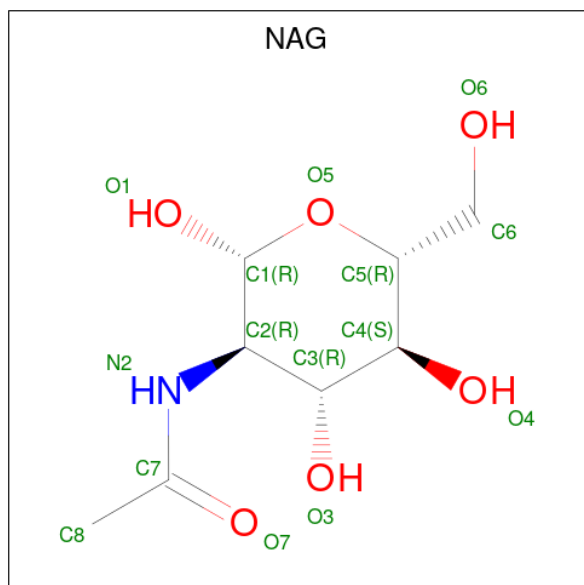
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



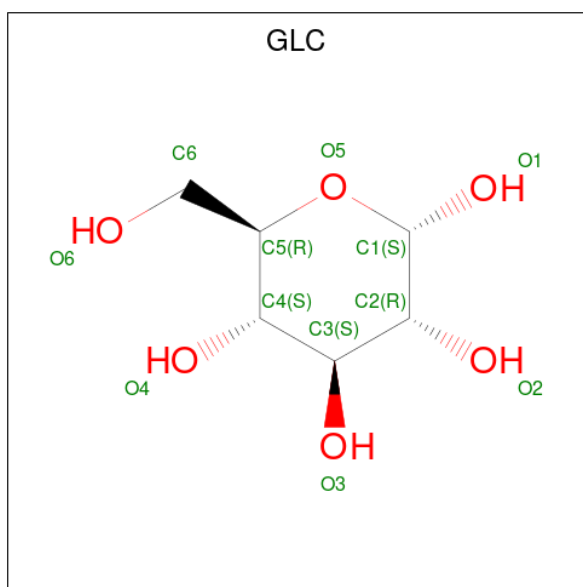
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



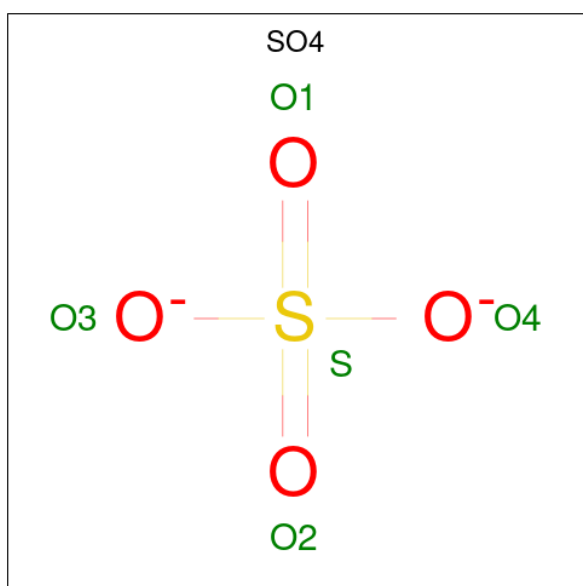
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		
8	A	1	Total	C	O	0	0
			12	6	6		

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



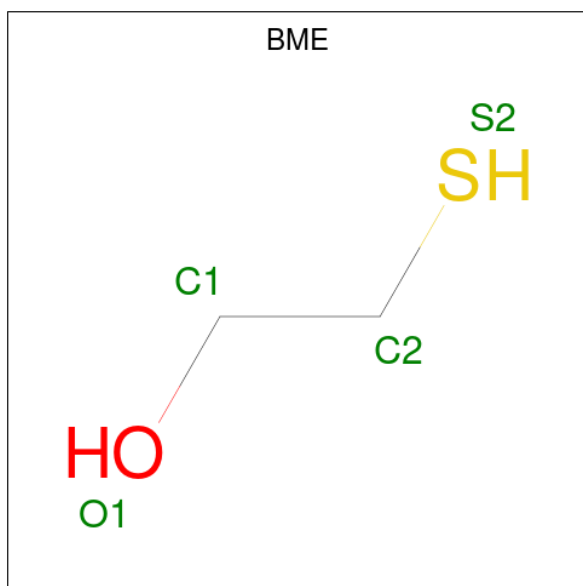
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 10 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			4	2	1	1		

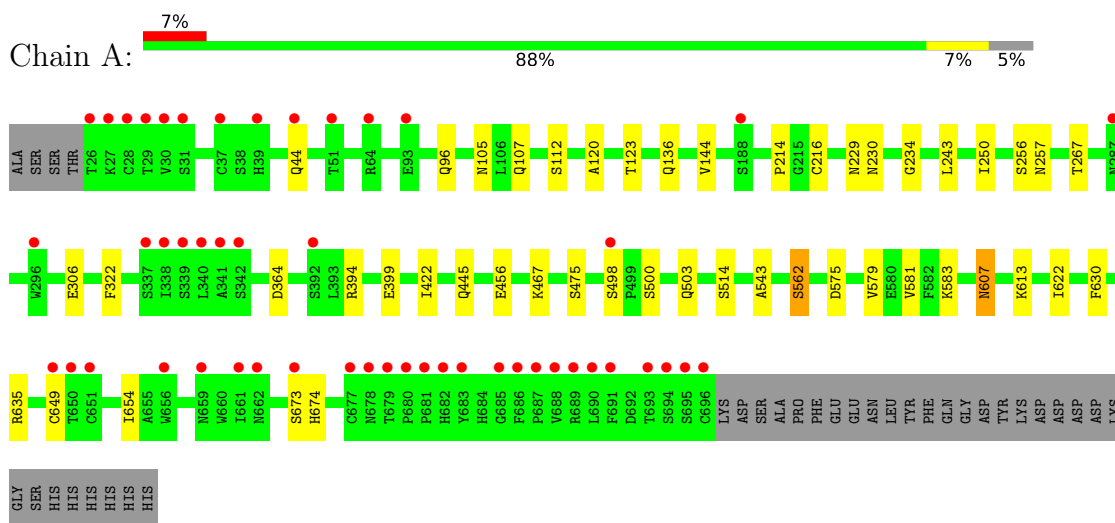
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	363	Total	O	0	0
			363	363		

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: Toll-like receptor 3



- 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





- 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 3: 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[beta-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 6: 2-acetamido-2-deoxy- α -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  50% 50%

MAC1
JUGZ

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.60Å 160.79Å 122.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.42	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-2.40) 93.5 (50.00-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.232 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6183	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: GLC, SO4, BME, NAG, BMA, NDG, FUC, 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	0.78	0/5533	1.06	29/7511 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	HIS	N-CA-C	8.30	122.72	112.59
1	A	673	SER	N-CA-C	7.22	120.57	111.69
1	A	394	ARG	N-CA-C	7.19	119.12	111.28
1	A	607	ASN	N-CA-C	6.84	119.58	111.71
1	A	622	ILE	N-CA-C	6.65	117.67	108.89
1	A	581	VAL	N-CA-C	6.31	118.97	111.09
1	A	500	SER	N-CA-C	6.22	116.75	109.60
1	A	216	CYS	N-CA-C	6.21	118.85	111.33
1	A	250	ILE	N-CA-C	6.04	117.22	109.30
1	A	144	VAL	N-CA-C	6.00	118.55	111.05
1	A	635	ARG	N-CA-C	5.93	121.09	111.37
1	A	120	ALA	N-CA-C	5.72	118.29	111.71
1	A	562	SER	N-CA-C	5.72	119.36	112.38
1	A	630	PHE	N-CA-C	5.69	120.22	113.28
1	A	456	GLU	N-CA-C	5.69	120.06	113.18
1	A	475	SER	N-CA-C	5.69	118.21	111.33
1	A	364	ASP	N-CA-C	5.62	118.05	111.02
1	A	234	GLY	CA-C-N	5.60	125.06	119.24
1	A	234	GLY	C-N-CA	5.60	125.06	119.24
1	A	649	CYS	N-CA-C	5.53	117.51	109.71
1	A	583	LYS	N-CA-C	5.48	117.68	111.11
1	A	322	PHE	N-CA-C	5.44	119.66	113.19
1	A	579	VAL	N-CA-C	5.35	118.55	111.17
1	A	123	THR	N-CA-C	5.33	119.05	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLU	N-CA-C	5.31	117.57	110.35
1	A	112	SER	N-CA-C	5.14	118.01	111.69
1	A	514	SER	N-CA-C	5.11	117.27	110.53
1	A	267	THR	N-CA-C	5.05	117.17	111.11
1	A	543	ALA	N-CA-C	5.02	119.65	111.37

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	5420	0	5399	15	1
2	B	28	0	25	1	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	E	39	0	34	0	0
4	H	37	0	32	1	0
4	J	38	0	34	2	0
5	I	61	0	52	0	0
6	K	28	0	24	0	0
7	A	14	0	13	0	0
8	A	24	0	24	0	0
9	A	15	0	0	0	0
10	A	4	0	5	0	0
11	A	363	0	0	1	0
All	All	6183	0	5742	19	1

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 2.

All (19) 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:422:ILE:H	1:A:445:GLN:HE22	1.23	0.86
4:J:1:NAG:H61	4:J:2:NAG:H82	1.72	0.70
1:A:230[A]:ASN:ND2	1:A:257:ASN:HD22	1.95	0.64
1:A:422:ILE:N	1:A:445:GLN:HE22	1.98	0.56
1:A:230[A]:ASN:HD22	1:A:257:ASN:HD22	1.52	0.55
1:A:230[A]:ASN:HD22	1:A:257:ASN:ND2	2.06	0.54
1:A:399:GLU:OE2	4:H:1:NAG:H83	2.08	0.52
1:A:422:ILE:H	1:A:445:GLN:NE2	2.02	0.52
1:A:229[A]:ASN:HD22	1:A:256:SER:H	1.57	0.51
1:A:562:SER:HB3	11:A:6550:HOH:O	2.11	0.51
1:A:229[A]:ASN:ND2	1:A:256:SER:H	2.09	0.51
4:J:1:NAG:H61	4:J:2:NAG:C8	2.42	0.47
1:A:44:GLN:OE1	2:C:2:NAG:H62	2.16	0.46
1:A:105:ASN:C	1:A:105:ASN:HD22	2.23	0.46
2:D:1:NAG:H82	2:D:1:NAG:H3	1.99	0.45
1:A:105:ASN:HD22	1:A:107:GLN:H	1.65	0.44
1:A:105:ASN:ND2	1:A:107:GLN:H	2.16	0.43
2:B:1:NAG:H61	2:B:2:NAG:N2	2.33	0.42
1:A:105:ASN:HD21	1:A:107:GLN:HG2	1.86	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASP:OD2	1:A:575:ASP:OD2[4_555]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	674/705 (96%)	634 (94%)	40 (6%)	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	631/656 (96%)	621 (98%)	10 (2%)	55 76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	136	GLN
1	A	214	PRO
1	A	243	LEU
1	A	467	LYS
1	A	498	SER
1	A	503	GLN
1	A	607	ASN
1	A	613	LYS
1	A	654	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	62	GLN
1	A	105	ASN
1	A	108	HIS
1	A	169	GLN
1	A	229[A]	ASN
1	A	259	GLN
1	A	309	ASN
1	A	311	GLN
1	A	445	GLN
1	A	494	ASN
1	A	515	ASN
1	A	539	HIS
1	A	550	ASN
1	A	607	ASN

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Mol	Chain	Res	Type
1	A	618	GLN
1	A	659	ASN
1	A	678	ASN
1	A	682	HIS

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 ⓘ

26 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	B	1	1,2	14,14,15	0.70	0	17,19,21	0.54	0
2	NAG	B	2	2	14,14,15	0.57	0	17,19,21	0.70	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	0.50	0
2	NAG	D	1	1,2	14,14,15	0.60	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.59	0	17,19,21	0.66	0
3	NAG	E	1	1,3	14,14,15	0.48	0	17,19,21	0.69	0
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
3	BMA	E	3	3	11,11,12	0.55	0	15,15,17	0.21	0
2	NAG	F	1	1,2	14,14,15	0.60	0	17,19,21	0.67	0
2	NAG	F	2	2	14,14,15	0.61	0	17,19,21	0.68	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.52	0	17,19,21	0.63	0
2	NAG	G	2	2	14,14,15	0.58	0	17,19,21	0.59	0
4	NAG	H	1	1,9,4	13,13,15	1.07	1 (7%)	15,17,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	2	4	14,14,15	0.60	0	17,19,21	0.73	1 (5%)
4	FUC	H	3	4	10,10,11	0.63	0	14,14,16	0.31	0
5	NAG	I	1	1,5	14,14,15	0.52	0	17,19,21	0.65	0
5	NAG	I	2	5	14,14,15	0.56	0	17,19,21	0.66	0
5	BMA	I	3	5	11,11,12	0.63	0	15,15,17	0.48	0
5	MAN	I	4	5	11,11,12	0.69	0	15,15,17	0.57	0
5	BMA	I	5	5	11,11,12	0.64	0	15,15,17	0.44	0
4	NAG	J	1	1,4	14,14,15	0.61	0	17,19,21	0.77	0
4	NAG	J	2	4	14,14,15	0.71	0	17,19,21	0.80	0
4	FUC	J	3	4	10,10,11	0.69	0	14,14,16	0.35	0
6	NAG	K	1	1,6	14,14,15	1.07	1 (7%)	17,19,21	0.68	0
6	NDG	K	2	6	14,14,15	0.69	0	17,19,21	0.67	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
2	NAG	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,9,4	-	2/6/19/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	1/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	C1-C2	3.16	1.55	1.51
6	K	1	NAG	C1-C2	2.22	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C2-N2-C7	-2.20	119.95	122.90
3	E	2	NAG	C2-N2-C7	-2.10	120.08	122.90
2	F	2	NAG	C2-N2-C7	-2.09	120.10	122.90
2	B	2	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C3-C2-N2-C7
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
6	K	1	NAG	C3-C2-N2-C7
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	K	2	NDG	C8-C7-N2-C2
6	K	2	NDG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
5	I	3	BMA	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
4	J	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
6	K	2	NDG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
6	K	2	NDG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6

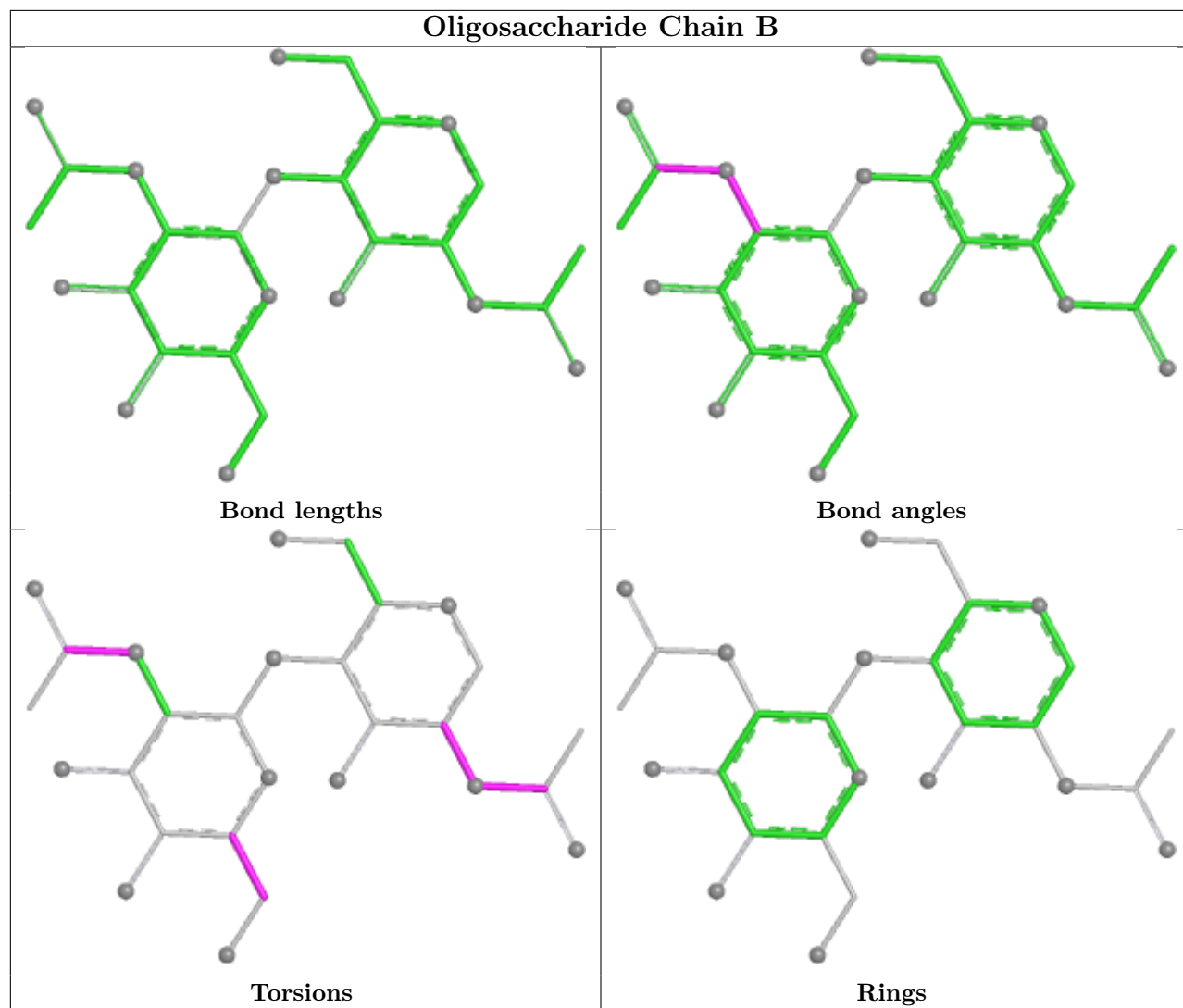
All (1) ring outliers are listed below:

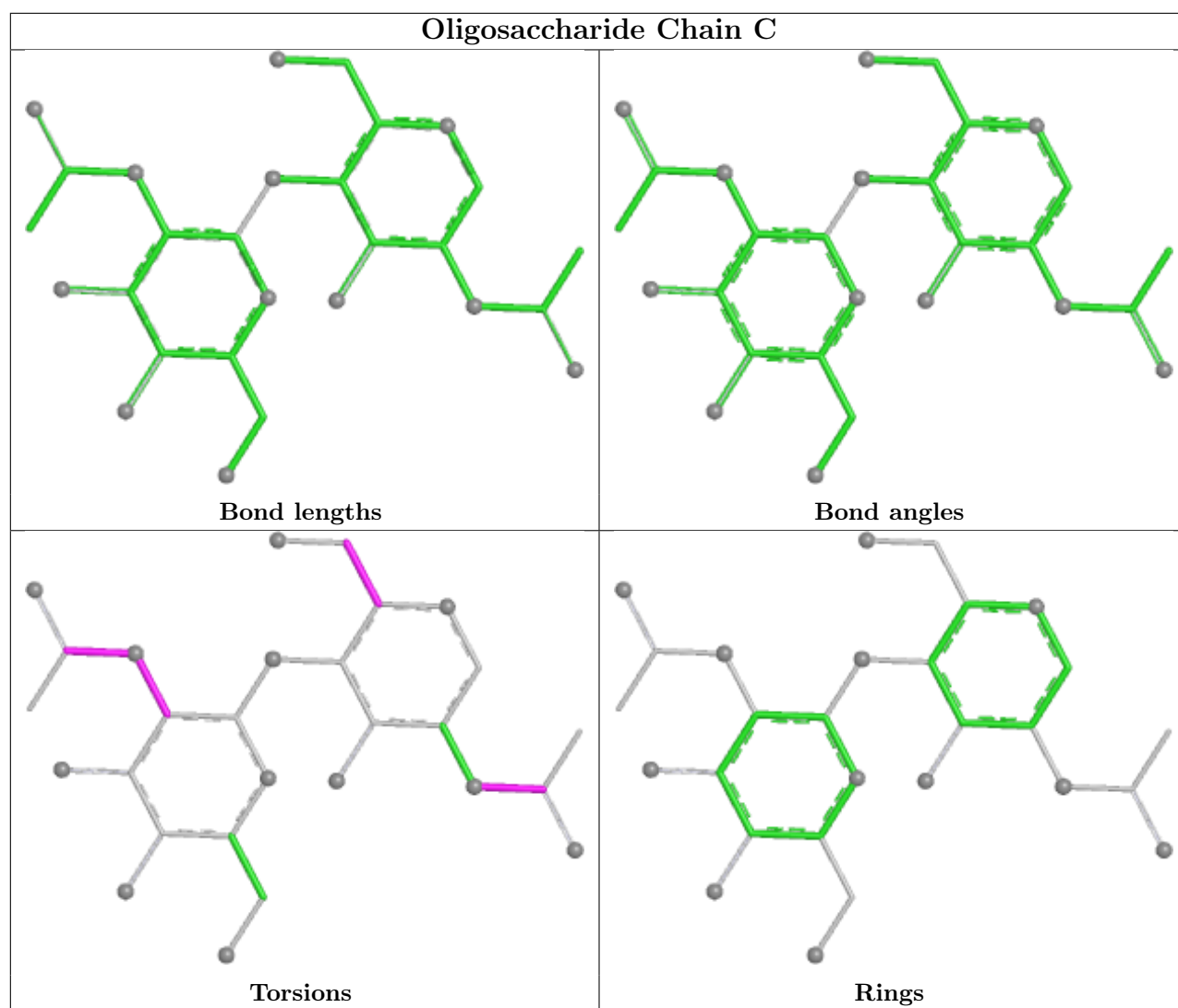
Mol	Chain	Res	Type	Atoms
5	I	4	MAN	C1-C2-C3-C4-C5-O5

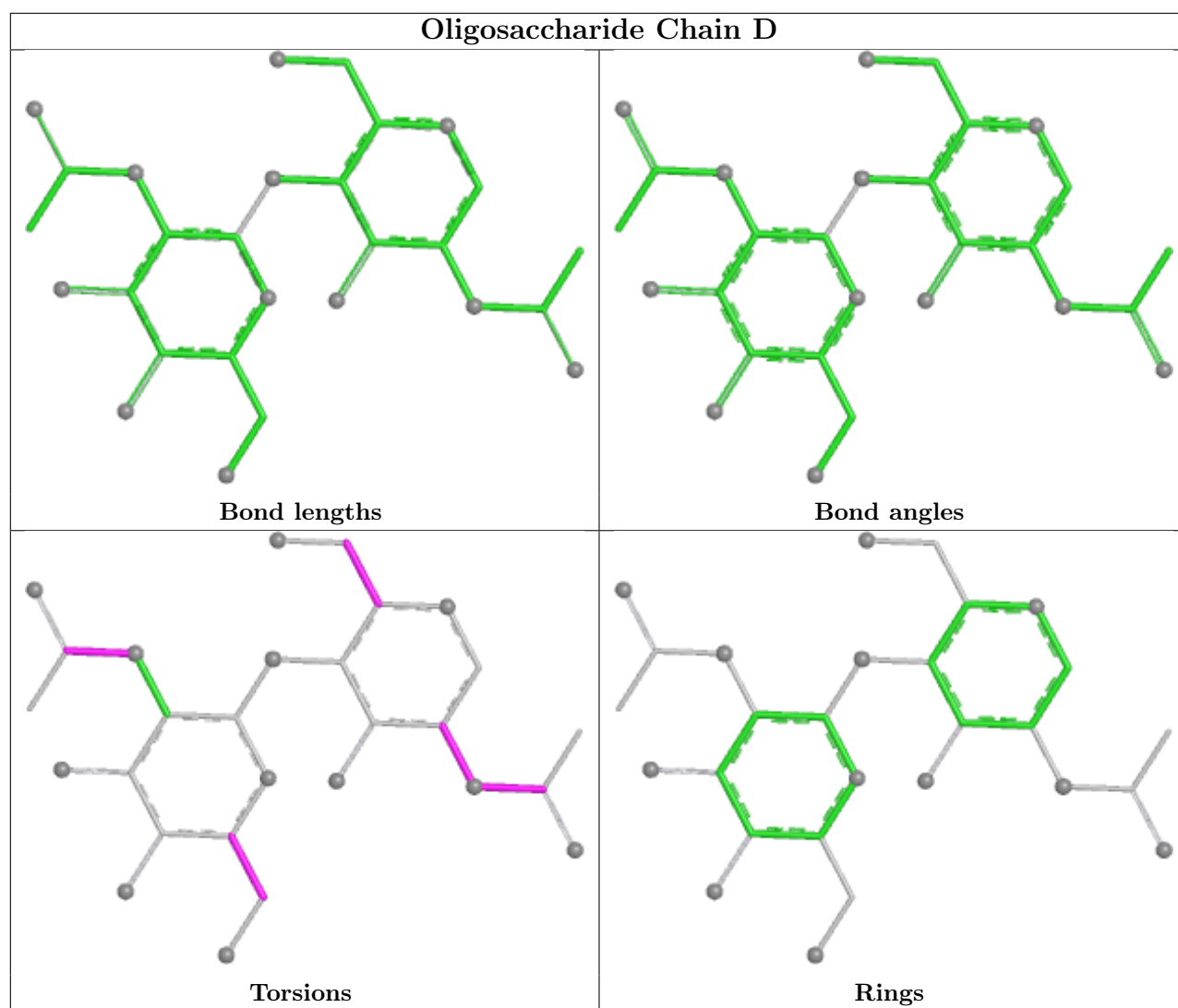
7 monomers are involved in 6 short contacts:

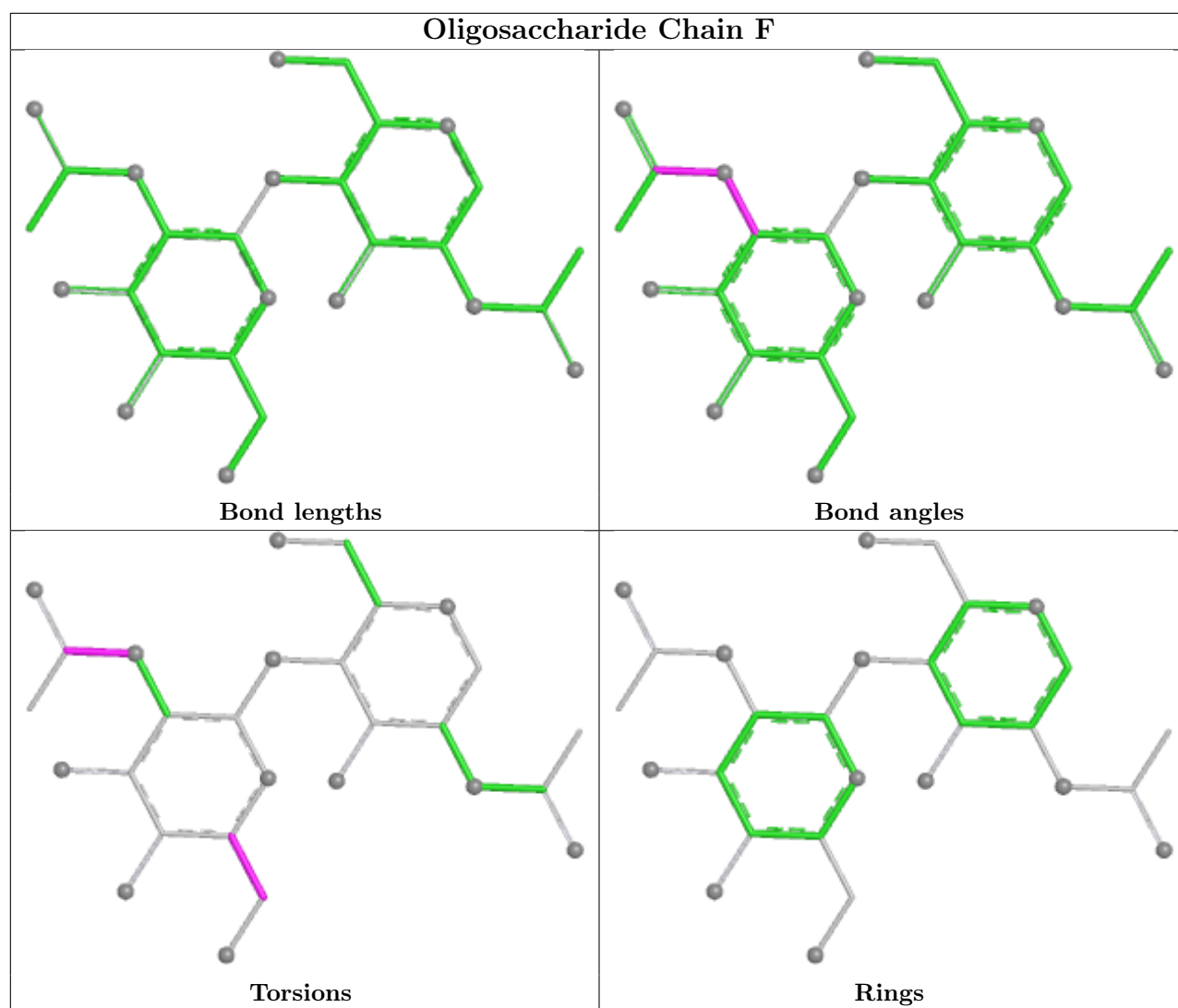
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
4	J	2	NAG	2	0
4	H	1	NAG	1	0
2	B	2	NAG	1	0
4	J	1	NAG	2	0
2	C	2	NAG	1	0
2	D	1	NAG	1	0

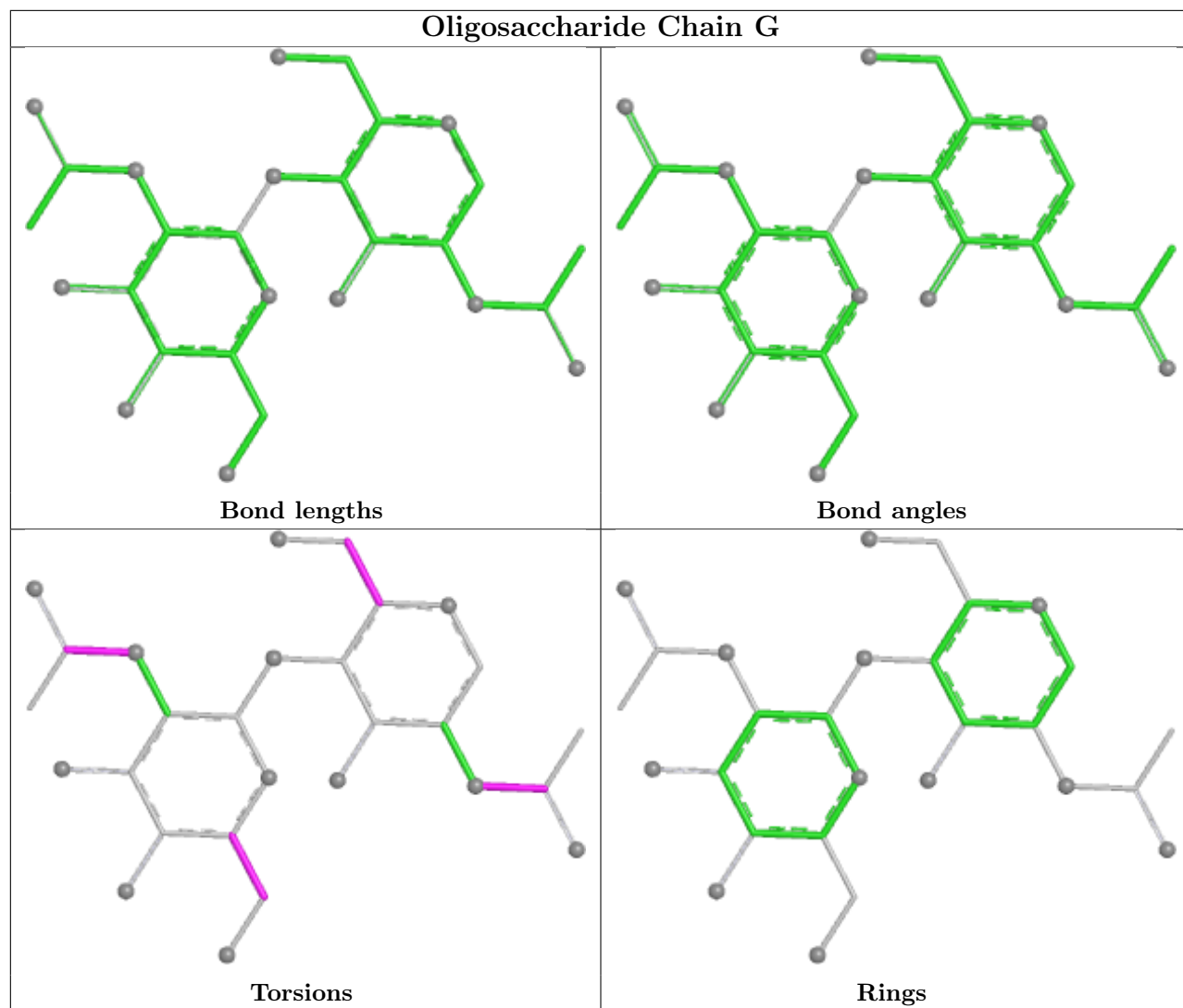
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

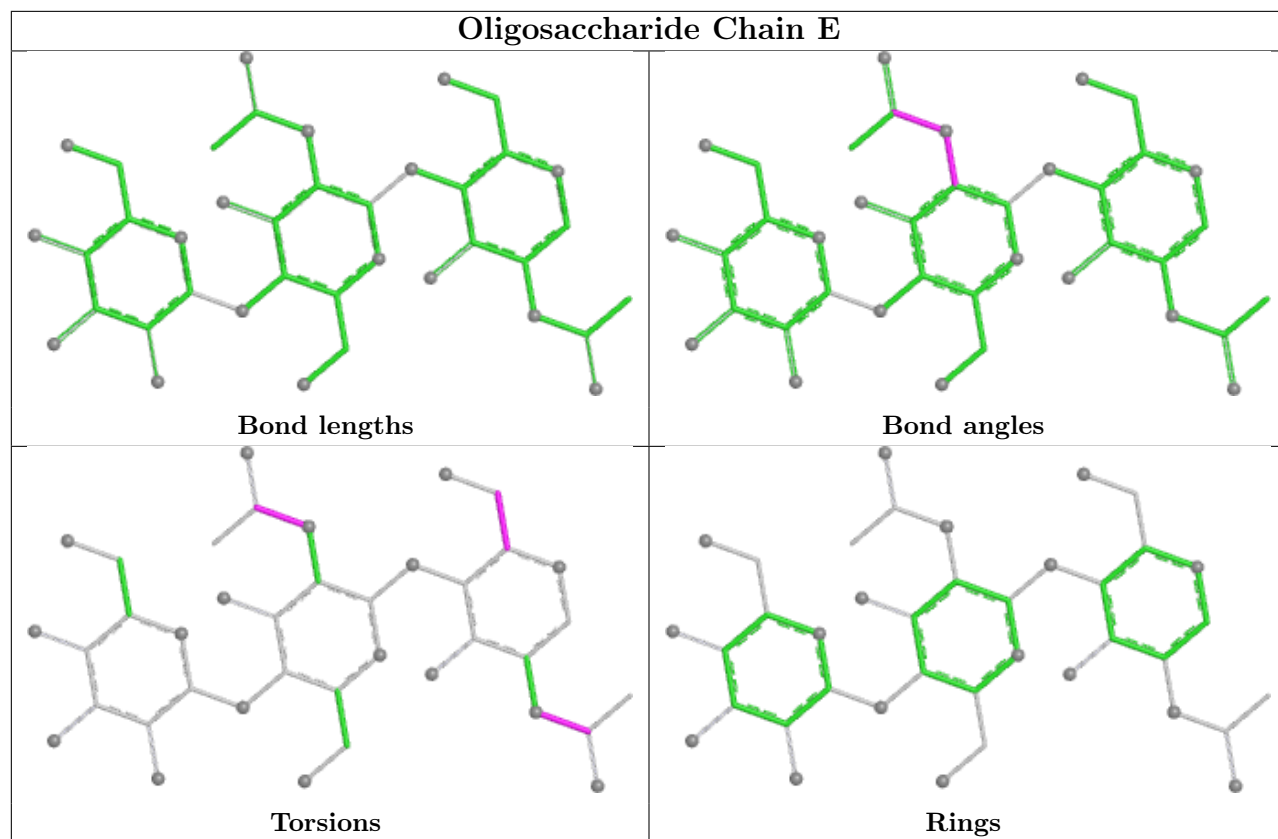


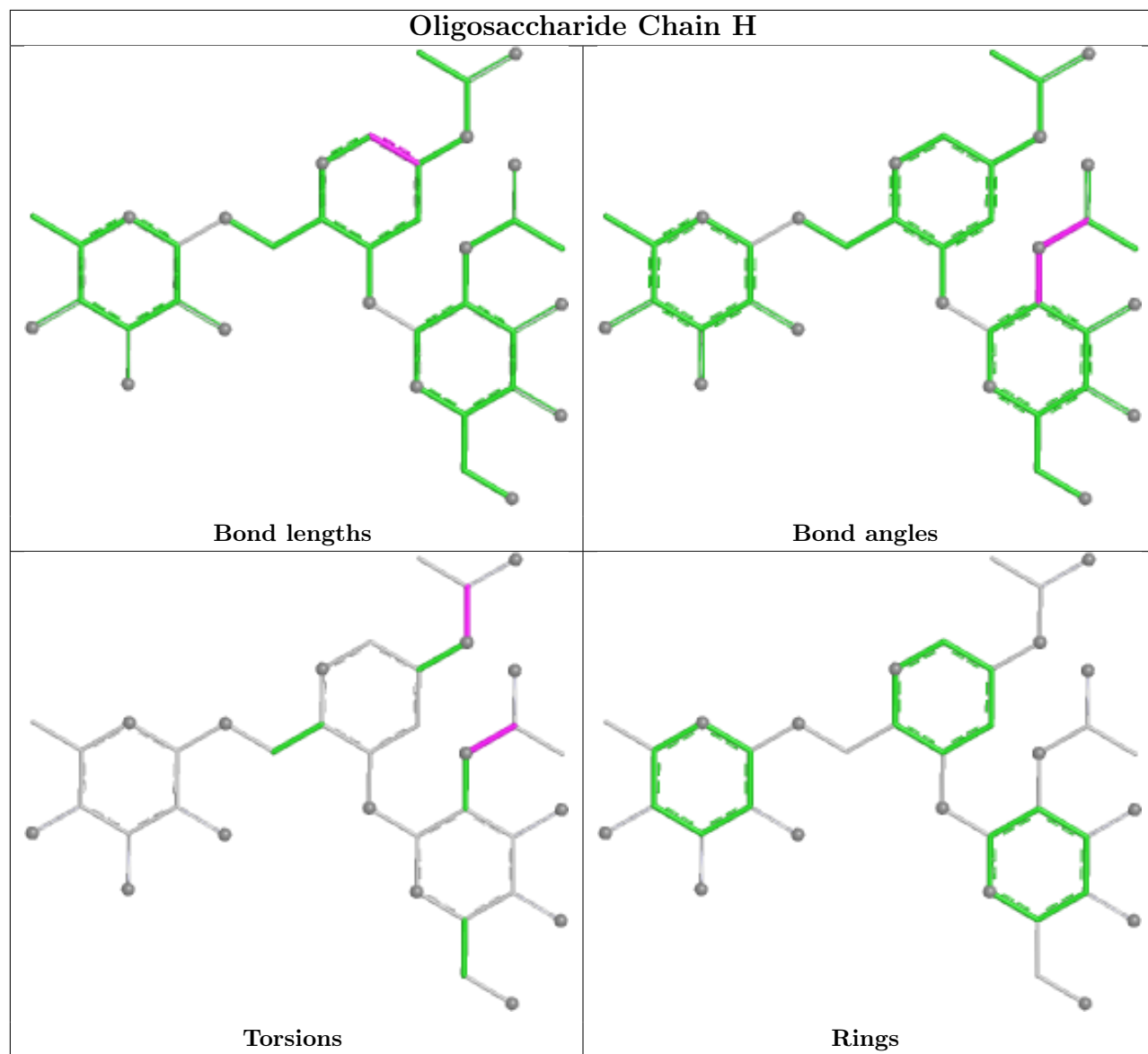


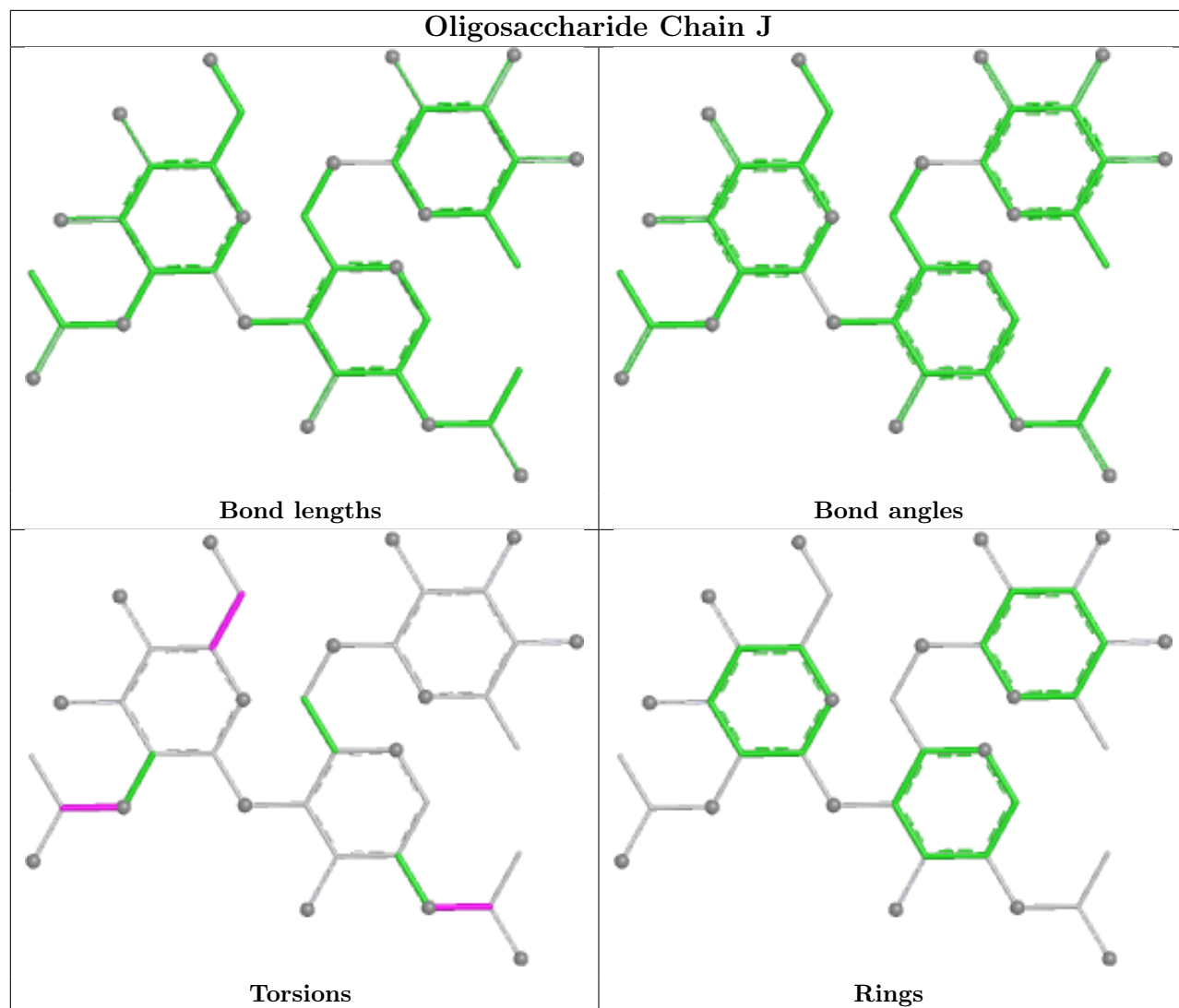


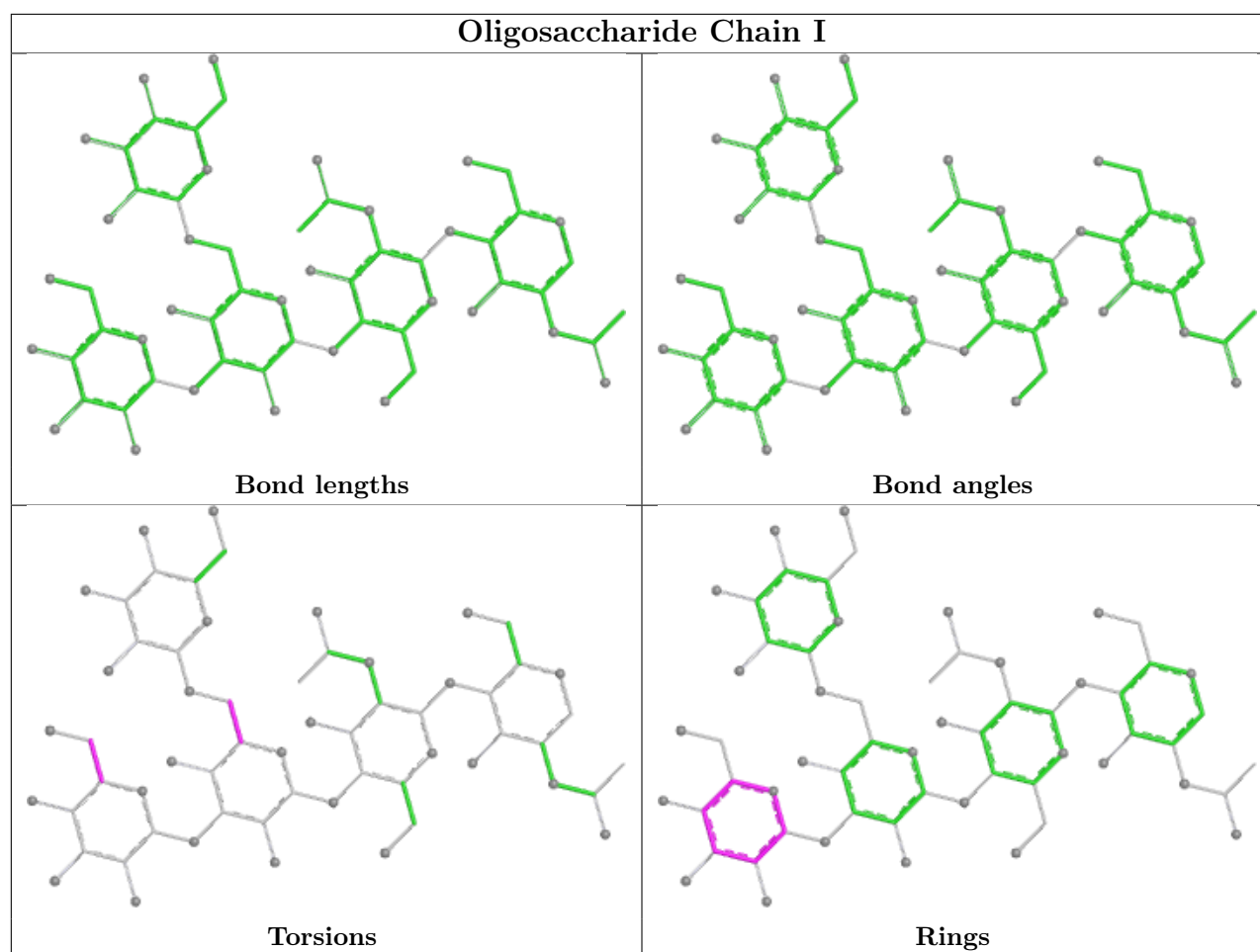


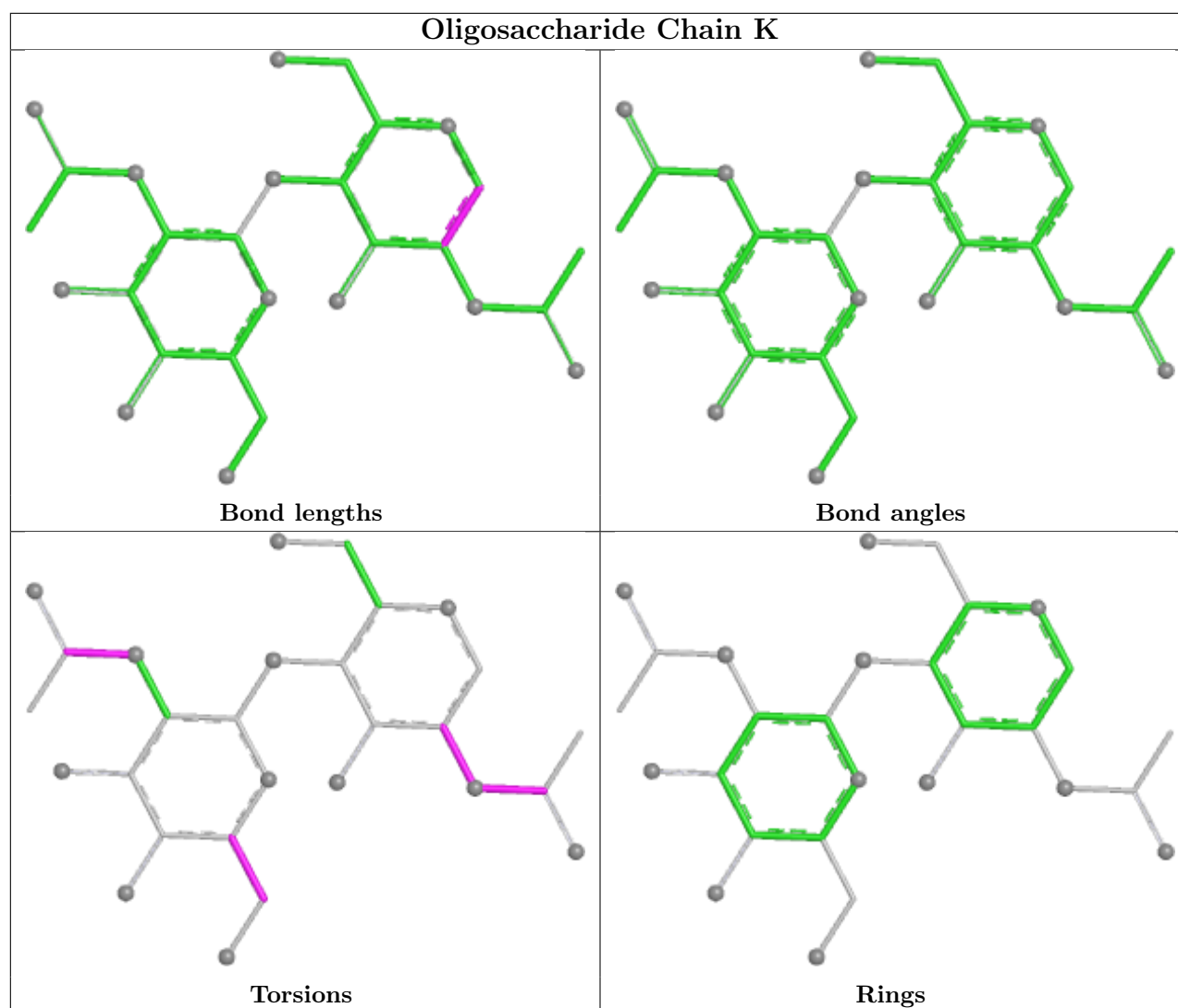












5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
9	SO4	A	750	-	4,4,4	0.35	0	6,6,6	0.13	0
9	SO4	A	751	-	4,4,4	0.36	0	6,6,6	0.08	0
7	NAG	A	1961	1	14,14,15	0.70	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	A	752	4	4,4,4	0.45	0	6,6,6	0.22	0
8	GLC	A	754	-	12,12,12	1.61	1 (8%)	17,17,17	1.55	3 (17%)
8	GLC	A	753	-	12,12,12	1.70	2 (16%)	17,17,17	1.60	4 (23%)
10	BME	A	1270	1	3,3,3	0.43	0	2,2,2	0.32	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
8	GLC	A	754	-	-	2/2/22/22	0/1/1/1
8	GLC	A	753	-	-	2/2/22/22	0/1/1/1
7	NAG	A	1961	1	-	2/6/23/26	0/1/1/1
10	BME	A	1270	1	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	753	GLC	O5-C1	4.67	1.54	1.42
8	A	754	GLC	O5-C1	4.62	1.54	1.42
8	A	753	GLC	C4-C5	2.13	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	754	GLC	O5-C5-C6	3.48	115.06	106.44
8	A	753	GLC	O5-C5-C6	3.39	114.83	106.44
8	A	753	GLC	C6-C5-C4	-3.33	104.83	113.02
8	A	754	GLC	C6-C5-C4	-3.28	104.95	113.02
8	A	753	GLC	O6-C6-C5	-2.41	103.13	111.33
8	A	754	GLC	O6-C6-C5	-2.18	103.92	111.33
7	A	1961	NAG	C2-N2-C7	-2.15	120.01	122.90
8	A	753	GLC	O1-C1-C2	2.09	115.04	108.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1961	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	1961	NAG	O7-C7-N2-C2
8	A	754	GLC	O5-C5-C6-O6
8	A	754	GLC	C4-C5-C6-O6
8	A	753	GLC	O5-C5-C6-O6
8	A	753	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	671/705 (95%)	0.36	49 (7%) 21 17	15, 39, 76, 95	5 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	696	CYS	7.0
1	A	340	LEU	6.9
1	A	338	ILE	6.2
1	A	26	THR	5.2
1	A	683	TYR	5.0
1	A	681	PRO	4.9
1	A	690	LEU	4.9
1	A	342	SER	4.9
1	A	337	SER	4.7
1	A	694	SER	4.7
1	A	339	SER	4.7
1	A	341	ALA	4.6
1	A	679	THR	4.6
1	A	691	PHE	3.8
1	A	686	PHE	3.7
1	A	689	ARG	3.7
1	A	695	SER	3.5
1	A	680	PRO	3.4
1	A	30	VAL	3.4
1	A	37	CYS	3.3
1	A	693	THR	3.3
1	A	28	CYS	3.3
1	A	392	SER	3.2
1	A	651	CYS	2.8
1	A	27	LYS	2.8
1	A	659	ASN	2.7
1	A	682	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	29	THR	2.5
1	A	687	PRO	2.5
1	A	93[A]	GLU	2.5
1	A	650	THR	2.5
1	A	685	GLY	2.5
1	A	688	VAL	2.4
1	A	498	SER	2.4
1	A	656	TRP	2.4
1	A	44	GLN	2.3
1	A	287[A]	ASN	2.2
1	A	649	CYS	2.3
1	A	661	ILE	2.2
1	A	51	THR	2.2
1	A	296	TRP	2.2
1	A	31	SER	2.2
1	A	39	HIS	2.1
1	A	64	ARG	2.1
1	A	188	SER	2.1
1	A	662	ASN	2.1
1	A	677	CYS	2.1
1	A	678	ASN	2.0
1	A	673	SER	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	K	1	14/15	0.33	0.27	79,85,87,91	0
2	NAG	C	2	14/15	0.36	0.24	97,99,100,100	0
2	NAG	G	2	14/15	0.44	0.26	88,90,92,92	0
5	BMA	I	5	11/12	0.48	0.20	99,99,100,100	0
5	MAN	I	4	11/12	0.51	0.20	97,99,100,100	0
6	NDG	K	2	14/15	0.56	0.18	95,97,98,98	0

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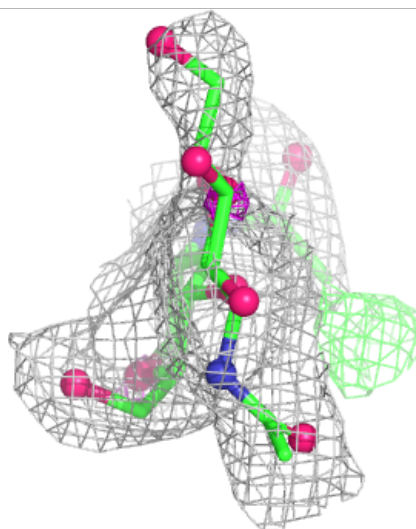
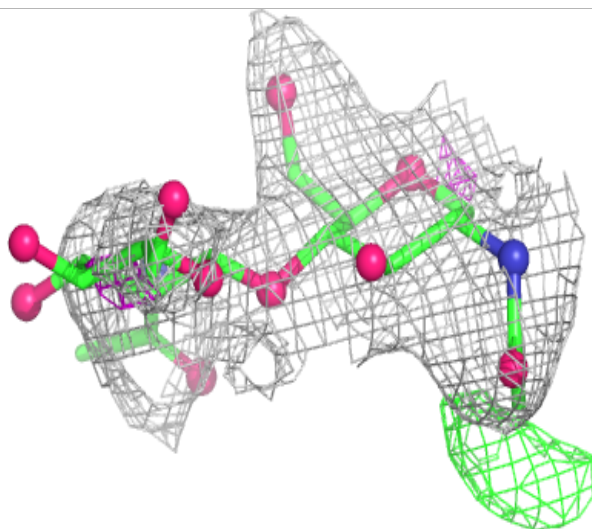
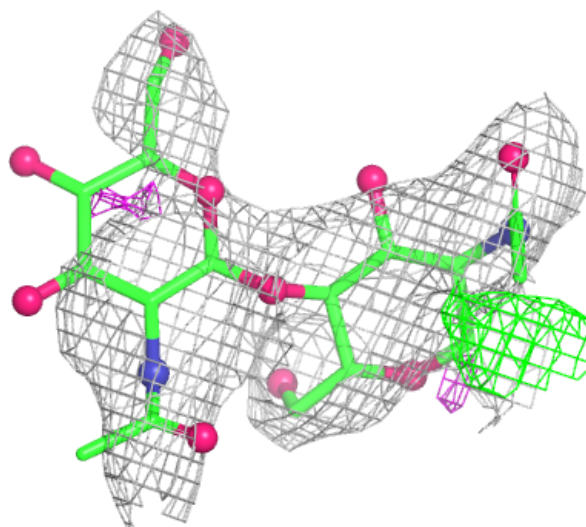
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	J	2	14/15	0.57	0.22	73,77,79,80	0
3	NAG	E	2	14/15	0.60	0.20	84,86,88,90	0
2	NAG	B	2	14/15	0.60	0.19	98,99,100,100	0
5	BMA	I	3	11/12	0.61	0.18	84,91,94,97	0
2	NAG	B	1	14/15	0.62	0.17	88,90,92,95	0
2	NAG	F	2	14/15	0.62	0.22	80,84,85,86	0
4	NAG	H	2	14/15	0.66	0.20	89,91,92,92	0
4	FUC	H	3	10/11	0.69	0.23	84,85,86,87	0
2	NAG	D	2	14/15	0.71	0.20	76,79,80,81	0
2	NAG	C	1	14/15	0.71	0.21	81,85,89,93	0
4	FUC	J	3	10/11	0.72	0.21	73,76,77,77	0
2	NAG	D	1	14/15	0.72	0.20	59,65,68,72	0
2	NAG	F	1	14/15	0.76	0.15	59,63,69,75	0
3	NAG	E	1	14/15	0.76	0.16	68,74,76,80	0
3	BMA	E	3	11/12	0.80	0.21	91,92,93,93	0
2	NAG	G	1	14/15	0.81	0.15	68,73,76,83	0
4	NAG	H	1	13/15	0.82	0.15	72,75,83,86	0
5	NAG	I	2	14/15	0.86	0.13	55,59,67,77	0
4	NAG	J	1	14/15	0.89	0.11	37,53,66,68	0
5	NAG	I	1	14/15	0.96	0.08	32,35,39,45	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.

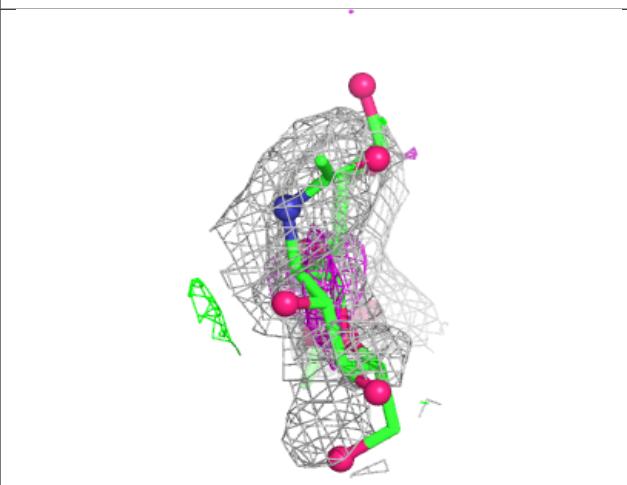
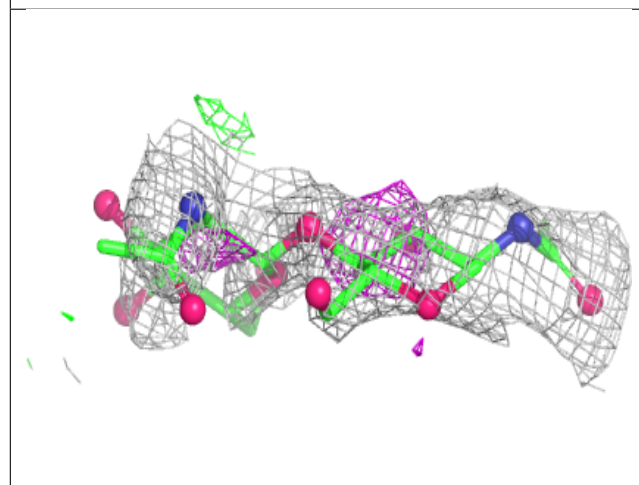
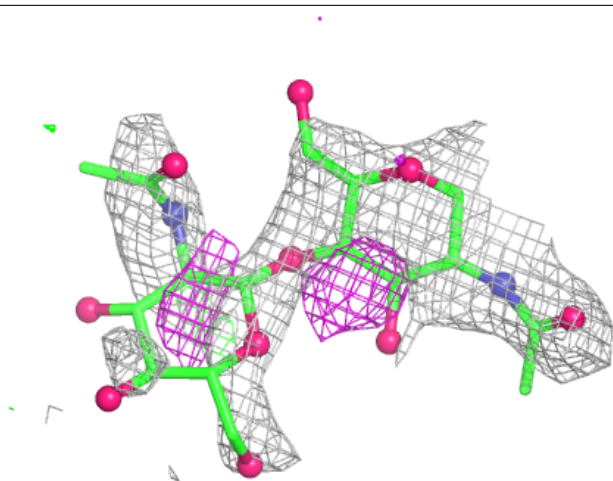
Electron density around Chain B:

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



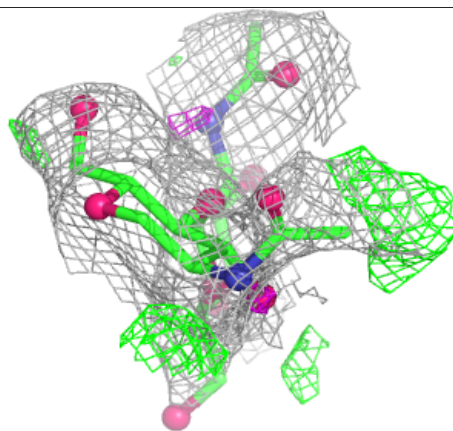
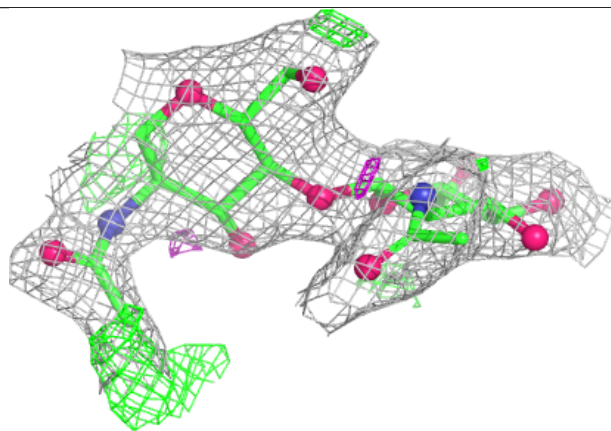
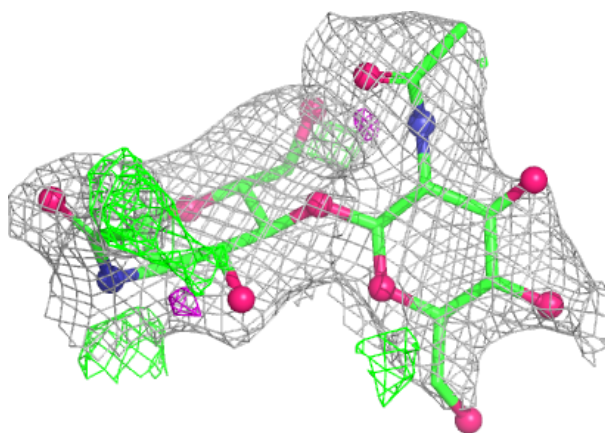
Electron density around Chain C:

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



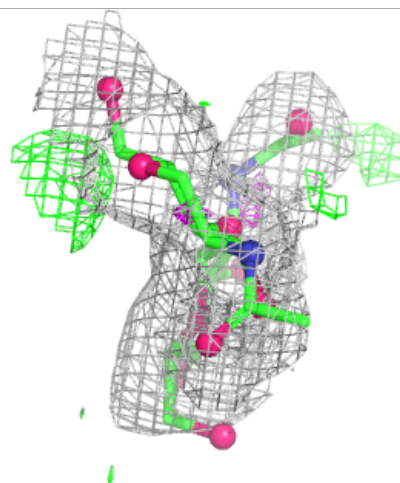
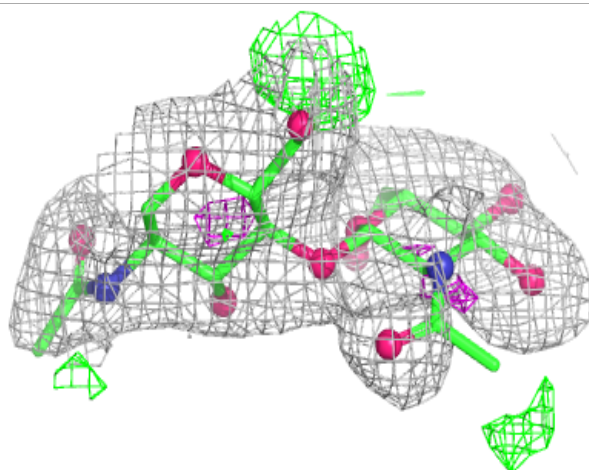
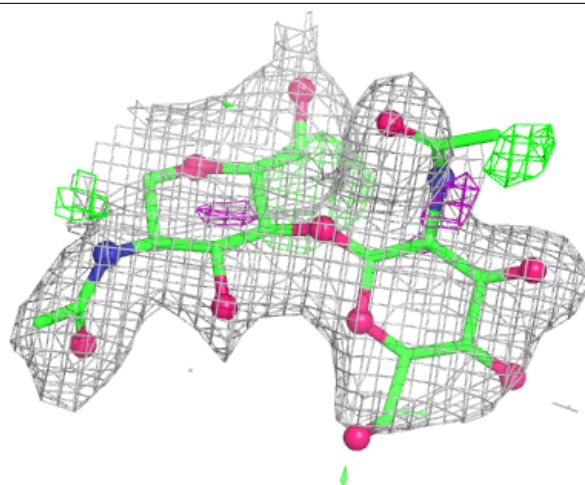
Electron density around Chain D:

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



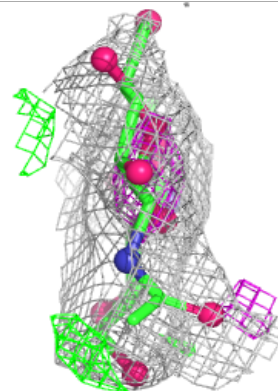
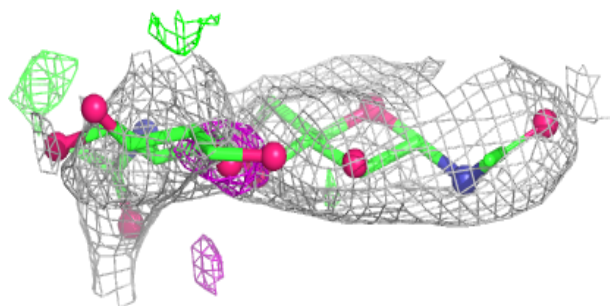
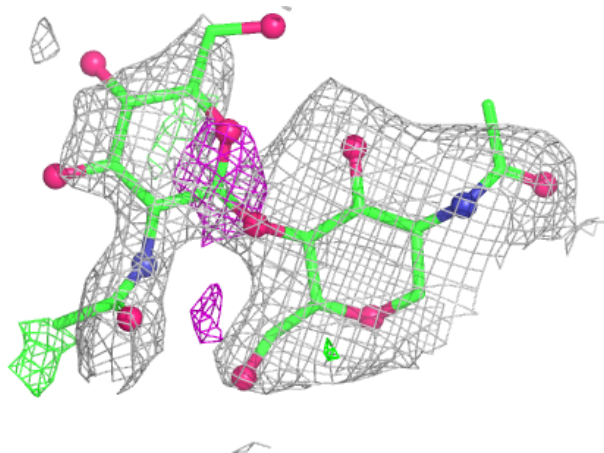
Electron density around Chain F:

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



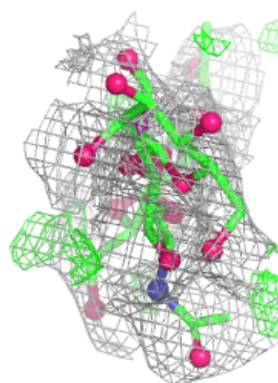
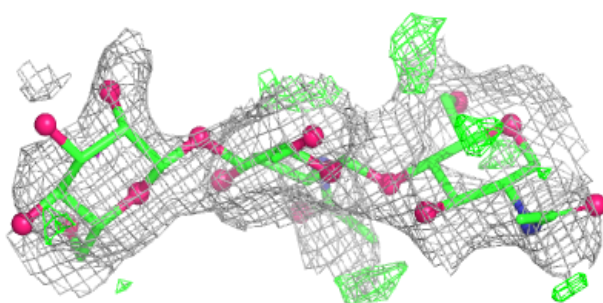
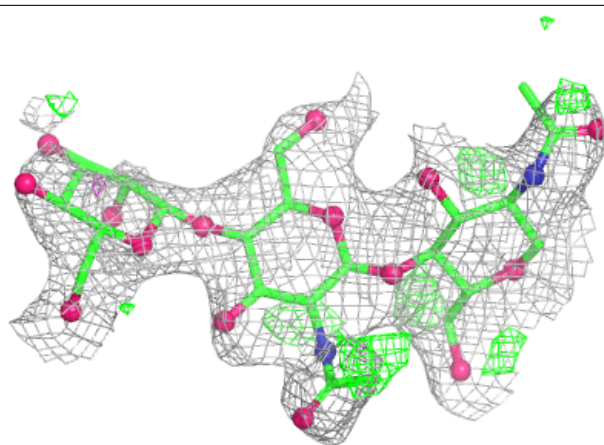
Electron density around Chain G:

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



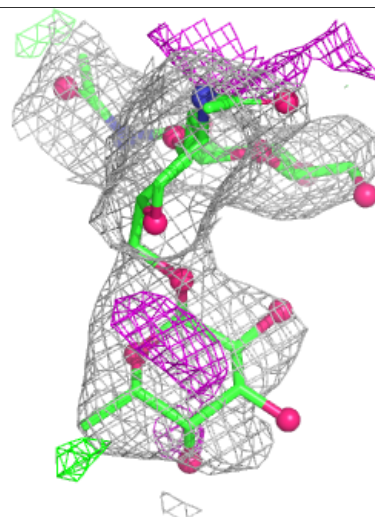
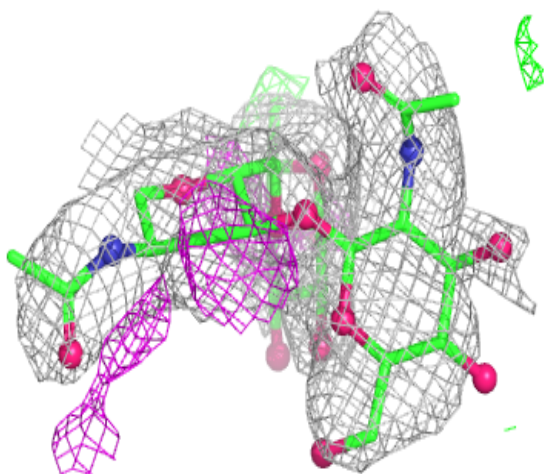
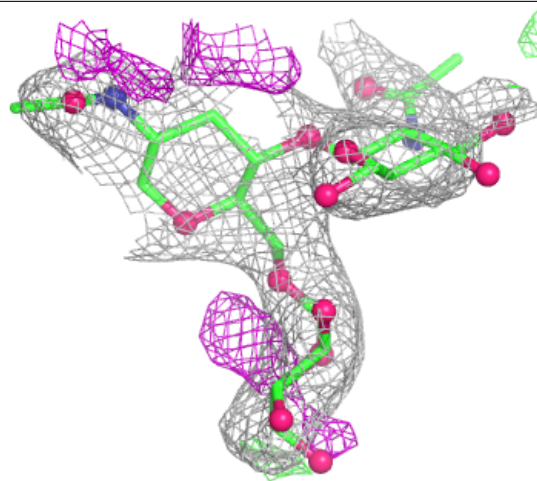
Electron density around Chain E:

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



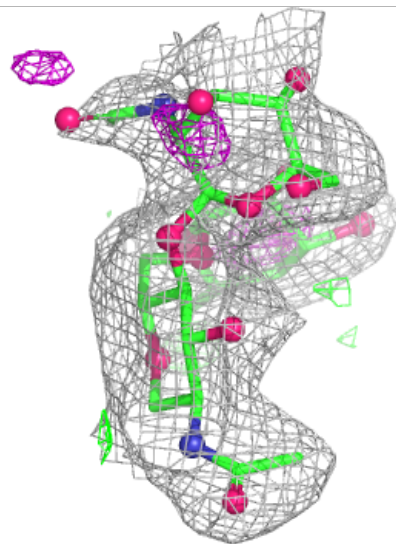
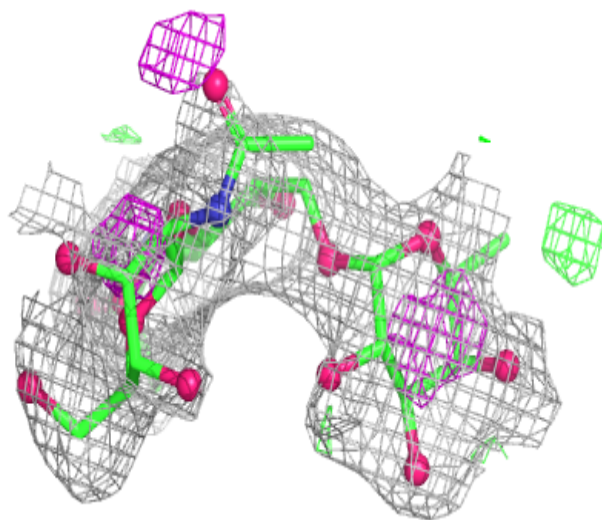
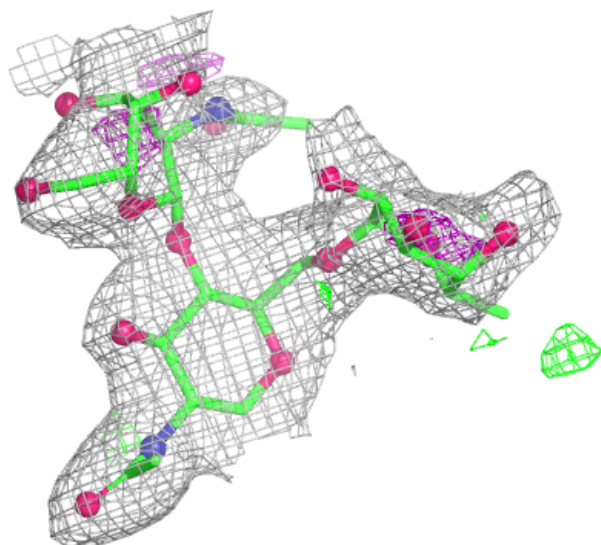
Electron density around Chain H:

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



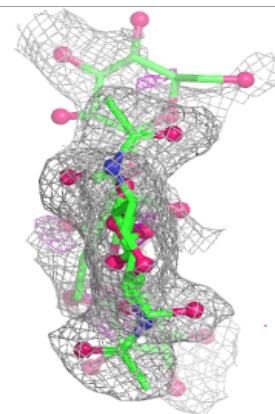
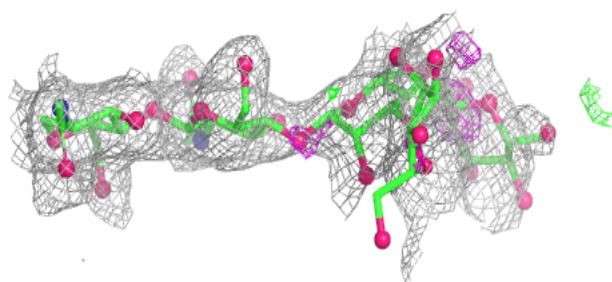
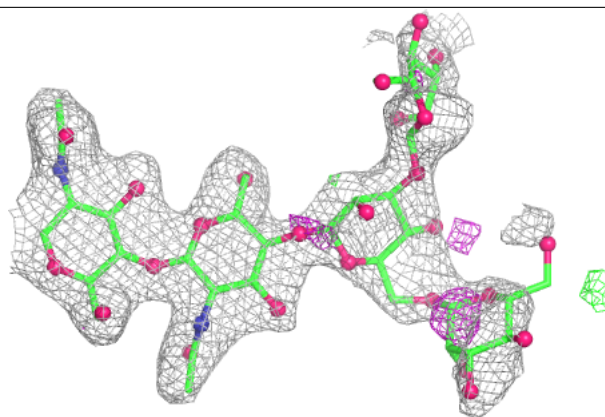
Electron density around Chain J:

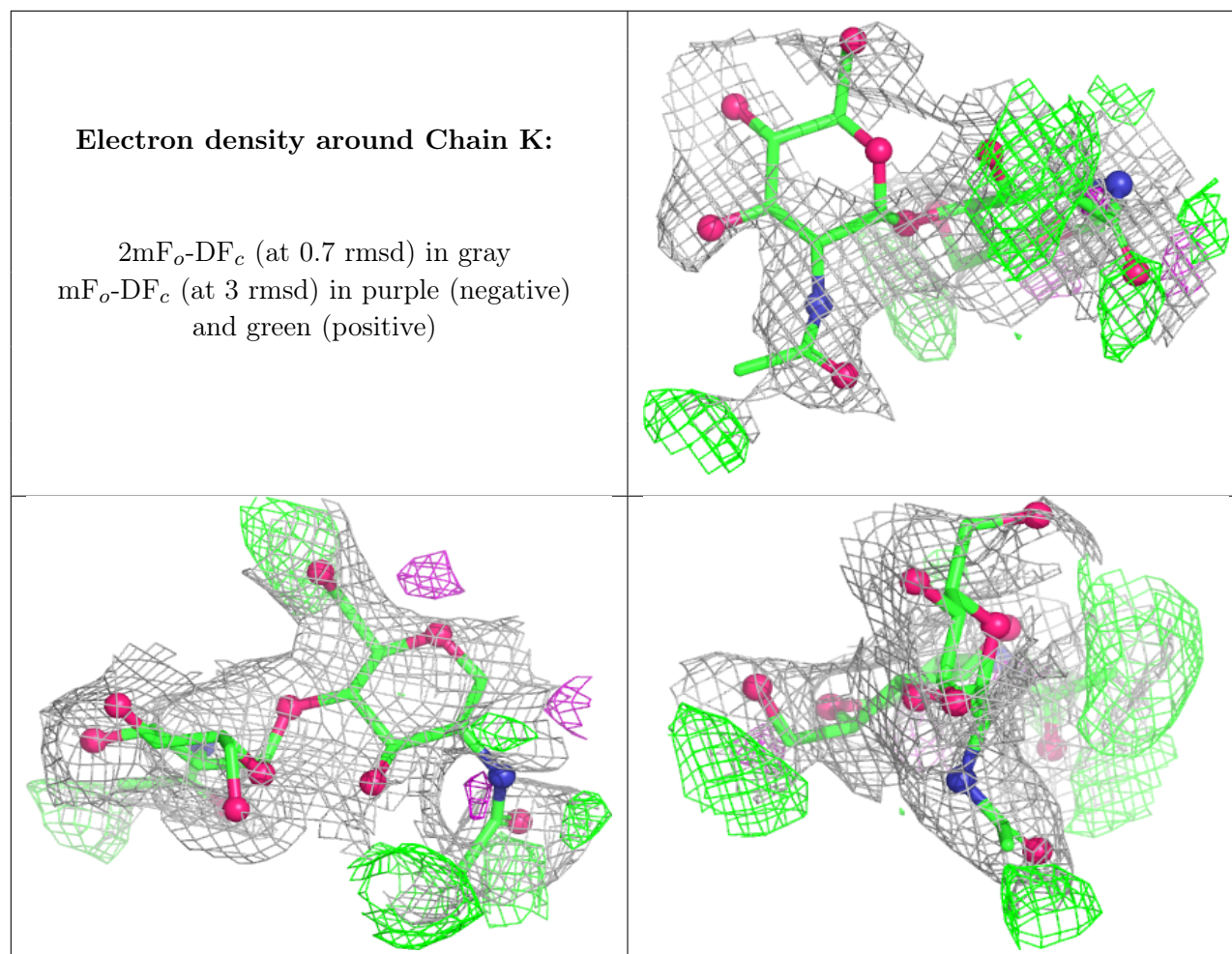
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (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
9	SO4	A	752	5/5	0.37	0.19	88,92,92,93	0
7	NAG	A	1961	14/15	0.60	0.20	74,78,79,81	0
8	GLC	A	754	12/12	0.66	0.26	99,100,100,100	0
8	GLC	A	753	12/12	0.71	0.21	54,59,62,67	0
10	BME	A	1270	4/4	0.81	0.24	57,57,61,64	0
9	SO4	A	751	5/5	0.94	0.13	67,69,69,70	0
9	SO4	A	750	5/5	0.96	0.09	43,44,46,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.