



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2025 – 02:20 PM JST

PDB ID : 9KO7 / pdb_00009ko7
Title : Crystal structure of chicken ACE2
Authors : Lan, J.; Wang, C.H.
Deposited on : 2024-11-20
Resolution : 3.27 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

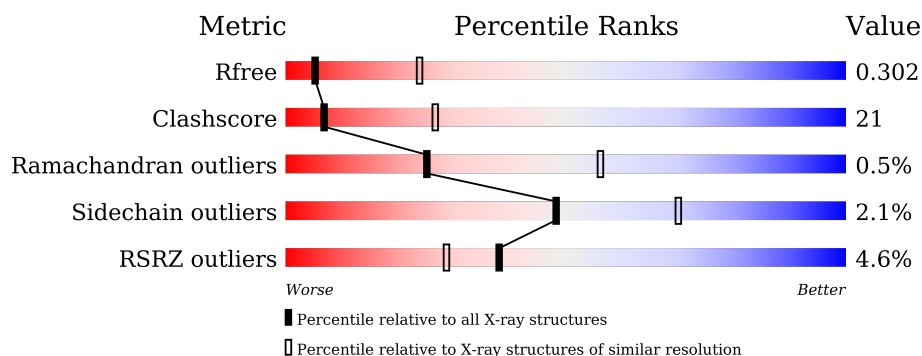
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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}	164625	1214 (3.30-3.26)
Clashscore	180529	1265 (3.30-3.26)
Ramachandran outliers	177936	1264 (3.30-3.26)
Sidechain outliers	177891	1263 (3.30-3.26)
RSRZ outliers	164620	1215 (3.30-3.26)

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	597	<div> <div>2%</div> <div>59%</div> <div>39%</div> <div>.</div> </div>
1	B	597	<div> <div>6%</div> <div>57%</div> <div>39%</div> <div>..</div> </div>
1	C	597	<div> <div>6%</div> <div>58%</div> <div>39%</div> <div>..</div> </div>
2	D	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
2	L	4	<div> <div>25%</div> <div>75%</div> </div>
3	E	3	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	3	 33% 67%
3	J	3	 33% 67%
3	K	3	 100%
4	F	2	 100%
4	G	2	 100%
4	I	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15044 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	596	Total	C	N	O	S	0	0	0
			4874	3102	817	925	30			
1	C	596	Total	C	N	O	S	0	0	0
			4874	3102	817	925	30			
1	A	596	Total	C	N	O	S	0	0	0
			4874	3102	817	925	30			

There are 3 discrepancies between the modelled and reference sequences:

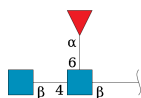
Chain	Residue	Modelled	Actual	Comment	Reference
B	395	ASN	ASP	conflict	UNP A0A5J6CU64
C	395	ASN	ASP	conflict	UNP A0A5J6CU64
A	395	ASN	ASP	conflict	UNP A0A5J6CU64

- Molecule 2 is an oligosaccharide called 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
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



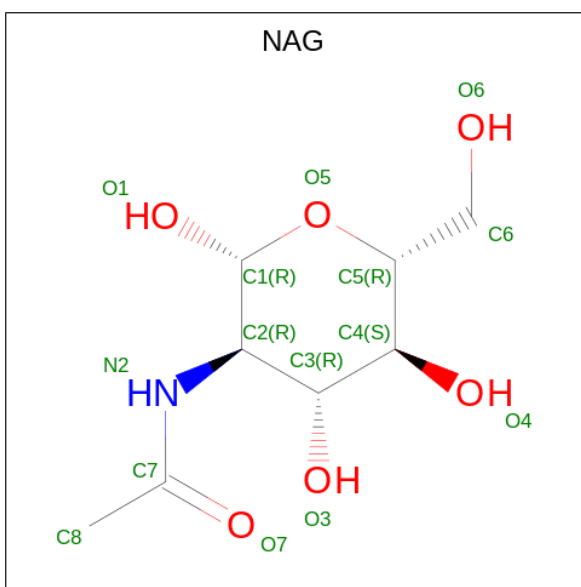
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



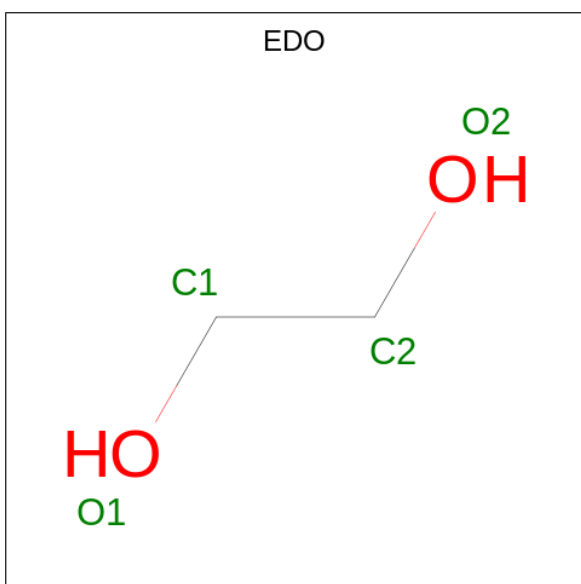
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

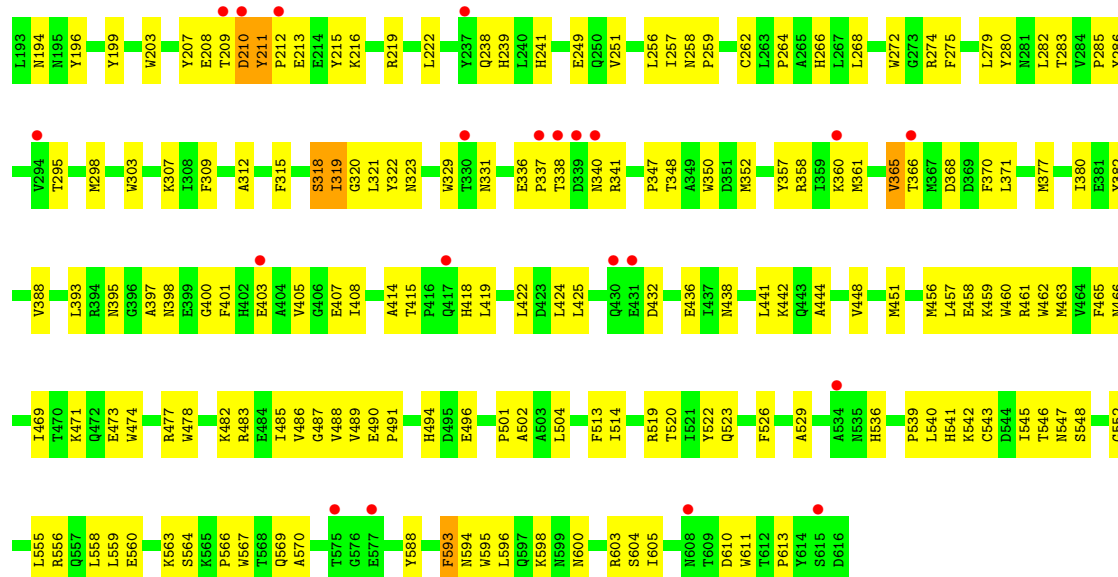


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

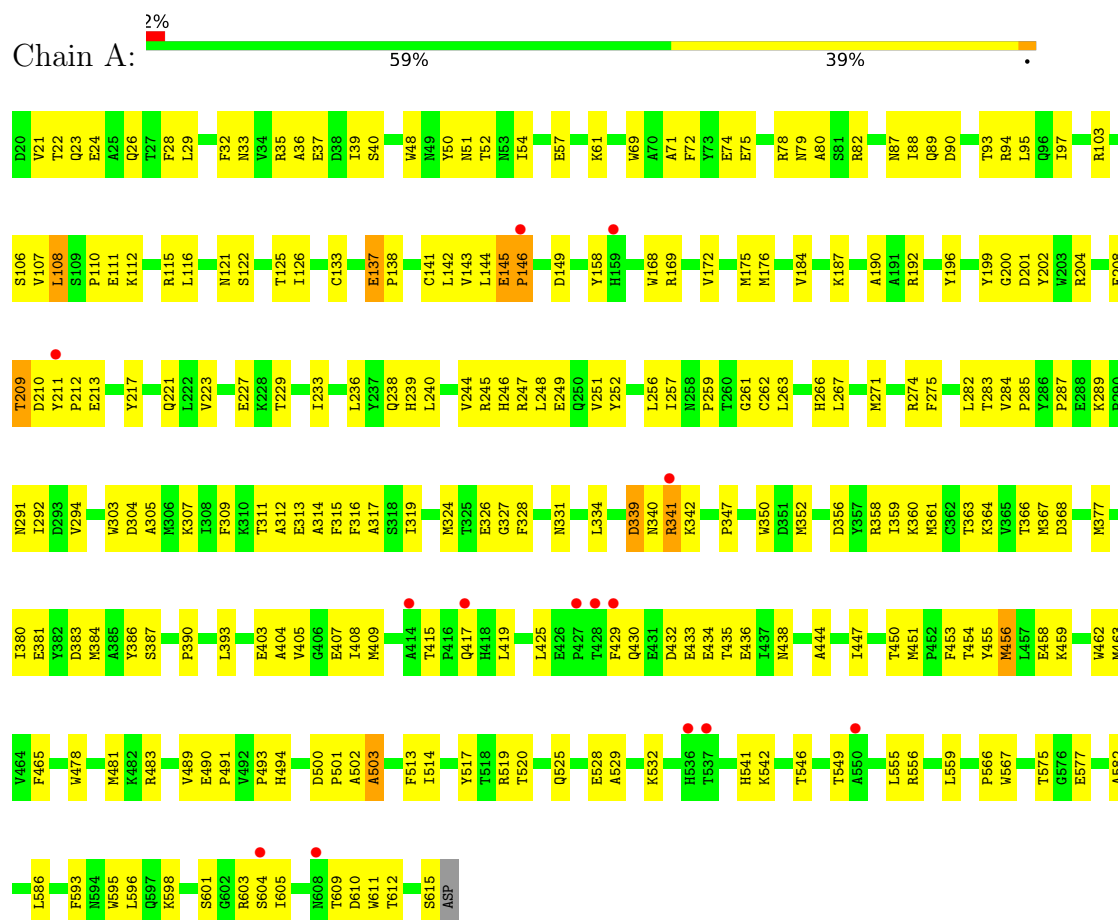
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0



- Molecule 1: Angiotensin-converting enzyme



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



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



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



- Molecule 3: 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)-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 G:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.98Å 92.78Å 152.71Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	44.27 – 3.27 44.27 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.27-3.27) 98.3 (44.27-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.239 , 0.296 0.252 , 0.302	Depositor DCC
R_{free} test set	2013 reflections (5.44%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15044	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 3.71% 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: MAN, FUC, EDO, BMA, NAG

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	0.53	0/5011	0.82	4/6812 (0.1%)
1	B	0.57	2/5011 (0.0%)	0.88	6/6812 (0.1%)
1	C	0.56	0/5011	0.89	6/6812 (0.1%)
All	All	0.55	2/15033 (0.0%)	0.86	16/20436 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	SER	C-O	10.36	1.37	1.24
1	B	105	SER	N-CA	5.86	1.53	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ILE	N-CA-C	-12.36	100.91	111.91
1	B	104	GLY	O-C-N	-7.98	112.33	122.70
1	C	138	PRO	N-CA-C	-6.91	98.24	112.47
1	A	339	ASP	CB-CA-C	-6.64	102.46	111.89
1	C	146	PRO	N-CA-CB	-6.40	96.53	103.25

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	GLY	Mainchain
1	B	192	ARG	Sidechain
1	C	318	SER	Mainchain
1	C	483	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4874	0	4619	192	0
1	B	4874	0	4620	207	1
1	C	4874	0	4619	216	0
2	D	50	0	43	1	0
2	L	50	0	43	0	0
3	E	38	0	34	2	0
3	H	38	0	34	1	0
3	J	38	0	34	0	0
3	K	38	0	34	0	0
4	F	28	0	25	0	0
4	G	28	0	25	3	0
4	I	28	0	25	2	0
5	A	28	0	26	1	0
5	B	28	0	26	1	0
5	C	14	0	13	0	0
6	B	8	0	12	1	0
6	C	8	0	12	1	0
All	All	15044	0	14244	611	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 21.

The worst 5 of 611 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:403:GLU:HB3	1:A:519:ARG:HD3	1.39	1.01
1:B:105:SER:O	1:B:108:LEU:HD23	1.63	0.97
1:B:105:SER:O	1:B:108:LEU:CD2	2.17	0.92
1:B:326:GLU:HG2	1:C:163:TRP:CD1	2.04	0.92
1:C:134:LYS:HG3	1:C:135:ALA:H	1.35	0.91

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:B:192:ARG:O	1:B:601:SER:O[4_446]	1.75	0.45

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	594/597 (100%)	543 (91%)	49 (8%)	2 (0%)	37	67
1	B	594/597 (100%)	534 (90%)	56 (9%)	4 (1%)	19	49
1	C	594/597 (100%)	533 (90%)	58 (10%)	3 (0%)	25	56
All	All	1782/1791 (100%)	1610 (90%)	163 (9%)	9 (0%)	25	56

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	TYR
1	C	137	GLU
1	A	137	GLU
1	B	137	GLU
1	A	146	PRO

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	521/522 (100%)	515 (99%)	6 (1%)	67	81
1	B	521/522 (100%)	507 (97%)	14 (3%)	40	65
1	C	521/522 (100%)	508 (98%)	13 (2%)	42	66
All	All	1563/1566 (100%)	1530 (98%)	33 (2%)	48	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	339	ASP
1	A	456	MET
1	B	601	SER
1	B	548	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	527	GLN
1	A	597	GLN
1	A	417	GLN
1	C	89	GLN
1	C	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	D	1	1,2	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
2	NAG	D	2	2	14,14,15	0.40	0	17,19,21	0.62	0
2	BMA	D	3	2	11,11,12	0.94	0	15,15,17	1.11	1 (6%)
2	MAN	D	4	2	11,11,12	1.69	3 (27%)	15,15,17	1.37	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.65	0
3	NAG	E	2	3	14,14,15	0.75	1 (7%)	17,19,21	0.61	0
3	FUC	E	3	3	10,10,11	2.04	3 (30%)	14,14,16	2.28	7 (50%)
4	NAG	F	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.85	0
4	NAG	F	2	4	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
4	NAG	G	1	1,4	14,14,15	0.35	0	17,19,21	0.67	0
4	NAG	G	2	4	14,14,15	0.54	0	17,19,21	0.55	0
3	NAG	H	1	3,1	14,14,15	0.98	1 (7%)	17,19,21	0.66	0
3	NAG	H	2	3	14,14,15	0.59	1 (7%)	17,19,21	0.58	0
3	FUC	H	3	3	10,10,11	2.23	4 (40%)	14,14,16	1.36	3 (21%)
4	NAG	I	1	1,4	14,14,15	0.27	0	17,19,21	0.60	0
4	NAG	I	2	4	14,14,15	0.44	0	17,19,21	0.58	0
3	NAG	J	1	3,1	14,14,15	0.63	0	17,19,21	0.78	0
3	NAG	J	2	3	14,14,15	0.66	1 (7%)	17,19,21	1.13	1 (5%)
3	FUC	J	3	3	10,10,11	1.61	2 (20%)	14,14,16	2.00	4 (28%)
3	NAG	K	1	3,1	14,14,15	0.56	0	17,19,21	0.70	1 (5%)
3	NAG	K	2	3	14,14,15	0.61	1 (7%)	17,19,21	0.77	1 (5%)
3	FUC	K	3	3	10,10,11	1.78	1 (10%)	14,14,16	1.59	4 (28%)
2	NAG	L	1	1,2	14,14,15	0.42	0	17,19,21	0.59	0
2	NAG	L	2	2	14,14,15	0.66	1 (7%)	17,19,21	1.02	2 (11%)
2	BMA	L	3	2	11,11,12	1.10	1 (9%)	15,15,17	0.95	0
2	MAN	L	4	2	11,11,12	1.40	2 (18%)	15,15,17	1.22	1 (6%)

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	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	FUC	J	3	3	-	-	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	1/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	FUC	C2-C3	-5.25	1.44	1.52
3	K	3	FUC	C2-C3	4.57	1.59	1.52
3	E	3	FUC	C2-C3	-4.43	1.46	1.52
3	E	3	FUC	C1-C2	3.46	1.60	1.52
2	D	4	MAN	C1-C2	3.39	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	3	FUC	C1-C2-C3	-4.76	103.81	109.67
3	E	3	FUC	O2-C2-C1	4.63	118.63	109.15
2	D	4	MAN	C1-O5-C5	3.97	117.56	112.19
3	E	3	FUC	O3-C3-C2	-3.69	102.92	109.99
3	J	2	NAG	C1-O5-C5	3.47	116.89	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

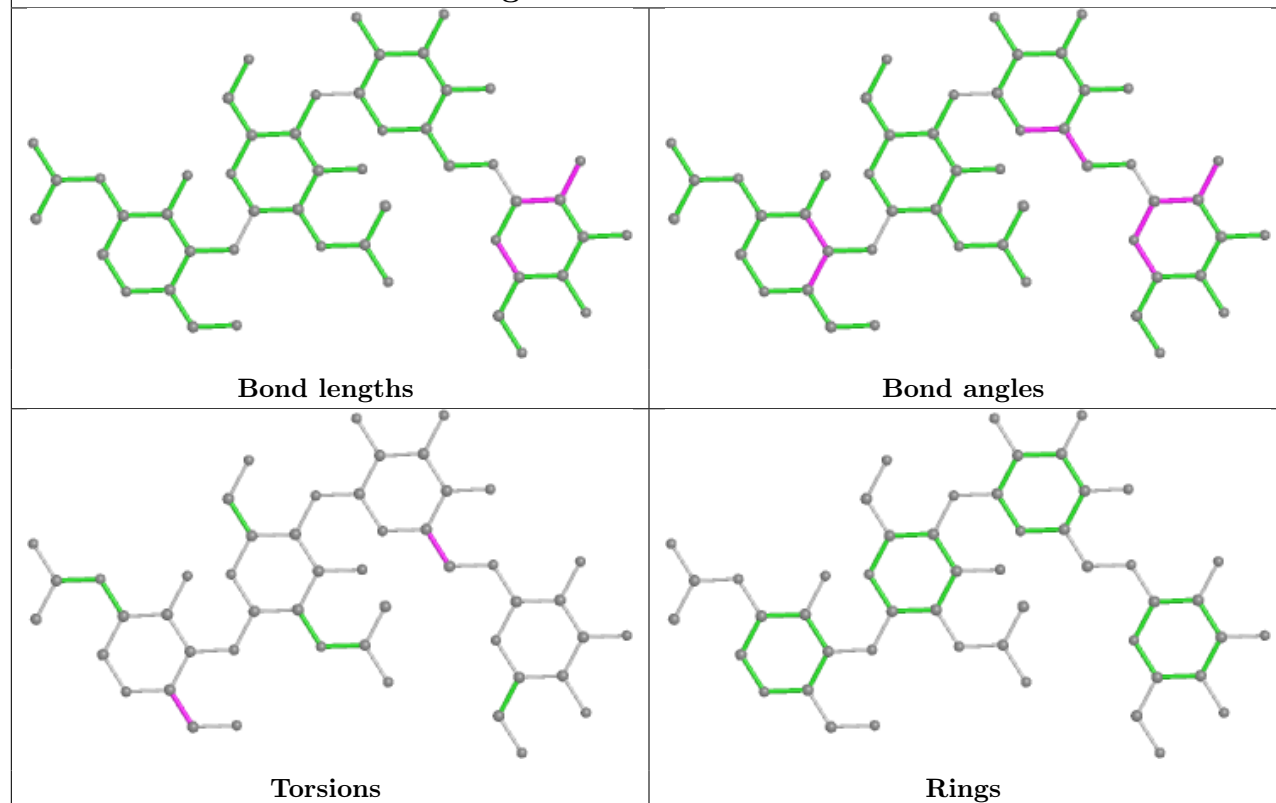
There are no ring outliers.

8 monomers are involved in 9 short contacts:

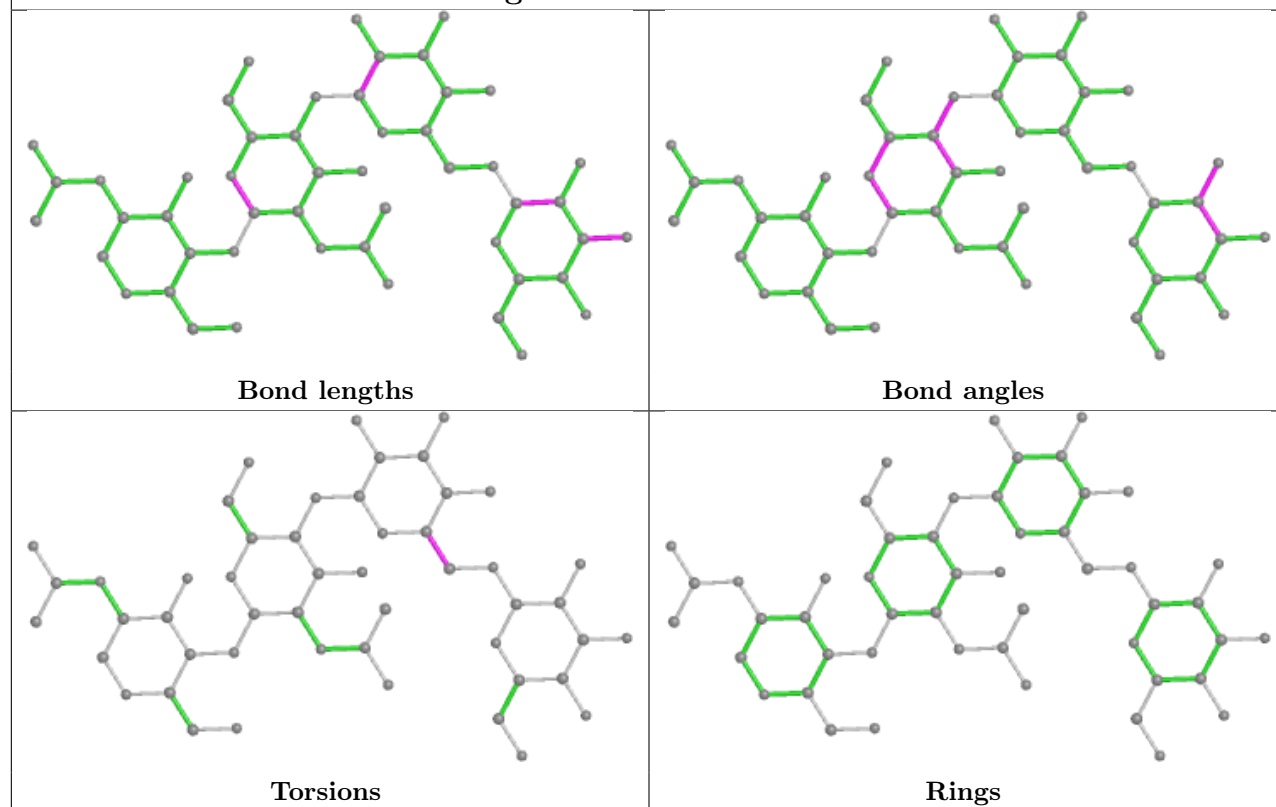
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	H	3	FUC	1	0
3	E	1	NAG	1	0
4	I	1	NAG	2	0
2	D	4	MAN	1	0
4	G	1	NAG	2	0
3	E	3	FUC	2	0
4	G	2	NAG	1	0

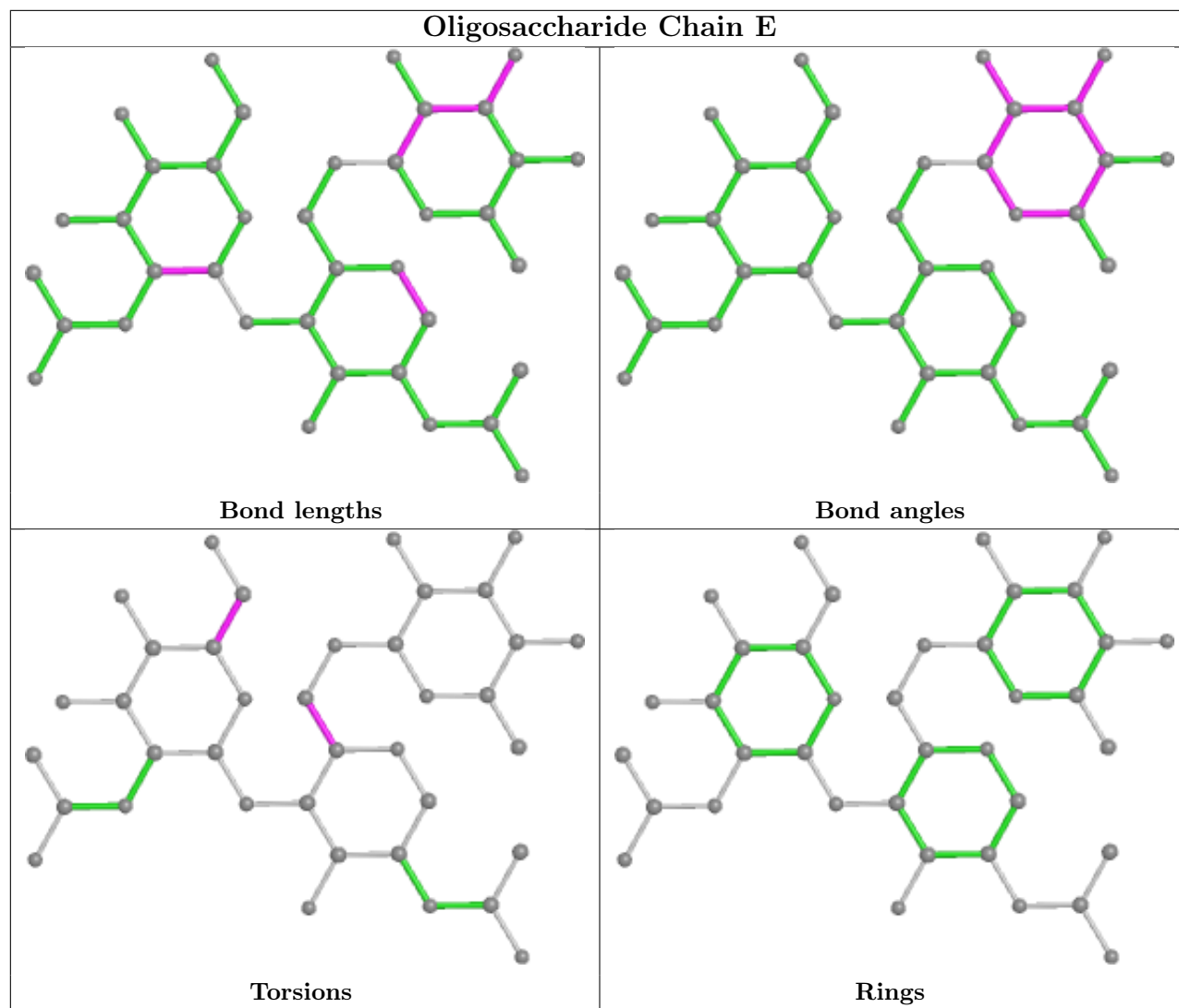
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

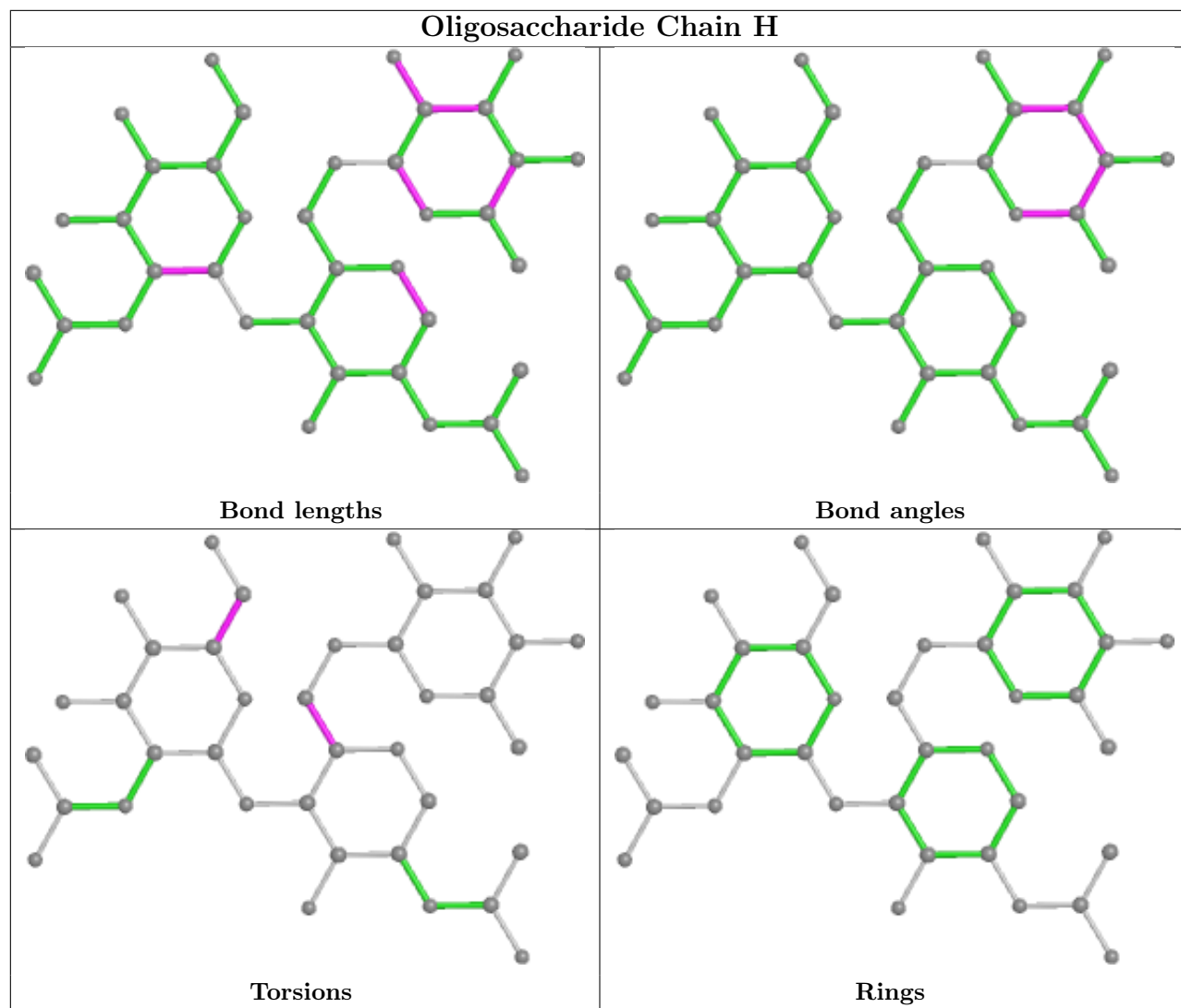
Oligosaccharide Chain D

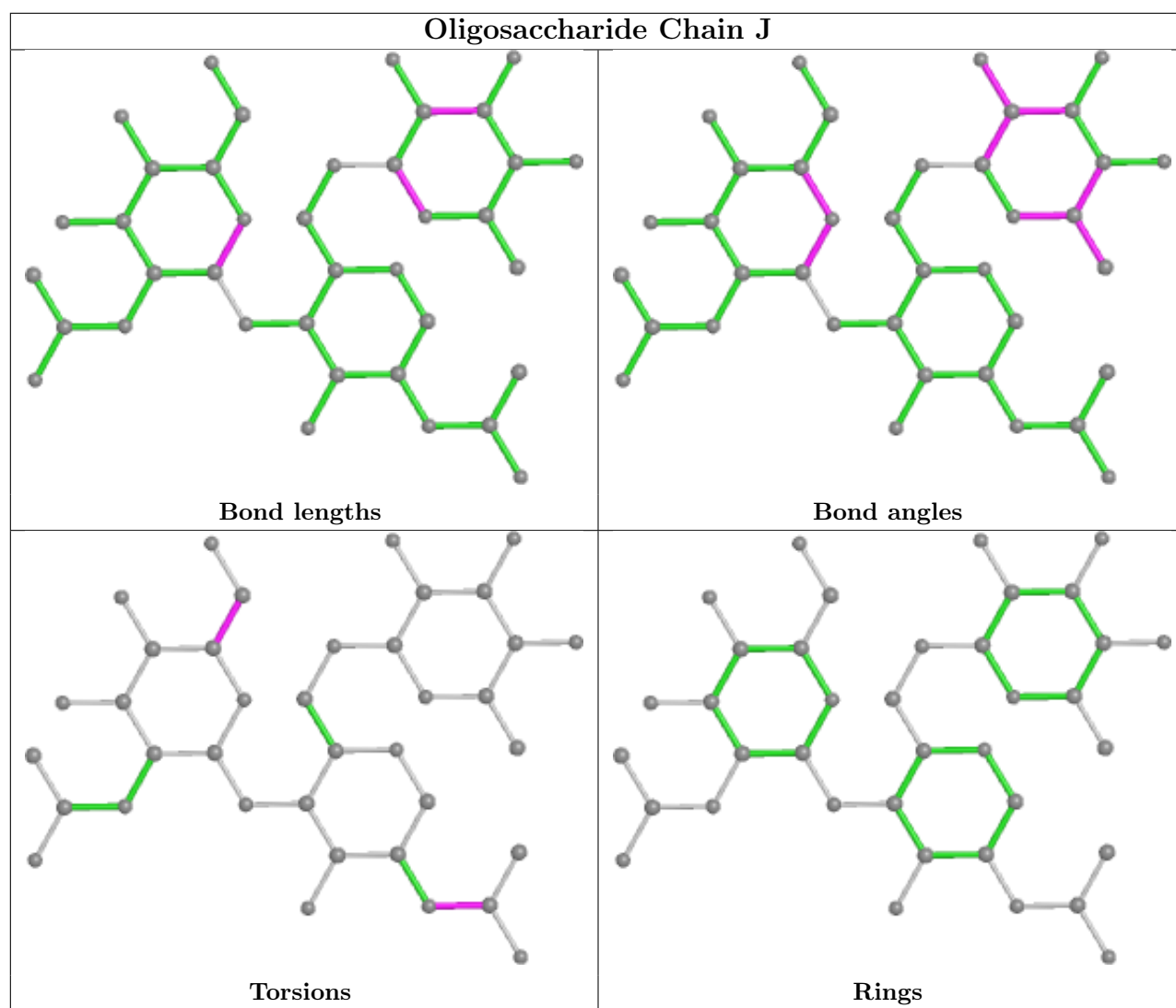


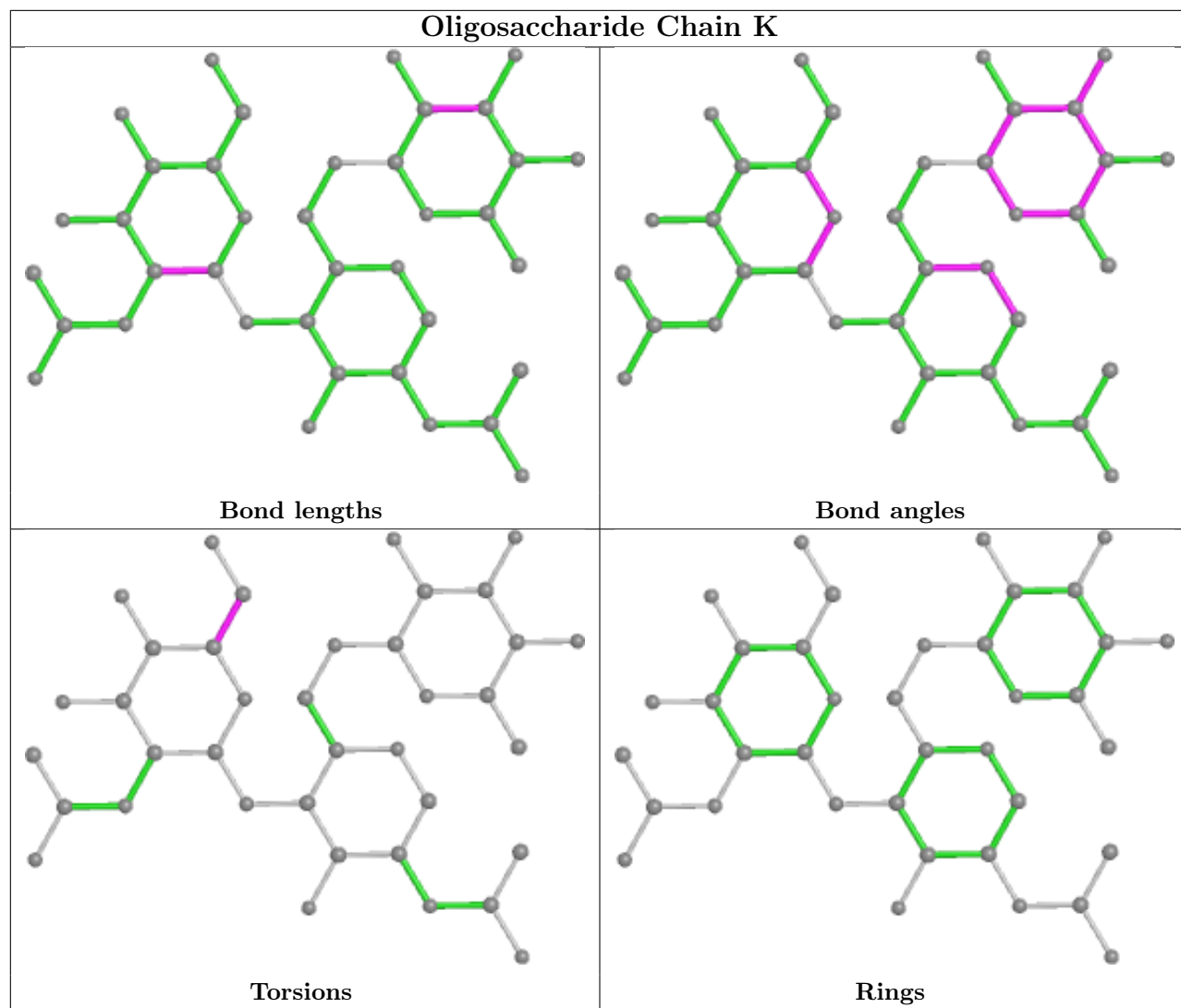
Oligosaccharide Chain L

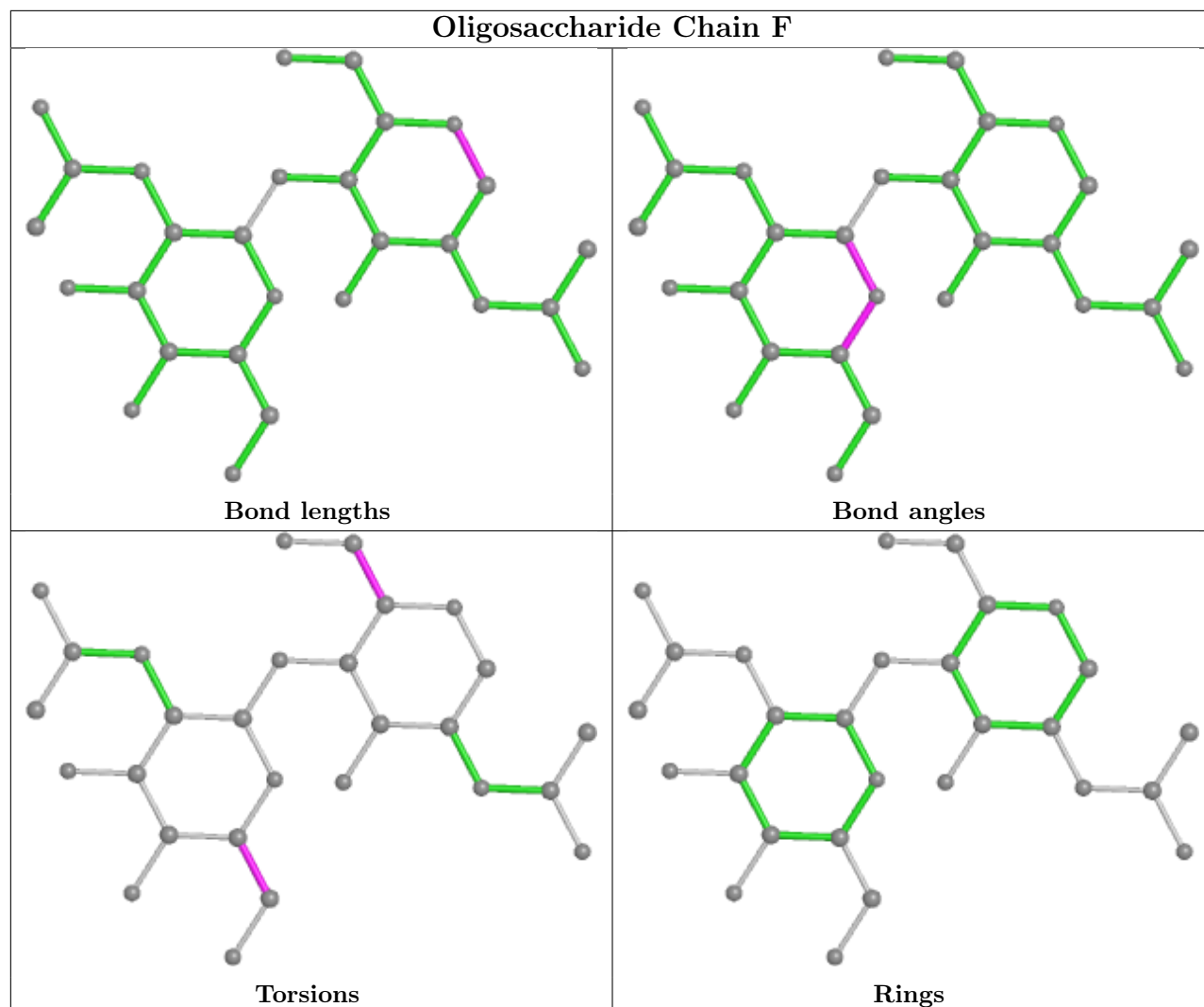


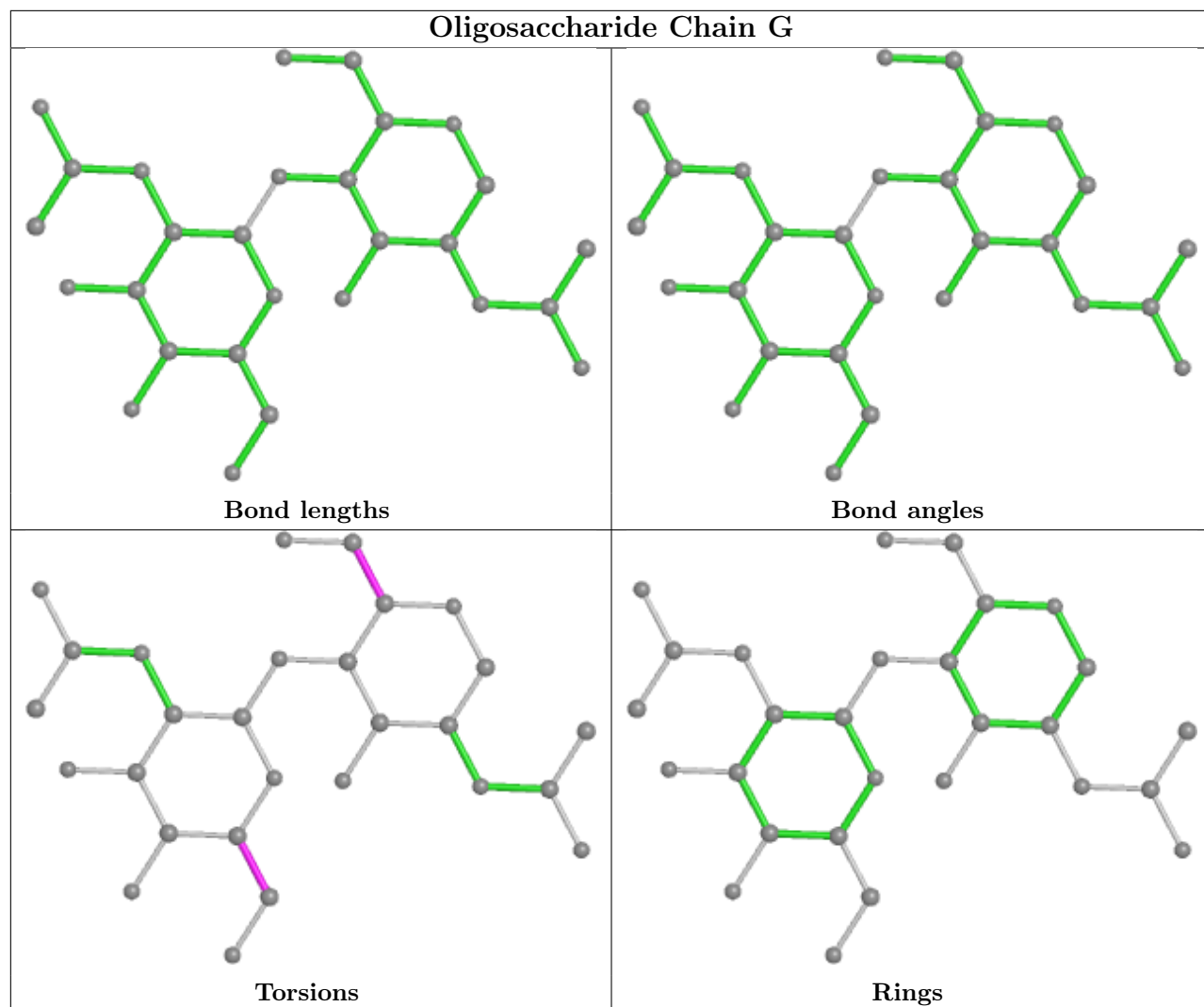


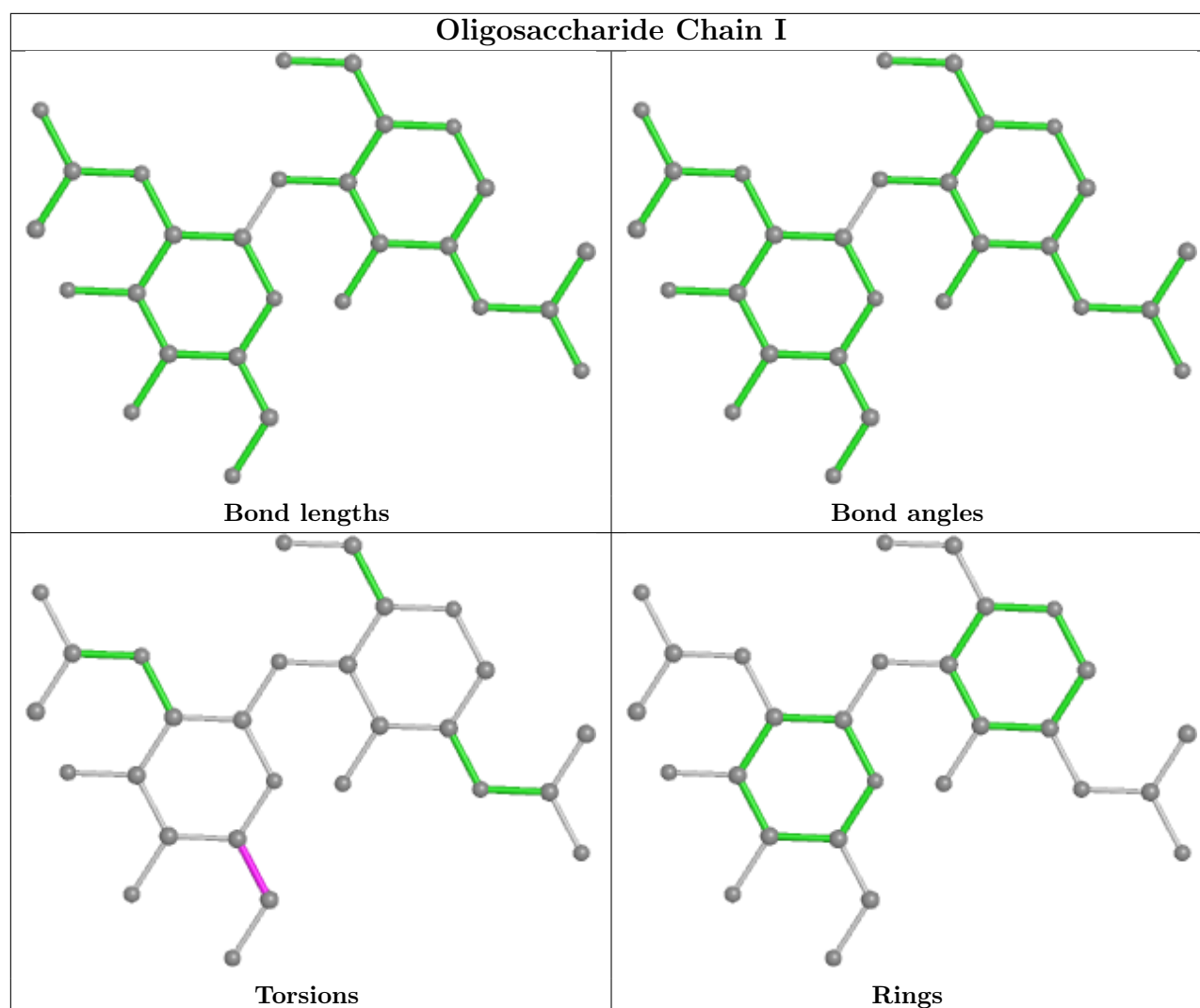












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
6	EDO	B	704	-	3,3,3	0.39	0	2,2,2	0.57	0
5	NAG	B	701	1	14,14,15	0.47	0	17,19,21	0.63	0
5	NAG	A	702	1	14,14,15	0.72	1 (7%)	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.35	0
5	NAG	A	701	1	14,14,15	0.73	1 (7%)	17,19,21	0.67	0
5	NAG	B	702	1	14,14,15	0.45	0	17,19,21	0.43	0
5	NAG	C	701	1	14,14,15	0.76	1 (7%)	17,19,21	1.14	1 (5%)
6	EDO	C	703	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	C	702	-	3,3,3	0.66	0	2,2,2	0.37	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
6	EDO	B	704	-	-	1/1/1/1	-
5	NAG	B	701	1	-	4/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	EDO	B	703	-	-	0/1/1/1	-
5	NAG	A	701	1	-	4/6/23/26	0/1/1/1
5	NAG	B	702	1	-	0/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
6	EDO	C	703	-	-	1/1/1/1	-
6	EDO	C	702	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	NAG	O5-C1	2.68	1.48	1.43
5	A	702	NAG	O5-C1	2.57	1.47	1.43
5	A	701	NAG	C1-C2	2.04	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	NAG	C1-O5-C5	4.09	117.73	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	701	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	701	NAG	O5-C5-C6-O6
5	B	701	NAG	C8-C7-N2-C2
5	B	701	NAG	O7-C7-N2-C2
5	A	701	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	NAG	1	0
6	B	703	EDO	1	0
5	A	701	NAG	1	0
6	C	703	EDO	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 [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	596/597 (99%)	0.34	14 (2%) 61 46	13, 41, 82, 151	0
1	B	596/597 (99%)	0.38	36 (6%) 29 23	11, 41, 86, 147	0
1	C	596/597 (99%)	0.43	33 (5%) 32 25	14, 41, 81, 138	0
All	All	1788/1791 (99%)	0.38	83 (4%) 38 29	11, 41, 83, 151	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	TYR	6.5
1	A	211	TYR	6.0
1	C	212	PRO	5.5
1	B	292	ILE	5.2
1	B	608	ASN	4.8

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	I	2	14/15	0.14	0.18	72,85,92,98	0
4	NAG	I	1	14/15	0.44	0.17	73,88,93,96	0
2	BMA	D	3	11/12	0.44	0.17	75,84,90,92	0

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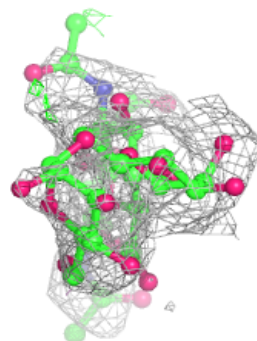
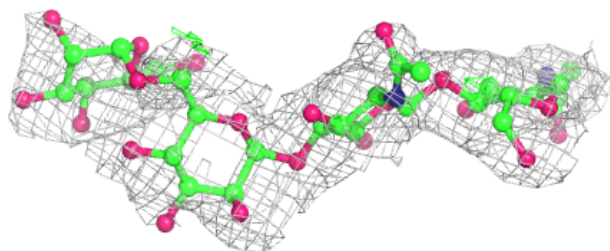
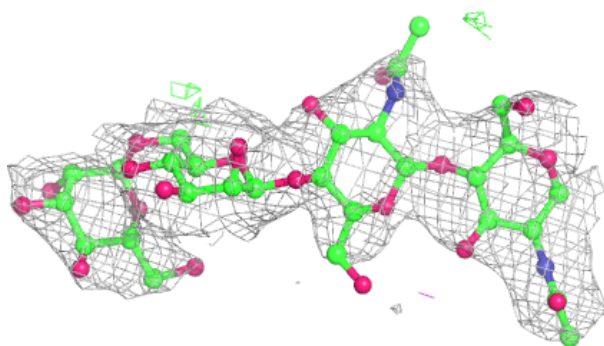
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	K	2	14/15	0.54	0.17	74,81,100,110	0
2	MAN	L	4	11/12	0.56	0.15	65,87,95,98	0
2	NAG	D	2	14/15	0.62	0.13	51,71,80,88	0
4	NAG	F	2	14/15	0.64	0.16	66,77,85,90	0
4	NAG	G	2	14/15	0.64	0.13	60,72,81,90	0
3	NAG	H	2	14/15	0.68	0.15	57,69,78,79	0
4	NAG	F	1	14/15	0.71	0.14	43,61,73,78	0
3	NAG	E	2	14/15	0.72	0.15	38,68,77,83	0
2	BMA	L	3	11/12	0.74	0.10	78,83,89,90	0
3	NAG	J	2	14/15	0.76	0.14	44,59,74,80	0
3	NAG	K	1	14/15	0.76	0.12	40,59,72,80	0
2	NAG	L	2	14/15	0.77	0.16	68,81,95,98	0
3	FUC	K	3	10/11	0.78	0.15	54,63,71,72	0
2	MAN	D	4	11/12	0.78	0.17	59,73,89,97	0
4	NAG	G	1	14/15	0.80	0.12	53,61,72,73	0
2	NAG	L	1	14/15	0.83	0.15	65,77,86,96	0
2	NAG	D	1	14/15	0.84	0.13	42,56,63,71	0
3	NAG	E	1	14/15	0.85	0.12	39,46,58,60	0
3	FUC	H	3	10/11	0.85	0.16	30,36,46,51	0
3	NAG	H	1	14/15	0.87	0.13	30,41,49,60	0
3	FUC	E	3	10/11	0.88	0.13	28,31,39,40	0
3	NAG	J	1	14/15	0.89	0.10	32,40,48,50	0
3	FUC	J	3	10/11	0.94	0.09	34,38,41,41	0

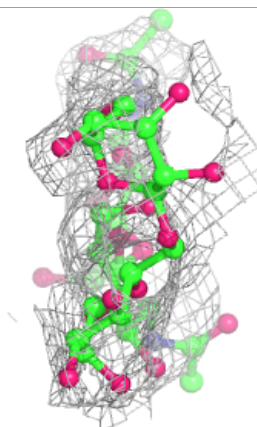
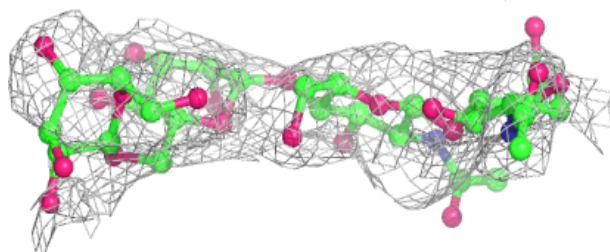
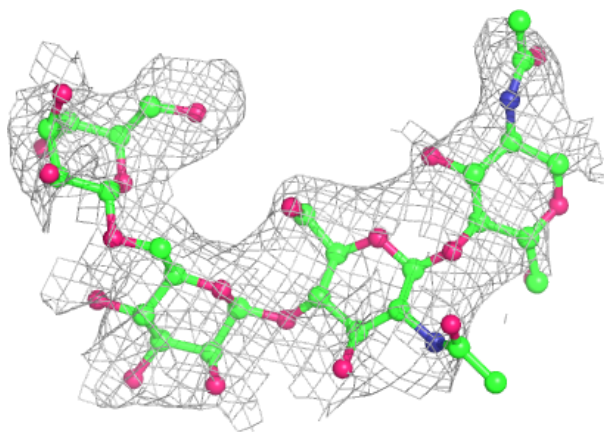
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

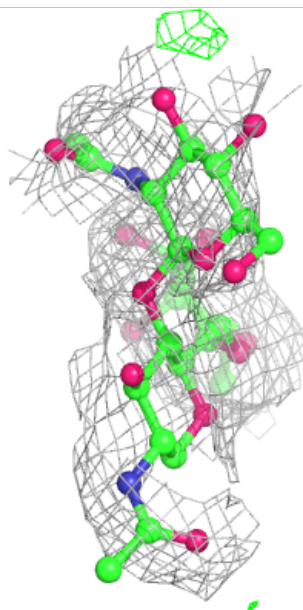
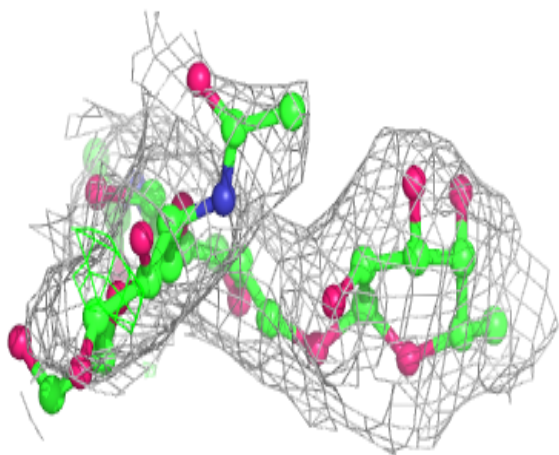
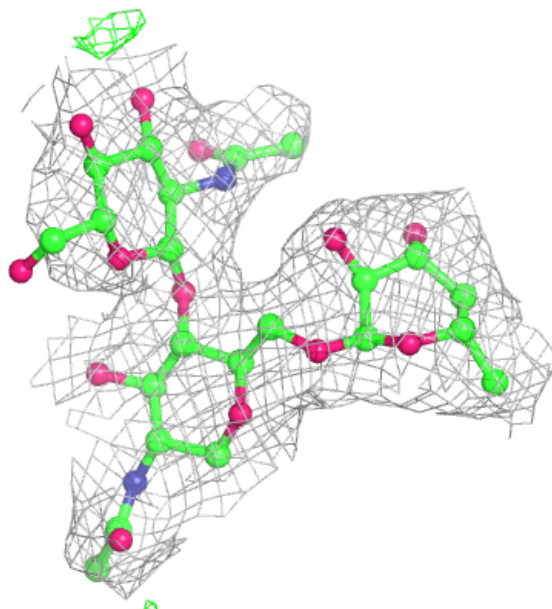
**Electron density around Chain L:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



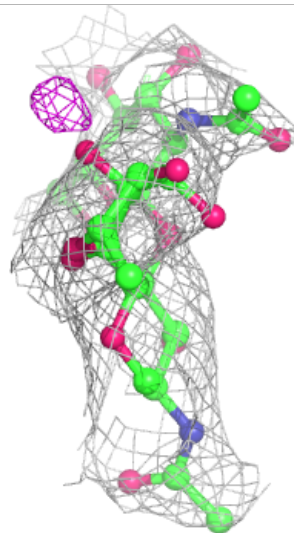
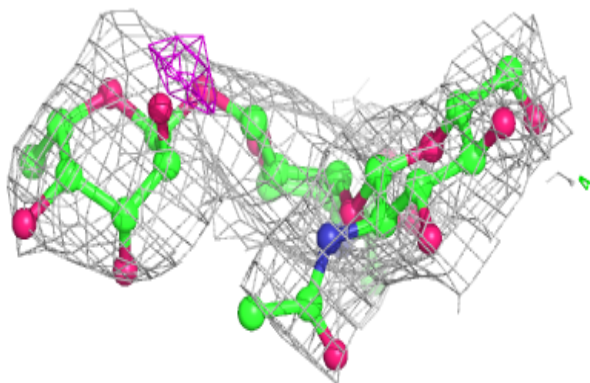
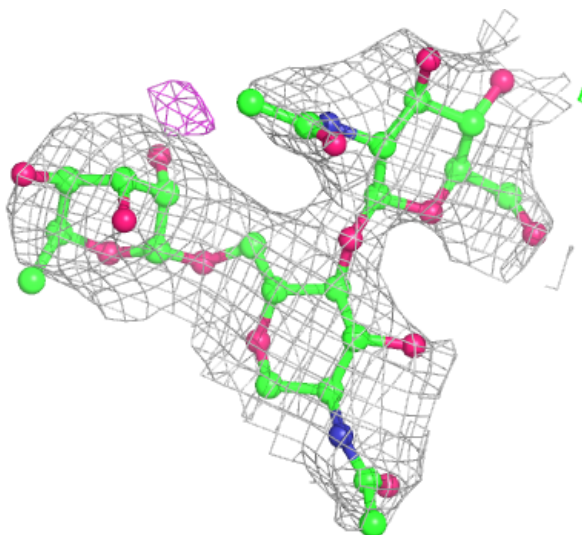
Electron density around Chain E:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



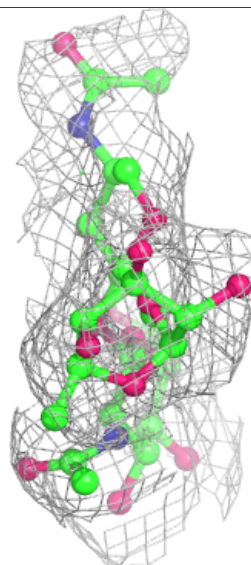
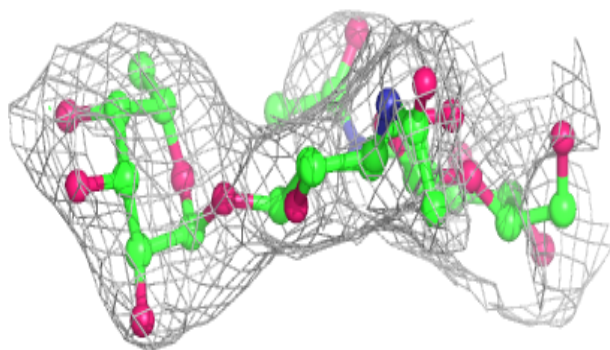
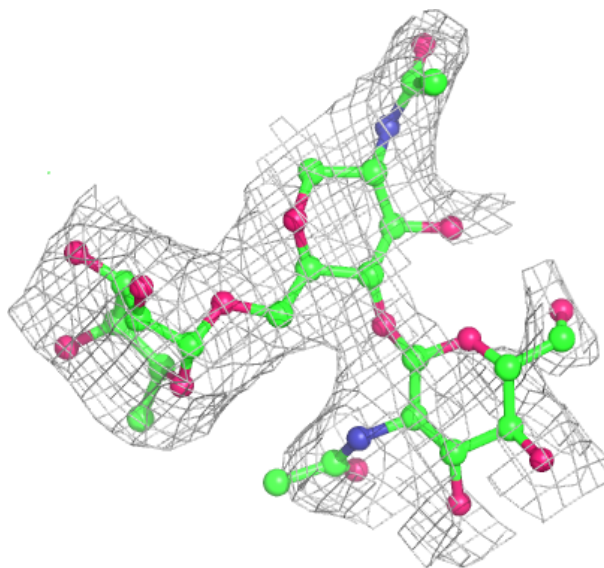
Electron density around Chain H:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



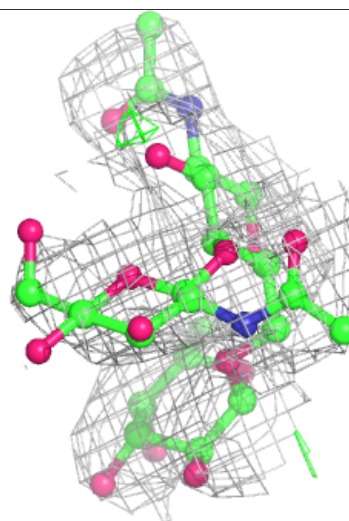
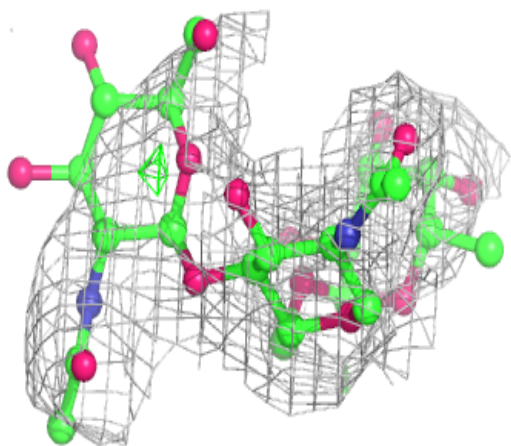
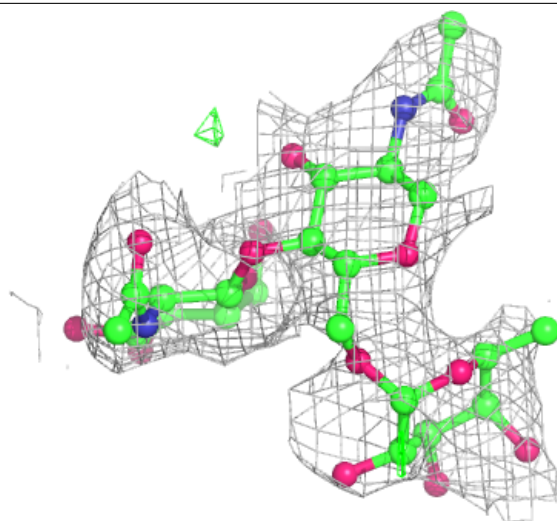
Electron density around Chain J:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



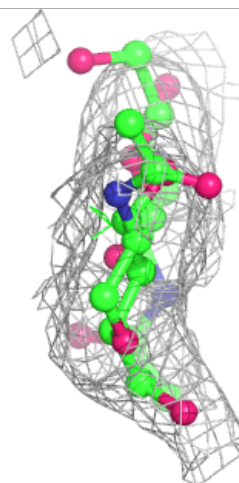
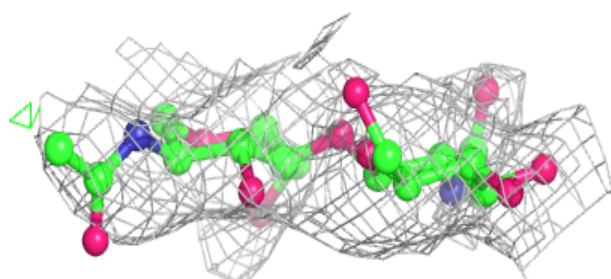
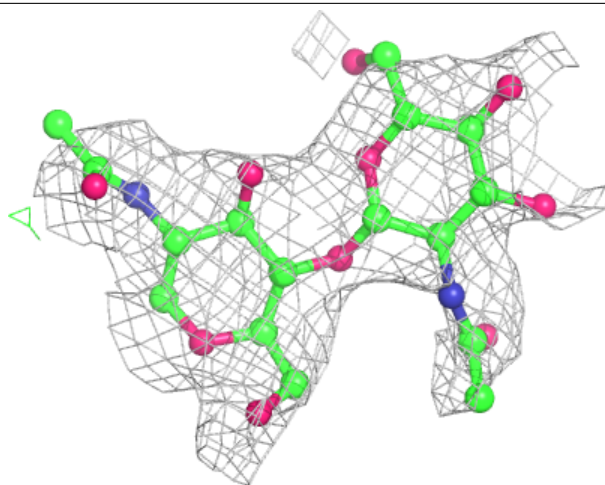
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



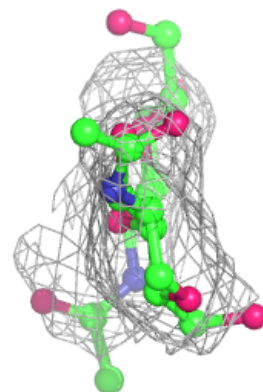
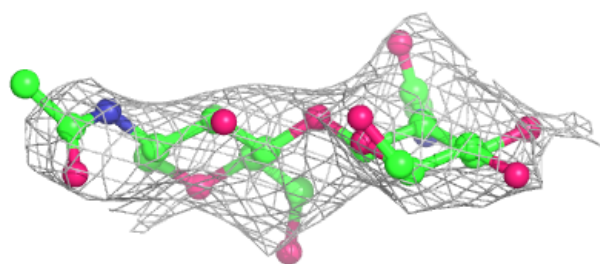
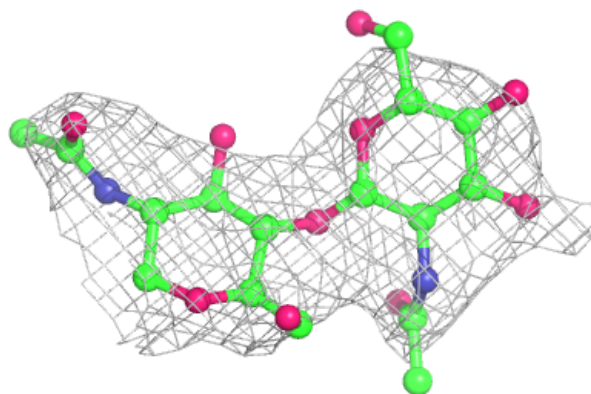
Electron density around Chain F:

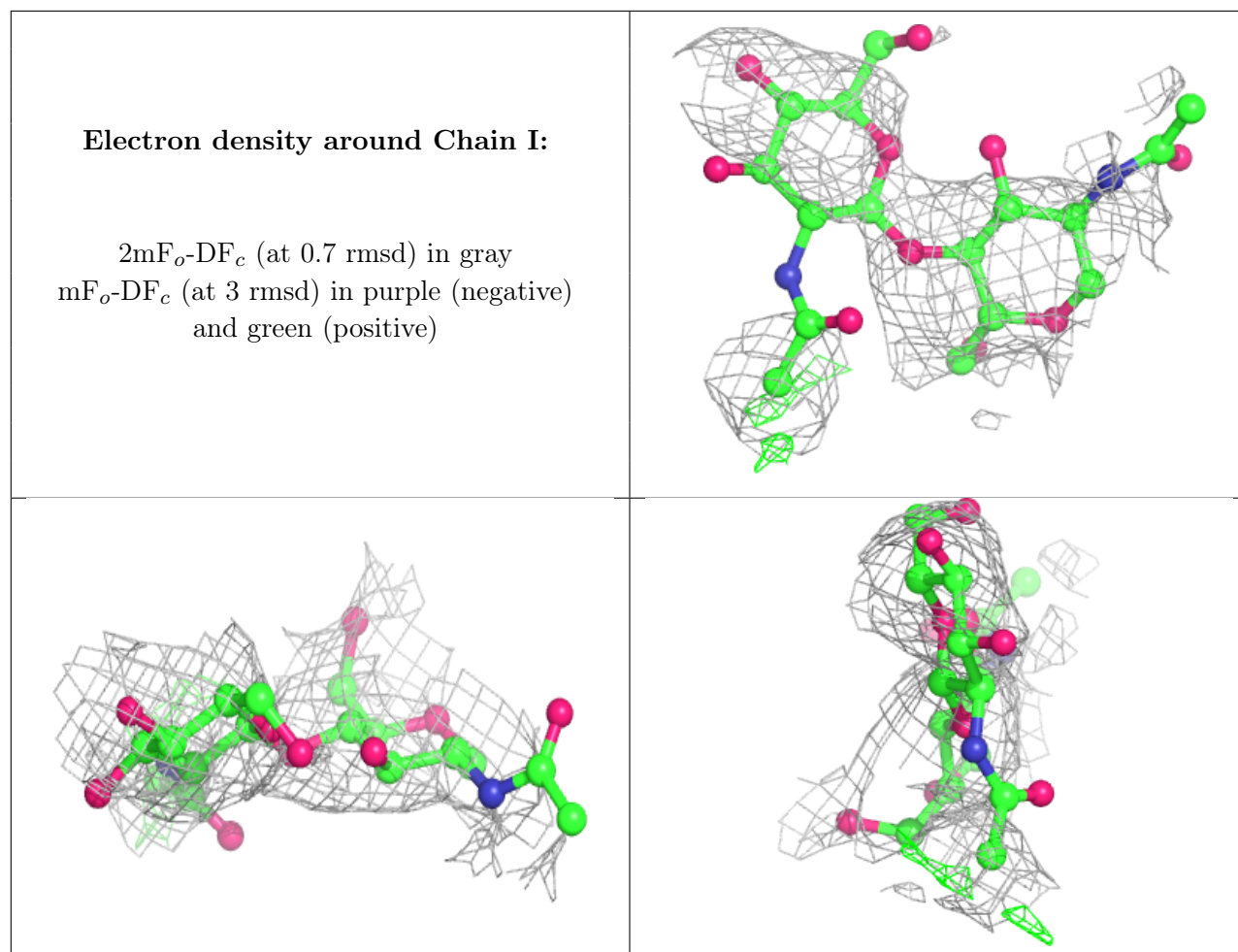
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	NAG	B	702	14/15	0.51	0.14	66,77,81,82	0
5	NAG	A	701	14/15	0.57	0.18	51,61,68,72	0
5	NAG	C	701	14/15	0.58	0.15	54,65,78,82	0
5	NAG	B	701	14/15	0.58	0.17	71,80,84,88	0
5	NAG	A	702	14/15	0.61	0.17	71,78,82,85	0
6	EDO	C	702	4/4	0.77	0.12	18,28,29,32	0
6	EDO	B	703	4/4	0.78	0.19	31,35,36,50	0
6	EDO	C	703	4/4	0.79	0.16	23,31,36,36	0
6	EDO	B	704	4/4	0.89	0.10	23,30,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.