



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 2C10 / pdb_00002c10
Title : The structure of a truncated, soluble version of semicarbazide- sensitive amine oxidase
Authors : Jakobsson, E.; Kleywegt, G.J.
Deposited on : 2005-09-09
Resolution : 2.50 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

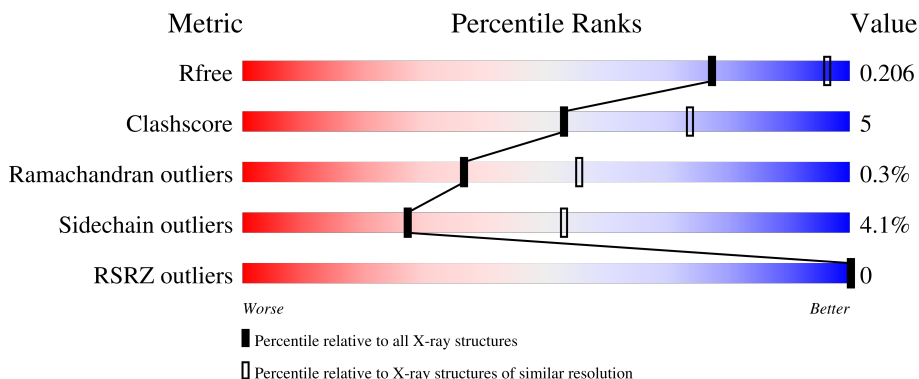
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	735	80% 15% . .
1	B	735	83% 12% . .
1	C	735	83% 12% . .
1	D	735	84% 11% . .
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	H	3	 33% 67%
2	K	3	 100%
3	F	3	 100%
3	L	3	 33% 67%
4	G	2	 100%
4	J	2	 100%
4	M	2	 100%
4	P	2	 100%
5	I	5	 80% 20%
5	O	5	 100%
6	N	4	 25% 75%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	X	-	-	-
3	FUC	F	3	X	-	-	-
3	NAG	L	1	X	-	-	-
3	FUC	L	3	X	-	-	-
5	NAG	I	1	X	-	-	-
5	FUC	I	5	X	-	-	-
5	NAG	O	1	X	-	-	-
5	FUC	O	5	X	-	-	-

2 Entry composition [i](#)

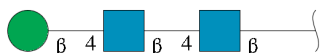
There are 11 unique types of molecules in this entry. The entry contains 23470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEMBRANE COPPER AMINE OXIDASE.

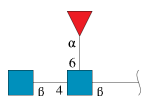
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	706	Total 5563	C 3571	N 960	O 1011	S 21	0	0	1
1	B	709	Total 5587	C 3587	N 965	O 1014	S 21	0	0	1
1	C	706	Total 5563	C 3571	N 960	O 1011	S 21	0	0	1
1	D	709	Total 5587	C 3587	N 965	O 1014	S 21	0	0	1

- Molecule 2 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
			Total	C	N	O			
2	E	3	Total 39	C 22	N 2	O 15	0	0	0
2	H	3	Total 39	C 22	N 2	O 15	0	0	0
2	K	3	Total 39	C 22	N 2	O 15	0	0	0

- 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.



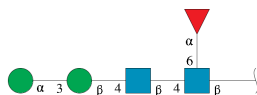
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	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			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



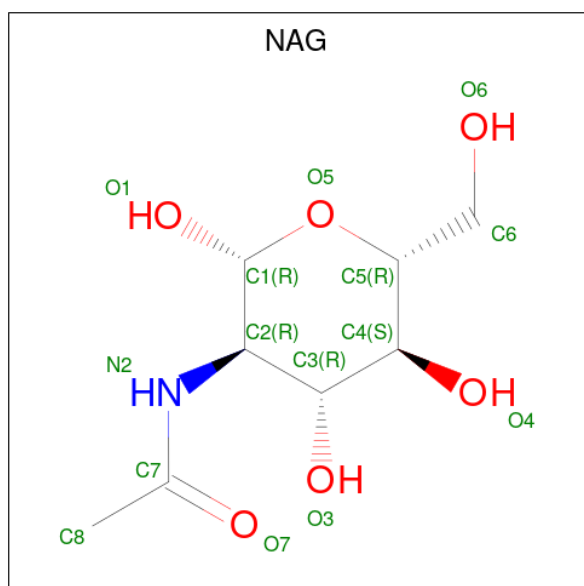
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	O	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 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
			Total	C	N	O			
6	N	4	50	28	2	20	0	0	0

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



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Ca 2 2	0	0
8	B	2	Total Ca 2 2	0	0
8	C	2	Total Ca 2 2	0	0
8	D	2	Total Ca 2 2	0	0

- Molecule 9 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cu 1 1	0	0
9	B	1	Total Cu 1 1	0	0
9	C	1	Total Cu 1 1	0	0
9	D	1	Total Cu 1 1	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Cl 2 2	0	0
10	B	2	Total Cl 2 2	0	0
10	C	2	Total Cl 2 2	0	0
10	D	2	Total Cl 2 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	141	Total O 141 141	0	0
11	B	139	Total O 139 139	0	0
11	C	141	Total O 141 141	0	0

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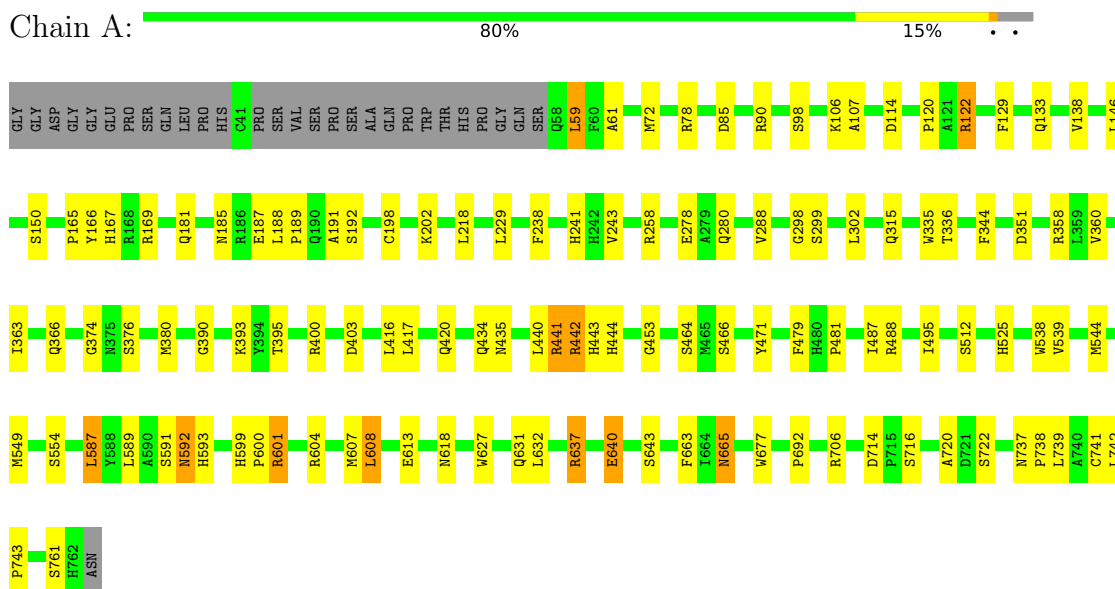
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	142	Total 142	O 142	0	0

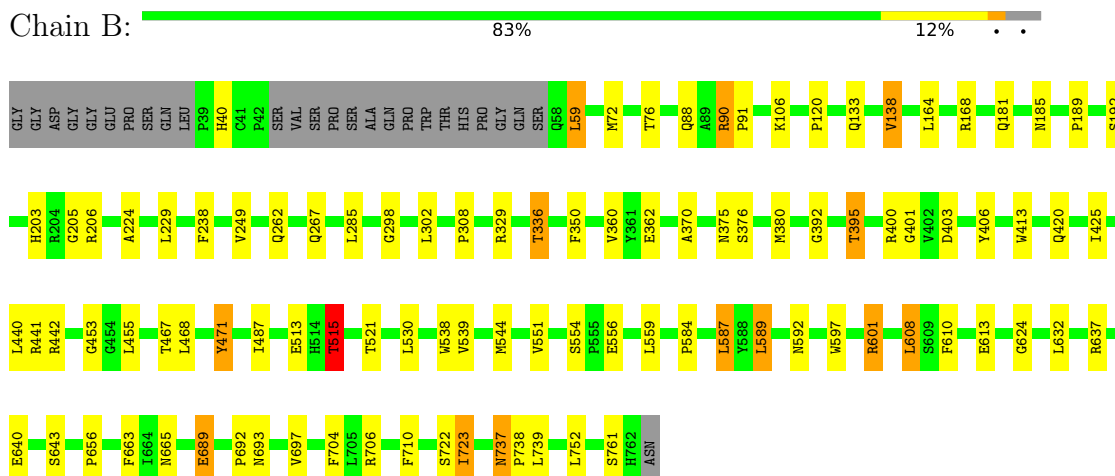
3 Residue-property plots [i](#)

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.

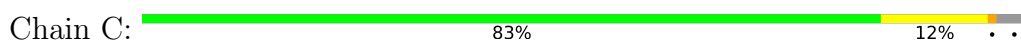
- Molecule 1: MEMBRANE COPPER AMINE OXIDASE

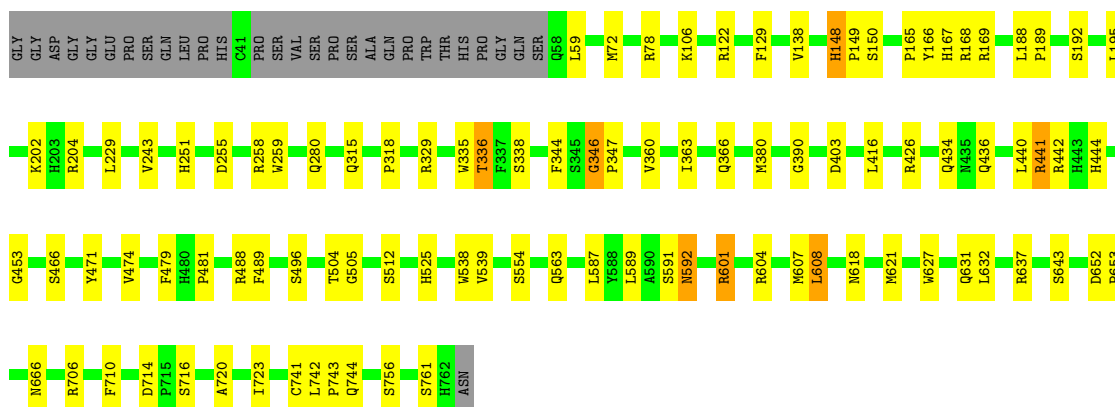


- Molecule 1: MEMBRANE COPPER AMINE OXIDASE



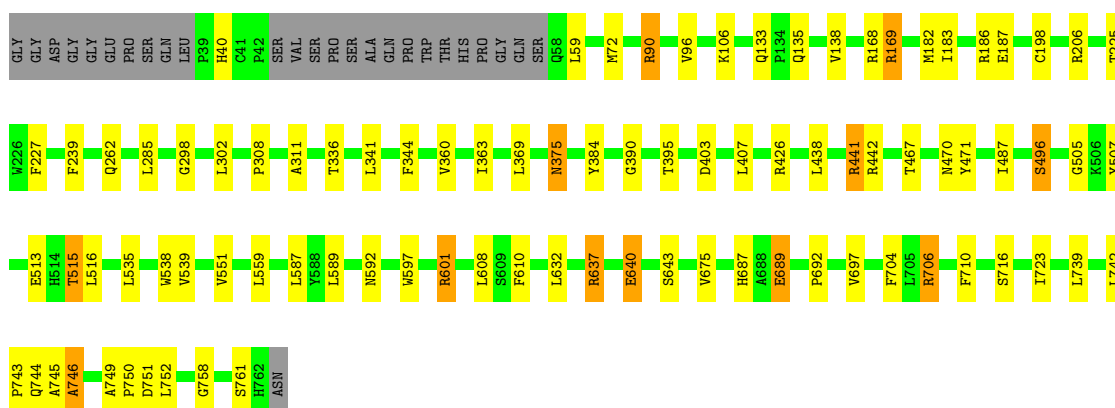
- Molecule 1: MEMBRANE COPPER AMINE OXIDASE





- Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain D: 84% 11%



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

Chain E: 100%

MAG1
MAG2
BMA3

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

Chain H: 33% 67%

MAG1
MAG2
BMA3

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

Chain K: 100%

MAG1
MAG2
BMA3

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

Chain F: 100%

MAG1
MAG2
FUC3

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

Chain L: 33% 67%

MAG1
MAG2
FUC3

- 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 J: 100%

MAG1
MAG2

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

Chain M: 100%

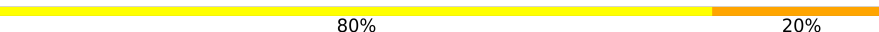
MAG1
MAG2

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

Chain P: 100%

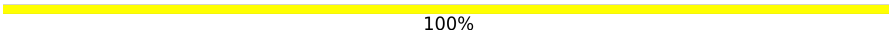
MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  80% 20%

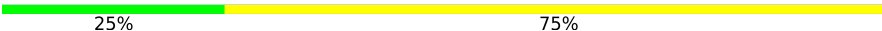
MAG1
MAG2
BMA3
MAN4
FUC5

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
BMA3
MAN4
FUC5

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

Chain N:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	130.24Å 130.24Å 221.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.50) 98.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.252 0.204 , 0.206	Depositor DCC
R_{free} test set	6351 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtrriage
Anisotropy	0.645	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 4.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23470	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: CA, CU, CL, FUC, MAN, TPQ, NAG, 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	0.60	1/5724 (0.0%)	0.84	6/7804 (0.1%)
1	B	0.60	1/5751 (0.0%)	0.85	6/7842 (0.1%)
1	C	0.60	1/5724 (0.0%)	0.85	9/7804 (0.1%)
1	D	0.59	1/5751 (0.0%)	0.84	1/7842 (0.0%)
All	All	0.60	4/22950 (0.0%)	0.85	22/31292 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	761	SER	C-N	-6.74	1.24	1.33
1	A	761	SER	C-N	-6.57	1.24	1.33
1	B	761	SER	C-N	-6.56	1.24	1.33
1	C	761	SER	C-N	-6.42	1.24	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	SER	CA-C-N	8.40	128.06	119.82
1	C	554	SER	C-N-CA	8.40	128.06	119.82
1	A	592	ASN	N-CA-C	-6.82	105.09	113.41
1	C	346	GLY	CA-C-N	6.22	126.25	119.90
1	C	346	GLY	C-N-CA	6.22	126.25	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	198	CYS	Peptide

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	5563	0	5311	78	0
1	B	5587	0	5333	54	0
1	C	5563	0	5311	52	0
1	D	5587	0	5332	59	0
2	E	39	0	34	0	0
2	H	39	0	34	1	0
2	K	39	0	34	0	0
3	F	38	0	34	0	0
3	L	38	0	34	1	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
5	I	60	0	52	2	0
5	O	60	0	52	0	0
6	N	50	0	43	0	0
7	A	14	0	13	1	0
7	B	42	0	39	1	0
7	C	14	0	13	0	0
7	D	42	0	39	1	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	2	0	0	0	0
10	C	2	0	0	0	0
10	D	2	0	0	0	0
11	A	141	0	0	9	0
11	B	139	0	0	4	0
11	C	141	0	0	5	0
11	D	142	0	0	5	0
All	All	23470	0	21808	224	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 5.

The worst 5 of 224 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:D:360:VAL:HG11	1:D:363:ILE:HG13	1.38	1.04
1:A:360:VAL:HG11	1:A:363:ILE:HG13	1.56	0.85
1:D:426:ARG:HE	1:D:758:GLY:HA3	1.49	0.78
1:A:538:TRP:CZ3	1:A:592:ASN:HB2	2.19	0.77
1:A:488:ARG:HH12	1:A:608:LEU:CD1	1.98	0.77

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	702/735 (96%)	671 (96%)	30 (4%)	1 (0%)	48 68
1	B	704/735 (96%)	675 (96%)	27 (4%)	2 (0%)	36 55
1	C	702/735 (96%)	668 (95%)	32 (5%)	2 (0%)	36 55
1	D	704/735 (96%)	675 (96%)	26 (4%)	3 (0%)	30 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2812/2940 (96%)	2689 (96%)	115 (4%)	8 (0%)	36	55

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	ALA
1	C	744	GLN
1	B	59	LEU
1	C	204	ARG
1	B	205	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/609 (96%)	558 (95%)	27 (5%)	24	48
1	B	588/609 (97%)	563 (96%)	25 (4%)	26	51
1	C	585/609 (96%)	562 (96%)	23 (4%)	28	55
1	D	588/609 (97%)	566 (96%)	22 (4%)	30	57
All	All	2346/2436 (96%)	2249 (96%)	97 (4%)	27	53

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	202	LYS
1	C	666	ASN
1	C	243	VAL
1	C	441	ARG
1	D	59	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	757	HIS
1	C	315	GLN
1	D	375	ASN
1	C	241	HIS
1	C	560	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPQ	D	471	1	13,14,15	2.22	2 (15%)	13,19,21	1.50	3 (23%)
1	TPQ	A	471	1	13,14,15	2.16	3 (23%)	13,19,21	1.57	4 (30%)
1	TPQ	C	471	1	13,14,15	2.19	2 (15%)	13,19,21	1.48	3 (23%)
1	TPQ	B	471	1	13,14,15	2.21	3 (23%)	13,19,21	1.64	3 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	D	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	A	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	C	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	4/5/22/24	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	TPQ	O5-C5	4.88	1.37	1.24
1	C	471	TPQ	O5-C5	4.88	1.37	1.24
1	B	471	TPQ	O5-C5	4.80	1.37	1.24
1	A	471	TPQ	O5-C5	4.61	1.36	1.24
1	C	471	TPQ	O2-C2	4.54	1.36	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	C6-C1-C2	3.19	120.92	118.66
1	C	471	TPQ	C6-C1-C2	3.05	120.83	118.66
1	D	471	TPQ	C6-C5-C4	2.74	121.59	116.80
1	A	471	TPQ	C1-C6-C5	-2.65	118.13	122.59
1	A	471	TPQ	C6-C5-C4	2.64	121.43	116.80

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C6-C1-CB-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	1	0

5.5 Carbohydrates [i](#)

37 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	E	1	1,2	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.18	1 (5%)
2	BMA	E	3	2	11,11,12	0.49	0	15,15,17	1.18	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.67	0	17,19,21	1.74	3 (17%)
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.82	4 (23%)
3	FUC	F	3	3	10,10,11	0.68	0	14,14,16	1.50	2 (14%)
4	NAG	G	1	4,1	14,14,15	0.58	0	17,19,21	1.05	2 (11%)
4	NAG	G	2	4	14,14,15	0.63	0	17,19,21	1.43	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.67	0	17,19,21	1.26	2 (11%)
2	NAG	H	2	2	14,14,15	0.50	0	17,19,21	1.16	1 (5%)
2	BMA	H	3	2	11,11,12	0.73	0	15,15,17	0.91	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.60	0	17,19,21	1.79	2 (11%)
5	NAG	I	2	5	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
5	BMA	I	3	5	11,11,12	0.69	0	15,15,17	1.74	3 (20%)
5	MAN	I	4	5	11,11,12	0.55	0	15,15,17	1.13	1 (6%)
5	FUC	I	5	5	10,10,11	0.71	0	14,14,16	0.89	0
4	NAG	J	1	4,1	14,14,15	0.65	0	17,19,21	0.99	1 (5%)
4	NAG	J	2	4	14,14,15	0.61	0	17,19,21	1.58	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
2	NAG	K	2	2	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
2	BMA	K	3	2	11,11,12	0.60	0	15,15,17	0.85	1 (6%)
3	NAG	L	1	3,1	14,14,15	0.63	0	17,19,21	2.05	4 (23%)
3	NAG	L	2	3	14,14,15	0.55	0	17,19,21	1.42	4 (23%)
3	FUC	L	3	3	10,10,11	0.79	0	14,14,16	1.39	3 (21%)
4	NAG	M	1	4,1	14,14,15	0.54	0	17,19,21	1.54	3 (17%)
4	NAG	M	2	4	14,14,15	0.65	0	17,19,21	1.69	1 (5%)
6	NAG	N	1	6,1	14,14,15	0.56	0	17,19,21	1.01	0
6	NAG	N	2	6	14,14,15	0.56	0	17,19,21	2.00	8 (47%)
6	BMA	N	3	6	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
6	MAN	N	4	6	11,11,12	0.60	0	15,15,17	1.38	2 (13%)
5	NAG	O	1	1,5	14,14,15	0.51	0	17,19,21	2.33	3 (17%)
5	NAG	O	2	5	14,14,15	0.49	0	17,19,21	1.93	3 (17%)
5	BMA	O	3	5	11,11,12	0.88	0	15,15,17	1.94	3 (20%)
5	MAN	O	4	5	11,11,12	0.60	0	15,15,17	2.52	3 (20%)
5	FUC	O	5	5	10,10,11	0.76	0	14,14,16	1.36	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	P	1	4,1	14,14,15	0.58	0	17,19,21	0.95	2 (11%)
4	NAG	P	2	4	14,14,15	0.65	0	17,19,21	1.12	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	1/1/4/5	-	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	1/2/19/22	0/1/1/1
5	FUC	I	5	5	1/1/4/5	-	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
3	NAG	L	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	FUC	L	3	3	1/1/4/5	-	0/1/1/1
4	NAG	M	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
5	NAG	O	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	MAN	O	4	5	-	2/2/19/22	0/1/1/1
5	FUC	O	5	5	1/1/4/5	-	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	4	MAN	C1-O5-C5	8.39	123.42	112.19
5	O	2	NAG	C1-O5-C5	5.99	120.22	112.19
5	O	1	NAG	C1-O5-C5	5.84	120.02	112.19
5	O	1	NAG	O5-C1-C2	5.83	120.32	111.29
5	O	3	BMA	C1-C2-C3	5.74	118.00	109.64

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	1	NAG	C1
3	F	3	FUC	C1
3	L	1	NAG	C1
3	L	3	FUC	C1
5	I	1	NAG	C1

5 of 63 torsion outliers are listed below:

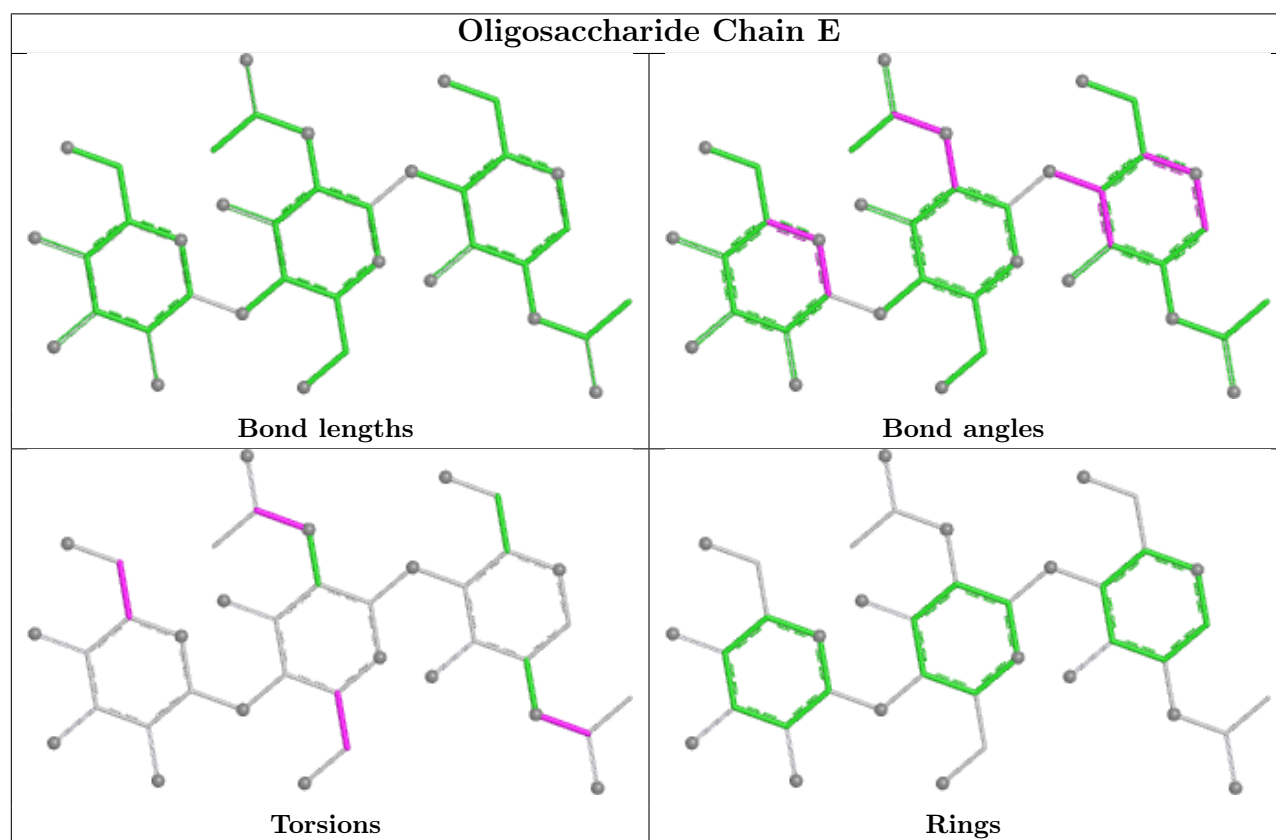
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2

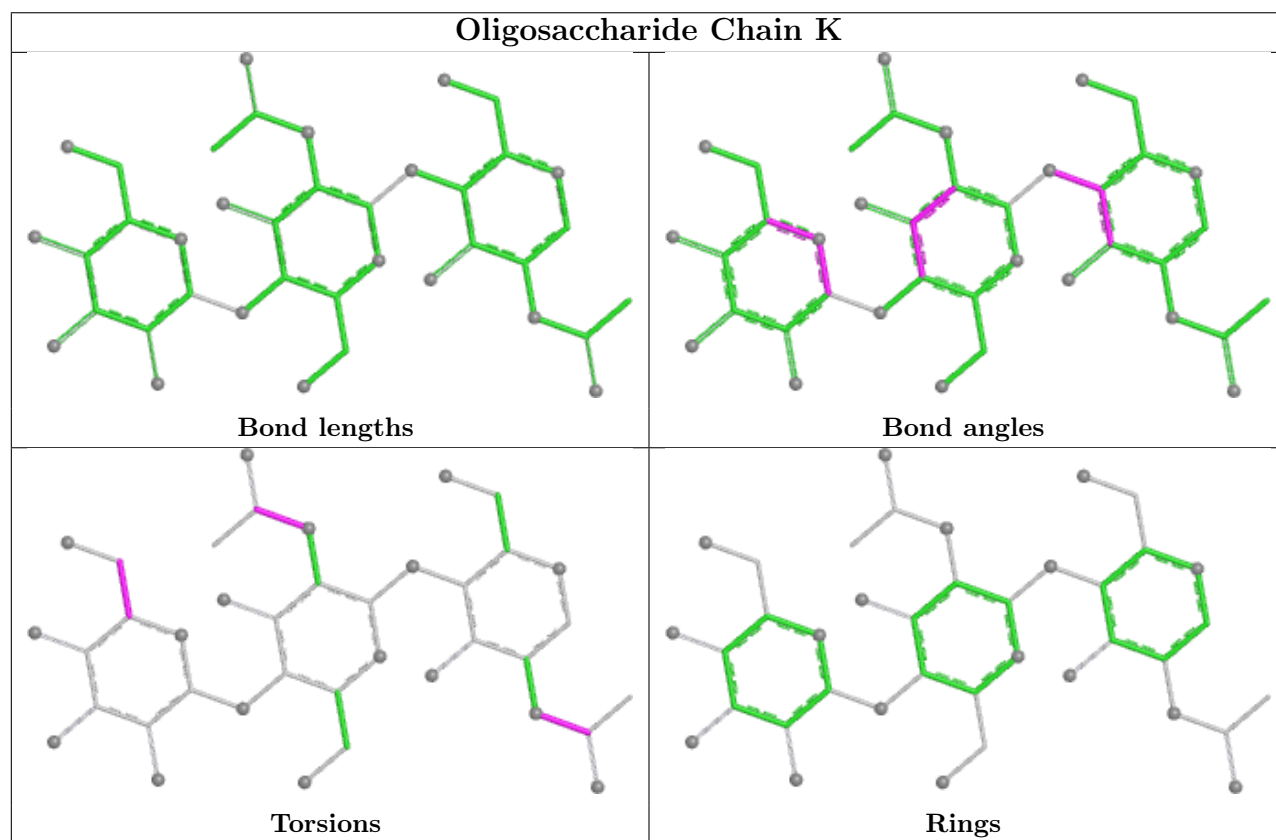
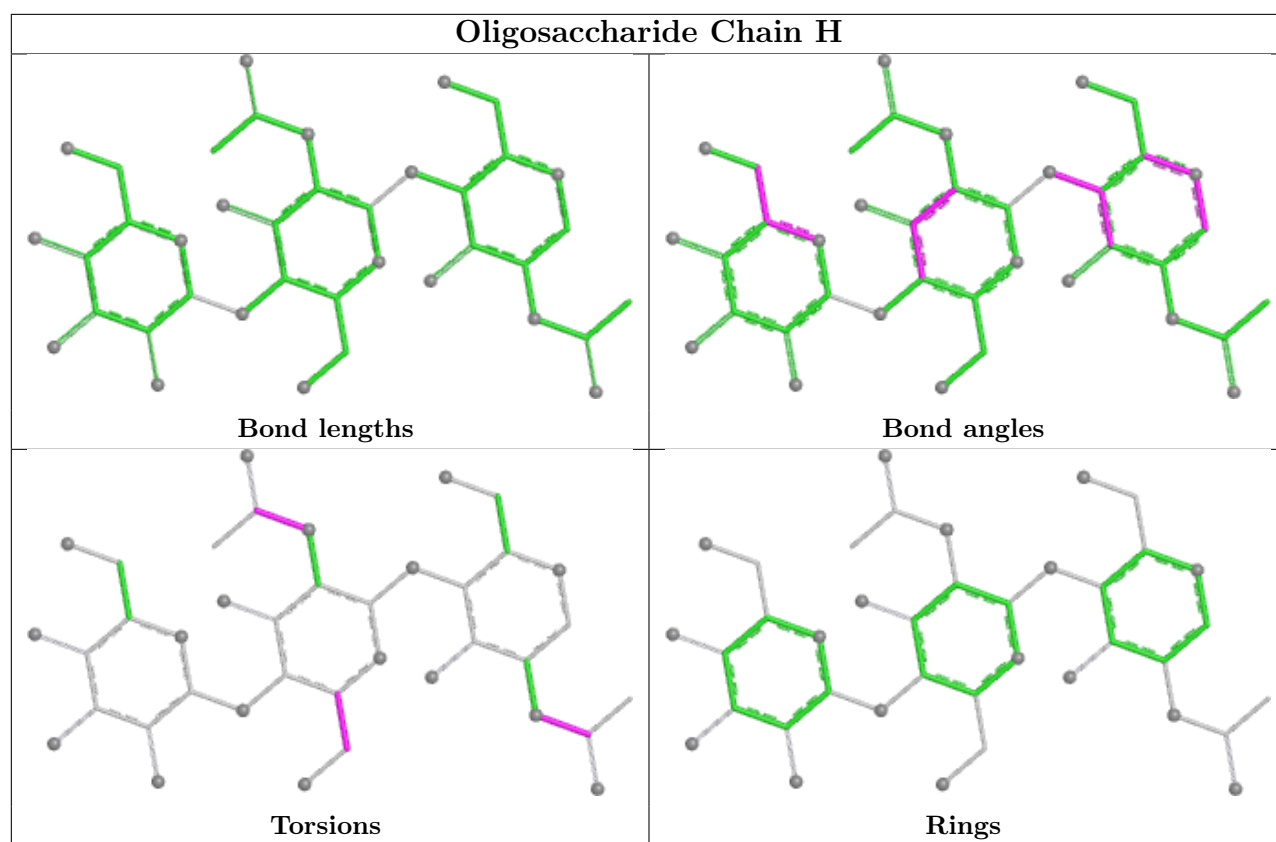
There are no ring outliers.

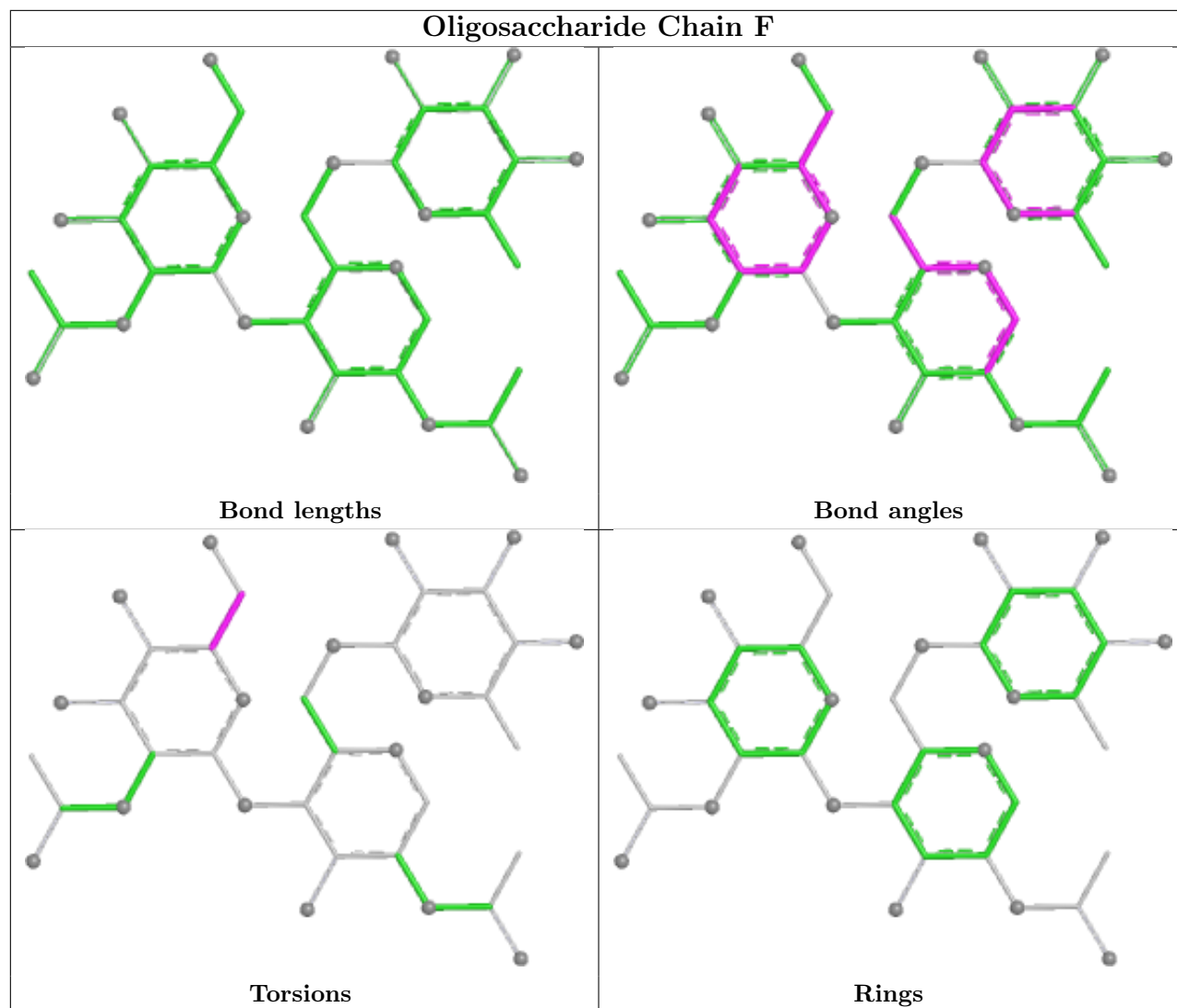
6 monomers are involved in 4 short contacts:

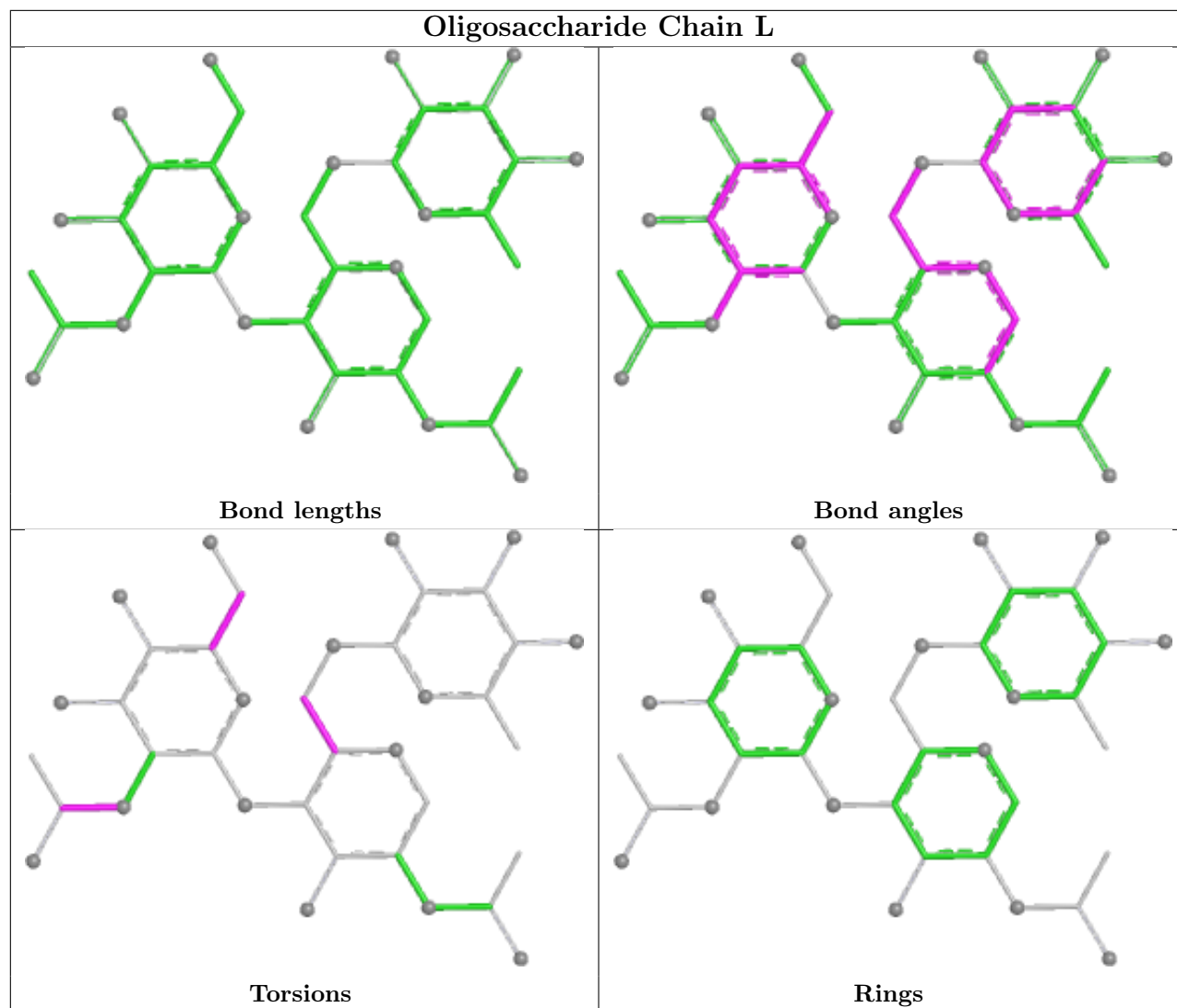
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0
5	I	2	NAG	2	0
3	L	1	NAG	1	0
2	H	3	BMA	1	0
5	I	5	FUC	1	0
3	L	2	NAG	1	0

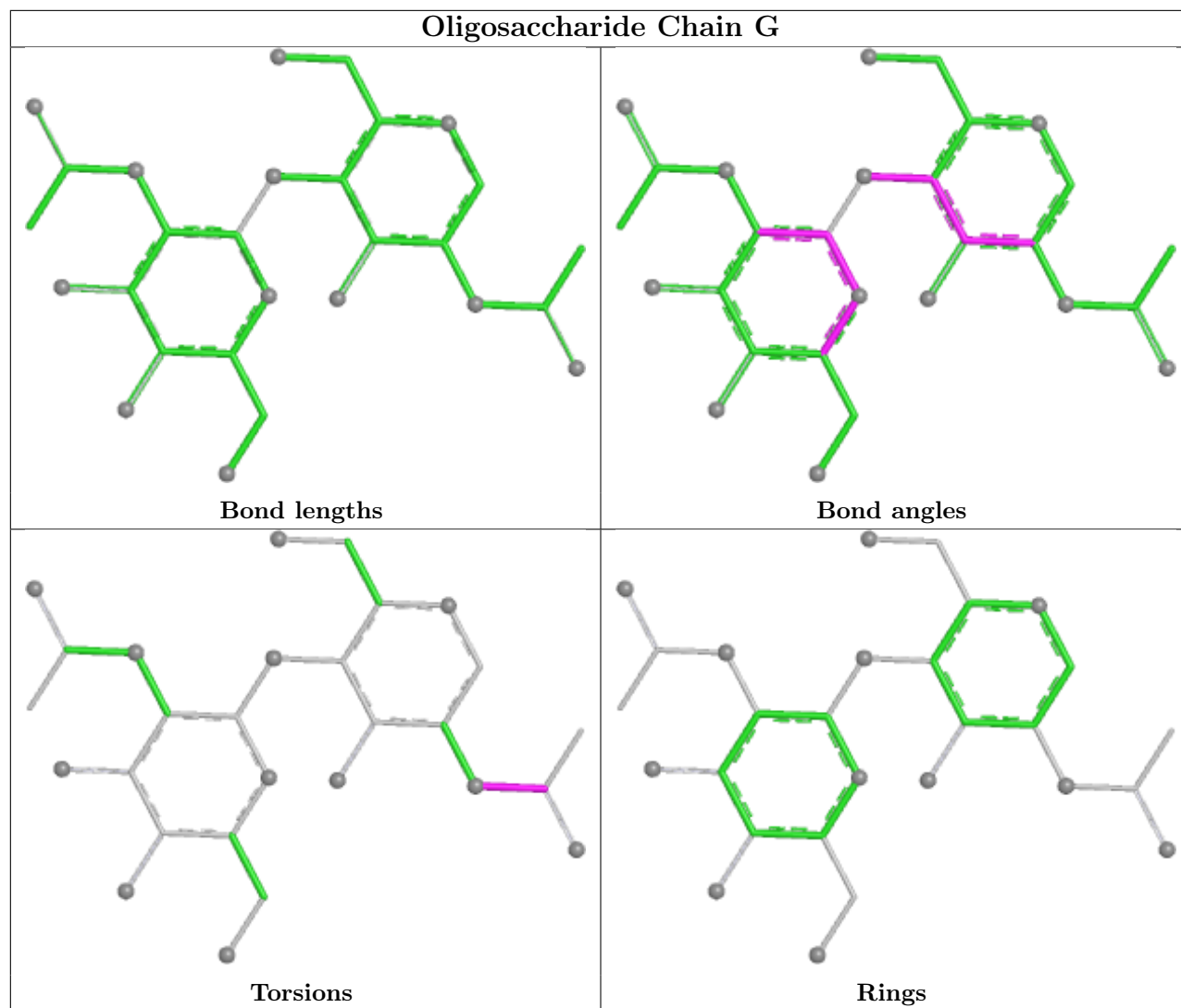
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

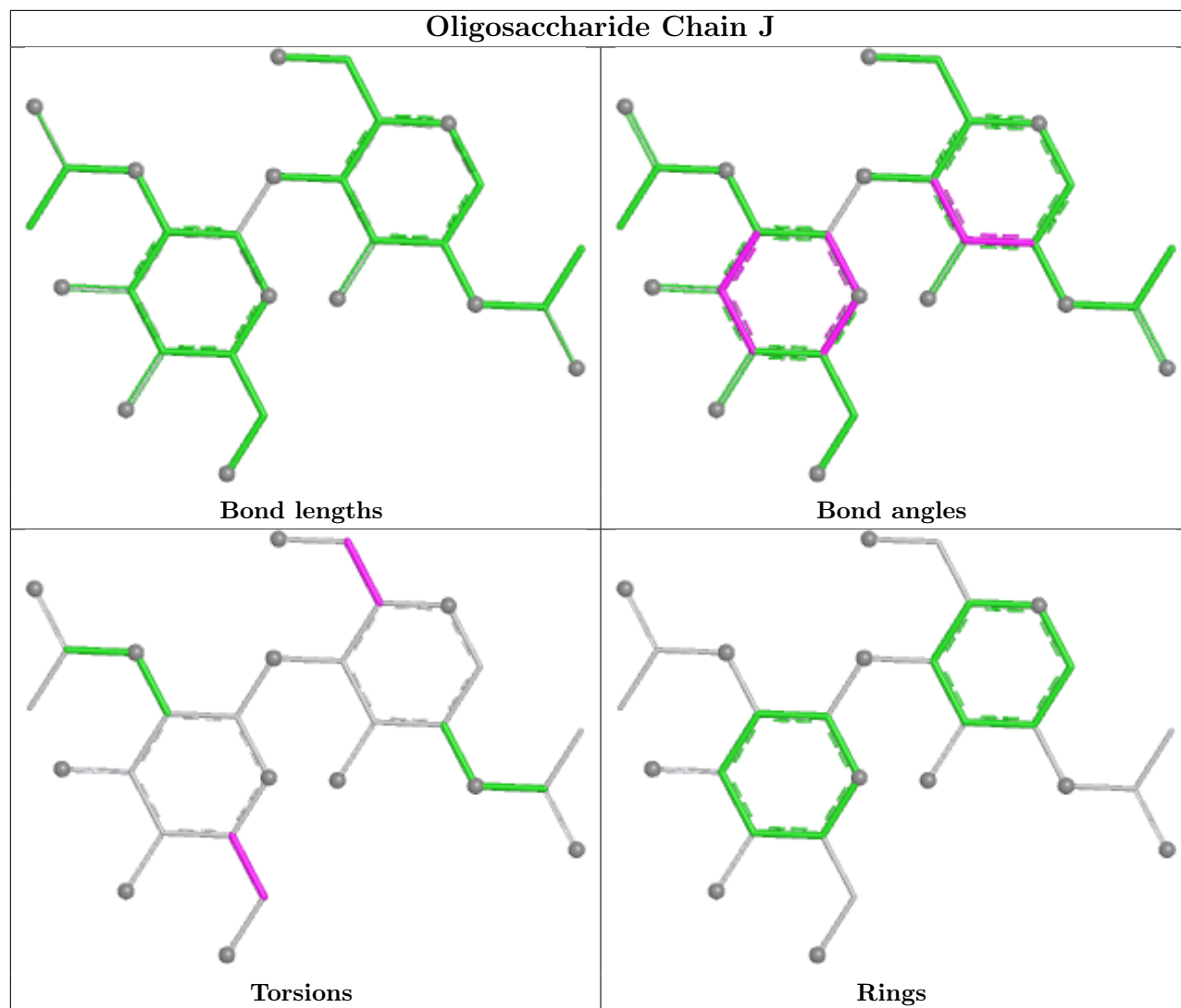


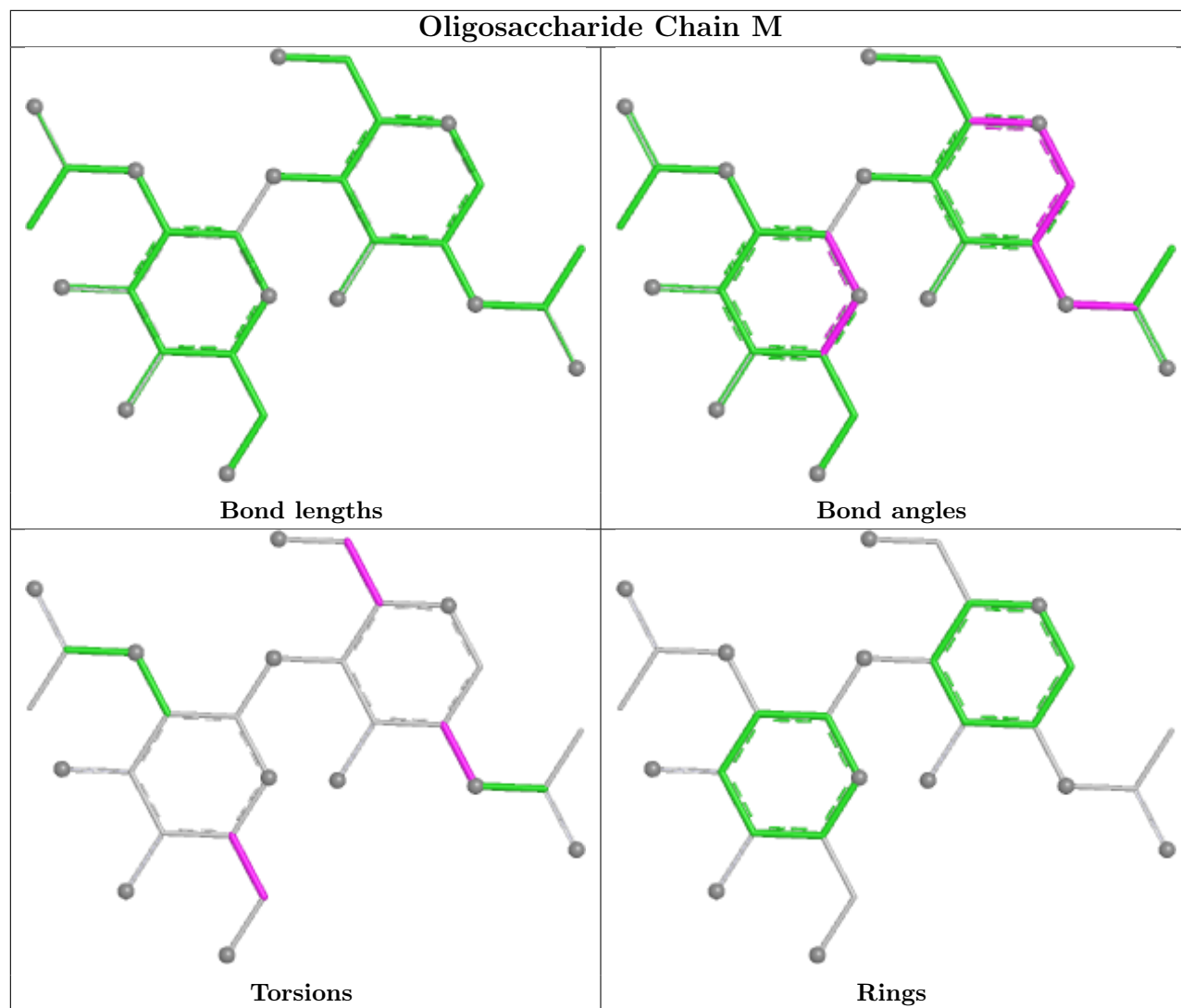


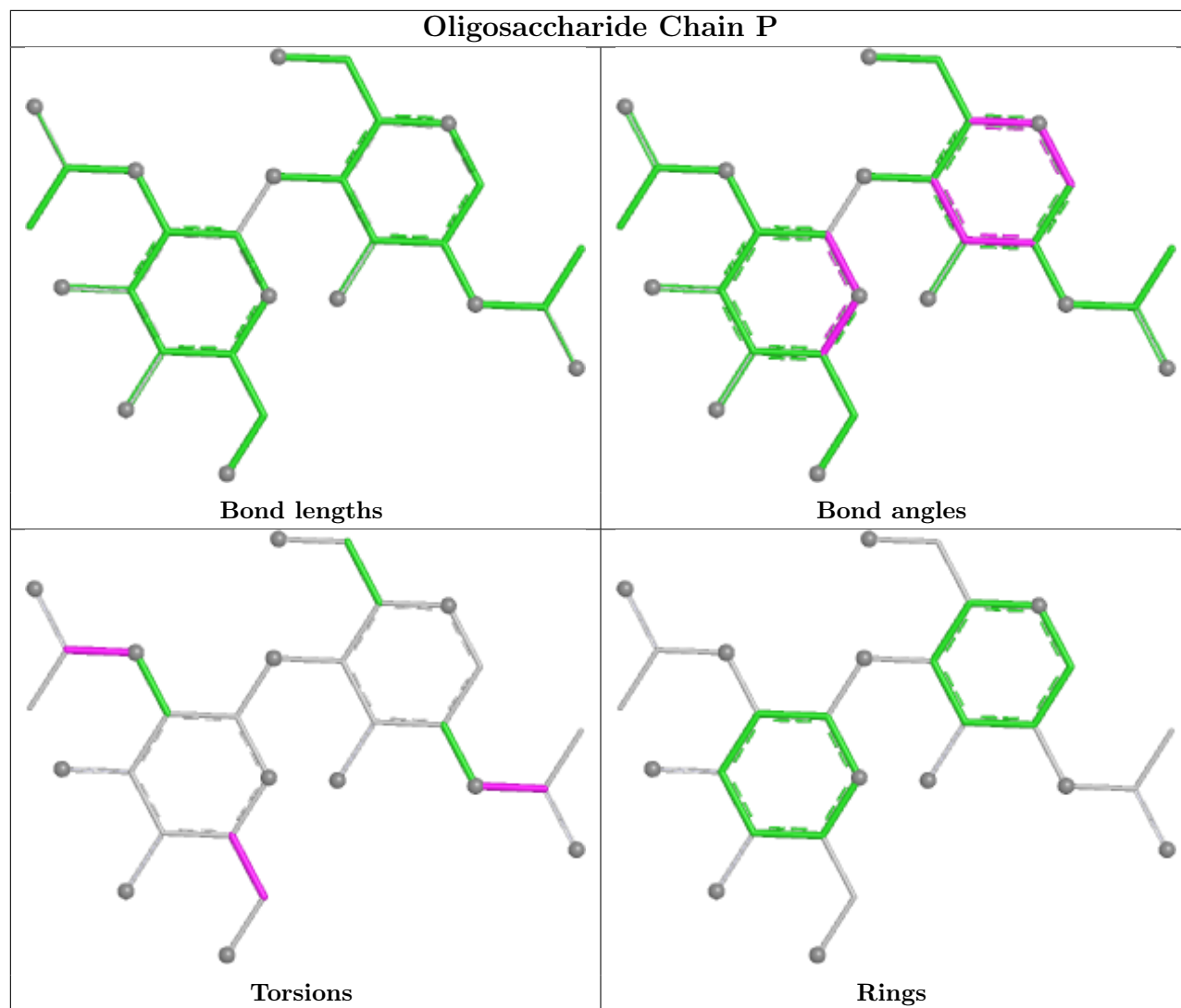


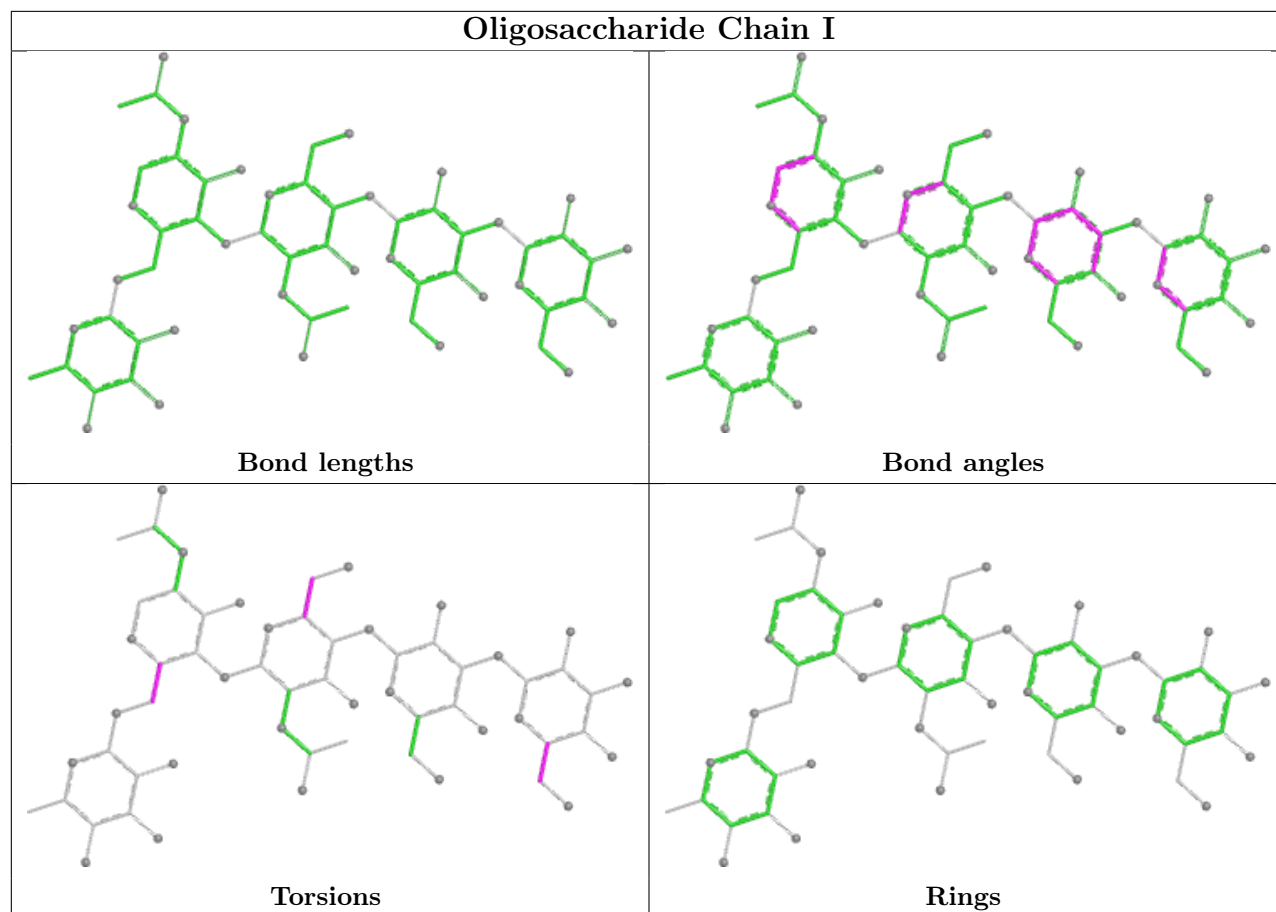


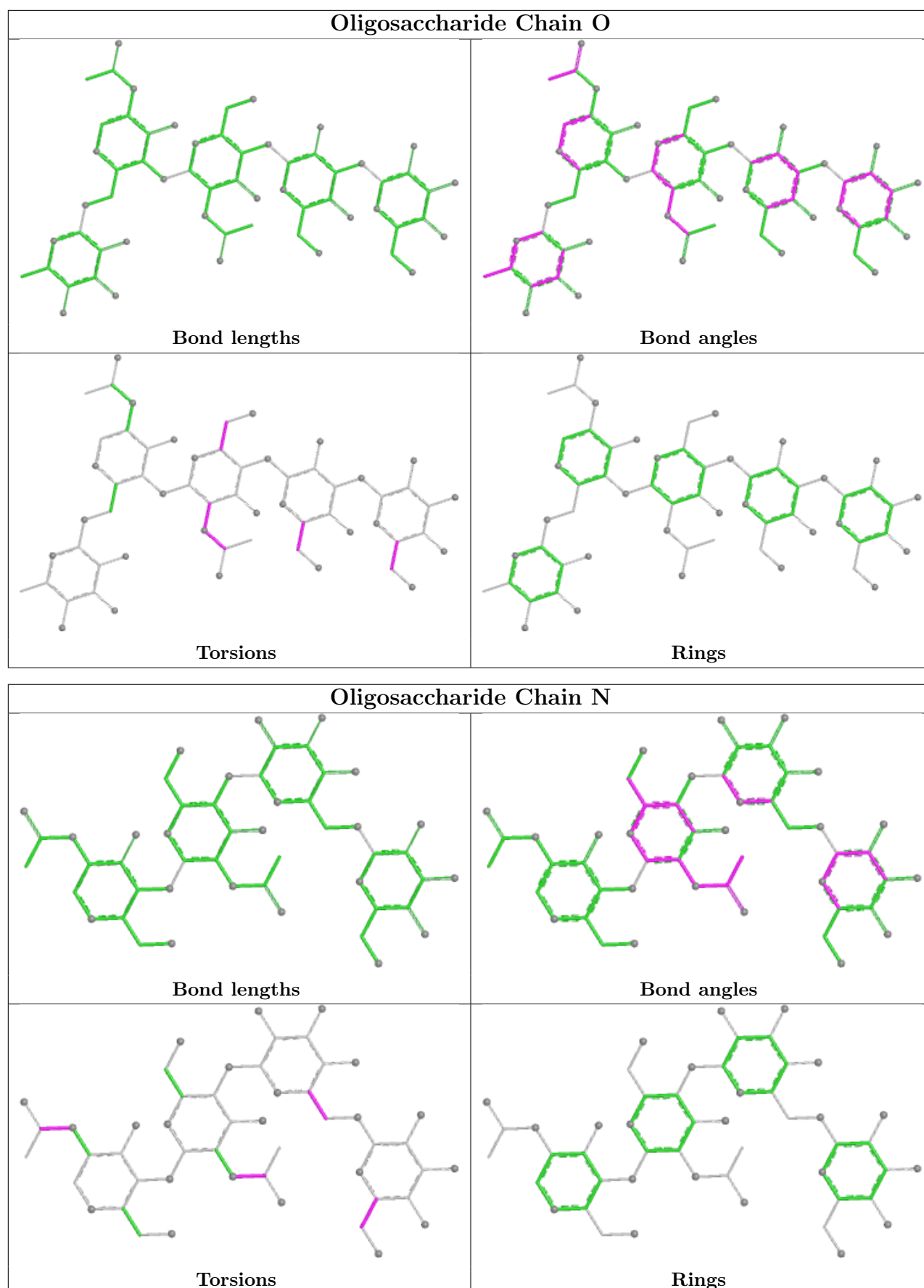












5.6 Ligand geometry

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 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	C	1768	1	14,14,15	0.62	0	17,19,21	0.78	0
7	NAG	D	1770	1	14,14,15	0.68	0	17,19,21	1.29	2 (11%)
7	NAG	B	1770	1	14,14,15	0.65	0	17,19,21	2.74	6 (35%)
7	NAG	D	1774	-	14,14,15	0.64	0	17,19,21	1.59	3 (17%)
7	NAG	D	1768	1	14,14,15	0.59	0	17,19,21	1.55	3 (17%)
7	NAG	B	1773	-	14,14,15	0.62	0	17,19,21	1.90	4 (23%)
7	NAG	A	1768	1	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
7	NAG	B	1768	1	14,14,15	0.55	0	17,19,21	1.51	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
7	NAG	C	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1770	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1770	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1774	-	-	3/6/23/26	0/1/1/1
7	NAG	D	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1773	-	-	4/6/23/26	0/1/1/1
7	NAG	A	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1768	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1770	NAG	C1-O5-C5	8.34	123.36	112.19
7	B	1768	NAG	C1-O5-C5	5.35	119.35	112.19
7	B	1773	NAG	C2-N2-C7	5.03	129.64	122.90
7	D	1774	NAG	C2-N2-C7	4.21	128.54	122.90
7	B	1770	NAG	C4-C3-C2	4.03	116.92	111.02

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1768	NAG	C8-C7-N2-C2
7	B	1768	NAG	O7-C7-N2-C2
7	B	1773	NAG	C1-C2-N2-C7
7	D	1774	NAG	C3-C2-N2-C7
7	D	1774	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1774	NAG	1	0
7	B	1773	NAG	1	0
7	A	1768	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	705/735 (95%)	-1.49	0 100 100	26, 34, 64, 88	0
1	B	708/735 (96%)	-1.50	0 100 100	24, 34, 67, 99	0
1	C	705/735 (95%)	-1.49	0 100 100	25, 35, 64, 84	0
1	D	708/735 (96%)	-1.49	0 100 100	24, 34, 68, 101	0
All	All	2826/2940 (96%)	-1.50	0 100 100	24, 34, 67, 101	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPQ	A	471	14/15	0.99	0.04	40,48,51,52	0
1	TPQ	B	471	14/15	0.99	0.05	39,47,49,50	0
1	TPQ	C	471	14/15	0.99	0.04	38,46,49,49	0
1	TPQ	D	471	14/15	0.99	0.05	38,46,49,49	0

6.3 Carbohydrates [i](#)

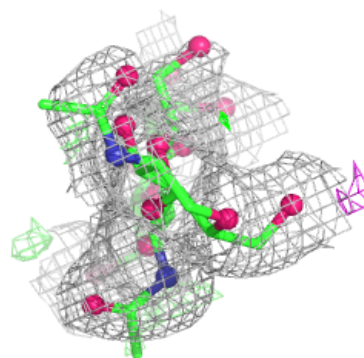
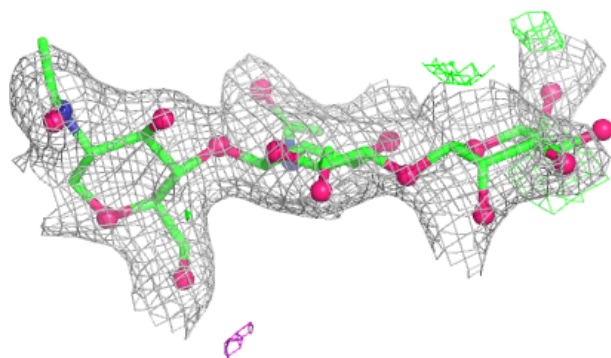
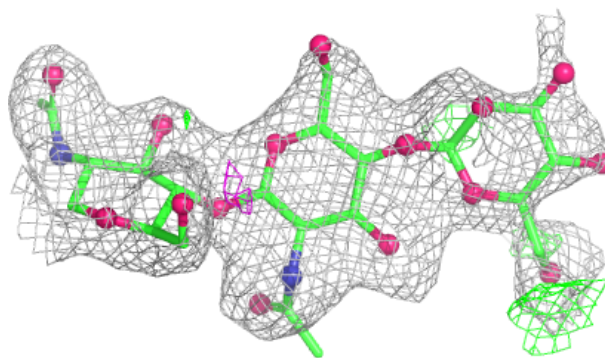
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	K	3	11/12	0.94	0.05	73,75,75,76	0
2	BMA	H	3	11/12	0.95	0.05	79,82,82,82	0
2	BMA	E	3	11/12	0.95	0.06	72,74,75,75	0
3	NAG	L	2	14/15	0.95	0.07	62,65,69,69	0
4	NAG	M	2	14/15	0.95	0.06	76,79,80,81	0
6	BMA	N	3	11/12	0.95	0.04	79,82,86,88	0
5	BMA	I	3	11/12	0.96	0.05	69,70,72,75	0
5	MAN	O	4	11/12	0.96	0.06	79,81,82,82	0
4	NAG	G	2	14/15	0.96	0.07	77,81,81,82	0
6	MAN	N	4	11/12	0.96	0.05	89,90,91,91	0
5	MAN	I	4	11/12	0.97	0.05	78,79,80,81	0
5	BMA	O	3	11/12	0.97	0.04	67,70,72,76	0
3	NAG	F	2	14/15	0.97	0.05	57,61,62,62	0
4	NAG	P	2	14/15	0.97	0.05	74,75,77,77	0
4	NAG	J	2	14/15	0.97	0.05	71,73,73,74	0
4	NAG	P	1	14/15	0.98	0.04	59,66,68,71	0
3	NAG	L	1	14/15	0.98	0.03	42,48,53,58	0
5	NAG	I	2	14/15	0.98	0.04	54,61,67,68	0
2	NAG	K	1	14/15	0.98	0.04	43,49,51,55	0
2	NAG	K	2	14/15	0.98	0.04	59,61,66,70	0
5	FUC	I	5	10/11	0.98	0.05	53,55,56,57	0
5	NAG	O	2	14/15	0.98	0.04	55,59,62,66	0
4	NAG	J	1	14/15	0.98	0.04	58,63,65,68	0
2	NAG	H	2	14/15	0.98	0.04	62,66,70,75	0
5	FUC	O	5	10/11	0.98	0.05	52,55,57,58	0
6	NAG	N	2	14/15	0.98	0.04	61,64,68,74	0
4	NAG	M	1	14/15	0.98	0.04	58,64,66,72	0
2	NAG	E	2	14/15	0.98	0.04	59,63,65,69	0
5	NAG	O	1	14/15	0.99	0.03	34,43,52,52	0
4	NAG	G	1	14/15	0.99	0.04	58,64,67,73	0
2	NAG	H	1	14/15	0.99	0.03	39,43,48,55	0
5	NAG	I	1	14/15	0.99	0.03	39,45,51,54	0
3	FUC	F	3	10/11	0.99	0.04	50,51,52,52	0
6	NAG	N	1	14/15	0.99	0.04	40,44,49,55	0
2	NAG	E	1	14/15	0.99	0.04	43,46,49,55	0
3	NAG	F	1	14/15	0.99	0.02	39,44,48,53	0
3	FUC	L	3	10/11	0.99	0.04	47,50,52,53	0

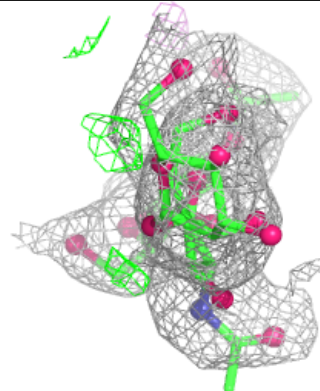
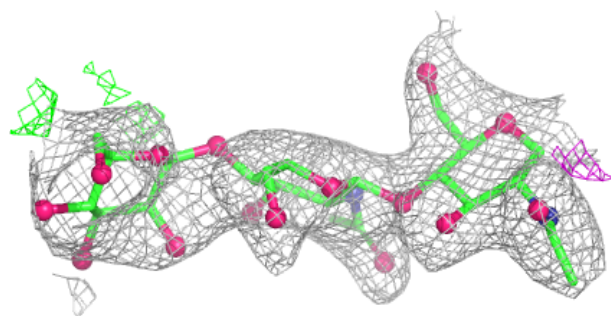
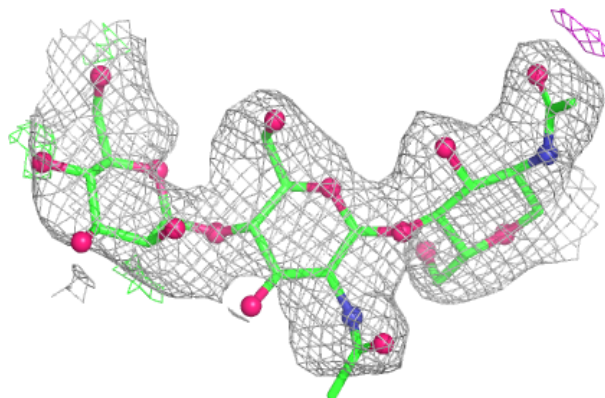
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

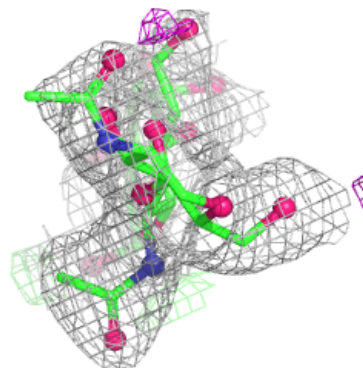
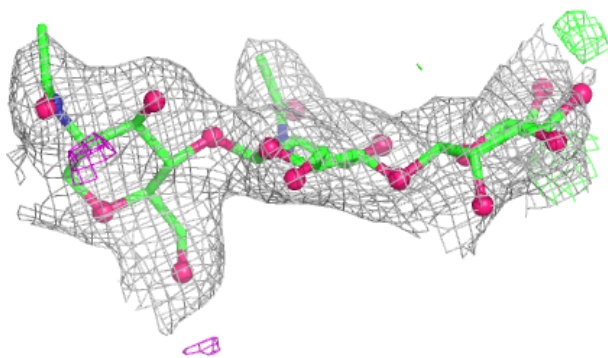
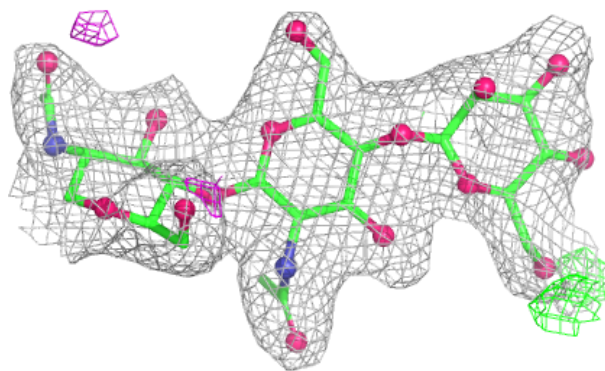
**Electron density around Chain H:**

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



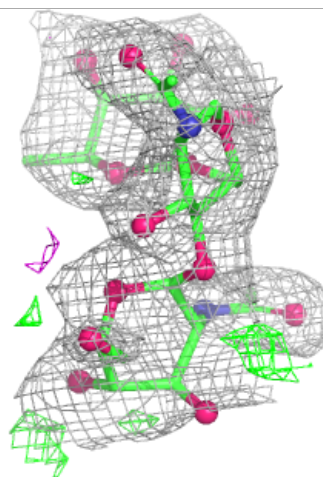
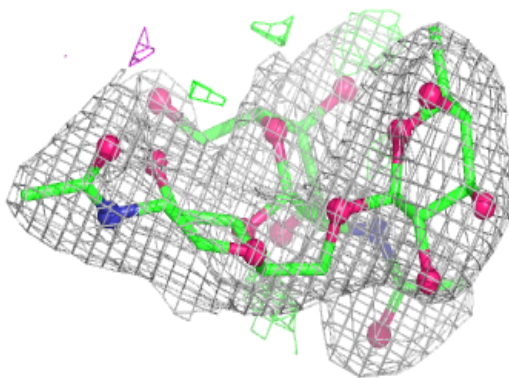
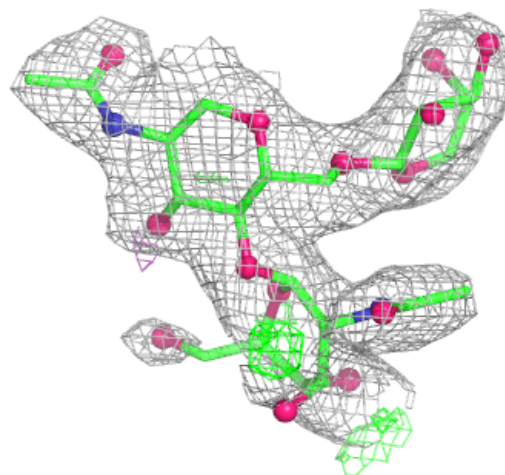
Electron density around Chain K:

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



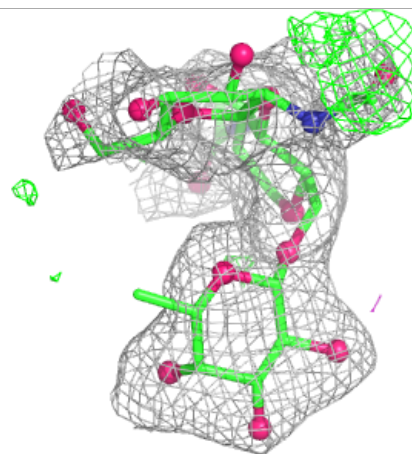
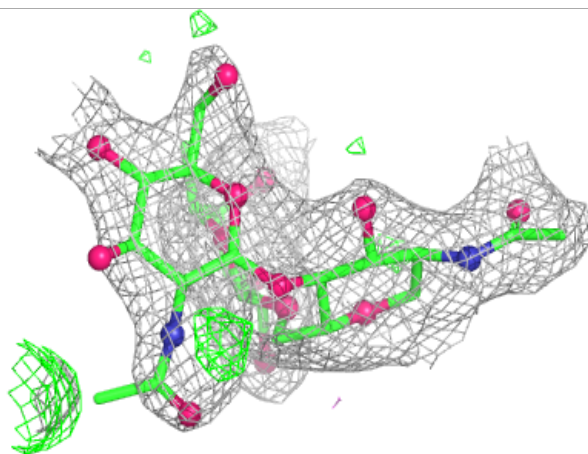
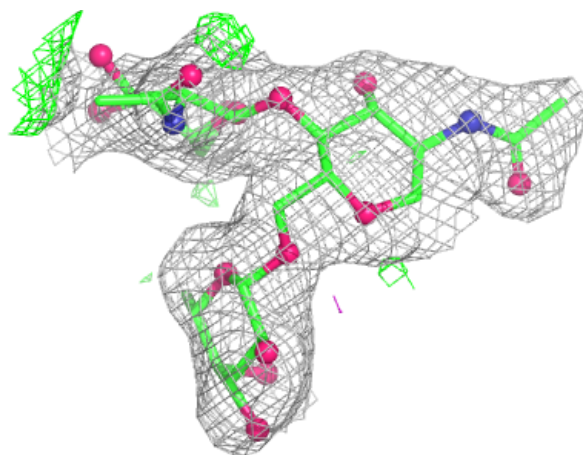
Electron density around Chain F:

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



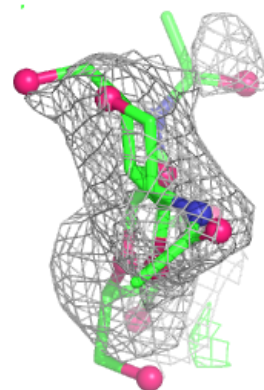
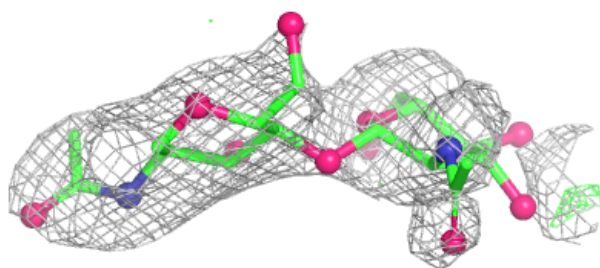
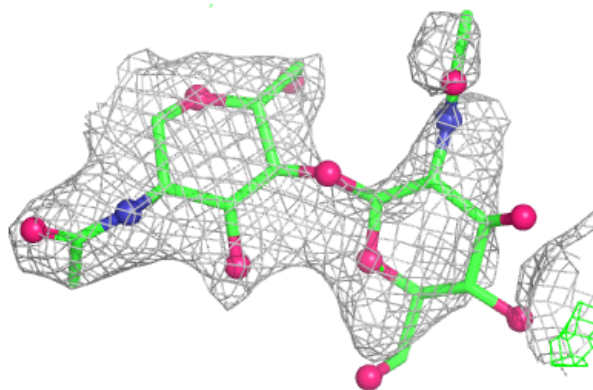
Electron density around Chain L:

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



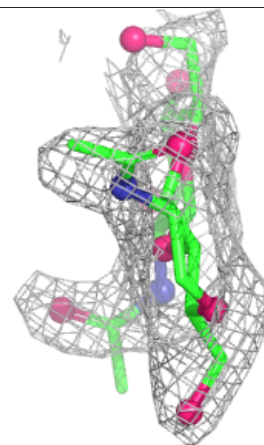
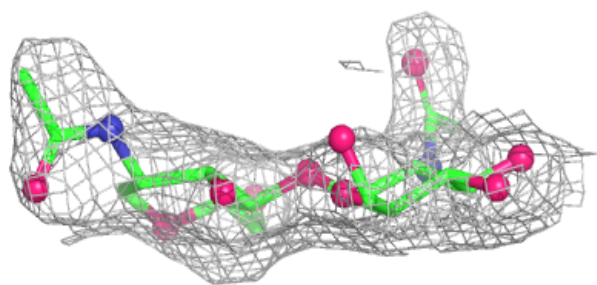
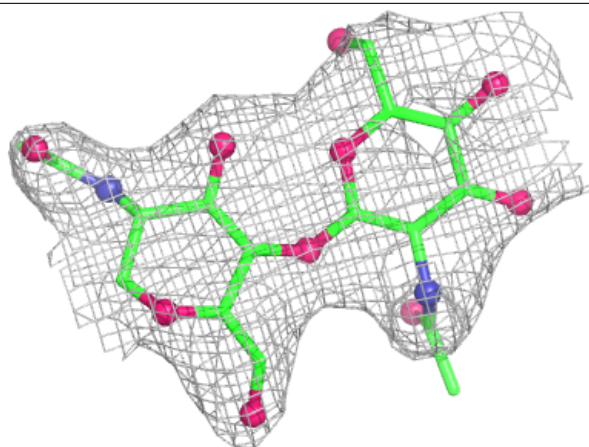
Electron density around Chain G:

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

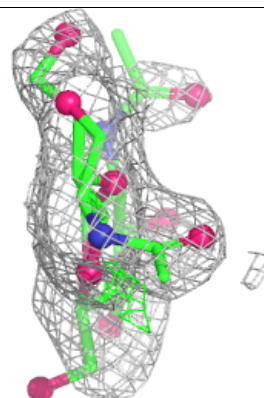
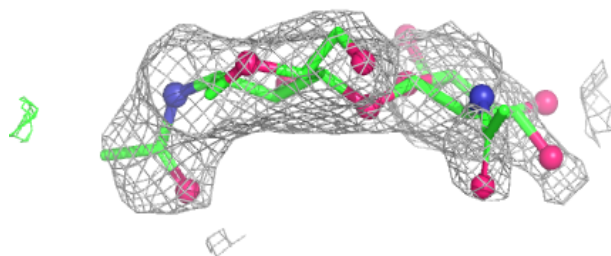
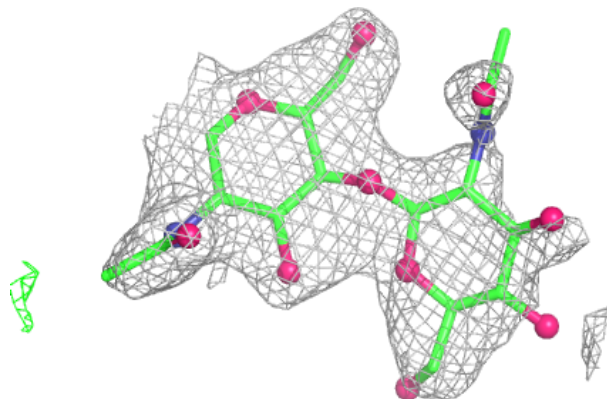


Electron density around Chain J:

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

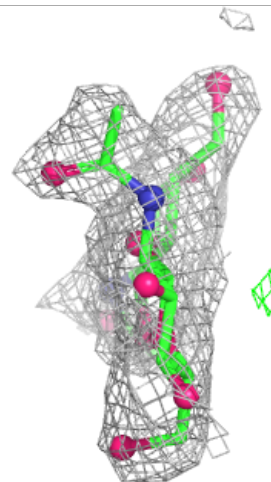
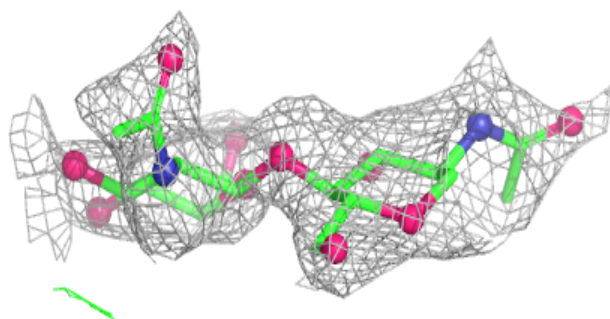
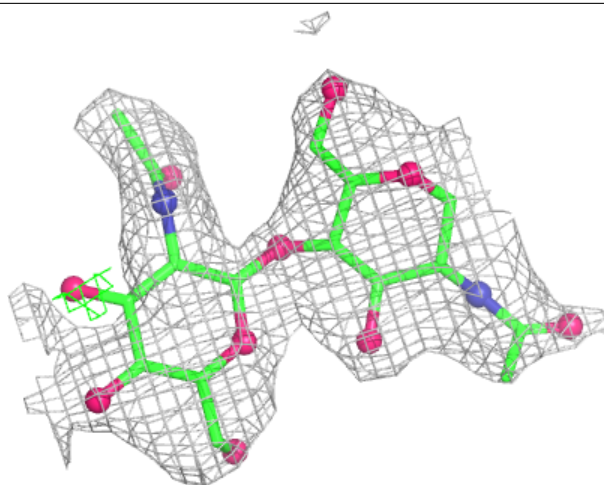
**Electron density around Chain M:**

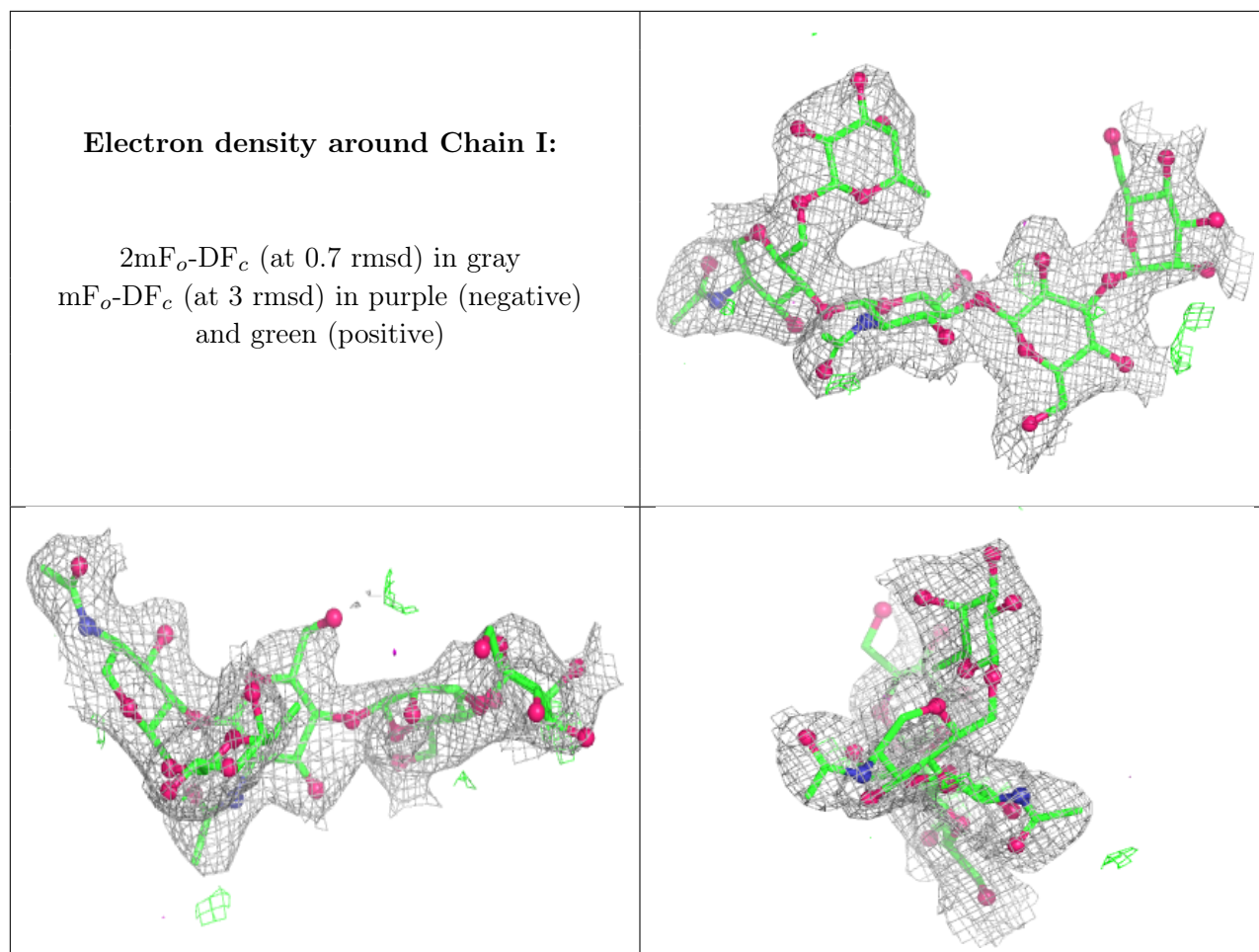
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

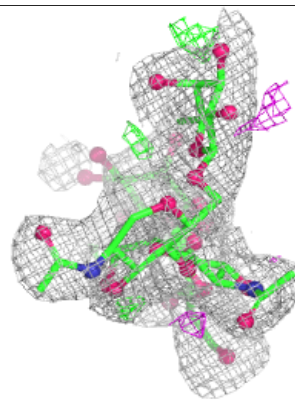
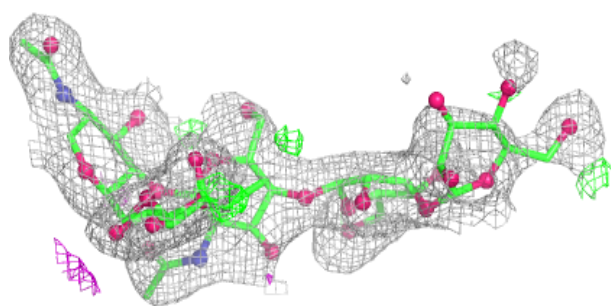
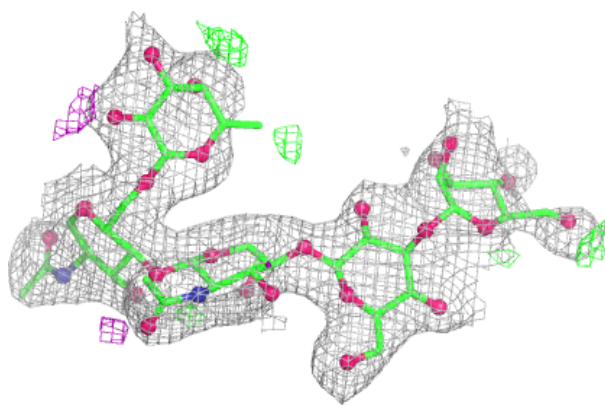
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



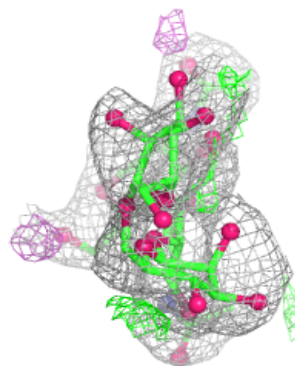
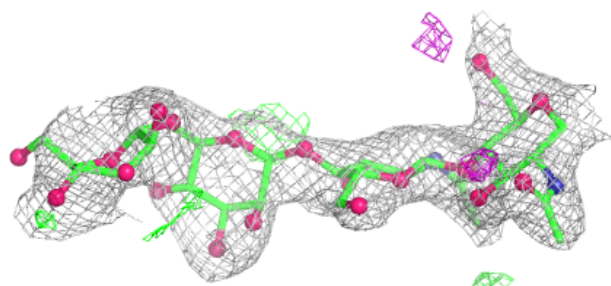
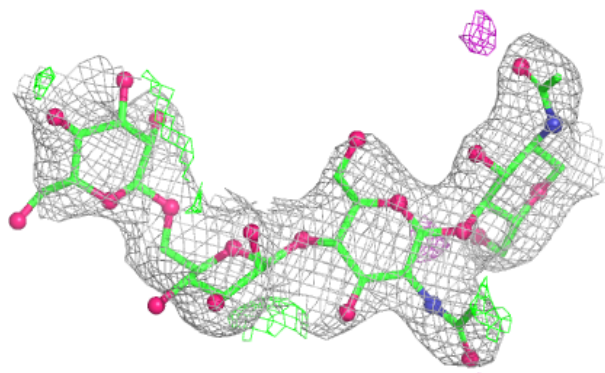


Electron density around Chain O:

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

**Electron density around Chain N:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1768	14/15	0.95	0.05	64,69,70,70	0
7	NAG	B	1770	14/15	0.95	0.04	60,65,66,66	0
7	NAG	D	1768	14/15	0.95	0.04	62,66,69,70	0
7	NAG	C	1768	14/15	0.96	0.04	61,66,66,68	0
7	NAG	B	1768	14/15	0.96	0.04	62,67,70,71	0
7	NAG	D	1774	14/15	0.96	0.05	83,86,87,87	0
7	NAG	D	1770	14/15	0.97	0.04	60,65,67,67	0
7	NAG	B	1773	14/15	0.97	0.04	77,78,78,79	0
8	CA	A	1773	1/1	0.99	0.01	40,40,40,40	0
8	CA	C	1773	1/1	0.99	0.02	42,42,42,42	0
10	CL	C	1775	1/1	0.99	0.05	24,24,24,24	1
10	CL	D	1780	1/1	0.99	0.03	21,21,21,21	1
8	CA	C	1771	1/1	1.00	0.02	28,28,28,28	0
8	CA	A	1771	1/1	1.00	0.03	29,29,29,29	0
8	CA	D	1776	1/1	1.00	0.02	25,25,25,25	0
8	CA	D	1778	1/1	1.00	0.02	29,29,29,29	0
9	CU	A	1772	1/1	1.00	0.01	33,33,33,33	0
9	CU	B	1776	1/1	1.00	0.01	35,35,35,35	0
9	CU	C	1772	1/1	1.00	0.02	36,36,36,36	0
9	CU	D	1777	1/1	1.00	0.01	35,35,35,35	0
10	CL	A	1774	1/1	1.00	0.01	19,19,19,19	0
10	CL	A	1775	1/1	1.00	0.03	24,24,24,24	1
10	CL	B	1778	1/1	1.00	0.02	18,18,18,18	0
10	CL	B	1779	1/1	1.00	0.02	18,18,18,18	1
10	CL	C	1774	1/1	1.00	0.01	15,15,15,15	0
8	CA	B	1775	1/1	1.00	0.03	27,27,27,27	0
10	CL	D	1779	1/1	1.00	0.01	16,16,16,16	0
8	CA	B	1777	1/1	1.00	0.01	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.