



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2024 – 12:05 PM EST

PDB ID : 2RI9
Title : Penicillium citrinum alpha-1,2-mannosidase in complex with a substrate analog
Authors : Lobsanov, Y.D.; Yoshida, T.; Desmet, T.; Nerinckx, W.; Yip, P.; Claeysens, M.; Herscovics, A.; Howell, P.L.
Deposited on : 2007-10-10
Resolution : 1.95 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

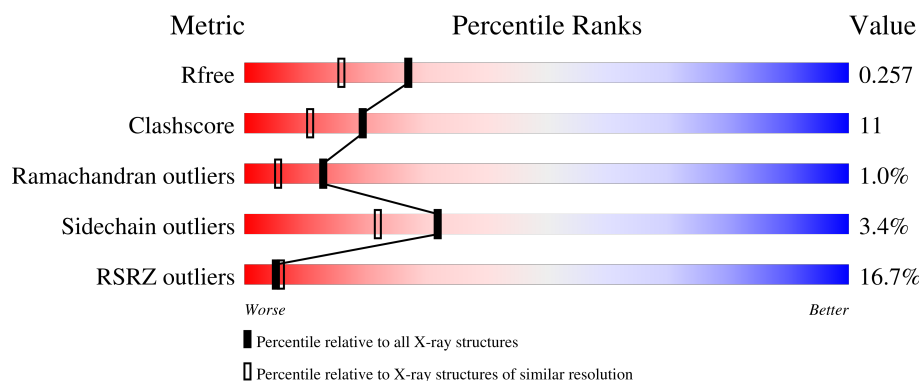
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	475	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	475	<div> <div>32%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	5	
3	H	5	
4	F	2	
4	J	2	
5	I	2	

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	MAN	D	3	X	-	-	-
3	MAN	H	3	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8503 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

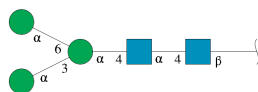
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	2	0
			3744	2370	624	741	9			
1	B	475	Total	C	N	O	S	0	1	0
			3736	2365	623	740	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	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 alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

- Molecule 4 is an oligosaccharide called alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	O		0	2	0
			22	12	10				
4	J	2	Total	C	O		0	2	0
			22	12	10				

- Molecule 5 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
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

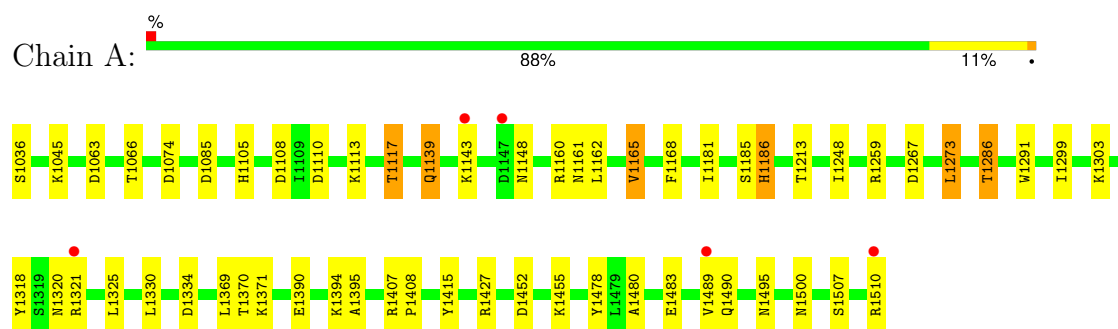
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	482	Total	O	0	1
			483	483		
8	B	235	Total	O	0	1
			236	236		

3 Residue-property plots

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: Mannosyl-oligosaccharide alpha-1,2-mannosidase



- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase



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

Chain C:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain D:  60% 20% 20%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain H:  60% 40%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 4: alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside

Chain F:  50% 50%

MAN1
LDY2

- Molecule 4: alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside

Chain J:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.49Å 111.00Å 86.23Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	49.83 – 1.95 49.83 – 1.97	Depositor EDS
% Data completeness (in resolution range)	93.9 (49.83-1.95) 94.0 (49.83-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.260 0.207 , 0.257	Depositor DCC
R_{free} test set	5018 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, MMA, MAN, GOL, LDY, NDG, CA

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	0.68	0/3839	0.73	2/5215 (0.0%)
1	B	0.45	0/3831	0.66	2/5205 (0.0%)
All	All	0.58	0/7670	0.69	4/10420 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1066	THR	N-CA-C	-5.76	95.45	111.00
1	B	2066	THR	N-CA-C	-5.46	96.25	111.00
1	A	1334	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	2462	TYR	CB-CA-C	-5.07	100.26	110.40

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	3744	0	3543	42	0
1	B	3736	0	3536	125	0
2	C	28	0	25	1	0
2	E	28	0	25	0	0
2	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	61	0	51	1	0
3	H	61	0	51	6	0
4	F	22	0	13	1	0
4	J	22	0	14	0	0
5	I	28	0	24	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	3	0	0
7	B	12	0	3	0	0
8	A	483	0	0	14	0
8	B	236	0	0	17	0
All	All	8503	0	7313	172	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 11.

The worst 5 of 172 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2330:LEU:HD21	1:B:2407[B]:ARG:NH2	1.86	0.89
1:A:1330:LEU:HD21	1:A:1407[B]:ARG:NH2	1.96	0.80
1:A:1139:GLN:HE21	1:A:1139:GLN:HA	1.49	0.78
1:A:1490:GLN:H	1:A:1495:ASN:HD21	1.32	0.78
1:B:2423:LYS:HE2	1:B:2423:LYS:HA	1.67	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	475/475 (100%)	457 (96%)	15 (3%)	3 (1%)	22 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/475 (100%)	429 (90%)	39 (8%)	6 (1%)	10	3
All	All	949/950 (100%)	886 (93%)	54 (6%)	9 (1%)	13	7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2215	ASP
1	A	1267	ASP
1	B	2148	ASN
1	B	2267	ASP
1	B	2216	GLU

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	402/400 (100%)	392 (98%)	10 (2%)	42	34
1	B	401/400 (100%)	384 (96%)	17 (4%)	25	15
All	All	803/800 (100%)	776 (97%)	27 (3%)	32	22

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2117	THR
1	B	2181	ILE
1	B	2408	PRO
1	B	2171	ASP
1	B	2243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1490	GLN
1	B	2490	GLN

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Mol	Chain	Res	Type
1	A	1495	ASN
1	B	2495	ASN
1	B	2348	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 ⓘ

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.60	0	17,19,21	0.85	0
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	0.76	0
3	NAG	D	1	3,1	14,14,15	1.19	1 (7%)	17,19,21	0.88	0
3	NDG	D	2	3	14,14,15	1.11	2 (14%)	17,19,21	0.93	1 (5%)
3	MAN	D	3	3	11,11,12	0.48	0	15,15,17	0.47	0
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	0.59	0
3	MAN	D	5	3	11,11,12	0.47	0	15,15,17	0.63	0
2	NAG	E	1	2,1	14,14,15	0.86	1 (7%)	17,19,21	0.80	0
2	NAG	E	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.70	0
4	MMA	F	1[A]	4	13,13,13	0.67	0	18,18,18	0.89	2 (11%)
4	LDY	F	2[A]	4,6	9,9,10	0.96	0	10,12,14	1.21	1 (10%)
2	NAG	G	1	2,1	14,14,15	0.68	0	17,19,21	0.72	1 (5%)
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.72	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.82	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDG	H	2	3	14,14,15	0.83	0	17,19,21	1.03	2 (11%)
3	MAN	H	3	3	11,11,12	0.52	0	15,15,17	0.45	0
3	MAN	H	4	3	11,11,12	0.43	0	15,15,17	0.66	1 (6%)
3	MAN	H	5	3	11,11,12	0.48	0	15,15,17	0.59	0
5	NAG	I	1	5,1	14,14,15	0.99	1 (7%)	17,19,21	0.71	0
5	NDG	I	2	5	14,14,15	0.81	0	17,19,21	0.85	1 (5%)
4	MMA	J	1[A]	4	13,13,13	0.64	0	18,18,18	0.76	0
4	LDY	J	2[A]	4,6	9,9,10	0.90	0	10,12,14	0.84	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NDG	D	2	3	-	3/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
4	MMA	F	1[A]	4	-	0/4/24/24	0/1/1/1
4	LDY	F	2[A]	4,6	-	-	0/1/1/1
2	NAG	G	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	4/6/23/26	0/1/1/1
3	NDG	H	2	3	-	4/6/23/26	0/1/1/1
3	MAN	H	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NDG	I	2	5	-	3/6/23/26	0/1/1/1
4	MMA	J	1[A]	4	-	2/4/24/24	0/1/1/1
4	LDY	J	2[A]	4,6	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.91	1.56	1.52
3	D	2	NDG	C1-C2	2.86	1.56	1.52
5	I	1	NAG	C1-C2	2.46	1.55	1.52
2	E	1	NAG	C1-C2	2.39	1.55	1.52
3	D	2	NDG	O5-C5	2.18	1.47	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2[A]	LDY	C1-C2-C3	3.20	114.31	109.64
3	H	2	NDG	C2-N2-C7	-2.66	119.33	122.90
3	H	2	NDG	C4-C3-C2	-2.51	107.34	111.02
3	D	2	NDG	C2-N2-C7	-2.51	119.54	122.90
5	I	2	NDG	C2-N2-C7	-2.39	119.70	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	3	MAN	C1
3	H	3	MAN	C1

5 of 31 torsion outliers are listed below:

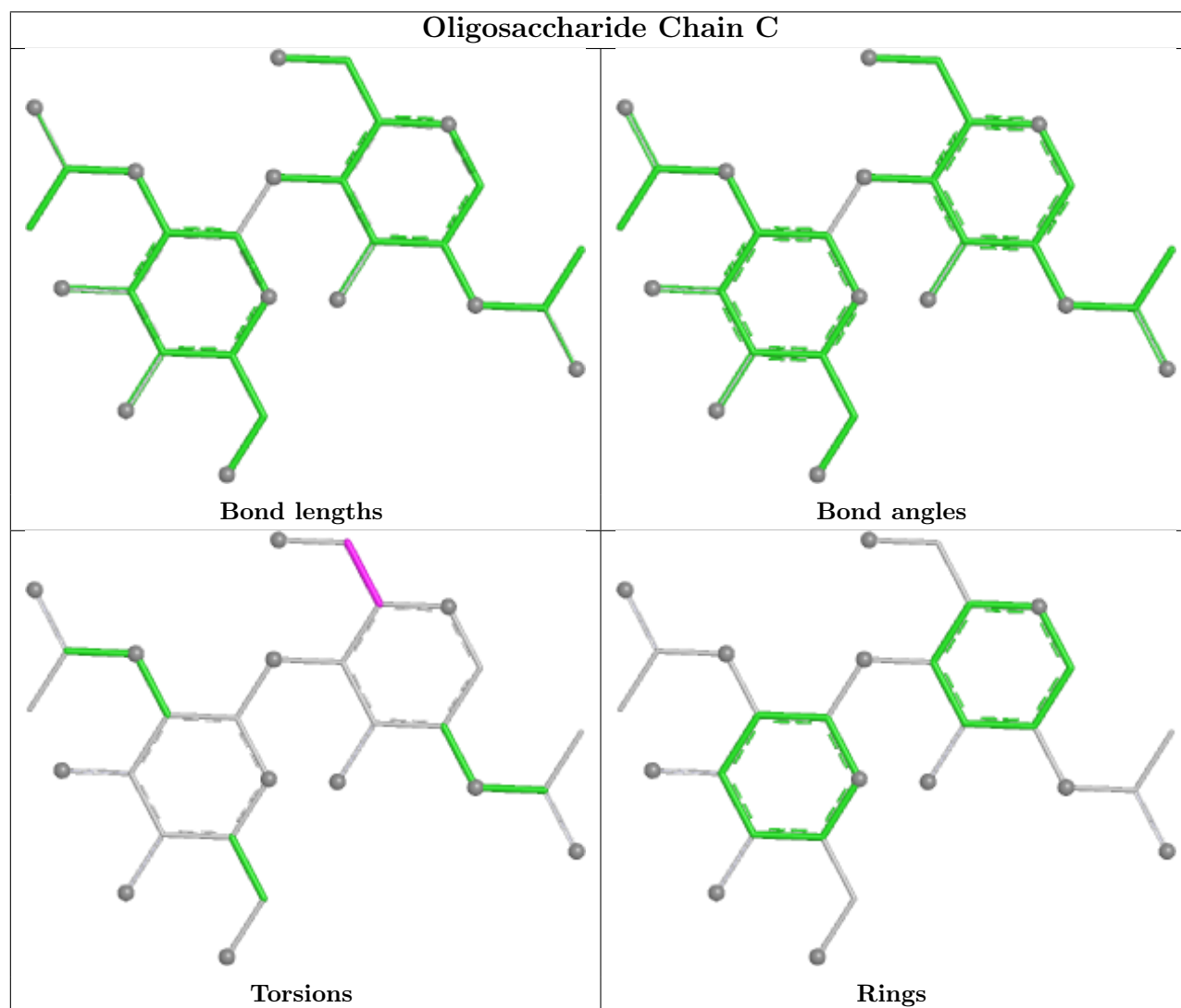
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
5	I	2	NDG	C3-C2-N2-C7

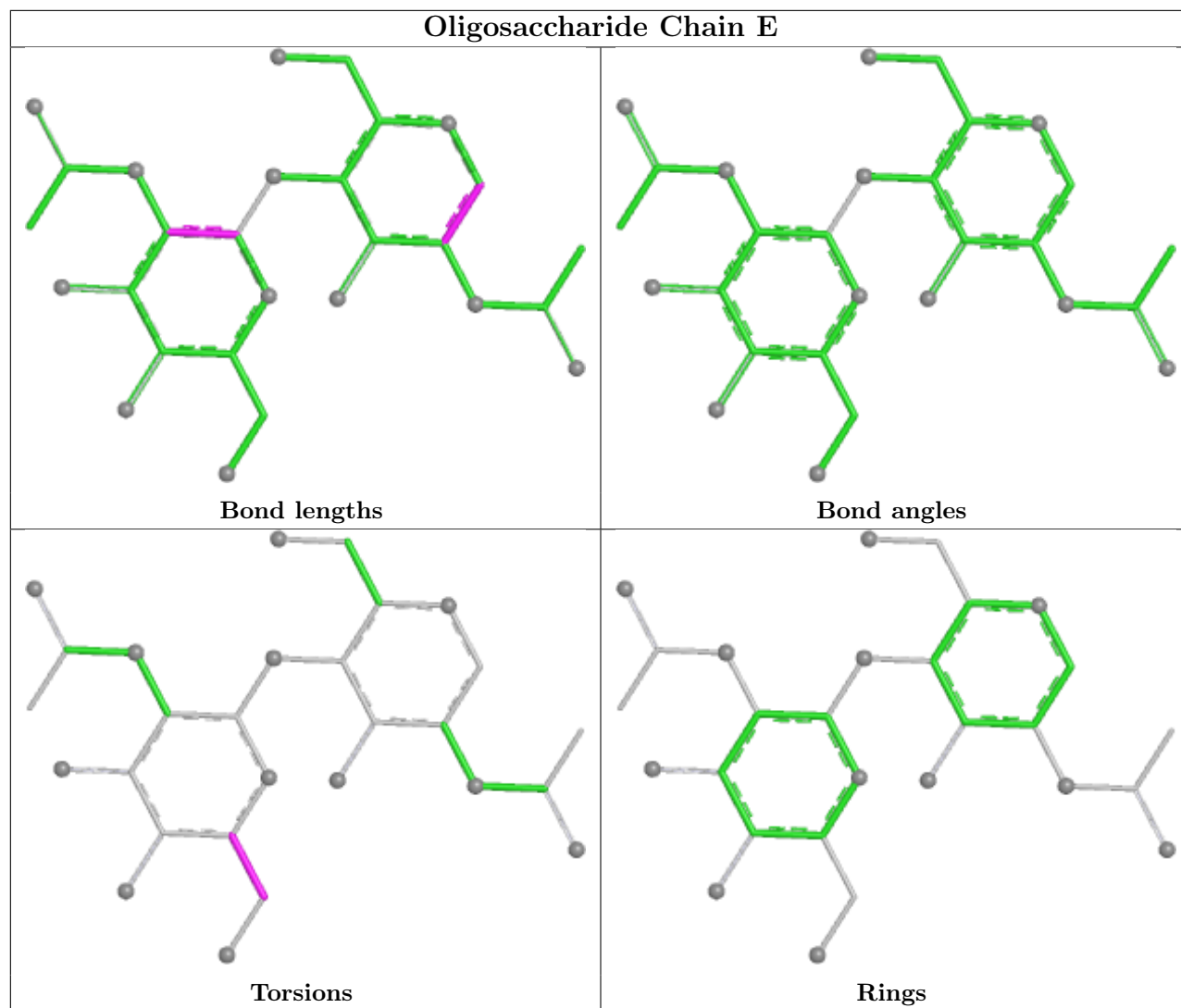
There are no ring outliers.

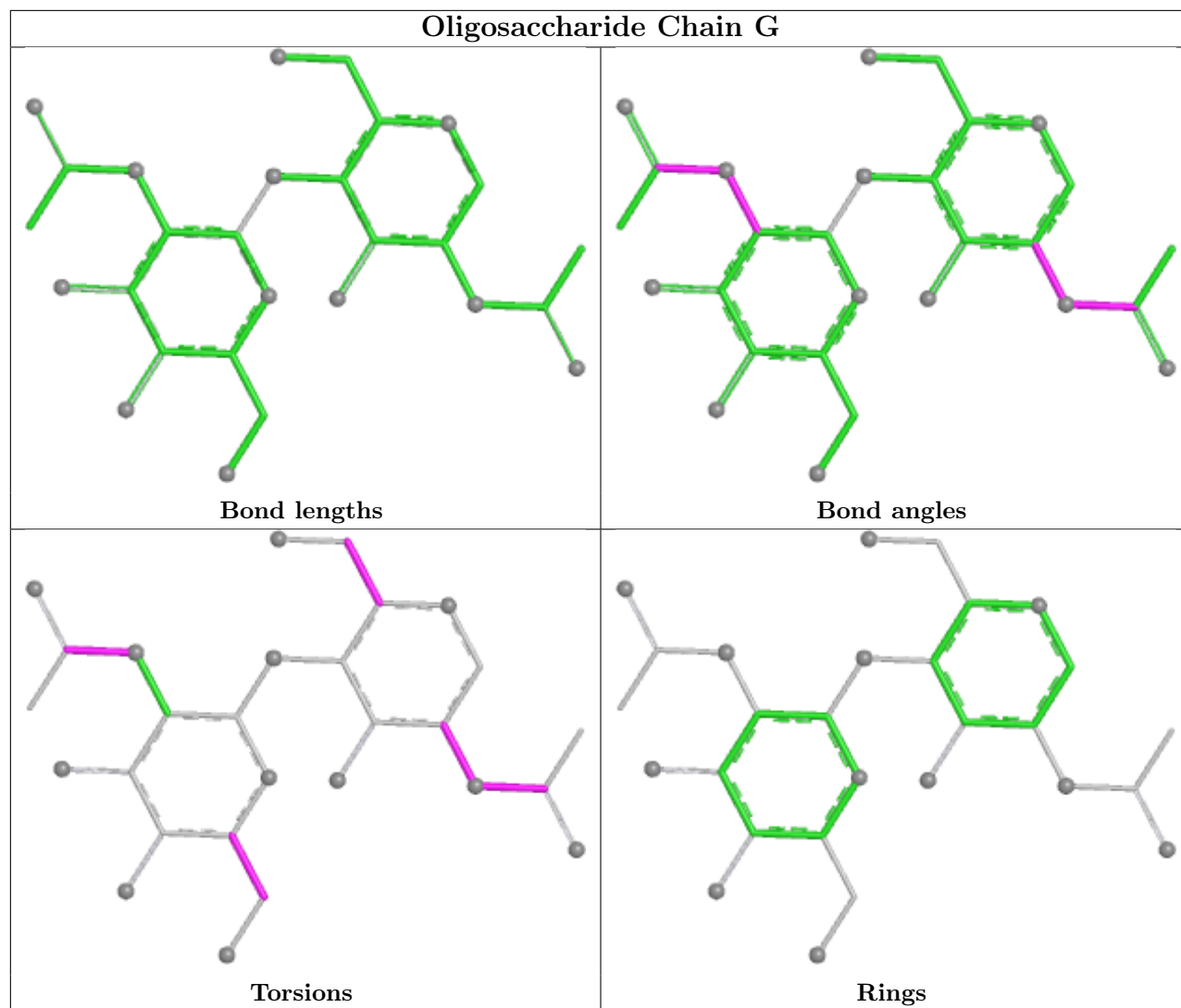
7 monomers are involved in 12 short contacts:

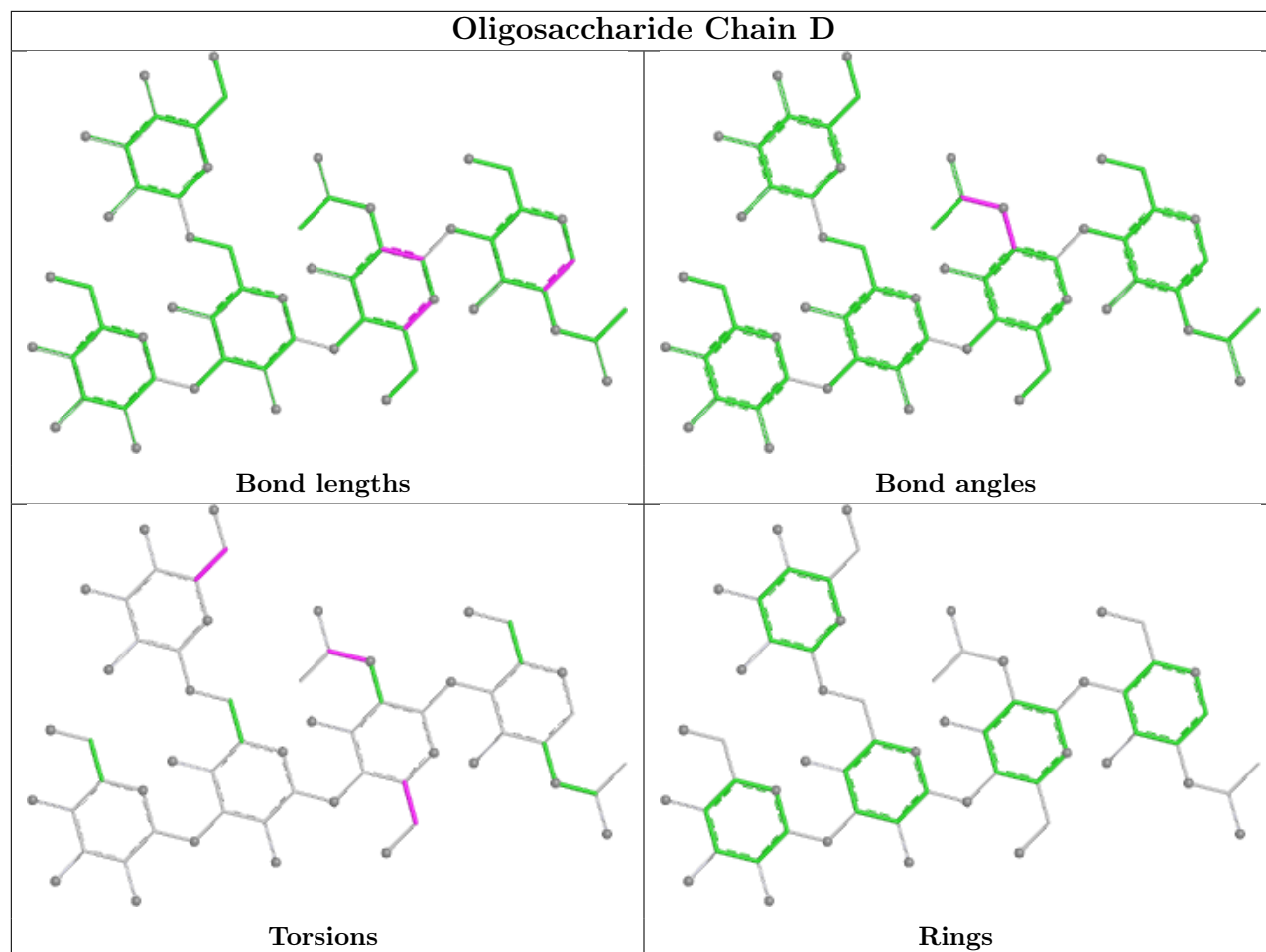
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0
2	C	1	NAG	1	0
5	I	2	NDG	1	0
4	F	2[A]	LDY	1	0
3	D	2	NDG	1	0
3	H	2	NDG	5	0
3	H	4	MAN	1	0

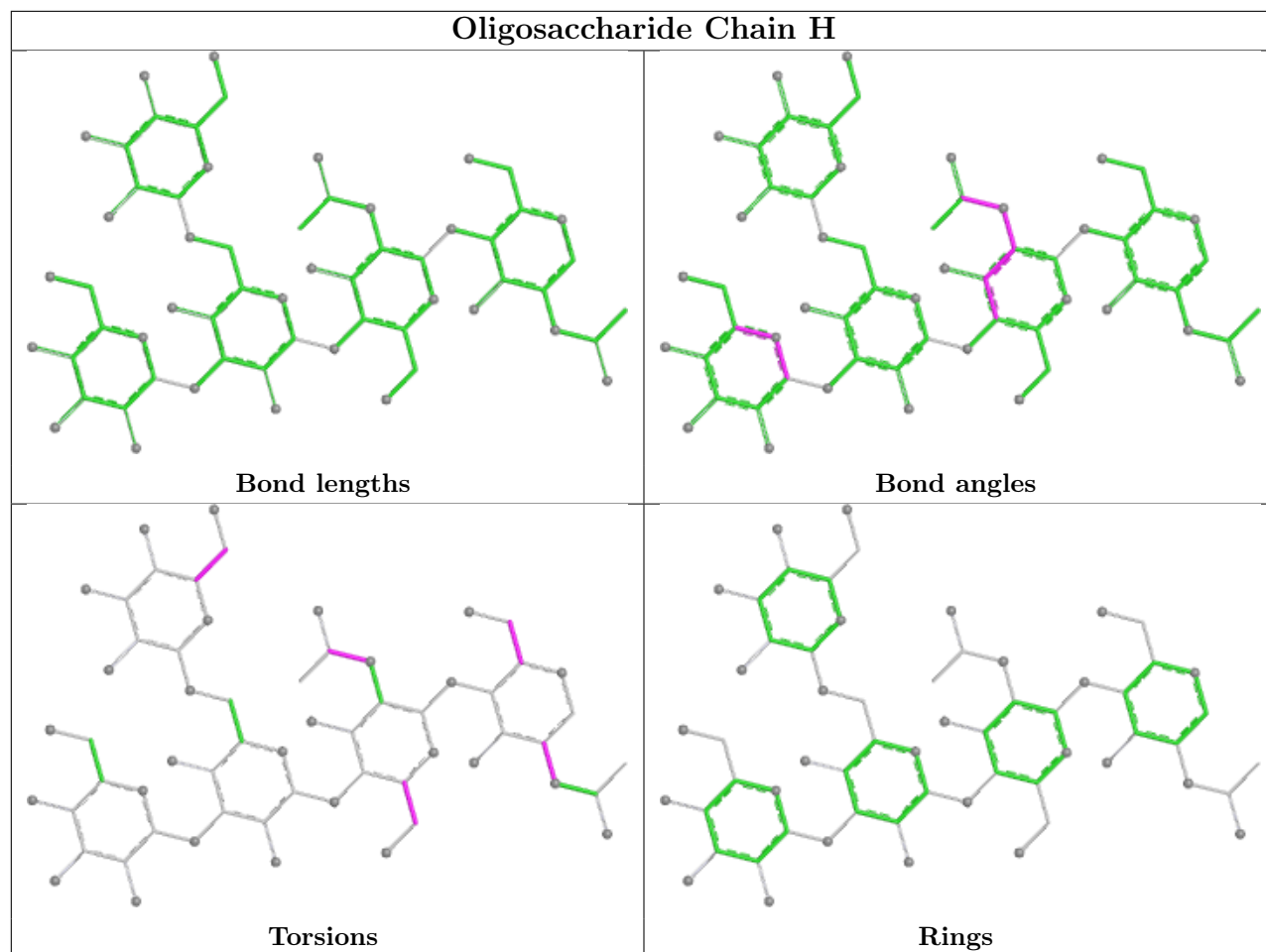
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

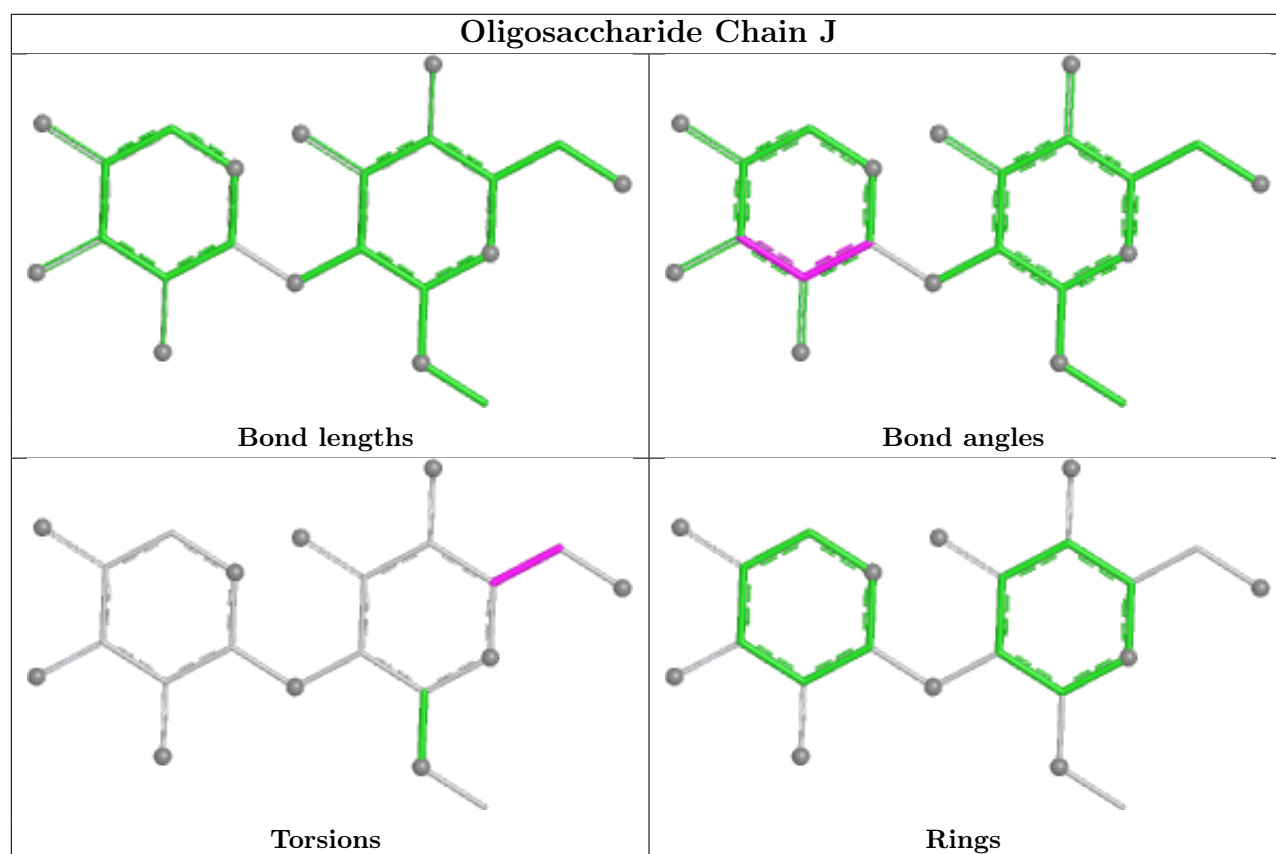
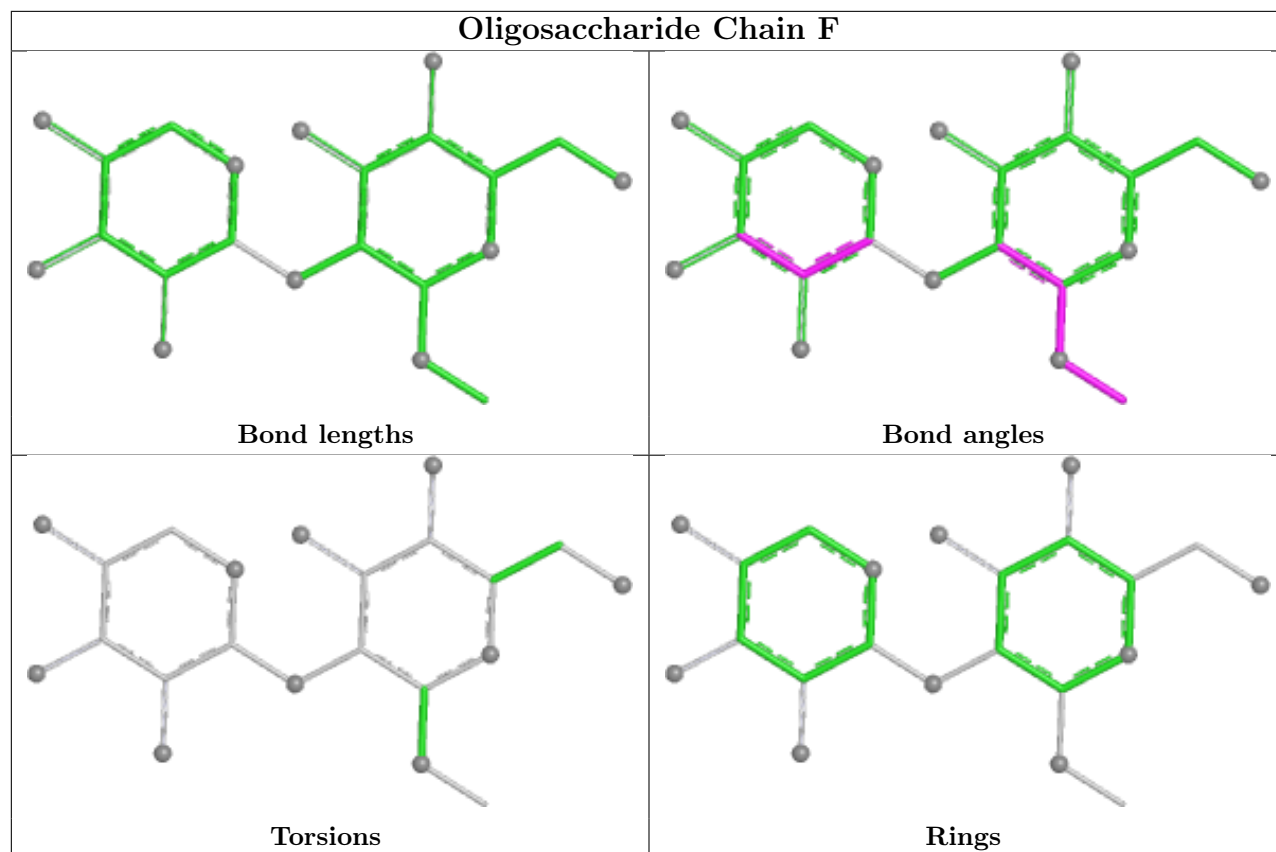


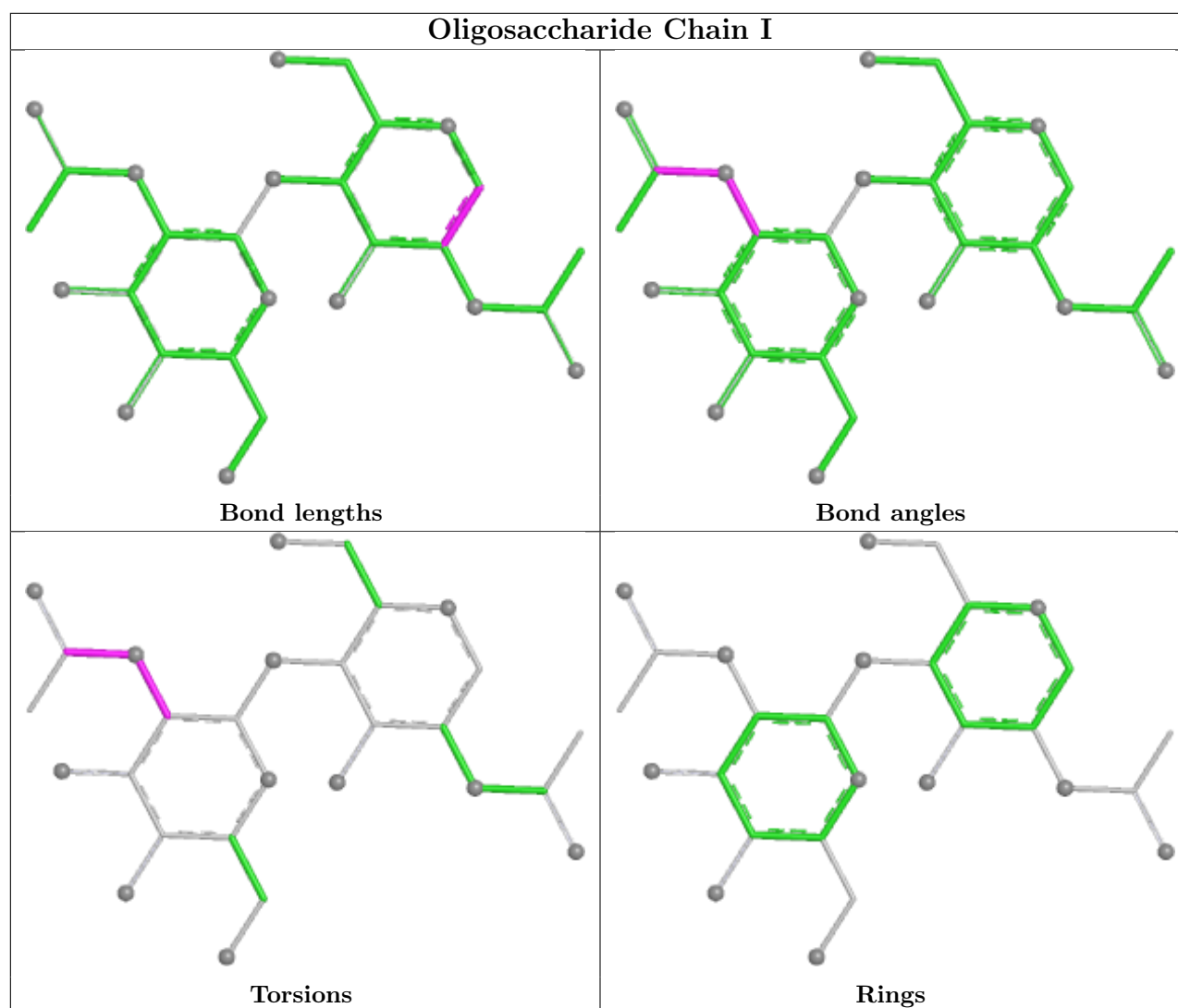












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GOL	A	1902[B]	-	5,5,5	0.34	0	5,5,5	0.34	0
7	GOL	B	2902[B]	-	5,5,5	0.25	0	5,5,5	0.30	0
7	GOL	B	2903[B]	6	5,5,5	0.33	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	1903[B]	6	5,5,5	0.27	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1902[B]	-	-	0/4/4/4	-
7	GOL	B	2902[B]	-	-	0/4/4/4	-
7	GOL	B	2903[B]	6	-	0/4/4/4	-
7	GOL	A	1903[B]	6	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/475 (100%)	-0.20	5 (1%) 77 82	5, 15, 32, 46	2 (0%)
1	B	475/475 (100%)	1.43	154 (32%) 1 1	8, 37, 62, 74	1 (0%)
All	All	950/950 (100%)	0.61	159 (16%) 5 6	5, 23, 58, 74	3 (0%)

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2256	ALA	6.1
1	B	2379	TRP	5.4
1	B	2384	VAL	5.2
1	B	2145	LEU	4.7
1	B	2302	LEU	4.7

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
2	NAG	G	2	14/15	0.58	0.16	70,71,72,73	0
2	NAG	G	1	14/15	0.59	0.19	60,62,65,68	0
3	MAN	H	5	11/12	0.66	0.15	58,59,60,60	11
3	MAN	D	5	11/12	0.67	0.17	42,46,48,48	11
3	NDG	H	2	14/15	0.74	0.16	53,54,56,56	0

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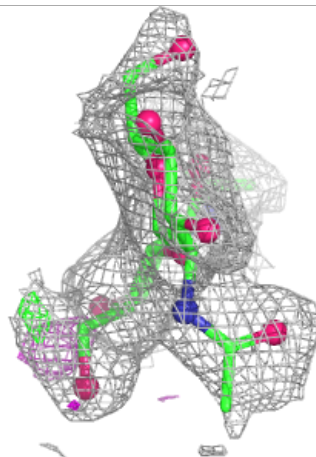
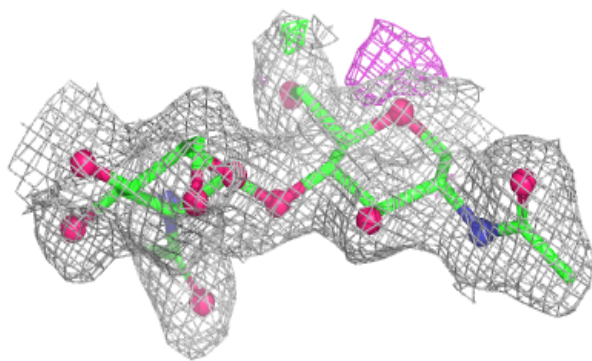
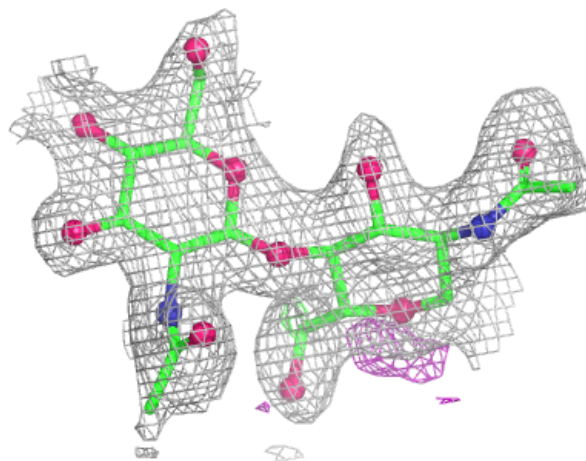
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	H	1	14/15	0.74	0.18	47,49,53,54	0
3	MAN	H	3	11/12	0.75	0.17	54,55,58,59	11
3	MAN	H	4	11/12	0.76	0.14	52,54,54,56	10
2	NAG	C	2	14/15	0.80	0.11	41,45,47,48	0
5	NDG	I	2	14/15	0.82	0.12	48,50,54,55	0
5	NAG	I	1	14/15	0.84	0.11	30,35,40,44	0
2	NAG	E	2	14/15	0.84	0.10	31,35,39,40	0
4	MMA	J	1[A]	13/13	0.85	0.11	24,26,29,29	13
3	MAN	D	4	11/12	0.86	0.11	25,29,31,33	10
2	NAG	C	1	14/15	0.86	0.11	26,29,32,35	0
3	NDG	D	2	14/15	0.89	0.10	21,25,30,30	0
4	MMA	F	1[A]	13/13	0.90	0.09	13,15,19,20	13
3	MAN	D	3	11/12	0.90	0.11	25,29,33,38	11
3	NAG	D	1	14/15	0.92	0.10	18,20,28,29	0
4	LDY	J	2[A]	9/10	0.92	0.10	15,18,20,22	9
2	NAG	E	1	14/15	0.95	0.06	15,18,21,25	0
4	LDY	F	2[A]	9/10	0.97	0.06	4,10,13,16	9

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.

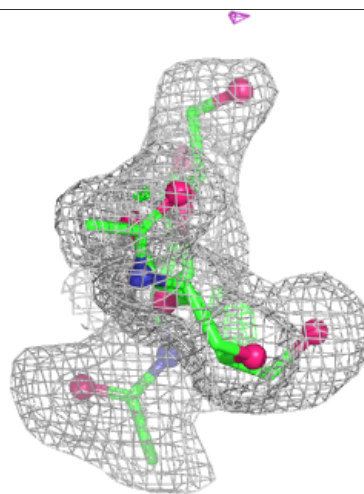
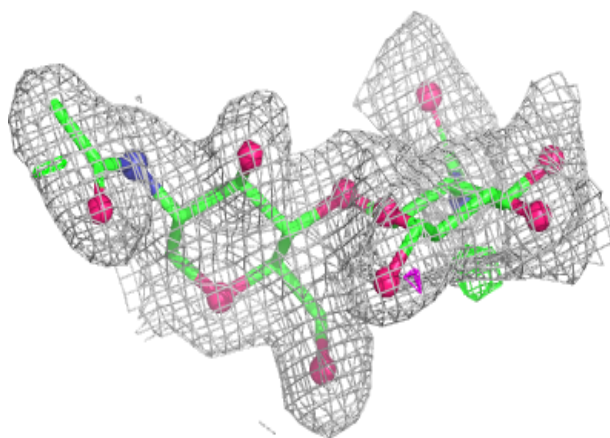
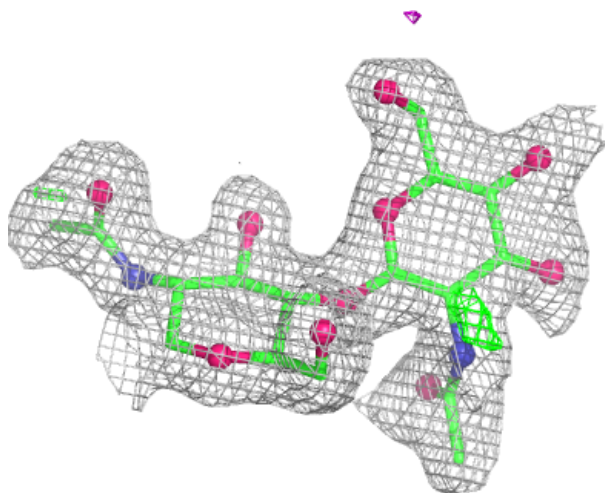
Electron density around Chain C:

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



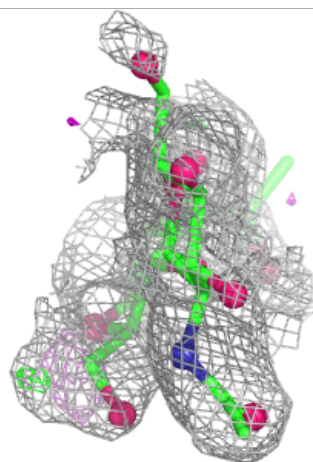
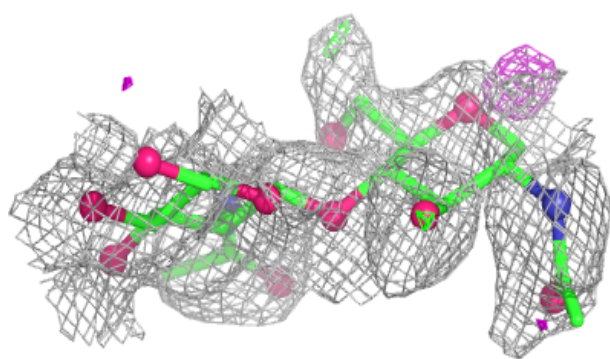
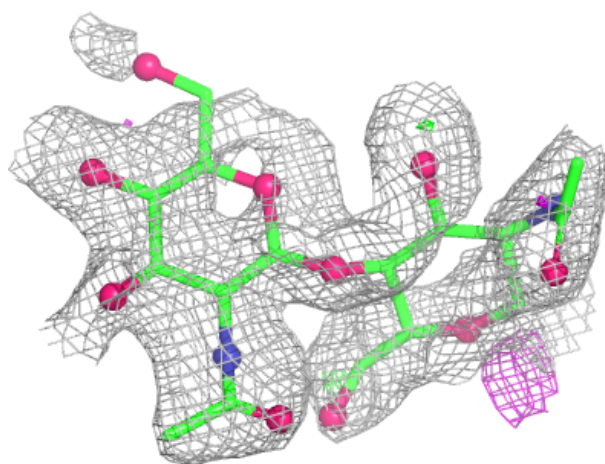
Electron density around Chain E:

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



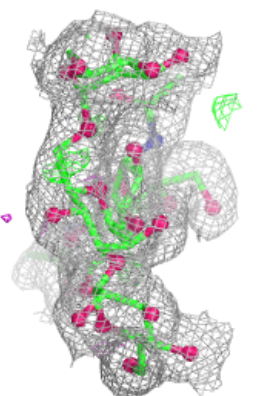
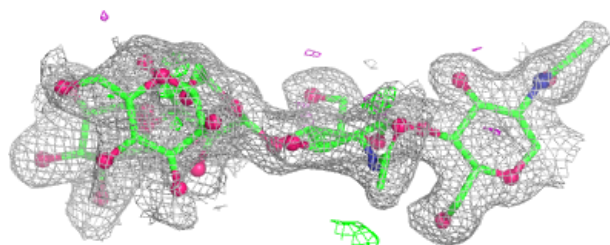
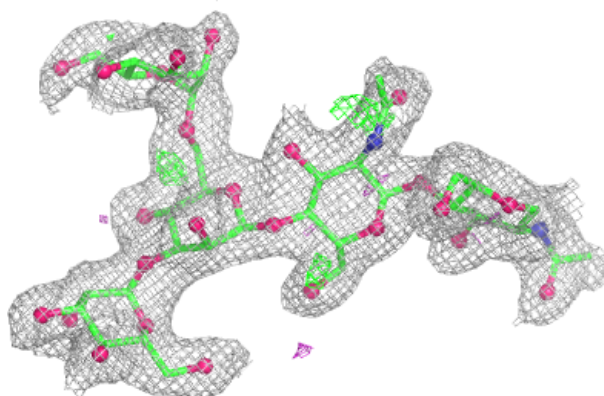
Electron density around Chain G:

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



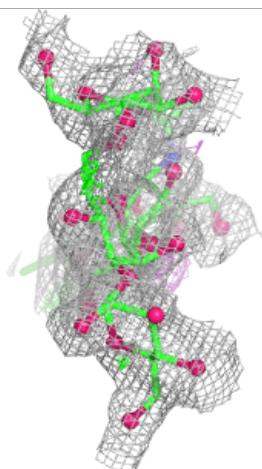
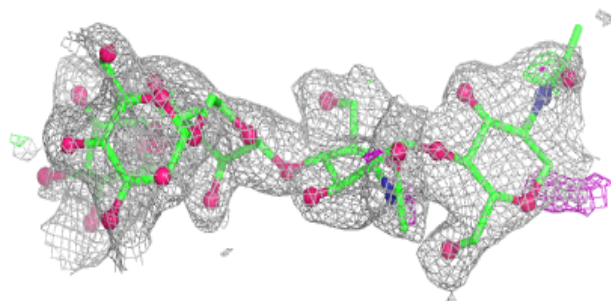
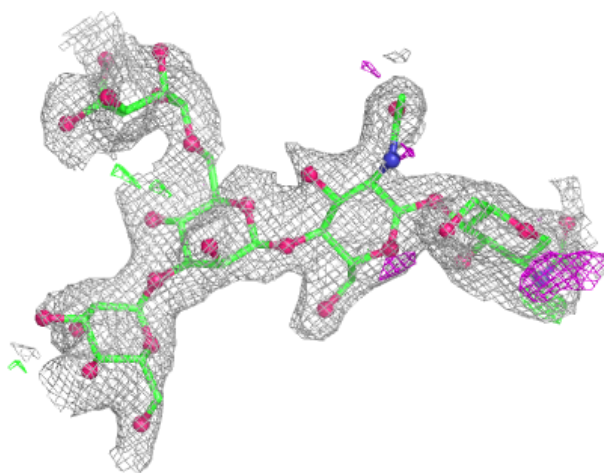
Electron density around Chain D:

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



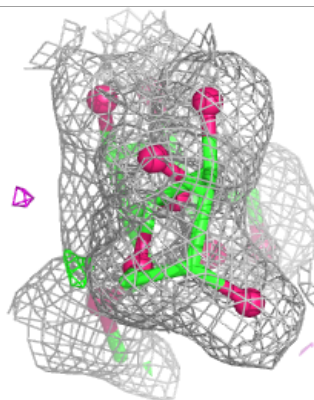
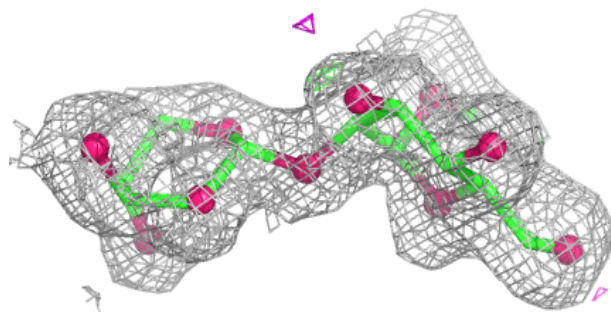
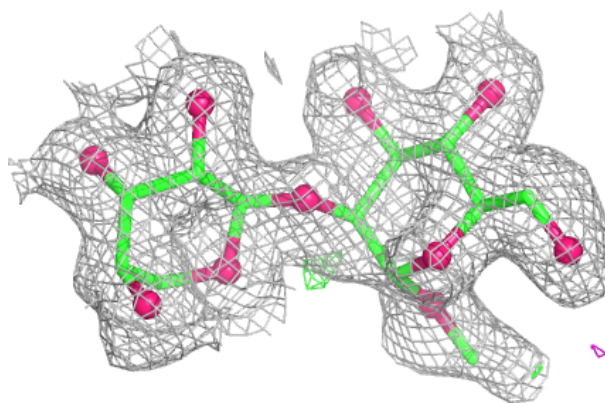
Electron density around Chain H:

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

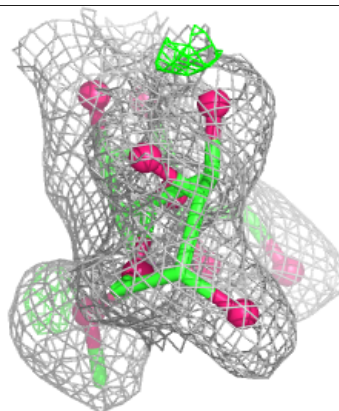
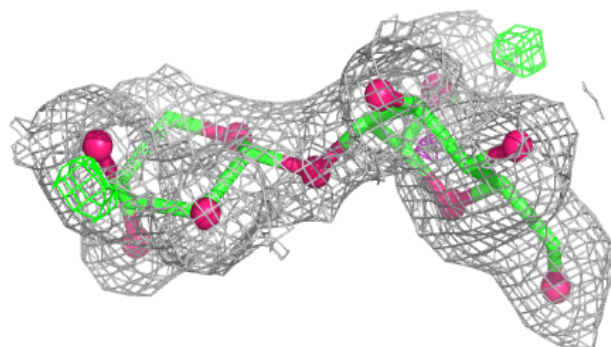
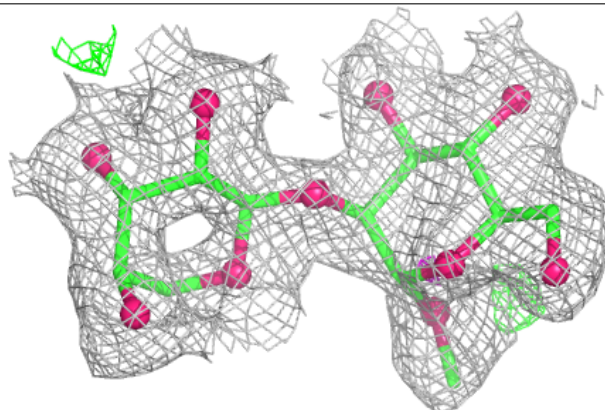


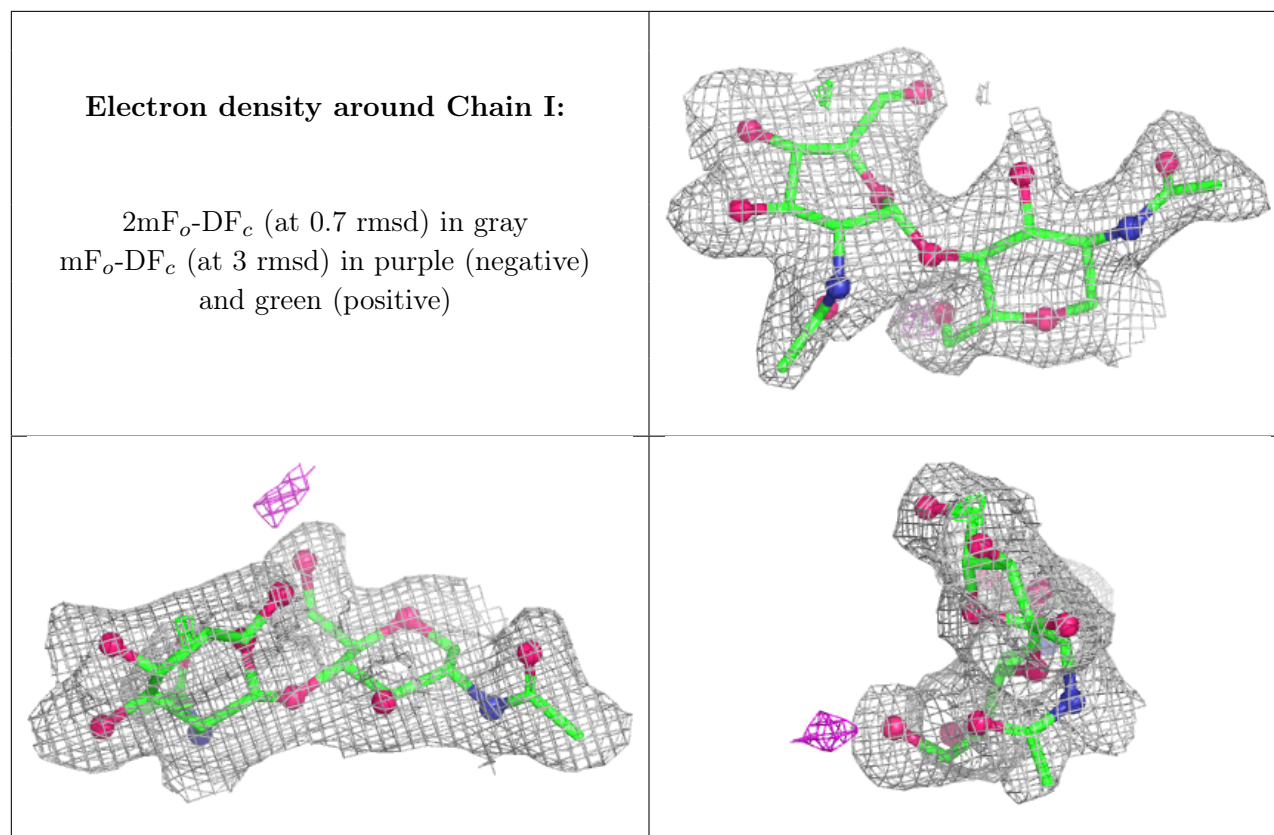
Electron density around Chain F:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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
7	GOL	A	1902[B]	6/6	0.77	0.14	25,26,27,27	6
7	GOL	B	2902[B]	6/6	0.88	0.11	34,35,35,35	6
7	GOL	B	2903[B]	6/6	0.93	0.07	11,11,12,12	6
7	GOL	A	1903[B]	6/6	0.96	0.05	6,7,7,7	6
6	CA	B	2551	1/1	0.98	0.03	15,15,15,15	0
6	CA	A	1550	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.