Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 10:27 am GMT

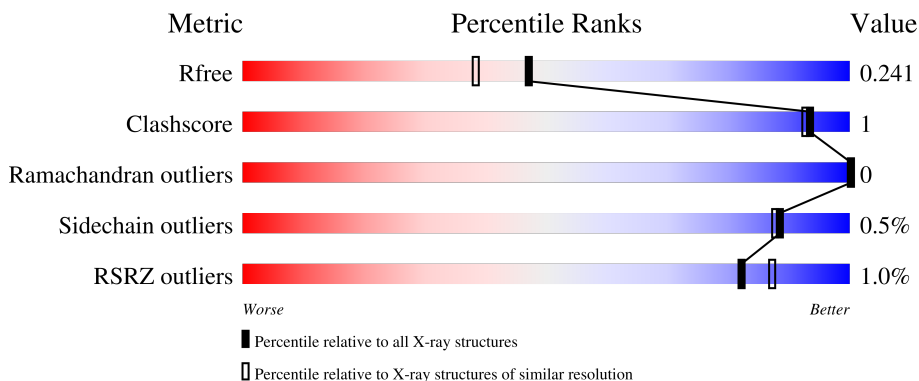|		
PDB ID	:	4UP4
Title	:	Structure of the recombinant lectin PVL from Psathyrella velutina in complex with GlcNAcb-D-1,3Galactoside
Authors	:	Audfray, A.; Beljoudi, M.; Hurbin, A.; Varrot, A.; Breiman, A.; Busser, B.; Lependu, J.; Coll, J.L.; Imberty, A.
Deposited on	:	2014-06-12
Resolution	:	1.95 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
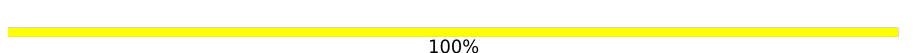*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.241
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	401	97%
1	B	401	96%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	50% 50%
2	J	2	100%
2	K	2	100%
2	L	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7251 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.
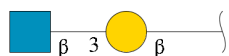
- Molecule 1 is a protein called LECTIN PVL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	3033	1924	545	555	9	0	0	0
1	B	399	Total	C	N	O	S	0	4	0
			3057	1937	551	560	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	SEE REMARK 999	UNP Q309D1
A	2	VAL	-	SEE REMARK 999	UNP Q309D1
A	3	VAL	-	SEE REMARK 999	UNP Q309D1
A	4	VAL	-	SEE REMARK 999	UNP Q309D1
A	5	ILE	-	SEE REMARK 999	UNP Q309D1
A	6	SER	-	SEE REMARK 999	UNP Q309D1
A	72	PRO	SER	conflict	UNP Q309D1
A	201	GLY	SER	conflict	UNP Q309D1
A	376	GLN	LYS	conflict	UNP Q309D1
B	1	SER	-	SEE REMARK 999	UNP Q309D1
B	2	VAL	-	SEE REMARK 999	UNP Q309D1
B	3	VAL	-	SEE REMARK 999	UNP Q309D1
B	4	VAL	-	SEE REMARK 999	UNP Q309D1
B	5	ILE	-	SEE REMARK 999	UNP Q309D1
B	6	SER	-	SEE REMARK 999	UNP Q309D1
B	72	PRO	SER	conflict	UNP Q309D1
B	201	GLY	SER	conflict	UNP Q309D1
B	376	GLN	LYS	conflict	UNP Q309D1

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total 26	C 14	N 1	O 11	0	0	0
2	D	2	Total 26	C 14	N 1	O 11	0	0	0
2	E	2	Total 26	C 14	N 1	O 11	0	0	0
2	F	2	Total 26	C 14	N 1	O 11	0	0	0
2	G	2	Total 26	C 14	N 1	O 11	0	0	0
2	H	2	Total 26	C 14	N 1	O 11	0	0	0
2	I	2	Total 26	C 14	N 1	O 11	0	0	0
2	J	2	Total 26	C 14	N 1	O 11	0	0	0
2	K	2	Total 26	C 14	N 1	O 11	0	0	0
2	L	2	Total 26	C 14	N 1	O 11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).
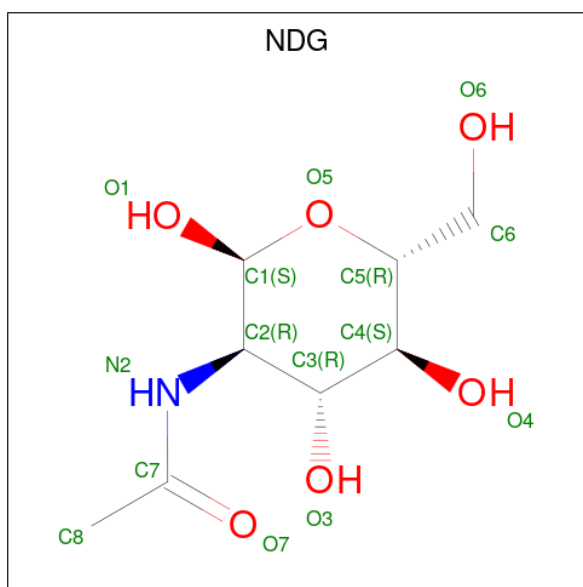
NDG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			15	8	1	6		

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	453	Total O 453 453	0	0
6	B	397	Total O 397 397	0	0

# 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.
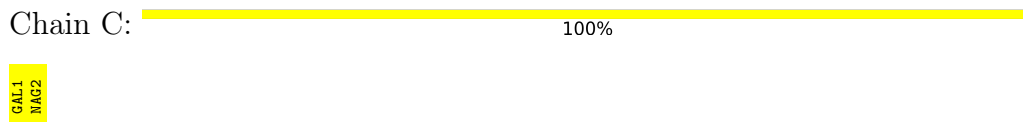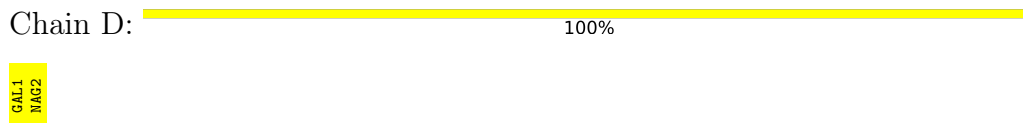
• Molecule 1: LECTIN PVL
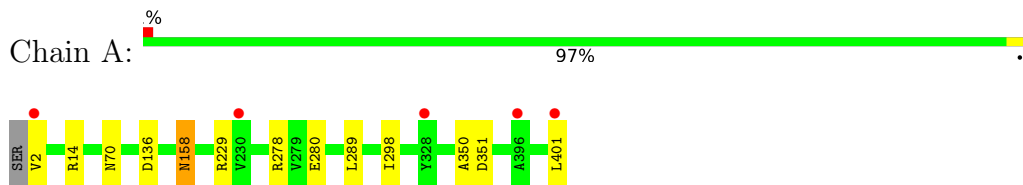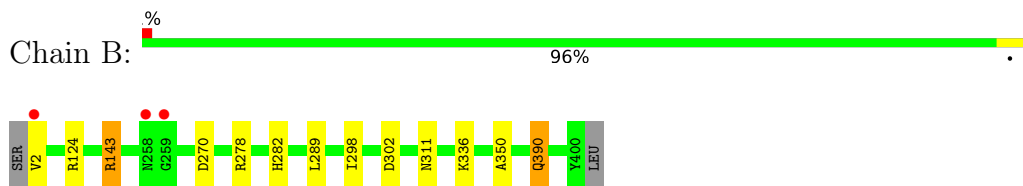
Chain A:

• Molecule 1: LECTIN PVL

Chain B:

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

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose
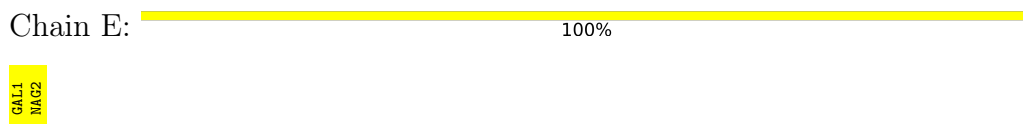
Chain D:

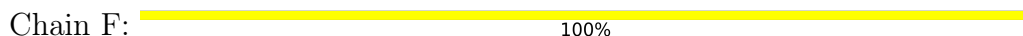• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain E:

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

Chain F:

GAL1 NAG2

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

Chain G:

100%

GAL1 NAG2

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

Chain H:

100%

GAL1 NAG2

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

Chain I:

50%	50%

GAL1 NAG2

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

Chain J:

100%

GAL1 NAG2

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

Chain K:

100%

GAL1 NAG2

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

Chain L:

100%

GAL1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.81Å 97.47Å 158.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.95) 99.8 (30.00-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.190 , 0.237 0.198 , 0.241	Depositor DCC
R_{free} test set	3069 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.4	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, GAL, NDG

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	0.83	0/3101	0.87	4/4210 (0.1%)
1	B	0.80	0/3125	0.84	2/4243 (0.0%)
All	All	0.81	0/6226	0.85	6/8453 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	270	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	278	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	143	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	136	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	229	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3033	0	2960	8	0
1	B	3057	0	2980	10	0
2	C	26	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	26	0	24	0	0
2	E	26	0	24	0	0
2	F	26	0	24	0	0
2	G	26	0	24	0	0
2	H	26	0	24	0	0
2	I	26	0	24	0	0
2	J	26	0	24	0	0
2	K	26	0	24	0	0
2	L	26	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	12	0	0
4	B	15	0	12	0	0
5	A	15	0	15	0	0
6	A	453	0	0	2	0
6	B	397	0	0	2	0
All	All	7251	0	6219	18	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 1.

All (18) 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:280:GLU:OE2	6:A:2312:HOH:O	2.00	0.80
1:A:70:ASN:O	1:A:401:LEU:HB2	1.93	0.68
1:B:278:ARG:H	1:B:282:HIS:HD2	1.42	0.67
1:B:124:ARG:CZ	1:B:143:ARG:HG3	2.29	0.62
1:A:158:ASN:HD22	1:A:158:ASN:H	1.48	0.58
1:B:311:ASN:ND2	6:B:2317:HOH:O	2.38	0.56
1:B:2:VAL:O	1:B:2:VAL:HG13	2.06	0.55
1:A:2:VAL:HG21	6:A:2324:HOH:O	2.12	0.50
1:B:282:HIS:HE1	1:B:302:ASP:OD1	1.94	0.50
1:A:14:ARG:HG3	1:A:401:LEU:HD21	1.94	0.48
1:A:298:ILE:HD12	1:A:298:ILE:N	2.32	0.44
1:B:289:LEU:HD23	1:B:350:ALA:HB3	1.99	0.44
1:B:390[A]:GLN:CD	1:B:390[A]:GLN:N	2.71	0.44
1:A:158:ASN:HD22	1:A:158:ASN:N	2.13	0.43
1:B:298:ILE:HD12	1:B:298:ILE:N	2.35	0.41
1:B:124:ARG:CZ	1:B:143:ARG:CG	2.99	0.40
1:A:289:LEU:HD23	1:A:350:ALA:HB3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:HA	6:B:2005:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/401 (99%)	392 (98%)	6 (2%)	0	100	100
1	B	401/401 (100%)	392 (98%)	9 (2%)	0	100	100
All	All	799/802 (100%)	784 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/311 (100%)	309 (100%)	1 (0%)	92	92
1	B	313/311 (101%)	310 (99%)	3 (1%)	76	74
All	All	623/622 (100%)	619 (99%)	4 (1%)	88	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	B	336	LYS
1	B	390[A]	GLN
1	B	390[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	158	ASN
1	A	256	ASN
1	B	80	ASN
1	B	88	ASN
1	B	192	ASN
1	B	256	ASN
1	B	282	HIS
1	B	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	GAL	C	1	2	12,12,12	0.84	0	17,17,17	1.52	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	C	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.92	0
2	GAL	D	1	2	12,12,12	0.72	0	17,17,17	1.71	3 (17%)
2	NAG	D	2	2	14,14,15	1.25	2 (14%)	17,19,21	1.49	3 (17%)
2	GAL	E	1	2	12,12,12	0.86	0	17,17,17	1.41	2 (11%)
2	NAG	E	2	2	14,14,15	0.77	0	17,19,21	1.32	2 (11%)
2	GAL	F	1	2	12,12,12	0.60	0	17,17,17	1.43	4 (23%)
2	NAG	F	2	2	14,14,15	0.83	0	17,19,21	1.80	3 (17%)
2	GAL	G	1	2	12,12,12	0.88	0	17,17,17	1.44	3 (17%)
2	NAG	G	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.65	5 (29%)
2	GAL	H	1	2	12,12,12	0.63	0	17,17,17	1.32	3 (17%)
2	NAG	H	2	2	14,14,15	1.26	2 (14%)	17,19,21	1.05	1 (5%)
2	GAL	I	1	2	12,12,12	0.69	0	17,17,17	0.96	0
2	NAG	I	2	2	14,14,15	0.90	0	17,19,21	1.48	3 (17%)
2	GAL	J	1	2	12,12,12	0.59	0	17,17,17	0.96	1 (5%)
2	NAG	J	2	2	14,14,15	0.77	0	17,19,21	1.14	1 (5%)
2	GAL	K	1	2	12,12,12	0.59	0	17,17,17	1.19	1 (5%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	1.45	3 (17%)
2	GAL	L	1	2	12,12,12	0.72	0	17,17,17	1.76	4 (23%)
2	NAG	L	2	2	14,14,15	0.79	0	17,19,21	1.56	4 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	C	1	2	-	0/2/22/22	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	GAL	D	1	2	-	1/2/22/22	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	GAL	E	1	2	-	0/2/22/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	GAL	F	1	2	-	1/2/22/22	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	GAL	G	1	2	-	1/2/22/22	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	GAL	H	1	2	-	0/2/22/22	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	I	1	2	-	1/2/22/22	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	GAL	J	1	2	-	1/2/22/22	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	GAL	K	1	2	-	0/2/22/22	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	GAL	L	1	2	-	0/2/22/22	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	-3.35	1.38	1.43
2	D	2	NAG	O7-C7	2.97	1.30	1.23
2	H	2	NAG	O5-C1	-2.74	1.39	1.43
2	C	2	NAG	C1-C2	2.38	1.55	1.52
2	G	2	NAG	C1-C2	2.17	1.55	1.52
2	H	2	NAG	C4-C5	2.02	1.57	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C5-C6	4.65	114.50	107.20
2	L	2	NAG	O5-C5-C6	4.51	114.28	107.20
2	F	2	NAG	C6-C5-C4	-3.78	104.15	113.00
2	C	1	GAL	O5-C5-C4	3.38	115.84	109.69
2	E	1	GAL	O2-C2-C1	3.30	116.80	109.16
2	D	2	NAG	C1-O5-C5	3.18	116.51	112.19
2	L	1	GAL	O3-C3-C2	-3.16	103.03	110.35
2	L	1	GAL	C4-C3-C2	-3.12	105.38	110.82
2	G	2	NAG	O5-C5-C6	3.05	111.98	107.20
2	D	1	GAL	O1-C1-C2	-2.97	100.68	109.03
2	G	2	NAG	C2-N2-C7	2.96	127.12	122.90
2	E	2	NAG	O5-C1-C2	-2.88	106.73	111.29
2	J	2	NAG	C4-C3-C2	-2.88	106.80	111.02
2	H	2	NAG	C4-C3-C2	-2.86	106.82	111.02
2	L	1	GAL	O4-C4-C3	-2.86	103.74	110.35
2	F	1	GAL	O5-C5-C6	2.81	113.43	106.44
2	D	1	GAL	O5-C5-C4	2.80	114.79	109.69
2	I	2	NAG	O4-C4-C5	2.79	116.22	109.30
2	D	1	GAL	C6-C5-C4	-2.77	106.52	113.00
2	D	2	NAG	O5-C5-C6	2.76	111.53	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C6-C5-C4	2.74	119.43	113.00
2	G	2	NAG	O3-C3-C2	2.64	114.93	109.47
2	G	2	NAG	O7-C7-N2	2.64	126.80	121.95
2	G	2	NAG	O7-C7-C8	-2.59	117.25	122.06
2	G	1	GAL	O3-C3-C2	-2.58	104.39	110.35
2	K	2	NAG	O7-C7-N2	2.55	126.63	121.95
2	L	1	GAL	O5-C5-C4	-2.54	105.09	109.69
2	H	1	GAL	O5-C1-C2	-2.48	105.86	110.28
2	F	1	GAL	C1-O5-C5	-2.47	108.99	113.66
2	C	1	GAL	O4-C4-C5	2.47	115.43	109.30
2	H	1	GAL	O5-C5-C4	2.46	114.17	109.69
2	F	1	GAL	C4-C3-C2	2.35	114.92	110.82
2	C	1	GAL	C1-O5-C5	2.31	118.02	113.66
2	E	1	GAL	C1-C2-C3	2.27	115.03	110.31
2	K	2	NAG	O3-C3-C4	-2.25	105.15	110.35
2	K	1	GAL	O5-C5-C4	2.22	113.72	109.69
2	G	1	GAL	O2-C2-C3	-2.20	105.27	110.35
2	L	2	NAG	C4-C3-C2	-2.15	107.86	111.02
2	E	2	NAG	C6-C5-C4	-2.14	107.99	113.00
2	H	1	GAL	C1-C2-C3	-2.13	105.90	110.31
2	F	2	NAG	C1-O5-C5	2.09	115.02	112.19
2	G	1	GAL	C4-C3-C2	-2.09	107.18	110.82
2	L	2	NAG	O3-C3-C2	2.07	113.76	109.47
2	F	1	GAL	O4-C4-C3	-2.05	105.61	110.35
2	D	2	NAG	C8-C7-N2	-2.03	112.65	116.10
2	J	1	GAL	O3-C3-C2	-2.02	105.67	110.35
2	L	2	NAG	C6-C5-C4	-2.02	108.28	113.00
2	K	2	NAG	O7-C7-C8	-2.01	118.33	122.06
2	I	2	NAG	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	1	GAL	O5-C5-C6-O6
2	F	1	GAL	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	1	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	1	GAL	O5-C5-C6-O6
2	G	1	GAL	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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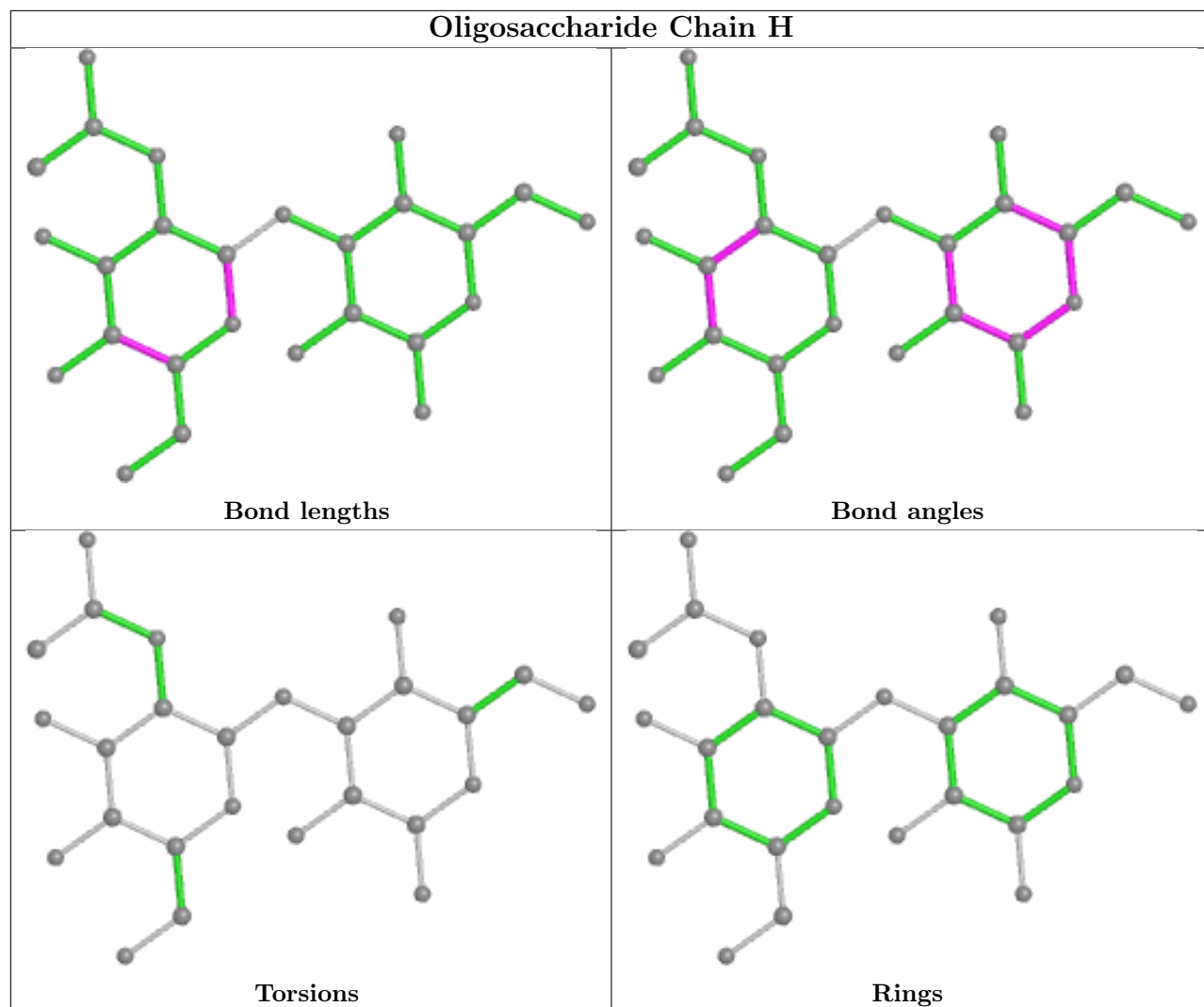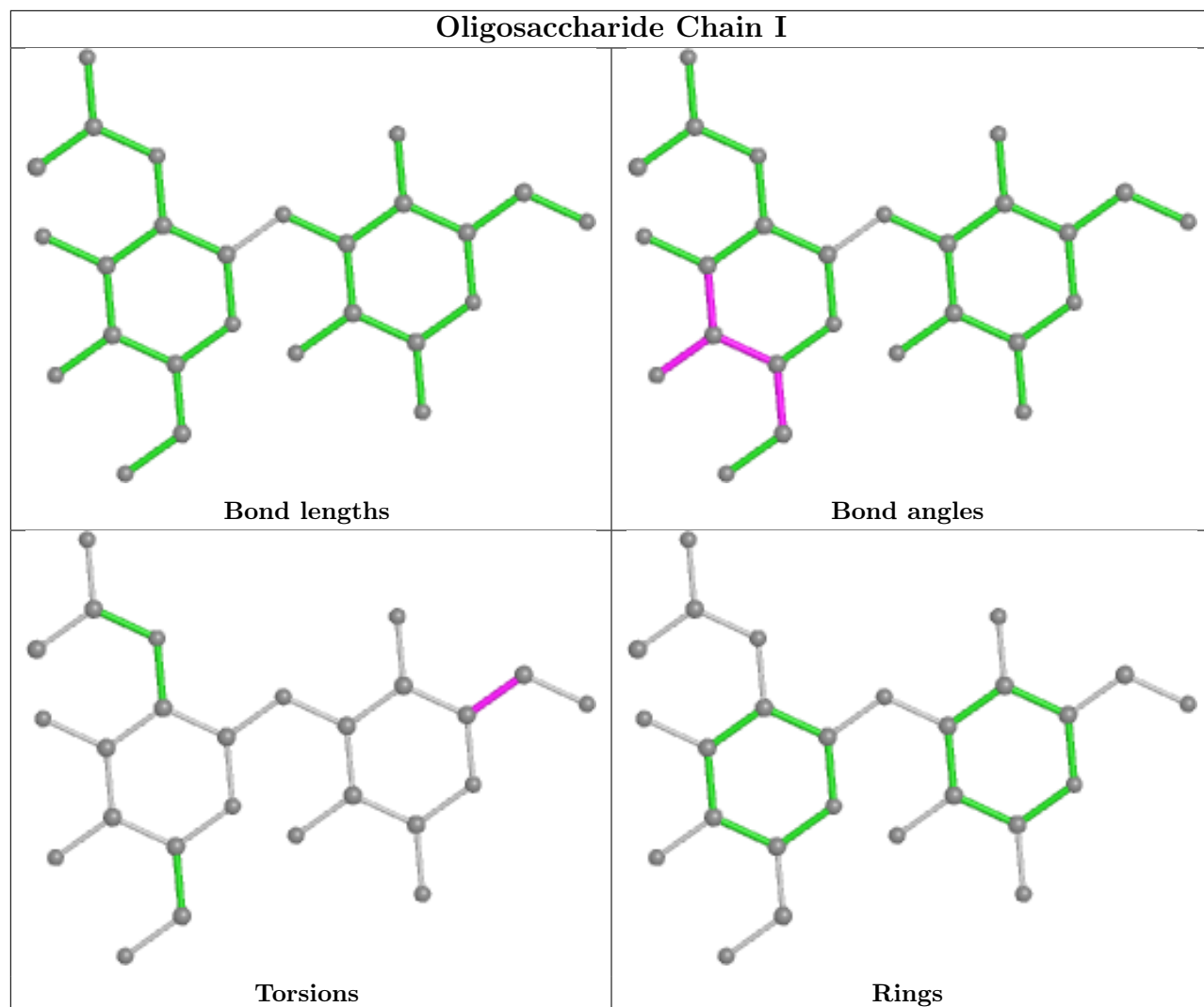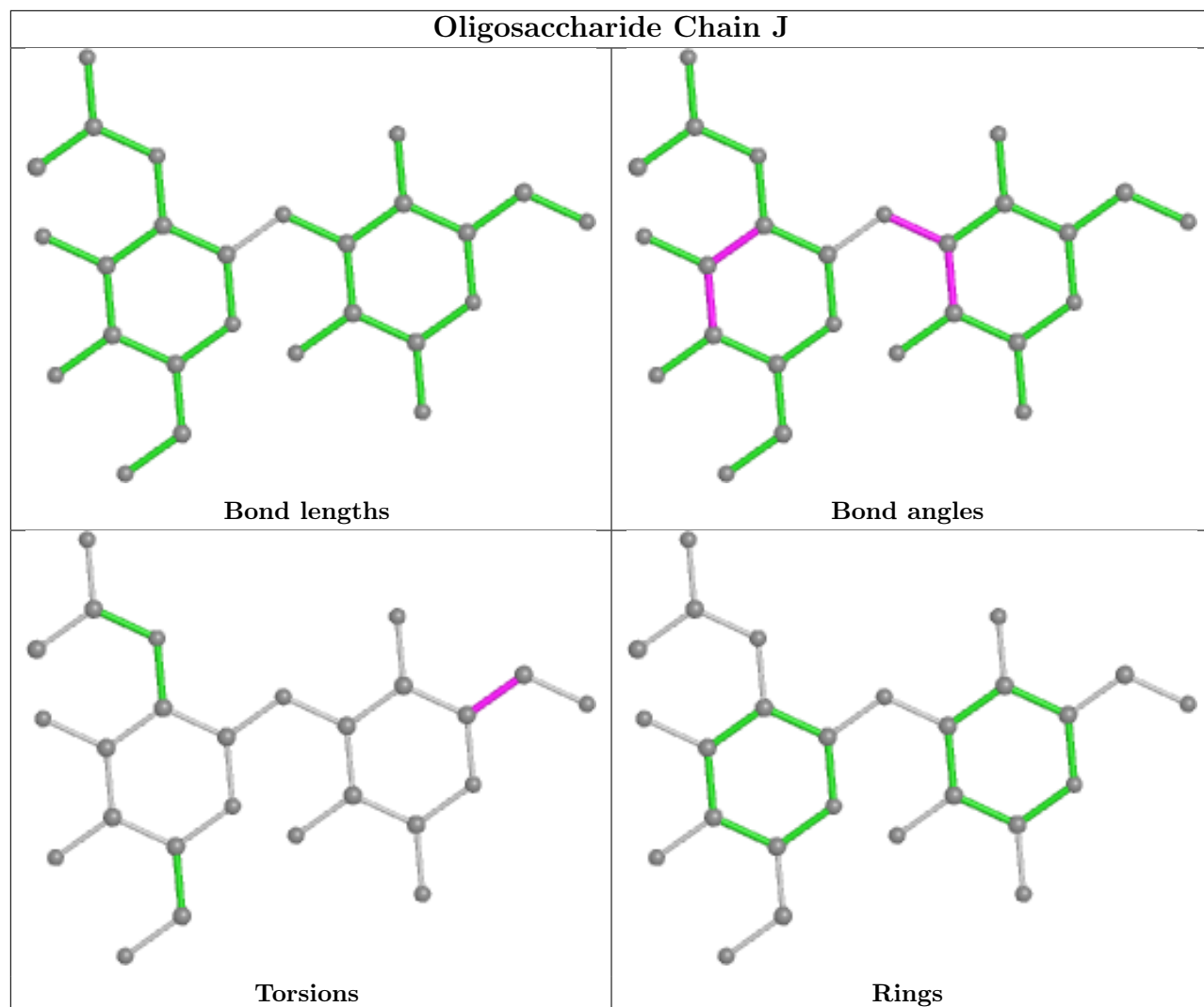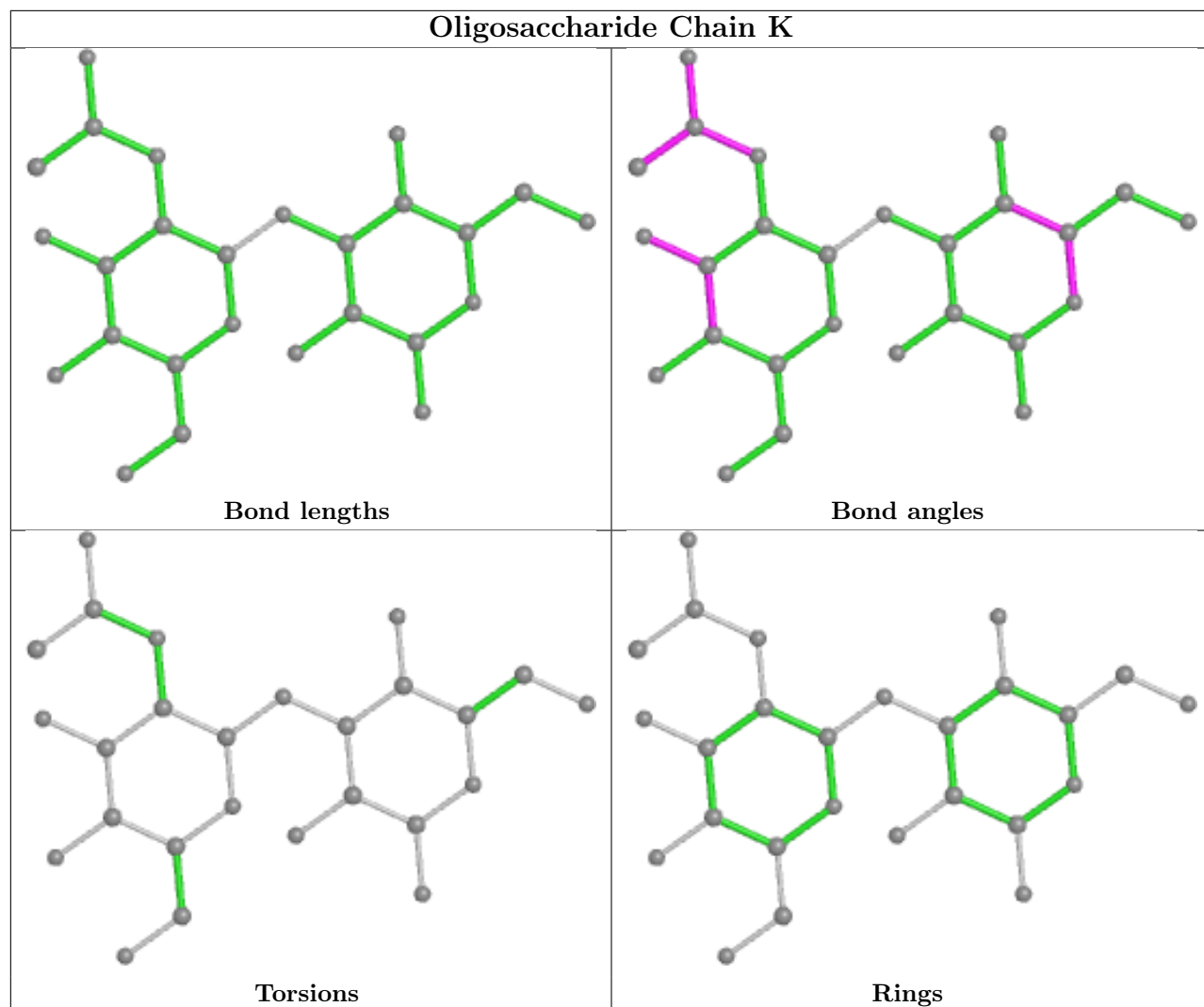

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

5.6　Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	#$|Z| > 2$
4	NDG	A	562[A]	-	15,15,15	0.45	0	21,21,21	2.51	6 (28%)
5	NAG	A	563[B]	-	15,15,15	0.40	0	21,21,21	1.27	2 (9%)
4	NDG	B	562	-	15,15,15	0.90	1 (6%)	21,21,21	1.62	5 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	A	562[A]	-	-	1/6/26/26	0/1/1/1
5	NAG	A	563[B]	-	-	0/6/26/26	0/1/1/1
4	NDG	B	562	-	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	562	NDG	O7-C7	2.03	1.27	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	562[A]	NDG	O1-C1-O5	-7.54	87.74	110.38
4	A	562[A]	NDG	C1-O5-C5	4.61	122.36	113.66
4	B	562	NDG	O5-C5-C6	3.57	115.30	106.44
5	A	563[B]	NAG	O3-C3-C2	3.43	116.59	109.66
4	A	562[A]	NDG	C1-C2-N2	-3.29	106.92	110.73
4	A	562[A]	NDG	O1-C1-C2	3.24	115.95	109.22
4	B	562	NDG	O5-C1-C2	-3.12	106.38	109.52
4	A	562[A]	NDG	O3-C3-C2	3.05	115.82	109.66
4	A	562[A]	NDG	O5-C1-C2	2.45	111.98	109.52
4	B	562	NDG	O3-C3-C2	2.32	114.34	109.66
4	B	562	NDG	C3-C2-N2	2.14	114.66	110.62
5	A	563[B]	NAG	C3-C2-N2	2.12	114.62	110.62
4	B	562	NDG	O1-C1-O5	2.03	116.49	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	562[A]	NDG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	400/401 (99%)	0.06	5 (1%)	77	83	8, 15, 24, 37	2 (0%)
1	B	399/401 (99%)	0.13	3 (0%)	86	90	9, 17, 25, 34	3 (0%)
All	All	799/802 (99%)	0.10	8 (1%)	82	87	8, 16, 25, 37	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	3.5
1	B	2	VAL	3.4
1	B	259	GLY	2.2
1	A	396	ALA	2.2
1	A	328	TYR	2.1
1	B	258	ASN	2.1
1	A	230	VAL	2.1
1	A	2	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å²)	Q<0.9
2	GAL	E	1	12/12	0.73	0.25	28,35,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	F	1	12/12	0.82	0.17	22,27,30,32	12
2	NAG	J	2	14/15	0.82	0.15	21,25,29,31	0
2	GAL	I	1	12/12	0.87	0.17	21,25,27,31	0
2	GAL	J	1	12/12	0.88	0.16	29,37,42,46	0
2	GAL	K	1	12/12	0.89	0.19	24,29,32,36	0
2	GAL	C	1	12/12	0.90	0.13	19,22,26,33	0
2	GAL	G	1	12/12	0.90	0.14	18,22,24,27	0
2	NAG	E	2	14/15	0.91	0.14	13,19,25,26	0
2	GAL	L	1	12/12	0.91	0.17	22,29,31,35	0
2	GAL	H	1	12/12	0.92	0.14	20,24,27,29	0
2	GAL	D	1	12/12	0.92	0.12	15,21,25,31	0
2	NAG	F	2	14/15	0.93	0.11	16,20,26,29	0
2	NAG	I	2	14/15	0.93	0.09	15,19,23,27	0
2	NAG	H	2	14/15	0.94	0.10	14,17,18,19	0
2	NAG	C	2	14/15	0.95	0.09	13,15,17,19	0
2	NAG	K	2	14/15	0.95	0.09	15,21,24,24	0
2	NAG	G	2	14/15	0.95	0.08	13,15,18,24	0
2	NAG	D	2	14/15	0.96	0.09	10,12,17,24	0
2	NAG	L	2	14/15	0.96	0.11	17,19,22,27	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.
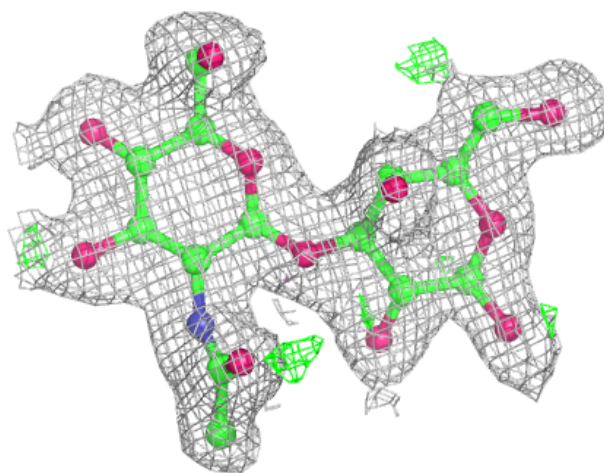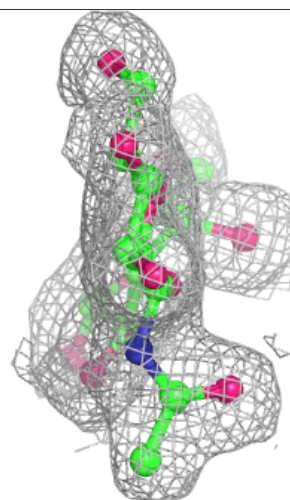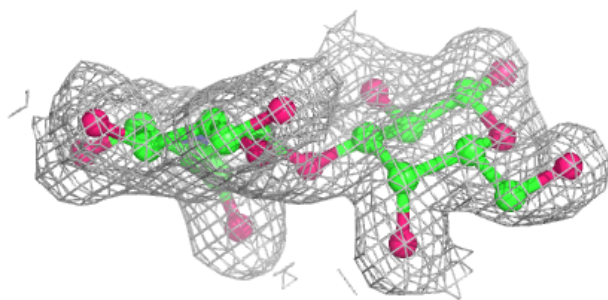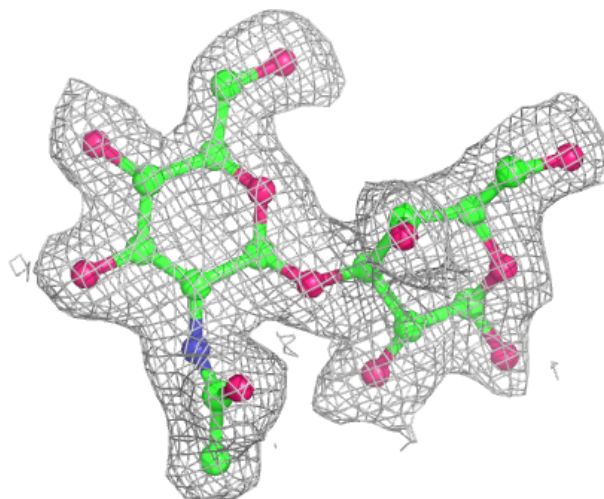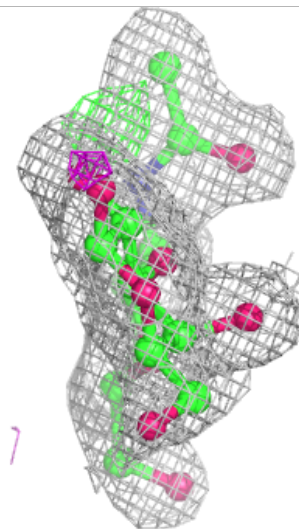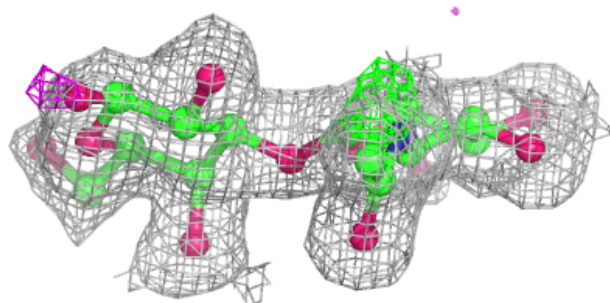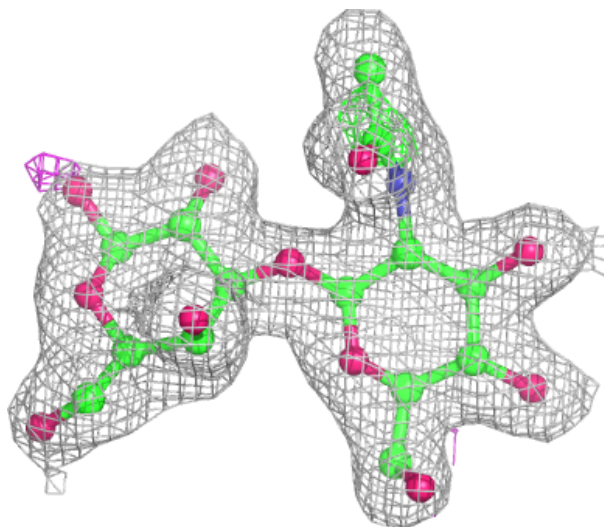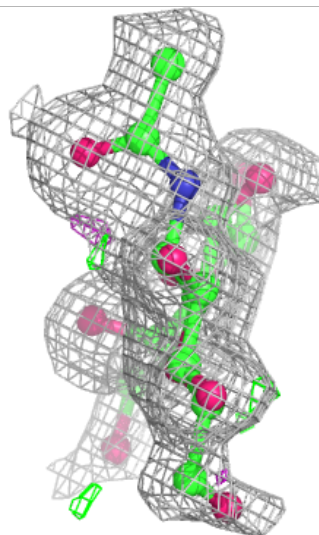
Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
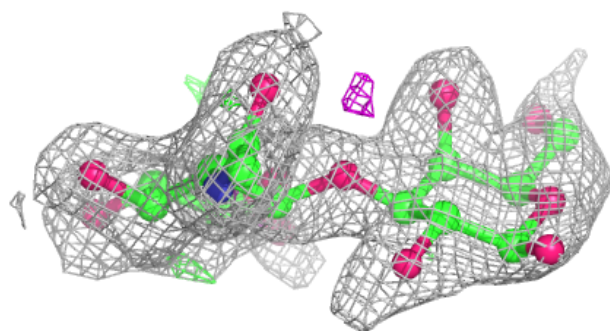and green (positive)
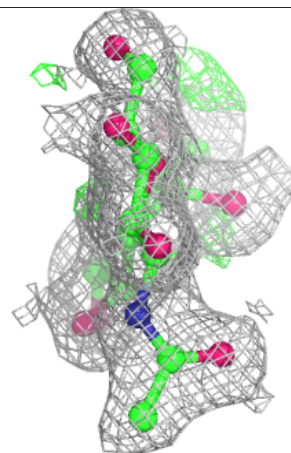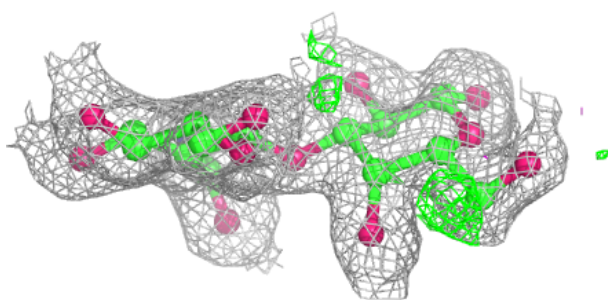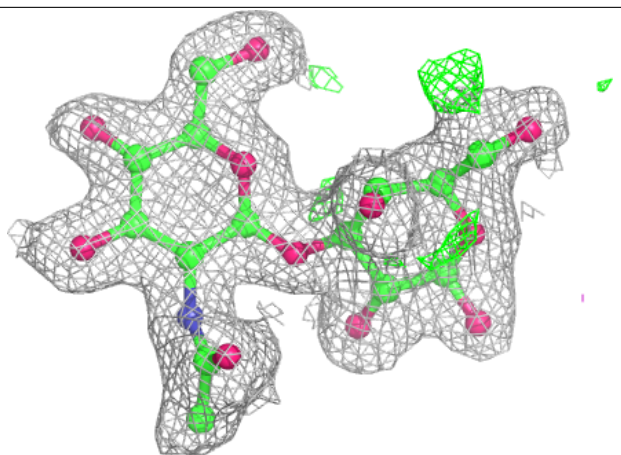
Electron density around Chain D:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
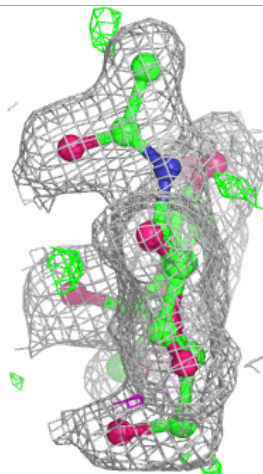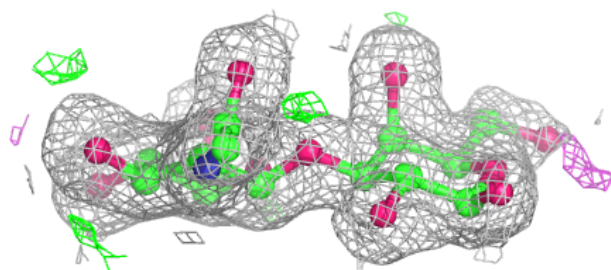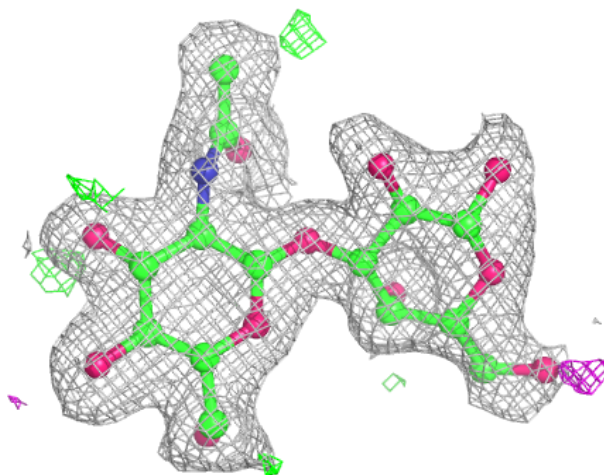
Electron density around Chain E:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
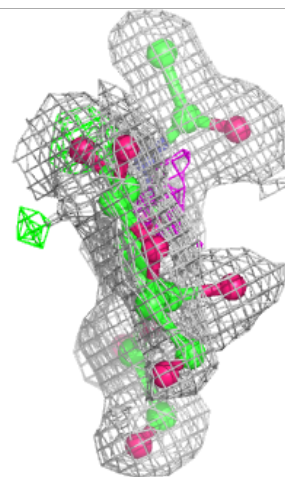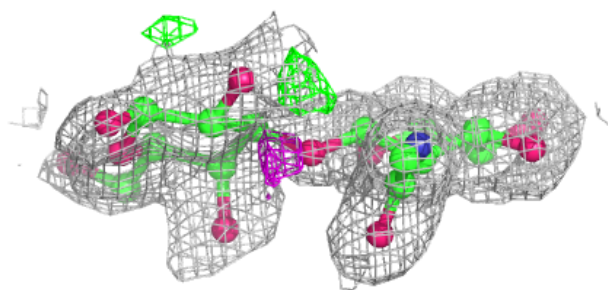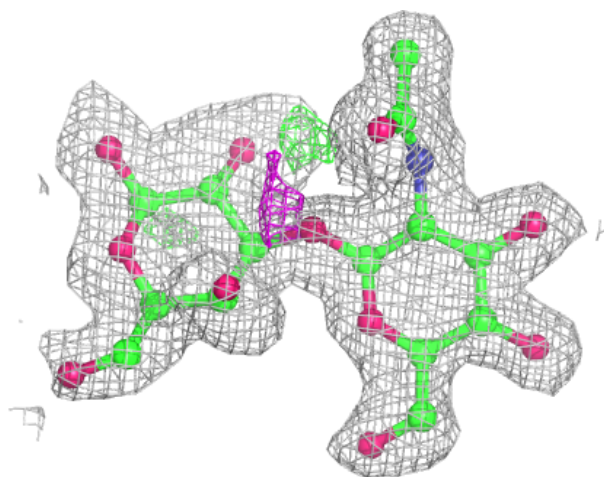
Electron density around Chain F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
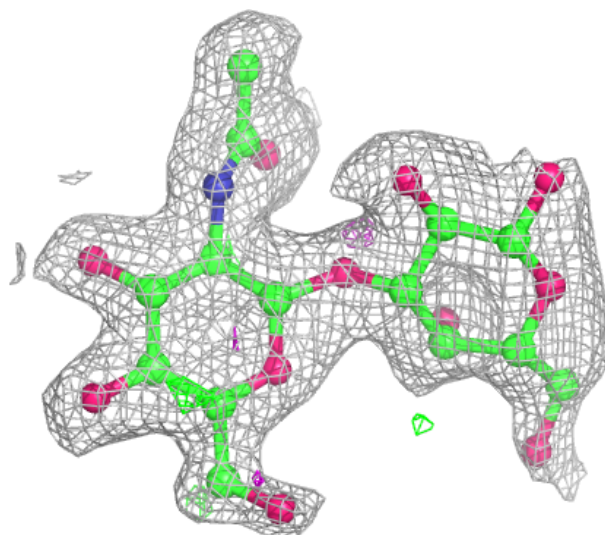and green (positive)
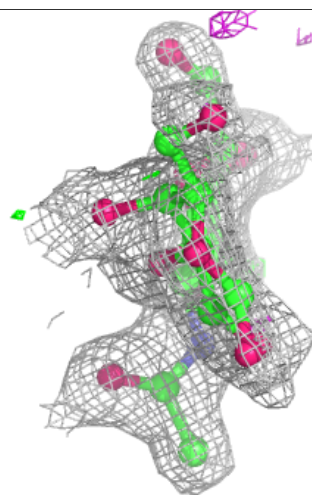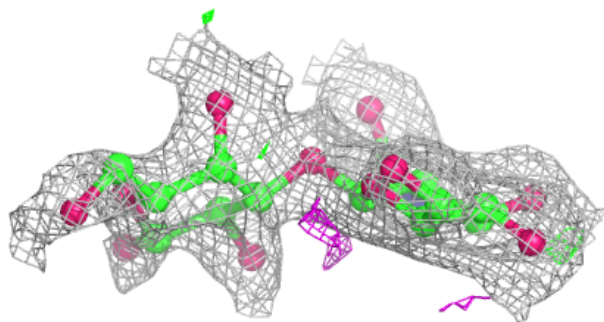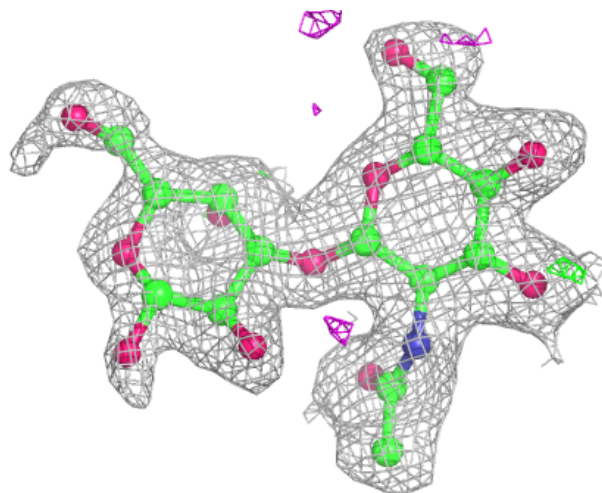
Electron density around Chain G:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
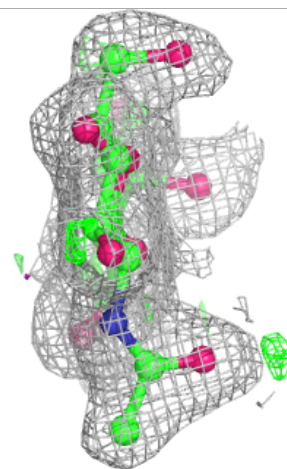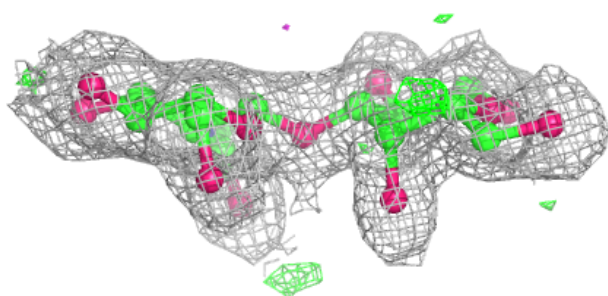
Electron density around Chain H:

$2mF_o$-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 I:

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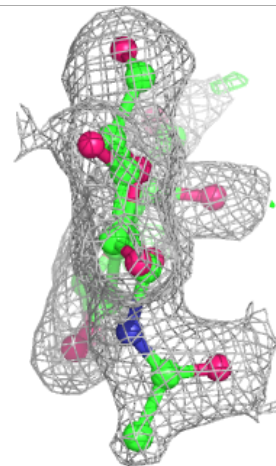mF_o-DF_c (at 3 rmsd) in purple (negative)
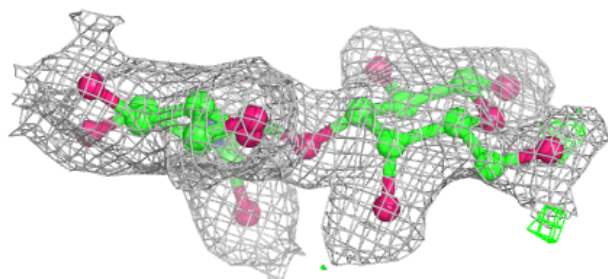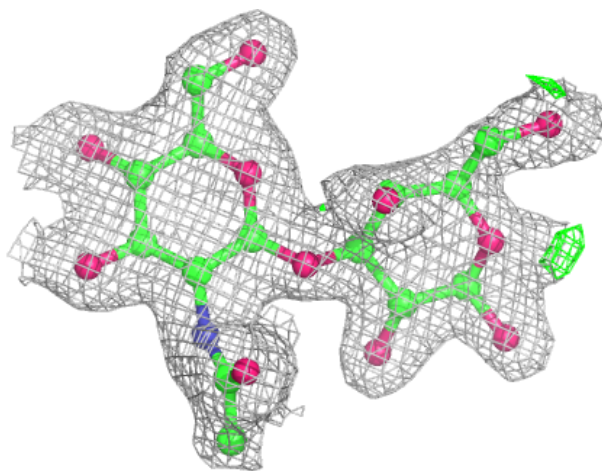and green (positive)

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 K:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
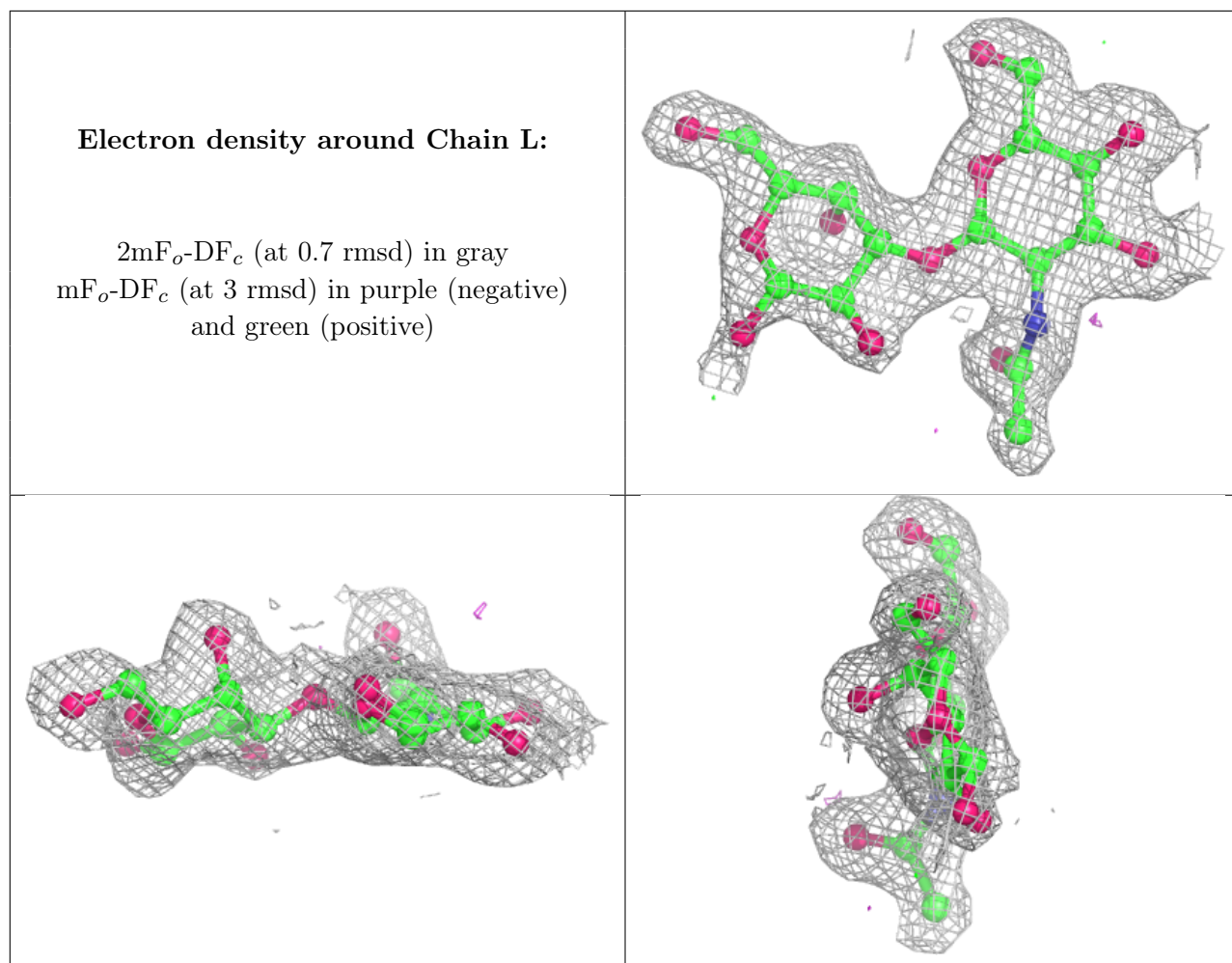and green (positive)

Electron density around Chain L:

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

6.4 Ligands ⓘ

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	NDG	A	562[A]	15/15	0.94	0.11	16,17,21,23	15
5	NAG	A	563[B]	15/15	0.94	0.11	16,18,22,24	15
4	NDG	B	562	15/15	0.95	0.11	17,18,20,20	0
3	CA	B	501	1/1	0.97	0.17	33,33,33,33	0
3	CA	A	502	1/1	0.98	0.19	29,29,29,29	0
3	CA	A	501	1/1	0.98	0.15	24,24,24,24	0
3	CA	B	502	1/1	0.98	0.20	30,30,30,30	0
3	CA	B	500	1/1	1.00	0.03	15,15,15,15	0
3	CA	A	500	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.