



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 04:29 PM BST

PDB ID : 6S6Q
Title : Crystal structure of the LRR ectodomain of the plant membrane receptor kinase GASSHO1/SCHENGEN3 from Arabidopsis thaliana in complex with CASPARIAN STRIP INTEGRITY FACTOR 2.
Authors : Okuda, S.; Moretti, A.; Hothorn, M.
Deposited on : 2019-07-03
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

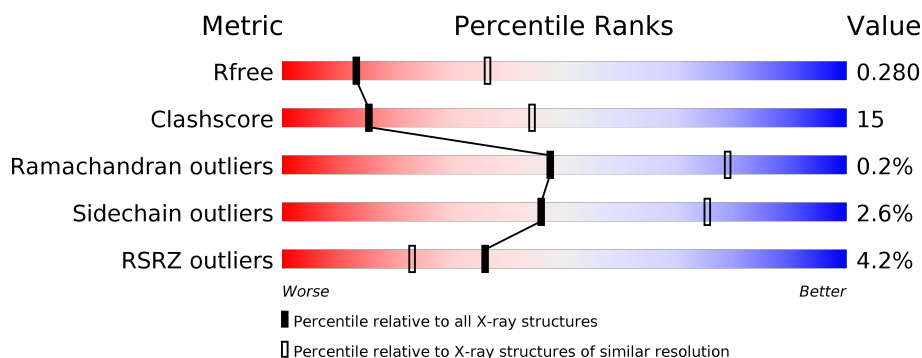
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on 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	863	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>••</div> </div> </div>
1	B	863	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>••</div> </div> </div>
2	C	21	<div> <div>24%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>19%</div> </div> </div>
2	D	21	<div> <div>19%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>10%</div> </div> </div>
3	E	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	K	2	<div><div></div><div>100%</div><div></div></div>
4	H	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>
4	J	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
5	I	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13575 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 LRR receptor-like serine/threonine-protein kinase GSO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6362	4011	1081	1246	24			
1	B	833	Total	C	N	O	S	0	0	0
			6370	4014	1079	1253	24			

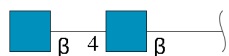
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP C0LGQ5
A	15	SER	-	expression tag	UNP C0LGQ5
A	16	SER	-	expression tag	UNP C0LGQ5
A	17	MET	-	expression tag	UNP C0LGQ5
A	871	GLU	-	expression tag	UNP C0LGQ5
A	872	ASN	-	expression tag	UNP C0LGQ5
A	873	LEU	-	expression tag	UNP C0LGQ5
A	874	TYR	-	expression tag	UNP C0LGQ5
A	875	PHE	-	expression tag	UNP C0LGQ5
A	876	GLN	-	expression tag	UNP C0LGQ5
B	14	GLY	-	expression tag	UNP C0LGQ5
B	15	SER	-	expression tag	UNP C0LGQ5
B	16	SER	-	expression tag	UNP C0LGQ5
B	17	MET	-	expression tag	UNP C0LGQ5
B	871	GLU	-	expression tag	UNP C0LGQ5
B	872	ASN	-	expression tag	UNP C0LGQ5
B	873	LEU	-	expression tag	UNP C0LGQ5
B	874	TYR	-	expression tag	UNP C0LGQ5
B	875	PHE	-	expression tag	UNP C0LGQ5
B	876	GLN	-	expression tag	UNP C0LGQ5

- Molecule 2 is a protein called Protein CASPARIAN STRIP INTEGRITY FACTOR 2.

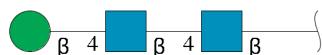
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	S	0	0	0
			174	112	30	31	1			
2	D	21	Total	C	N	O	S	0	0	0
			174	112	30	31	1			

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



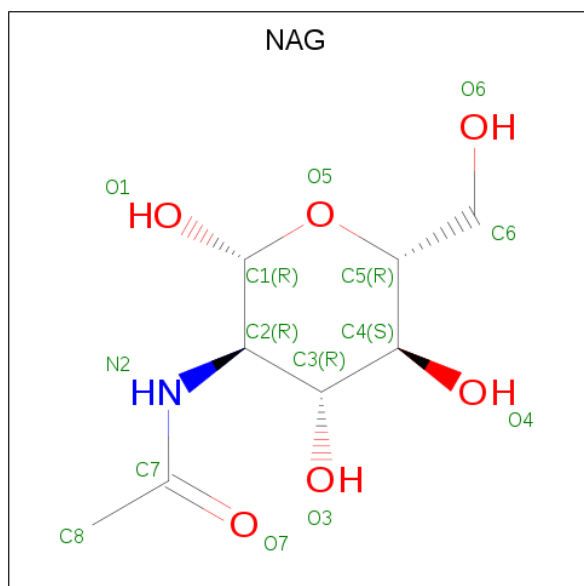
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(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
			25	14	1	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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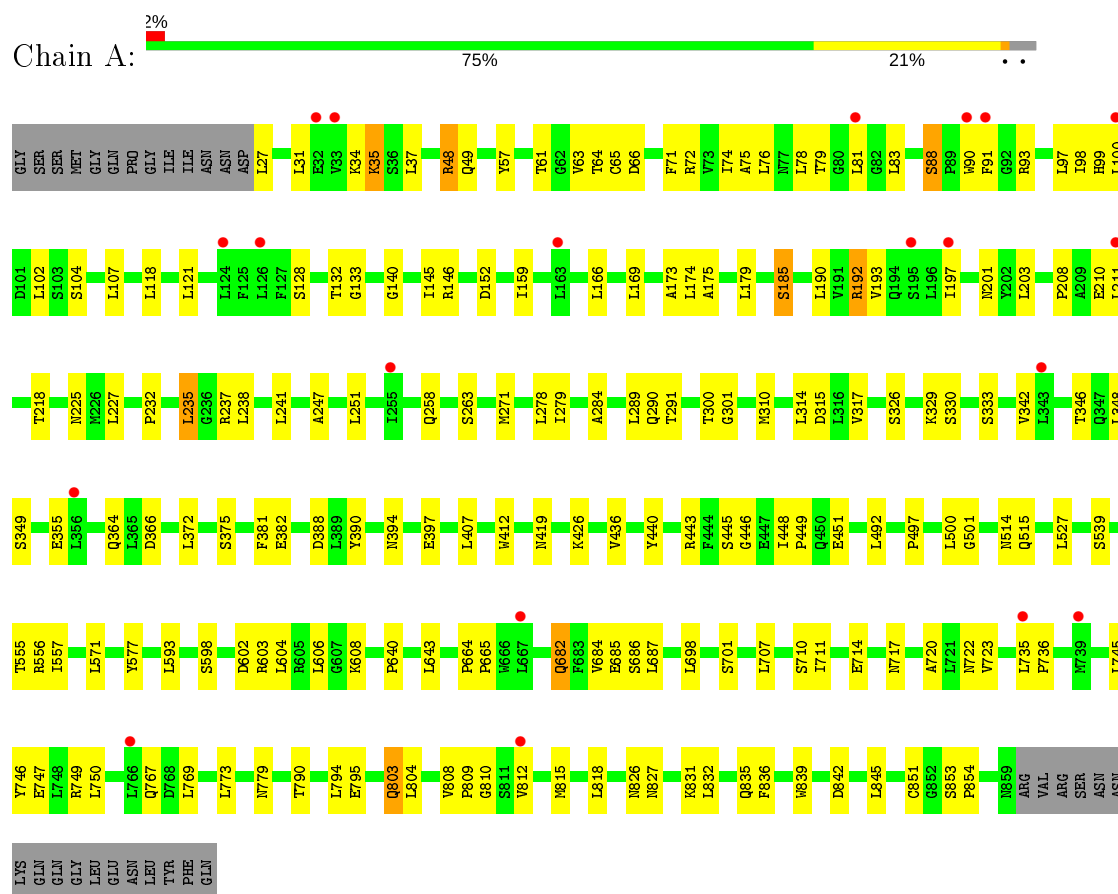
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
	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

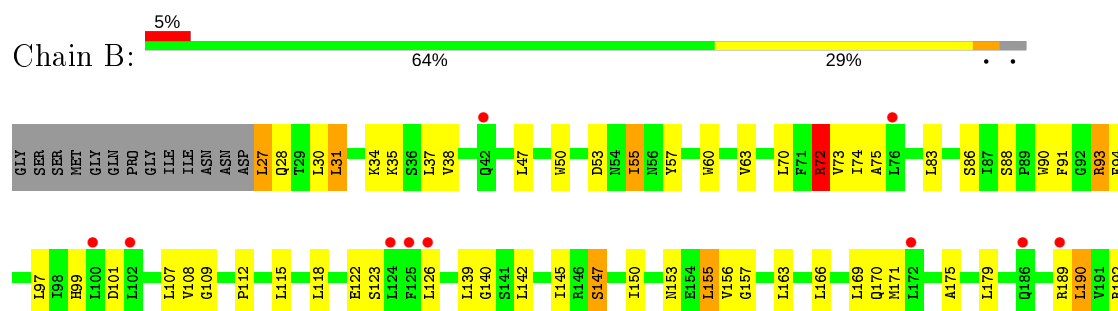
3 Residue-property plots [i](#)

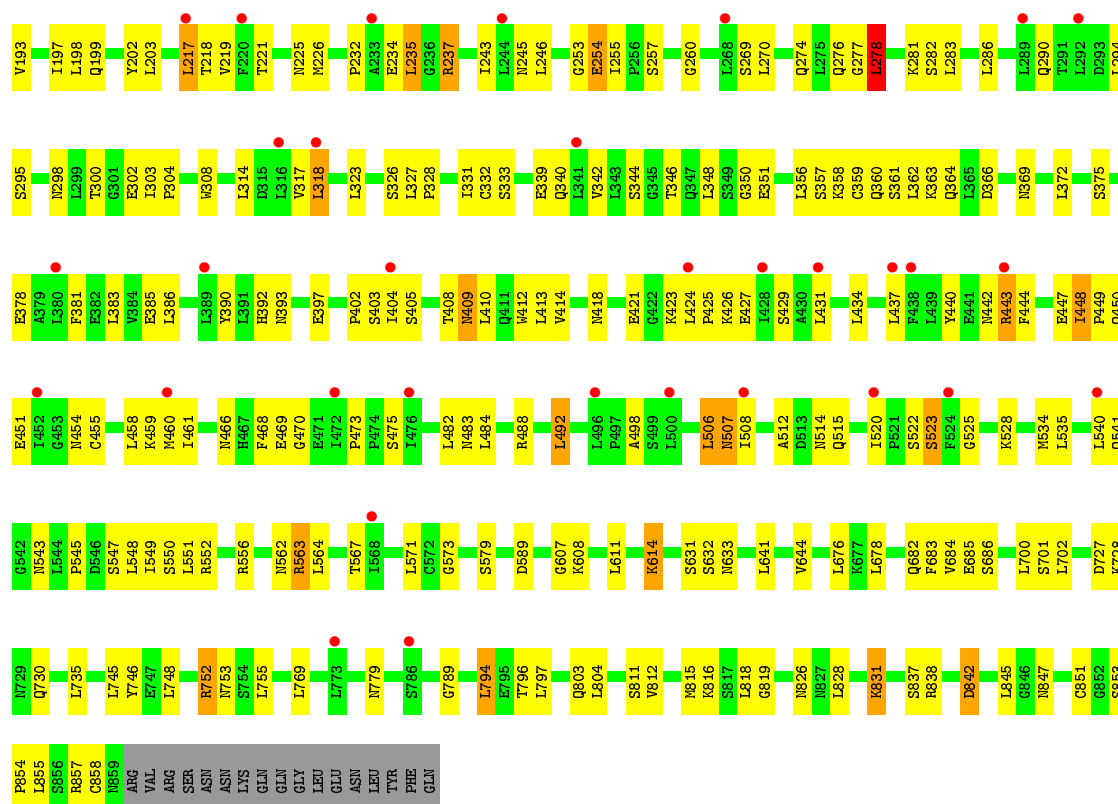
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LRR receptor-like serine/threonine-protein kinase GSO1

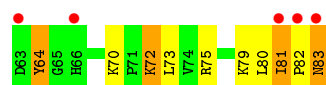


- Molecule 1: LRR receptor-like serine/threonine-protein kinase GSO1





• Molecule 2: Protein CASPARIAN STRIP INTEGRITY FACTOR 2



• Molecule 2: Protein CASPARIAN STRIP INTEGRITY FACTOR 2



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

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

Chain J:  67% 33%

MAG1
MAG2
BMA3

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

Chain I:  100%

MAG1
BMA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	192.36 Å 192.36 Å 149.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.95 48.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.30-2.95) 100.0 (48.32-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.96 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.280 0.209 , 0.280	Depositor DCC
R_{free} test set	2962 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	88.9	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13575	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: BMA, NAG, TYS

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	0.52	1/6464 (0.0%)	0.78	2/8785 (0.0%)
1	B	0.61	4/6472 (0.1%)	1.06	34/8796 (0.4%)
2	C	0.64	0/163	0.89	0/218
2	D	0.50	0/163	0.78	0/218
All	All	0.57	5/13262 (0.0%)	0.93	36/18017 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	LEU	CG-CD2	8.97	1.85	1.51
1	A	65	CYS	CB-SG	-7.32	1.69	1.82
1	B	254	GLU	CD-OE1	6.55	1.32	1.25
1	B	72	ARG	CZ-NH1	-5.87	1.25	1.33
1	B	72	ARG	CG-CD	-5.63	1.37	1.51

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	NE-CZ-NH2	30.25	135.42	120.30
1	B	237	ARG	NE-CZ-NH2	-29.13	105.73	120.30
1	B	72	ARG	NE-CZ-NH1	-12.48	114.06	120.30
1	B	237	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	B	217	LEU	CB-CG-CD2	-9.36	95.08	111.00

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	6362	0	6411	152	0
1	B	6370	0	6417	241	1
2	C	174	0	175	13	0
2	D	174	0	173	10	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	K	28	0	25	1	0
4	H	39	0	34	0	0
4	J	39	0	34	1	0
5	I	25	0	22	0	0
6	A	168	0	156	5	0
6	B	112	0	104	2	0
All	All	13575	0	13626	405	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 405 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:235:LEU:CD2	1:B:235:LEU:CG	1.85	1.54
1:B:346:THR:HG23	1:B:348:LEU:CD1	1.72	1.17
1:B:346:THR:CG2	1:B:348:LEU:HD13	1.75	1.15
1:A:34:LYS:HE3	1:A:90:TRP:CZ2	1.81	1.14
1:A:842:ASP:HA	1:A:845:LEU:HD13	1.34	1.10

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:NH2	1:B:237:ARG:NH2[8_555]	2.10	0.10

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	831/863 (96%)	766 (92%)	65 (8%)	0	100	100
1	B	831/863 (96%)	762 (92%)	68 (8%)	1 (0%)	51	83
2	C	18/21 (86%)	16 (89%)	1 (6%)	1 (6%)	2	8
2	D	18/21 (86%)	14 (78%)	3 (17%)	1 (6%)	2	8
All	All	1698/1768 (96%)	1558 (92%)	137 (8%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	ILE
2	D	80	LEU
1	B	475	SER

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	735/765 (96%)	723 (98%)	12 (2%)	62	84
1	B	738/765 (96%)	715 (97%)	23 (3%)	40	71
2	C	19/19 (100%)	17 (90%)	2 (10%)	7	24
2	D	19/19 (100%)	16 (84%)	3 (16%)	2	10
All	All	1511/1568 (96%)	1471 (97%)	40 (3%)	46	75

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	LEU
1	B	507	ASN
2	C	83	ASN
1	B	351	GLU
1	B	523	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	803	GLN
1	A	827	ASN
1	B	411	GLN
1	A	767	GLN
1	B	467	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
2	TYS	D	64	2	15,16,17	2.05	3 (20%)	18,22,24	3.08	5 (27%)
2	TYS	C	64	1,2	15,16,17	1.62	3 (20%)	18,22,24	1.97	3 (16%)

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	TYS	D	64	2	-	5/10/11/13	0/1/1/1
2	TYS	C	64	1,2	-	6/10/11/13	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)
2	D	64	TYS	OH-S	-4.75	1.51	1.58
2	C	64	TYS	OH-S	-4.34	1.51	1.58
2	D	64	TYS	O1-S	4.11	1.62	1.45
2	D	64	TYS	OH-CZ	-3.86	1.36	1.42
2	C	64	TYS	OH-CZ	-3.11	1.37	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	TYS	CB-CA-C	8.18	126.80	111.47
2	D	64	TYS	CG-CB-CA	6.97	128.22	114.10
2	C	64	TYS	O3-S-OH	6.44	121.33	105.83
2	D	64	TYS	CB-CG-CD1	-4.50	111.97	120.91
2	D	64	TYS	CD2-CG-CD1	3.57	123.78	118.17

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	64	TYS	N-CA-CB-CG
2	D	64	TYS	C-CA-CB-CG
2	D	64	TYS	CE1-CZ-OH-S
2	C	64	TYS	C-CA-CB-CG
2	C	64	TYS	CZ-OH-S-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	64	TYS	3	0
2	C	64	TYS	1	0

5.5 Carbohydrates

16 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	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	E	2	3	14,14,15	0.67	1 (7%)	17,19,21	0.65	0
3	NAG	F	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.11	2 (11%)
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.97	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.69	0	17,19,21	0.78	1 (5%)
3	NAG	G	2	3	14,14,15	0.41	0	17,19,21	0.49	0
4	NAG	H	1	1,4	14,14,15	0.52	0	17,19,21	0.60	0
4	NAG	H	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.51	0
4	BMA	H	3	4	11,11,12	1.55	2 (18%)	15,15,17	1.01	2 (13%)
5	NAG	I	1	1,5	14,14,15	0.21	0	17,19,21	0.91	1 (5%)
5	BMA	I	2	5	11,11,12	1.31	2 (18%)	15,15,17	1.04	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
4	NAG	J	2	4	14,14,15	0.72	1 (7%)	17,19,21	1.09	1 (5%)
4	BMA	J	3	4	11,11,12	1.22	2 (18%)	15,15,17	1.03	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.31	0	17,19,21	0.90	0
3	NAG	K	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.19	2 (11%)

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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	NAG	C1-C2	4.79	1.59	1.52
4	H	3	BMA	C2-C3	3.38	1.57	1.52
3	F	1	NAG	O5-C1	-3.05	1.38	1.43
4	H	2	NAG	O5-C1	-2.82	1.39	1.43
5	I	2	BMA	C1-C2	2.79	1.58	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	NAG	O5-C1-C2	-3.55	105.68	111.29
4	J	2	NAG	C1-O5-C5	3.42	116.82	112.19
5	I	1	NAG	C1-O5-C5	3.11	116.41	112.19
4	J	1	NAG	C1-O5-C5	3.05	116.32	112.19
3	F	2	NAG	C1-O5-C5	2.81	116.00	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

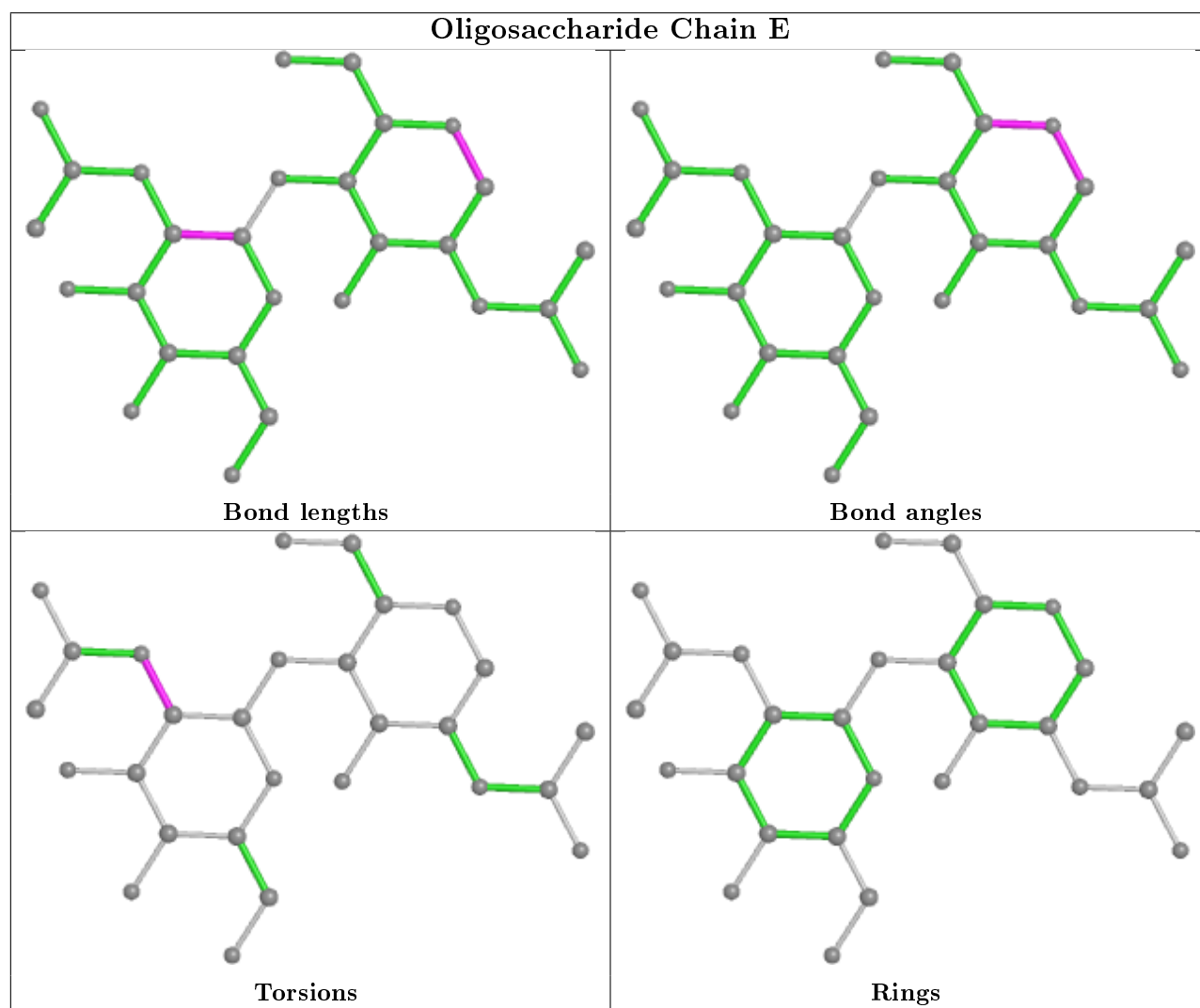
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6

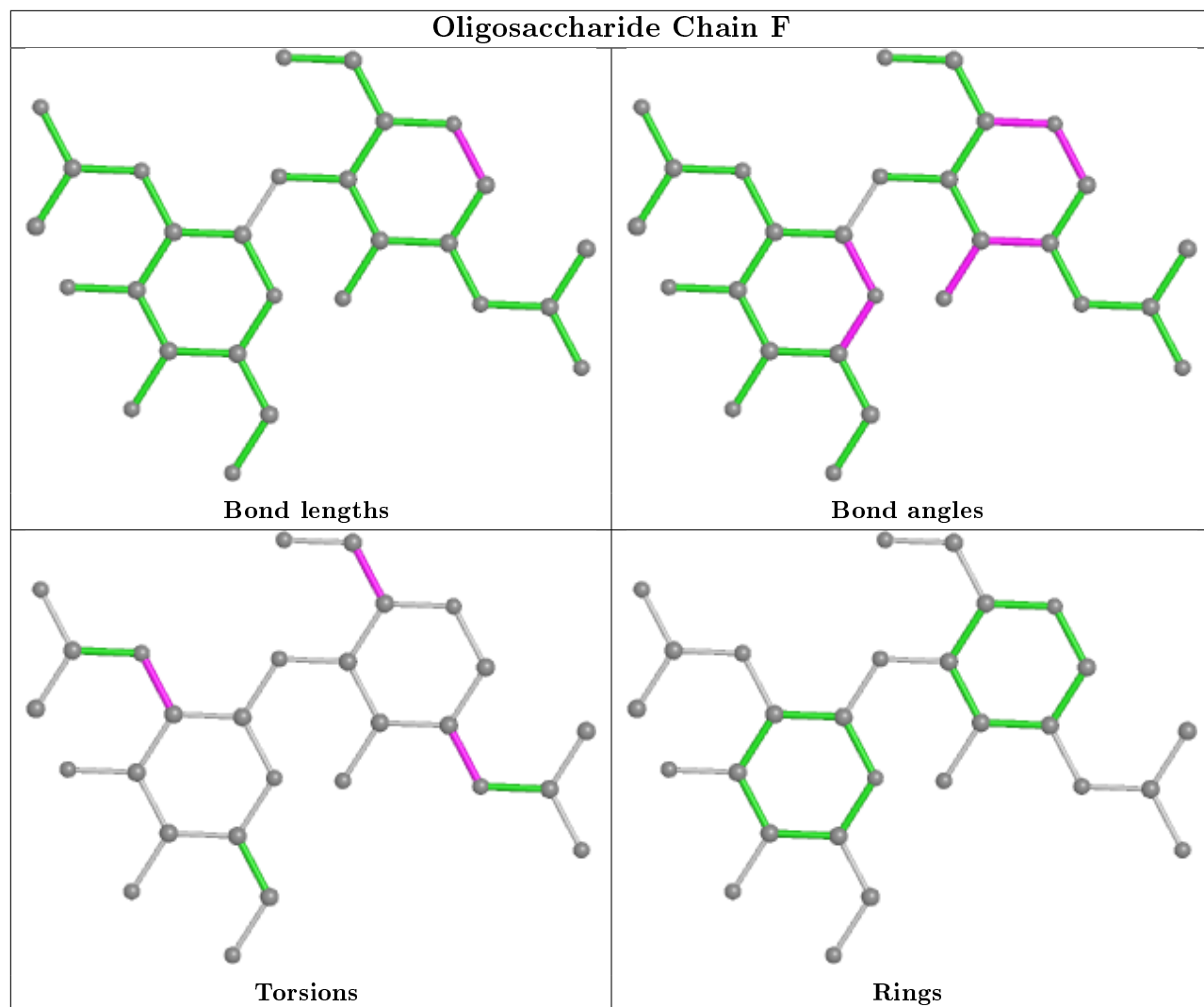
There are no ring outliers.

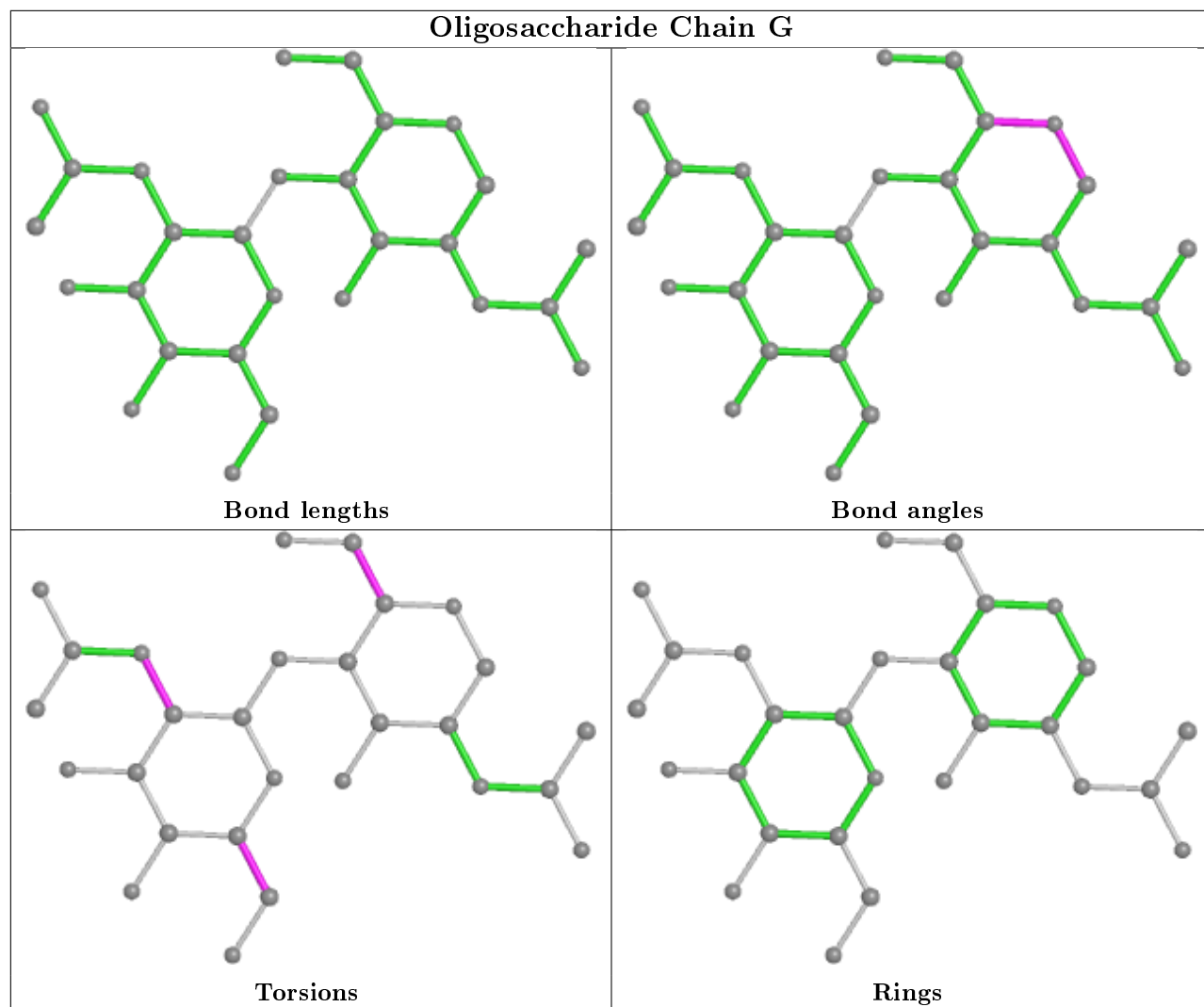
4 monomers are involved in 3 short contacts:

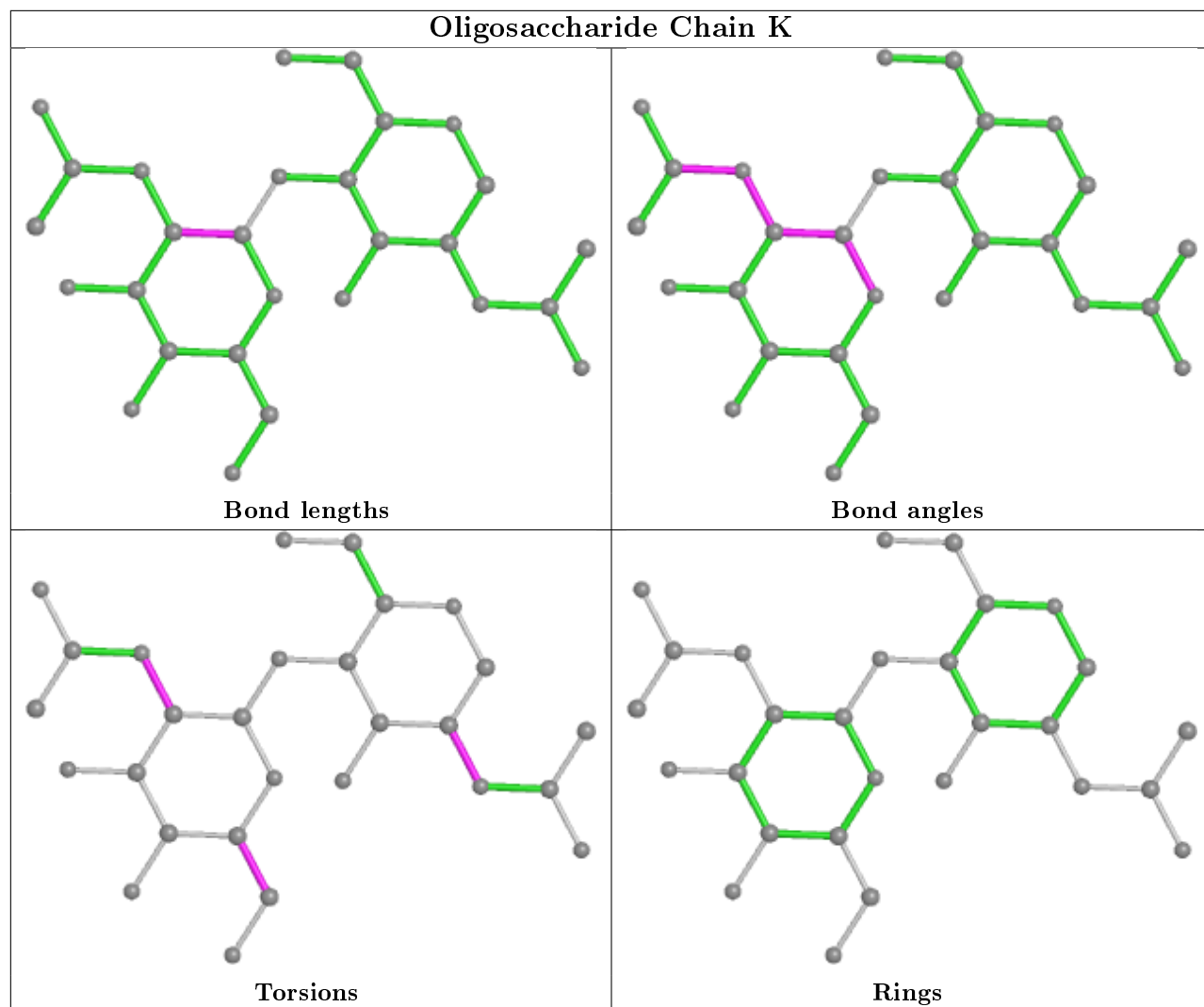
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	E	1	NAG	1	0
4	J	2	NAG	1	0
3	K	1	NAG	1	0

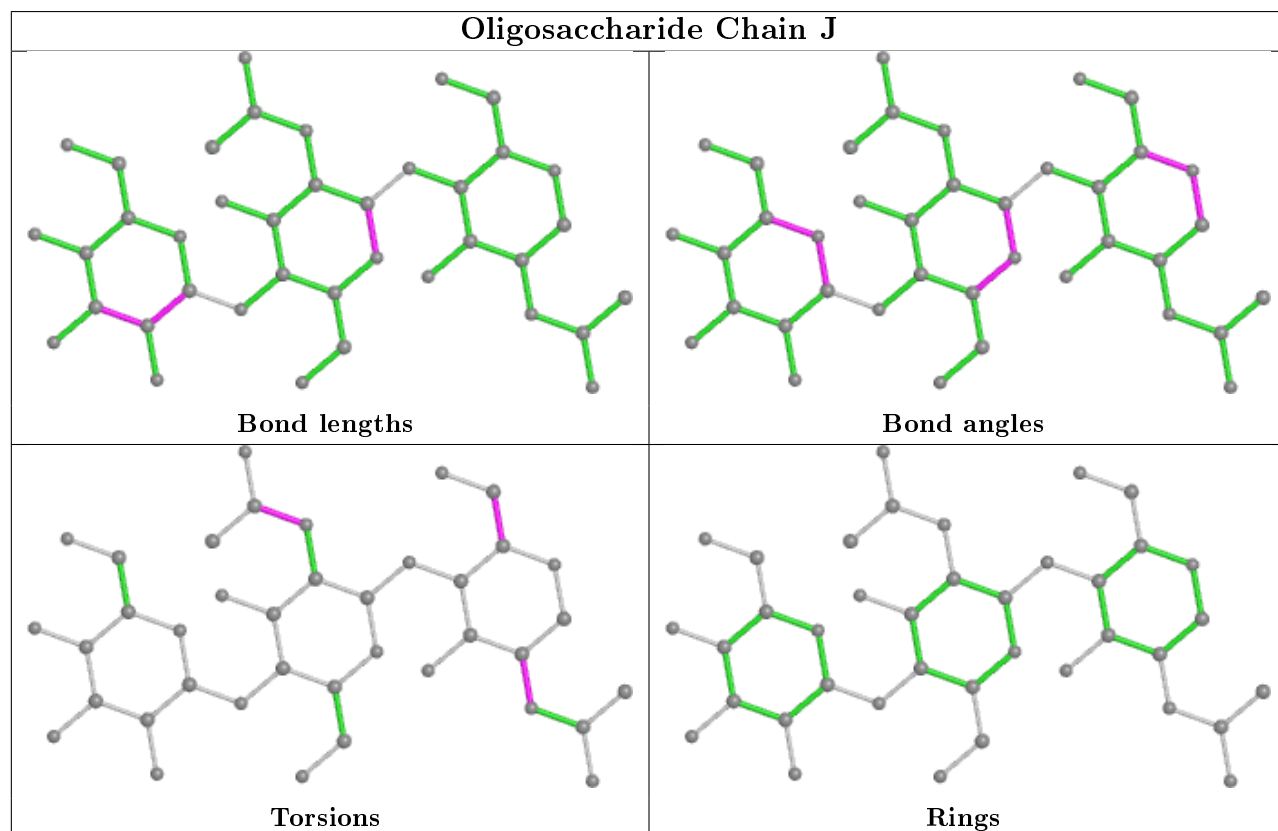
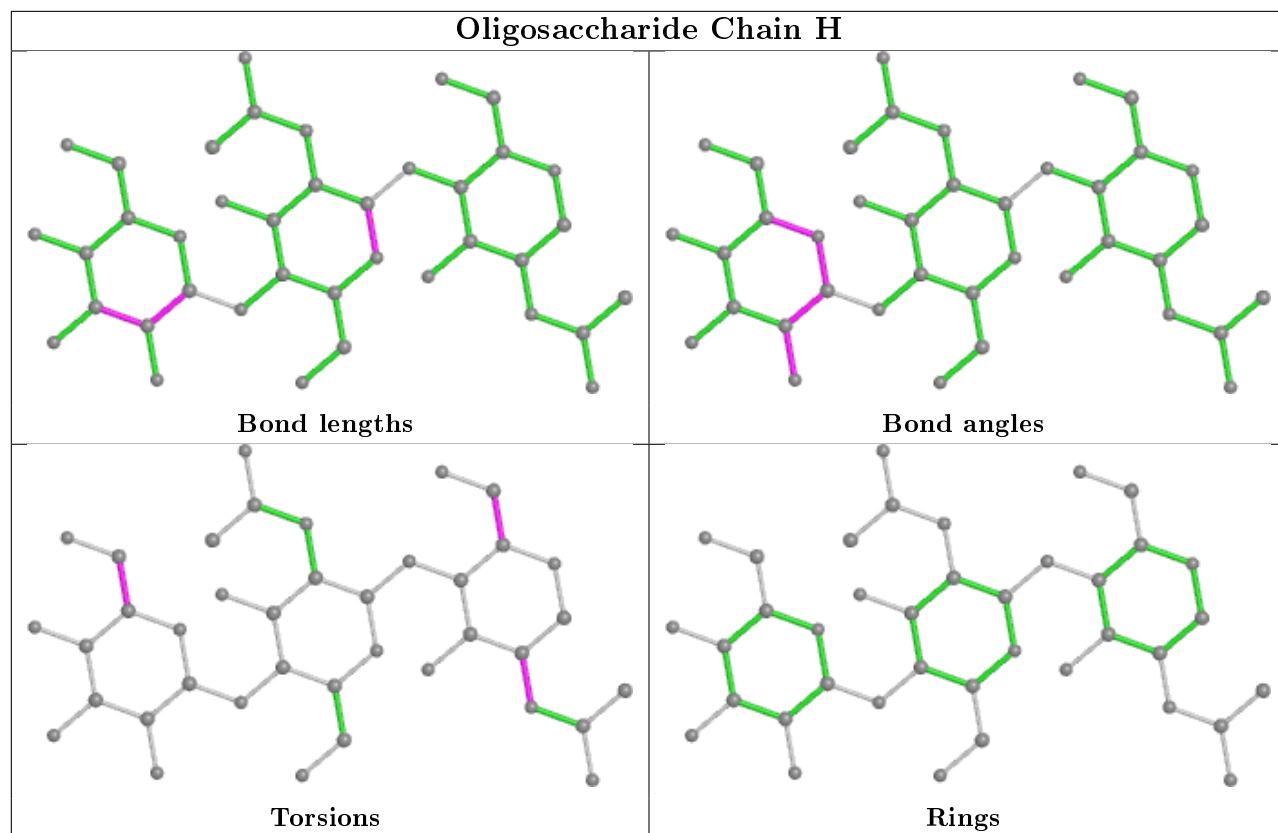
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

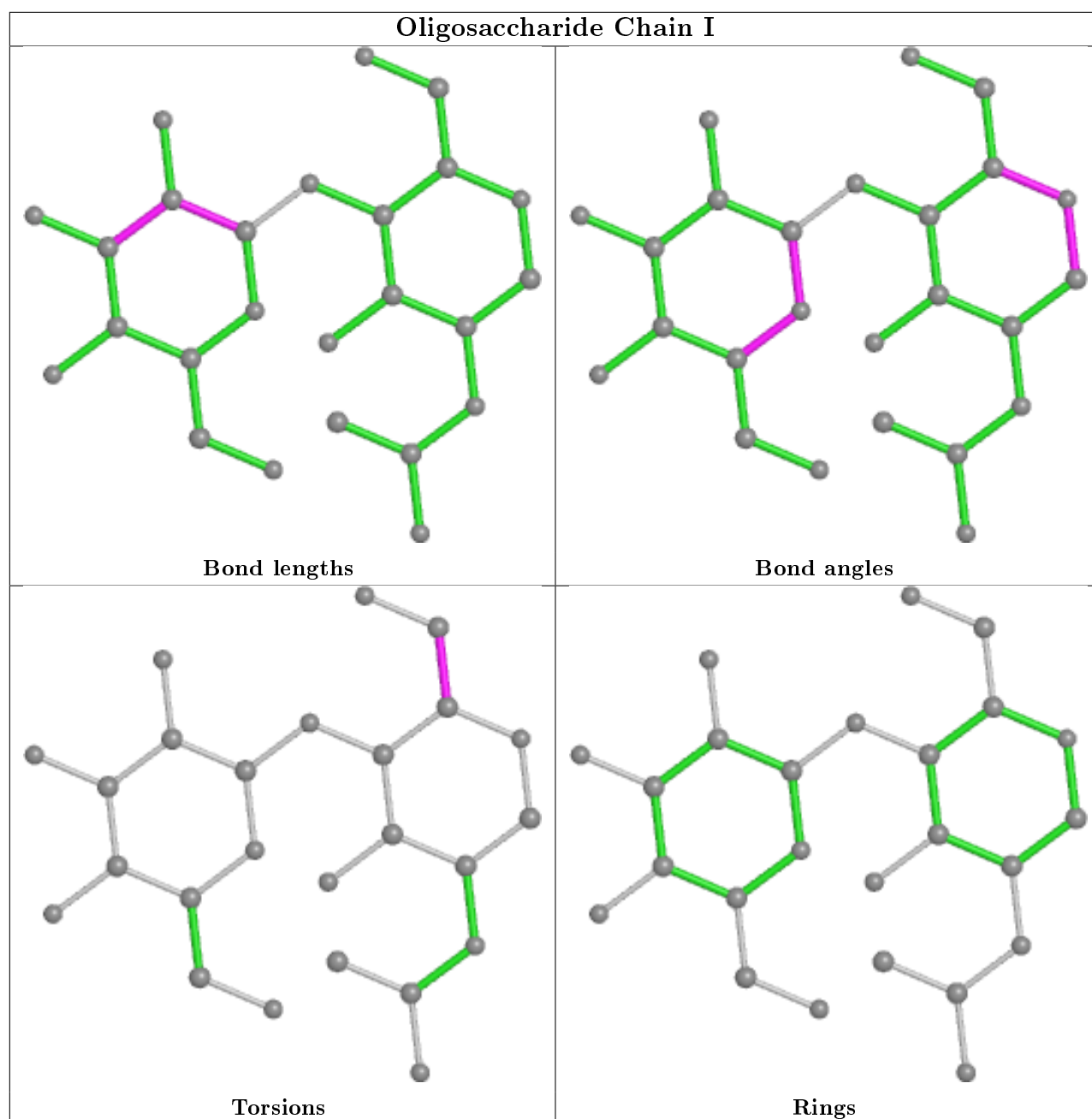












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	904	1	14,14,15	1.69	2 (14%)	17,19,21	0.89	1 (5%)
6	NAG	A	904	1	14,14,15	0.31	0	17,19,21	0.62	0
6	NAG	A	916	1	14,14,15	0.56	0	17,19,21	0.59	0
6	NAG	A	911	1	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	B	900	1	14,14,15	1.11	2 (14%)	17,19,21	2.13	4 (23%)
6	NAG	A	900	1	14,14,15	0.25	0	17,19,21	1.31	2 (11%)
6	NAG	B	911	1	14,14,15	0.72	0	17,19,21	0.75	1 (5%)
6	NAG	A	913	1	14,14,15	0.64	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	B	915	1	14,14,15	0.62	0	17,19,21	0.71	1 (5%)
6	NAG	B	912	1	14,14,15	0.96	2 (14%)	17,19,21	0.96	1 (5%)
6	NAG	A	903	1	14,14,15	0.67	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	A	917	1	14,14,15	0.85	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	A	910	1	14,14,15	0.84	1 (7%)	17,19,21	0.54	0
6	NAG	B	910	1	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
6	NAG	A	909	1	14,14,15	0.46	0	17,19,21	1.14	1 (5%)
6	NAG	A	914	1	14,14,15	0.63	1 (7%)	17,19,21	0.50	0
6	NAG	B	914	1	14,14,15	0.83	1 (7%)	17,19,21	0.53	0
6	NAG	A	915	1	14,14,15	0.64	0	17,19,21	0.59	0
6	NAG	B	913	1	14,14,15	0.34	0	17,19,21	0.52	0
6	NAG	A	912	1	14,14,15	0.43	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	904	1	-	2/6/23/26	0/1/1/1
6	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	NAG	A	916	1	-	2/6/23/26	0/1/1/1
6	NAG	A	911	1	-	2/6/23/26	0/1/1/1
6	NAG	B	900	1	-	5/6/23/26	0/1/1/1
6	NAG	A	900	1	-	1/6/23/26	0/1/1/1
6	NAG	B	911	1	-	1/6/23/26	0/1/1/1
6	NAG	A	913	1	-	3/6/23/26	0/1/1/1
6	NAG	B	915	1	-	1/6/23/26	0/1/1/1
6	NAG	B	912	1	-	1/6/23/26	0/1/1/1
6	NAG	A	903	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	917	1	-	1/6/23/26	0/1/1/1
6	NAG	A	910	1	-	3/6/23/26	0/1/1/1
6	NAG	B	910	1	-	2/6/23/26	0/1/1/1
6	NAG	A	909	1	-	3/6/23/26	0/1/1/1
6	NAG	A	914	1	-	2/6/23/26	0/1/1/1
6	NAG	B	914	1	-	2/6/23/26	0/1/1/1
6	NAG	A	915	1	-	0/6/23/26	0/1/1/1
6	NAG	B	913	1	-	2/6/23/26	0/1/1/1
6	NAG	A	912	1	-	1/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	904	NAG	O5-C1	5.01	1.51	1.43
6	B	904	NAG	C1-C2	3.69	1.57	1.52
6	B	900	NAG	C1-C2	-3.08	1.47	1.52
6	A	917	NAG	O5-C1	2.89	1.48	1.43
6	B	912	NAG	O5-C1	2.82	1.48	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	900	NAG	C2-N2-C7	6.83	132.63	122.90
6	A	909	NAG	C2-N2-C7	4.18	128.86	122.90
6	B	910	NAG	C1-O5-C5	3.81	117.35	112.19
6	A	900	NAG	C1-O5-C5	3.59	117.06	112.19
6	A	913	NAG	C1-O5-C5	3.29	116.64	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	900	NAG	C3-C2-N2-C7
6	A	900	NAG	C3-C2-N2-C7
6	A	909	NAG	C3-C2-N2-C7
6	B	914	NAG	O5-C5-C6-O6
6	B	913	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	916	NAG	1	0
6	B	900	NAG	1	0
6	A	909	NAG	2	0
6	B	914	NAG	1	0
6	A	915	NAG	2	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	833/863 (96%)	0.09	20 (2%) 59 42	51, 92, 143, 208	0
1	B	833/863 (96%)	0.23	42 (5%) 28 18	57, 106, 152, 186	0
2	C	20/21 (95%)	0.94	5 (25%) 0 0	65, 97, 165, 179	0
2	D	20/21 (95%)	1.23	4 (20%) 1 0	89, 127, 153, 164	0
All	All	1706/1768 (96%)	0.18	71 (4%) 36 23	51, 99, 150, 208	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	LEU	6.4
1	B	452	ILE	4.7
1	B	380	LEU	4.6
1	B	524	PHE	4.6
2	D	63	ASP	4.0

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
2	TYS	D	64	16/17	0.94	0.27	101,116,150,171	0
2	TYS	C	64	16/17	0.94	0.29	100,111,128,141	0

6.3 Carbohydrates ⓘ

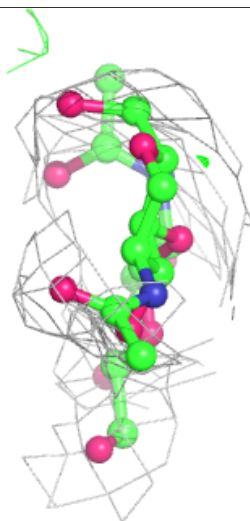
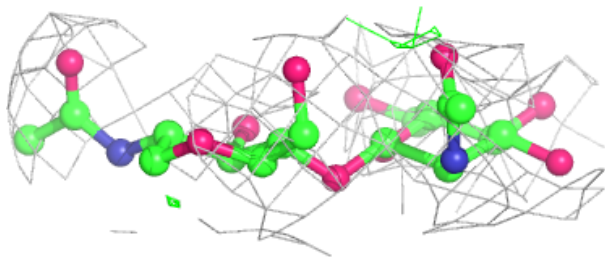
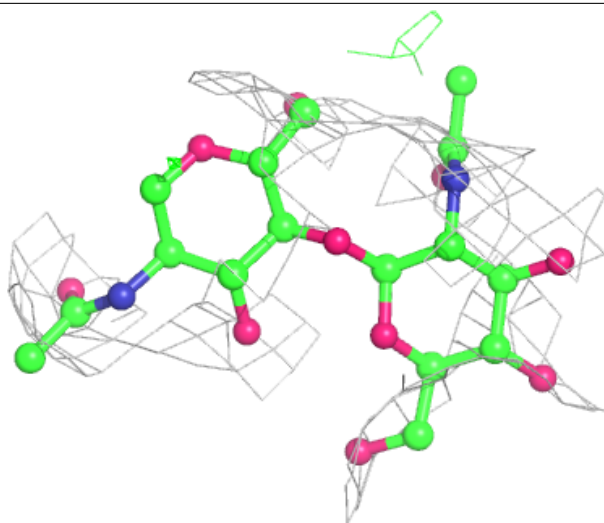
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.72	0.20	172,181,190,190	0
3	NAG	G	2	14/15	0.77	0.37	140,161,169,170	0
4	NAG	H	2	14/15	0.77	0.33	156,170,175,175	0
4	BMA	J	3	11/12	0.79	0.17	164,169,177,177	0
4	BMA	H	3	11/12	0.79	0.28	144,153,165,166	0
3	NAG	K	2	14/15	0.80	0.30	142,151,186,187	0
3	NAG	F	2	14/15	0.83	0.21	116,129,133,138	0
5	BMA	I	2	11/12	0.84	0.18	129,141,148,148	0
3	NAG	E	1	14/15	0.86	0.13	137,152,168,175	0
4	NAG	J	2	14/15	0.86	0.26	110,158,167,168	0
4	NAG	H	1	14/15	0.87	0.14	116,134,146,163	0
4	NAG	J	1	14/15	0.89	0.30	75,106,122,137	0
3	NAG	K	1	14/15	0.91	0.20	86,115,126,141	0
5	NAG	I	1	14/15	0.92	0.21	60,86,104,120	0
3	NAG	G	1	14/15	0.97	0.17	38,75,92,108	0
3	NAG	F	1	14/15	0.97	0.18	72,82,92,98	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.

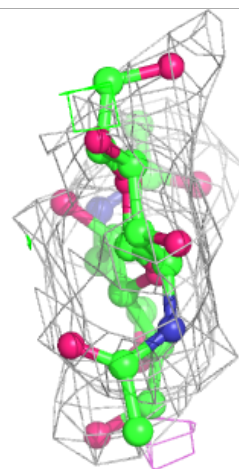
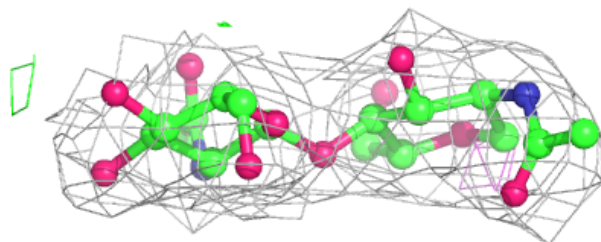
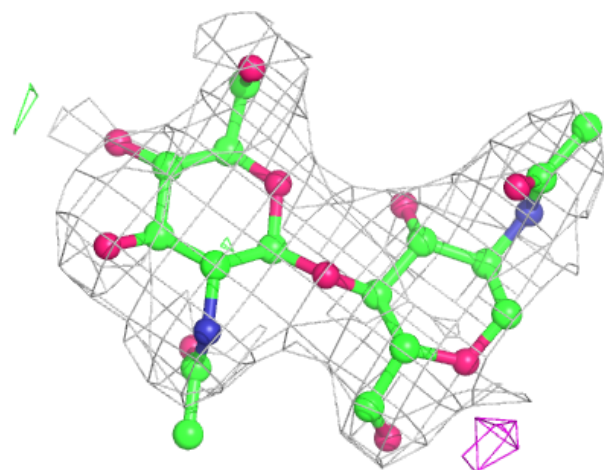
Electron density around Chain E:

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



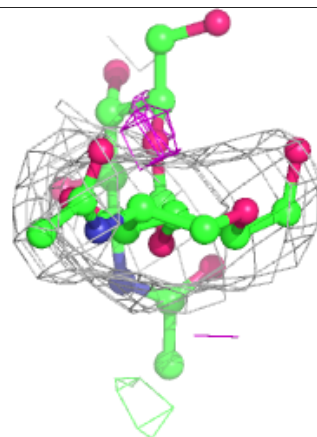
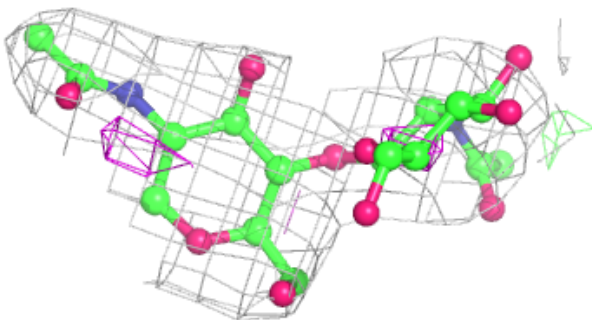
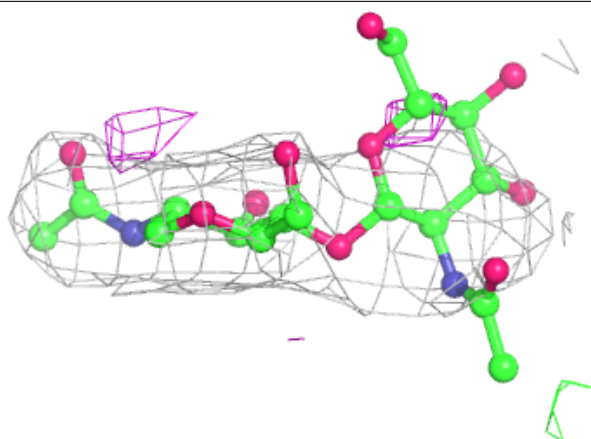
Electron density around Chain F:

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



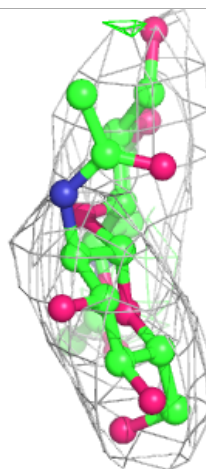
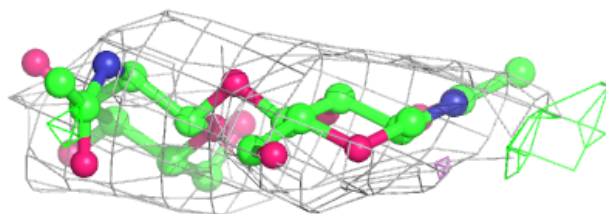
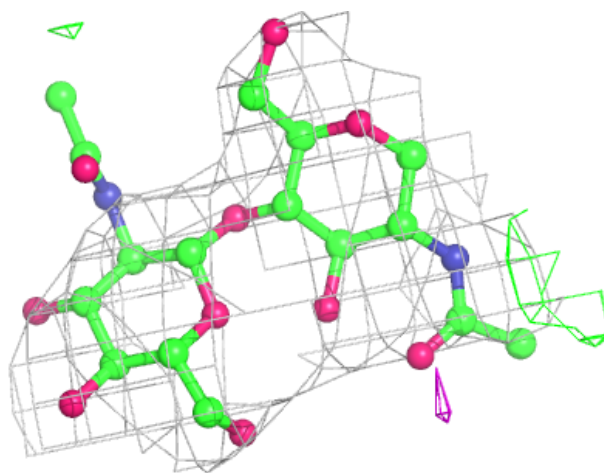
Electron density around Chain G:

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



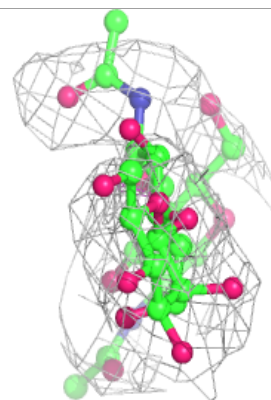
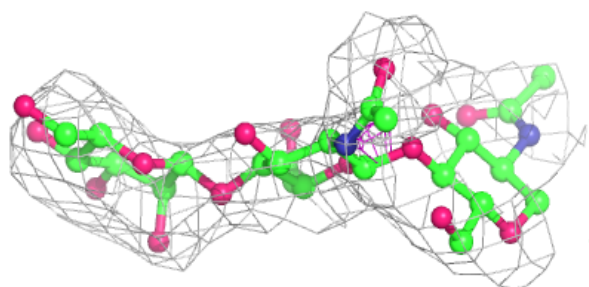
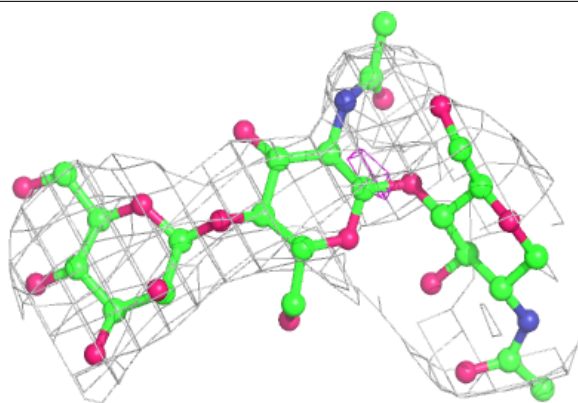
Electron density around Chain K:

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

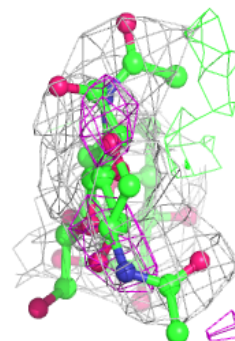
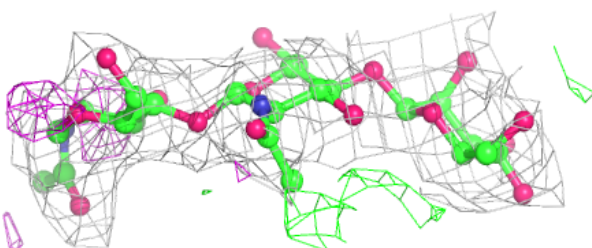
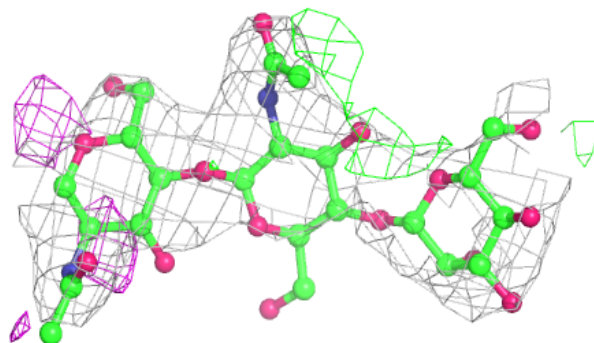


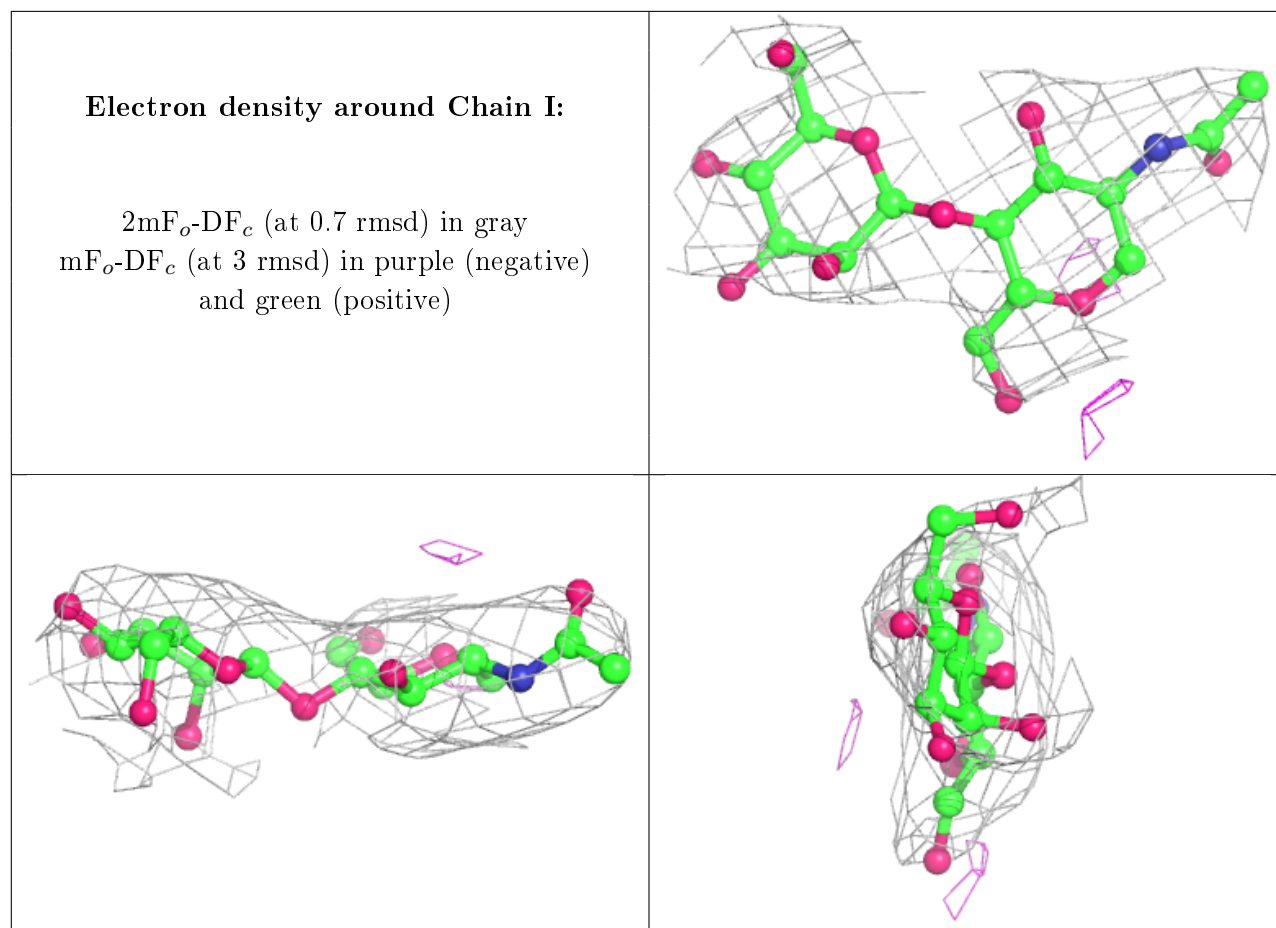
Electron density around Chain H:

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

**Electron density around Chain J:**

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





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
6	NAG	B	915	14/15	0.64	0.37	157,165,177,181	0
6	NAG	A	904	14/15	0.68	0.21	116,136,148,152	0
6	NAG	B	904	14/15	0.74	0.18	122,140,146,146	0
6	NAG	A	903	14/15	0.78	0.35	120,140,149,152	0
6	NAG	A	917	14/15	0.81	0.15	114,133,140,142	0
6	NAG	B	911	14/15	0.84	0.23	104,119,128,135	0
6	NAG	A	916	14/15	0.85	0.18	129,140,149,153	0
6	NAG	A	913	14/15	0.87	0.15	98,122,134,134	0
6	NAG	A	909	14/15	0.87	0.19	109,138,154,160	0
6	NAG	B	913	14/15	0.88	0.20	107,126,135,137	0
6	NAG	A	910	14/15	0.89	0.23	86,110,147,153	0
6	NAG	B	910	14/15	0.89	0.20	90,120,126,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	912	14/15	0.89	0.28	78,114,125,127	0
6	NAG	B	914	14/15	0.92	0.23	86,122,132,134	0
6	NAG	B	912	14/15	0.92	0.12	107,120,129,132	0
6	NAG	A	911	14/15	0.92	0.22	92,113,130,130	0
6	NAG	A	900	14/15	0.93	0.15	65,86,103,104	0
6	NAG	B	900	14/15	0.93	0.15	80,91,116,118	0
6	NAG	A	914	14/15	0.93	0.11	95,126,136,138	0
6	NAG	A	915	14/15	0.94	0.15	77,104,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.