



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:33 PM BST

PDB ID : 3DKH
Title : L559A mutant of Melanocarpus albomyces laccase
Authors : Hakulinen, N.; Rouvinen, J.
Deposited on : 2008-06-25
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

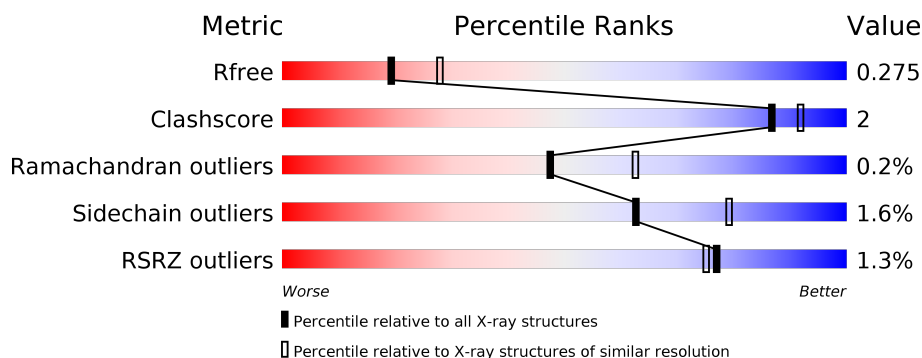
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	559	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	559	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	C	4	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
3	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>
3	G	2	<div> <div></div> <div>100%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	2	-	-	-	X
4	BMA	I	3	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9856 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.

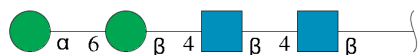
- Molecule 1 is a protein called Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4357	2756	758	828	15			
1	B	558	Total	C	N	O	S	0	0	0
			4357	2756	758	828	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	LEU	engineered mutation	UNP Q70KY3
B	559	ALA	LEU	engineered mutation	UNP Q70KY3

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



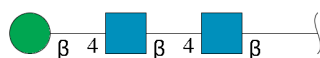
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	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	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cu	0	0
			4	4		
6	A	4	Total	Cu	0	0
			4	4		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

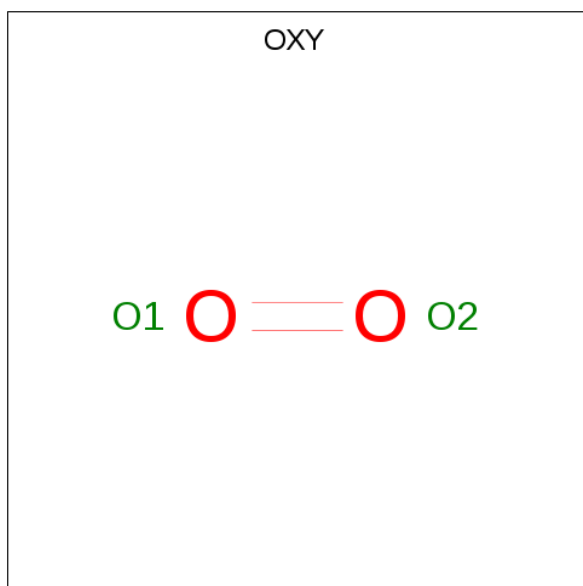
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



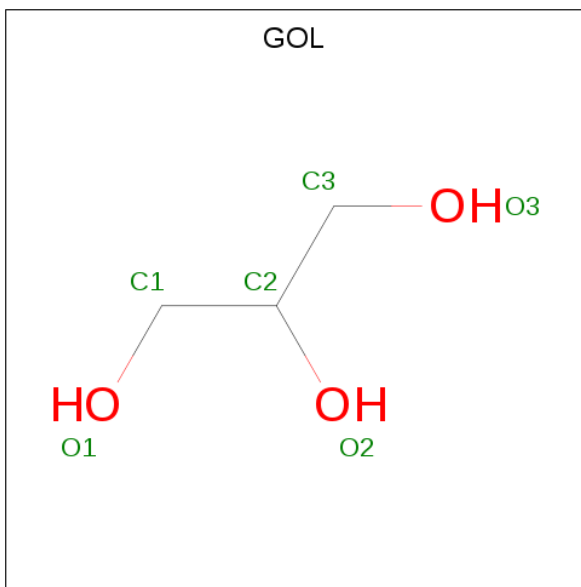
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 2 2	0	0
9	B	1	Total O 2 2	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

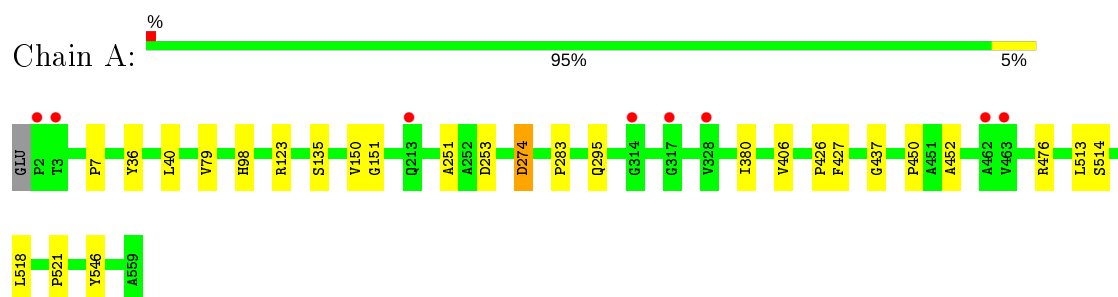
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	368	Total O 368 368	0	0
11	B	338	Total O 338 338	0	0

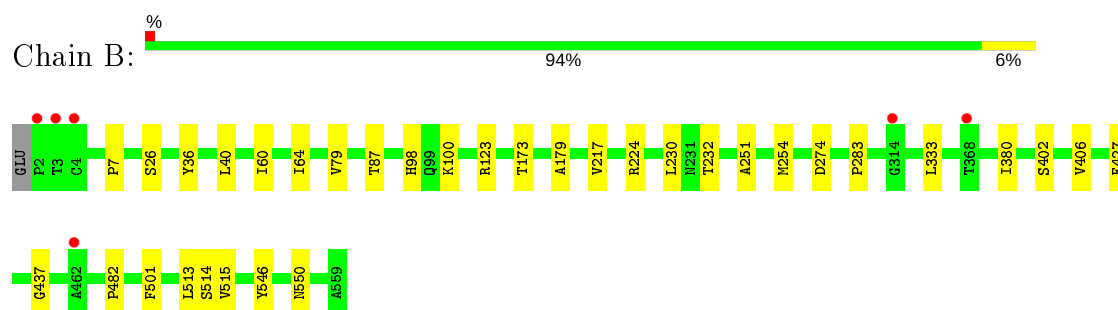
3 Residue-property plots

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.

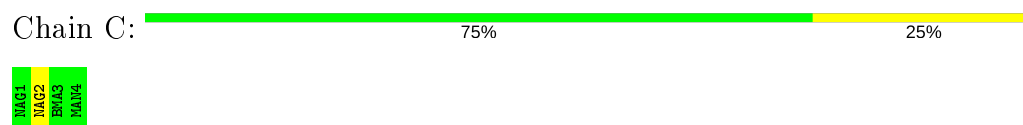
- Molecule 1: Laccase-1



- Molecule 1: Laccase-1



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



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

Chain F:  100%

NA01
NA02

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

Chain G:  100%

NA01
NA02

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

Chain K:  50% 50%

NA01
NA02

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

Chain E:  67% 33%

NA01
NA02
B/A3

- 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:  67% 33%

NA01
NA02
B/A3

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

Chain I:  100%

NA01
NA02
B/A3

- 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%

NA01
NA02
B/A3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.51Å 62.02Å 125.67Å 90.00° 99.92° 90.00°	Depositor
Resolution (Å)	19.82 – 2.40 19.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.82-2.40) 97.7 (19.82-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.282 0.219 , 0.275	Depositor DCC
R_{free} test set	2532 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9856	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: GOL, BMA, NAG, CL, OXY, SO4, CU, MAN

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	0.65	0/4494	0.76	1/6174 (0.0%)
1	B	0.65	0/4494	0.76	0/6174
All	All	0.65	0/8988	0.76	1/12348 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	546	TYR	Sidechain
1	B	546	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4357	0	4097	14	0
1	B	4357	0	4095	14	0
2	C	50	0	43	1	0
3	D	28	0	25	3	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	K	28	0	25	1	0
4	E	39	0	34	1	0
4	H	39	0	34	1	0
4	I	39	0	34	0	0
4	J	39	0	34	1	0
5	A	28	0	26	0	0
5	B	56	0	52	4	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	B	6	0	8	3	0
11	A	368	0	0	4	0
11	B	338	0	0	5	0
All	All	9856	0	8557	37	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 2.

All (37) 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)
11:A:1206:HOH:O	4:E:2:NAG:H3	1.89	0.71
5:B:770:NAG:H81	11:B:912:HOH:O	1.92	0.69
1:B:217:VAL:HG13	5:B:760:NAG:H81	1.77	0.66
1:A:295:GLN:HE21	1:A:452:ALA:H	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:700:NAG:H5	11:B:992:HOH:O	1.97	0.65
1:B:406:VAL:HG13	3:K:1:NAG:H81	1.80	0.62
1:B:380:ILE:HG21	1:B:514:SER:HB3	1.81	0.61
3:D:1:NAG:O6	3:D:2:NAG:H82	2.02	0.59
3:D:1:NAG:C6	3:D:2:NAG:H82	2.34	0.58
1:B:251:ALA:HB3	1:B:274:ASP:HB2	1.87	0.57
11:A:1068:HOH:O	2:C:2:NAG:H4	2.08	0.53
1:A:427:PHE:CE2	10:B:810:GOL:H2	2.44	0.52
1:A:253:ASP:OD2	1:A:476:ARG:HB2	2.10	0.51
1:A:427:PHE:CZ	10:B:810:GOL:H2	2.45	0.51
1:A:380:ILE:HG21	1:A:514:SER:HB3	1.93	0.51
1:B:87:THR:HB	1:B:550:ASN:HD21	1.78	0.49
1:B:36:TYR:HB2	1:B:79:VAL:HG22	1.95	0.48
5:B:770:NAG:H5	11:B:1050:HOH:O	2.13	0.48
11:B:1010:HOH:O	4:J:2:NAG:H3	2.14	0.48
1:B:173:THR:HB	1:B:232:THR:OG1	2.14	0.48
1:A:251:ALA:HB3	1:A:274:ASP:HB2	1.96	0.47
1:B:501:PHE:HB3	1:B:515:VAL:HG23	1.95	0.47
1:A:150:VAL:HG12	1:A:151:GLY:N	2.28	0.47
1:A:36:TYR:HB2	1:A:79:VAL:HG22	1.97	0.46
1:A:426:PRO:HD2	11:A:1160:HOH:O	2.14	0.46
1:A:518:LEU:HG	1:A:521:PRO:HG3	1.97	0.46
3:D:1:NAG:H62	3:D:2:NAG:H82	1.99	0.43
1:B:427:PHE:CE2	10:B:810:GOL:H32	2.53	0.43
1:B:230:LEU:HB3	11:B:1042:HOH:O	2.18	0.43
1:B:179:ALA:CB	4:H:2:NAG:H81	2.50	0.42
1:B:333:LEU:HD21	1:B:482:PRO:HB3	2.01	0.42
1:A:150:VAL:HG12	1:A:151:GLY:H	1.85	0.41
1:A:98:HIS:O	1:A:437:GLY:HA2	2.20	0.41
1:B:40:LEU:HD22	1:B:60:ILE:HG12	2.03	0.41
1:A:521:PRO:HD2	11:A:930:HOH:O	2.20	0.41
1:B:98:HIS:O	1:B:437:GLY:HA2	2.20	0.41
1:A:406:VAL:HG13	3:F:1:NAG:H81	2.03	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	556/559 (100%)	534 (96%)	21 (4%)	1 (0%)	47	62
1	B	556/559 (100%)	535 (96%)	20 (4%)	1 (0%)	47	62
All	All	1112/1118 (100%)	1069 (96%)	41 (4%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	PRO
1	B	283	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	476/477 (100%)	470 (99%)	6 (1%)	69	84
1	B	476/477 (100%)	467 (98%)	9 (2%)	57	75
All	All	952/954 (100%)	937 (98%)	15 (2%)	62	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	123	ARG
1	A	135	SER
1	A	274	ASP

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Mol	Chain	Res	Type
1	A	450	PRO
1	A	513	LEU
1	B	7	PRO
1	B	26	SER
1	B	64	ILE
1	B	100	LYS
1	B	123	ARG
1	B	224	ARG
1	B	254	MET
1	B	402	SER
1	B	513	LEU

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

Mol	Chain	Res	Type
1	A	99	GLN
1	A	244	ASN
1	A	295	GLN
1	A	550	ASN
1	B	99	GLN
1	B	109	ASN
1	B	189	ASN
1	B	311	HIS
1	B	550	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 ⓘ

24 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	1,2	14,14,15	0.45	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.57	0
2	BMA	C	3	2	11,11,12	0.60	0	15,15,17	0.43	0
2	MAN	C	4	2	11,11,12	0.59	0	15,15,17	0.63	0
3	NAG	D	1	1,3	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
3	NAG	D	2	3	14,14,15	0.60	0	17,19,21	0.71	0
4	NAG	E	1	1,4	14,14,15	0.54	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	0.68	0
4	BMA	E	3	4	11,11,12	0.56	0	15,15,17	0.32	0
3	NAG	F	1	1,3	14,14,15	0.58	0	17,19,21	0.67	0
3	NAG	F	2	3	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.47	0	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	0.60	0
4	NAG	H	1	1,4	14,14,15	0.42	0	17,19,21	0.77	0
4	NAG	H	2	4	14,14,15	0.42	0	17,19,21	0.58	0
4	BMA	H	3	4	11,11,12	0.60	0	15,15,17	0.25	0
4	NAG	I	1	1,4	14,14,15	0.56	0	17,19,21	0.80	0
4	NAG	I	2	4	14,14,15	0.57	0	17,19,21	0.64	0
4	BMA	I	3	4	11,11,12	0.56	0	15,15,17	0.31	0
4	NAG	J	1	1,4	14,14,15	0.52	0	17,19,21	0.64	0
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	0.68	0
4	BMA	J	3	4	11,11,12	0.55	0	15,15,17	0.28	0
3	NAG	K	1	1,3	14,14,15	0.56	0	17,19,21	0.87	0
3	NAG	K	2	3	14,14,15	0.56	0	17,19,21	0.62	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	-2.31	119.61	122.90
3	D	1	NAG	C2-N2-C7	-2.01	120.03	122.90

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2

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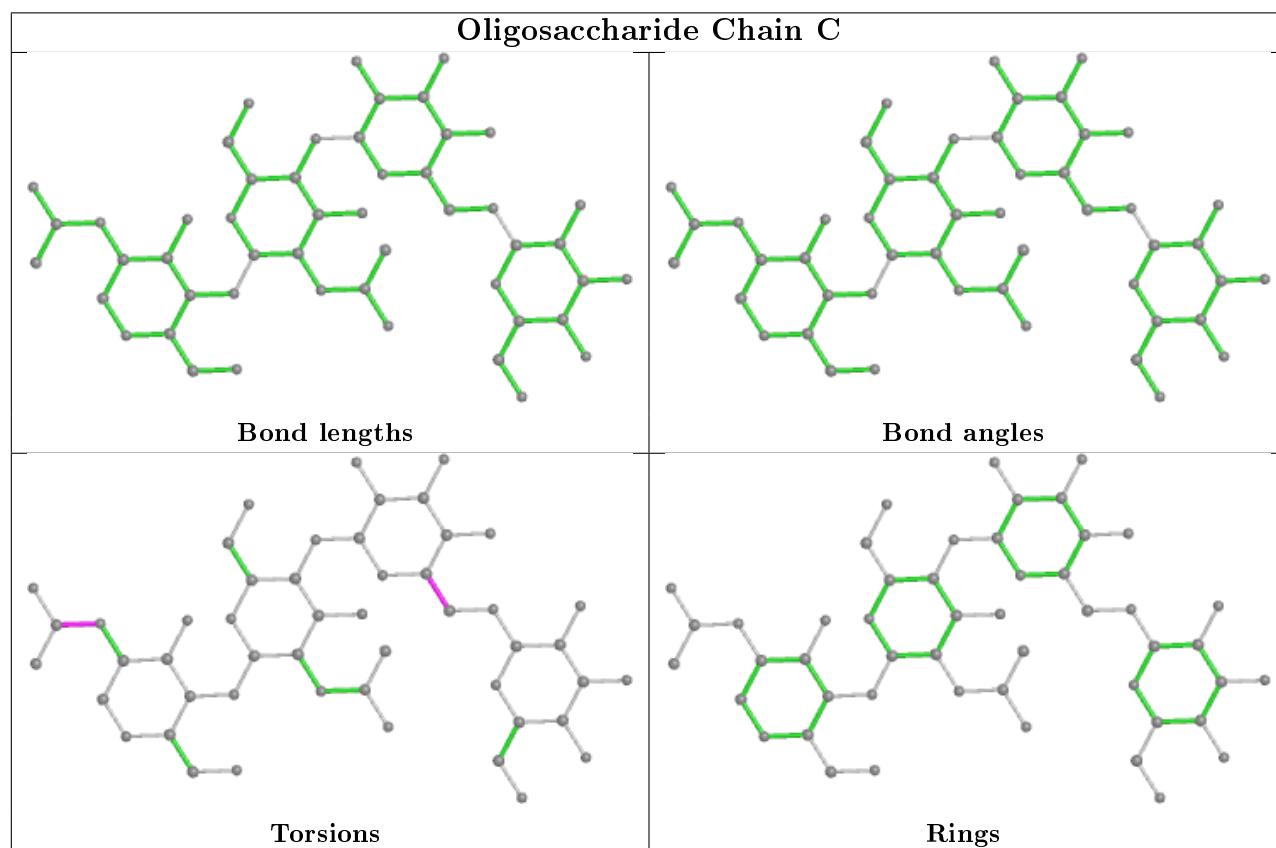
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C8-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
4	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
4	J	3	BMA	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O7-C7-N2-C2
4	J	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O7-C7-N2-C2
2	C	3	BMA	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2

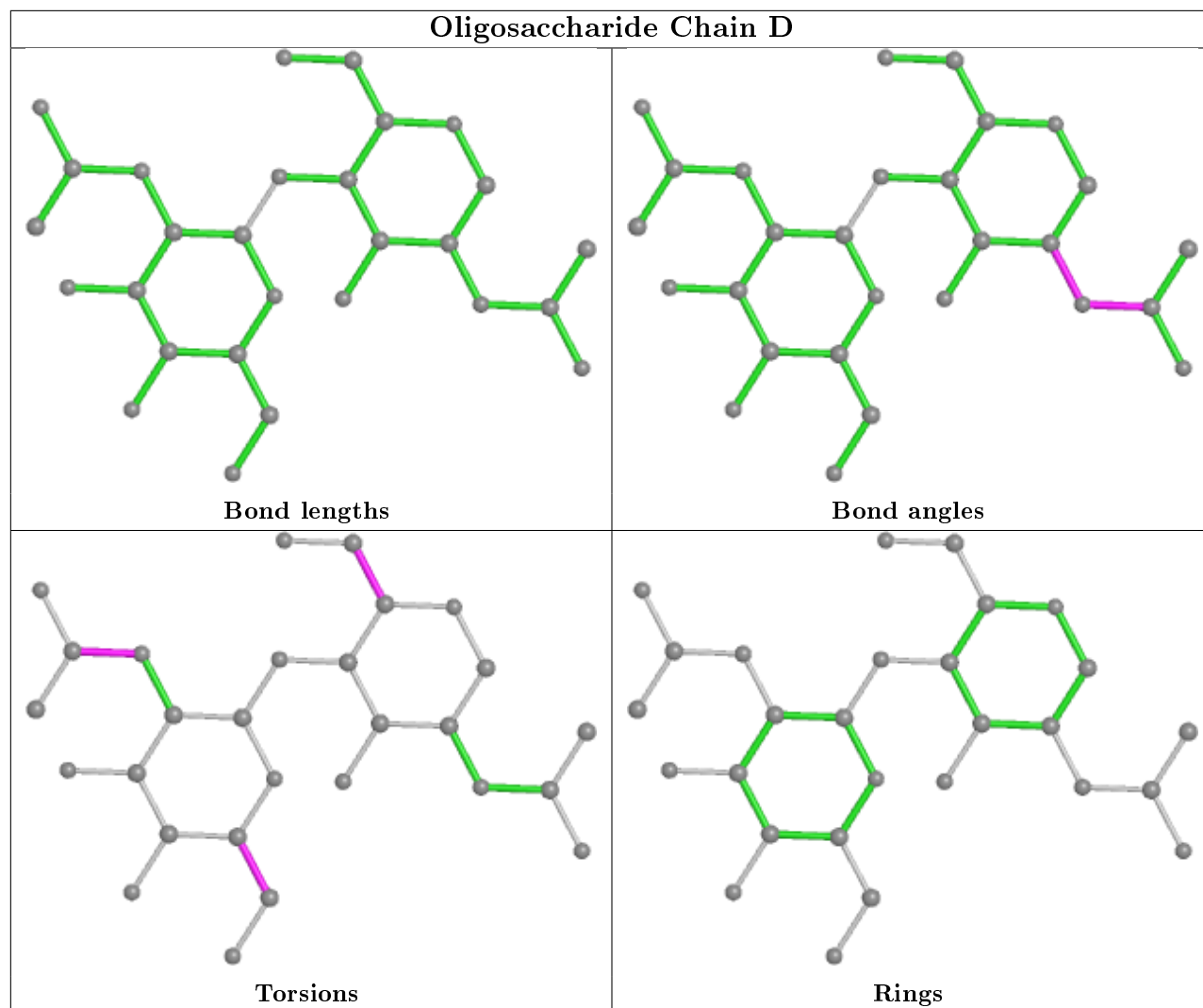
There are no ring outliers.

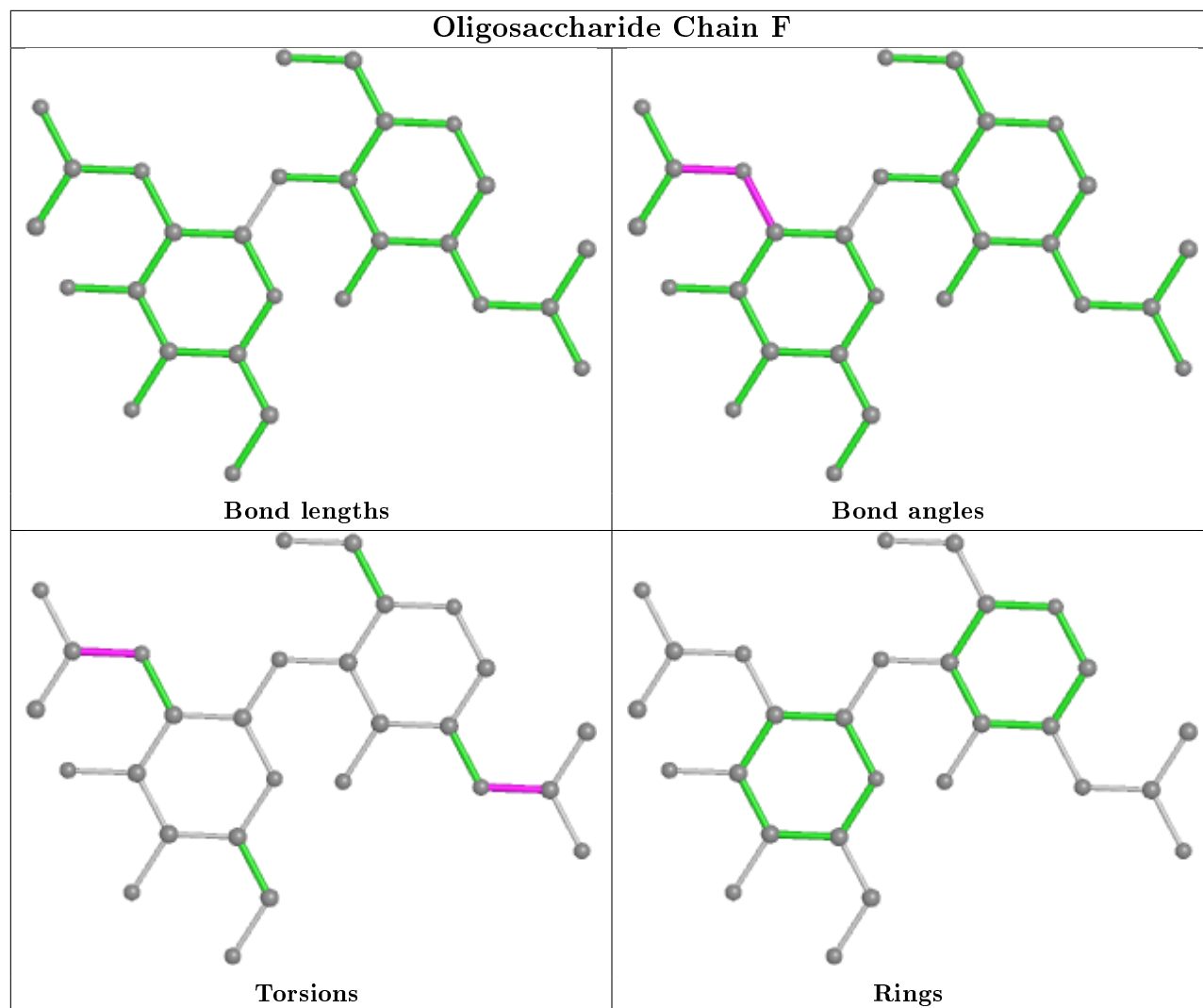
8 monomers are involved in 9 short contacts:

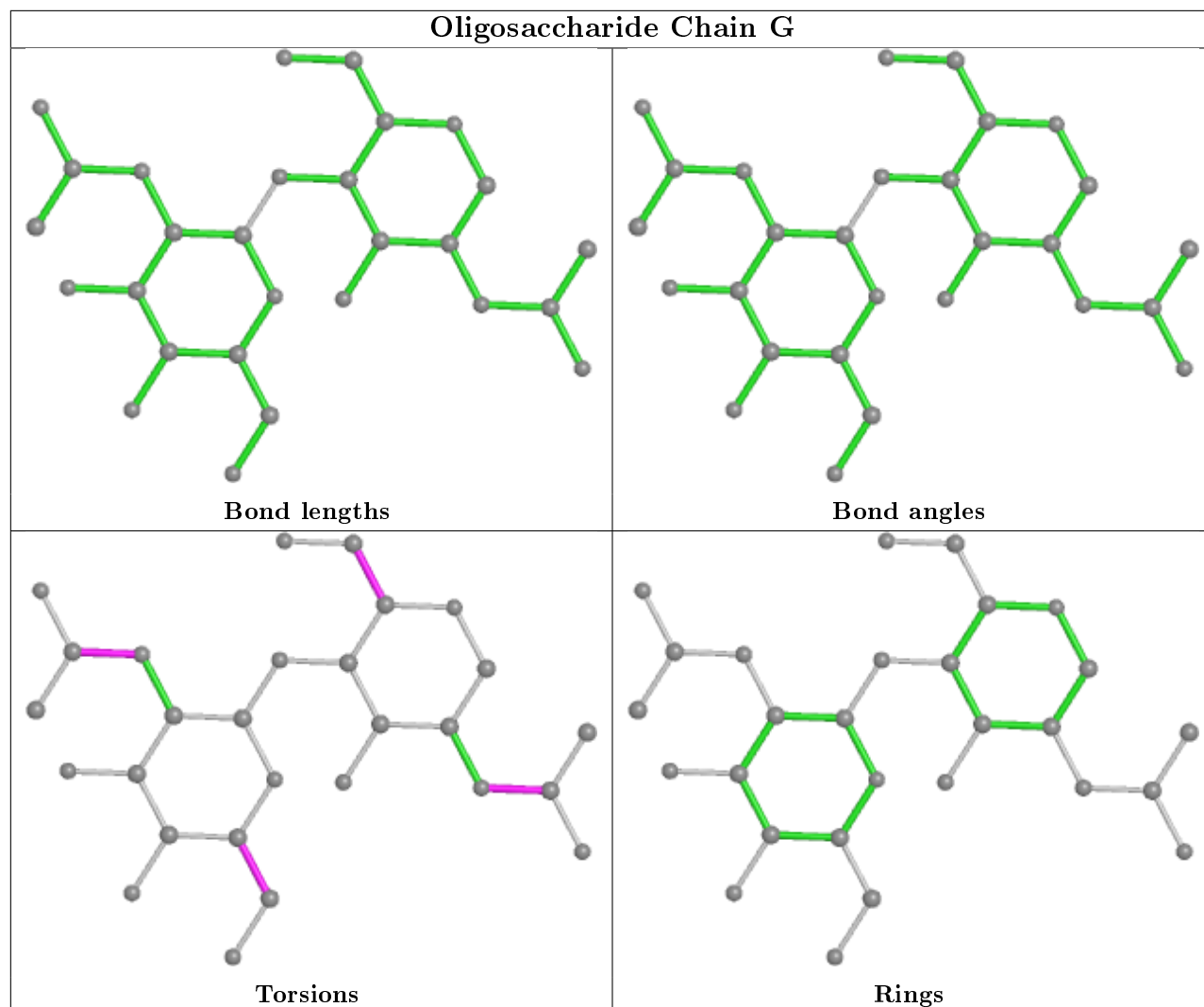
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
3	D	1	NAG	3	0
3	D	2	NAG	3	0
3	K	1	NAG	1	0
4	H	2	NAG	1	0
4	E	2	NAG	1	0
4	J	2	NAG	1	0
3	F	1	NAG	1	0

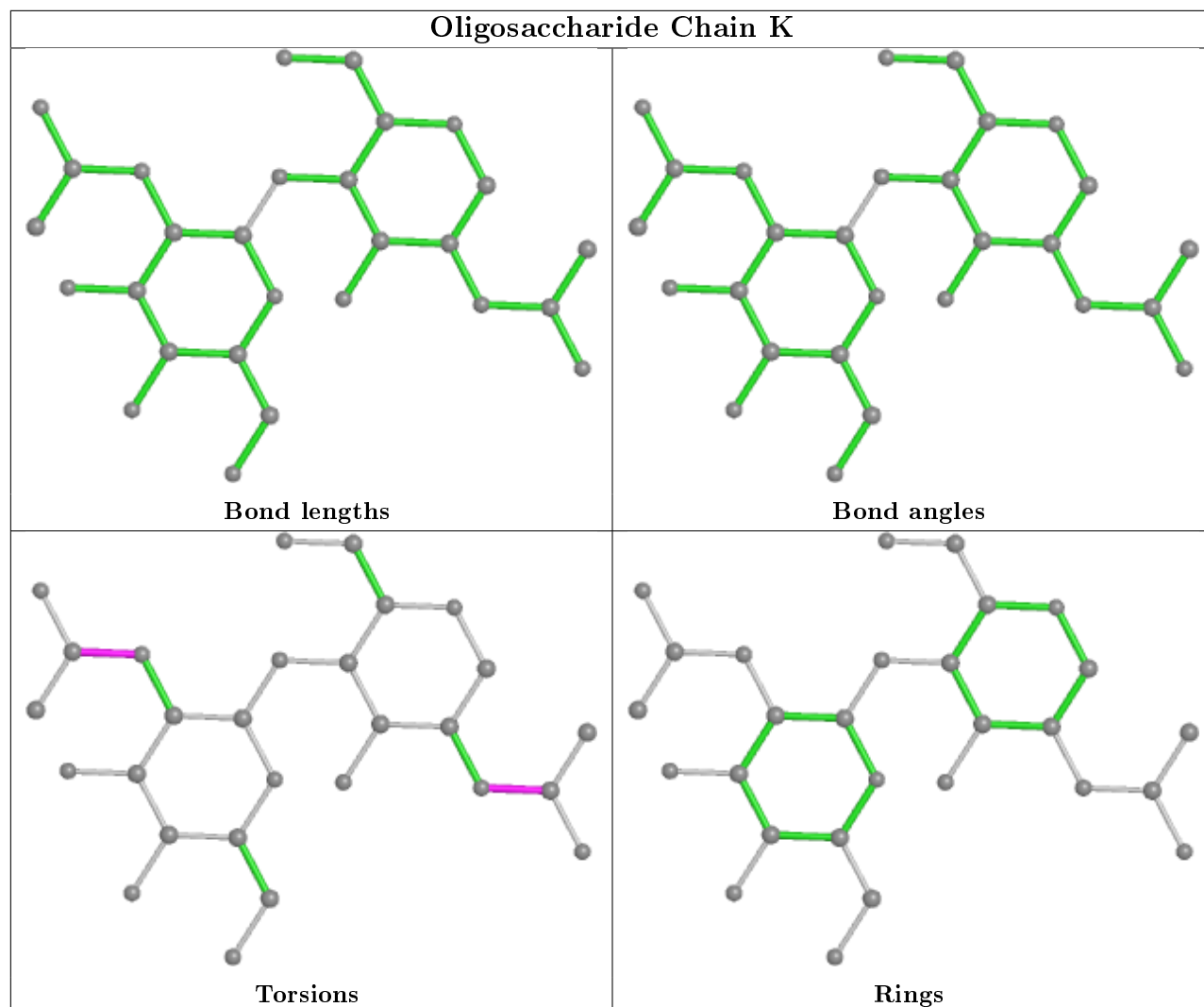
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

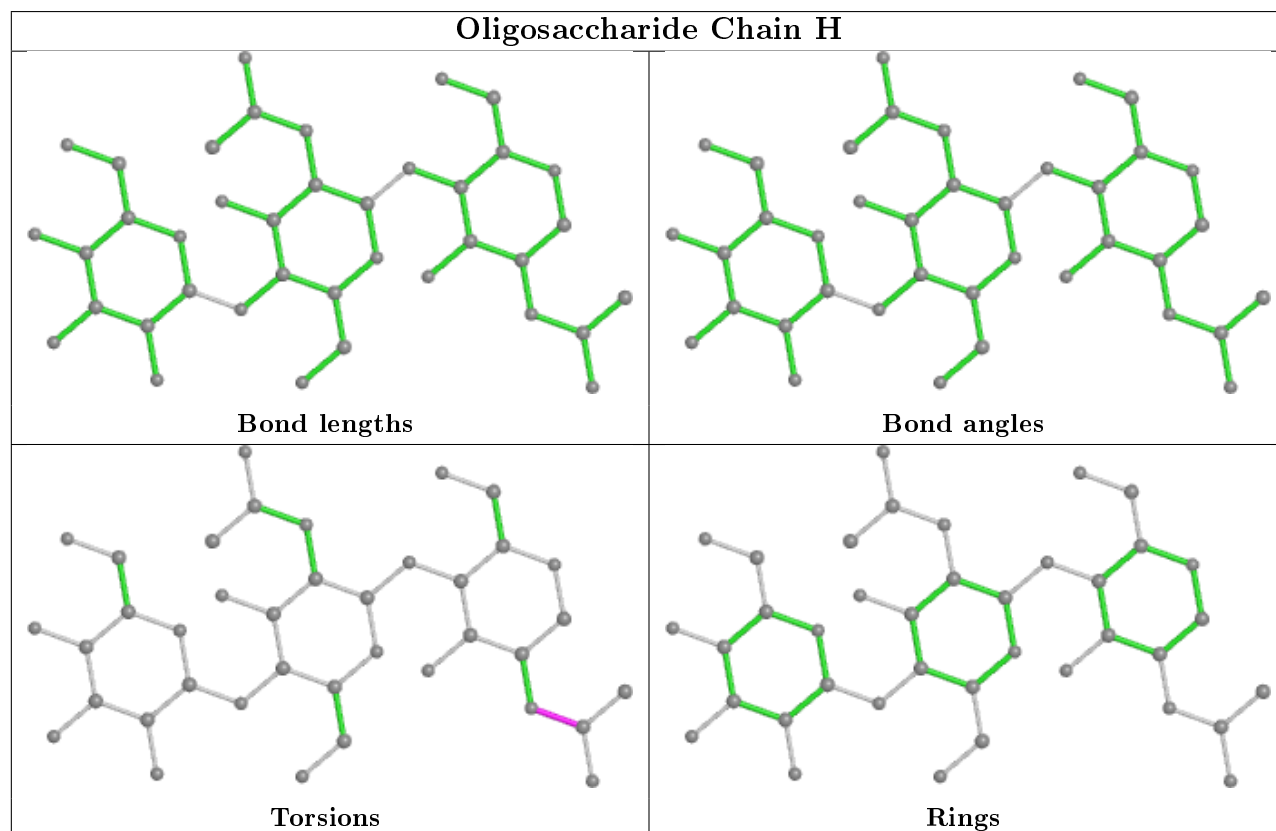
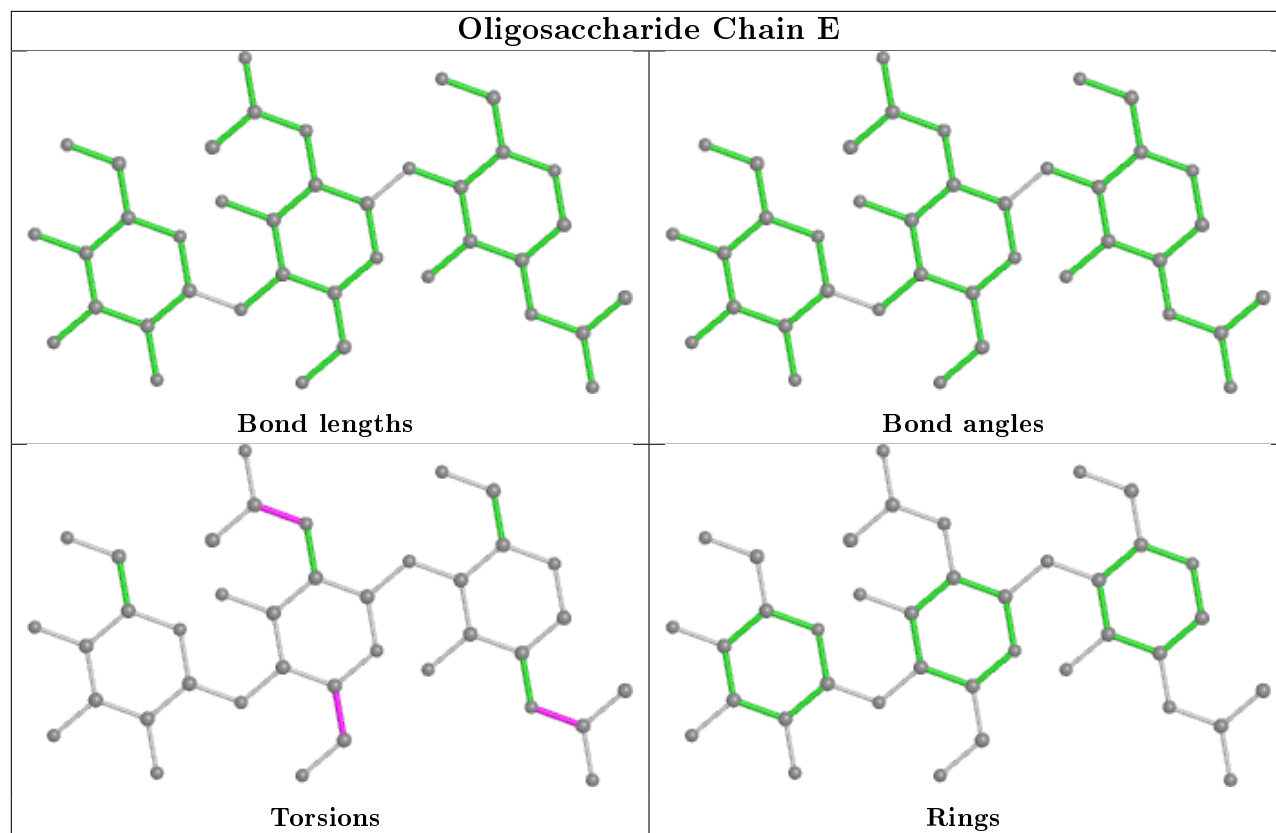


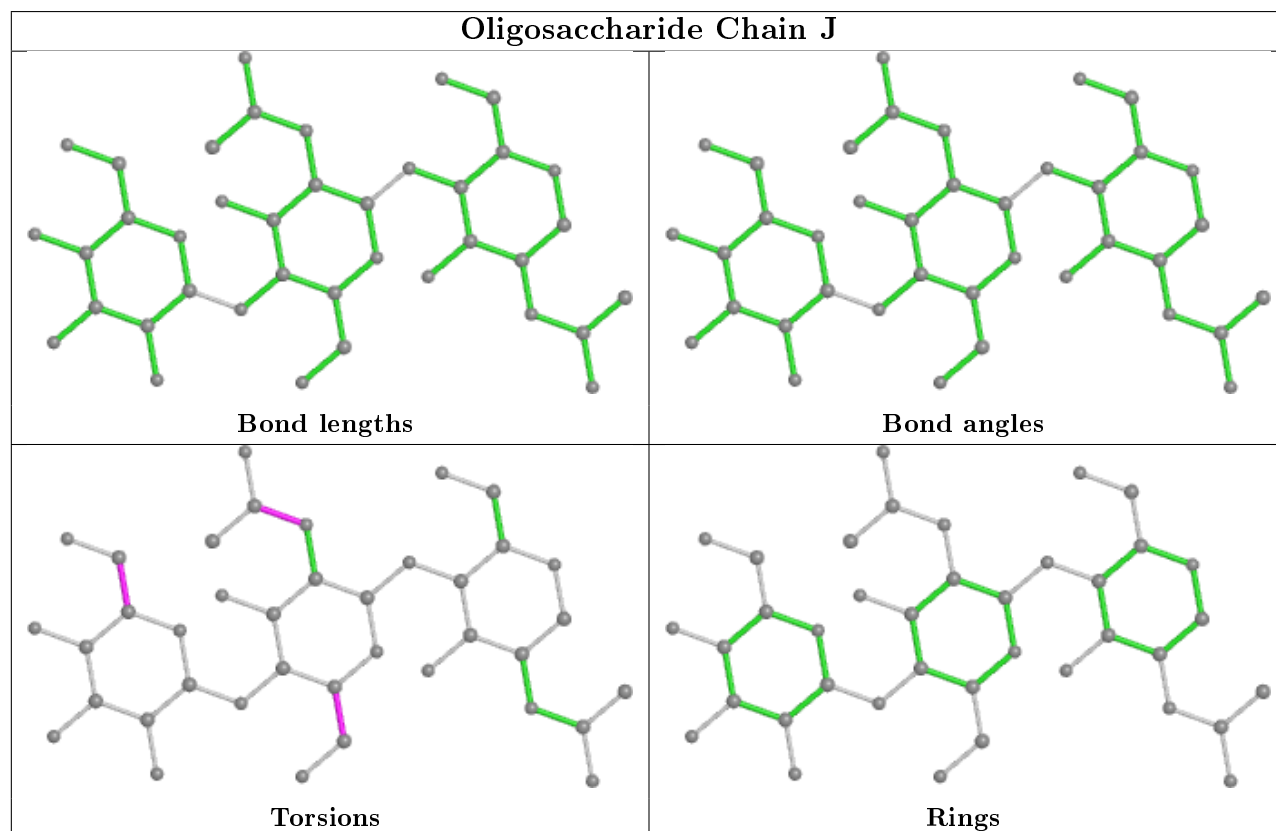
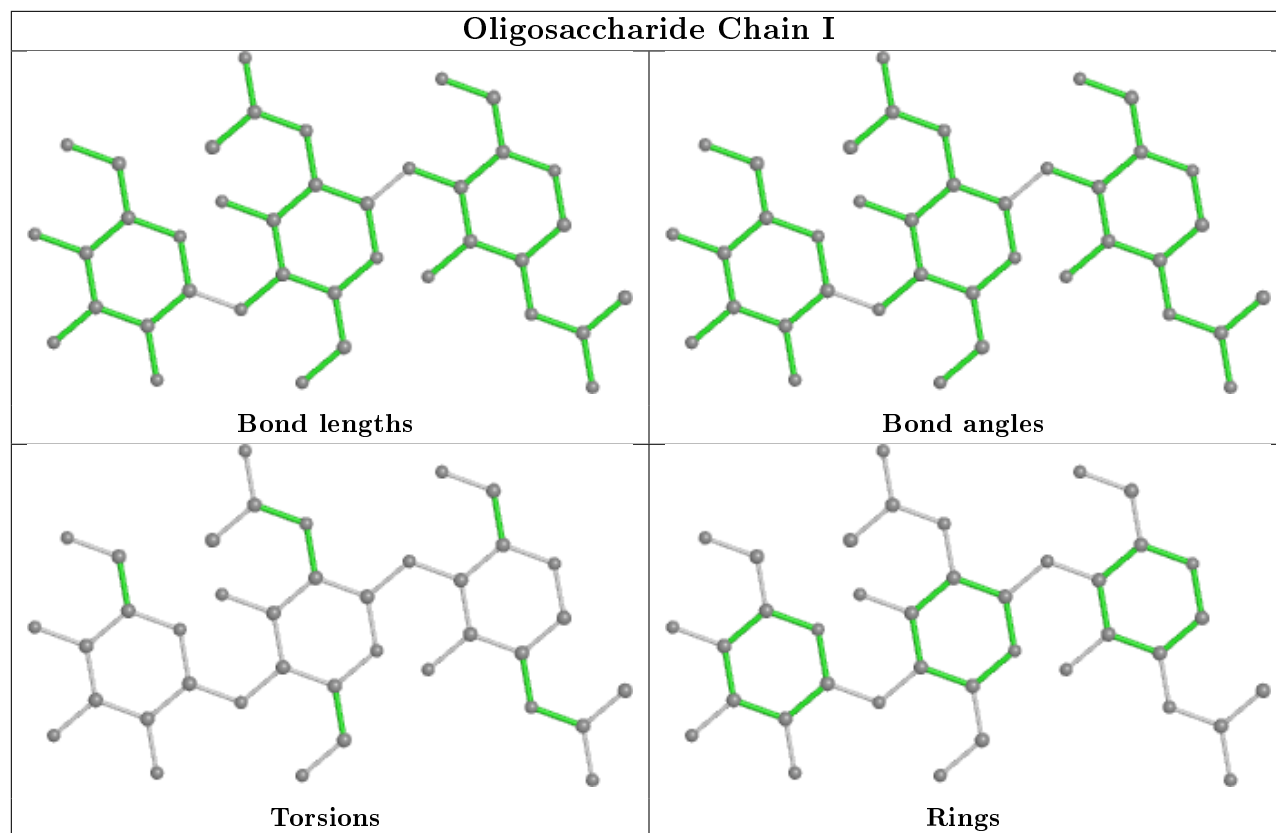












5.6 Ligand geometry

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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
5	NAG	B	700	1	14,14,15	0.45	0	17,19,21	0.66	0
5	NAG	B	750	1	14,14,15	0.62	0	17,19,21	0.57	0
8	SO4	A	802	-	4,4,4	0.22	0	6,6,6	0.09	0
8	SO4	B	801	-	4,4,4	0.27	0	6,6,6	0.04	0
10	GOL	B	810	-	5,5,5	0.25	0	5,5,5	0.33	0
5	NAG	A	700	1	14,14,15	0.51	0	17,19,21	0.71	1 (5%)
5	NAG	B	760	1	14,14,15	0.66	0	17,19,21	0.68	0
5	NAG	A	750	1	14,14,15	0.54	0	17,19,21	0.62	0
9	OXY	A	900	6	1,1,1	0.28	0	-		
5	NAG	B	770	1	14,14,15	0.75	1 (7%)	17,19,21	0.69	0
8	SO4	A	800	-	4,4,4	0.24	0	6,6,6	0.05	0
9	OXY	B	901	6	1,1,1	0.29	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
5	NAG	B	700	1	-	2/6/23/26	0/1/1/1
5	NAG	B	750	1	-	2/6/23/26	0/1/1/1
10	GOL	B	810	-	-	0/4/4/4	-
5	NAG	A	700	1	-	2/6/23/26	0/1/1/1
5	NAG	B	760	1	-	4/6/23/26	0/1/1/1
5	NAG	A	750	1	-	2/6/23/26	0/1/1/1
5	NAG	B	770	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	770	NAG	C1-C2	2.16	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	NAG	C2-N2-C7	-2.16	119.82	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	760	NAG	C8-C7-N2-C2
5	B	760	NAG	O7-C7-N2-C2
5	B	770	NAG	C8-C7-N2-C2
5	B	770	NAG	O7-C7-N2-C2
5	A	750	NAG	C8-C7-N2-C2
5	A	750	NAG	O7-C7-N2-C2
5	B	760	NAG	O5-C5-C6-O6
5	B	760	NAG	C4-C5-C6-O6
5	A	700	NAG	C8-C7-N2-C2
5	B	700	NAG	C8-C7-N2-C2
5	B	700	NAG	O7-C7-N2-C2
5	A	700	NAG	O7-C7-N2-C2
5	B	750	NAG	C8-C7-N2-C2
5	B	750	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	NAG	1	0
10	B	810	GOL	3	0
5	B	760	NAG	1	0
5	B	770	NAG	2	0

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 [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	558/559 (99%)	0.04	8 (1%) 75 73	3, 18, 36, 60	0
1	B	558/559 (99%)	0.07	6 (1%) 80 79	4, 20, 36, 63	0
All	All	1116/1118 (99%)	0.06	14 (1%) 77 75	3, 19, 36, 63	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	GLY	4.7
1	B	462	ALA	3.8
1	A	328	VAL	3.7
1	A	2	PRO	3.6
1	B	3	THR	3.3
1	B	314	GLY	2.8
1	A	462	ALA	2.7
1	B	4	CYS	2.5
1	A	213	GLN	2.5
1	A	463	VAL	2.3
1	B	368	THR	2.2
1	B	2	PRO	2.2
1	A	3	THR	2.1
1	A	317	GLY	2.1

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,

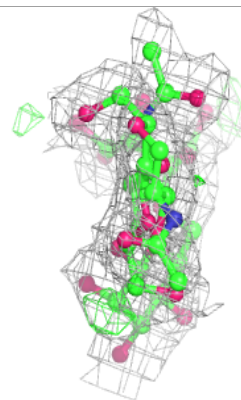
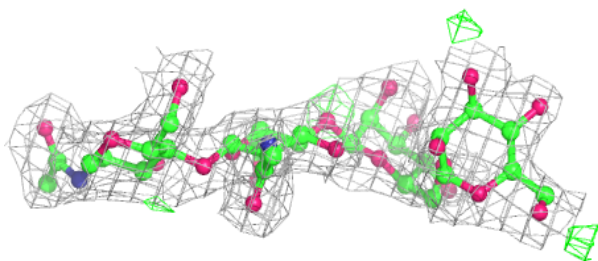
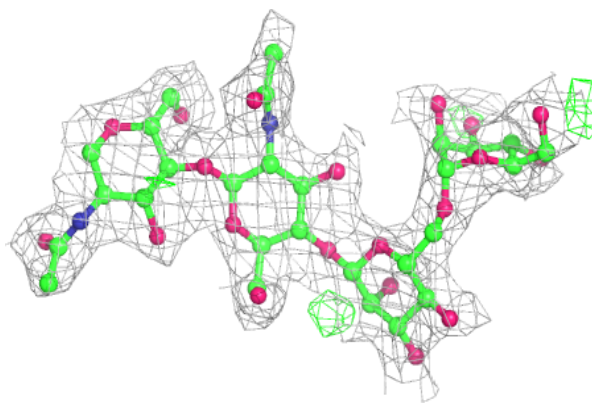
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.73	0.50	60,62,66,68	0
4	BMA	H	3	11/12	0.73	0.27	35,39,40,41	0
4	BMA	I	3	11/12	0.75	0.40	62,65,66,66	0
2	BMA	C	3	11/12	0.76	0.28	38,42,46,48	0
2	MAN	C	4	11/12	0.77	0.25	45,49,49,50	0
3	NAG	G	1	14/15	0.78	0.27	42,47,53,56	0
4	BMA	E	3	11/12	0.78	0.36	46,49,51,53	0
4	NAG	I	1	14/15	0.79	0.25	37,40,44,47	0
4	NAG	I	2	14/15	0.81	0.24	48,53,56,60	0
3	NAG	K	2	14/15	0.83	0.33	49,50,52,52	0
4	BMA	J	3	11/12	0.84	0.36	43,44,46,46	0
4	NAG	J	2	14/15	0.85	0.29	29,33,35,40	0
3	NAG	K	1	14/15	0.88	0.24	36,40,42,46	0
4	NAG	E	2	14/15	0.89	0.20	31,33,37,42	0
3	NAG	F	2	14/15	0.90	0.34	40,42,43,44	0
3	NAG	F	1	14/15	0.90	0.21	29,31,35,39	0
3	NAG	D	2	14/15	0.90	0.25	33,36,38,39	0
4	NAG	J	1	14/15	0.91	0.14	12,18,23,24	0
4	NAG	E	1	14/15	0.91	0.16	23,24,27,30	0
2	NAG	C	2	14/15	0.92	0.17	19,22,27,32	0
3	NAG	D	1	14/15	0.92	0.18	26,29,31,32	0
4	NAG	H	1	14/15	0.93	0.15	17,19,22,24	0
2	NAG	C	1	14/15	0.93	0.13	11,19,21,22	0
4	NAG	H	2	14/15	0.94	0.14	21,27,30,33	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.

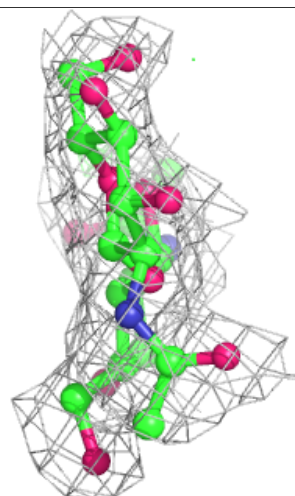
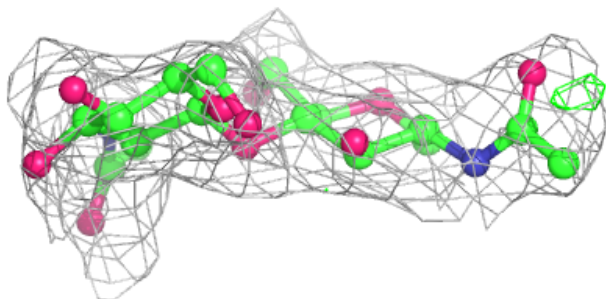
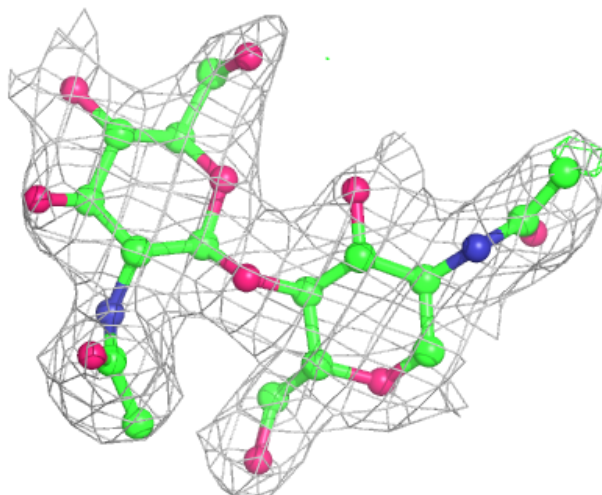
Electron density around Chain C:

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



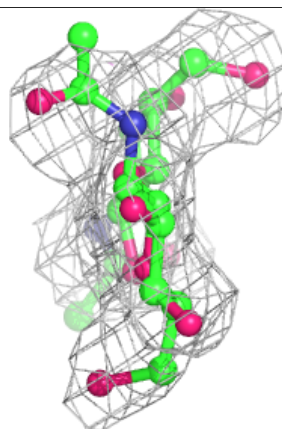
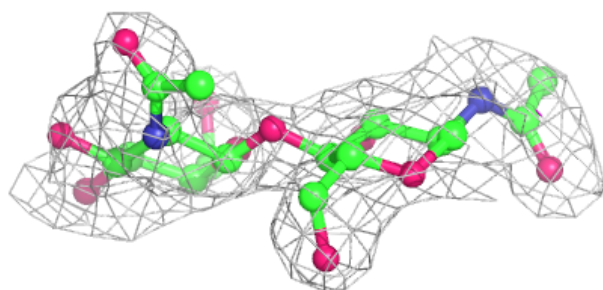
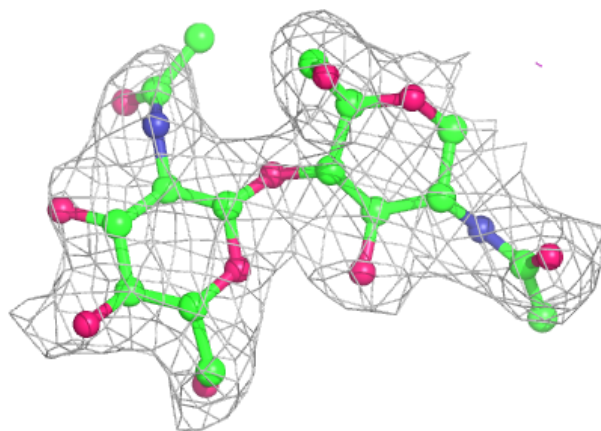
Electron density around Chain D:

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



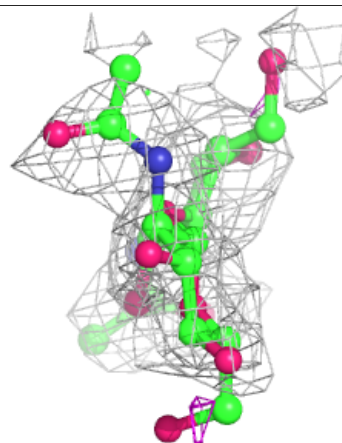
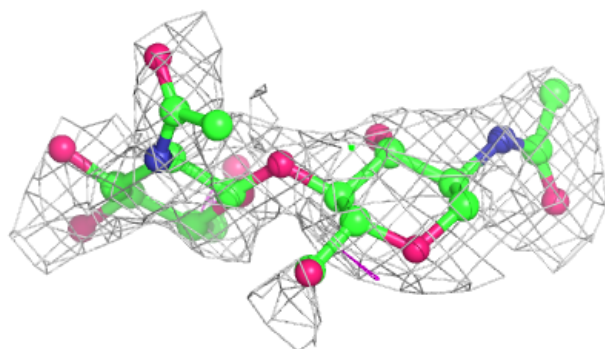
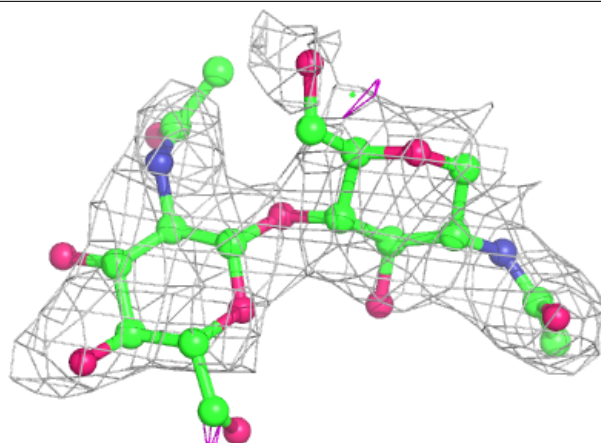
Electron density around Chain F:

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

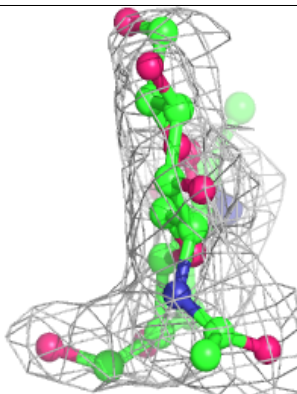
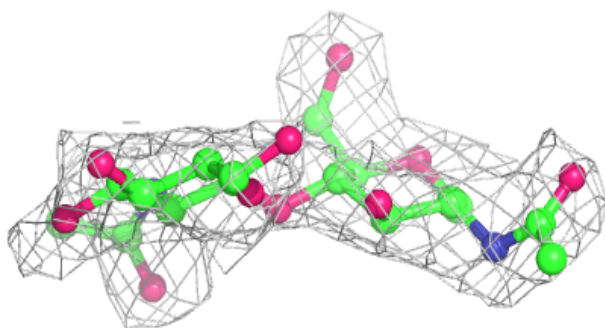
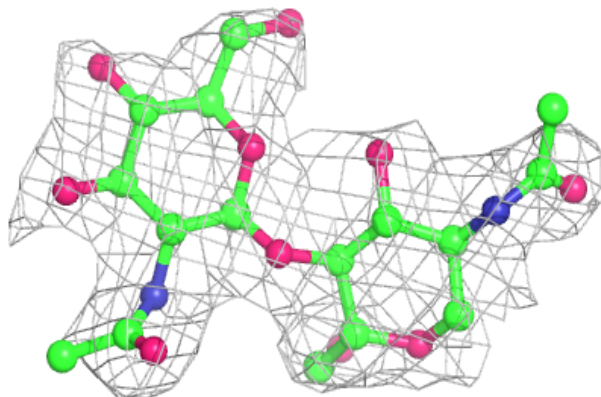


Electron density around Chain G:

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

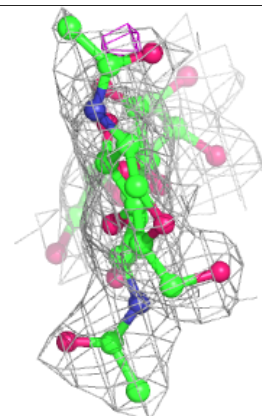
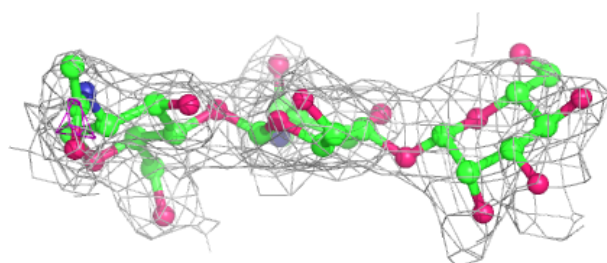
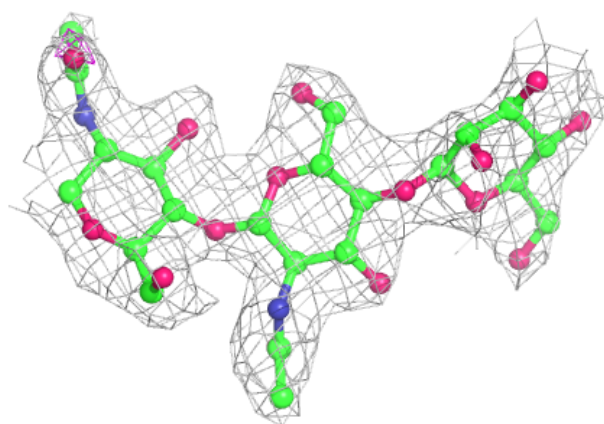
**Electron density around Chain K:**

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

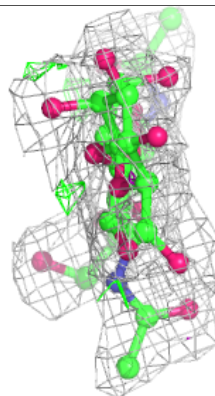
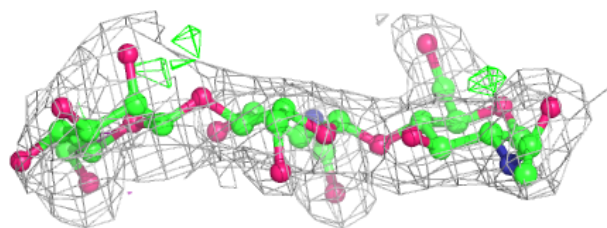
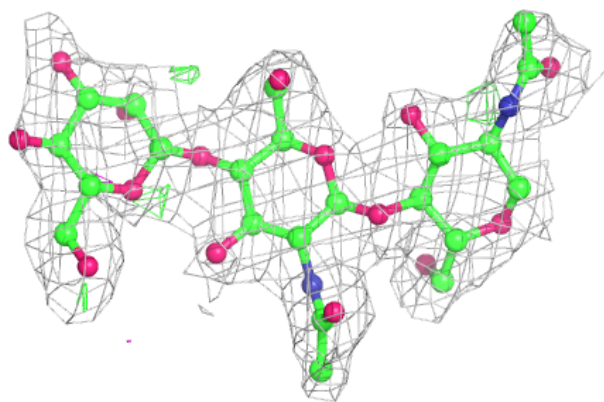


Electron density around Chain E:

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

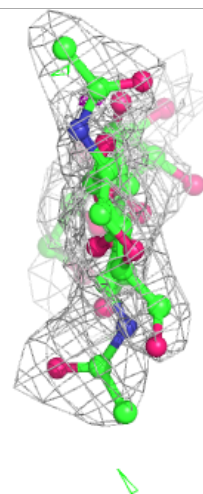
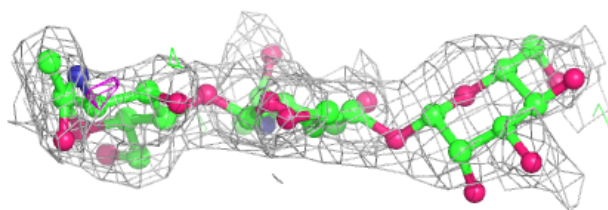
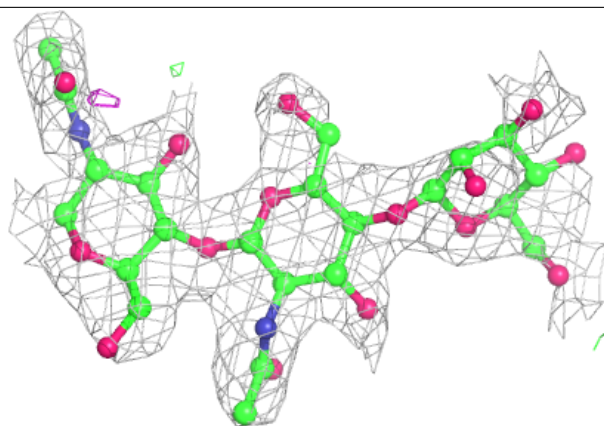
**Electron density around Chain H:**

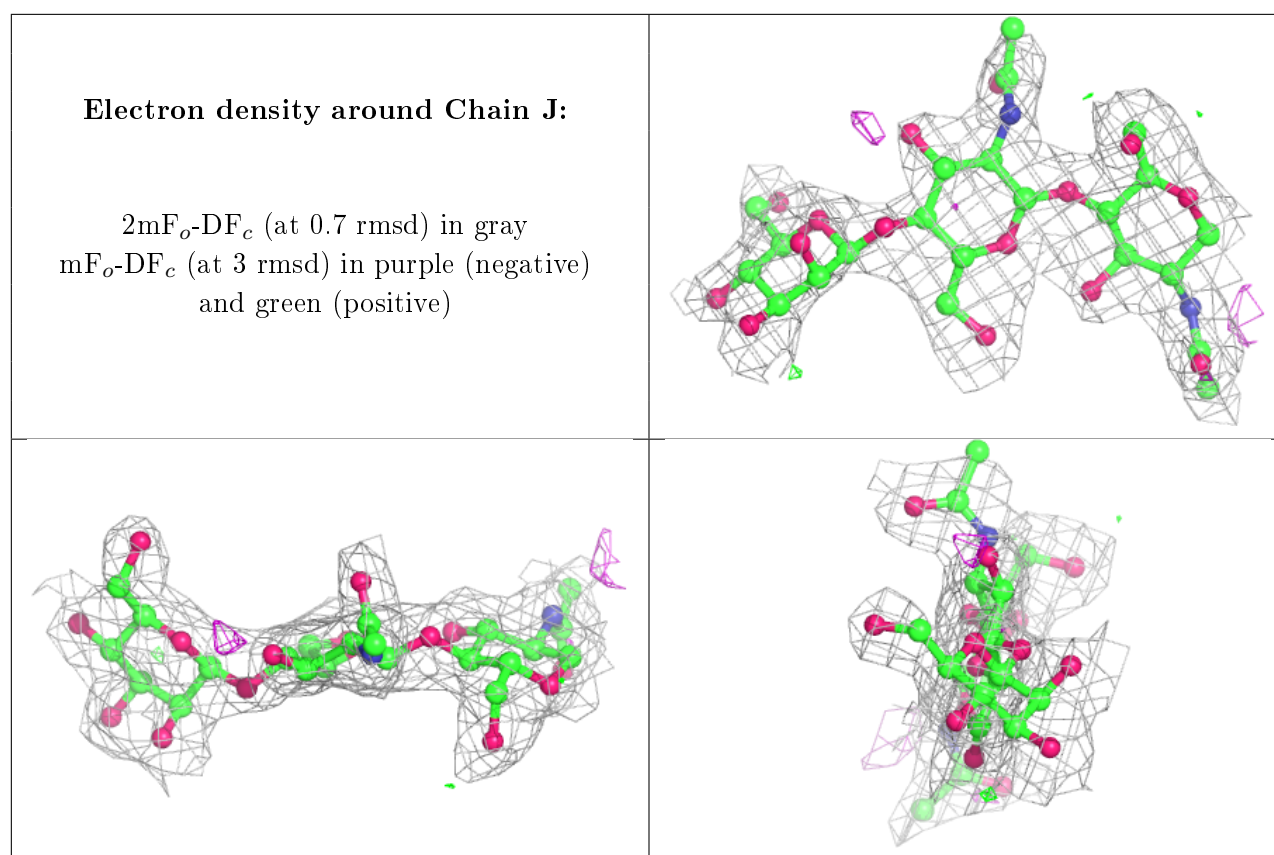
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (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
10	GOL	B	810	6/6	0.66	0.36	41,42,43,45	0
5	NAG	B	760	14/15	0.75	0.33	42,45,48,51	0
5	NAG	B	770	14/15	0.75	0.32	49,53,56,56	0
7	CL	A	610	1/1	0.78	0.25	49,49,49,49	0
5	NAG	B	700	14/15	0.85	0.21	24,28,30,34	0
5	NAG	A	700	14/15	0.87	0.19	22,25,26,29	0
8	SO4	A	802	5/5	0.90	0.18	59,60,60,61	0
8	SO4	B	801	5/5	0.90	0.17	77,77,77,77	0
8	SO4	A	800	5/5	0.90	0.15	84,84,85,85	0
5	NAG	B	750	14/15	0.91	0.19	19,22,26,26	0
5	NAG	A	750	14/15	0.91	0.20	33,35,38,38	0
9	OXY	B	901	2/2	0.96	0.12	8,8,8,9	0
6	CU	B	604	1/1	0.98	0.06	58,58,58,58	0
9	OXY	A	900	2/2	0.98	0.14	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CU	A	604	1/1	0.98	0.11	47,47,47,47	0
6	CU	B	602	1/1	0.99	0.03	22,22,22,22	0
6	CU	B	601	1/1	0.99	0.03	14,14,14,14	0
6	CU	B	603	1/1	0.99	0.03	25,25,25,25	0
6	CU	A	602	1/1	0.99	0.06	26,26,26,26	0
6	CU	A	603	1/1	1.00	0.08	15,15,15,15	0
6	CU	A	601	1/1	1.00	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.