



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:44 AM BST

PDB ID : 1L1Y
Title : The Crystal Structure and Catalytic Mechanism of Cellobiohydrolase CelS, the Major Enzymatic Component of the Clostridium thermocellum cellulosome
Authors : Guimaraes, B.G.; Souchon, H.; Lytle, B.L.; Wu, J.H.D.; Alzari, P.M.
Deposited on : 2002-02-20
Resolution : 2.40 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

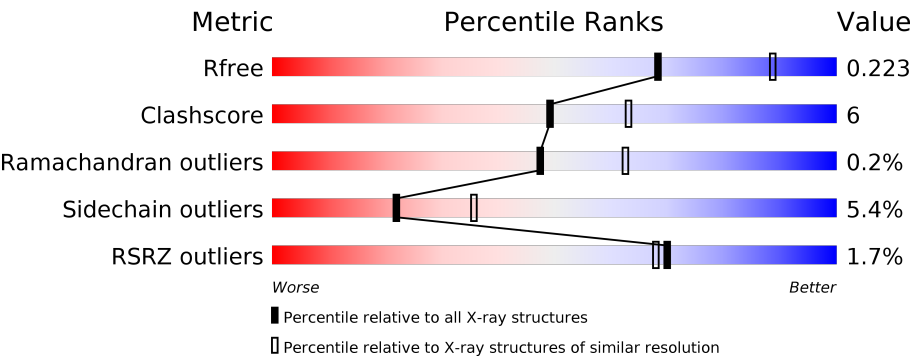
1 Overall quality at a glance i

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.



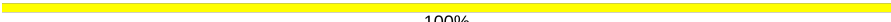

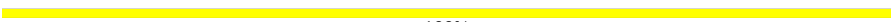
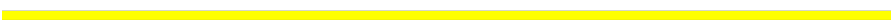


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	678	<div><div>3%</div><div><div></div><div>78%</div><div>15%</div><div>• 5%</div></div></div>
1	B	678	<div><div>2%</div><div><div></div><div>81%</div><div>11%</div><div>• 5%</div></div></div>
1	C	678	<div><div>2%</div><div><div></div><div>78%</div><div>15%</div><div>• 5%</div></div></div>
1	D	678	<div><div>%</div><div><div></div><div>81%</div><div>12%</div><div>• 5%</div></div></div>
1	E	678	<div><div>%</div><div><div></div><div>81%</div><div>12%</div><div>• 5%</div></div></div>
1	F	678	<div><div>%</div><div><div></div><div>81%</div><div>11%</div><div>• 5%</div></div></div>

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32457 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 cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5103	3285	825	973	20			
1	B	642	Total	C	N	O	S	0	0	0
			5128	3299	835	974	20			
1	C	642	Total	C	N	O	S	0	0	0
			5109	3287	832	970	20			
1	D	642	Total	C	N	O	S	0	0	0
			5136	3303	836	977	20			
1	E	642	Total	C	N	O	S	0	0	0
			5124	3298	832	974	20			
1	F	642	Total	C	N	O	S	0	0	0
			5130	3300	833	977	20			

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

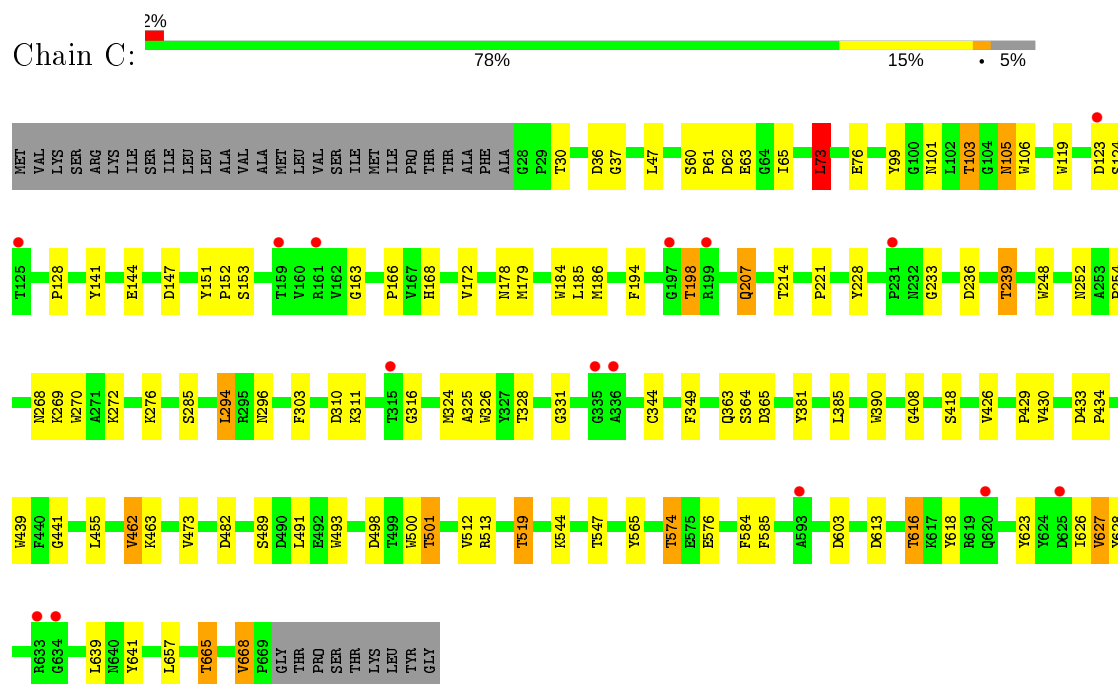


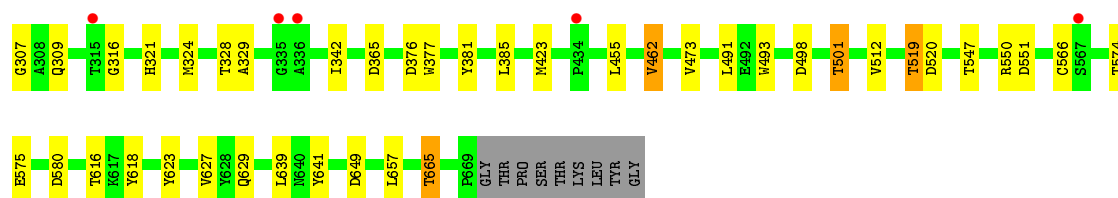
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			22	12	10			
2	H	2	Total	C	O	0	0	0
			22	12	10			
2	I	2	Total	C	O	0	0	0
			22	12	10			
2	J	2	Total	C	O	0	0	0
			22	12	10			
2	K	2	Total	C	O	0	0	0
			22	12	10			
2	L	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is water.

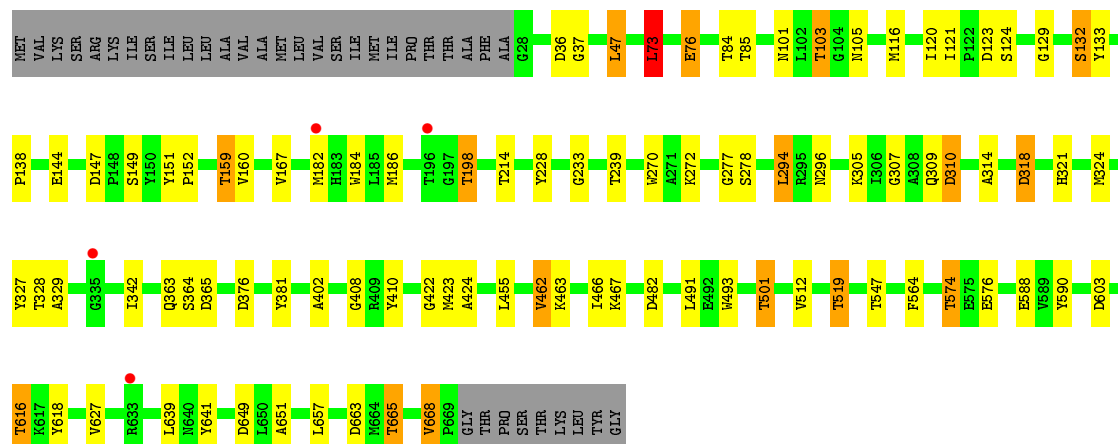
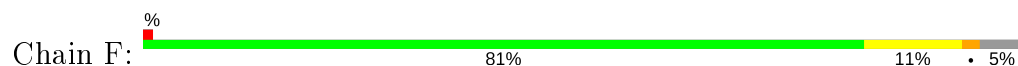
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 169	O 169	0	0
3	B	204	Total 204	O 204	0	0
3	C	214	Total 214	O 214	0	0
3	D	326	Total 326	O 326	0	0
3	E	286	Total 286	O 286	0	0
3	F	396	Total 396	O 396	0	0

- Molecule 1: cellobiohydrolase





- Molecule 1: cellobiohydrolase



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



BGC1
BGC2

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



BGC1
BGC2

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



BGC1
BGC2

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



BGC1
BGC2

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

Chain K:  100%

BG C1
BG C2

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

Chain L:  50% 50%

BG C1
BG C2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	147.24Å 207.20Å 213.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.40) 99.9 (14.99-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.189 , 0.224 0.188 , 0.223	Depositor DCC
R_{free} test set	12676 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32457	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: BGC

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	0.56	0/5282	0.77	11/7213 (0.2%)
1	B	0.55	0/5307	0.75	9/7241 (0.1%)
1	C	0.54	0/5288	0.76	8/7218 (0.1%)
1	D	0.62	1/5315 (0.0%)	0.79	11/7251 (0.2%)
1	E	0.60	0/5303	0.78	12/7236 (0.2%)
1	F	0.64	0/5309	0.79	8/7244 (0.1%)
All	All	0.59	1/31804 (0.0%)	0.77	59/43403 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	MET	SD-CE	-5.16	1.49	1.77

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ASP	CB-CG-OD2	7.01	124.61	118.30
1	C	62	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	147	ASP	CB-CG-OD2	6.65	124.28	118.30
1	C	73	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ASP	CB-CG-OD2	6.48	124.13	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	327	TYR	Peptide
1	F	327	TYR	Peptide

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	5103	0	4667	67	0
1	B	5128	0	4727	58	0
1	C	5109	0	4686	64	0
1	D	5136	0	4737	54	0
1	E	5124	0	4720	55	0
1	F	5130	0	4726	73	0
2	G	22	0	19	0	0
2	H	22	0	19	0	0
2	I	22	0	19	0	0
2	J	22	0	19	0	0
2	K	22	0	19	0	0
2	L	22	0	19	0	0
3	A	169	0	0	8	0
3	B	204	0	0	4	0
3	C	214	0	0	10	0
3	D	326	0	0	5	0
3	E	286	0	0	7	0
3	F	396	0	0	13	0
All	All	32457	0	28377	350	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 6.

The worst 5 of 350 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:574:THR:HG21	1:A:576:GLU:OE1	1.58	1.03
1:A:105:ASN:HB2	3:A:840:HOH:O	1.62	0.97
3:C:703:HOH:O	1:E:169:ASN:HB3	1.66	0.95
1:C:103:THR:HG22	1:C:105:ASN:H	1.35	0.91
1:C:294:LEU:HG	1:C:324:MET:HE1	1.55	0.86

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	640/678 (94%)	607 (95%)	30 (5%)	3 (0%)	29	41
1	B	640/678 (94%)	623 (97%)	17 (3%)	0	100	100
1	C	640/678 (94%)	618 (97%)	22 (3%)	0	100	100
1	D	640/678 (94%)	622 (97%)	16 (2%)	2 (0%)	41	55
1	E	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	47	62
1	F	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	47	62
All	All	3840/4068 (94%)	3716 (97%)	117 (3%)	7 (0%)	47	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	335	GLY
1	E	77	ALA
1	A	600	PRO
1	D	278	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	512/556 (92%)	480 (94%)	32 (6%)	18	28
1	B	519/556 (93%)	494 (95%)	25 (5%)	25	41
1	C	513/556 (92%)	481 (94%)	32 (6%)	18	29
1	D	521/556 (94%)	491 (94%)	30 (6%)	20	32
1	E	518/556 (93%)	494 (95%)	24 (5%)	27	43
1	F	520/556 (94%)	495 (95%)	25 (5%)	25	41
All	All	3103/3336 (93%)	2935 (95%)	168 (5%)	22	36

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	473	VAL
1	D	167	VAL
1	F	462	VAL
1	C	501	THR
1	C	627	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	178	ASN
1	C	363	GLN
1	F	101	ASN
1	C	207	GLN
1	C	268	ASN

5.3.3 RNA [i](#)

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 ⓘ

12 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	BGC	G	1	2	11,11,12	0.65	0	15,15,17	1.35	2 (13%)
2	BGC	G	2	2	11,11,12	0.51	0	15,15,17	0.86	1 (6%)
2	BGC	H	1	2	11,11,12	0.47	0	15,15,17	1.27	2 (13%)
2	BGC	H	2	2	11,11,12	0.61	0	15,15,17	0.82	0
2	BGC	I	1	2	11,11,12	0.82	0	15,15,17	1.34	2 (13%)
2	BGC	I	2	2	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
2	BGC	J	1	2	11,11,12	0.75	0	15,15,17	1.96	3 (20%)
2	BGC	J	2	2	11,11,12	0.77	0	15,15,17	1.10	1 (6%)
2	BGC	K	1	2	11,11,12	0.77	0	15,15,17	1.25	2 (13%)
2	BGC	K	2	2	11,11,12	0.76	0	15,15,17	1.15	1 (6%)
2	BGC	L	1	2	11,11,12	0.72	0	15,15,17	1.59	1 (6%)
2	BGC	L	2	2	11,11,12	0.72	0	15,15,17	0.69	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	BGC	G	1	2	-	0/2/19/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/19/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/19/22	0/1/1/1
2	BGC	J	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	1	2	-	0/2/19/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	L	1	2	-	0/2/19/22	0/1/1/1
2	BGC	L	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	BGC	O5-C1-C2	-6.09	101.37	110.77
2	L	1	BGC	O5-C1-C2	-5.12	102.87	110.77
2	K	1	BGC	O5-C1-C2	-3.92	104.72	110.77
2	G	1	BGC	O5-C1-C2	-3.82	104.87	110.77
2	J	2	BGC	C1-O5-C5	3.60	117.06	112.19

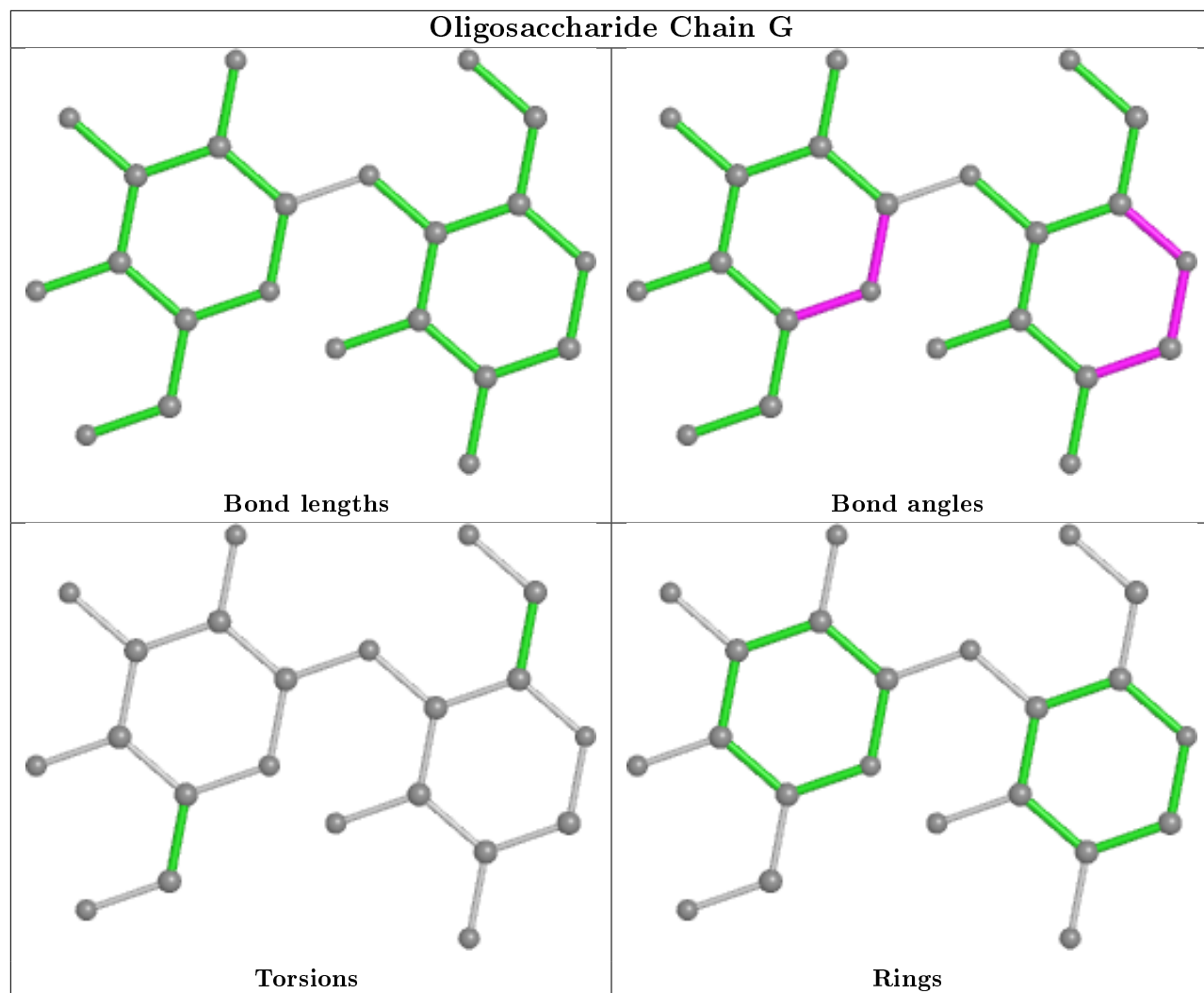
There are no chirality outliers.

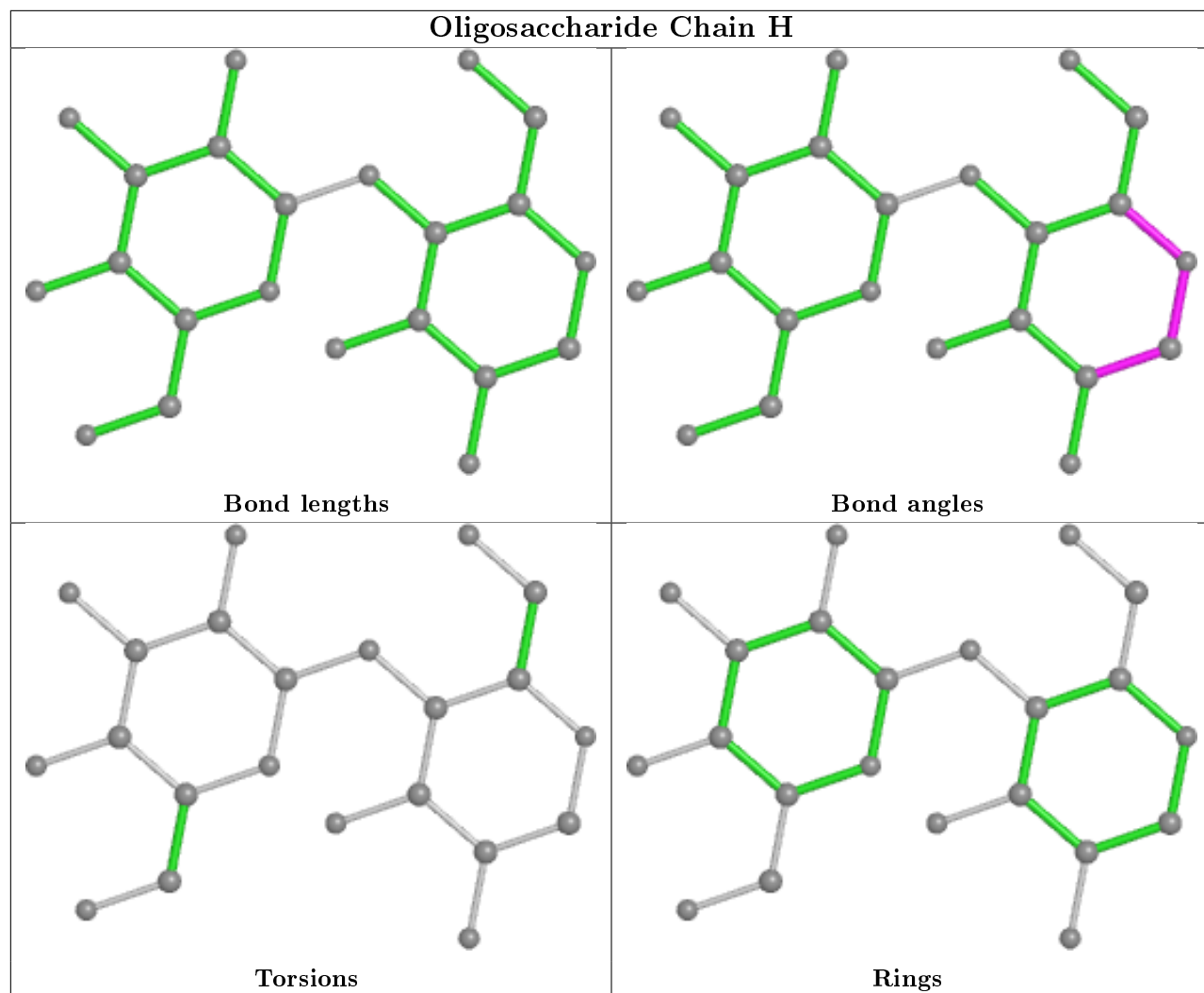
There are no torsion outliers.

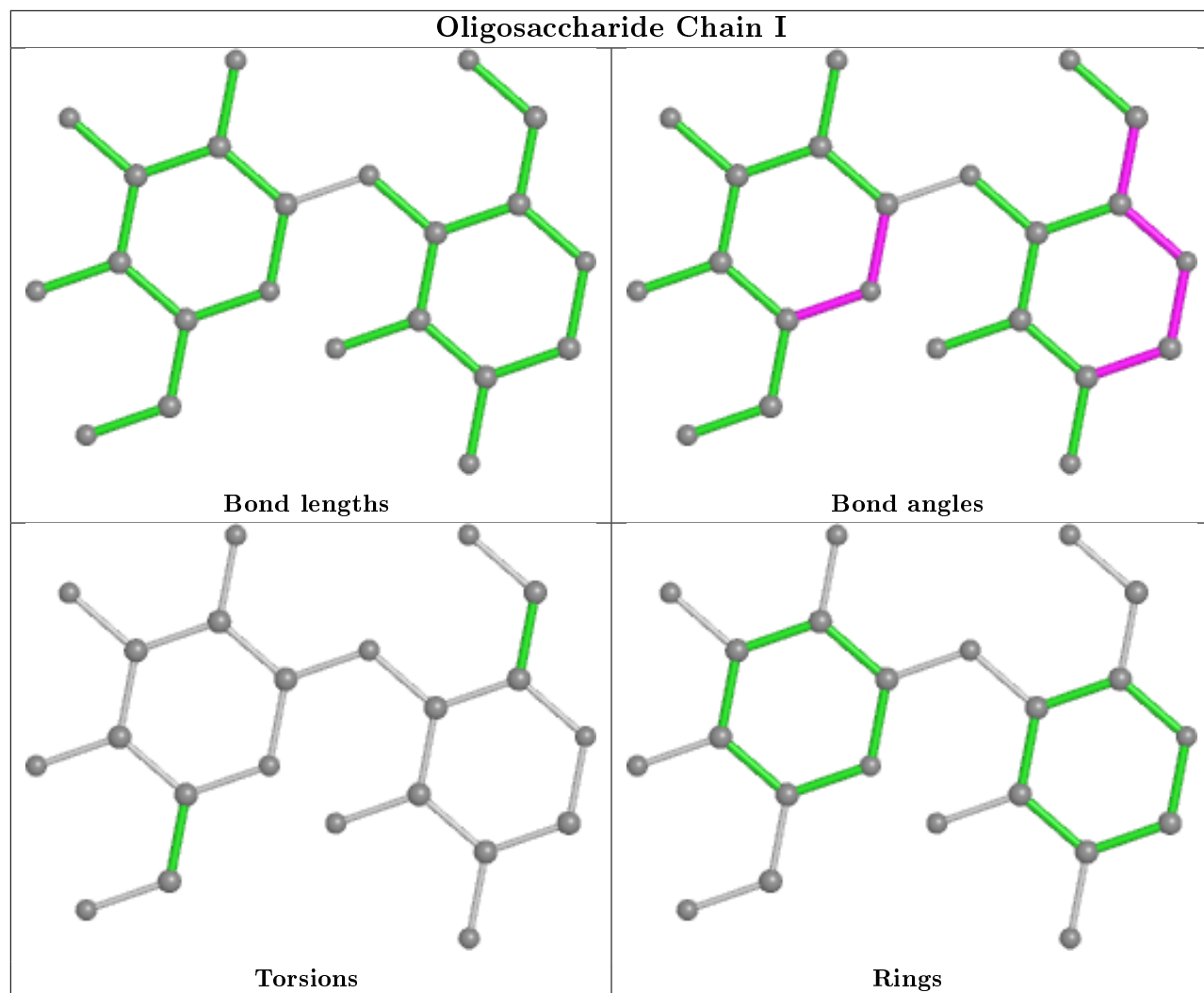
There are no ring outliers.

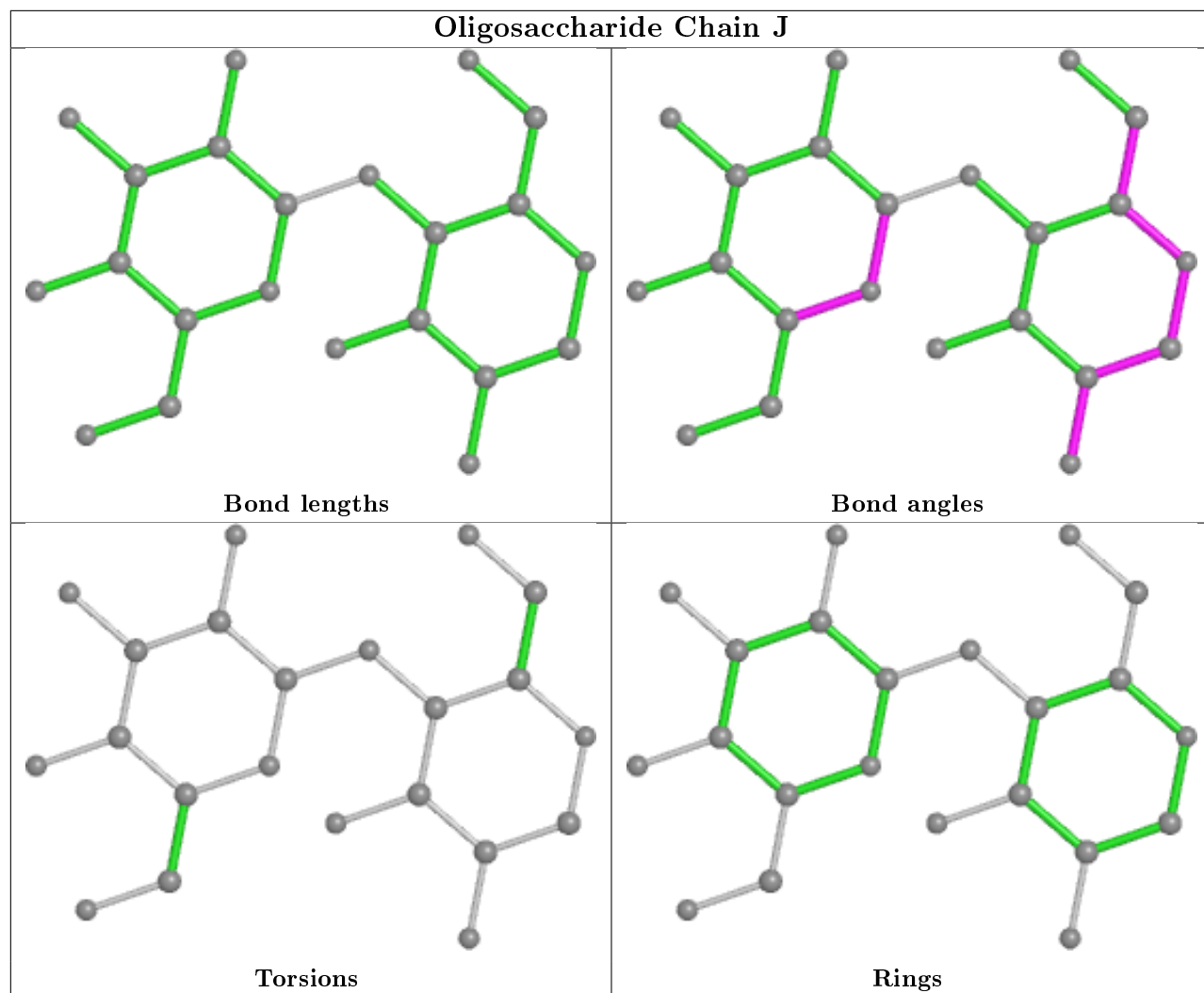
No monomer is involved in short contacts.

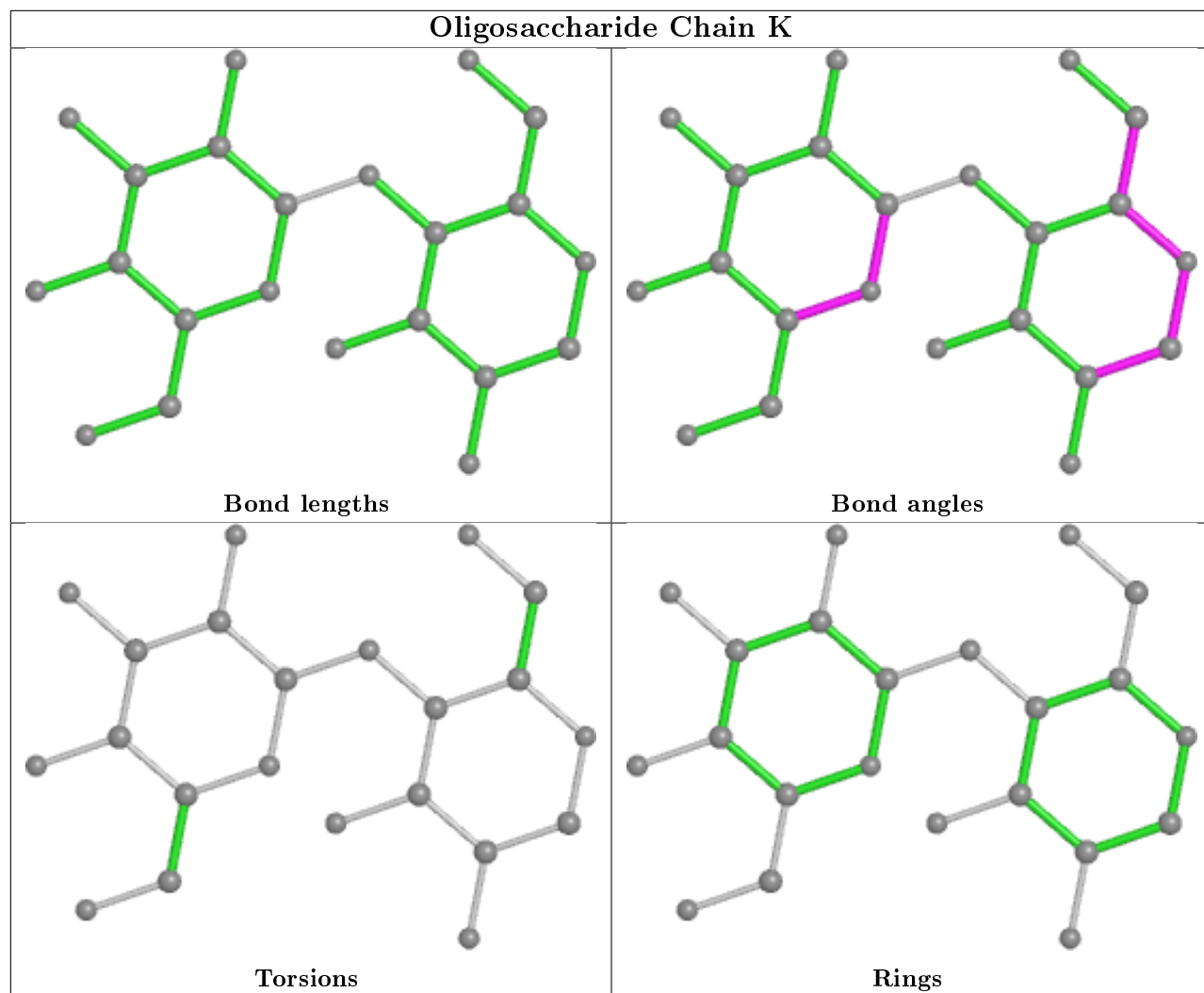
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

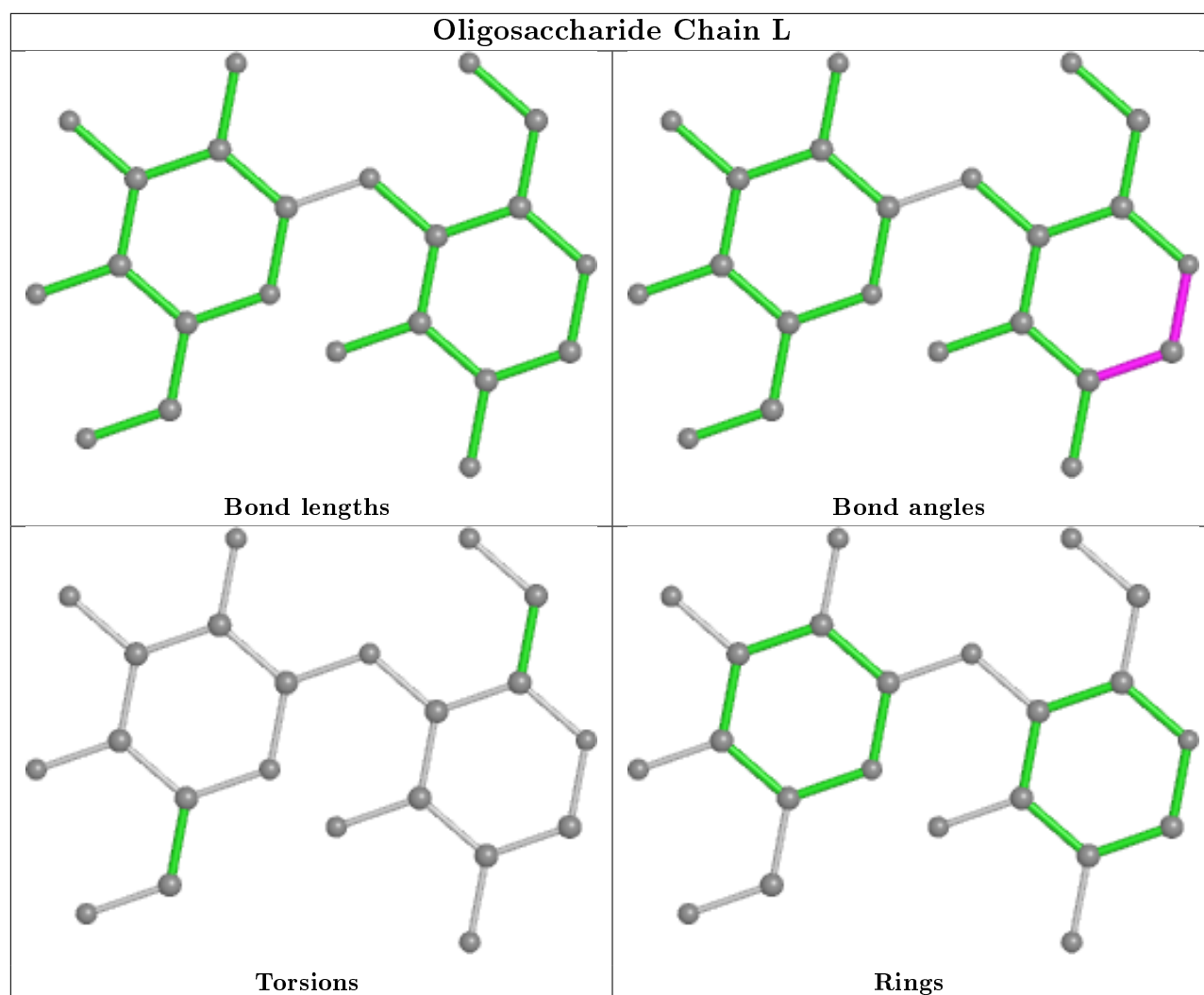












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

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(Å ²)	Q<0.9
1	A	642/678 (94%)	-0.20	19 (2%) 50 49	23, 40, 65, 73	0
1	B	642/678 (94%)	-0.44	12 (1%) 66 64	23, 37, 55, 69	0
1	C	642/678 (94%)	-0.37	15 (2%) 60 58	20, 37, 63, 73	0
1	D	642/678 (94%)	-0.54	8 (1%) 79 77	20, 31, 47, 55	0
1	E	642/678 (94%)	-0.68	6 (0%) 84 82	18, 29, 43, 56	0
1	F	642/678 (94%)	-0.80	4 (0%) 89 88	17, 26, 38, 53	0
All	All	3852/4068 (94%)	-0.50	64 (1%) 70 68	17, 32, 58, 73	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	5.8
1	A	336	ALA	4.8
1	A	335	GLY	4.1
1	D	567	SER	3.5
1	A	415	ALA	3.5

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

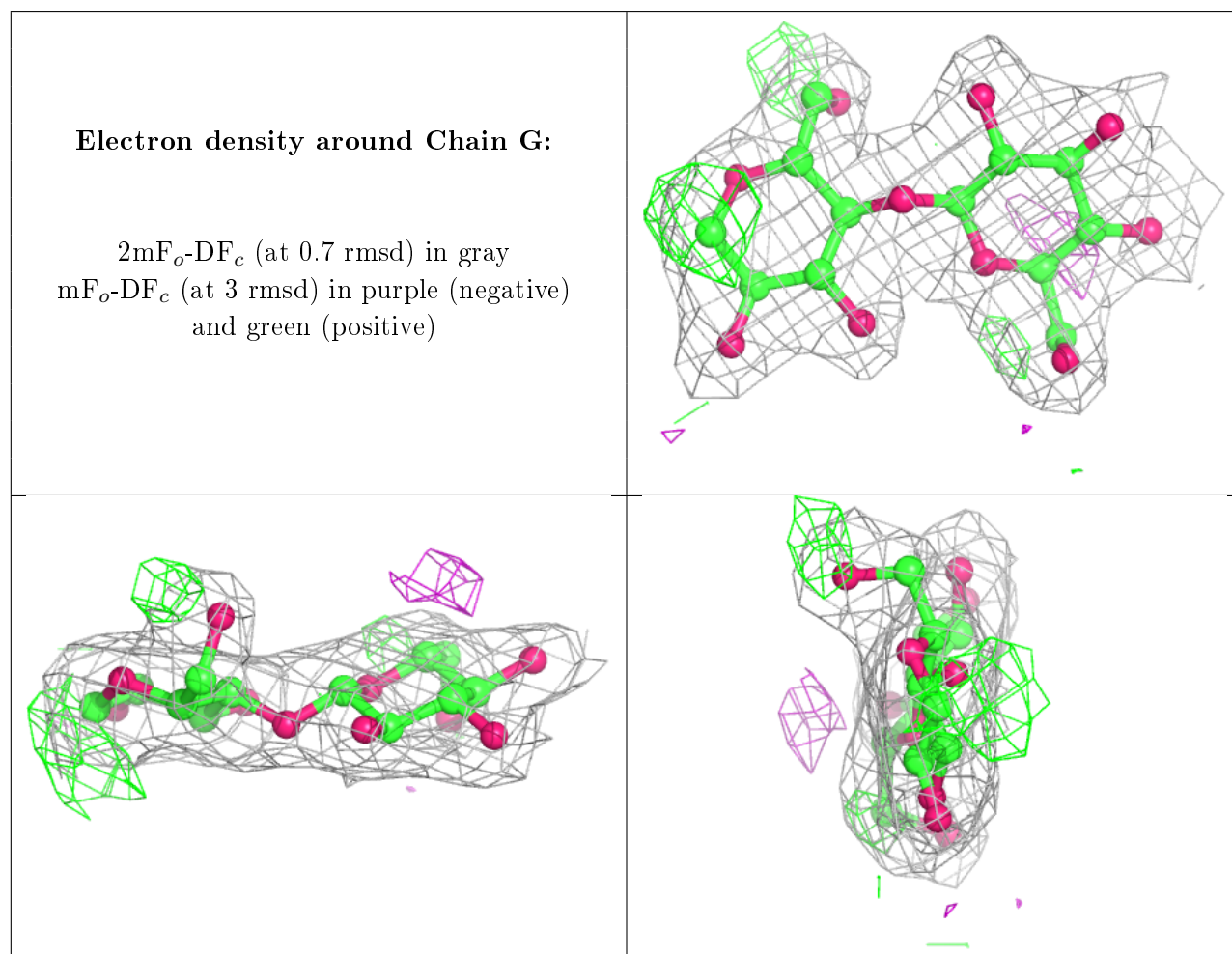
There are no non-standard protein/DNA/RNA residues in this entry.

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.

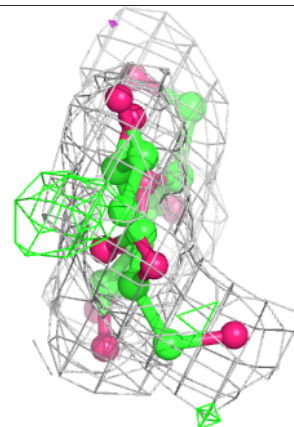
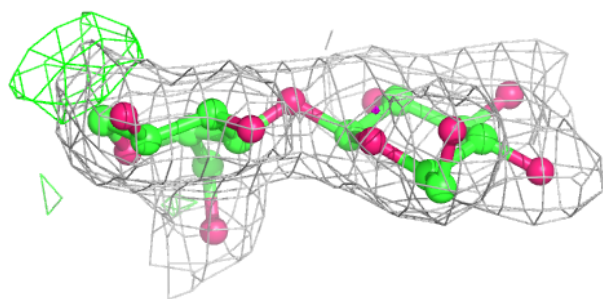
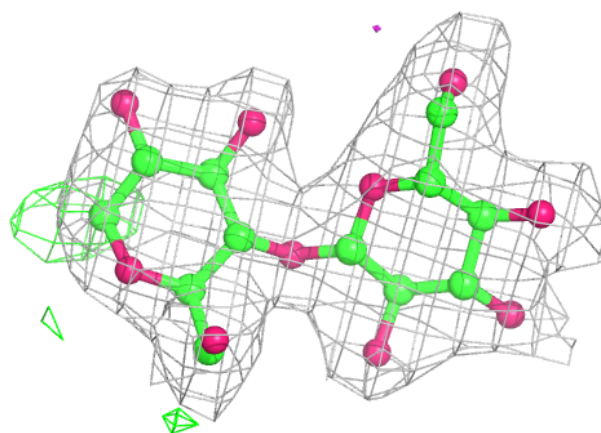
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	K	1	11/12	0.93	0.12	26,29,34,34	0
2	BGC	H	1	11/12	0.93	0.12	38,38,41,41	0
2	BGC	J	1	11/12	0.93	0.13	35,37,43,44	0
2	BGC	G	1	11/12	0.93	0.11	34,35,37,37	0
2	BGC	G	2	11/12	0.94	0.10	33,34,35,35	0
2	BGC	I	1	11/12	0.95	0.12	30,36,39,40	0
2	BGC	L	1	11/12	0.95	0.10	28,31,36,37	0
2	BGC	J	2	11/12	0.97	0.07	30,31,32,33	0
2	BGC	K	2	11/12	0.97	0.08	24,25,26,27	0
2	BGC	H	2	11/12	0.97	0.07	31,33,34,35	0
2	BGC	L	2	11/12	0.98	0.07	24,27,29,30	0
2	BGC	I	2	11/12	0.98	0.07	31,32,33,35	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.

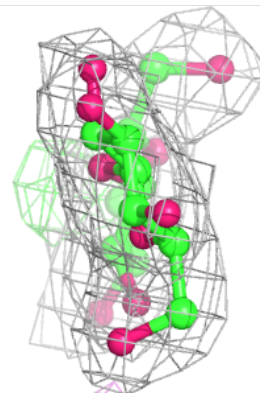
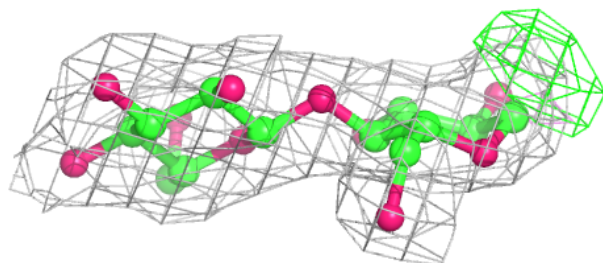
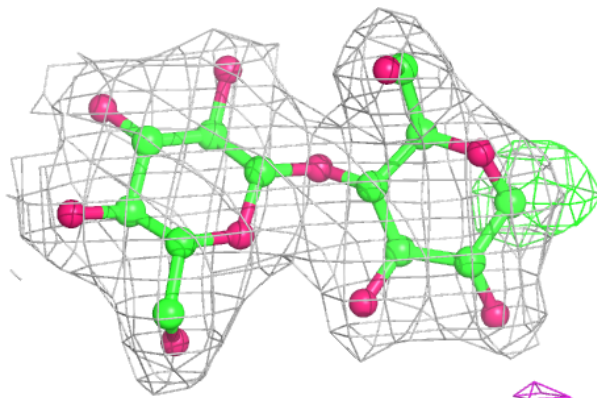


Electron density around Chain H:

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

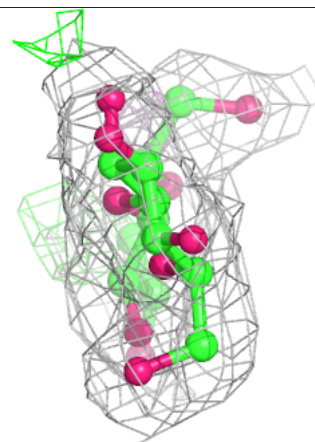
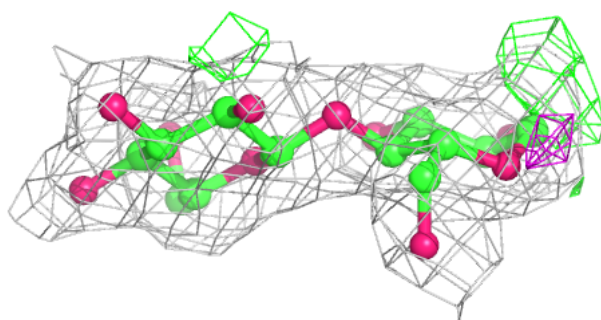
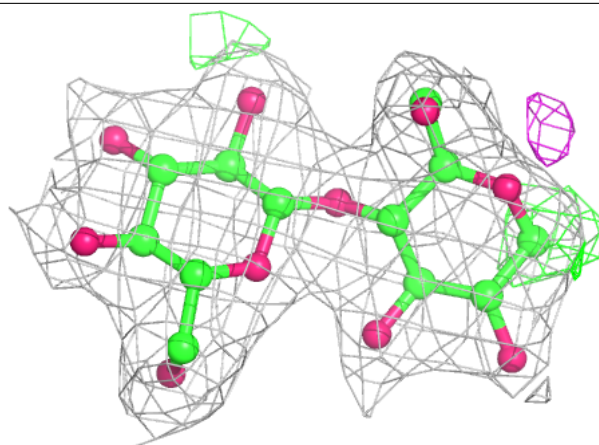
**Electron density around Chain I:**

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

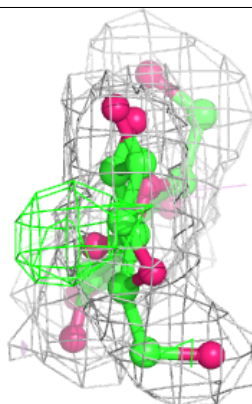
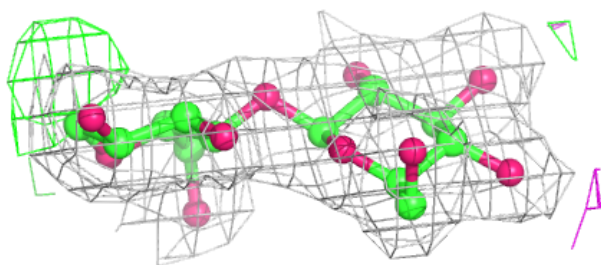
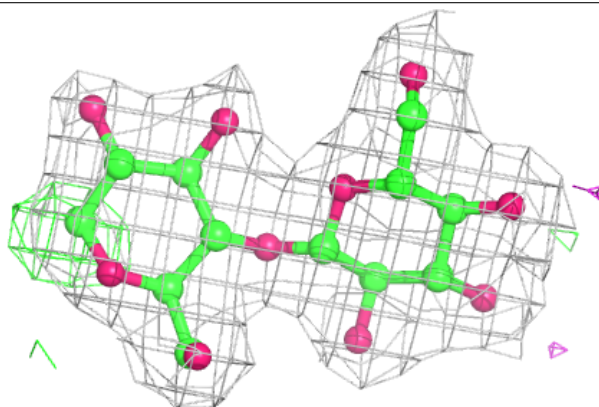


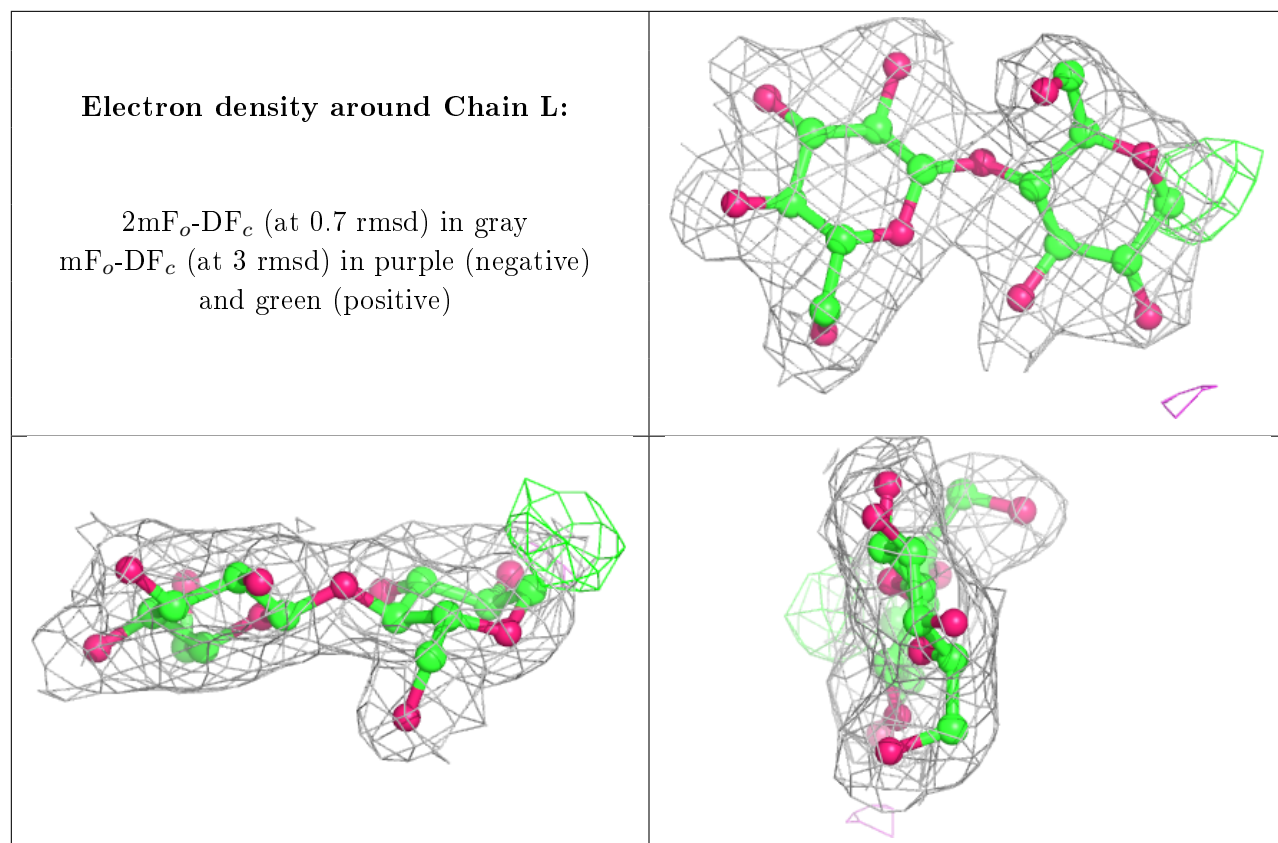
Electron density around Chain J:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.