



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2024 – 10:31 pm BST

PDB ID : 2C3H  
Title : Structure of CBM26 from *Bacillus halodurans* amylase in complex with maltose  
Authors : Boraston, A.B.; Healey, M.; Klassen, J.; Ficko-Blean, E.; Lammerts van Bueren, A.; Law, V.  
Deposited on : 2005-10-07  
Resolution : 2.24 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

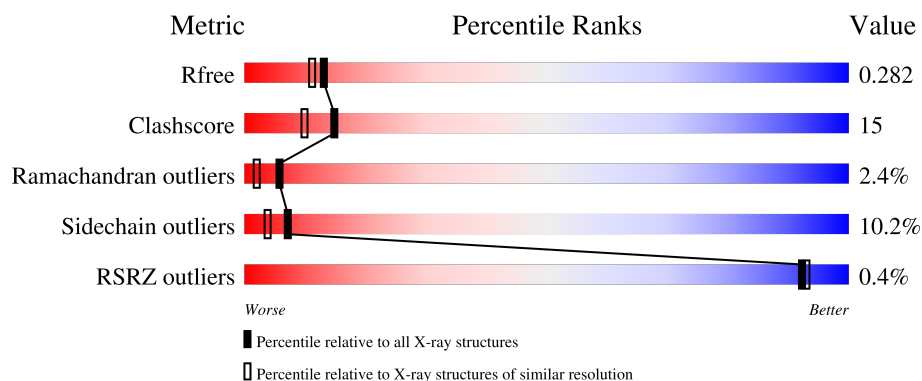
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	98	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>7%</div> <div>• 5%</div> </div> </div>
1	B	98	<div> <div></div> <div> <div>61%</div> <div>26%</div> <div>7%</div> <div>• •</div> </div> </div>
1	C	98	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>• • 7%</div> </div> </div>
1	D	98	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>• 6%</div> </div> </div>
1	E	98	<div> <div></div> <div> <div>70%</div> <div>19%</div> <div>• • 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	98	 59% 27% 5% • 7%
1	G	98	 68% 20% • • 6%
1	H	98	 53% 34% 6% • 6%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	P	2	 100%

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	SO4	A	1099	-	-	X	-
4	GLC	D	300	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7264 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 ALPHA-AMYLASE G-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	0	0
			783	505	127	150	1			
1	B	94	Total	C	N	O	S	0	0	0
			788	508	128	151	1			
1	C	91	Total	C	N	O	S	0	0	0
			770	497	125	147	1			
1	D	92	Total	C	N	O	S	0	0	0
			777	502	126	148	1			
1	E	92	Total	C	N	O	S	0	0	0
			777	502	126	148	1			
1	F	91	Total	C	N	O	S	0	0	0
			770	497	125	147	1			
1	G	92	Total	C	N	O	S	0	0	0
			777	502	126	148	1			
1	H	92	Total	C	N	O	S	0	0	0
			777	502	126	148	1			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



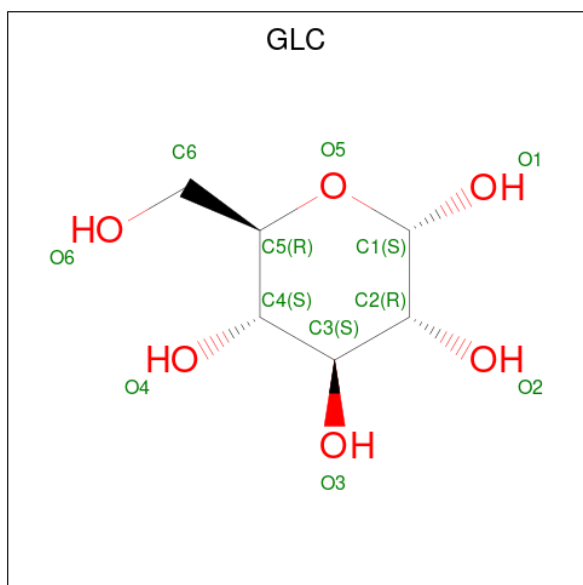
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	101	Total	O	0	0
			101	101		
5	C	106	Total	O	0	0
			106	106		
5	D	103	Total	O	0	0
			103	103		
5	E	103	Total	O	0	0
			103	103		
5	F	86	Total	O	0	0
			86	86		

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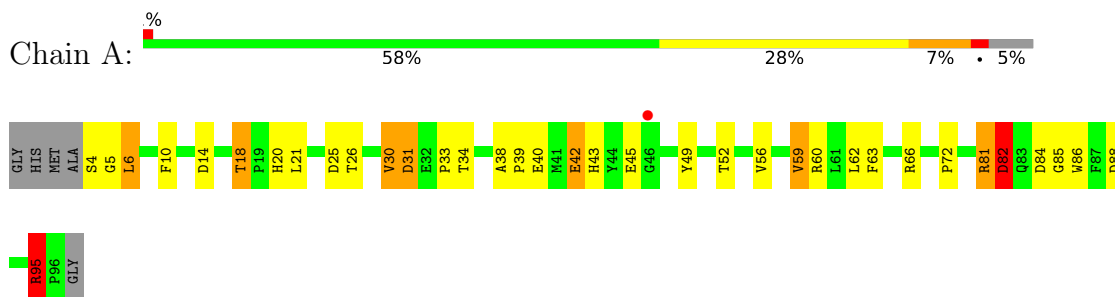
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	86	Total 86	O 86	0	0
5	H	118	Total 118	O 118	0	0

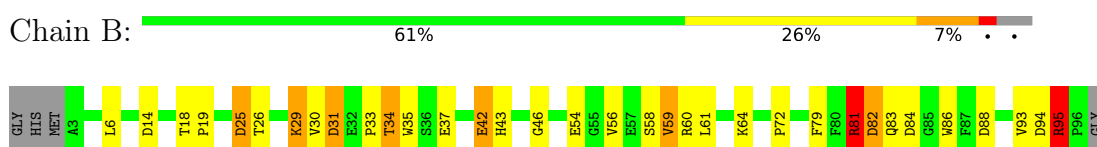
### 3 Residue-property plots [i](#)

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.

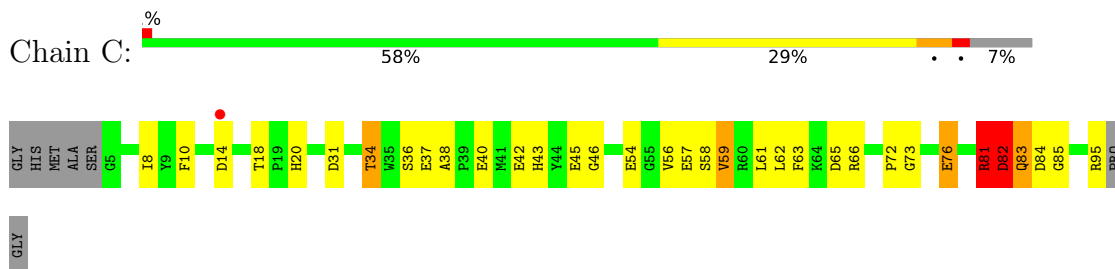
- Molecule 1: ALPHA-AMYLASE G-6



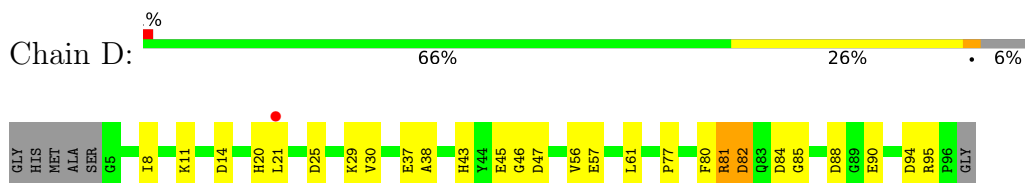
- Molecule 1: ALPHA-AMYLASE G-6



- Molecule 1: ALPHA-AMYLASE G-6



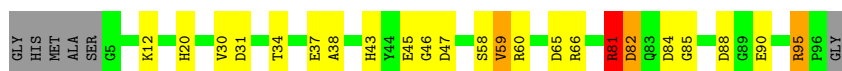
- Molecule 1: ALPHA-AMYLASE G-6



- Molecule 1: ALPHA-AMYLASE G-6







- Molecule 1: ALPHA-AMYLASE G-6

Chain F: 59% 27% 5% 7%



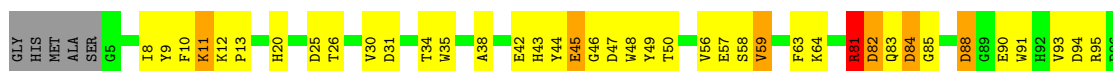
- Molecule 1: ALPHA-AMYLASE G-6

Chain G: 68% 20% 6%



- Molecule 1: ALPHA-AMYLASE G-6

Chain H: 53% 34% 6% 6%



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

Chain I: 100%



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

Chain J: 100%



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

Chain K: 100%



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

Chain L: 100%

GLC1  
GLC2

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

Chain M:  100%GLC1  
GLC2

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

Chain N:  100%GLC1  
GLC2

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

Chain O:  100%GLC1  
GLC2

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

Chain P:  100%GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.20Å 108.20Å 180.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.24 19.94 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.24) 98.6 (19.94-2.24)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.75 (at 2.23Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.203 , 0.279 0.209 , 0.282	Depositor DCC
$R_{free}$ test set	2964 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SO4

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	0.87	0/818	1.14	9/1119 (0.8%)
1	B	0.94	0/823	1.20	8/1126 (0.7%)
1	C	0.88	0/804	1.24	10/1099 (0.9%)
1	D	0.87	0/812	1.08	7/1111 (0.6%)
1	E	0.91	0/812	1.13	6/1111 (0.5%)
1	F	0.90	0/804	1.14	10/1099 (0.9%)
1	G	0.79	0/812	1.08	4/1111 (0.4%)
1	H	0.84	0/812	1.04	4/1111 (0.4%)
All	All	0.88	0/6497	1.13	58/8887 (0.7%)

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	C	1	0
1	D	0	1
1	F	0	1
1	G	0	1
All	All	1	3

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ASP	CB-CG-OD2	10.79	128.02	118.30
1	G	81	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	E	84	ASP	CB-CG-OD2	9.81	127.13	118.30
1	F	84	ASP	CB-CG-OD2	9.78	127.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASP	CB-CG-OD2	8.77	126.19	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	82	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	81	ARG	Peptide
1	F	81	ARG	Peptide
1	G	81	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	783	0	686	33	0
1	B	788	0	691	23	0
1	C	770	0	674	30	0
1	D	777	0	681	18	0
1	E	777	0	681	29	0
1	F	770	0	674	16	0
1	G	777	0	681	15	0
1	H	777	0	681	31	0
2	I	23	0	21	1	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
3	A	20	0	0	3	0
3	C	10	0	0	1	0
3	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	10	0	0	1	0
4	D	12	0	12	0	0
5	A	101	0	0	13	0
5	B	101	0	0	8	0
5	C	106	0	0	12	0
5	D	103	0	0	4	0
5	E	103	0	0	14	0
5	F	86	0	0	4	1
5	G	86	0	0	7	0
5	H	118	0	0	8	0
All	All	7264	0	5629	183	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 183 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:33:PRO:HG2	5:A:2031:HOH:O	1.40	1.21
1:H:34:THR:HG21	5:H:2045:HOH:O	1.38	1.20
1:E:31:ASP:HB3	5:E:2029:HOH:O	1.48	1.12
1:B:94:ASP:O	1:B:95:ARG:HB3	1.53	1.05
1:E:66:ARG:HB2	5:E:2060:HOH:O	1.64	0.96

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)
5:F:2055:HOH:O	5:F:2084:HOH:O[4_556]	2.11	0.09

## 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	91/98 (93%)	86 (94%)	3 (3%)	2 (2%)	6	2
1	B	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	6	2
1	C	89/98 (91%)	85 (96%)	2 (2%)	2 (2%)	6	2
1	D	90/98 (92%)	82 (91%)	6 (7%)	2 (2%)	6	2
1	E	90/98 (92%)	88 (98%)	0	2 (2%)	6	2
1	F	89/98 (91%)	83 (93%)	4 (4%)	2 (2%)	6	2
1	G	90/98 (92%)	84 (93%)	4 (4%)	2 (2%)	6	2
1	H	90/98 (92%)	85 (94%)	2 (2%)	3 (3%)	4	1
All	All	721/784 (92%)	676 (94%)	28 (4%)	17 (2%)	6	2

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	ASP
1	B	95	ARG
1	D	82	ASP
1	E	82	ASP
1	F	82	ASP

### 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	82/84 (98%)	73 (89%)	9 (11%)	6	3
1	B	82/84 (98%)	70 (85%)	12 (15%)	3	1
1	C	80/84 (95%)	69 (86%)	11 (14%)	3	1
1	D	81/84 (96%)	79 (98%)	2 (2%)	47	54
1	E	81/84 (96%)	77 (95%)	4 (5%)	25	25
1	F	80/84 (95%)	68 (85%)	12 (15%)	3	1
1	G	81/84 (96%)	74 (91%)	7 (9%)	10	7
1	H	81/84 (96%)	72 (89%)	9 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	648/672 (96%)	582 (90%)	66 (10%)	<b>7</b> <b>4</b>

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	LYS
1	H	30	VAL
1	H	95	ARG
1	C	54	GLU
1	C	42	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	43	HIS
1	F	43	HIS
1	H	43	HIS
1	F	20	HIS
1	F	69	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 ⓘ

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
2	GLC	I	1	2	12,12,12	0.46	0	17,17,17	1.03	1 (5%)
2	GLC	I	2	2	11,11,12	0.77	0	15,15,17	1.58	2 (13%)
2	GLC	J	1	2	12,12,12	0.54	0	17,17,17	1.29	3 (17%)
2	GLC	J	2	2	11,11,12	0.86	1 (9%)	15,15,17	1.39	1 (6%)
2	GLC	K	1	2	12,12,12	0.41	0	17,17,17	1.21	2 (11%)
2	GLC	K	2	2	11,11,12	0.52	0	15,15,17	1.23	1 (6%)
2	GLC	L	1	2	12,12,12	0.68	0	17,17,17	1.47	2 (11%)
2	GLC	L	2	2	11,11,12	0.96	0	15,15,17	1.53	3 (20%)
2	GLC	M	1	2	12,12,12	0.65	0	17,17,17	1.32	3 (17%)
2	GLC	M	2	2	11,11,12	0.71	0	15,15,17	1.62	4 (26%)
2	GLC	N	1	2	12,12,12	0.50	0	17,17,17	1.14	2 (11%)
2	GLC	N	2	2	11,11,12	0.87	1 (9%)	15,15,17	0.76	0
2	GLC	O	1	2	12,12,12	0.82	1 (8%)	17,17,17	1.44	4 (23%)
2	GLC	O	2	2	11,11,12	0.93	0	15,15,17	1.72	3 (20%)
2	GLC	P	1	2	12,12,12	0.60	0	17,17,17	0.89	1 (5%)
2	GLC	P	2	2	11,11,12	0.74	0	15,15,17	1.25	1 (6%)

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	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1	2	-	0/2/22/22	0/1/1/1
2	GLC	N	2	2	-	0/2/19/22	0/1/1/1
2	GLC	O	1	2	-	0/2/22/22	0/1/1/1
2	GLC	O	2	2	-	0/2/19/22	0/1/1/1
2	GLC	P	1	2	-	0/2/22/22	0/1/1/1
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	GLC	C2-C3	2.32	1.55	1.52
2	N	2	GLC	O5-C1	-2.17	1.40	1.43
2	O	1	GLC	O4-C4	-2.08	1.38	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	GLC	C1-O5-C5	4.61	118.43	112.19
2	I	2	GLC	C1-O5-C5	4.14	117.80	112.19
2	O	2	GLC	C1-O5-C5	4.05	117.67	112.19
2	L	2	GLC	O3-C3-C2	-3.78	102.75	109.99
2	K	2	GLC	C1-O5-C5	3.56	117.01	112.19

There are no chirality outliers.

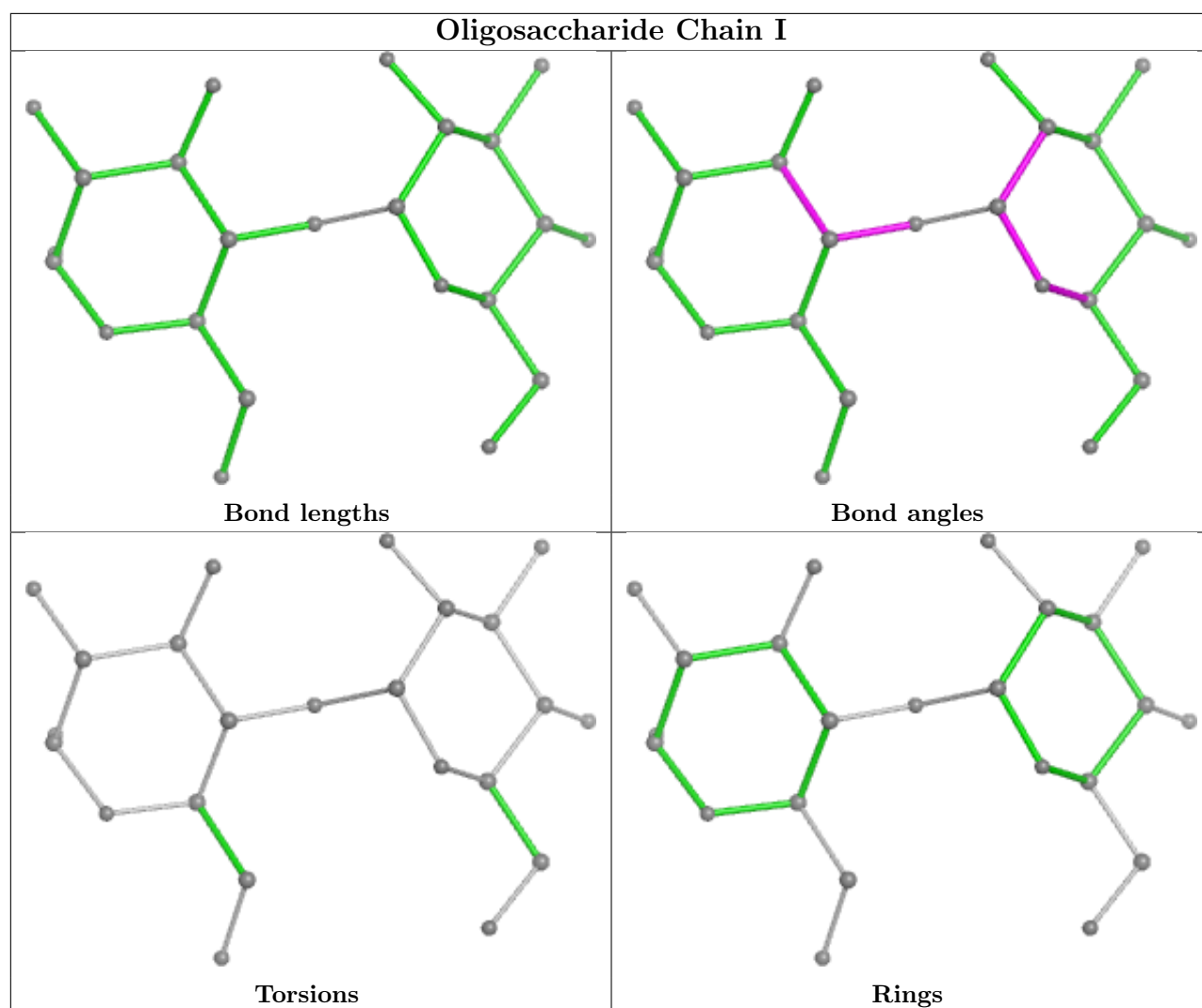
There are no torsion outliers.

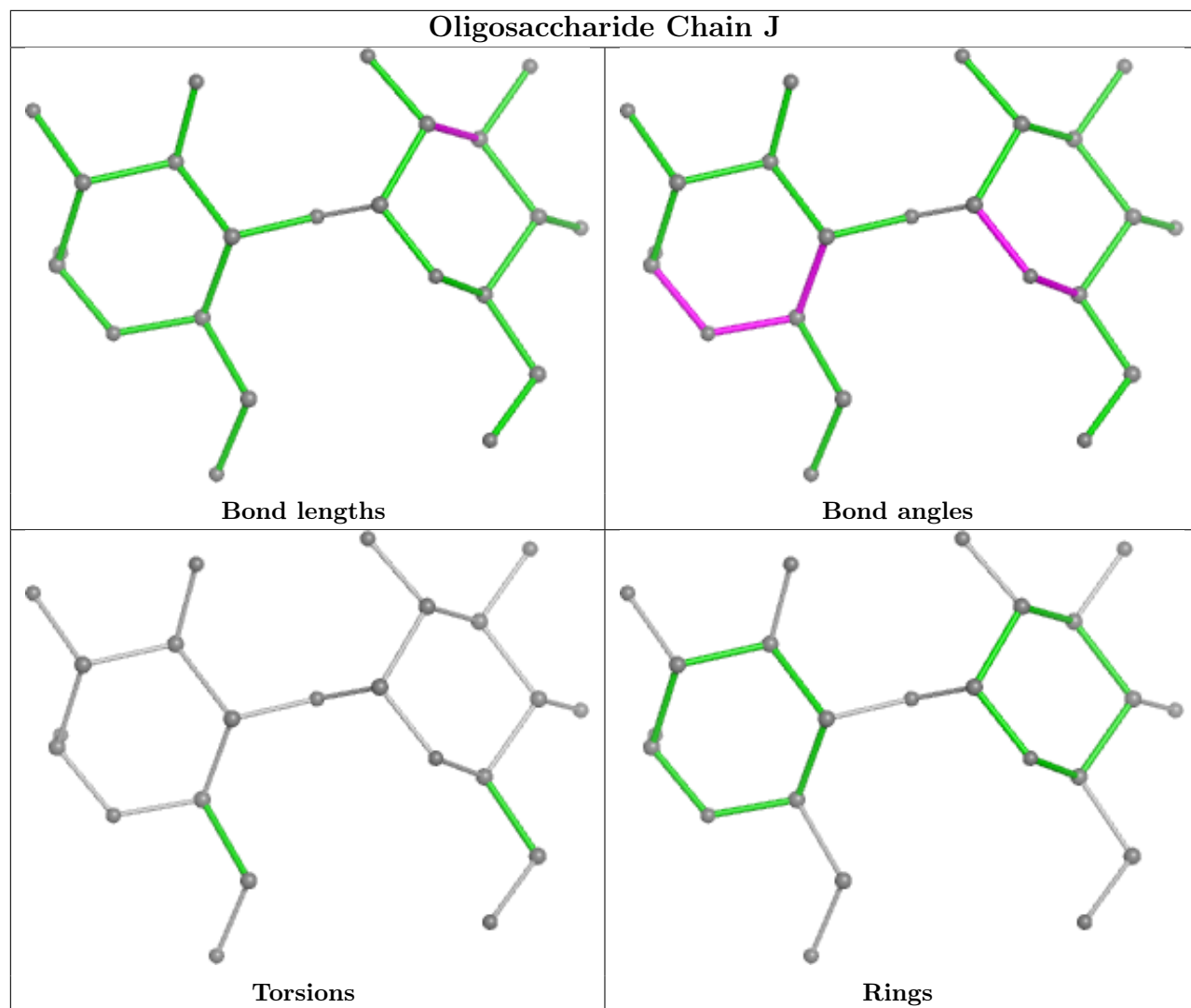
There are no ring outliers.

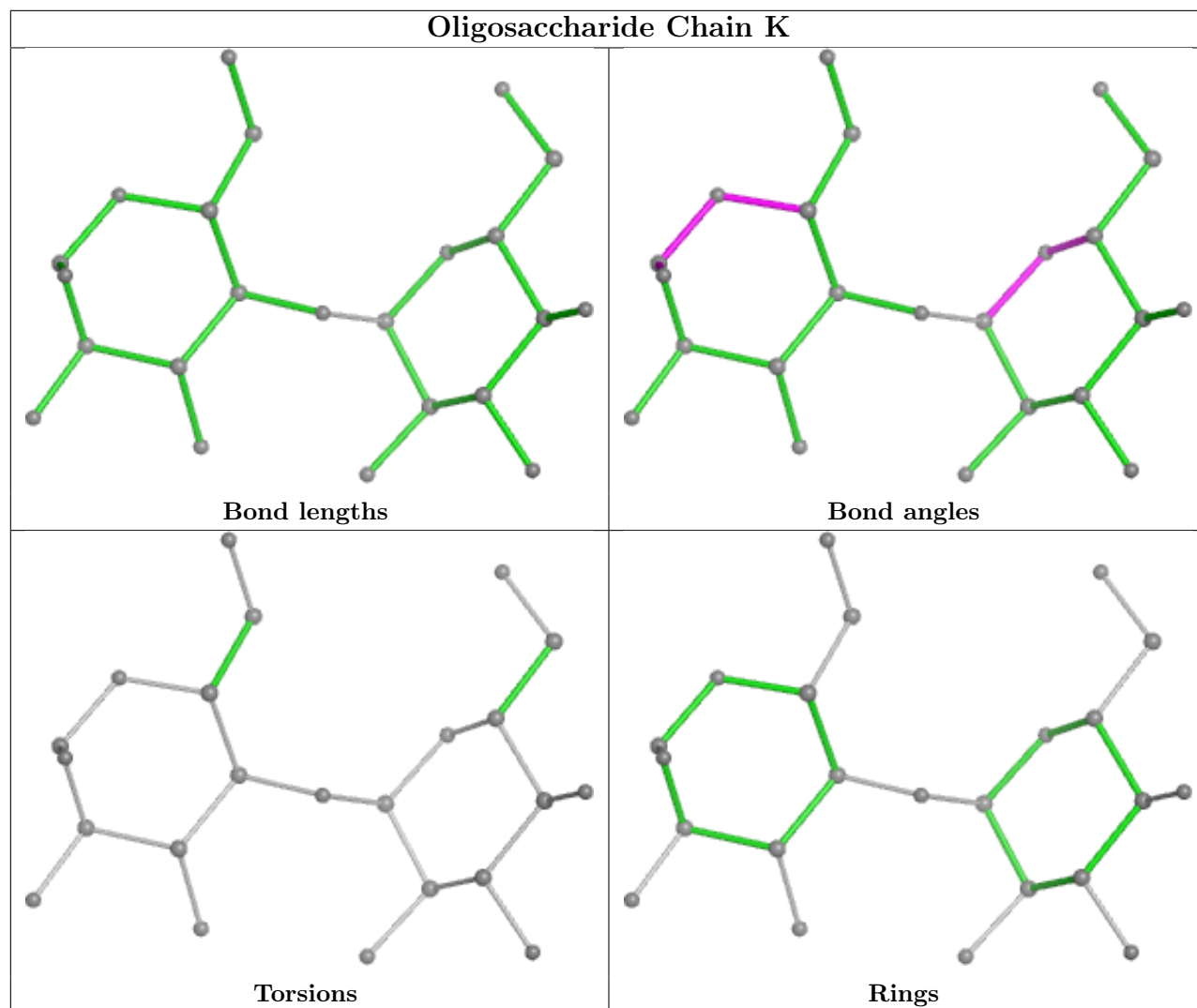
2 monomers are involved in 1 short contact:

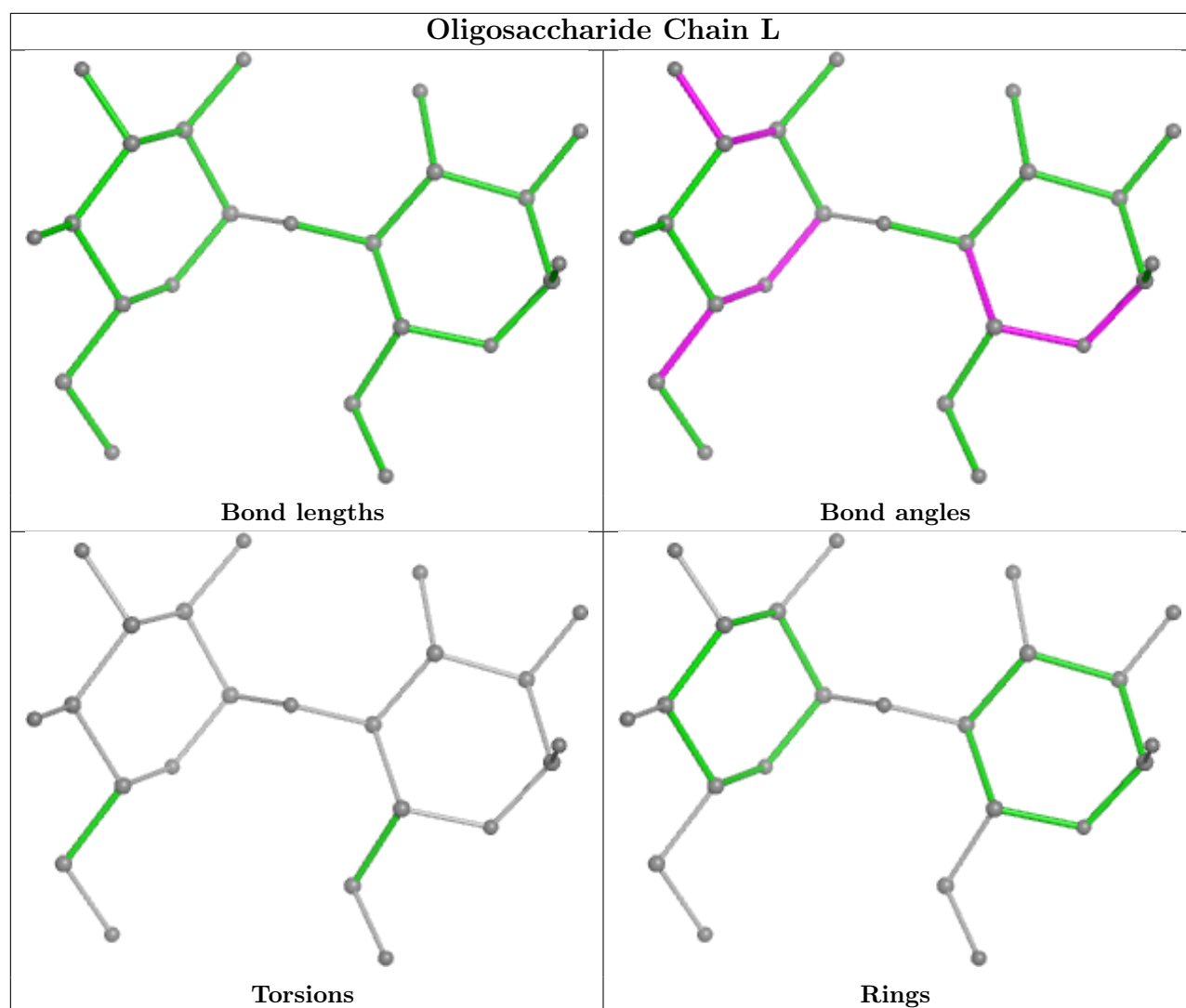
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GLC	1	0
2	I	1	GLC	1	0

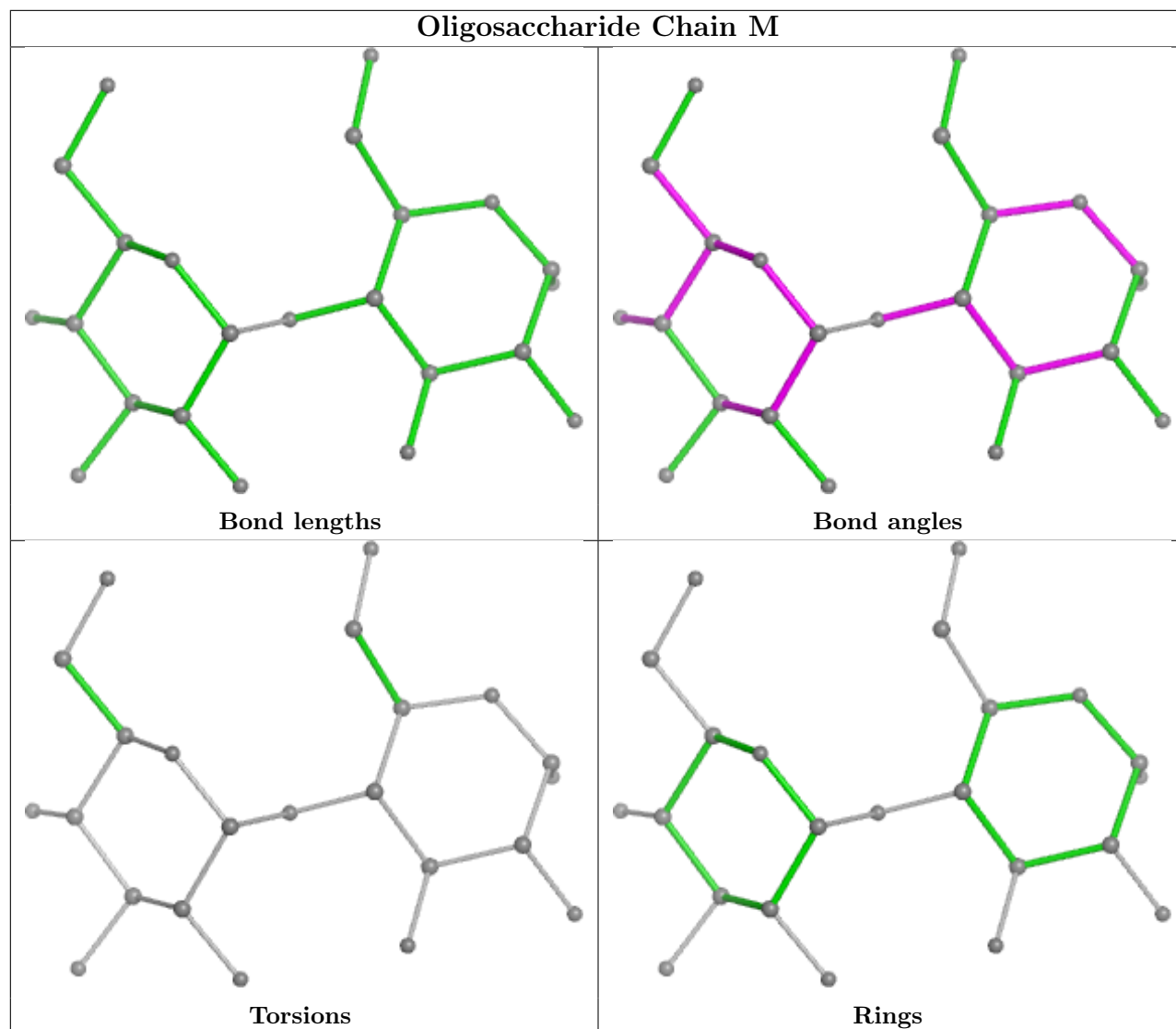
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

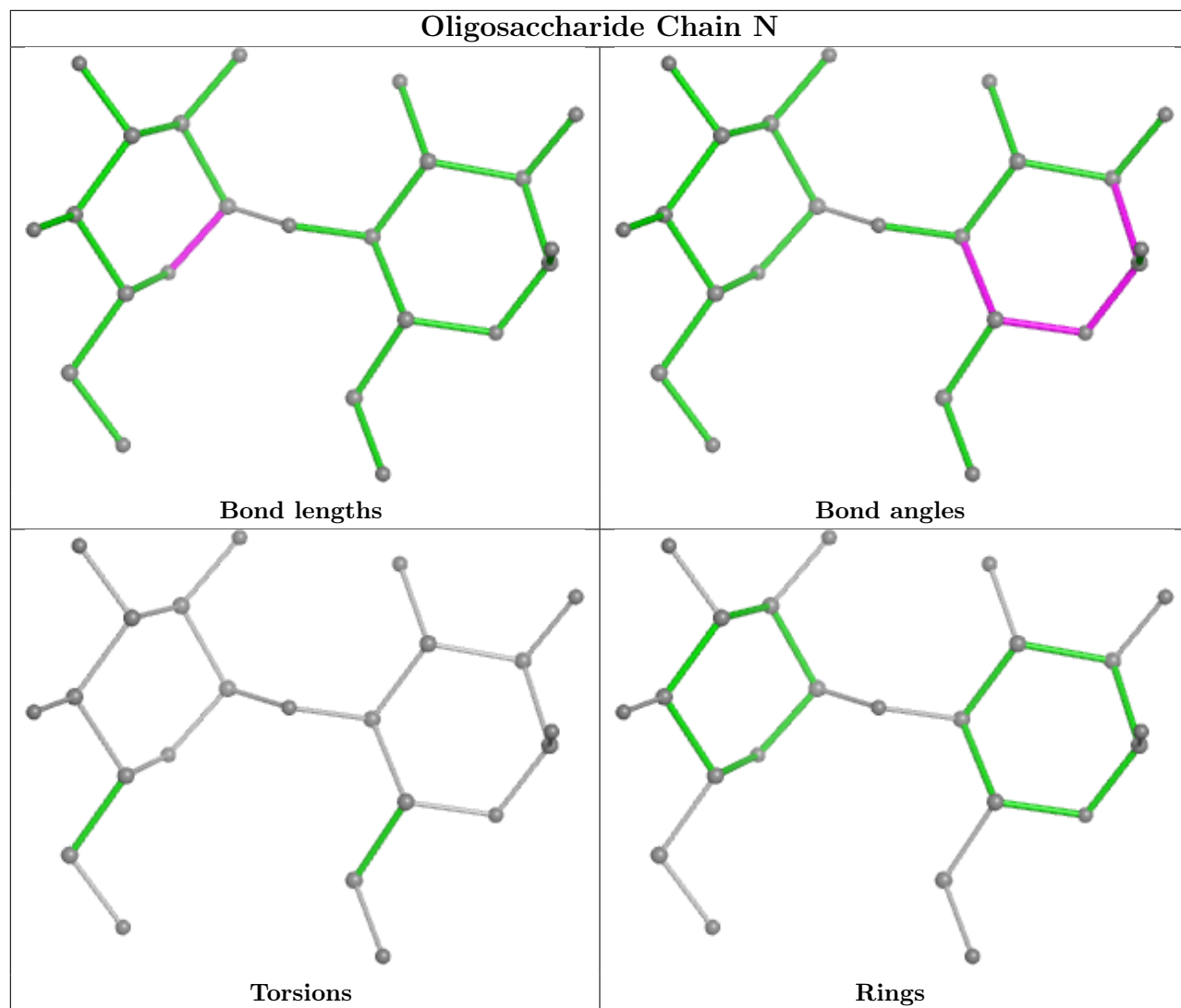




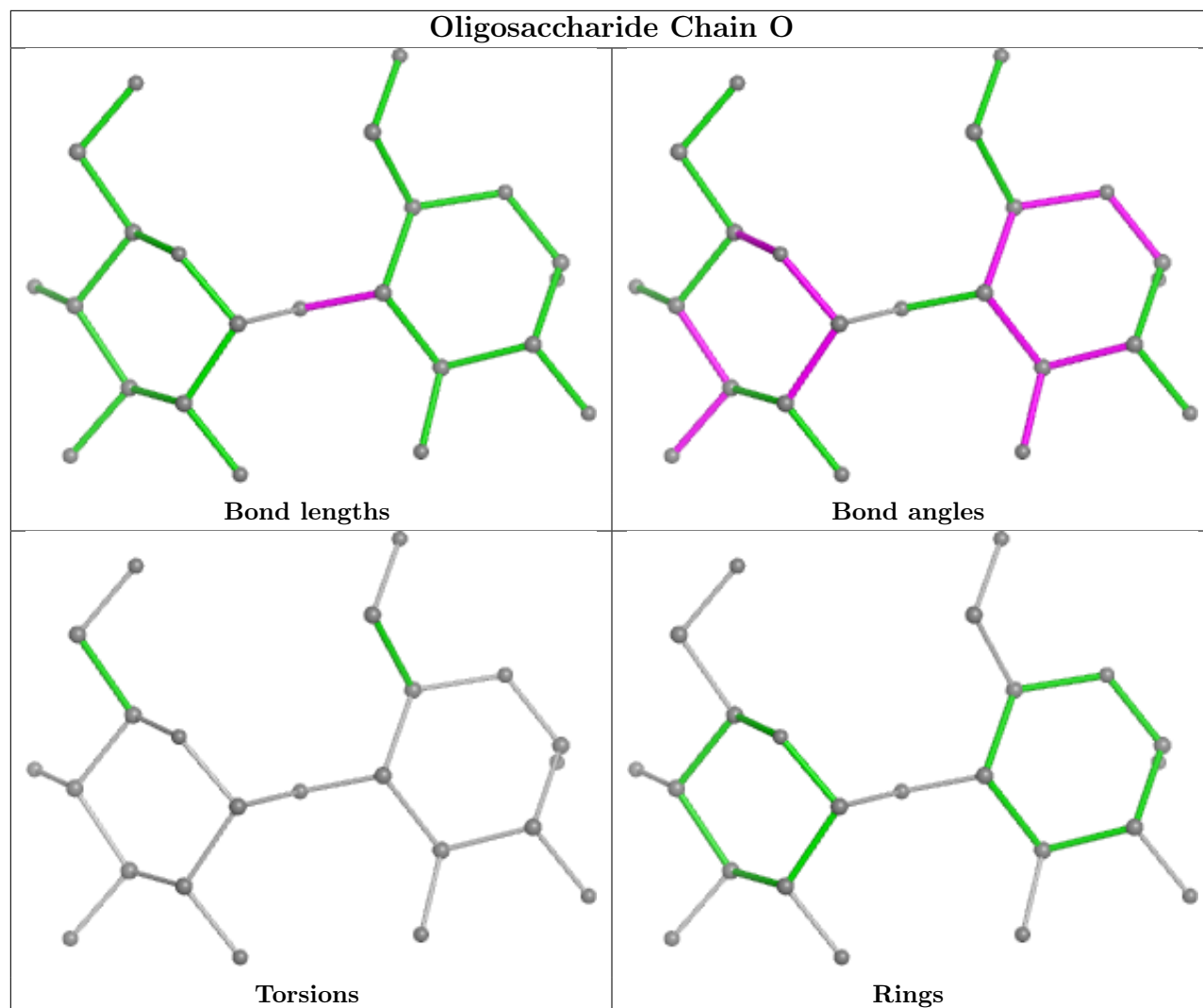


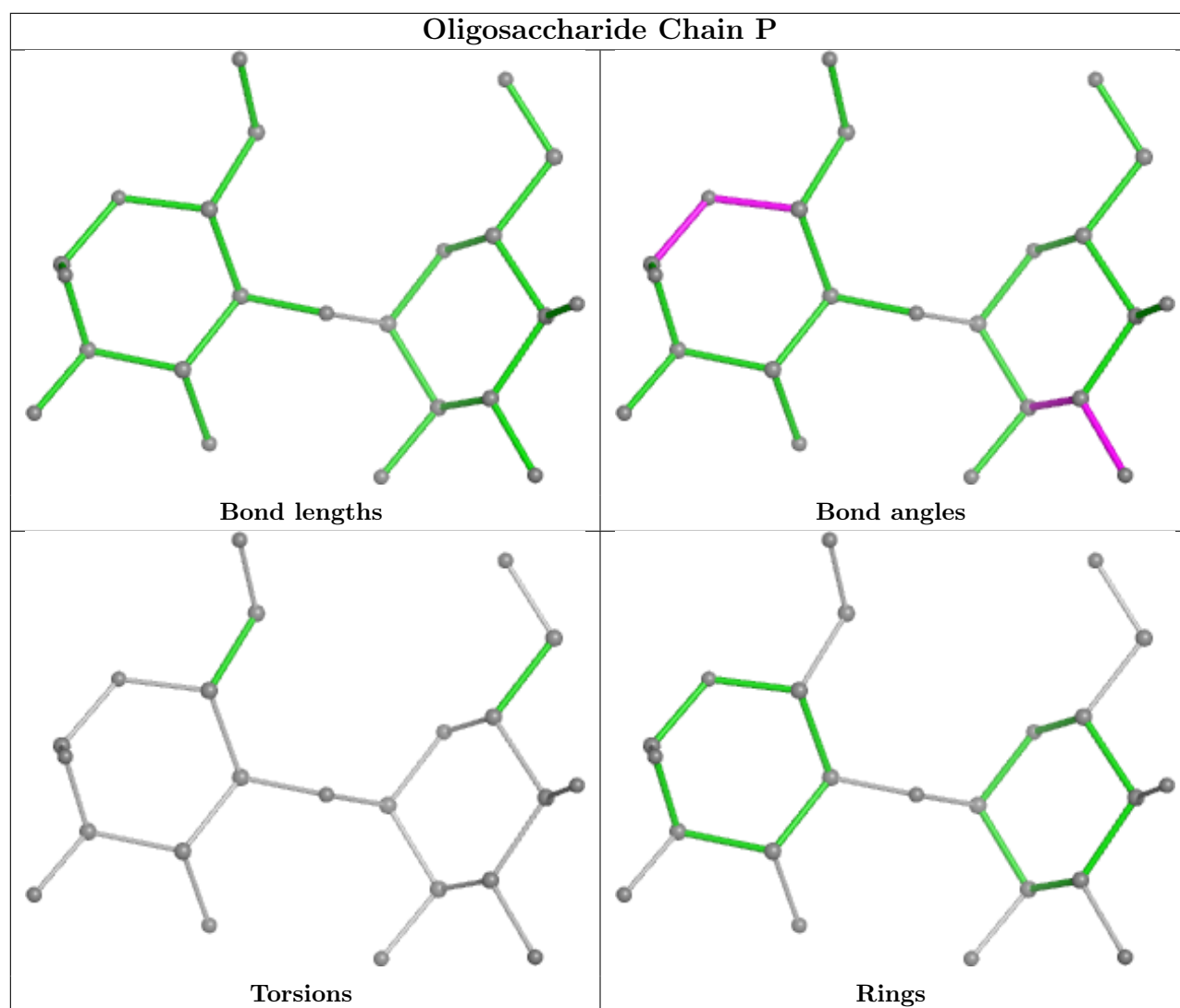












## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
3	SO4	G	1097	-	4,4,4	0.72	0	6,6,6	1.03	0
3	SO4	C	1096	-	4,4,4	0.54	0	6,6,6	1.35	1 (16%)
3	SO4	A	1097	-	4,4,4	0.26	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	F	1096	-	4,4,4	0.83	0	6,6,6	0.52	0
3	SO4	G	1098	-	4,4,4	0.21	0	6,6,6	0.48	0
4	GLC	D	300	-	12,12,12	0.64	0	17,17,17	0.81	0
3	SO4	A	1099	-	4,4,4	0.13	0	6,6,6	0.44	0
3	SO4	A	1100	-	4,4,4	0.19	0	6,6,6	0.36	0
3	SO4	A	1098	-	4,4,4	0.17	0	6,6,6	0.51	0
3	SO4	C	1097	-	4,4,4	0.31	0	6,6,6	0.37	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
4	GLC	D	300	-	1/1/5/5	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1096	SO4	O4-S-O3	2.12	118.09	109.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	300	GLC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1097	SO4	1	0
3	A	1097	SO4	1	0
3	A	1099	SO4	2	0
3	C	1097	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	93/98 (94%)	-0.18	1 (1%) 80 81	26, 37, 50, 59	0
1	B	94/98 (95%)	-0.23	0 100 100	27, 35, 46, 57	0
1	C	91/98 (92%)	-0.27	1 (1%) 80 81	26, 35, 45, 48	0
1	D	92/98 (93%)	-0.16	1 (1%) 80 81	29, 41, 51, 54	0
1	E	92/98 (93%)	-0.41	0 100 100	26, 33, 47, 52	0
1	F	91/98 (92%)	-0.16	0 100 100	29, 38, 52, 66	0
1	G	92/98 (93%)	-0.26	0 100 100	29, 40, 52, 55	0
1	H	92/98 (93%)	-0.13	0 100 100	26, 37, 53, 56	0
All	All	737/784 (94%)	-0.23	3 (0%) 92 93	26, 37, 51, 66	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	ASP	2.2
1	A	46	GLY	2.2
1	D	21	LEU	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](#)

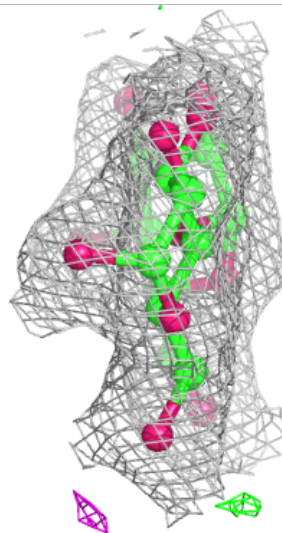
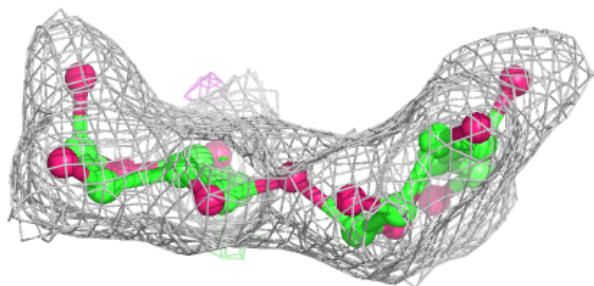
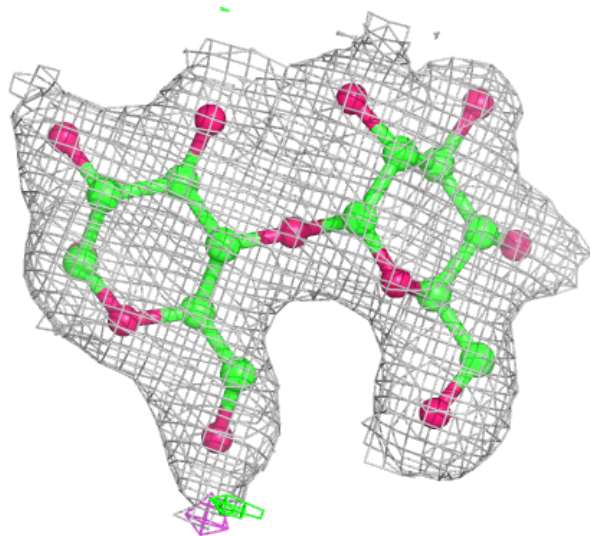
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	J	2	11/12	0.96	0.09	25,28,31,34	0
2	GLC	K	2	11/12	0.96	0.08	24,27,30,31	0
2	GLC	O	2	11/12	0.96	0.07	30,35,36,39	0
2	GLC	P	2	11/12	0.96	0.08	26,30,35,36	0
2	GLC	L	2	11/12	0.97	0.07	24,29,30,32	0
2	GLC	P	1	12/12	0.97	0.07	28,30,32,34	0
2	GLC	M	2	11/12	0.97	0.07	25,27,30,30	0
2	GLC	J	1	12/12	0.98	0.07	24,29,33,33	0
2	GLC	M	1	12/12	0.98	0.07	22,26,30,33	0
2	GLC	I	1	12/12	0.98	0.07	24,30,33,34	0
2	GLC	N	1	12/12	0.98	0.07	26,28,31,34	0
2	GLC	N	2	11/12	0.98	0.07	29,30,31,32	0
2	GLC	O	1	12/12	0.98	0.07	27,32,33,34	0
2	GLC	K	1	12/12	0.98	0.07	28,32,35,39	0
2	GLC	I	2	11/12	0.98	0.07	25,31,33,36	0
2	GLC	L	1	12/12	0.98	0.07	27,30,32,34	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.

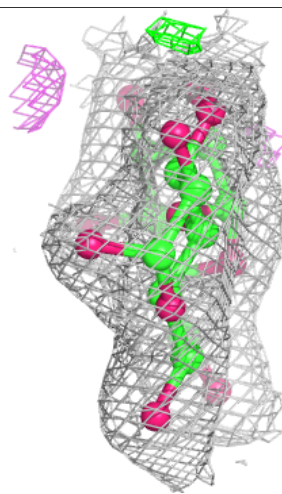
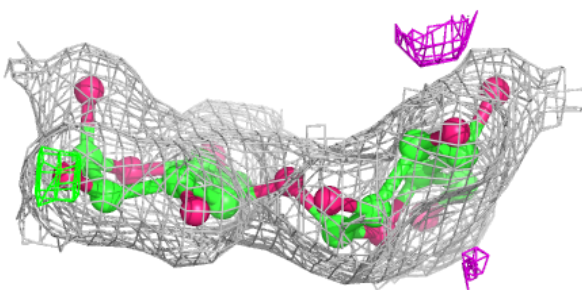
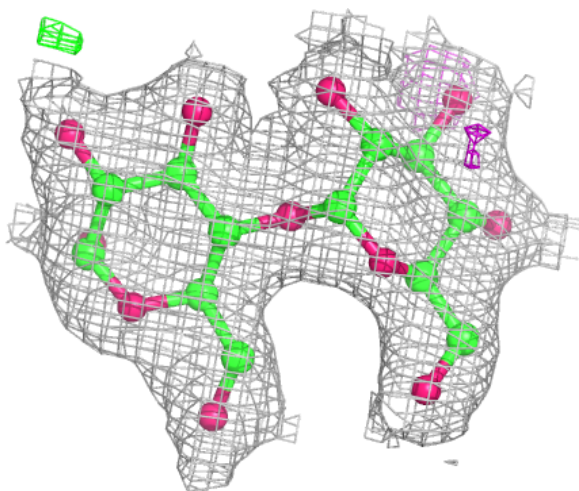
**Electron density around Chain I:**

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



**Electron density around Chain J:**

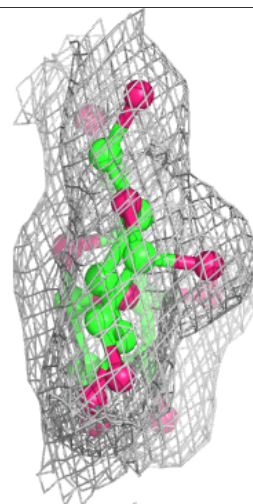
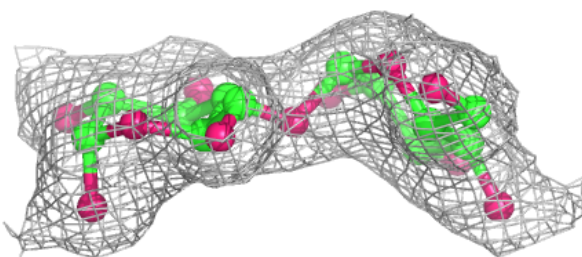
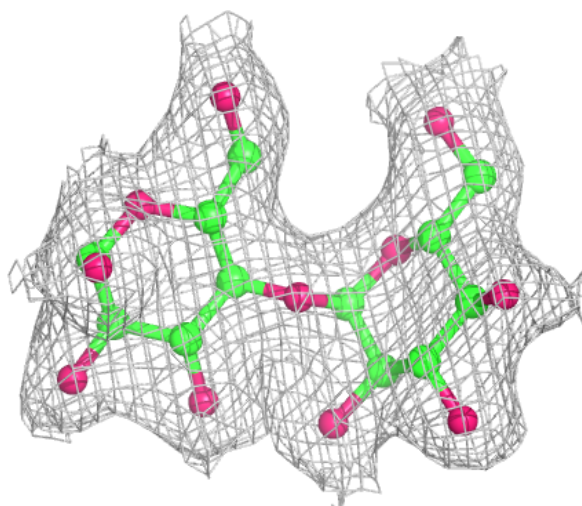
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





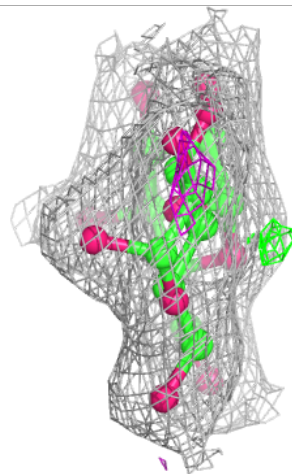
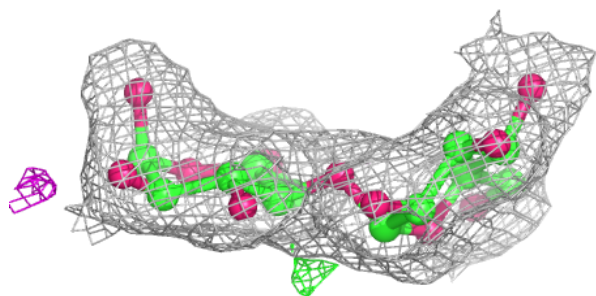
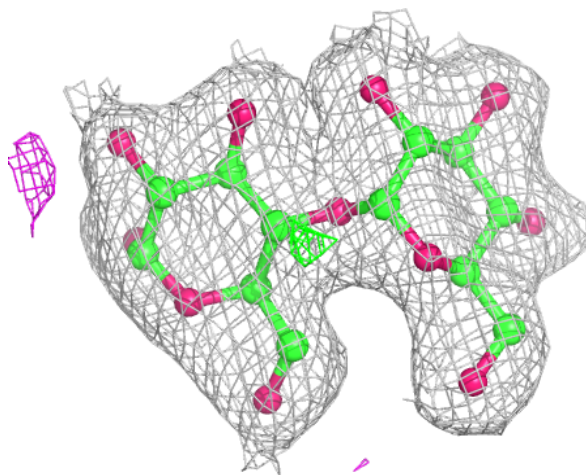
**Electron density around Chain K:**

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



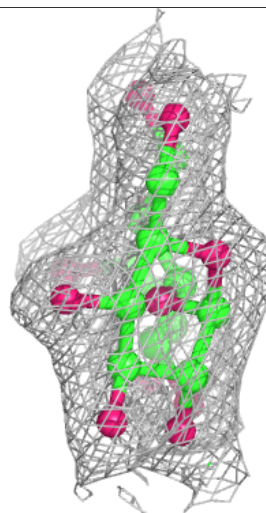
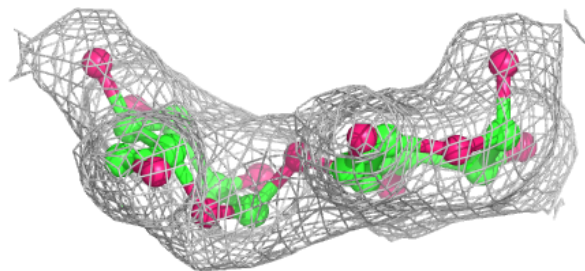
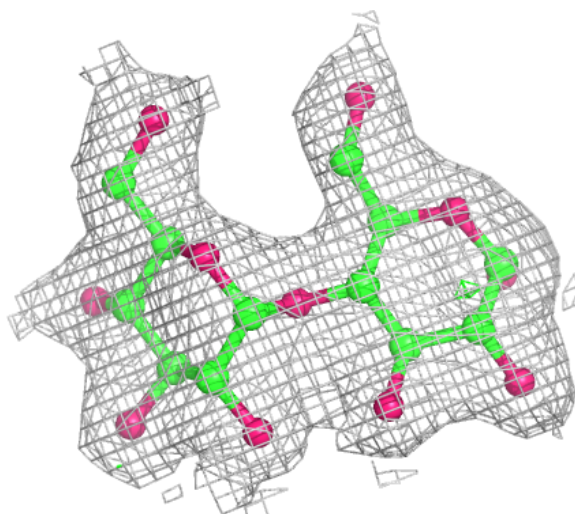
**Electron density around Chain L:**

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



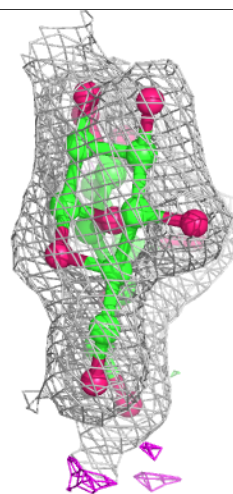
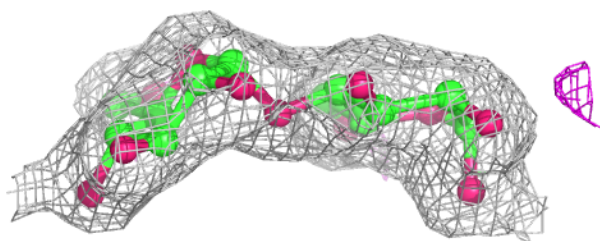
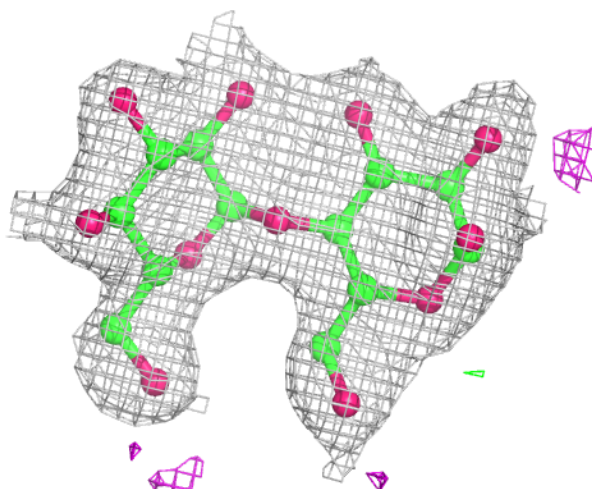
**Electron density around Chain M:**

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



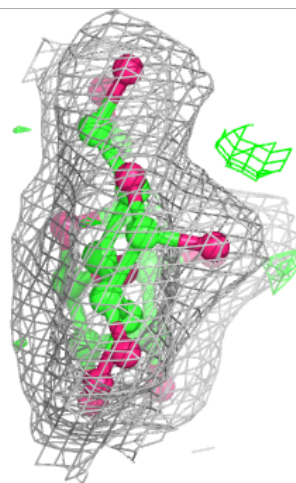
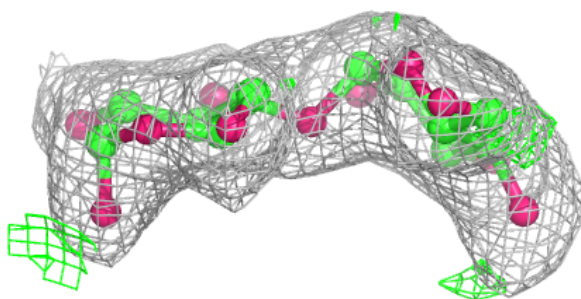
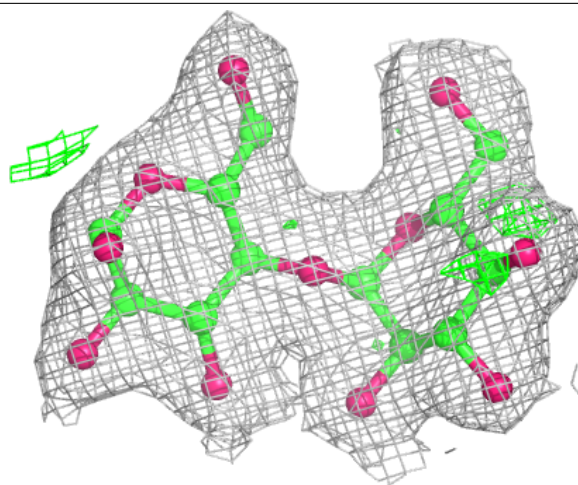
**Electron density around Chain N:**

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

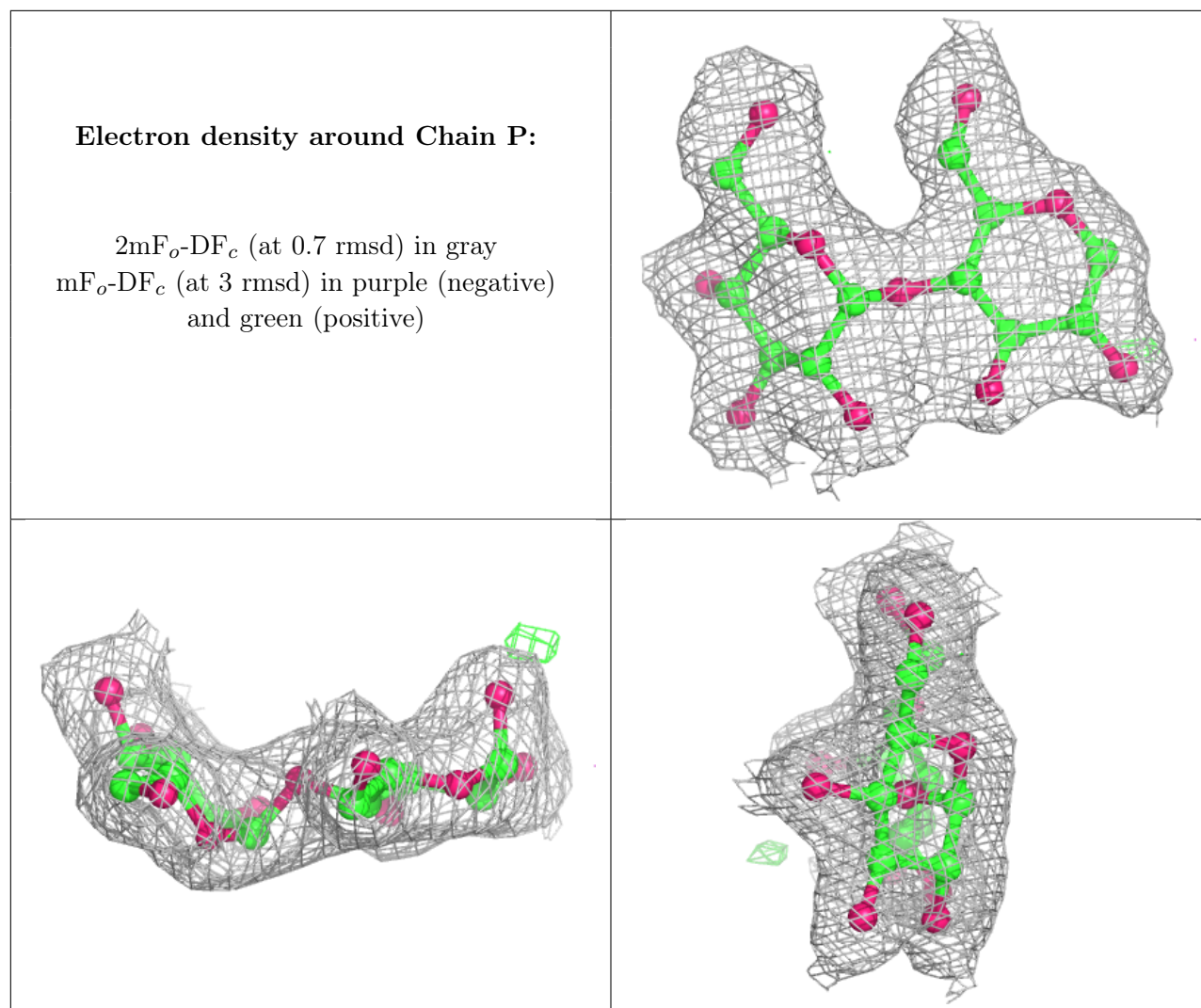


**Electron density around Chain O:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GLC	D	300	12/12	0.56	0.28	93,95,95,95	0
3	SO4	F	1096	5/5	0.93	0.17	48,49,51,53	0
3	SO4	A	1098	5/5	0.96	0.16	64,65,66,67	0
3	SO4	G	1098	5/5	0.96	0.22	68,70,70,70	0
3	SO4	C	1097	5/5	0.96	0.22	53,54,57,58	0
3	SO4	A	1097	5/5	0.97	0.19	57,61,62,62	0
3	SO4	A	1099	5/5	0.97	0.27	60,61,64,64	0
3	SO4	C	1096	5/5	0.98	0.10	38,38,42,42	0

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*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	G	1097	5/5	0.98	0.15	33,38,43,45	0
3	SO4	A	1100	5/5	0.99	0.06	49,51,53,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.