



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 05:37 AM EDT

PDB ID : 6QUG  
Title : GHK tagged MBP-Nup98(1-29)  
Authors : Huyton, T.; Gorlich, D.  
Deposited on : 2019-02-27  
Resolution : 2.70 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](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

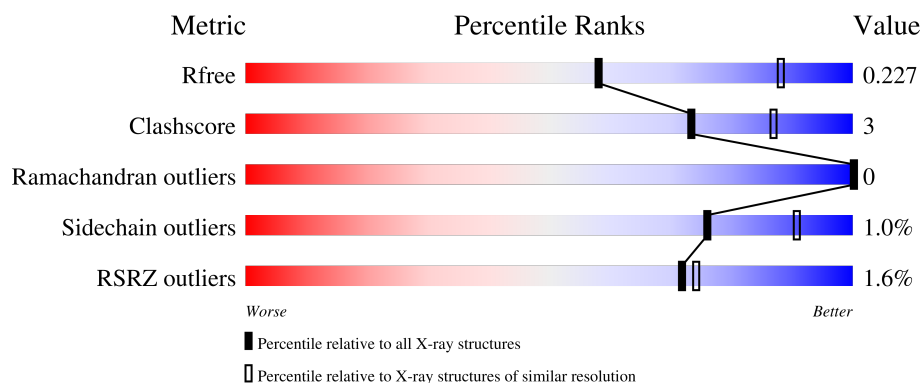
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.














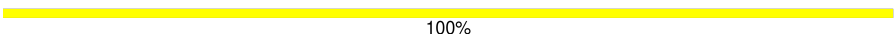
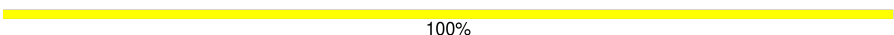
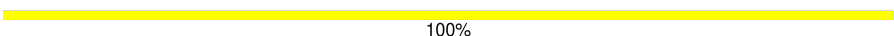

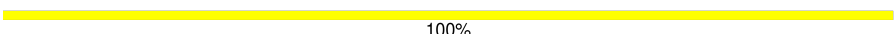
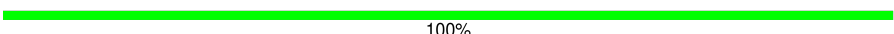
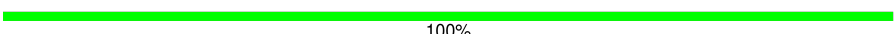

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	402	
1	B	402	
1	C	402	
1	D	402	
1	E	402	

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Mol	Chain	Length	Quality of chain
1	F	402	
1	G	402	
1	H	402	
1	I	402	
1	J	402	
1	K	402	
1	L	402	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34893 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 Maltodextrin-binding protein,Nucleoporin, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	B	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	C	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	D	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	E	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	F	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	G	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	H	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	I	372	Total	C	N	O	S	0	0	0
			2854	1839	467	542	6			
1	J	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	K	373	Total	C	N	O	S	0	0	0
			2859	1842	468	543	6			
1	L	372	Total	C	N	O	S	0	0	0
			2854	1839	467	542	6			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A376KDN7
A	-1	HIS	-	expression tag	UNP A0A376KDN7
A	0	LYS	-	expression tag	UNP A0A376KDN7
A	82	ALA	ASP	conflict	UNP A0A376KDN7
A	83	ALA	LYS	conflict	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	172	ALA	GLU	conflict	UNP A0A376KDN7
A	173	ALA	ASN	conflict	UNP A0A376KDN7
A	239	ALA	LYS	conflict	UNP A0A376KDN7
A	362	ALA	LYS	conflict	UNP A0A376KDN7
A	363	ALA	ASP	conflict	UNP A0A376KDN7
A	367	ASN	-	linker	UNP A0A376KDN7
A	368	ALA	-	linker	UNP A0A376KDN7
A	369	ALA	-	linker	UNP A0A376KDN7
A	370	ALA	-	linker	UNP A0A376KDN7
B	-2	GLY	-	expression tag	UNP A0A376KDN7
B	-1	HIS	-	expression tag	UNP A0A376KDN7
B	0	LYS	-	expression tag	UNP A0A376KDN7
B	82	ALA	ASP	conflict	UNP A0A376KDN7
B	83	ALA	LYS	conflict	UNP A0A376KDN7
B	172	ALA	GLU	conflict	UNP A0A376KDN7
B	173	ALA	ASN	conflict	UNP A0A376KDN7
B	239	ALA	LYS	conflict	UNP A0A376KDN7
B	362	ALA	LYS	conflict	UNP A0A376KDN7
B	363	ALA	ASP	conflict	UNP A0A376KDN7
B	367	ASN	-	linker	UNP A0A376KDN7
B	368	ALA	-	linker	UNP A0A376KDN7
B	369	ALA	-	linker	UNP A0A376KDN7
B	370	ALA	-	linker	UNP A0A376KDN7
C	-2	GLY	-	expression tag	UNP A0A376KDN7
C	-1	HIS	-	expression tag	UNP A0A376KDN7
C	0	LYS	-	expression tag	UNP A0A376KDN7
C	82	ALA	ASP	conflict	UNP A0A376KDN7
C	83	ALA	LYS	conflict	UNP A0A376KDN7
C	172	ALA	GLU	conflict	UNP A0A376KDN7
C	173	ALA	ASN	conflict	UNP A0A376KDN7
C	239	ALA	LYS	conflict	UNP A0A376KDN7
C	362	ALA	LYS	conflict	UNP A0A376KDN7
C	363	ALA	ASP	conflict	UNP A0A376KDN7
C	367	ASN	-	linker	UNP A0A376KDN7
C	368	ALA	-	linker	UNP A0A376KDN7
C	369	ALA	-	linker	UNP A0A376KDN7
C	370	ALA	-	linker	UNP A0A376KDN7
D	-2	GLY	-	expression tag	UNP A0A376KDN7
D	-1	HIS	-	expression tag	UNP A0A376KDN7
D	0	LYS	-	expression tag	UNP A0A376KDN7
D	82	ALA	ASP	conflict	UNP A0A376KDN7
D	83	ALA	LYS	conflict	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	172	ALA	GLU	conflict	UNP A0A376KDN7
D	173	ALA	ASN	conflict	UNP A0A376KDN7
D	239	ALA	LYS	conflict	UNP A0A376KDN7
D	362	ALA	LYS	conflict	UNP A0A376KDN7
D	363	ALA	ASP	conflict	UNP A0A376KDN7
D	367	ASN	-	linker	UNP A0A376KDN7
D	368	ALA	-	linker	UNP A0A376KDN7
D	369	ALA	-	linker	UNP A0A376KDN7
D	370	ALA	-	linker	UNP A0A376KDN7
E	-2	GLY	-	expression tag	UNP A0A376KDN7
E	-1	HIS	-	expression tag	UNP A0A376KDN7
E	0	LYS	-	expression tag	UNP A0A376KDN7
E	82	ALA	ASP	conflict	UNP A0A376KDN7
E	83	ALA	LYS	conflict	UNP A0A376KDN7
E	172	ALA	GLU	conflict	UNP A0A376KDN7
E	173	ALA	ASN	conflict	UNP A0A376KDN7
E	239	ALA	LYS	conflict	UNP A0A376KDN7
E	362	ALA	LYS	conflict	UNP A0A376KDN7
E	363	ALA	ASP	conflict	UNP A0A376KDN7
E	367	ASN	-	linker	UNP A0A376KDN7
E	368	ALA	-	linker	UNP A0A376KDN7
E	369	ALA	-	linker	UNP A0A376KDN7
E	370	ALA	-	linker	UNP A0A376KDN7
F	-2	GLY	-	expression tag	UNP A0A376KDN7
F	-1	HIS	-	expression tag	UNP A0A376KDN7
F	0	LYS	-	expression tag	UNP A0A376KDN7
F	82	ALA	ASP	conflict	UNP A0A376KDN7
F	83	ALA	LYS	conflict	UNP A0A376KDN7
F	172	ALA	GLU	conflict	UNP A0A376KDN7
F	173	ALA	ASN	conflict	UNP A0A376KDN7
F	239	ALA	LYS	conflict	UNP A0A376KDN7
F	362	ALA	LYS	conflict	UNP A0A376KDN7
F	363	ALA	ASP	conflict	UNP A0A376KDN7
F	367	ASN	-	linker	UNP A0A376KDN7
F	368	ALA	-	linker	UNP A0A376KDN7
F	369	ALA	-	linker	UNP A0A376KDN7
F	370	ALA	-	linker	UNP A0A376KDN7
G	-2	GLY	-	expression tag	UNP A0A376KDN7
G	-1	HIS	-	expression tag	UNP A0A376KDN7
G	0	LYS	-	expression tag	UNP A0A376KDN7
G	82	ALA	ASP	conflict	UNP A0A376KDN7
G	83	ALA	LYS	conflict	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	172	ALA	GLU	conflict	UNP A0A376KDN7
G	173	ALA	ASN	conflict	UNP A0A376KDN7
G	239	ALA	LYS	conflict	UNP A0A376KDN7
G	362	ALA	LYS	conflict	UNP A0A376KDN7
G	363	ALA	ASP	conflict	UNP A0A376KDN7
G	367	ASN	-	linker	UNP A0A376KDN7
G	368	ALA	-	linker	UNP A0A376KDN7
G	369	ALA	-	linker	UNP A0A376KDN7
G	370	ALA	-	linker	UNP A0A376KDN7
H	-2	GLY	-	expression tag	UNP A0A376KDN7
H	-1	HIS	-	expression tag	UNP A0A376KDN7
H	0	LYS	-	expression tag	UNP A0A376KDN7
H	82	ALA	ASP	conflict	UNP A0A376KDN7
H	83	ALA	LYS	conflict	UNP A0A376KDN7
H	172	ALA	GLU	conflict	UNP A0A376KDN7
H	173	ALA	ASN	conflict	UNP A0A376KDN7
H	239	ALA	LYS	conflict	UNP A0A376KDN7
H	362	ALA	LYS	conflict	UNP A0A376KDN7
H	363	ALA	ASP	conflict	UNP A0A376KDN7
H	367	ASN	-	linker	UNP A0A376KDN7
H	368	ALA	-	linker	UNP A0A376KDN7
H	369	ALA	-	linker	UNP A0A376KDN7
H	370	ALA	-	linker	UNP A0A376KDN7
I	-2	GLY	-	expression tag	UNP A0A376KDN7
I	-1	HIS	-	expression tag	UNP A0A376KDN7
I	0	LYS	-	expression tag	UNP A0A376KDN7
I	82	ALA	ASP	conflict	UNP A0A376KDN7
I	83	ALA	LYS	conflict	UNP A0A376KDN7
I	172	ALA	GLU	conflict	UNP A0A376KDN7
I	173	ALA	ASN	conflict	UNP A0A376KDN7
I	239	ALA	LYS	conflict	UNP A0A376KDN7
I	362	ALA	LYS	conflict	UNP A0A376KDN7
I	363	ALA	ASP	conflict	UNP A0A376KDN7
I	367	ASN	-	linker	UNP A0A376KDN7
I	368	ALA	-	linker	UNP A0A376KDN7
I	369	ALA	-	linker	UNP A0A376KDN7
I	370	ALA	-	linker	UNP A0A376KDN7
J	-2	GLY	-	expression tag	UNP A0A376KDN7
J	-1	HIS	-	expression tag	UNP A0A376KDN7
J	0	LYS	-	expression tag	UNP A0A376KDN7
J	82	ALA	ASP	conflict	UNP A0A376KDN7
J	83	ALA	LYS	conflict	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ALA	GLU	conflict	UNP A0A376KDN7
J	173	ALA	ASN	conflict	UNP A0A376KDN7
J	239	ALA	LYS	conflict	UNP A0A376KDN7
J	362	ALA	LYS	conflict	UNP A0A376KDN7
J	363	ALA	ASP	conflict	UNP A0A376KDN7
J	367	ASN	-	linker	UNP A0A376KDN7
J	368	ALA	-	linker	UNP A0A376KDN7
J	369	ALA	-	linker	UNP A0A376KDN7
J	370	ALA	-	linker	UNP A0A376KDN7
K	-2	GLY	-	expression tag	UNP A0A376KDN7
K	-1	HIS	-	expression tag	UNP A0A376KDN7
K	0	LYS	-	expression tag	UNP A0A376KDN7
K	82	ALA	ASP	conflict	UNP A0A376KDN7
K	83	ALA	LYS	conflict	UNP A0A376KDN7
K	172	ALA	GLU	conflict	UNP A0A376KDN7
K	173	ALA	ASN	conflict	UNP A0A376KDN7
K	239	ALA	LYS	conflict	UNP A0A376KDN7
K	362	ALA	LYS	conflict	UNP A0A376KDN7
K	363	ALA	ASP	conflict	UNP A0A376KDN7
K	367	ASN	-	linker	UNP A0A376KDN7
K	368	ALA	-	linker	UNP A0A376KDN7
K	369	ALA	-	linker	UNP A0A376KDN7
K	370	ALA	-	linker	UNP A0A376KDN7
L	-2	GLY	-	expression tag	UNP A0A376KDN7
L	-1	HIS	-	expression tag	UNP A0A376KDN7
L	0	LYS	-	expression tag	UNP A0A376KDN7
L	82	ALA	ASP	conflict	UNP A0A376KDN7
L	83	ALA	LYS	conflict	UNP A0A376KDN7
L	172	ALA	GLU	conflict	UNP A0A376KDN7
L	173	ALA	ASN	conflict	UNP A0A376KDN7
L	239	ALA	LYS	conflict	UNP A0A376KDN7
L	362	ALA	LYS	conflict	UNP A0A376KDN7
L	363	ALA	ASP	conflict	UNP A0A376KDN7
L	367	ASN	-	linker	UNP A0A376KDN7
L	368	ALA	-	linker	UNP A0A376KDN7
L	369	ALA	-	linker	UNP A0A376KDN7
L	370	ALA	-	linker	UNP A0A376KDN7

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





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			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			
2	U	2	Total	C	O	0	0	0
			23	12	11			
2	V	2	Total	C	O	0	0	0
			23	12	11			
2	W	2	Total	C	O	0	0	0
			23	12	11			
2	X	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

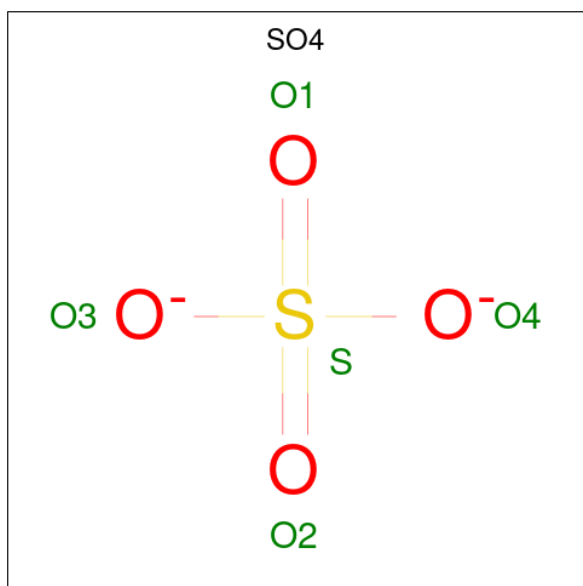
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	E	1	Total	Cu	0	0
			1	1		

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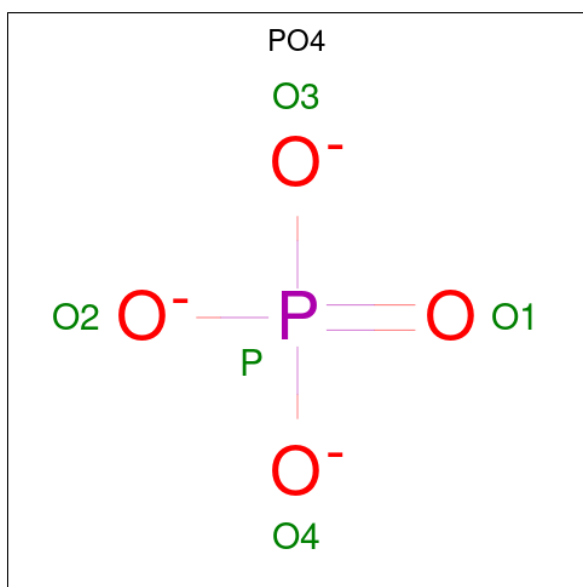
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Cu	0	0
			1	1		
3	G	1	Total	Cu	0	0
			1	1		
3	H	1	Total	Cu	0	0
			1	1		
3	I	1	Total	Cu	0	0
			1	1		
3	J	1	Total	Cu	0	0
			1	1		
3	K	1	Total	Cu	0	0
			1	1		
3	L	1	Total	Cu	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	I	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	18	Total	O	0	0
			18	18		
6	C	14	Total	O	0	0
			14	14		
6	D	18	Total	O	0	0
			18	18		
6	E	19	Total	O	0	0
			19	19		
6	F	21	Total	O	0	0
			21	21		
6	G	27	Total	O	0	0
			27	27		
6	H	17	Total	O	0	0
			17	17		

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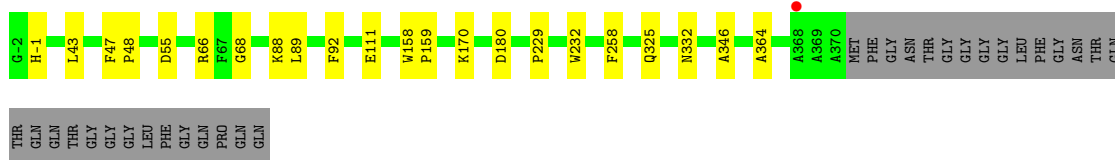
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	26	Total 26	O 26	0	0
6	J	33	Total 33	O 33	0	0
6	K	26	Total 26	O 26	0	0
6	L	23	Total 23	O 23	0	0

### 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.

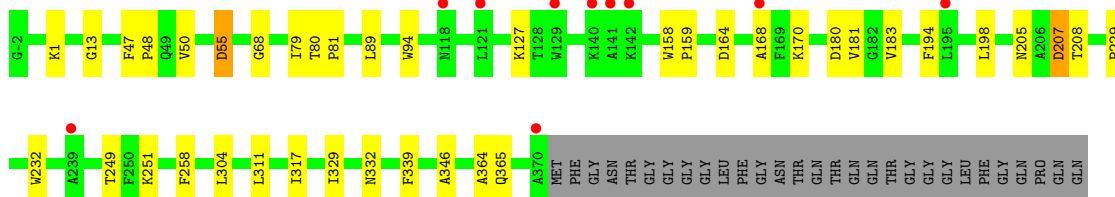
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

Chain A: 




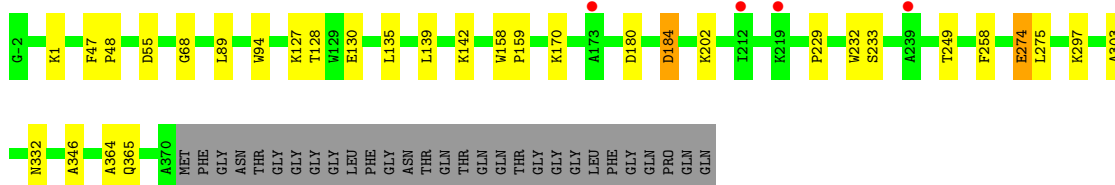
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

Chain B: 




- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

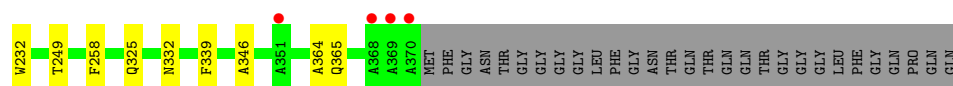
Chain C: 



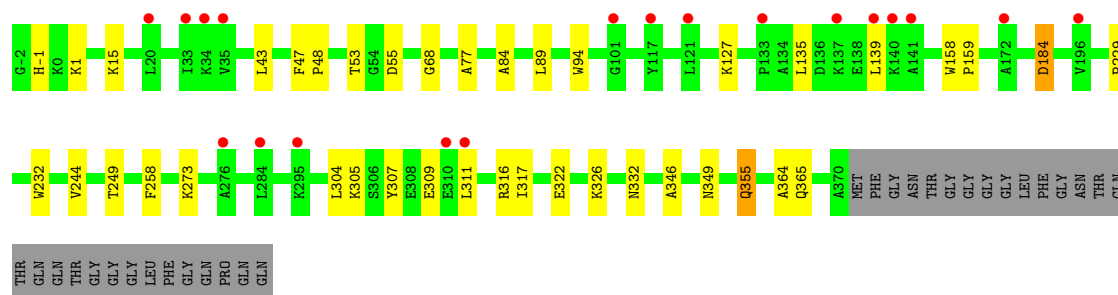
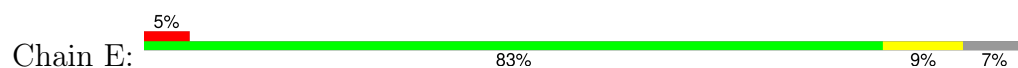
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

Chain D: 

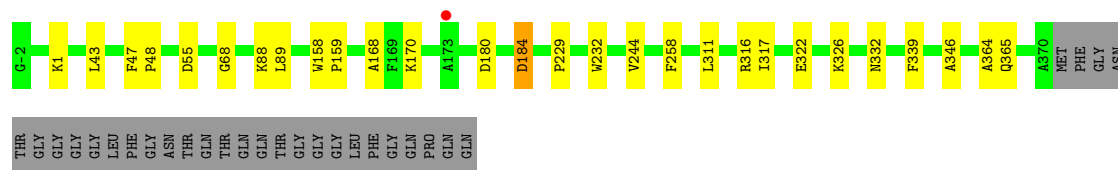




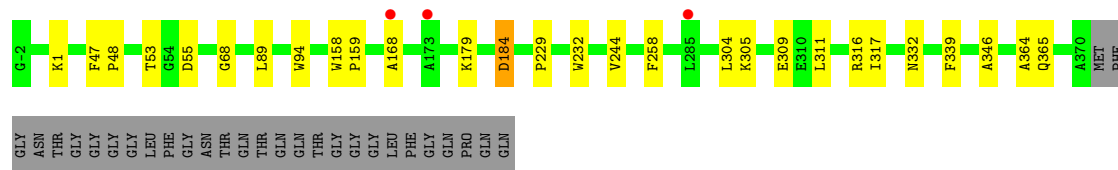
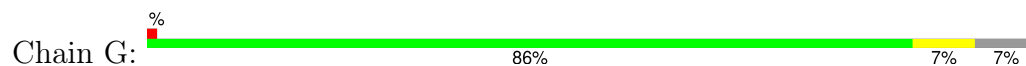
- Molecule 1: Maltodextrin-binding protein,Nucleoprin, putative



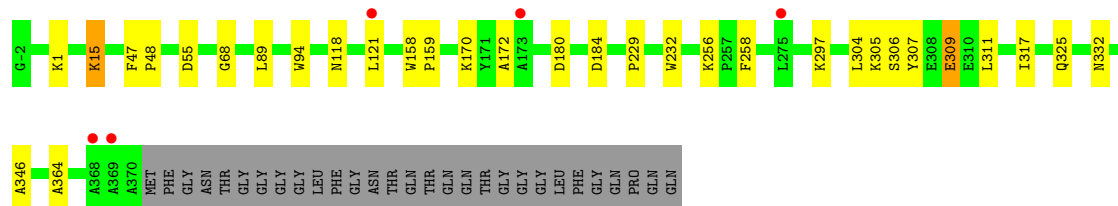
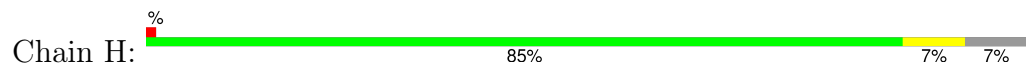
- Molecule 1: Maltodextrin-binding protein,Nucleoprin, putative



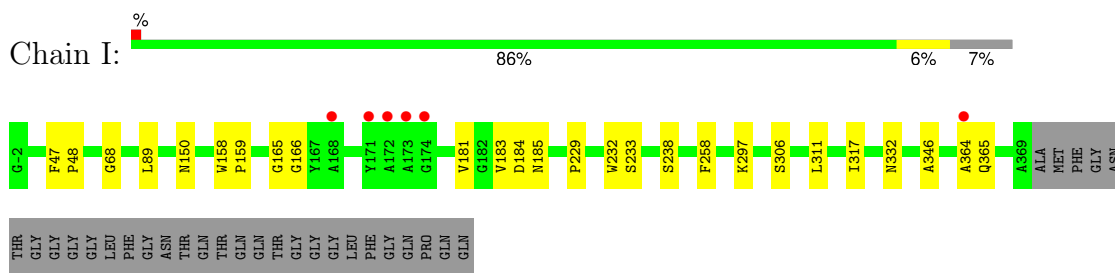
- Molecule 1: Maltodextrin-binding protein,Nucleoprin, putative



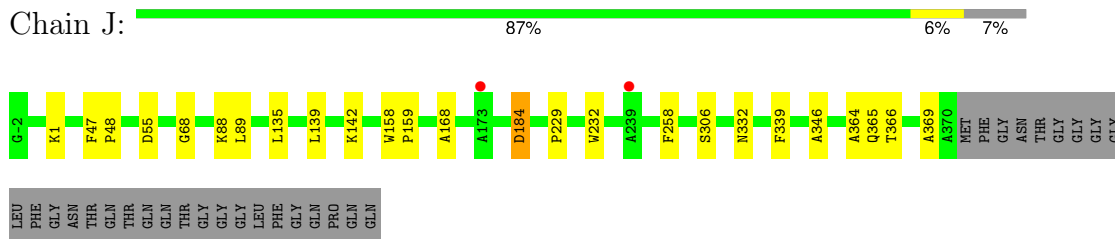
- Molecule 1: Maltodextrin-binding protein,Nucleoprin, putative



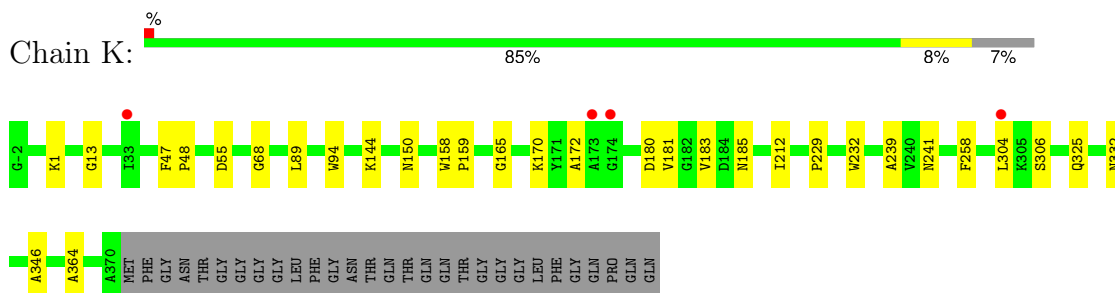
- Molecule 1: Maltodextrin-binding protein,Nucleoprin, putative



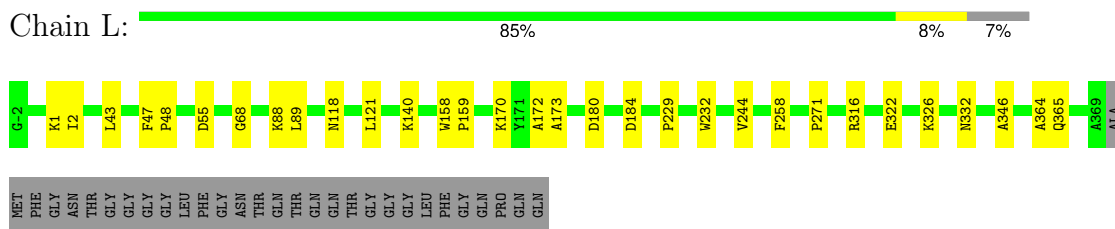
- Molecule 1: Maltodextrin-binding protein, Nucleoporin, putative



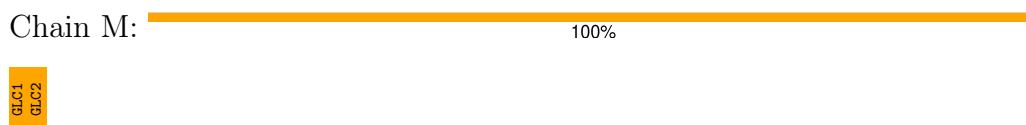
- Molecule 1: Maltodextrin-binding protein, Nucleoporin, putative



- Molecule 1: Maltodextrin-binding protein, Nucleoporin, putative



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



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





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

Chain O: 



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

Chain P: 

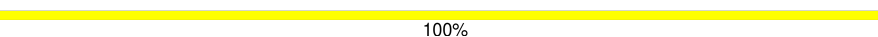


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q: 



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

Chain R: 



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

Chain S: 



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

Chain T: 



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

Chain U: 



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



Chain V:  100%



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

Chain W:  100%



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

Chain X:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.91Å 286.78Å 110.78Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.19 – 2.70 49.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.19-2.70) 100.0 (49.14-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.207 , 0.226 0.208 , 0.227	Depositor DCC
$R_{free}$ test set	7064 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PO4, GLC, CU

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	0.73	0/2929	0.74	0/3981
1	B	0.73	0/2929	0.74	0/3981
1	C	0.72	0/2929	0.74	0/3981
1	D	0.72	0/2929	0.73	0/3981
1	E	0.71	0/2929	0.73	0/3981
1	F	0.72	0/2929	0.73	0/3981
1	G	0.74	0/2929	0.74	0/3981
1	H	0.73	0/2929	0.74	0/3981
1	I	0.75	0/2924	0.74	0/3974
1	J	0.73	0/2929	0.74	0/3981
1	K	0.73	0/2929	0.74	0/3981
1	L	0.73	0/2924	0.73	0/3974
All	All	0.73	0/35138	0.74	0/47758

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2859	0	2833	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2859	0	2833	30	0
1	C	2859	0	2833	21	0
1	D	2859	0	2833	19	0
1	E	2859	0	2833	29	0
1	F	2859	0	2833	17	0
1	G	2859	0	2833	18	0
1	H	2859	0	2833	19	0
1	I	2854	0	2828	13	0
1	J	2859	0	2833	14	0
1	K	2859	0	2833	21	0
1	L	2854	0	2828	25	0
2	M	23	0	21	2	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
2	Q	23	0	21	0	0
2	R	23	0	21	0	0
2	S	23	0	21	0	0
2	T	23	0	21	0	0
2	U	23	0	21	0	0
2	V	23	0	21	0	0
2	W	23	0	21	0	0
2	X	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	C	5	0	0	0	0
4	K	5	0	0	1	0
4	L	5	0	0	0	0
5	D	10	0	0	0	0
5	I	5	0	0	1	0
5	J	5	0	0	0	0
6	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	0	0	0
6	C	14	0	0	0	0
6	D	18	0	0	0	0
6	E	19	0	0	0	0
6	F	21	0	0	0	0
6	G	27	0	0	0	0
6	H	17	0	0	0	0
6	I	26	0	0	0	0
6	J	33	0	0	0	0
6	K	26	0	0	2	0
6	L	23	0	0	1	0
All	All	34893	0	34238	225	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 3.

All (225) 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:D:115:LEU:HD11	1:D:224:MET:HE3	1.26	1.07
1:B:1:LYS:HD3	1:B:55:ASP:OD1	1.75	0.86
1:B:170:LYS:HD2	1:B:180:ASP:OD2	1.76	0.83
1:E:349:ASN:HB3	1:E:355:GLN:HG3	1.65	0.79
1:B:194:PHE:CE2	1:B:198:LEU:HD11	2.19	0.78
1:E:84:ALA:HB2	1:L:121:LEU:CD1	2.17	0.74
1:C:1:LYS:HA	1:C:55:ASP:OD1	1.87	0.74
1:A:325:GLN:HA	1:L:172:ALA:HB1	1.70	0.72
1:E:84:ALA:HB2	1:L:121:LEU:HD12	1.72	0.72
1:B:50:VAL:CG1	1:B:55:ASP:HB3	2.19	0.72
1:D:115:LEU:HD11	1:D:224:MET:CE	2.15	0.71
1:G:305:LYS:O	1:G:309:GLU:HG2	1.91	0.70
1:H:325:GLN:HA	1:K:172:ALA:HB1	1.72	0.70
1:E:1:LYS:HE3	1:E:53:THR:O	1.92	0.69
1:B:194:PHE:O	1:B:198:LEU:HD13	1.92	0.69
1:C:135:LEU:O	1:C:139:LEU:HD12	1.93	0.69
1:E:135:LEU:O	1:E:139:LEU:HD12	1.92	0.69
1:D:82:ALA:HA	1:K:239:ALA:HB1	1.75	0.69
1:E:307:TYR:O	1:E:311:LEU:HD13	1.93	0.68
1:H:307:TYR:O	1:H:311:LEU:HD13	1.93	0.67
1:D:135:LEU:O	1:D:139:LEU:HD12	1.94	0.66
1:I:150:ASN:ND2	5:I:402:PO4:O2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:135:LEU:O	1:J:139:LEU:HD12	1.95	0.65
1:E:305:LYS:O	1:E:309:GLU:HG2	1.96	0.65
1:G:168:ALA:HB2	1:G:339:PHE:CZ	2.32	0.64
1:K:1:LYS:HA	1:K:55:ASP:OD1	1.98	0.64
1:D:87:ASP:OD2	1:K:144:LYS:NZ	2.21	0.64
1:F:168:ALA:HB2	1:F:339:PHE:CZ	2.32	0.64
1:J:1:LYS:HA	1:J:55:ASP:OD1	1.98	0.64
1:C:274:GLU:CD	1:C:274:GLU:H	2.02	0.63
1:H:172:ALA:HB1	1:K:325:GLN:HA	1.82	0.62
1:K:181:VAL:HG12	1:K:183:VAL:HG13	1.82	0.62
1:D:1:LYS:HE2	1:D:53:THR:O	2.00	0.62
1:H:1:LYS:HA	1:H:55:ASP:OD1	2.00	0.62
1:H:307:TYR:CZ	1:H:311:LEU:HD11	2.35	0.61
1:D:115:LEU:CD1	1:D:224:MET:HE3	2.16	0.61
1:E:307:TYR:CZ	1:E:311:LEU:HD11	2.35	0.61
1:B:170:LYS:CD	1:B:180:ASP:OD2	2.48	0.60
1:B:50:VAL:HG12	1:B:55:ASP:HB3	1.82	0.60
1:C:89:LEU:HD23	1:C:303:ALA:CB	2.32	0.60
1:G:1:LYS:CE	1:G:53:THR:O	2.50	0.59
1:L:2:ILE:CG2	1:L:271:PRO:HD2	2.32	0.59
1:B:181:VAL:HG12	1:B:183:VAL:HG22	1.83	0.59
1:H:305:LYS:O	1:H:309:GLU:HG2	2.02	0.59
1:B:329:ILE:H	1:B:329:ILE:HD12	1.69	0.57
1:C:89:LEU:HD23	1:C:303:ALA:HB3	1.85	0.57
1:B:164:ASP:OD2	1:B:251:LYS:HE2	2.04	0.57
1:K:150:ASN:ND2	4:K:402:SO4:O3	2.38	0.56
1:C:128:THR:OG1	1:C:130:GLU:OE1	2.23	0.56
1:I:166:GLY:HA2	1:I:185:ASN:HD21	1.70	0.56
1:J:168:ALA:HB2	1:J:339:PHE:CZ	2.42	0.55
1:B:89:LEU:HD12	1:B:94:TRP:CZ2	2.41	0.55
1:I:165:GLY:O	1:I:185:ASN:ND2	2.40	0.55
1:E:77:ALA:HB2	1:E:273:LYS:HE2	1.88	0.55
1:E:89:LEU:HD12	1:E:94:TRP:CZ2	2.42	0.55
1:L:184:ASP:HB2	1:L:365:GLN:HB2	1.88	0.55
1:A:66:ARG:NH2	2:M:2:GLC:O4	2.38	0.54
1:B:183:VAL:CG2	1:B:365:GLN:HA	2.37	0.54
1:G:89:LEU:HD12	1:G:94:TRP:CZ2	2.43	0.54
1:I:68:GLY:HA3	1:I:332:ASN:O	2.08	0.54
1:E:307:TYR:CE1	1:E:311:LEU:HD11	2.43	0.54
1:K:89:LEU:HD12	1:K:94:TRP:CZ2	2.42	0.54
1:K:68:GLY:HA3	1:K:332:ASN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:GLY:HA3	1:D:332:ASN:O	2.08	0.53
1:C:68:GLY:HA3	1:C:332:ASN:O	2.08	0.53
1:L:68:GLY:HA3	1:L:332:ASN:O	2.08	0.53
1:B:68:GLY:HA3	1:B:332:ASN:O	2.09	0.53
1:E:68:GLY:HA3	1:E:332:ASN:O	2.09	0.53
1:G:1:LYS:HA	1:G:55:ASP:OD1	2.07	0.53
1:G:68:GLY:HA3	1:G:332:ASN:O	2.08	0.53
1:H:68:GLY:HA3	1:H:332:ASN:O	2.09	0.52
1:B:80:THR:N	1:B:81:PRO:HD3	2.24	0.52
1:L:2:ILE:HG22	1:L:271:PRO:HD2	1.90	0.52
1:J:68:GLY:HA3	1:J:332:ASN:O	2.09	0.52
1:E:1:LYS:HA	1:E:55:ASP:OD1	2.10	0.52
1:A:68:GLY:HA3	1:A:332:ASN:O	2.10	0.52
1:F:68:GLY:HA3	1:F:332:ASN:O	2.10	0.52
1:H:89:LEU:HD12	1:H:94:TRP:CZ2	2.44	0.52
1:K:165:GLY:O	1:K:185:ASN:ND2	2.43	0.52
1:F:1:LYS:HA	1:F:55:ASP:OD1	2.10	0.51
1:F:244:VAL:HG13	1:F:316:ARG:HG2	1.93	0.51
1:G:244:VAL:HG13	1:G:316:ARG:HG2	1.93	0.51
1:H:307:TYR:CE1	1:H:311:LEU:HD11	2.45	0.51
1:B:89:LEU:HD23	1:B:304:LEU:HA	1.93	0.51
1:G:168:ALA:CB	1:G:339:PHE:CE1	2.93	0.51
1:D:168:ALA:HB2	1:D:339:PHE:CZ	2.46	0.50
1:H:89:LEU:HD23	1:H:304:LEU:HA	1.93	0.50
1:D:127:LYS:O	1:D:249:THR:HG22	2.12	0.50
1:L:229:PRO:HA	1:L:232:TRP:CE2	2.47	0.50
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.47	0.50
1:G:229:PRO:HA	1:G:232:TRP:CE2	2.47	0.50
1:I:229:PRO:HA	1:I:232:TRP:CE2	2.46	0.50
1:E:43:LEU:HD23	1:E:43:LEU:C	2.32	0.50
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.47	0.50
1:A:43:LEU:C	1:A:43:LEU:HD23	2.31	0.50
1:F:229:PRO:HA	1:F:232:TRP:CE2	2.47	0.50
1:F:43:LEU:C	1:F:43:LEU:HD23	2.32	0.50
1:D:229:PRO:HA	1:D:232:TRP:CE2	2.47	0.49
1:B:79:ILE:C	1:B:81:PRO:HD3	2.33	0.49
1:E:244:VAL:HG13	1:E:316:ARG:HG2	1.94	0.49
1:K:229:PRO:HA	1:K:232:TRP:CE2	2.47	0.49
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.47	0.49
1:E:127:LYS:O	1:E:249:THR:HG22	2.13	0.49
1:H:229:PRO:HA	1:H:232:TRP:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:PRO:HA	1:J:232:TRP:CE2	2.47	0.49
1:K:89:LEU:HD23	1:K:304:LEU:HA	1.95	0.49
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.47	0.49
1:B:168:ALA:HB2	1:B:339:PHE:CZ	2.48	0.49
1:F:168:ALA:CB	1:F:339:PHE:CE1	2.96	0.49
1:L:43:LEU:HD23	1:L:43:LEU:C	2.32	0.49
1:C:233:SER:HB3	1:C:297:LYS:HZ2	1.78	0.49
1:E:89:LEU:HD23	1:E:304:LEU:HA	1.94	0.49
1:G:89:LEU:HD23	1:G:304:LEU:HA	1.94	0.49
1:J:366:THR:O	1:J:369:ALA:HB3	2.12	0.49
1:B:127:LYS:O	1:B:249:THR:HG22	2.13	0.48
1:C:127:LYS:O	1:C:249:THR:HG22	2.13	0.48
1:J:142:LYS:HG3	1:J:142:LYS:O	2.12	0.48
1:B:207:ASP:CG	1:D:207:ASP:OD1	2.52	0.48
1:G:1:LYS:HE3	1:G:53:THR:O	2.12	0.48
1:I:233:SER:HB3	1:I:297:LYS:HD3	1.95	0.48
1:K:170:LYS:HD3	1:K:180:ASP:OD2	2.14	0.48
1:E:307:TYR:CE2	1:E:311:LEU:HD21	2.48	0.48
1:B:50:VAL:HG12	1:B:55:ASP:CB	2.44	0.48
1:E:84:ALA:HB2	1:L:121:LEU:HD11	1.92	0.48
1:E:158:TRP:N	1:E:159:PRO:CD	2.77	0.48
1:L:346:ALA:HB2	1:L:364:ALA:HB2	1.96	0.48
1:H:346:ALA:HB2	1:H:364:ALA:HB2	1.96	0.47
1:E:-1:HIS:CD2	1:K:13:GLY:HA3	2.49	0.47
1:B:158:TRP:N	1:B:159:PRO:CD	2.77	0.47
1:B:50:VAL:CG1	1:B:55:ASP:CB	2.91	0.47
1:D:158:TRP:N	1:D:159:PRO:CD	2.78	0.47
1:B:183:VAL:HG23	1:B:365:GLN:HB2	1.97	0.47
1:L:2:ILE:HG21	1:L:271:PRO:HD2	1.96	0.47
1:A:158:TRP:N	1:A:159:PRO:CD	2.78	0.47
1:C:89:LEU:HD13	1:C:94:TRP:CZ2	2.49	0.47
1:H:118:ASN:ND2	1:H:121:LEU:HD13	2.30	0.47
1:E:84:ALA:CB	1:L:121:LEU:HD12	2.42	0.47
1:F:158:TRP:N	1:F:159:PRO:CD	2.78	0.47
1:L:244:VAL:HG13	1:L:316:ARG:HG2	1.97	0.47
1:C:158:TRP:N	1:C:159:PRO:CD	2.78	0.47
1:D:1:LYS:HA	1:D:55:ASP:OD2	2.14	0.47
1:G:158:TRP:N	1:G:159:PRO:CD	2.78	0.46
1:I:158:TRP:N	1:I:159:PRO:CD	2.78	0.46
1:J:158:TRP:N	1:J:159:PRO:CD	2.78	0.46
1:L:158:TRP:N	1:L:159:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:LYS:HG2	1:K:55:ASP:OD1	2.15	0.46
1:K:158:TRP:N	1:K:159:PRO:CD	2.78	0.46
1:K:346:ALA:HB2	1:K:364:ALA:HB2	1.98	0.46
1:G:346:ALA:HB2	1:G:364:ALA:HB2	1.98	0.46
1:H:170:LYS:HD3	1:H:180:ASP:OD2	2.15	0.46
1:C:170:LYS:HD3	1:C:180:ASP:OD2	2.16	0.46
1:C:202:LYS:HE2	1:K:212:ILE:CD1	2.46	0.46
1:H:158:TRP:N	1:H:159:PRO:CD	2.78	0.46
1:F:346:ALA:HB2	1:F:364:ALA:HB2	1.99	0.45
1:F:311:LEU:HB3	1:F:317:ILE:HD13	1.99	0.45
1:C:346:ALA:HB2	1:C:364:ALA:HB2	1.98	0.45
1:E:1:LYS:CE	1:E:53:THR:O	2.62	0.45
1:E:346:ALA:HB2	1:E:364:ALA:HB2	1.98	0.45
1:J:184:ASP:HB3	1:J:365:GLN:HB2	2.00	0.45
1:J:346:ALA:HB2	1:J:364:ALA:HB2	2.00	0.44
1:A:346:ALA:HB2	1:A:364:ALA:HB2	2.00	0.44
1:B:346:ALA:HB2	1:B:364:ALA:HB2	1.99	0.44
1:I:346:ALA:HB2	1:I:364:ALA:HB2	1.99	0.44
1:D:82:ALA:HB1	6:K:520:HOH:O	2.18	0.44
1:G:311:LEU:HB3	1:G:317:ILE:HD13	1.99	0.44
1:A:89:LEU:N	1:A:89:LEU:HD12	2.33	0.44
1:G:184:ASP:HB3	1:G:365:GLN:HB2	2.00	0.44
1:K:241:ASN:ND2	6:K:503:HOH:O	2.50	0.44
1:D:184:ASP:HB3	1:D:365:GLN:HB2	2.00	0.44
1:C:233:SER:HB3	1:C:297:LYS:NZ	2.33	0.44
1:F:47:PHE:HB3	1:F:48:PRO:HD3	2.00	0.43
1:D:346:ALA:HB2	1:D:364:ALA:HB2	1.99	0.43
1:L:140:LYS:HE2	6:L:522:HOH:O	2.18	0.43
1:A:-1:HIS:CD2	1:B:13:GLY:HA3	2.53	0.43
1:G:168:ALA:HB2	1:G:339:PHE:CE1	2.53	0.43
1:A:111:GLU:OE1	2:M:1:GLC:O2	2.33	0.43
1:I:89:LEU:HD12	1:I:89:LEU:N	2.34	0.43
1:A:170:LYS:HD2	1:A:180:ASP:OD2	2.18	0.42
1:C:274:GLU:HG2	1:C:275:LEU:HD12	2.01	0.42
1:H:47:PHE:HB3	1:H:48:PRO:HD3	2.02	0.42
1:A:92:PHE:CD2	1:L:173:ALA:O	2.72	0.42
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.01	0.42
1:F:89:LEU:N	1:F:89:LEU:HD12	2.35	0.42
1:F:184:ASP:HB3	1:F:365:GLN:HB2	2.01	0.42
1:L:47:PHE:HB3	1:L:48:PRO:HD3	2.01	0.42
1:J:89:LEU:N	1:J:89:LEU:HD12	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:LYS:HD2	1:L:180:ASP:OD2	2.19	0.42
1:G:244:VAL:CG1	1:G:316:ARG:HG2	2.50	0.42
1:L:89:LEU:HD12	1:L:89:LEU:N	2.34	0.42
1:E:184:ASP:HB3	1:E:365:GLN:HB2	2.02	0.42
1:J:47:PHE:HB3	1:J:48:PRO:HD3	2.02	0.42
1:A:88:LYS:C	1:A:89:LEU:HD12	2.41	0.41
1:F:170:LYS:HD2	1:F:180:ASP:OD2	2.20	0.41
1:G:47:PHE:HB3	1:G:48:PRO:HD3	2.01	0.41
1:A:47:PHE:HB3	1:A:48:PRO:HD3	2.02	0.41
1:B:47:PHE:HB3	1:B:48:PRO:HD3	2.02	0.41
1:F:88:LYS:C	1:F:89:LEU:HD12	2.41	0.41
1:L:118:ASN:ND2	1:L:121:LEU:HD13	2.35	0.41
1:C:47:PHE:HB3	1:C:48:PRO:HD3	2.02	0.41
1:H:256:LYS:HB3	1:H:256:LYS:HE2	1.91	0.41
1:I:311:LEU:HB3	1:I:317:ILE:HD13	2.02	0.41
1:D:89:LEU:HD12	1:D:89:LEU:N	2.35	0.41
1:B:311:LEU:HB3	1:B:317:ILE:HD13	2.01	0.41
1:C:142:LYS:HG3	1:C:142:LYS:O	2.20	0.41
1:C:202:LYS:HE2	1:K:212:ILE:HD13	2.03	0.41
1:J:168:ALA:CB	1:J:339:PHE:CE1	3.04	0.41
1:I:47:PHE:HB3	1:I:48:PRO:HD3	2.03	0.41
1:K:47:PHE:HB3	1:K:48:PRO:HD3	2.03	0.41
1:D:47:PHE:HB3	1:D:48:PRO:HD3	2.02	0.41
1:E:311:LEU:HB3	1:E:317:ILE:HD13	2.01	0.41
1:H:15:LYS:O	1:H:297:LYS:HD2	2.20	0.41
1:J:88:LYS:C	1:J:89:LEU:HD12	2.41	0.41
1:C:184:ASP:HB3	1:C:365:GLN:HB2	2.03	0.41
1:F:322:GLU:O	1:F:326:LYS:HG3	2.21	0.41
1:I:181:VAL:HG12	1:I:183:VAL:HG13	2.02	0.41
1:L:1:LYS:HA	1:L:55:ASP:OD1	2.21	0.41
1:L:88:LYS:C	1:L:89:LEU:HD12	2.41	0.41
1:B:168:ALA:CB	1:B:339:PHE:CE1	3.04	0.40
1:H:311:LEU:HB3	1:H:317:ILE:HD13	2.03	0.40
1:F:244:VAL:CG1	1:F:316:ARG:HG2	2.51	0.40
1:I:184:ASP:HB2	1:I:365:GLN:HB2	2.02	0.40
1:A:325:GLN:CA	1:L:172:ALA:HB1	2.44	0.40
1:B:205:ASN:HB3	1:B:208:THR:HG23	2.04	0.40
1:E:322:GLU:O	1:E:326:LYS:HG3	2.21	0.40
1:L:322:GLU:O	1:L:326:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/402 (92%)	365 (98%)	6 (2%)	0	100	100
1	B	371/402 (92%)	364 (98%)	7 (2%)	0	100	100
1	C	371/402 (92%)	365 (98%)	6 (2%)	0	100	100
1	D	371/402 (92%)	366 (99%)	5 (1%)	0	100	100
1	E	371/402 (92%)	366 (99%)	5 (1%)	0	100	100
1	F	371/402 (92%)	367 (99%)	4 (1%)	0	100	100
1	G	371/402 (92%)	366 (99%)	5 (1%)	0	100	100
1	H	371/402 (92%)	365 (98%)	6 (2%)	0	100	100
1	I	370/402 (92%)	366 (99%)	4 (1%)	0	100	100
1	J	371/402 (92%)	367 (99%)	4 (1%)	0	100	100
1	K	371/402 (92%)	365 (98%)	6 (2%)	0	100	100
1	L	370/402 (92%)	364 (98%)	6 (2%)	0	100	100
All	All	4450/4824 (92%)	4386 (99%)	64 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/307 (94%)	286 (99%)	2 (1%)	84	94
1	B	288/307 (94%)	285 (99%)	3 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/307 (94%)	285 (99%)	3 (1%)	76	91
1	D	288/307 (94%)	283 (98%)	5 (2%)	60	84
1	E	288/307 (94%)	284 (99%)	4 (1%)	67	86
1	F	288/307 (94%)	286 (99%)	2 (1%)	84	94
1	G	288/307 (94%)	285 (99%)	3 (1%)	76	91
1	H	288/307 (94%)	283 (98%)	5 (2%)	60	84
1	I	288/307 (94%)	285 (99%)	3 (1%)	76	91
1	J	288/307 (94%)	285 (99%)	3 (1%)	76	91
1	K	288/307 (94%)	286 (99%)	2 (1%)	84	94
1	L	288/307 (94%)	287 (100%)	1 (0%)	92	98
All	All	3456/3684 (94%)	3420 (99%)	36 (1%)	76	91

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	258	PHE
1	B	55	ASP
1	B	207	ASP
1	B	258	PHE
1	C	184	ASP
1	C	258	PHE
1	C	274	GLU
1	D	1	LYS
1	D	2	ILE
1	D	184	ASP
1	D	258	PHE
1	D	325	GLN
1	E	15	LYS
1	E	184	ASP
1	E	258	PHE
1	E	355	GLN
1	F	184	ASP
1	F	258	PHE
1	G	179	LYS
1	G	184	ASP
1	G	258	PHE
1	H	15	LYS

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Mol	Chain	Res	Type
1	H	184	ASP
1	H	258	PHE
1	H	306	SER
1	H	309	GLU
1	I	238	SER
1	I	258	PHE
1	I	306	SER
1	J	184	ASP
1	J	258	PHE
1	J	306	SER
1	K	258	PHE
1	K	306	SER
1	L	258	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	GLC	M	1	2	12,12,12	0.41	0	17,17,17	1.16	2 (11%)
2	GLC	M	2	2	11,11,12	0.43	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	N	1	2	12,12,12	0.47	0	17,17,17	0.62	0
2	GLC	N	2	2	11,11,12	0.52	0	15,15,17	0.95	2 (13%)
2	GLC	O	1	2	12,12,12	0.59	0	17,17,17	0.68	0
2	GLC	O	2	2	11,11,12	0.24	0	15,15,17	1.01	1 (6%)
2	GLC	P	1	2	12,12,12	0.55	0	17,17,17	0.74	0
2	GLC	P	2	2	11,11,12	0.49	0	15,15,17	0.99	0
2	GLC	Q	1	2	12,12,12	0.49	0	17,17,17	1.00	1 (5%)
2	GLC	Q	2	2	11,11,12	0.47	0	15,15,17	1.12	1 (6%)
2	GLC	R	1	2	12,12,12	0.44	0	17,17,17	1.24	2 (11%)
2	GLC	R	2	2	11,11,12	0.35	0	15,15,17	1.10	2 (13%)
2	GLC	S	1	2	12,12,12	0.54	0	17,17,17	0.90	2 (11%)
2	GLC	S	2	2	11,11,12	0.43	0	15,15,17	1.13	1 (6%)
2	GLC	T	1	2	12,12,12	0.68	0	17,17,17	0.79	0
2	GLC	T	2	2	11,11,12	0.40	0	15,15,17	0.84	0
2	GLC	U	1	2	12,12,12	0.52	0	17,17,17	1.00	1 (5%)
2	GLC	U	2	2	11,11,12	0.45	0	15,15,17	0.95	1 (6%)
2	GLC	V	1	2	12,12,12	0.50	0	17,17,17	0.73	0
2	GLC	V	2	2	11,11,12	0.24	0	15,15,17	0.81	0
2	GLC	W	1	2	12,12,12	0.52	0	17,17,17	0.92	0
2	GLC	W	2	2	11,11,12	0.37	0	15,15,17	0.98	0
2	GLC	X	1	2	12,12,12	0.38	0	17,17,17	1.17	1 (5%)
2	GLC	X	2	2	11,11,12	0.30	0	15,15,17	0.78	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	GLC	M	1	2	-	2/2/22/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1	2	-	1/2/22/22	0/1/1/1
2	GLC	N	2	2	-	1/2/19/22	0/1/1/1
2	GLC	O	1	2	-	2/2/22/22	0/1/1/1
2	GLC	O	2	2	-	2/2/19/22	0/1/1/1
2	GLC	P	1	2	-	2/2/22/22	0/1/1/1
2	GLC	P	2	2	-	2/2/19/22	0/1/1/1
2	GLC	Q	1	2	-	0/2/22/22	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	R	1	2	-	1/2/22/22	0/1/1/1
2	GLC	R	2	2	-	0/2/19/22	0/1/1/1
2	GLC	S	1	2	-	0/2/22/22	0/1/1/1
2	GLC	S	2	2	-	2/2/19/22	0/1/1/1
2	GLC	T	1	2	-	2/2/22/22	0/1/1/1
2	GLC	T	2	2	-	0/2/19/22	0/1/1/1
2	GLC	U	1	2	-	1/2/22/22	0/1/1/1
2	GLC	U	2	2	-	0/2/19/22	0/1/1/1
2	GLC	V	1	2	-	2/2/22/22	0/1/1/1
2	GLC	V	2	2	-	0/2/19/22	0/1/1/1
2	GLC	W	1	2	-	2/2/22/22	0/1/1/1
2	GLC	W	2	2	-	0/2/19/22	0/1/1/1
2	GLC	X	1	2	-	2/2/22/22	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	2	GLC	O5-C1-C2	-3.81	101.70	110.79
2	Q	2	GLC	C1-O5-C5	3.08	116.32	112.19
2	M	1	GLC	C1-O5-C5	3.02	119.49	113.65
2	R	1	GLC	C1-C2-C3	2.67	115.79	110.36
2	N	2	GLC	O5-C1-C2	-2.48	104.86	110.79
2	M	2	GLC	O2-C2-C1	2.47	114.88	109.22
2	U	1	GLC	C1-C2-C3	2.43	115.31	110.36
2	M	1	GLC	O5-C5-C4	2.43	114.07	109.70
2	R	2	GLC	C1-O5-C5	2.42	115.43	112.19
2	O	2	GLC	O5-C1-C2	-2.42	105.01	110.79
2	S	1	GLC	C1-O5-C5	2.36	118.22	113.65
2	U	2	GLC	O5-C1-C2	-2.27	105.37	110.79
2	Q	1	GLC	O4-C4-C3	-2.18	105.24	110.38
2	N	2	GLC	C1-O5-C5	2.15	115.07	112.19
2	R	1	GLC	C4-C3-C2	2.10	114.52	110.83
2	R	2	GLC	O5-C5-C6	-2.03	103.71	107.66
2	X	1	GLC	C4-C3-C2	2.02	114.37	110.83
2	S	1	GLC	O5-C5-C4	2.00	113.31	109.70

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	1	GLC	O5-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	V	1	GLC	C4-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	X	1	GLC	C4-C5-C6-O6
2	X	1	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6
2	M	1	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	O	1	GLC	O5-C5-C6-O6
2	O	2	GLC	C4-C5-C6-O6
2	W	1	GLC	C4-C5-C6-O6
2	P	2	GLC	O5-C5-C6-O6
2	M	1	GLC	O5-C5-C6-O6
2	S	2	GLC	O5-C5-C6-O6
2	W	1	GLC	O5-C5-C6-O6
2	O	2	GLC	O5-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	U	1	GLC	O5-C5-C6-O6
2	R	1	GLC	O5-C5-C6-O6

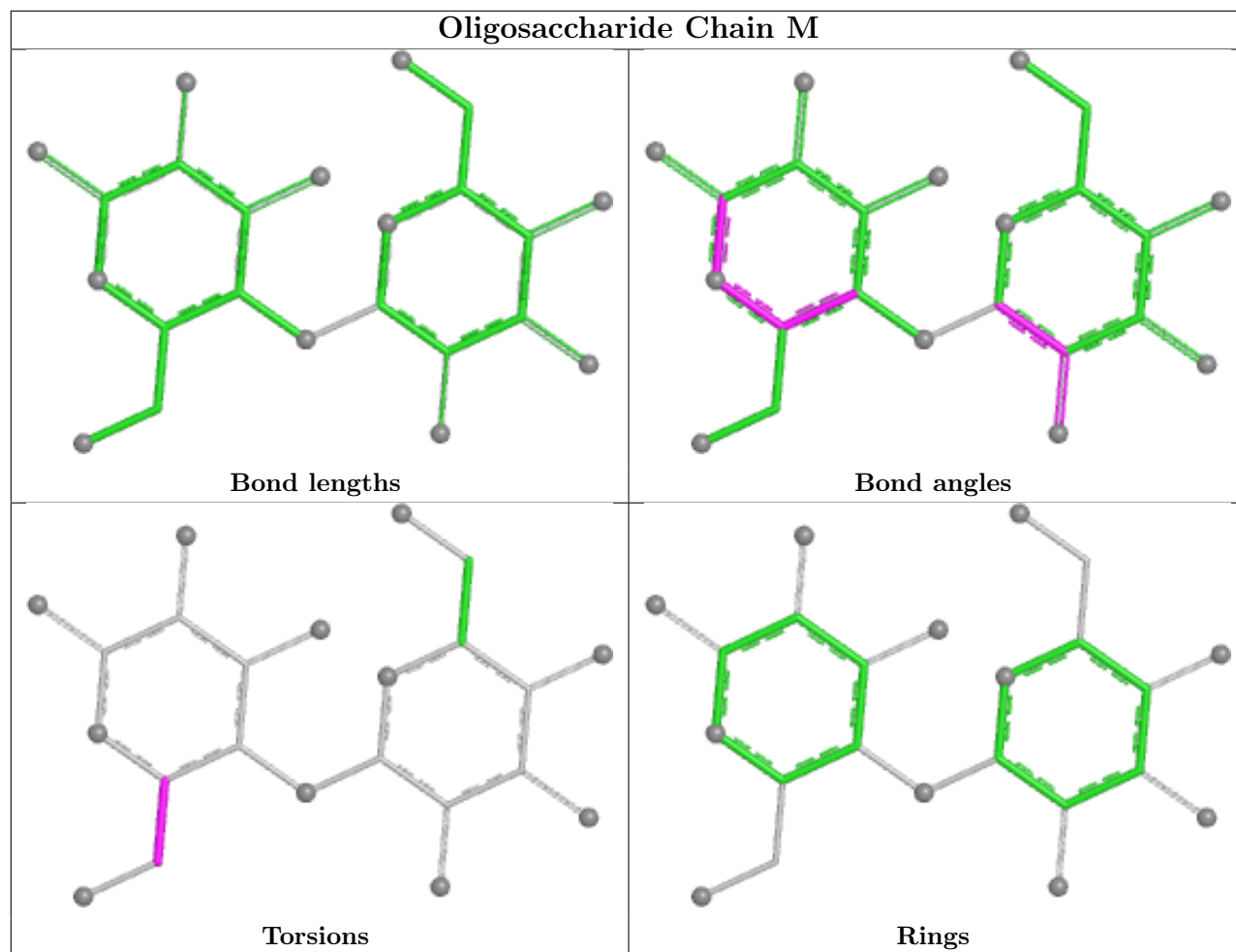
There are no ring outliers.

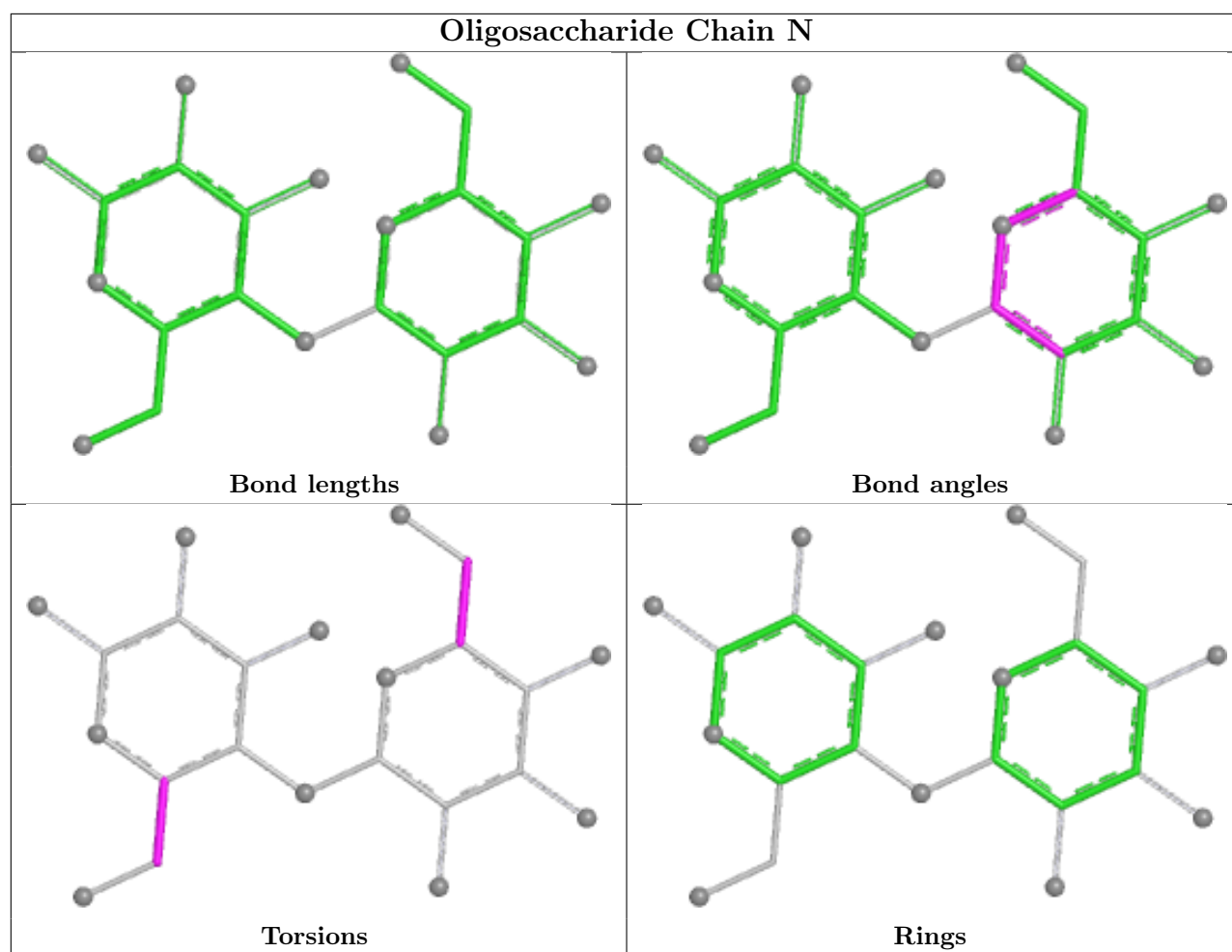
2 monomers are involved in 2 short contacts:

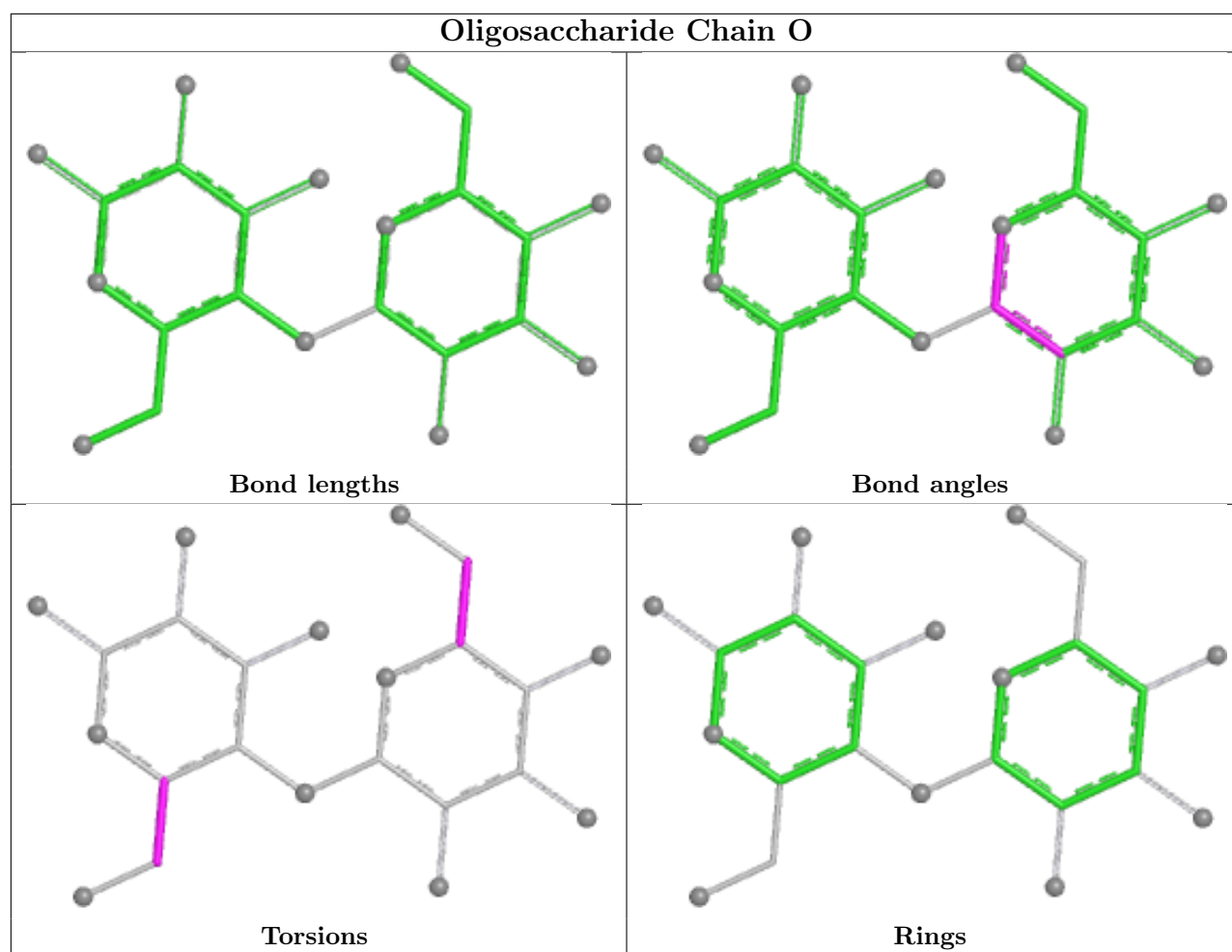
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	GLC	1	0
2	M	1	GLC	1	0

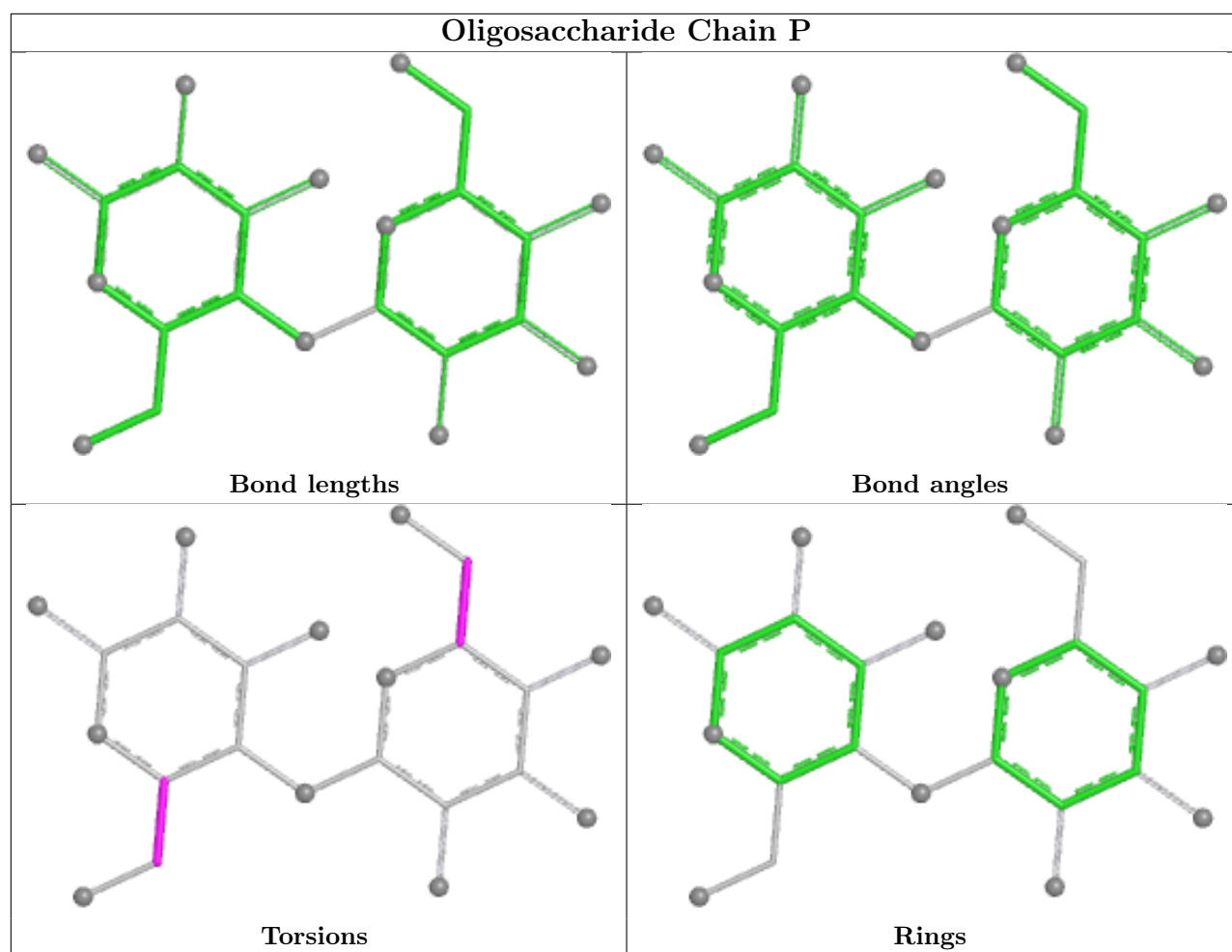
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

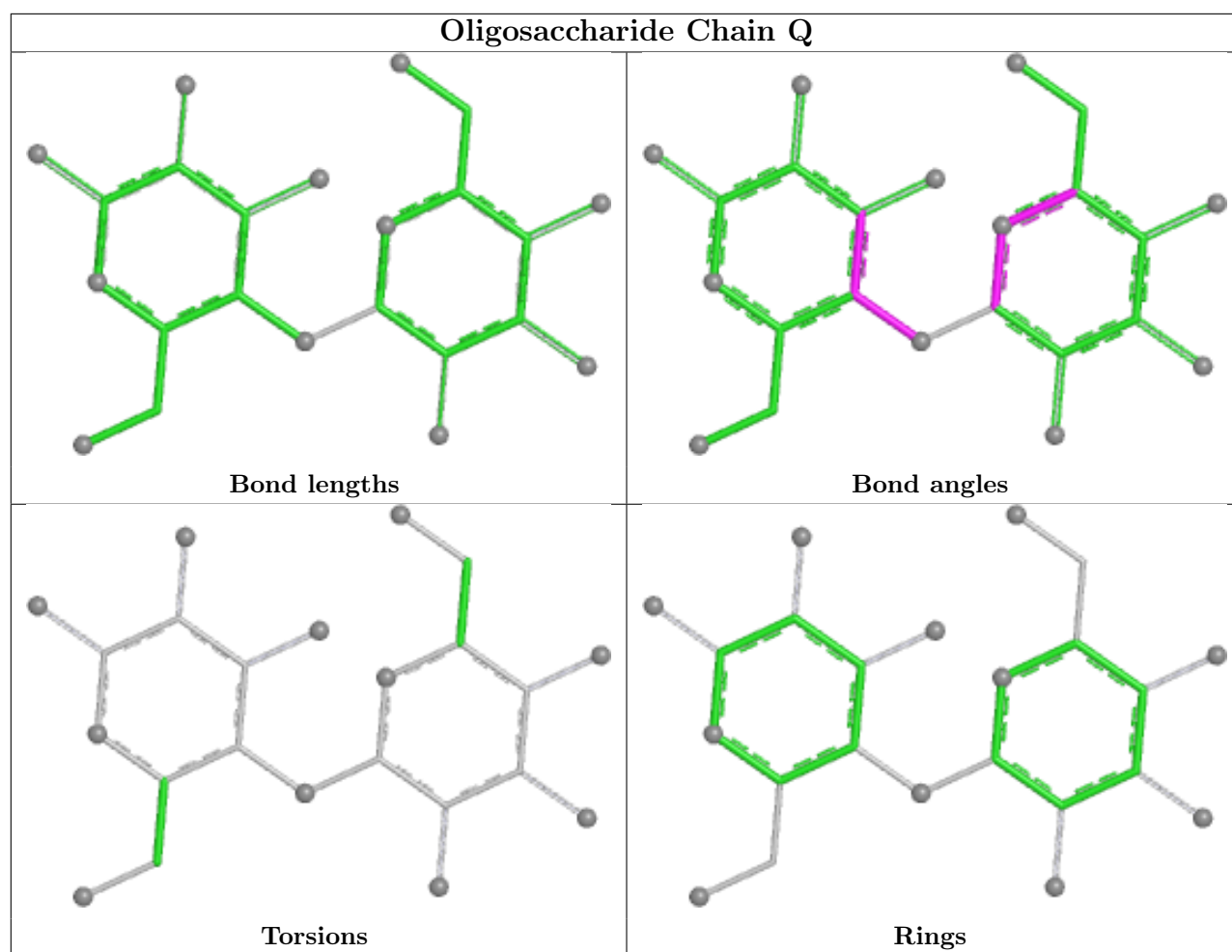


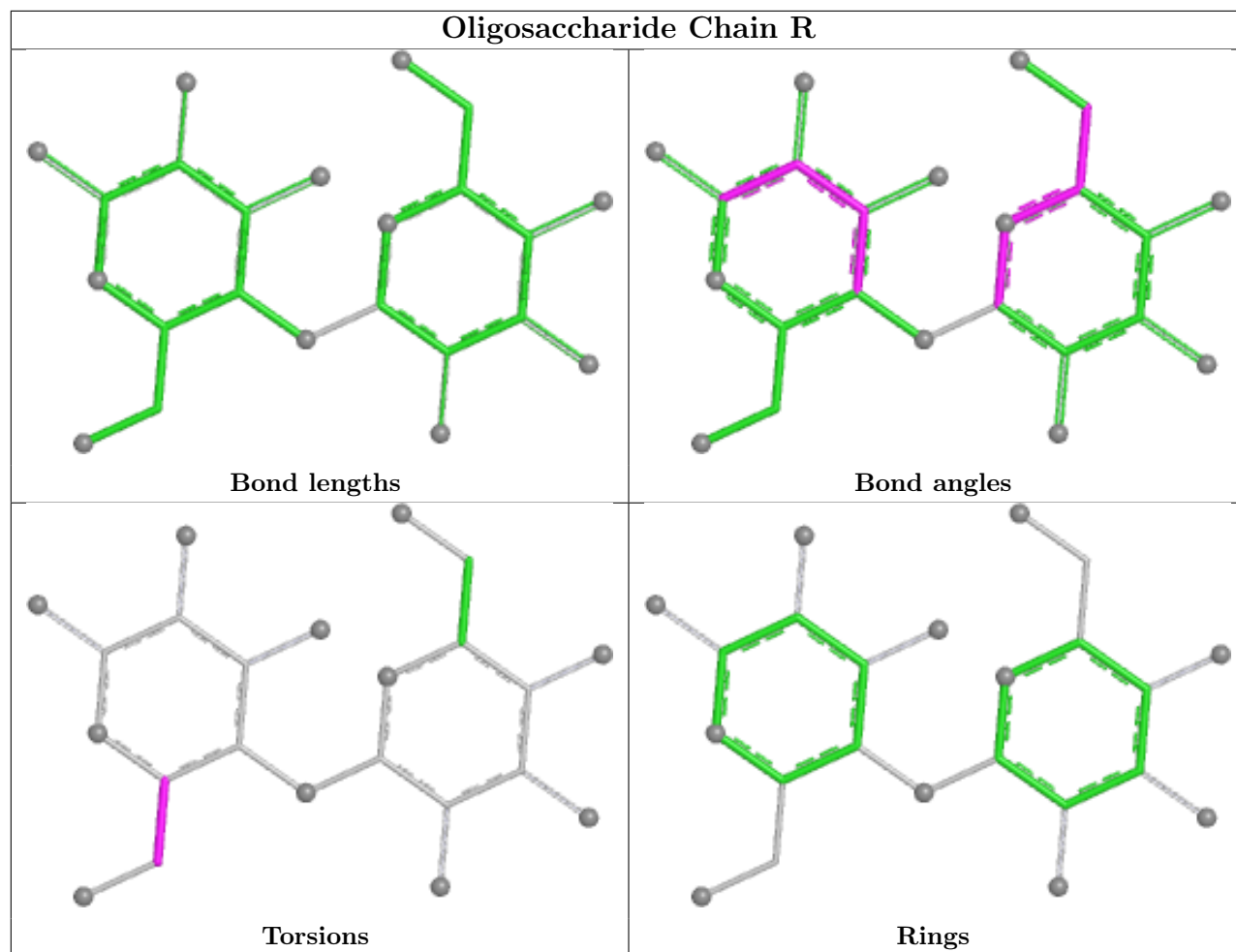


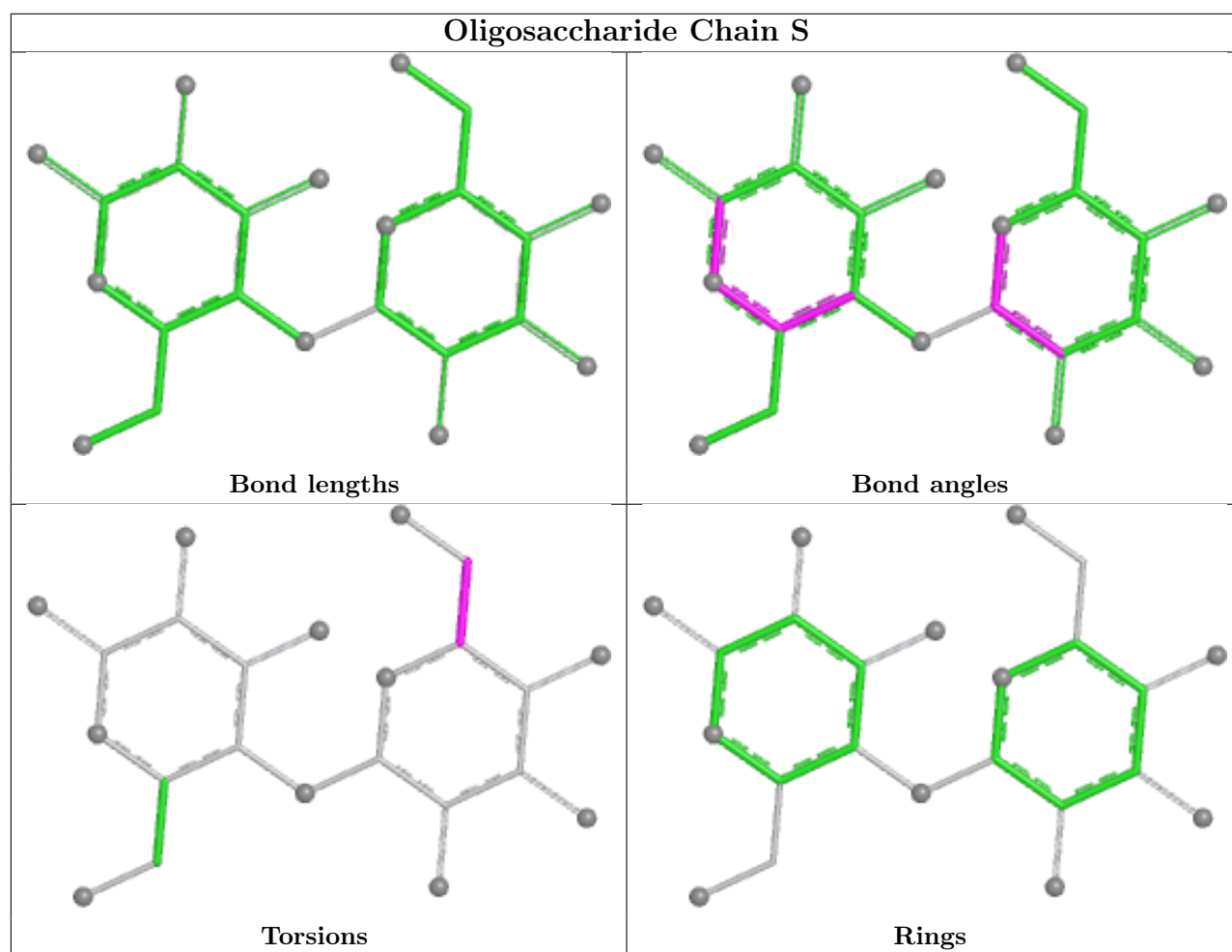


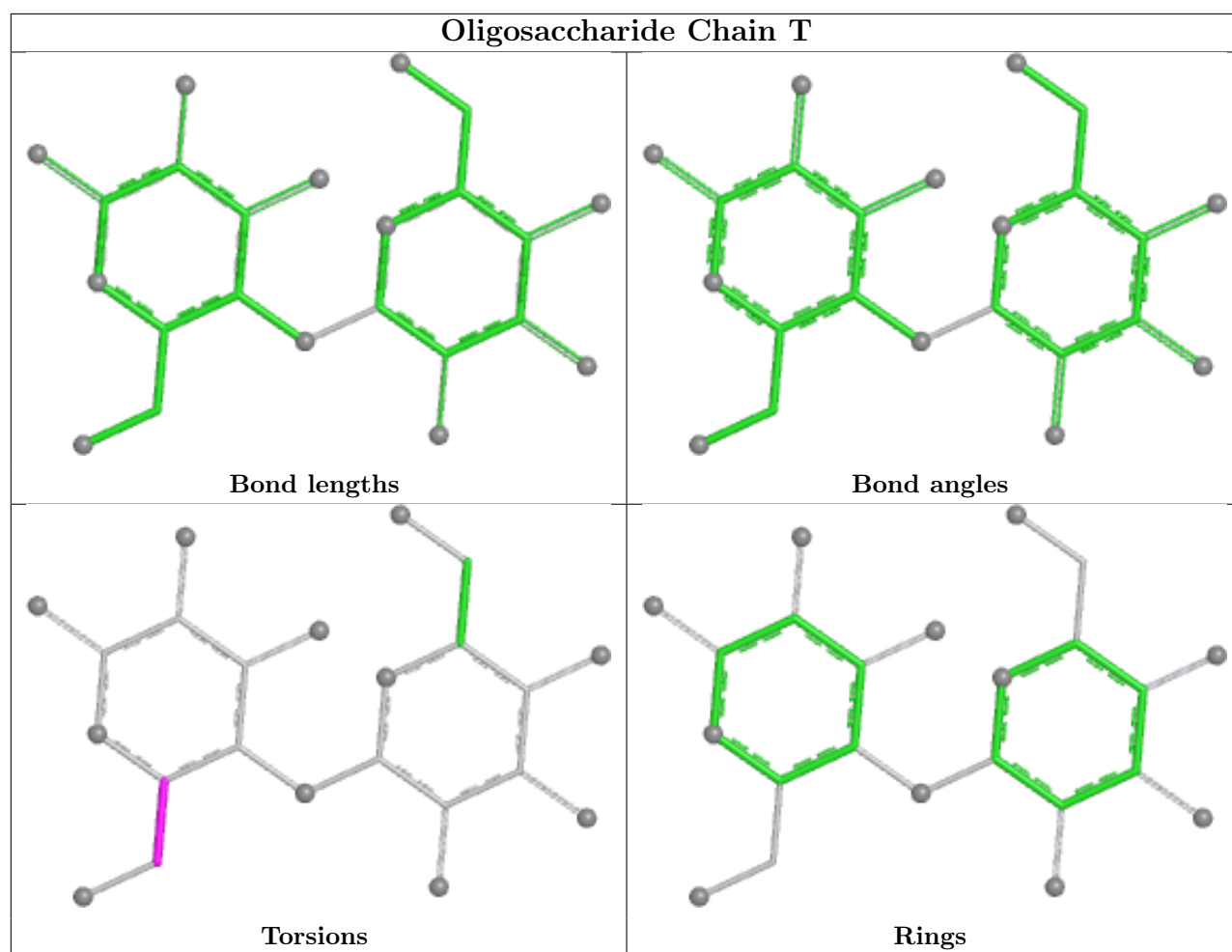




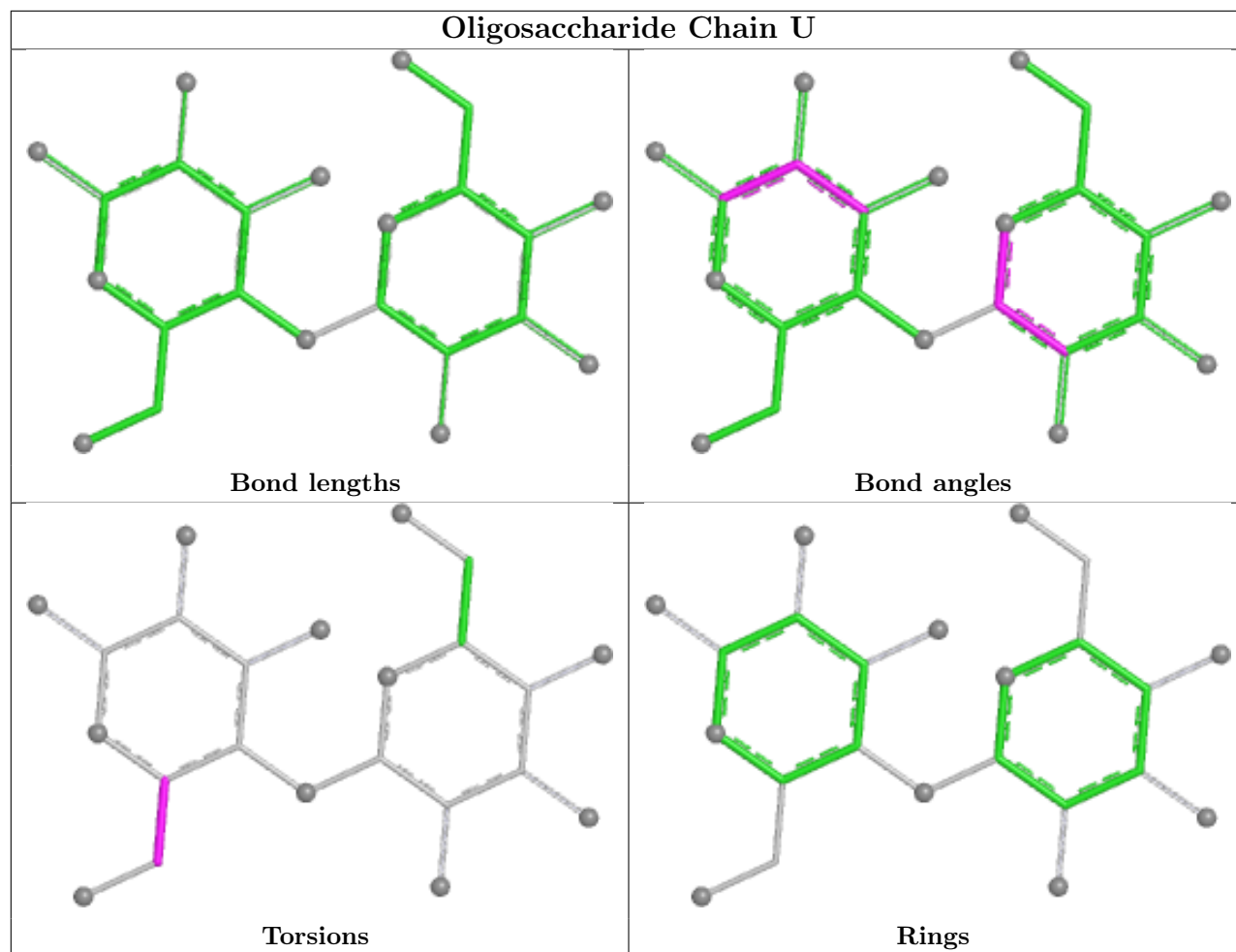


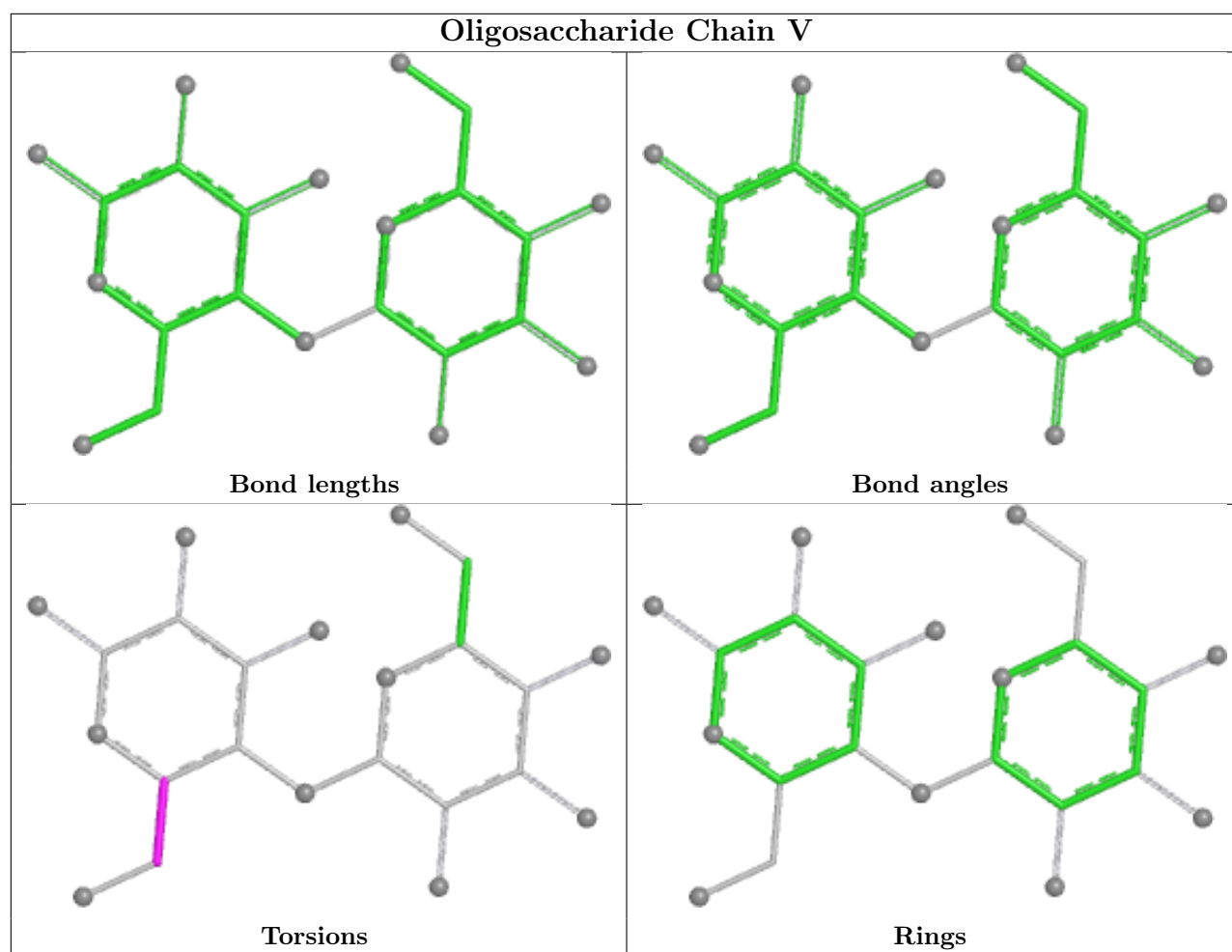


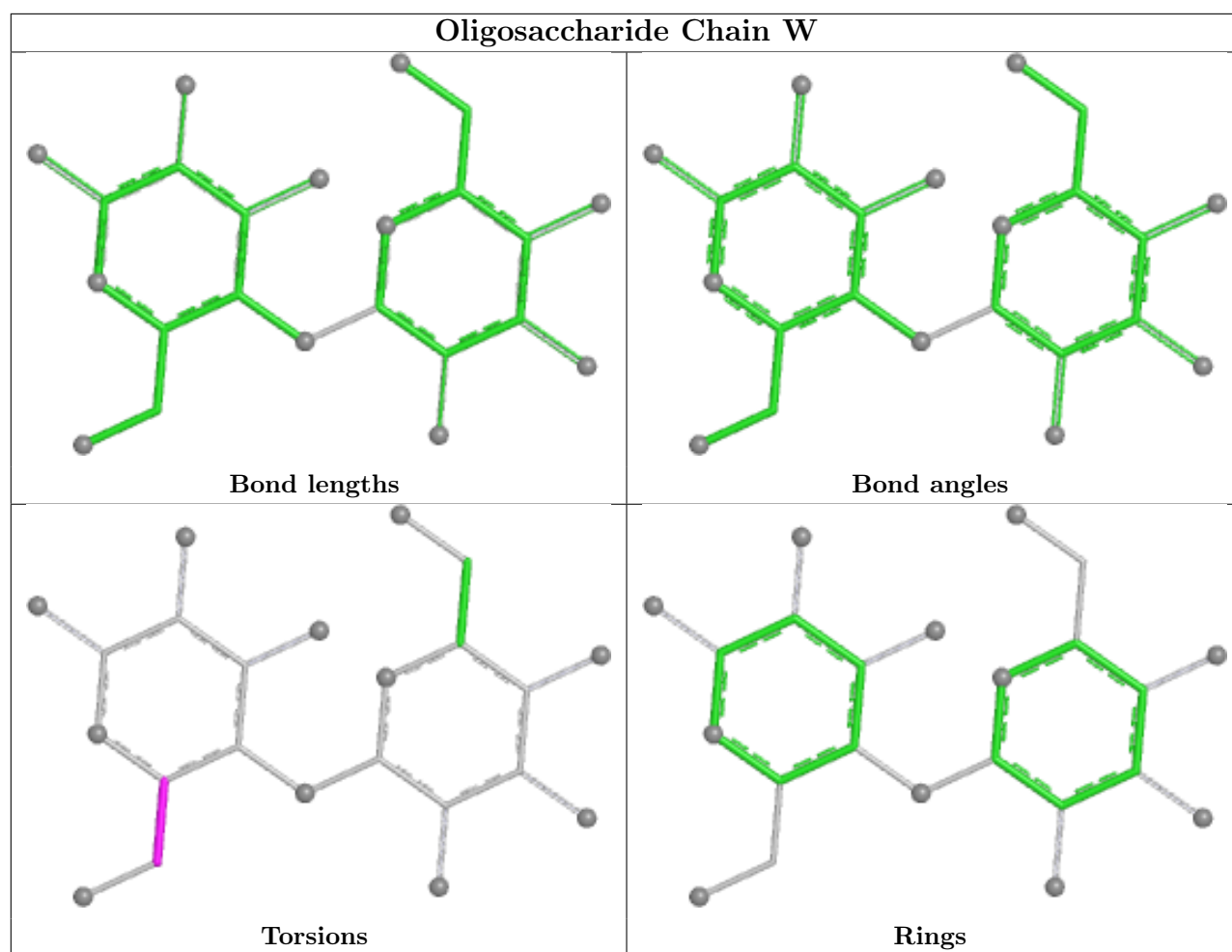


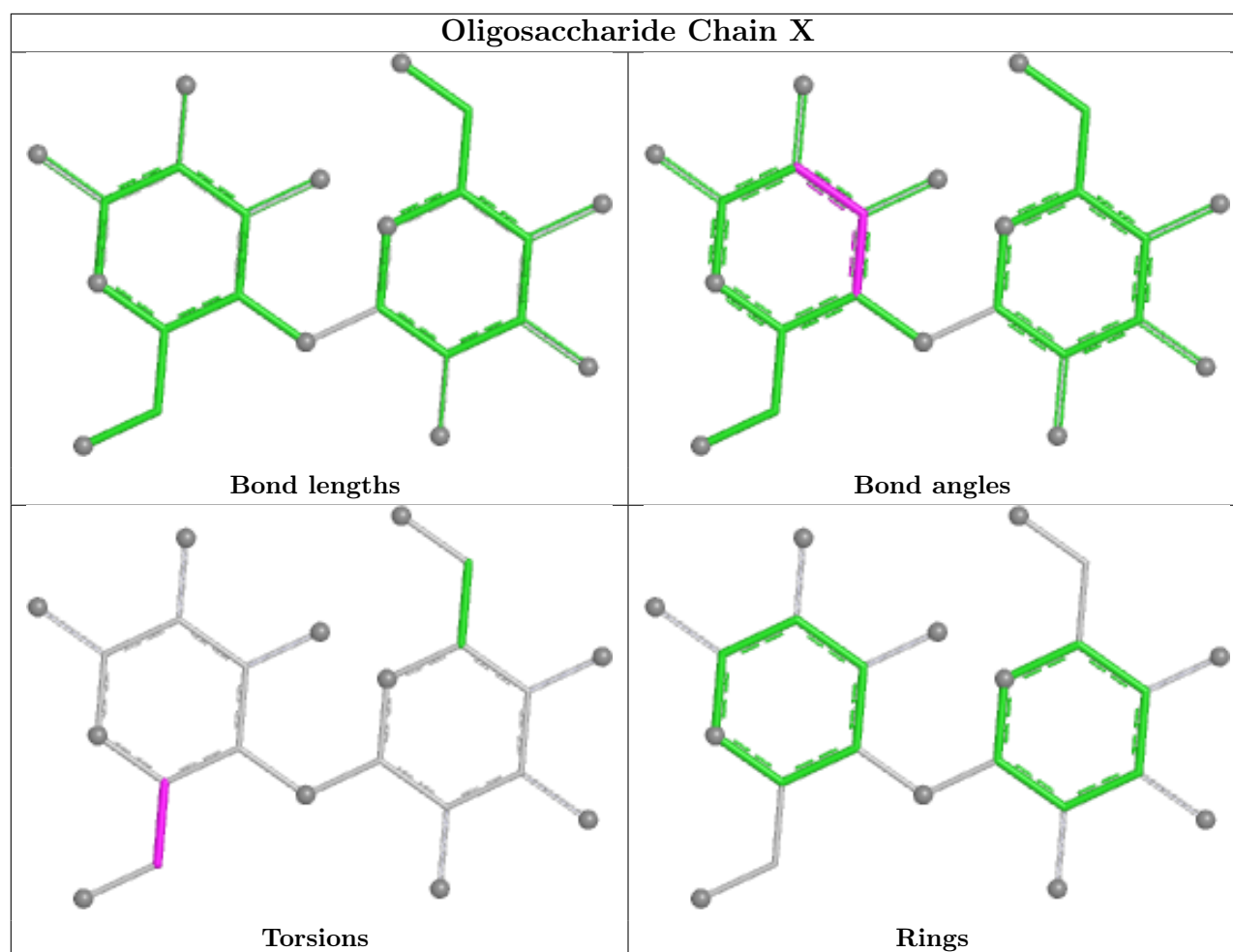












## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.13	0
5	PO4	J	402	-	4,4,4	0.77	0	6,6,6	0.46	0
5	PO4	I	402	-	4,4,4	0.87	0	6,6,6	0.47	0
4	SO4	L	402	-	4,4,4	0.30	0	6,6,6	0.12	0
4	SO4	K	402	-	4,4,4	0.35	0	6,6,6	0.07	0
5	PO4	D	402	-	4,4,4	0.75	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	D	403	-	4,4,4	0.71	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	402	PO4	1	0
4	K	402	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	373/402 (92%)	0.03	1 (0%) 94 95	44, 56, 79, 115	0
1	B	373/402 (92%)	0.25	10 (2%) 54 55	49, 76, 111, 142	0
1	C	373/402 (92%)	0.16	4 (1%) 80 82	50, 69, 97, 123	0
1	D	373/402 (92%)	0.23	16 (4%) 35 33	43, 70, 113, 146	0
1	E	373/402 (92%)	0.33	19 (5%) 28 26	50, 76, 117, 131	0
1	F	373/402 (92%)	0.10	1 (0%) 94 95	45, 65, 85, 123	0
1	G	373/402 (92%)	0.08	3 (0%) 86 87	43, 58, 85, 113	0
1	H	373/402 (92%)	0.20	5 (1%) 77 78	42, 61, 81, 134	0
1	I	372/402 (92%)	0.09	6 (1%) 72 74	44, 60, 89, 119	0
1	J	373/402 (92%)	0.02	2 (0%) 91 92	39, 58, 88, 119	0
1	K	373/402 (92%)	0.12	4 (1%) 80 82	39, 57, 85, 118	0
1	L	372/402 (92%)	0.11	0 100 100	42, 59, 88, 105	0
All	All	4474/4824 (92%)	0.14	71 (1%) 72 74	39, 63, 98, 146	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	ALA	4.9
1	B	129	TRP	4.1
1	G	173	ALA	4.0
1	E	34	LYS	3.8
1	E	35	VAL	3.7
1	K	33	ILE	3.6
1	D	122	LEU	3.5
1	D	140	LYS	3.4
1	D	141	ALA	3.3
1	I	168	ALA	3.3
1	I	173	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	173	ALA	3.3
1	E	140	LYS	3.0
1	C	212	ILE	2.9
1	E	121	LEU	2.9
1	E	311	LEU	2.9
1	B	168	ALA	2.9
1	E	20	LEU	2.8
1	E	33	ILE	2.8
1	D	370	ALA	2.7
1	K	174	GLY	2.7
1	I	171	TYR	2.7
1	E	295	LYS	2.7
1	D	200	LYS	2.6
1	C	219	LYS	2.6
1	B	118	ASN	2.6
1	B	121	LEU	2.6
1	K	173	ALA	2.5
1	A	368	ALA	2.5
1	D	171	TYR	2.5
1	D	194	PHE	2.5
1	D	351	ALA	2.4
1	B	239	ALA	2.4
1	D	33	ILE	2.4
1	H	173	ALA	2.4
1	H	368	ALA	2.4
1	I	172	ALA	2.4
1	B	140	LYS	2.4
1	D	34	LYS	2.4
1	B	141	ALA	2.3
1	D	368	ALA	2.3
1	B	370	ALA	2.3
1	I	364	ALA	2.2
1	G	285	LEU	2.2
1	E	141	ALA	2.2
1	K	304	LEU	2.2
1	J	173	ALA	2.2
1	H	275	LEU	2.2
1	B	142	LYS	2.2
1	E	172	ALA	2.2
1	D	173	ALA	2.1
1	E	137	LYS	2.1
1	B	195	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	7	LEU	2.1
1	E	310	GLU	2.1
1	H	369	ALA	2.1
1	E	101	GLY	2.1
1	E	139	LEU	2.1
1	E	284	LEU	2.1
1	J	239	ALA	2.1
1	E	276	ALA	2.1
1	D	174	GLY	2.1
1	D	369	ALA	2.1
1	I	174	GLY	2.1
1	D	121	LEU	2.0
1	E	133	PRO	2.0
1	E	196	VAL	2.0
1	F	173	ALA	2.0
1	G	168	ALA	2.0
1	H	121	LEU	2.0
1	E	117	TYR	2.0

## 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(Å <sup>2</sup> )	Q<0.9
2	GLC	O	1	12/12	0.94	0.13	53,58,65,70	0
2	GLC	P	2	11/12	0.94	0.15	44,47,49,50	0
2	GLC	X	2	11/12	0.94	0.20	38,41,43,43	0
2	GLC	Q	1	12/12	0.95	0.17	55,60,65,66	0
2	GLC	S	2	11/12	0.95	0.17	47,51,54,56	0
2	GLC	W	1	12/12	0.95	0.15	42,49,54,61	0
2	GLC	P	1	12/12	0.95	0.14	45,52,56,56	0
2	GLC	N	2	11/12	0.96	0.14	53,56,61,61	0
2	GLC	R	2	11/12	0.96	0.13	45,50,52,54	0
2	GLC	M	1	12/12	0.96	0.18	46,48,48,49	0

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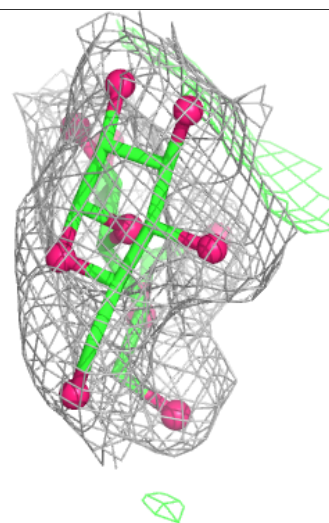
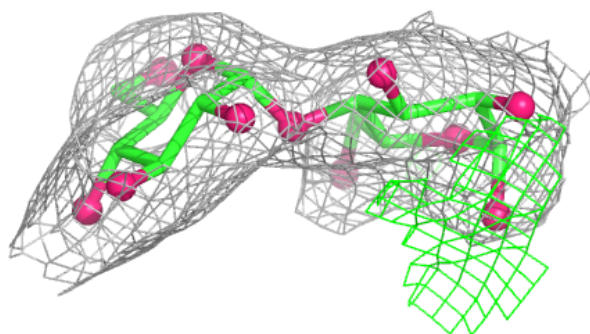
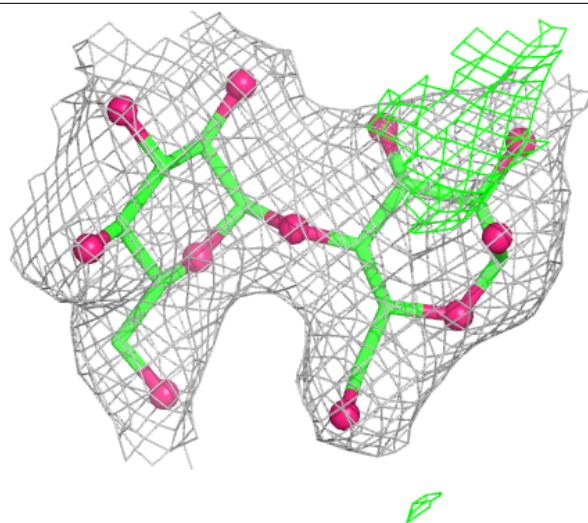
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	T	2	11/12	0.96	0.12	48,51,53,56	0
2	GLC	U	1	12/12	0.96	0.15	42,49,50,51	0
2	GLC	U	2	11/12	0.96	0.14	48,50,54,56	0
2	GLC	V	1	12/12	0.96	0.16	46,49,54,55	0
2	GLC	V	2	11/12	0.96	0.20	41,45,47,48	0
2	GLC	M	2	11/12	0.96	0.15	39,47,51,51	0
2	GLC	W	2	11/12	0.96	0.16	42,46,49,51	0
2	GLC	X	1	12/12	0.96	0.18	39,44,48,51	0
2	GLC	N	1	12/12	0.96	0.14	57,66,69,75	0
2	GLC	S	1	12/12	0.97	0.14	41,49,52,58	0
2	GLC	R	1	12/12	0.97	0.13	48,52,55,56	0
2	GLC	T	1	12/12	0.97	0.13	41,49,55,60	0
2	GLC	Q	2	11/12	0.97	0.12	48,53,55,56	0
2	GLC	O	2	11/12	0.98	0.13	47,48,52,52	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.

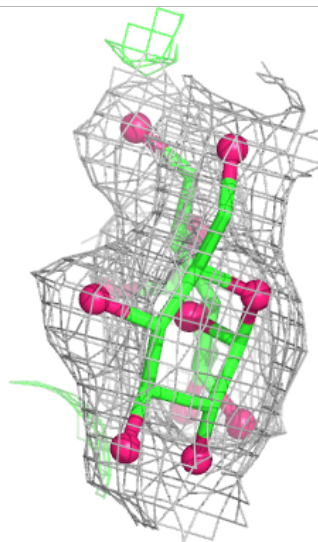
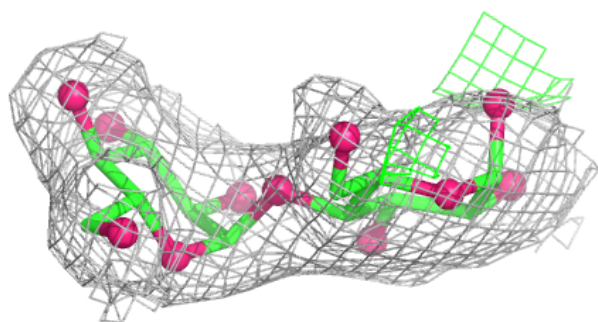
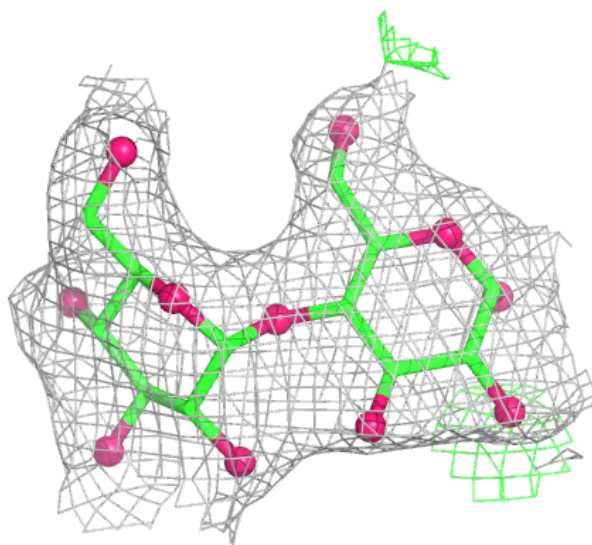
**Electron density around Chain M:**

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



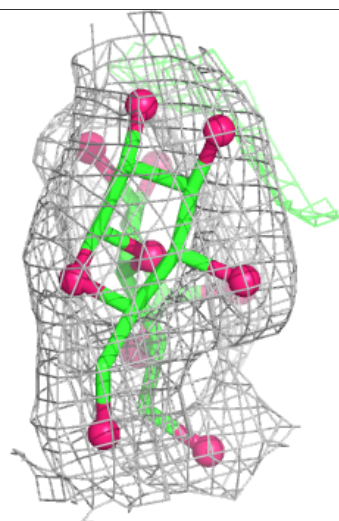
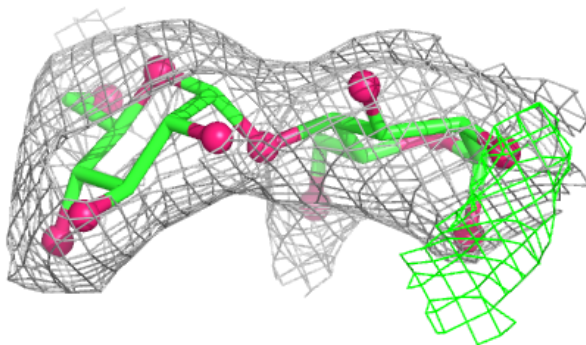
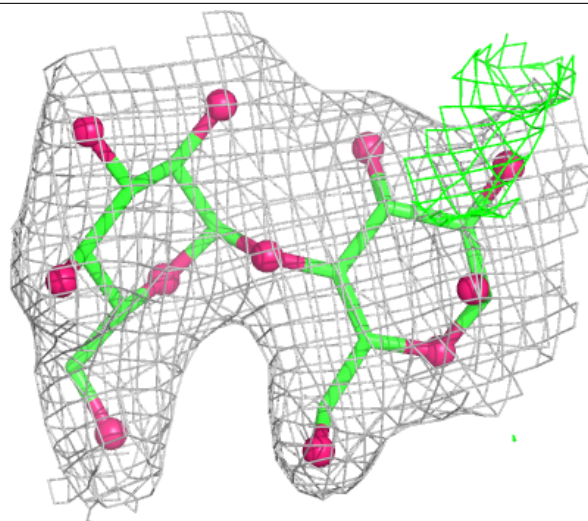
**Electron density around Chain N:**

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



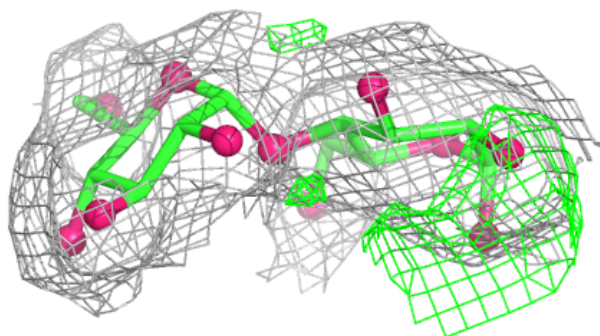
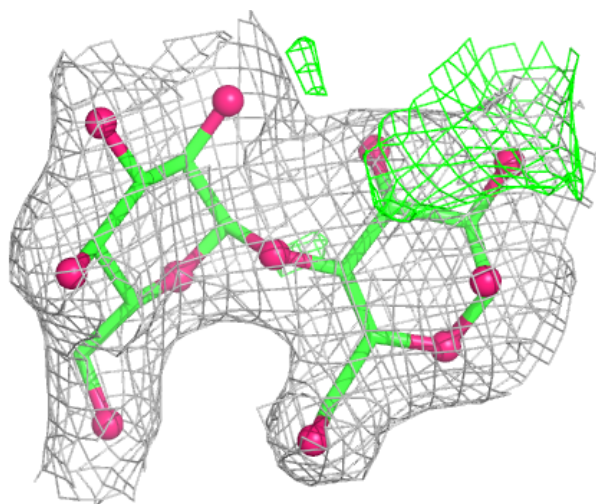
**Electron density around Chain O:**

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



**Electron density around Chain P:**

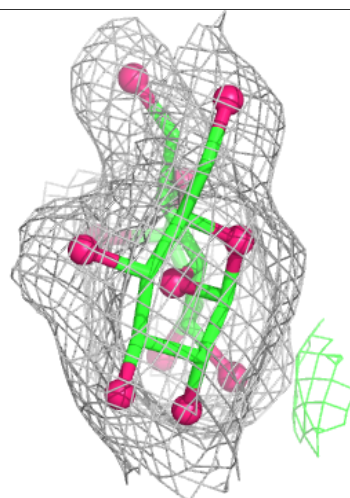
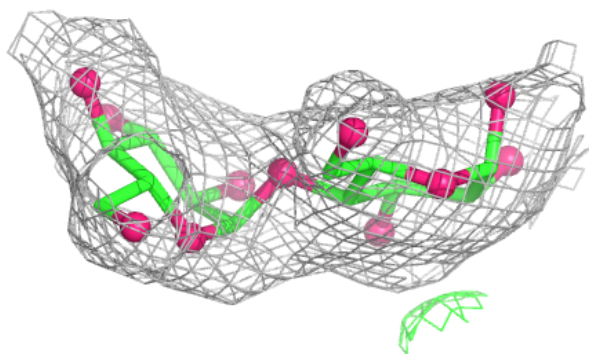
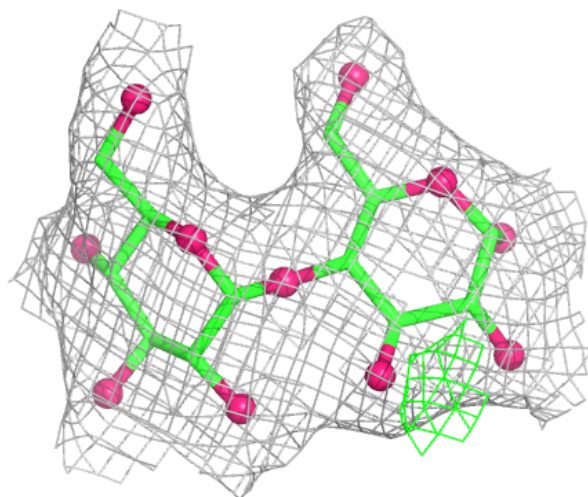
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





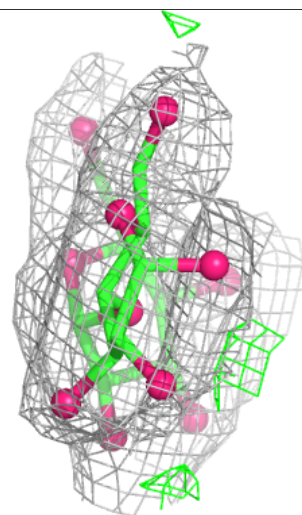
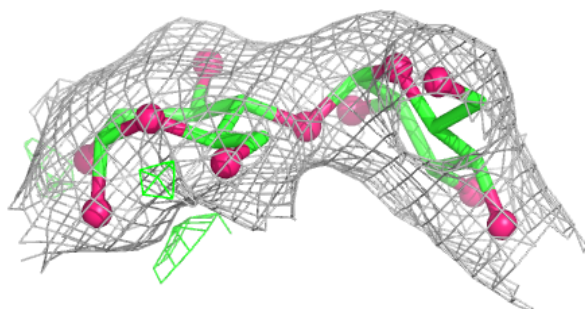
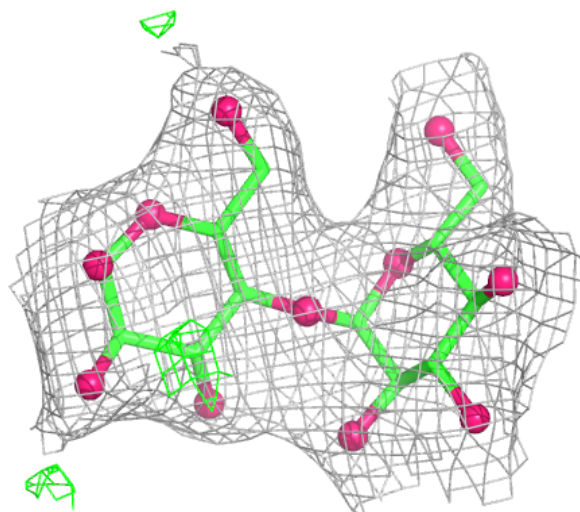
**Electron density around Chain Q:**

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



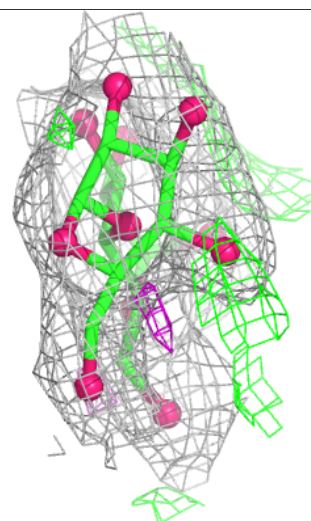
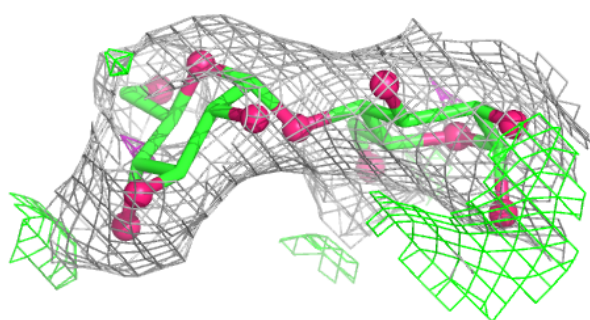
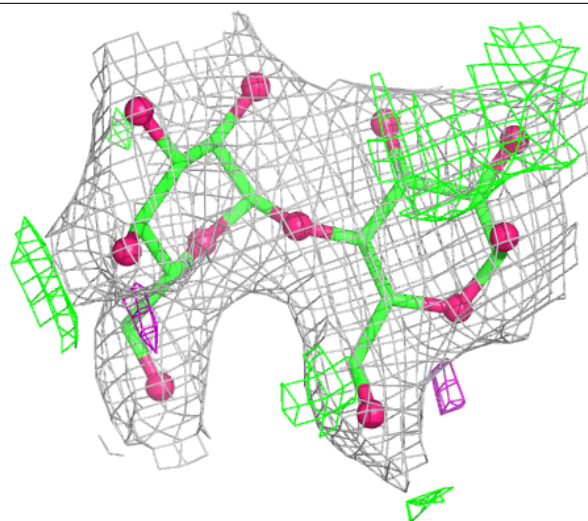
**Electron density around Chain R:**

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



**Electron density around Chain S:**

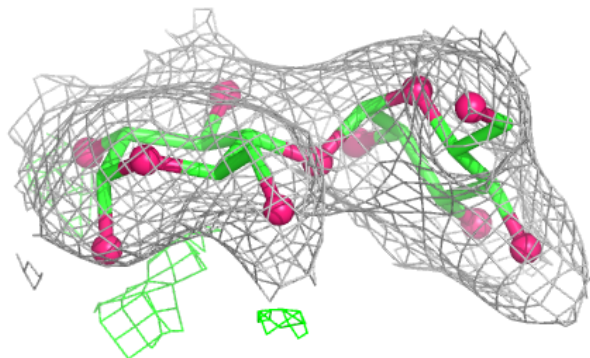
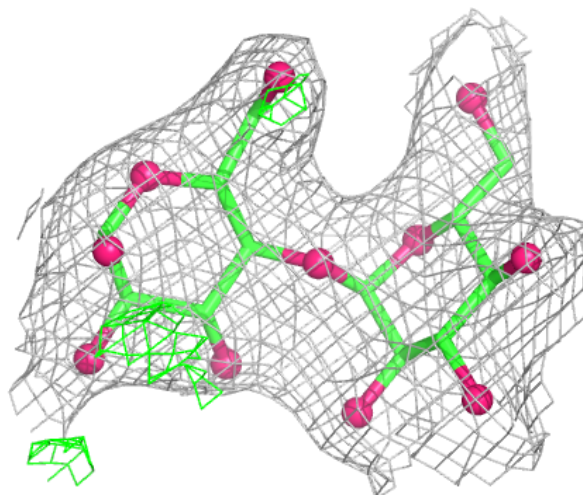
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





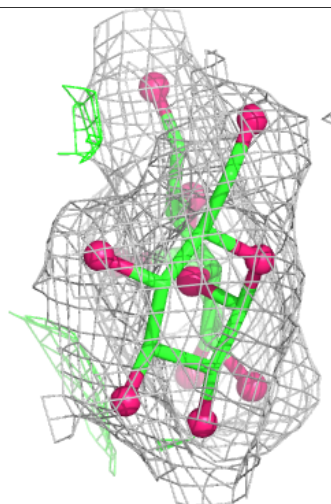
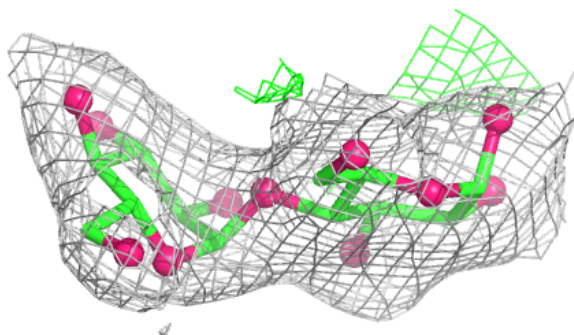
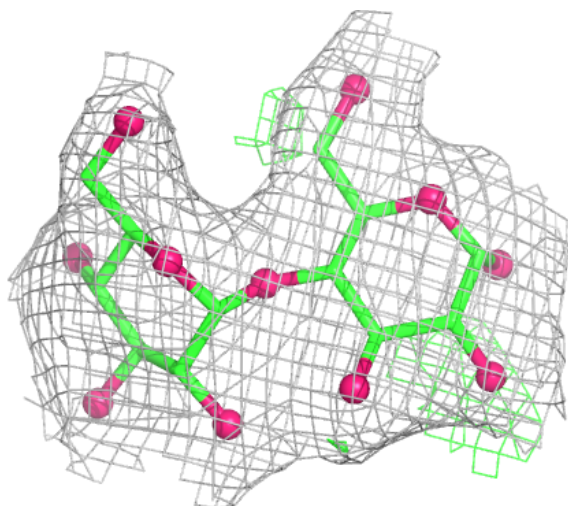
**Electron density around Chain T:**

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



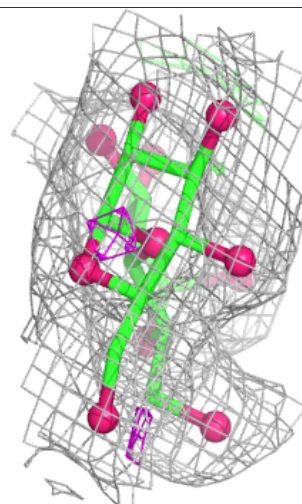
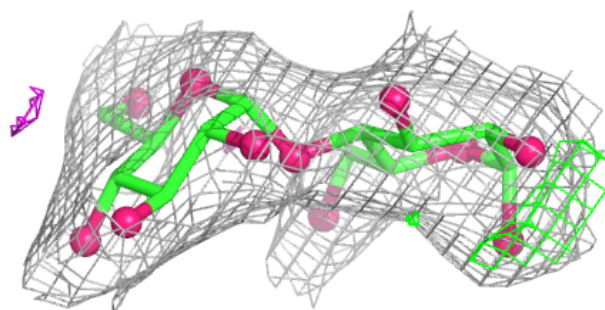
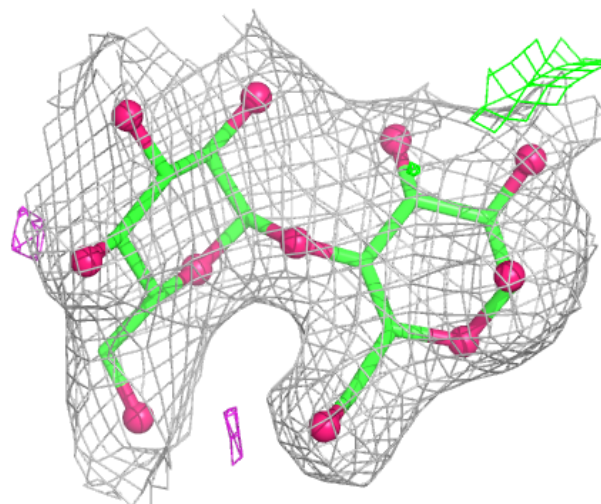
**Electron density around Chain U:**

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



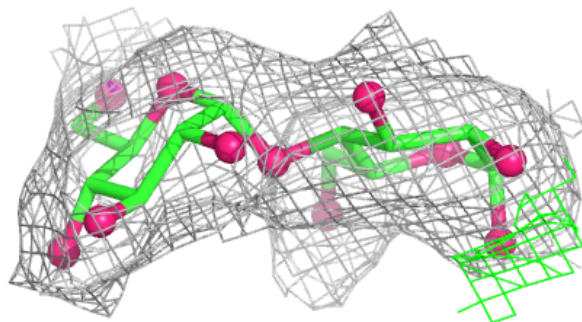
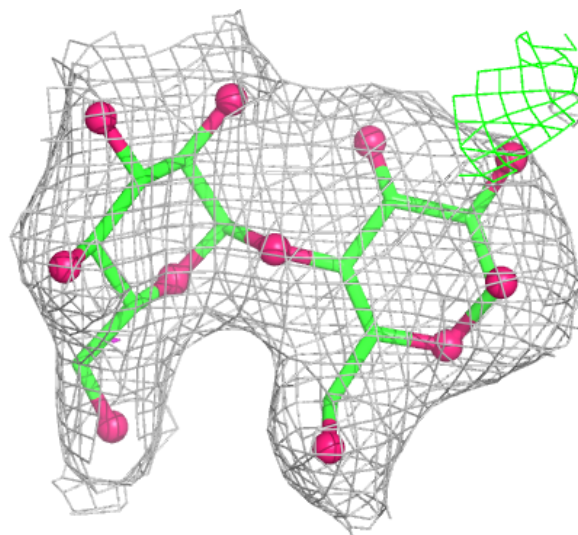
**Electron density around Chain V:**

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

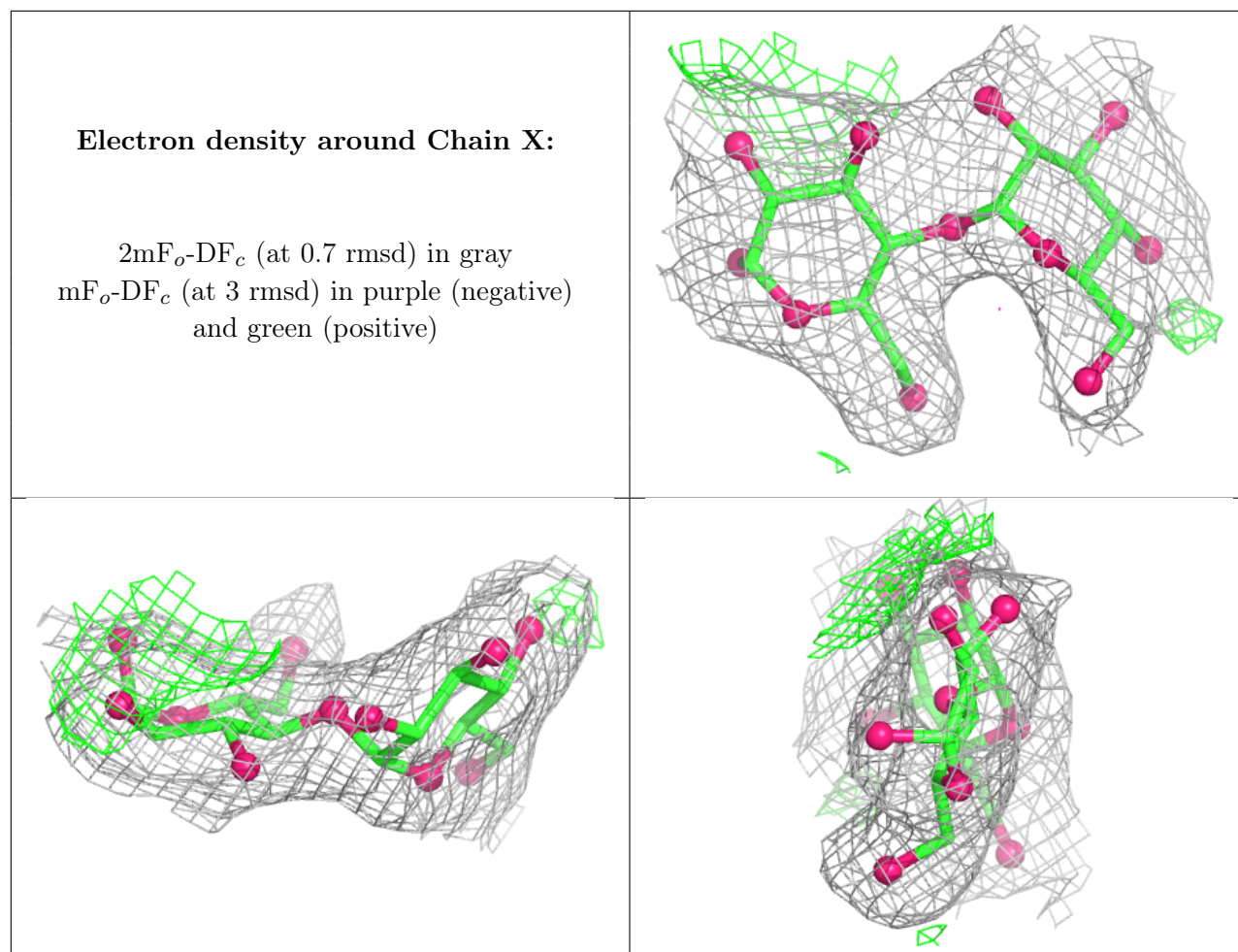


**Electron density around Chain W:**

$2mF_o-DF_c$  (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
5	PO4	D	403	5/5	0.72	0.22	70,71,73,75	1
3	CU	B	401	1/1	0.80	0.09	83,83,83,83	0
5	PO4	D	402	5/5	0.87	0.15	73,74,75,76	1
5	PO4	J	402	5/5	0.90	0.16	53,54,56,57	1
4	SO4	L	402	5/5	0.91	0.19	57,60,63,67	1
5	PO4	I	402	5/5	0.92	0.25	66,68,71,72	1
3	CU	A	401	1/1	0.92	0.04	74,74,74,74	0
3	CU	D	401	1/1	0.93	0.05	58,58,58,58	0
3	CU	J	401	1/1	0.94	0.05	53,53,53,53	0
4	SO4	K	402	5/5	0.95	0.12	60,62,66,74	1
3	CU	I	401	1/1	0.95	0.04	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	402	5/5	0.95	0.24	58,62,66,68	1
3	CU	K	401	1/1	0.97	0.05	67,67,67,67	0
3	CU	G	401	1/1	0.97	0.04	64,64,64,64	0
3	CU	L	401	1/1	0.98	0.04	71,71,71,71	0
3	CU	E	401	1/1	0.98	0.04	55,55,55,55	0
3	CU	C	401	1/1	0.98	0.04	65,65,65,65	0
3	CU	H	401	1/1	0.98	0.02	47,47,47,47	0
3	CU	F	401	1/1	0.99	0.05	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.