



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:43 PM UTC

PDB ID : 6QUG / pdb_00006qug
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

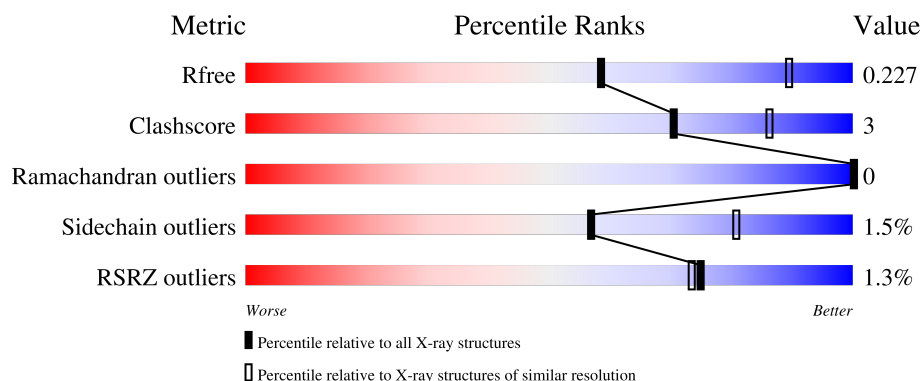
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	0% 87% 6% 7%
1	B	402	0% 82% 11% 7%
1	C	402	0% 85% 7% 7%
1	D	402	2% 84% 8% 7%
1	E	402	0% 83% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	402	 % 86% 6% 7%
1	G	402	 % 85% 7% 7%
1	H	402	 2% 84% 8% 7%
1	I	402	 86% 7% 7%
1	J	402	 % 86% 7% 7%
1	K	402	 % 85% 8% 7%
1	L	402	 % 84% 8% 7%
2	M	2	 100%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 100%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
2	V	2	 100%
2	W	2	 100%
2	X	2	 50% 50%

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
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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
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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 (CCD ID: CU) (formula: Cu).

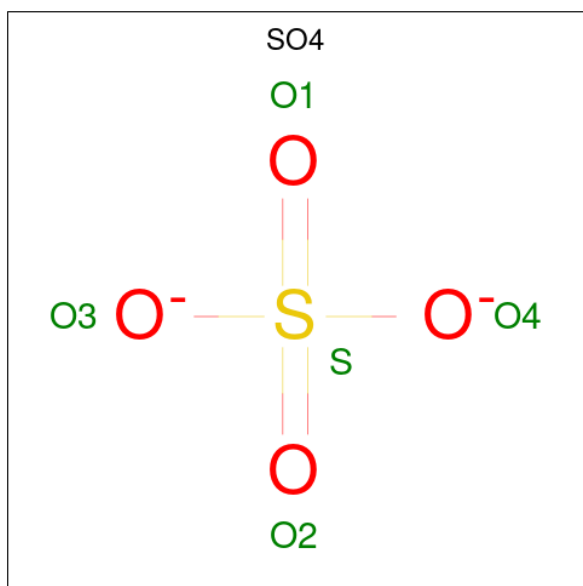
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	E	1	Total	Cu	0	0
			1	1		

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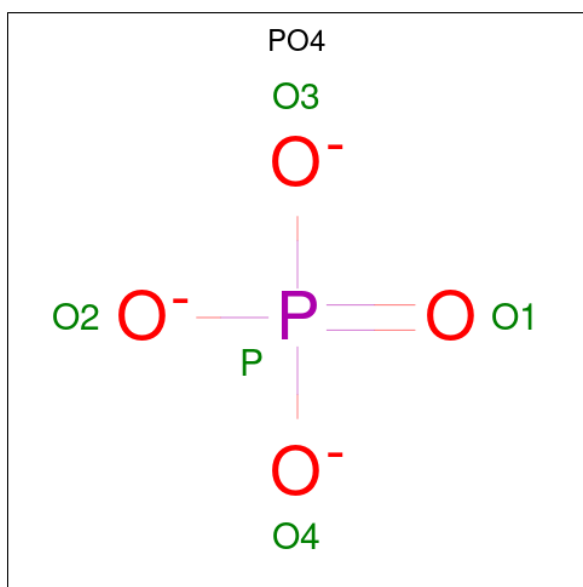
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Cu 1 1	0	0
3	G	1	Total Cu 1 1	0	0
3	H	1	Total Cu 1 1	0	0
3	I	1	Total Cu 1 1	0	0
3	J	1	Total Cu 1 1	0	0
3	K	1	Total Cu 1 1	0	0
3	L	1	Total Cu 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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		

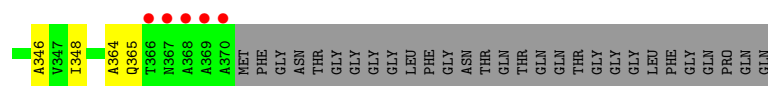
- Molecule 6 is water.

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		

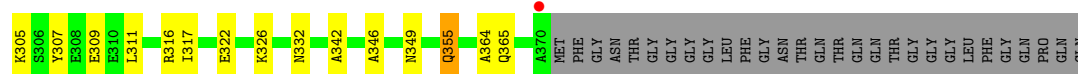
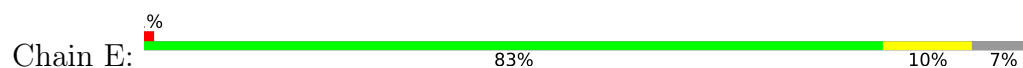
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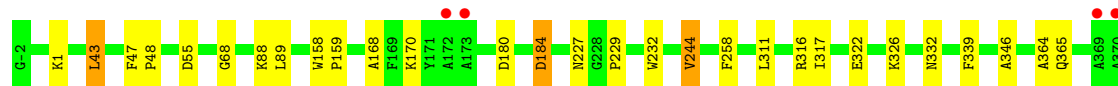
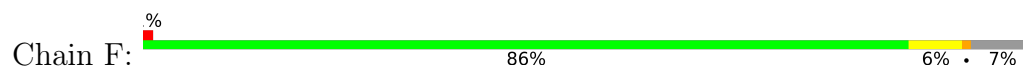
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	26	Total 26	O 26	0	0
6	J	33	Total 33	O 33	0	0
6	K	26	Total 26	O 26	0	0
6	L	23	Total 23	O 23	0	0



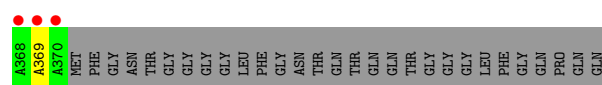
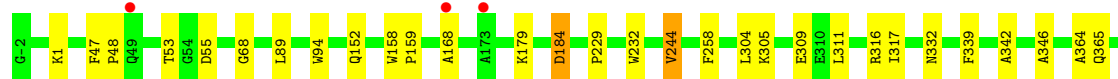
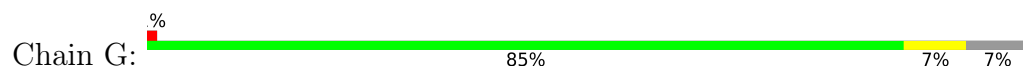
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative



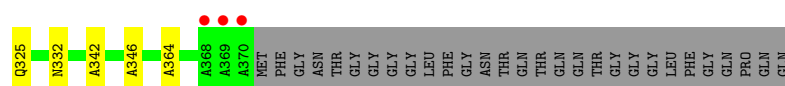
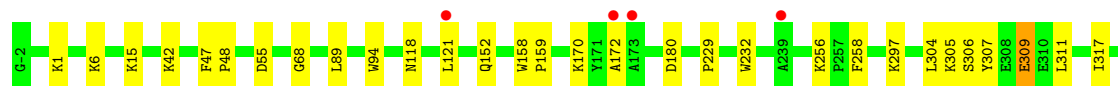
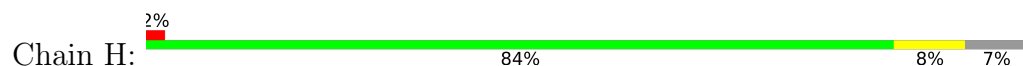
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative



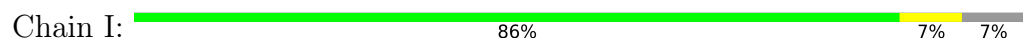
- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

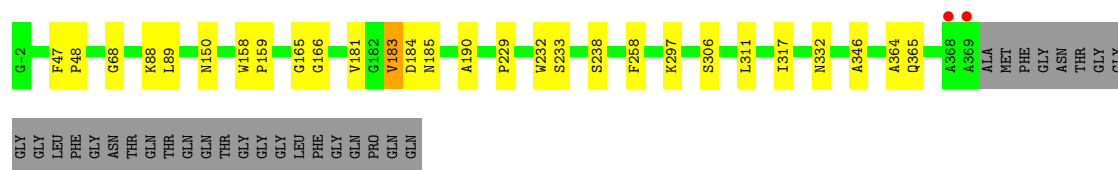


- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

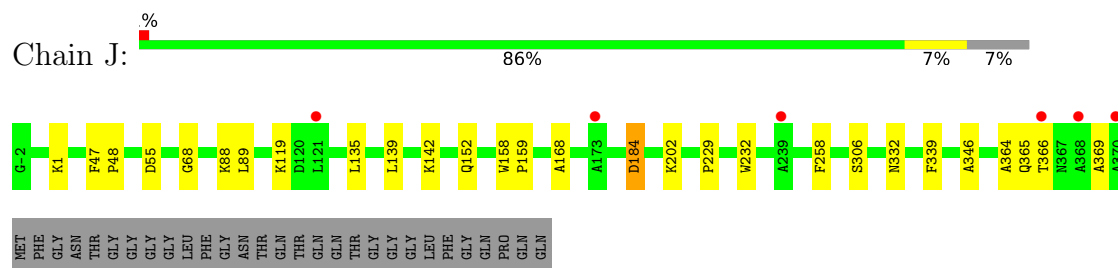


- Molecule 1: Maltodextrin-binding protein,Nucleoporin, putative

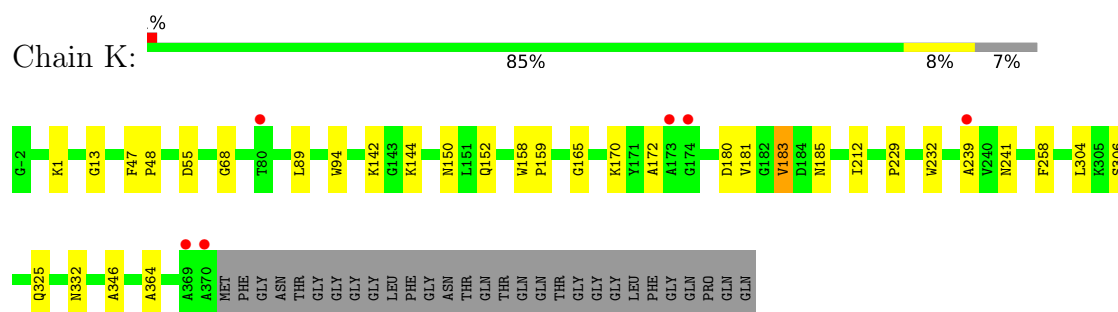




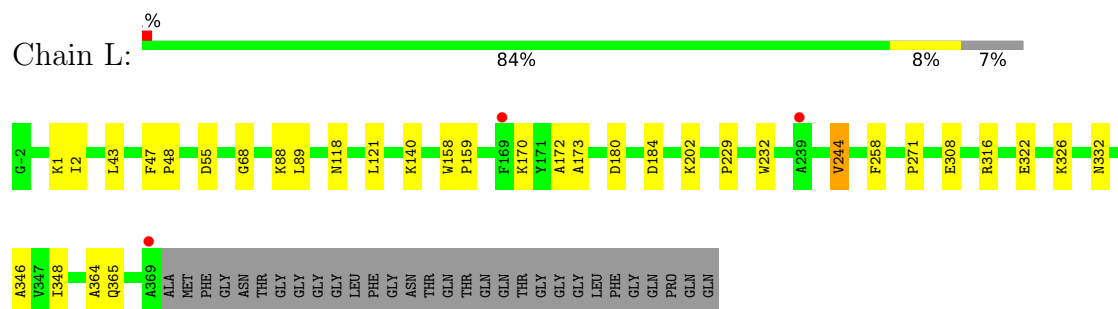
- Molecule 1: Maltodextrin-binding protein, Nucleoporin, putative



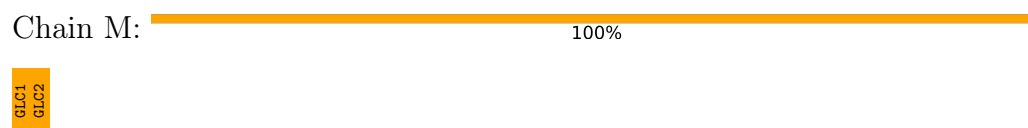
- Molecule 1: Maltodextrin-binding protein, Nucleoporin, putative



- 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

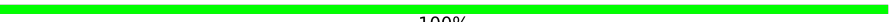


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  50% 50%

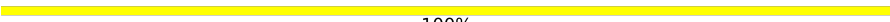


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  100%

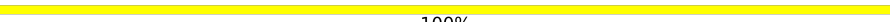


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:  100%

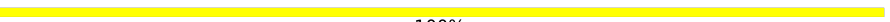


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:  100%

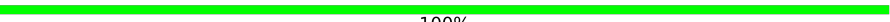


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain S:  100%

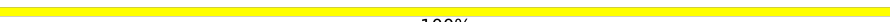


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain T:  100%



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

Chain U:  100%



- 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, α , β , γ	82.91Å 286.78Å 110.78Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.19 – 2.70 49.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.19-2.70) 100.0 (49.19-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	61.1	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.08	1/2929 (0.0%)	1.35	2/3981 (0.1%)
1	B	1.08	2/2929 (0.1%)	1.34	0/3981
1	C	1.07	0/2929	1.34	0/3981
1	D	1.07	1/2929 (0.0%)	1.34	3/3981 (0.1%)
1	E	1.06	1/2929 (0.0%)	1.34	0/3981
1	F	1.07	1/2929 (0.0%)	1.34	1/3981 (0.0%)
1	G	1.09	2/2929 (0.1%)	1.34	1/3981 (0.0%)
1	H	1.07	1/2929 (0.0%)	1.35	2/3981 (0.1%)
1	I	1.09	1/2924 (0.0%)	1.34	0/3974
1	J	1.07	0/2929	1.35	1/3981 (0.0%)
1	K	1.07	0/2929	1.35	0/3981
1	L	1.07	0/2924	1.34	1/3974 (0.0%)
All	All	1.07	10/35138 (0.0%)	1.34	11/47758 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	342	ALA	C-O	5.65	1.30	1.24
1	E	342	ALA	C-O	5.64	1.30	1.24
1	B	190	ALA	C-O	5.50	1.30	1.24
1	I	190	ALA	C-O	5.28	1.30	1.24
1	H	342	ALA	C-O	5.24	1.30	1.24
1	F	227	ASN	C-O	5.11	1.29	1.23
1	B	342	ALA	C-O	5.10	1.29	1.24
1	D	190	ALA	C-O	5.08	1.29	1.24
1	A	227	ASN	C-O	5.05	1.29	1.24
1	G	369	ALA	C-O	5.02	1.29	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	308	GLU	CB-CG-CD	7.08	124.64	112.60
1	D	184	ASP	CA-CB-CG	5.95	118.55	112.60
1	G	184	ASP	CA-CB-CG	5.52	118.12	112.60
1	F	184	ASP	CA-CB-CG	5.34	117.94	112.60
1	H	42	LYS	CA-C-N	5.12	128.51	120.82
1	H	42	LYS	C-N-CA	5.12	128.51	120.82
1	J	184	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	210	TYR	CA-C-N	5.01	126.96	120.44
1	D	210	TYR	C-N-CA	5.01	126.96	120.44
1	A	42	LYS	CA-C-N	5.00	128.32	120.82
1	A	42	LYS	C-N-CA	5.00	128.32	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2859	0	2833	15	0
1	B	2859	0	2833	30	0
1	C	2859	0	2833	21	0
1	D	2859	0	2833	22	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	21	0
1	I	2854	0	2828	14	0
1	J	2859	0	2833	14	0
1	K	2859	0	2833	21	0
1	L	2854	0	2828	26	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	232	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 (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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:D:115:LEU:HD21	1:D:224:MET:HE3	1.66	0.77
1:D:115:LEU:HD11	1:D:224:MET:CE	2.15	0.76
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:HE3	1.72	0.72
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:C:274:GLU:CD	1:C:274:GLU:H	2.02	0.67
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:115:LEU:HD11	1:D:224:MET:HE2	1.84	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:I:166:GLY:HA2	1:I:185:ASN:HD21	1.70	0.56
1:C:128:THR:OG1	1:C:130:GLU:OE1	2.23	0.55
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:E:43:LEU:HD23	1:E:43:LEU:C	2.32	0.55
1:L:184:ASP:HB2	1:L:365:GLN:HB2	1.88	0.55
1:F:43:LEU:C	1:F:43:LEU:HD23	2.32	0.54
1:A:66:ARG:NH2	2:M:2:GLC:O4	2.38	0.54
1:B:79:ILE:C	1:B:81:PRO:HD3	2.33	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:A:43:LEU:C	1:A:43:LEU:HD23	2.31	0.54
1:I:68:GLY:HA3	1:I:332:ASN:O	2.08	0.54
1:L:43:LEU:HD23	1:L:43:LEU:C	2.32	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
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:207:ASP:CG	1:D:207:ASP:OD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:PRO:HA	1:E:232:TRP:CE2	2.47	0.50
1:F:229:PRO:HA	1:F:232:TRP:CE2	2.47	0.50
1:D:229:PRO:HA	1:D:232:TRP:CE2	2.47	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:111:GLU:OE1	2:M:1:GLC:O2	2.33	0.46
1:L:158:TRP:N	1:L:159:PRO:CD	2.78	0.46
1:A:88:LYS:C	1:A:89:LEU:HD12	2.41	0.46
1:K:1:LYS:HG2	1:K:55:ASP:OD1	2.15	0.46
1:F:88:LYS:C	1:F:89:LEU:HD12	2.41	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:D:115:LEU:CD2	1:D:224:MET:HE3	2.42	0.46
1:J:88:LYS:C	1:J:89:LEU:HD12	2.41	0.46
1:L:88:LYS:C	1:L:89:LEU:HD12	2.41	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:LYS:C	1:I:89:LEU:HD12	2.43	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:D:88:LYS:C	1:D:89:LEU:HD12	2.42	0.44
1:G:311:LEU:HB3	1:G:317:ILE:HD13	1.99	0.44
1:A:89:LEU:HD12	1:A:89:LEU:N	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:L:118:ASN:CG	1:L:121:LEU:HD13	2.44	0.43
1:H:118:ASN:CG	1:H:121:LEU:HD13	2.44	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:HD12	1:F:89:LEU:N	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:HD12	1:J:89:LEU:N	2.33	0.42
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: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:L:118:ASN:ND2	1:L:121:LEU:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:15:LYS:C	1:H:297:LYS:HD2	2.45	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: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 [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	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%)	76	90
1	B	288/307 (94%)	282 (98%)	6 (2%)	47	75
1	C	288/307 (94%)	285 (99%)	3 (1%)	68	86
1	D	288/307 (94%)	282 (98%)	6 (2%)	47	75
1	E	288/307 (94%)	284 (99%)	4 (1%)	59	82
1	F	288/307 (94%)	285 (99%)	3 (1%)	68	86
1	G	288/307 (94%)	284 (99%)	4 (1%)	59	82
1	H	288/307 (94%)	283 (98%)	5 (2%)	53	79
1	I	288/307 (94%)	284 (99%)	4 (1%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	288/307 (94%)	283 (98%)	5 (2%)	53	79
1	K	288/307 (94%)	283 (98%)	5 (2%)	53	79
1	L	288/307 (94%)	284 (99%)	4 (1%)	59	82
All	All	3456/3684 (94%)	3405 (98%)	51 (2%)	57	81

All (51) 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	175	LYS
1	B	179	LYS
1	B	198	LEU
1	B	258	PHE
1	B	325	GLN
1	C	184	ASP
1	C	258	PHE
1	C	274	GLU
1	D	1	LYS
1	D	2	ILE
1	D	258	PHE
1	D	297	LYS
1	D	325	GLN
1	D	348	ILE
1	E	152	GLN
1	E	244	VAL
1	E	258	PHE
1	E	355	GLN
1	F	43	LEU
1	F	244	VAL
1	F	258	PHE
1	G	152	GLN
1	G	179	LYS
1	G	244	VAL
1	G	258	PHE
1	H	6	LYS
1	H	152	GLN
1	H	258	PHE
1	H	306	SER
1	H	309	GLU

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Mol	Chain	Res	Type
1	I	183	VAL
1	I	238	SER
1	I	258	PHE
1	I	306	SER
1	J	119	LYS
1	J	152	GLN
1	J	202	LYS
1	J	258	PHE
1	J	306	SER
1	K	142	LYS
1	K	152	GLN
1	K	183	VAL
1	K	258	PHE
1	K	306	SER
1	L	202	LYS
1	L	244	VAL
1	L	258	PHE
1	L	348	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	72	GLN
1	B	72	GLN
1	B	325	GLN
1	B	355	GLN
1	C	18	ASN
1	C	72	GLN
1	C	201	ASN
1	D	18	ASN
1	D	72	GLN
1	D	152	GLN
1	D	325	GLN
1	D	355	GLN
1	E	18	ASN
1	E	72	GLN
1	E	152	GLN
1	F	18	ASN
1	F	72	GLN
1	F	124	ASN
1	F	201	ASN

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Mol	Chain	Res	Type
1	F	234	ASN
1	G	18	ASN
1	G	72	GLN
1	G	152	GLN
1	H	72	GLN
1	H	152	GLN
1	I	18	ASN
1	I	72	GLN
1	J	72	GLN
1	J	152	GLN
1	K	18	ASN
1	K	72	GLN
1	K	152	GLN
1	K	355	GLN
1	L	18	ASN
1	L	72	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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:

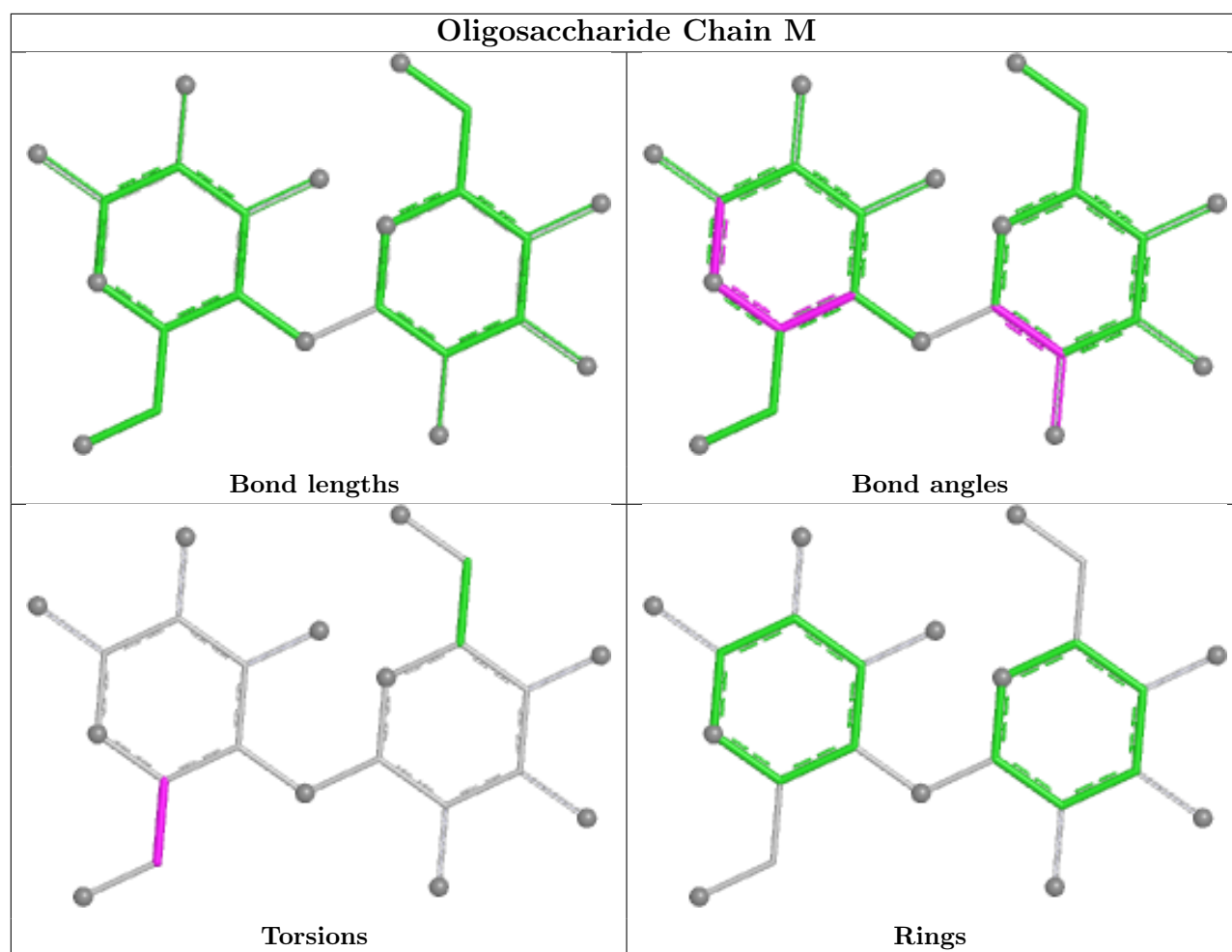
Mol	Chain	Res	Type	Atoms
2	V	1	GLC	O5-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	V	1	GLC	C4-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	X	1	GLC	C4-C5-C6-O6
2	X	1	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6
2	M	1	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	O	1	GLC	O5-C5-C6-O6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

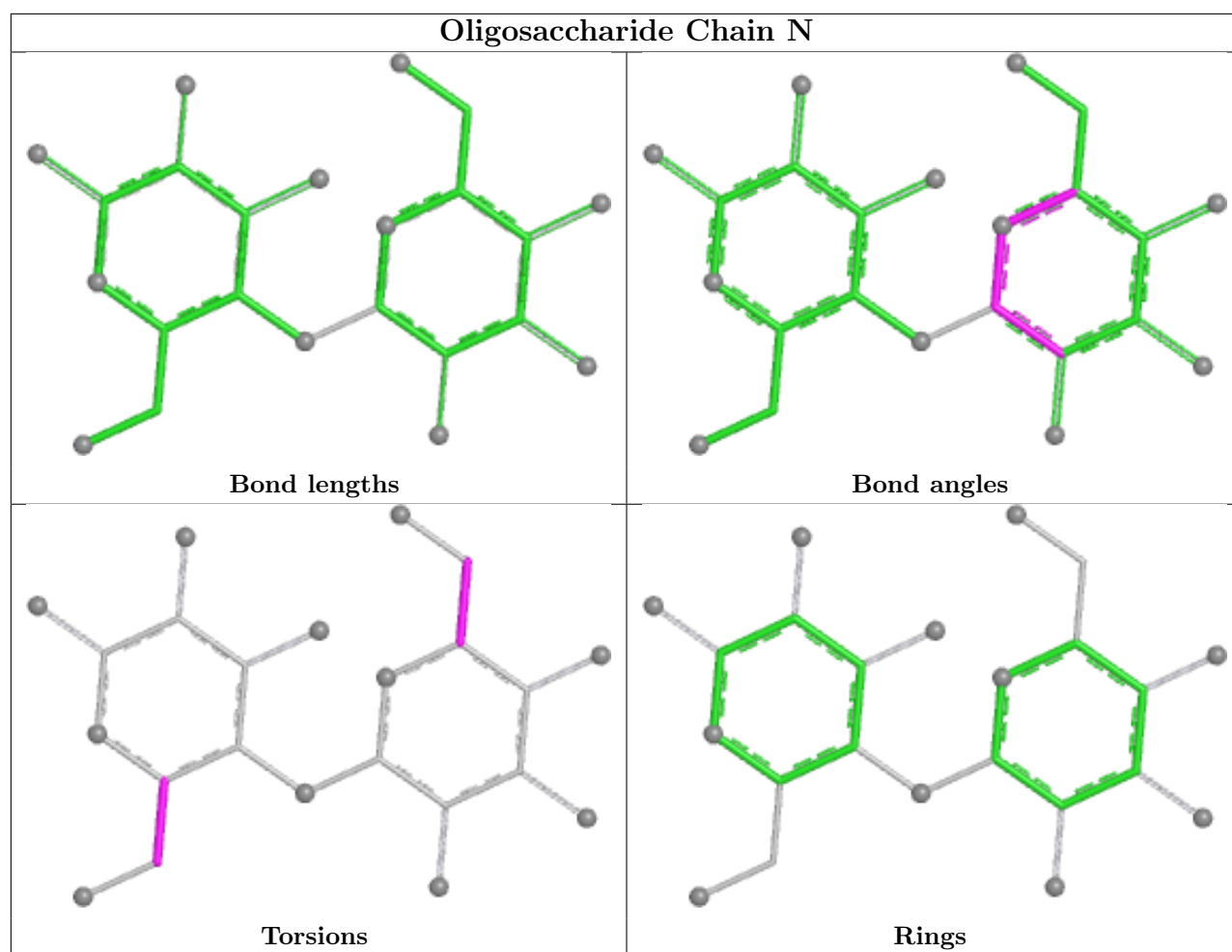
There are no ring outliers.

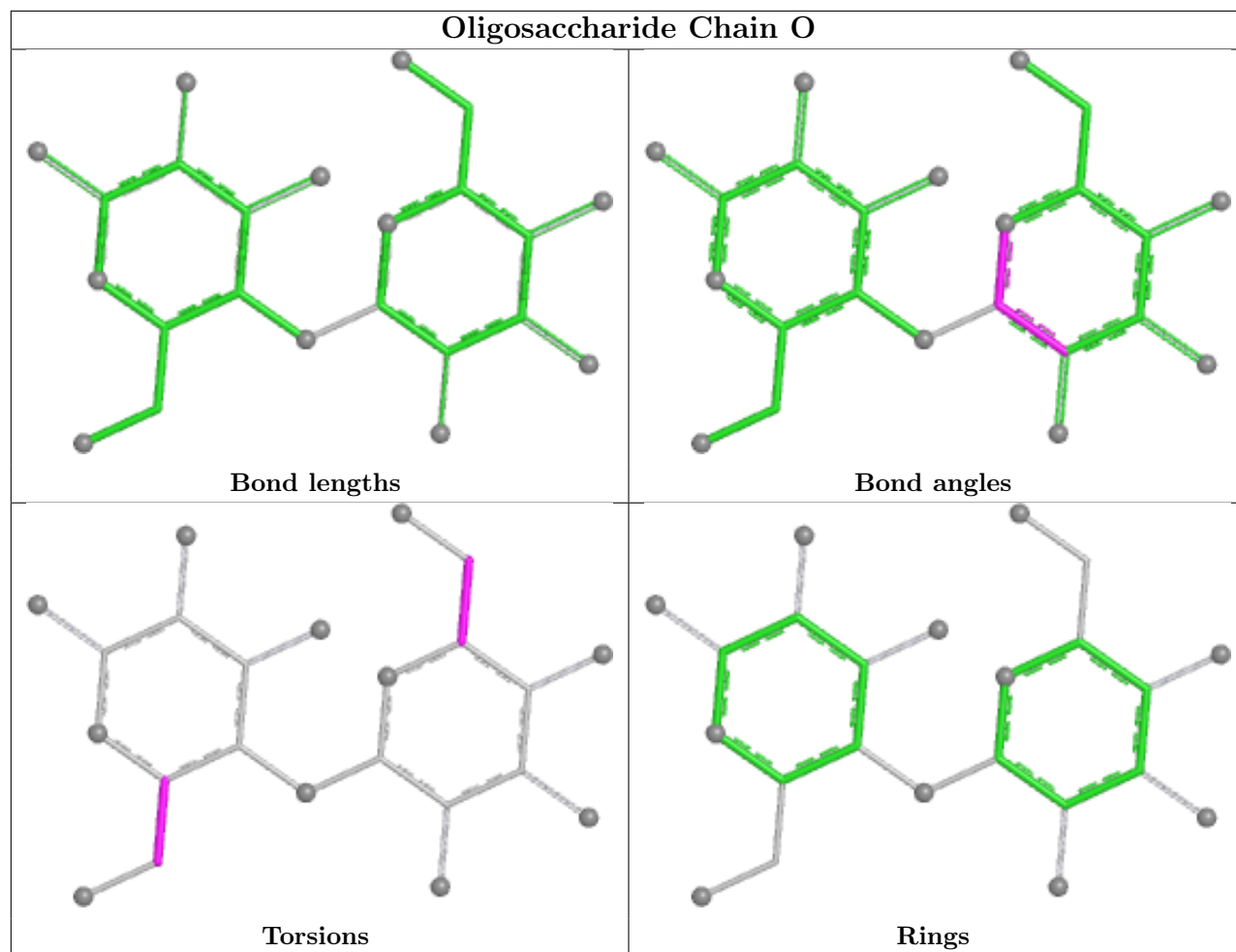
2 monomers are involved in 2 short contacts:

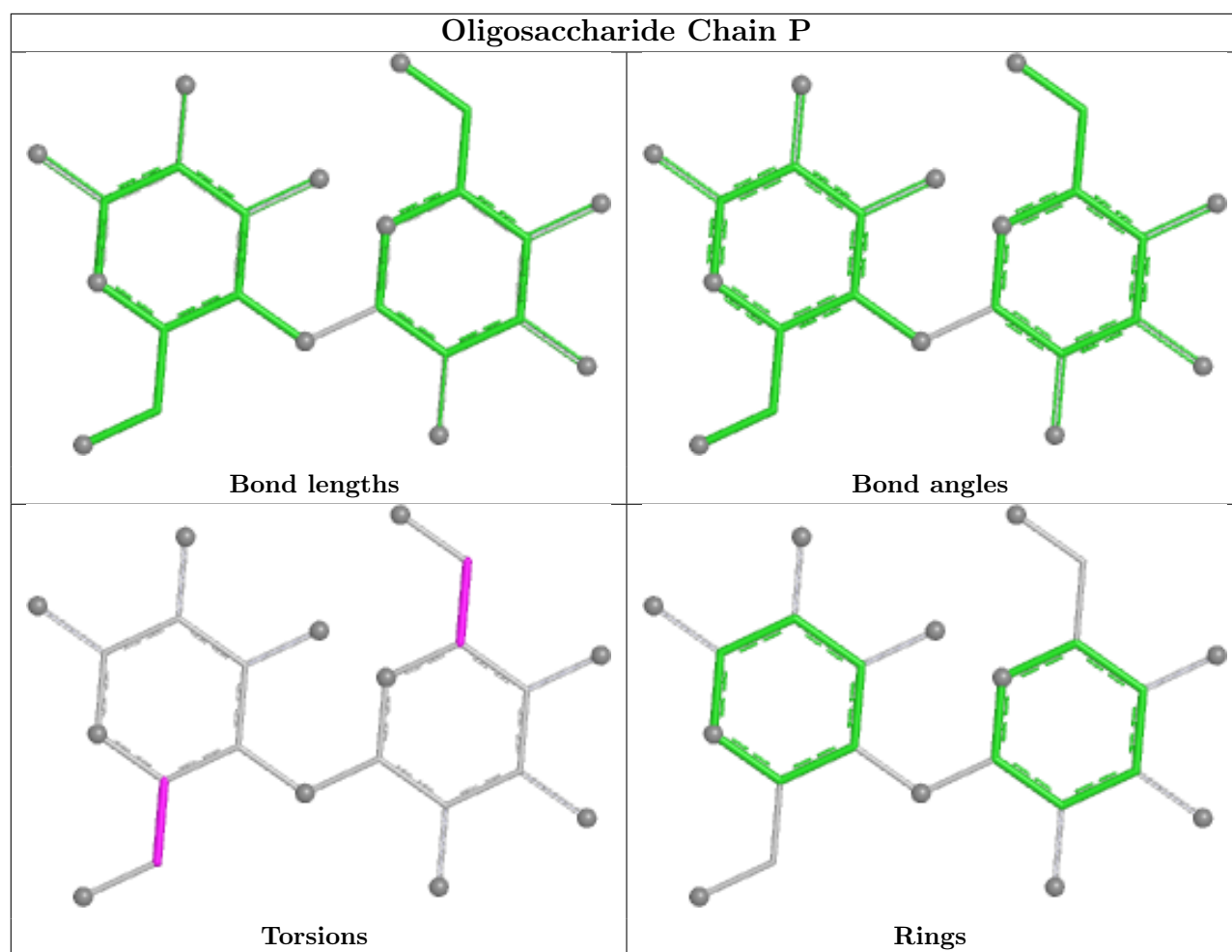
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	GLC	1	0
2	M	2	GLC	1	0

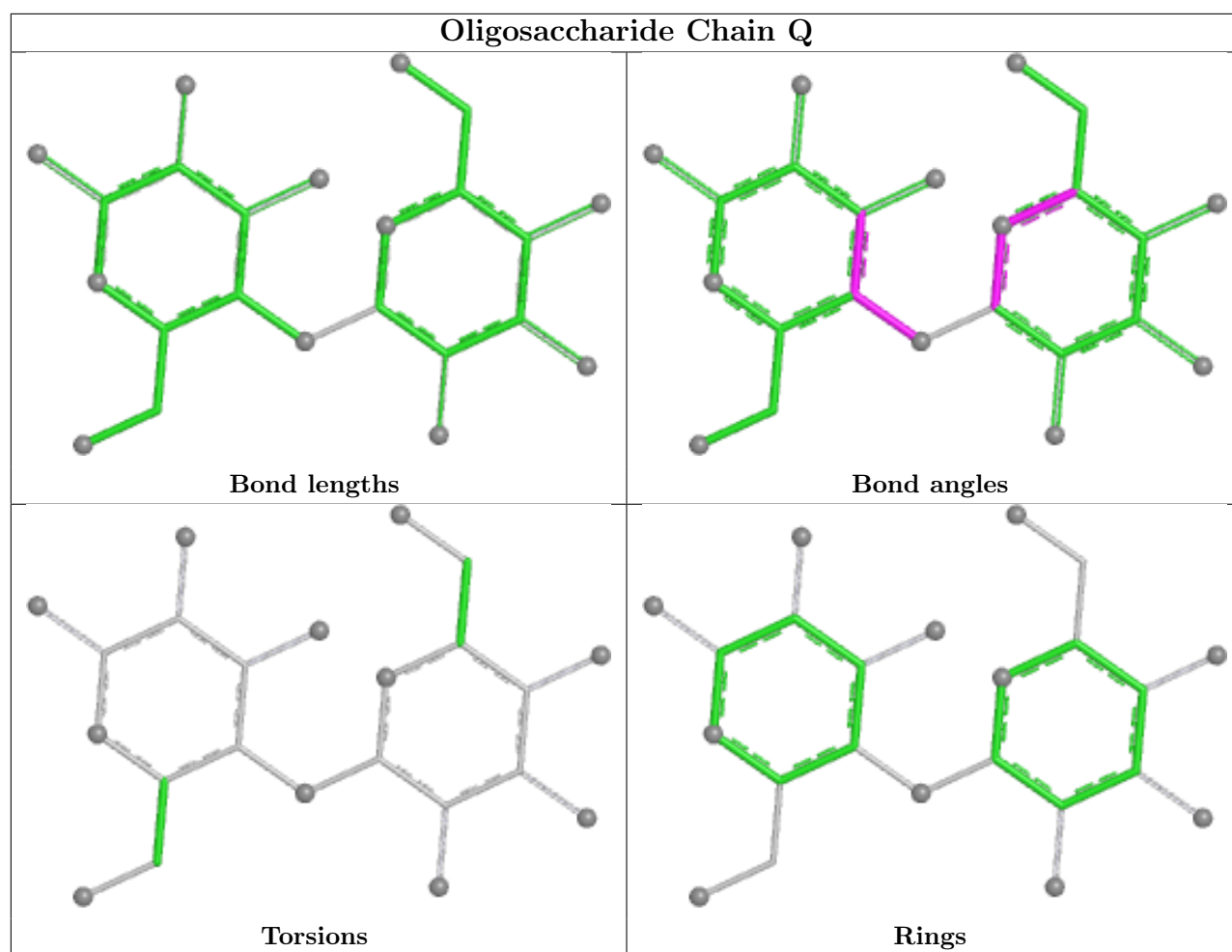
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

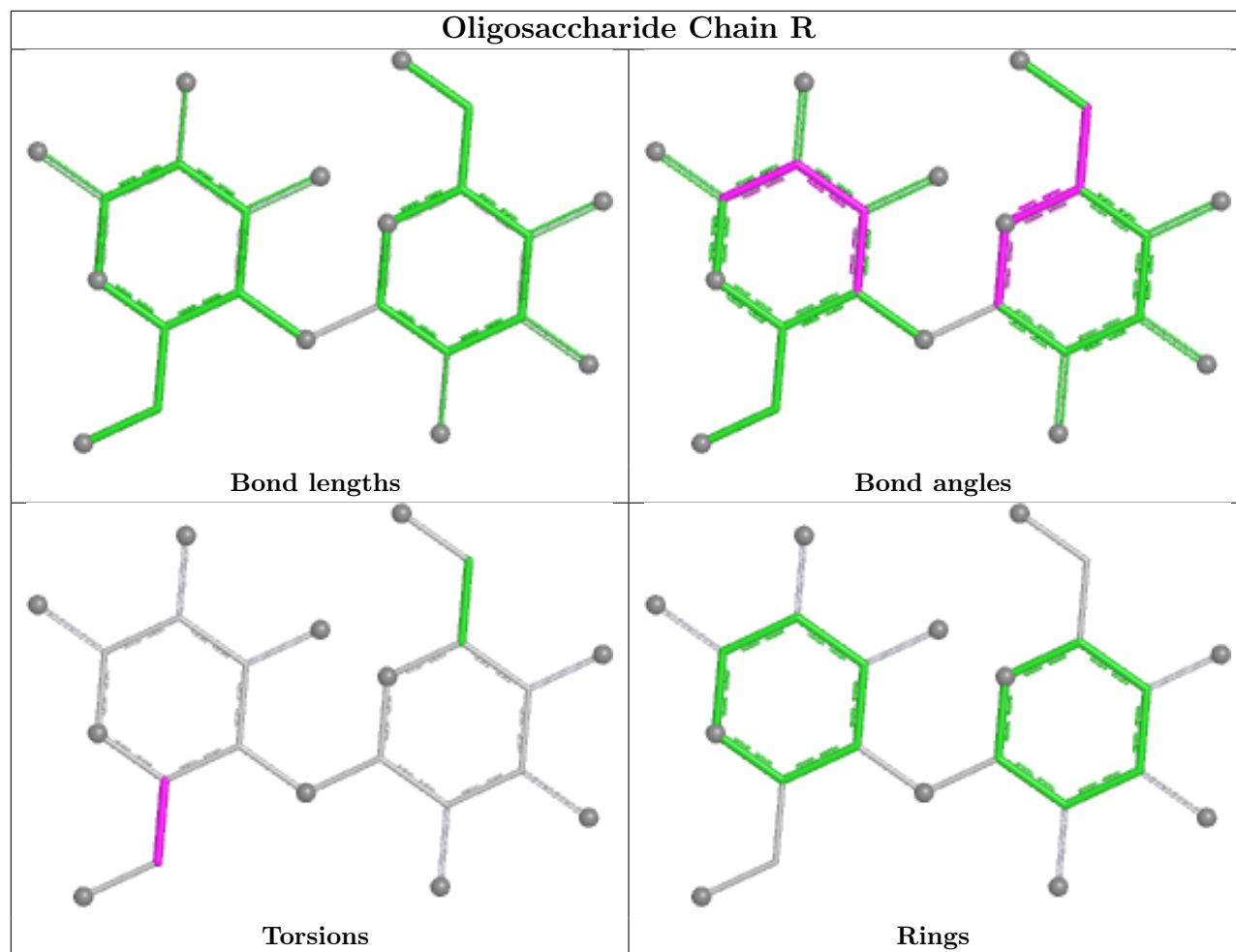


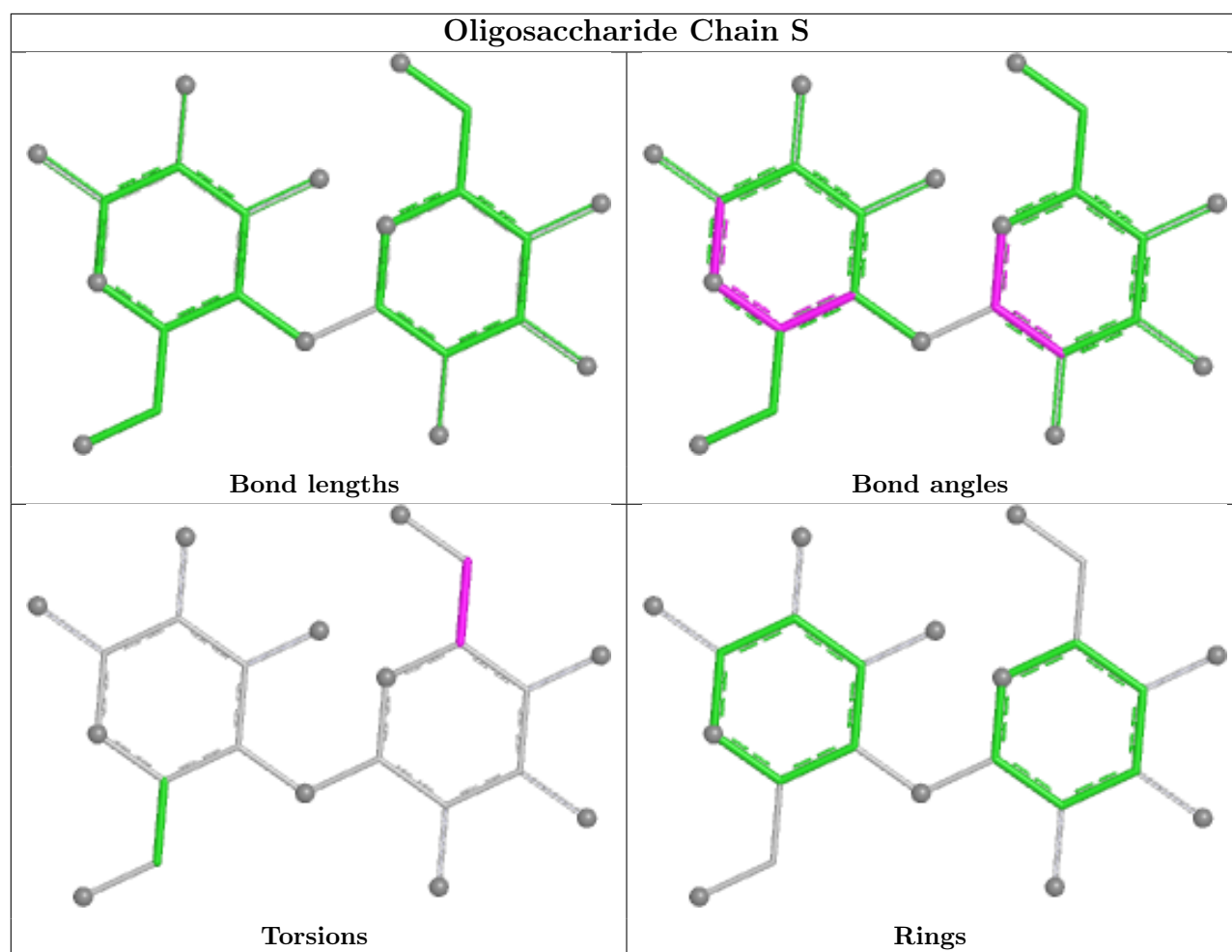


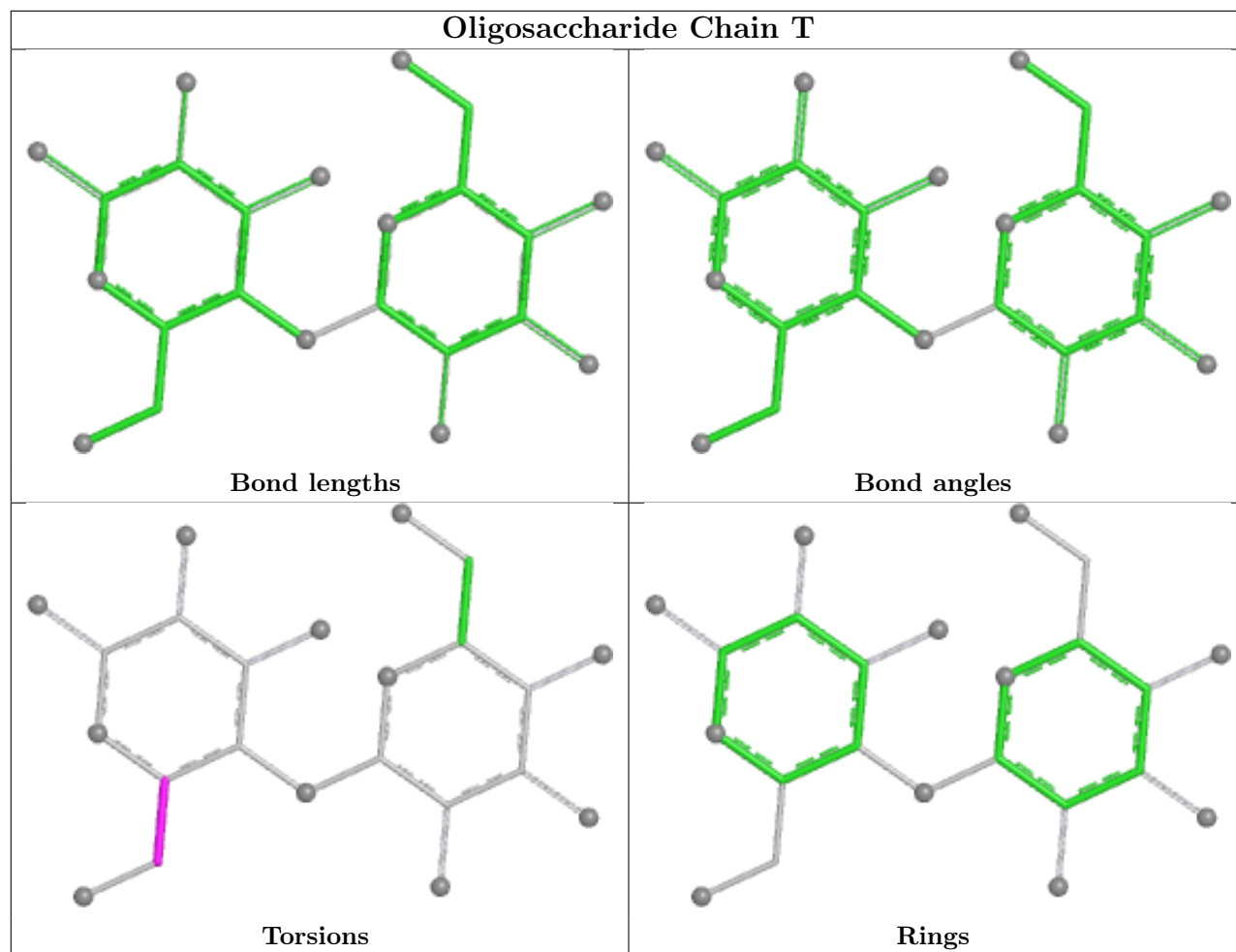


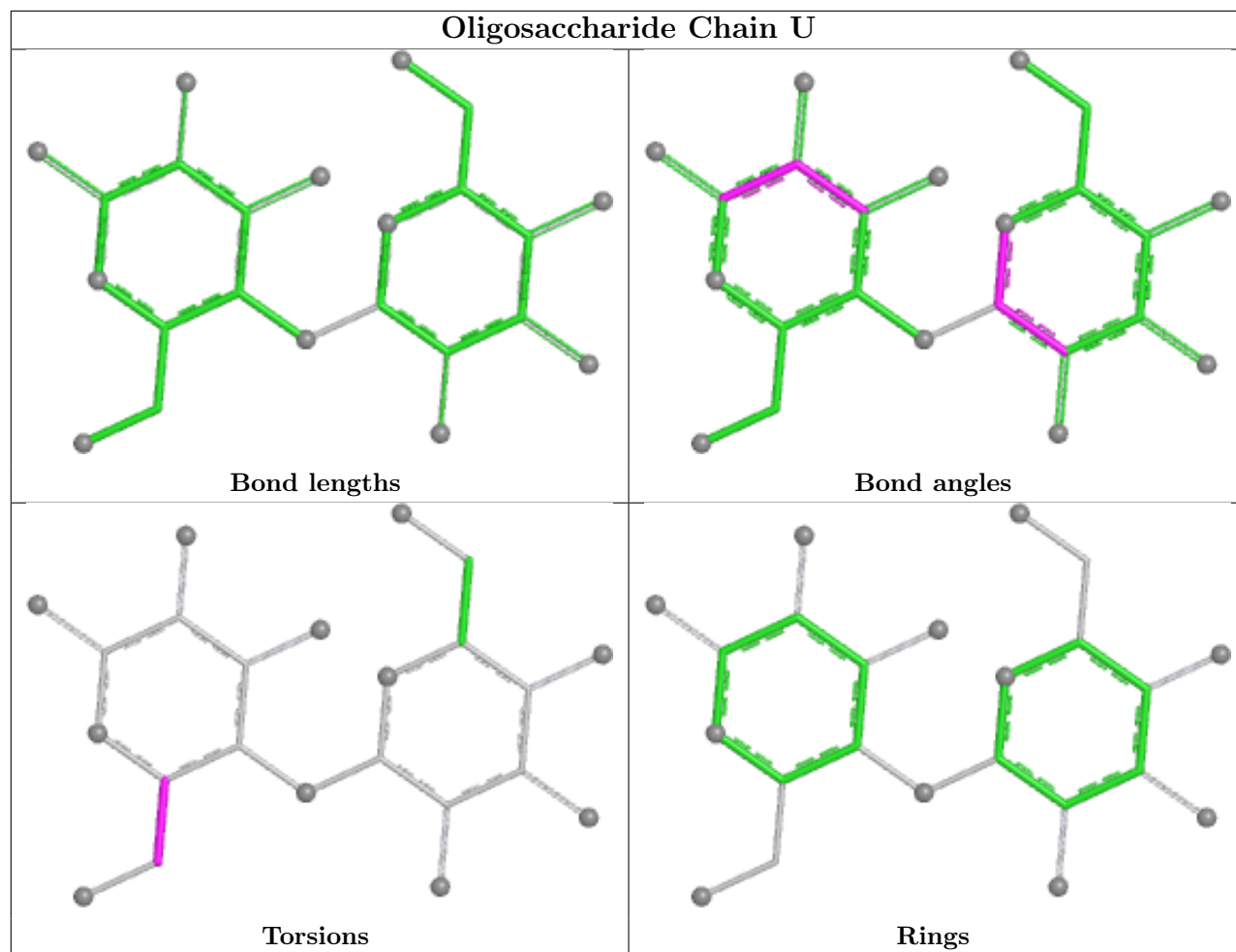


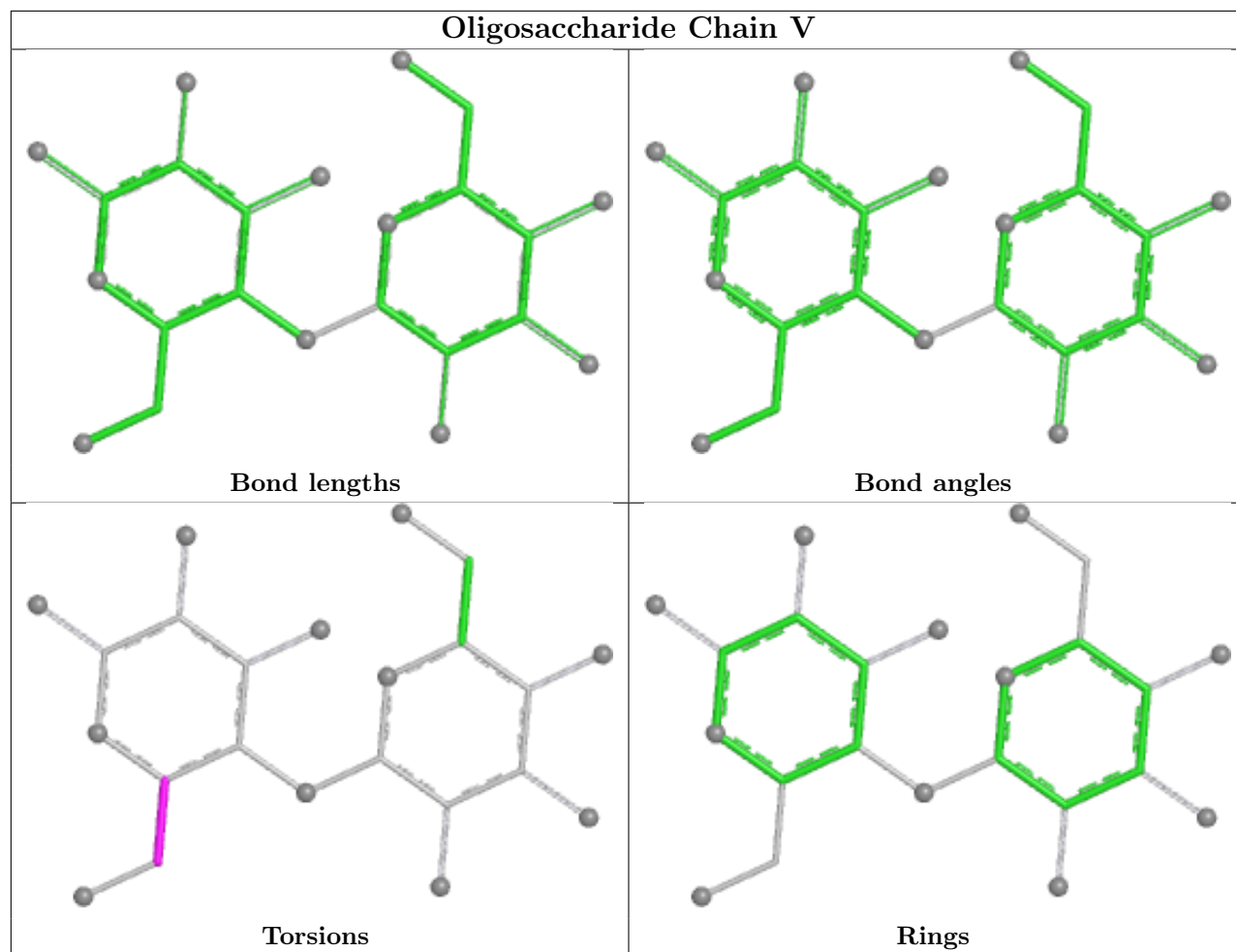


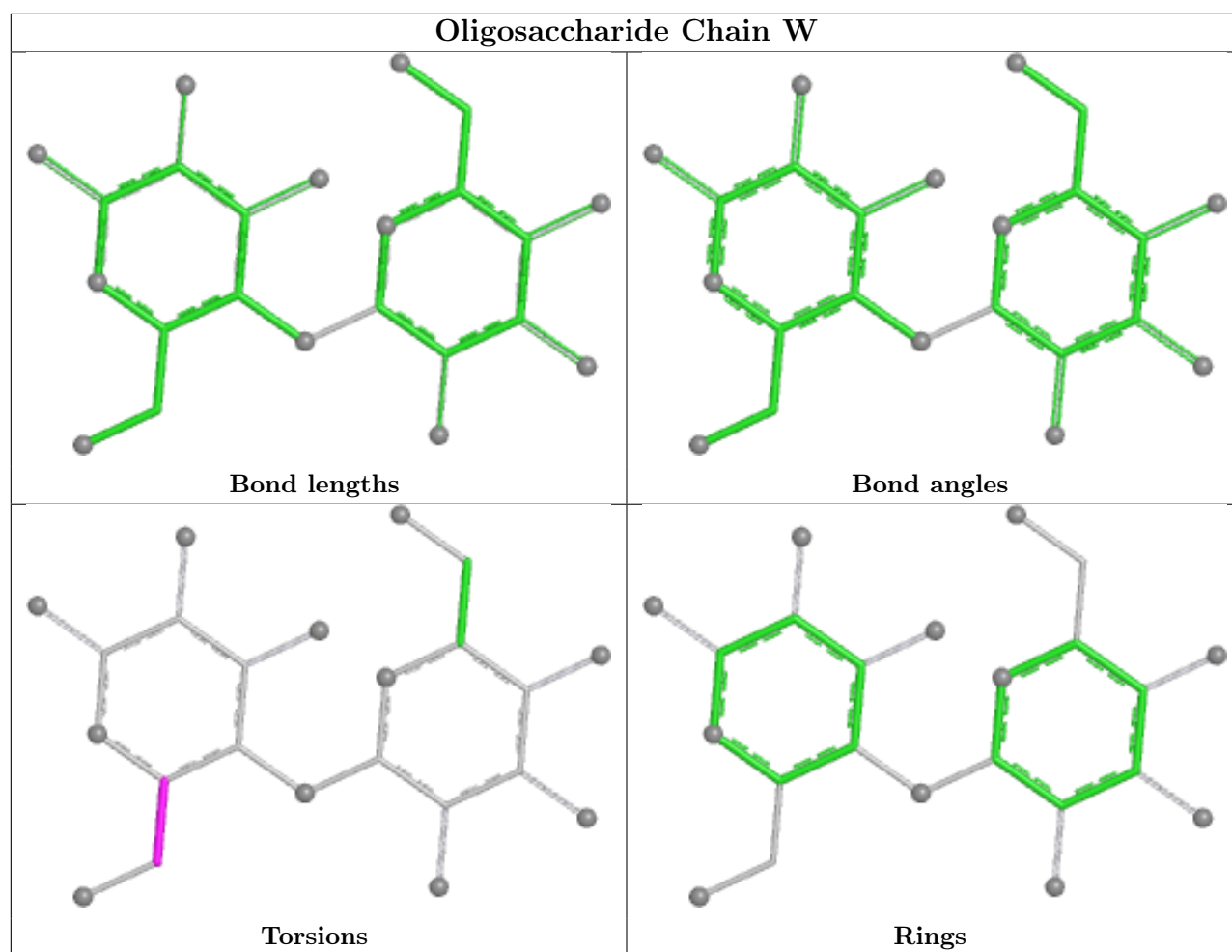


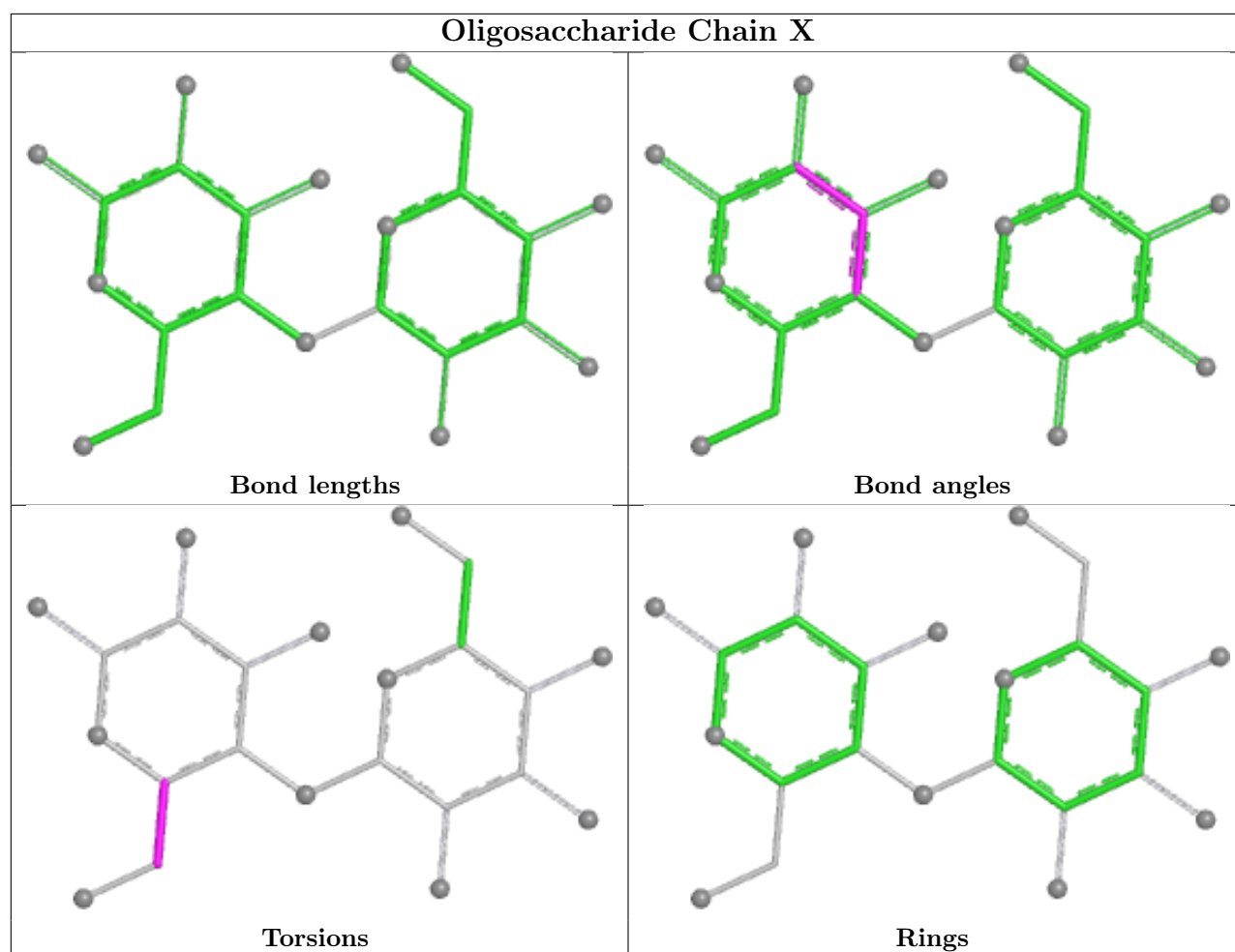












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	PO4	I	402	-	4,4,4	0.87	0	6,6,6	0.47	0
4	SO4	K	402	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	L	402	-	4,4,4	0.30	0	6,6,6	0.12	0
5	PO4	D	402	-	4,4,4	0.75	0	6,6,6	0.45	0
4	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.13	0
5	PO4	D	403	-	4,4,4	0.71	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	J	402	-	4,4,4	0.77	0	6,6,6	0.46	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	373/402 (92%)	-0.10	3 (0%) 82 81	43, 56, 79, 115	0
1	B	373/402 (92%)	0.32	5 (1%) 75 73	49, 76, 111, 142	0
1	C	373/402 (92%)	0.16	3 (0%) 82 81	50, 69, 97, 123	0
1	D	373/402 (92%)	0.21	8 (2%) 63 61	43, 70, 113, 146	0
1	E	373/402 (92%)	0.28	6 (1%) 70 68	50, 76, 117, 131	0
1	F	373/402 (92%)	0.02	4 (1%) 78 76	45, 65, 85, 123	0
1	G	373/402 (92%)	-0.02	6 (1%) 70 68	43, 58, 85, 113	0
1	H	373/402 (92%)	0.20	7 (1%) 66 63	42, 61, 81, 134	0
1	I	372/402 (92%)	0.01	2 (0%) 87 86	44, 60, 89, 119	0
1	J	373/402 (92%)	-0.05	6 (1%) 70 68	39, 58, 88, 119	0
1	K	373/402 (92%)	0.05	6 (1%) 70 68	39, 57, 85, 118	0
1	L	372/402 (92%)	0.00	3 (0%) 82 81	42, 59, 88, 105	0
All	All	4474/4824 (92%)	0.09	59 (1%) 75 73	39, 63, 98, 146	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	370	ALA	4.9
1	B	370	ALA	4.3
1	J	370	ALA	4.2
1	K	370	ALA	4.2
1	G	173	ALA	4.1
1	A	370	ALA	4.0
1	C	370	ALA	3.8
1	L	369	ALA	3.8
1	E	370	ALA	3.6
1	D	366	THR	3.5
1	C	239	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	370	ALA	3.4
1	K	174	GLY	3.2
1	H	369	ALA	3.2
1	B	178	ILE	3.2
1	H	173	ALA	3.2
1	J	239	ALA	3.0
1	A	173	ALA	3.0
1	H	172	ALA	2.8
1	I	369	ALA	2.8
1	J	368	ALA	2.8
1	G	369	ALA	2.8
1	K	239	ALA	2.7
1	D	370	ALA	2.7
1	J	173	ALA	2.7
1	A	369	ALA	2.7
1	E	172	ALA	2.7
1	K	173	ALA	2.7
1	G	368	ALA	2.6
1	E	121	LEU	2.5
1	B	369	ALA	2.5
1	K	369	ALA	2.5
1	L	169	PHE	2.4
1	H	121	LEU	2.4
1	F	173	ALA	2.4
1	G	168	ALA	2.4
1	E	237	THR	2.3
1	J	366	THR	2.3
1	D	141	ALA	2.3
1	D	207	ASP	2.3
1	H	239	ALA	2.2
1	B	366	THR	2.2
1	B	166	GLY	2.2
1	D	369	ALA	2.2
1	E	45	GLU	2.2
1	G	49	GLN	2.2
1	D	135	LEU	2.1
1	F	370	ALA	2.1
1	I	368	ALA	2.1
1	L	239	ALA	2.1
1	C	212	ILE	2.1
1	D	368	ALA	2.1
1	E	141	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	368	ALA	2.1
1	K	80	THR	2.1
1	J	121	LEU	2.1
1	D	367	ASN	2.1
1	F	172	ALA	2.0
1	F	369	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	P	1	12/12	0.88	0.10	45,52,56,56	0
2	GLC	Q	1	12/12	0.90	0.10	55,60,65,66	0
2	GLC	O	1	12/12	0.91	0.08	53,58,65,70	0
2	GLC	P	2	11/12	0.92	0.07	44,47,49,50	0
2	GLC	S	2	11/12	0.92	0.08	47,51,54,56	0
2	GLC	M	1	12/12	0.93	0.08	46,48,48,49	0
2	GLC	T	1	12/12	0.93	0.07	41,49,55,60	0
2	GLC	V	1	12/12	0.93	0.07	46,49,54,55	0
2	GLC	W	1	12/12	0.93	0.08	42,49,54,61	0
2	GLC	W	2	11/12	0.93	0.07	42,46,49,51	0
2	GLC	N	1	12/12	0.94	0.07	57,66,69,75	0
2	GLC	T	2	11/12	0.94	0.07	48,51,53,56	0
2	GLC	U	1	12/12	0.94	0.08	42,49,50,51	0
2	GLC	X	1	12/12	0.94	0.08	39,44,48,51	0
2	GLC	X	2	11/12	0.94	0.08	38,41,43,43	0
2	GLC	M	2	11/12	0.95	0.07	39,47,51,51	0
2	GLC	V	2	11/12	0.95	0.07	41,45,47,48	0
2	GLC	N	2	11/12	0.95	0.06	53,56,61,61	0
2	GLC	R	1	12/12	0.95	0.06	48,52,55,56	0
2	GLC	S	1	12/12	0.95	0.06	41,49,52,58	0
2	GLC	U	2	11/12	0.95	0.07	48,50,54,56	0
2	GLC	Q	2	11/12	0.96	0.07	48,53,55,56	0

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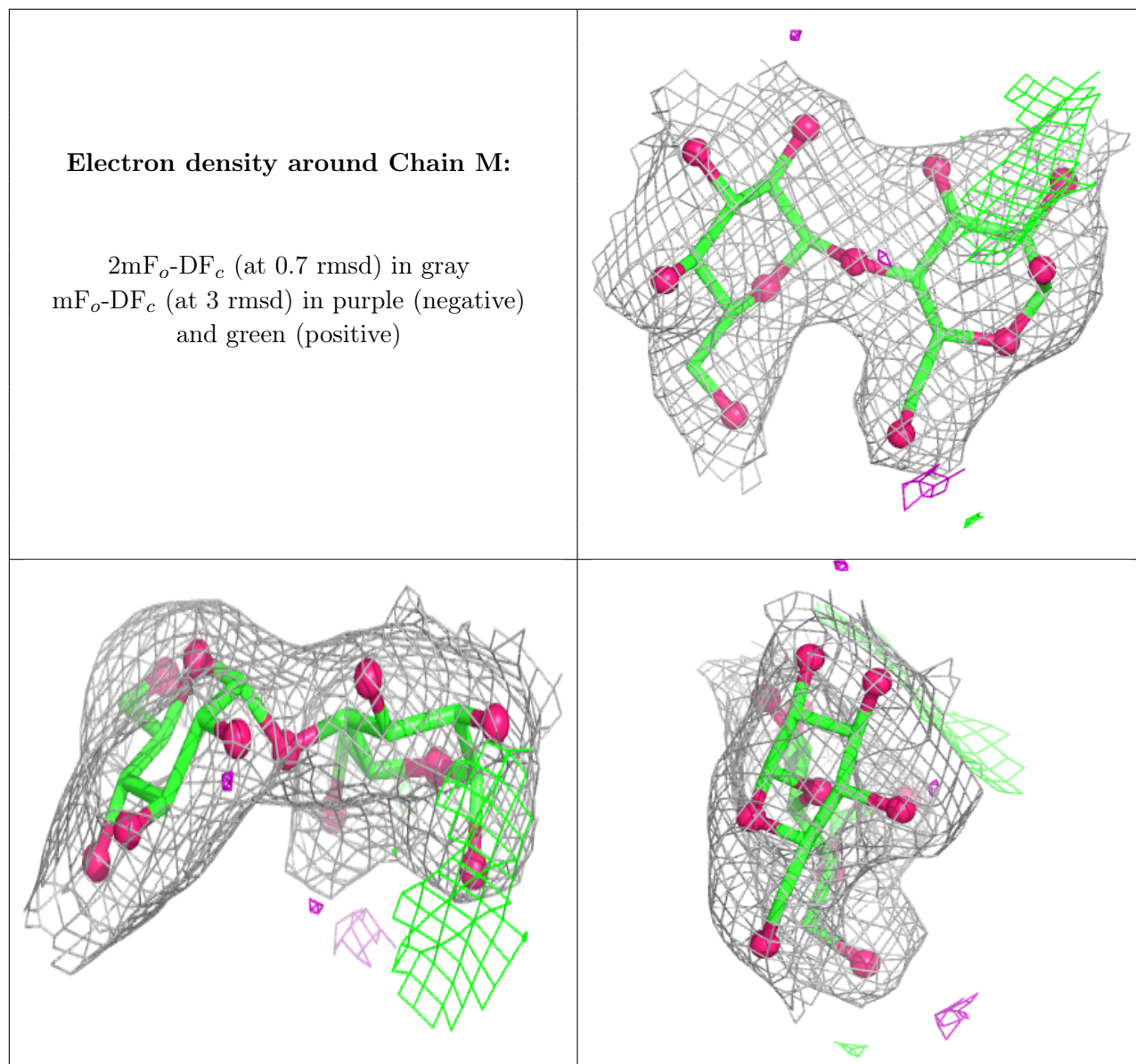
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	O	2	11/12	0.97	0.04	47,48,52,52	0
2	GLC	R	2	11/12	0.97	0.05	45,50,52,54	0

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.

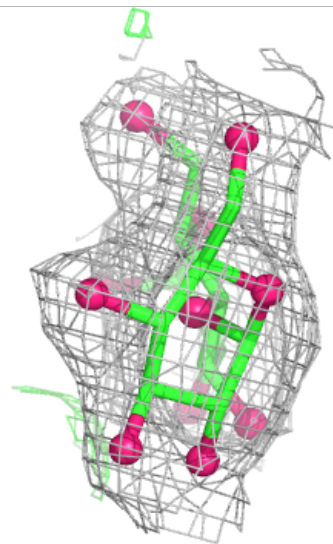
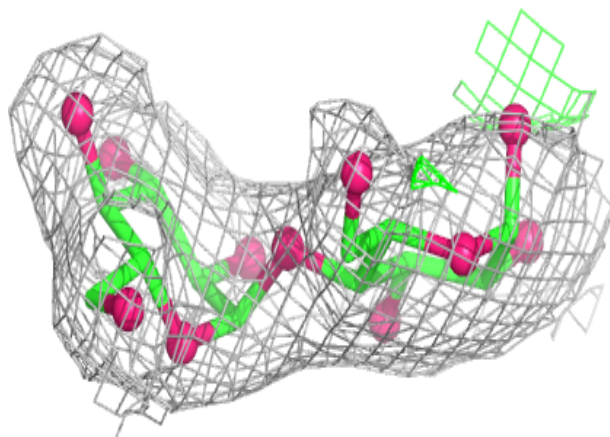
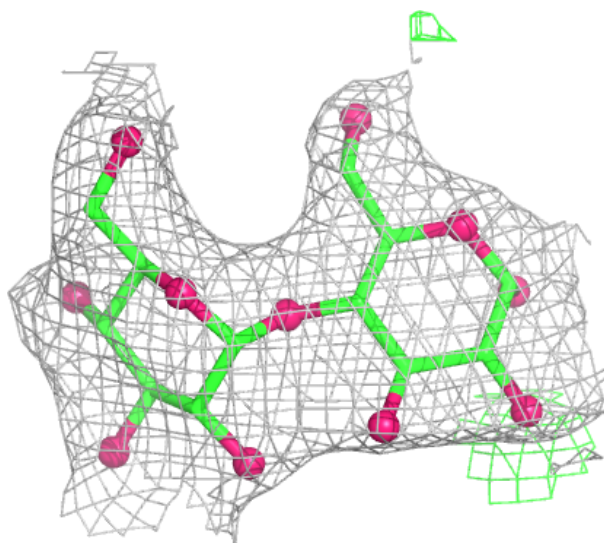
Electron density around Chain M:

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



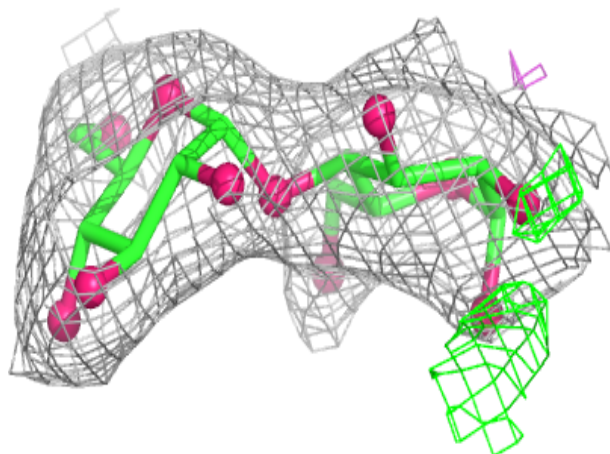
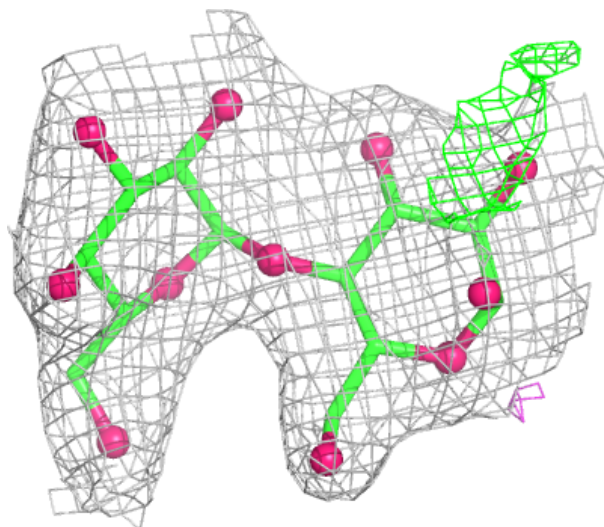
Electron density around Chain N:

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



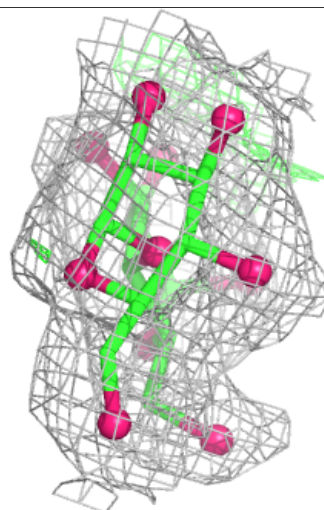
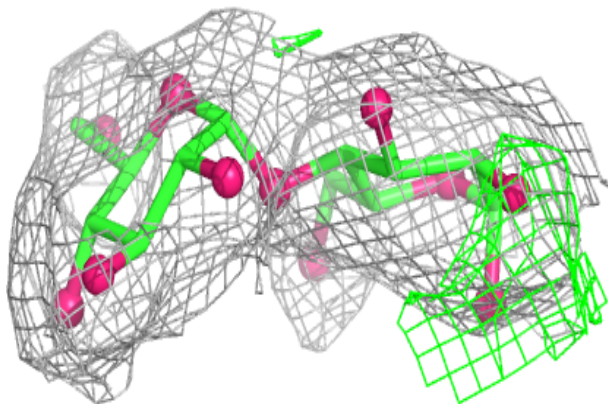
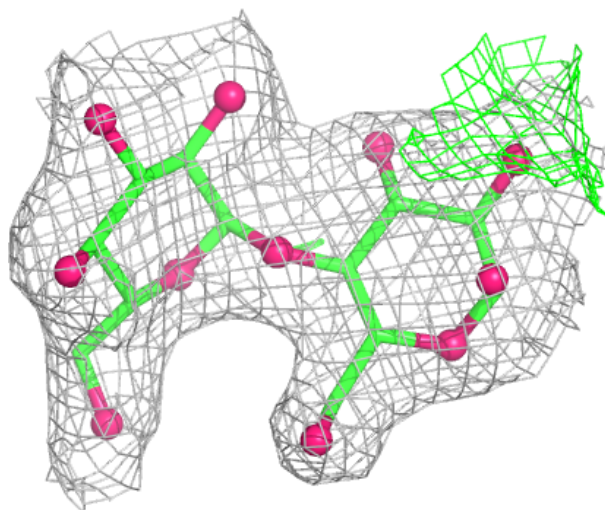
Electron density around Chain O:

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



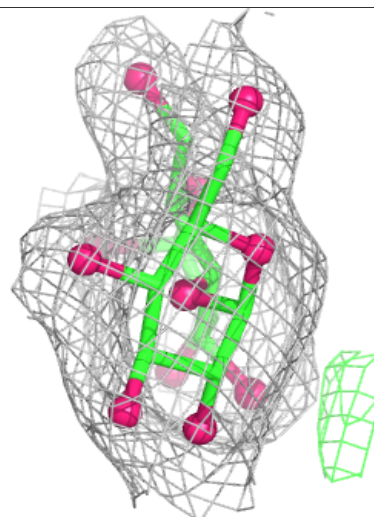
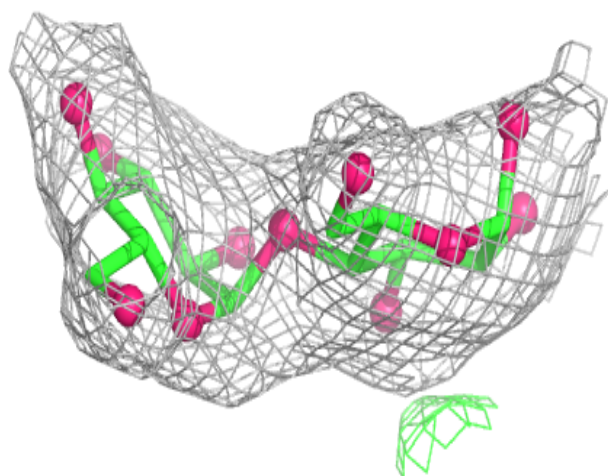
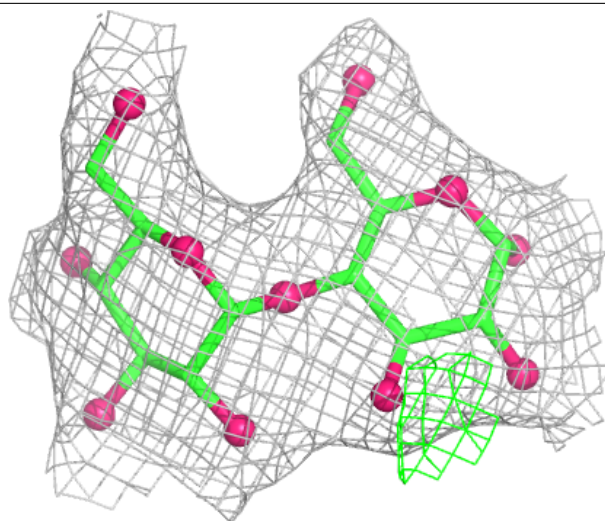
Electron density around Chain P:

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



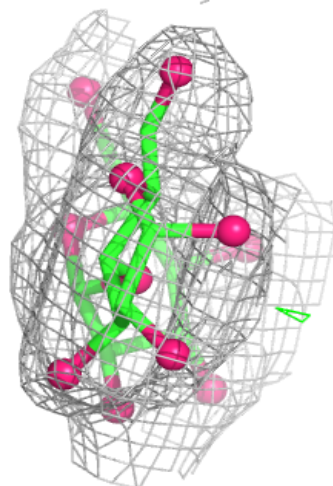
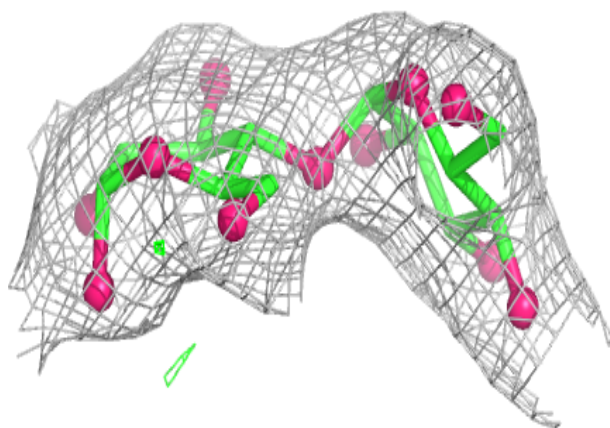
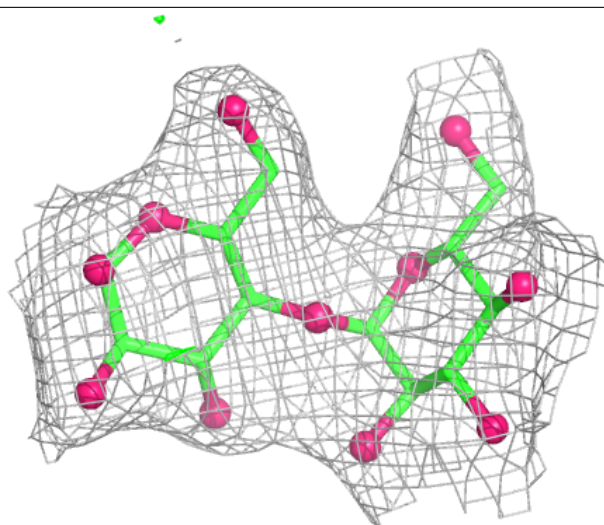
Electron density around Chain Q:

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and green (positive)



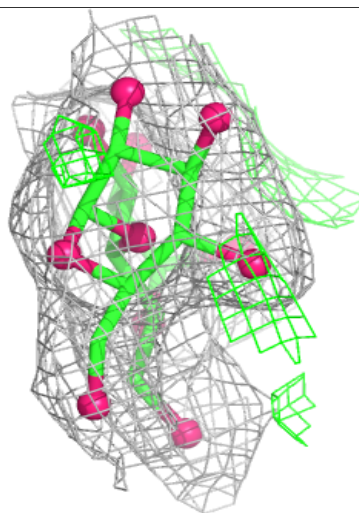
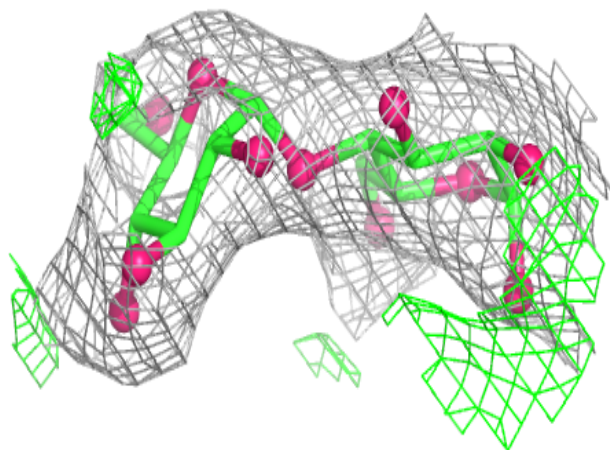
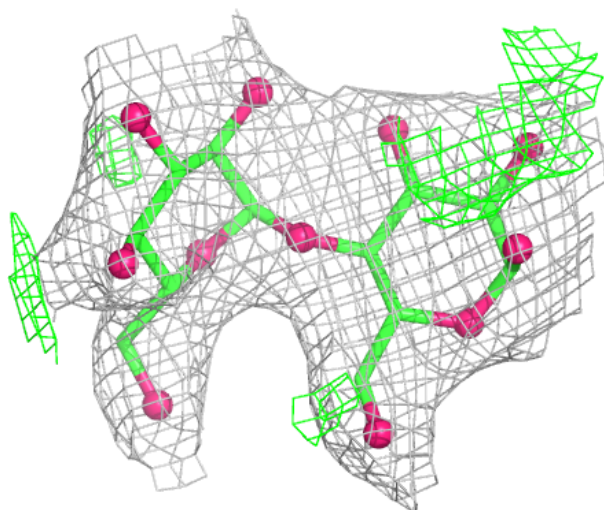
Electron density around Chain R:

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



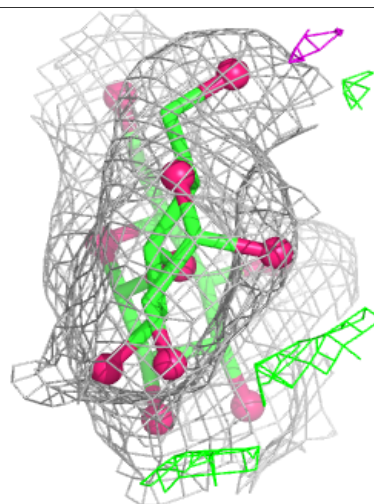
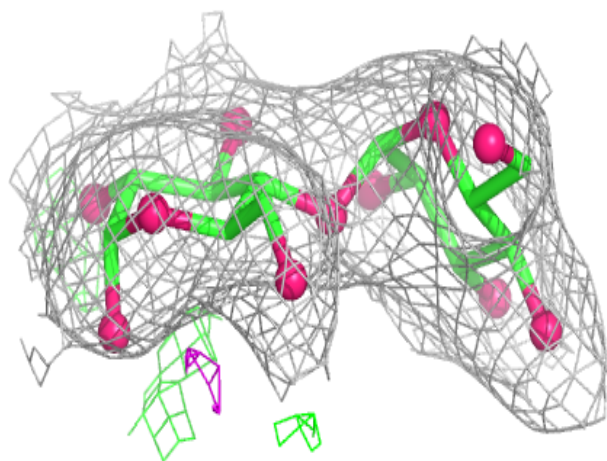
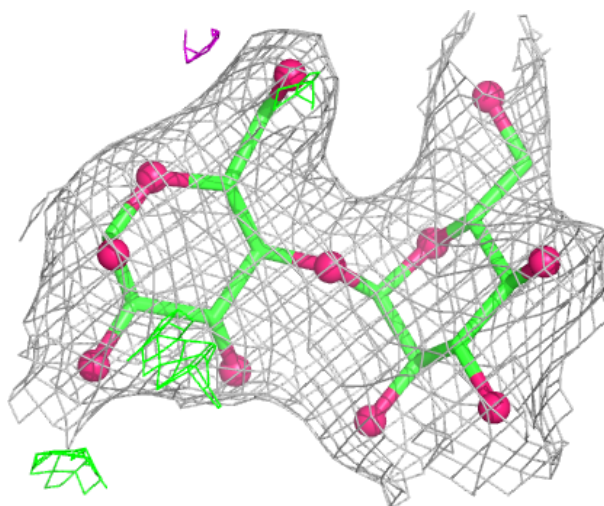
Electron density around Chain S:

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



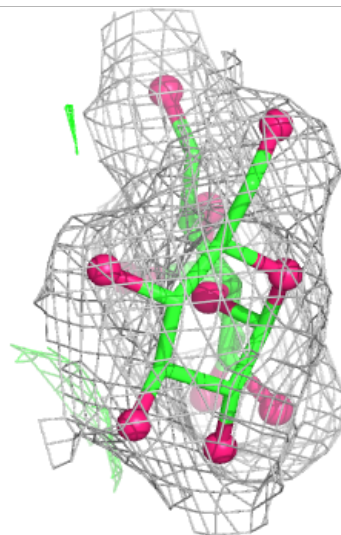
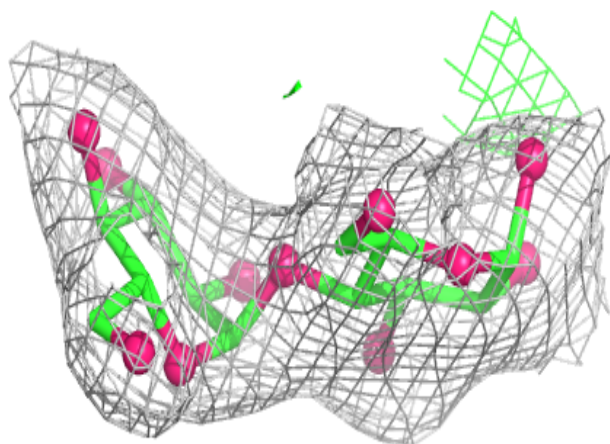
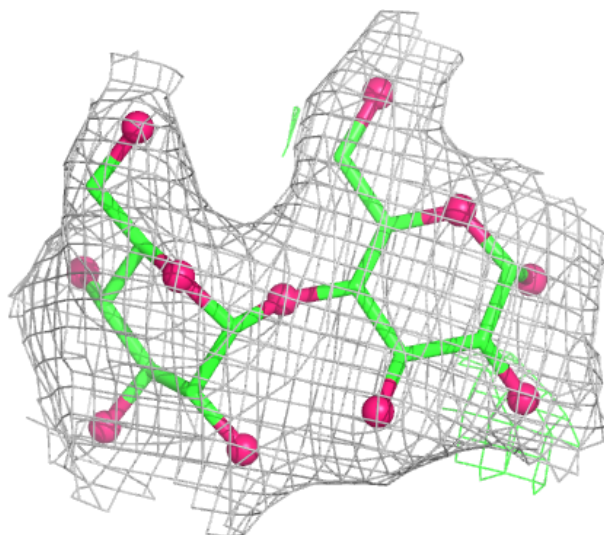
Electron density around Chain T:

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



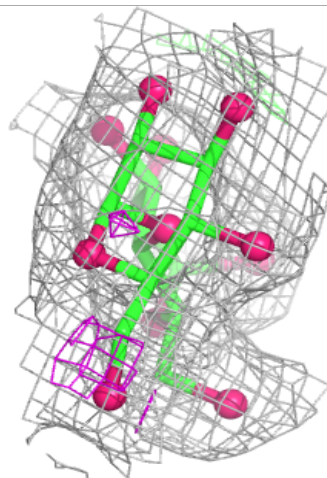
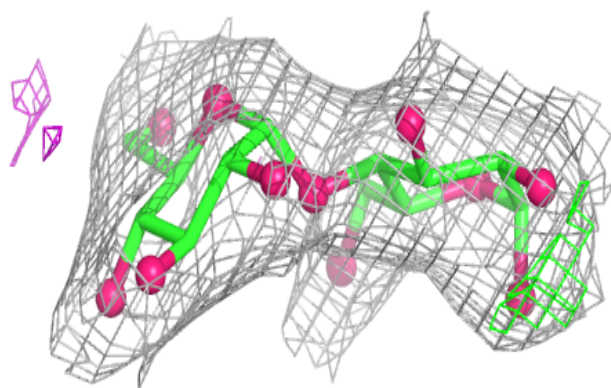
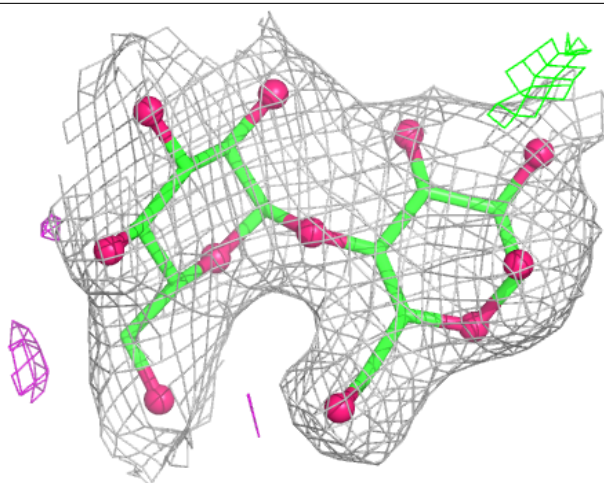
Electron density around Chain U:

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



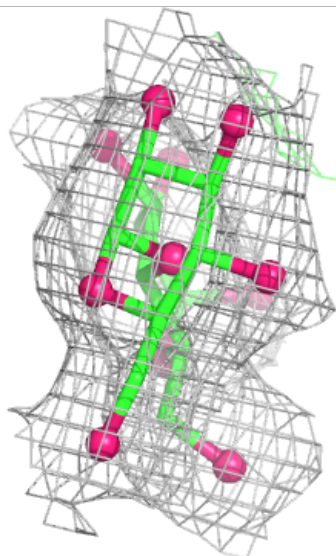
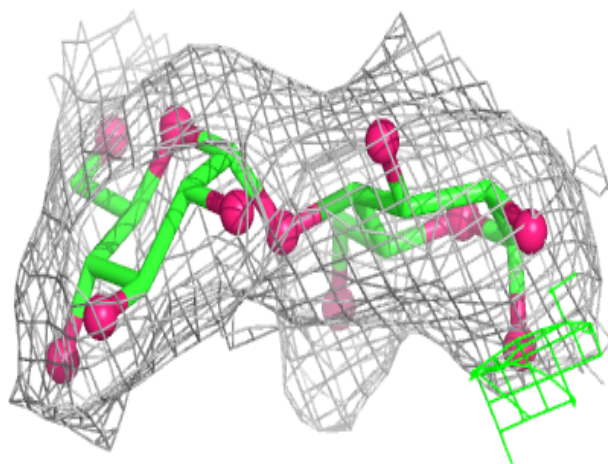
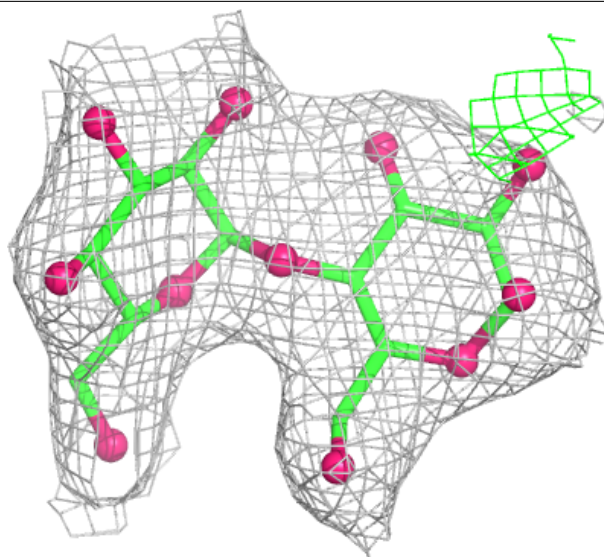
Electron density around Chain V:

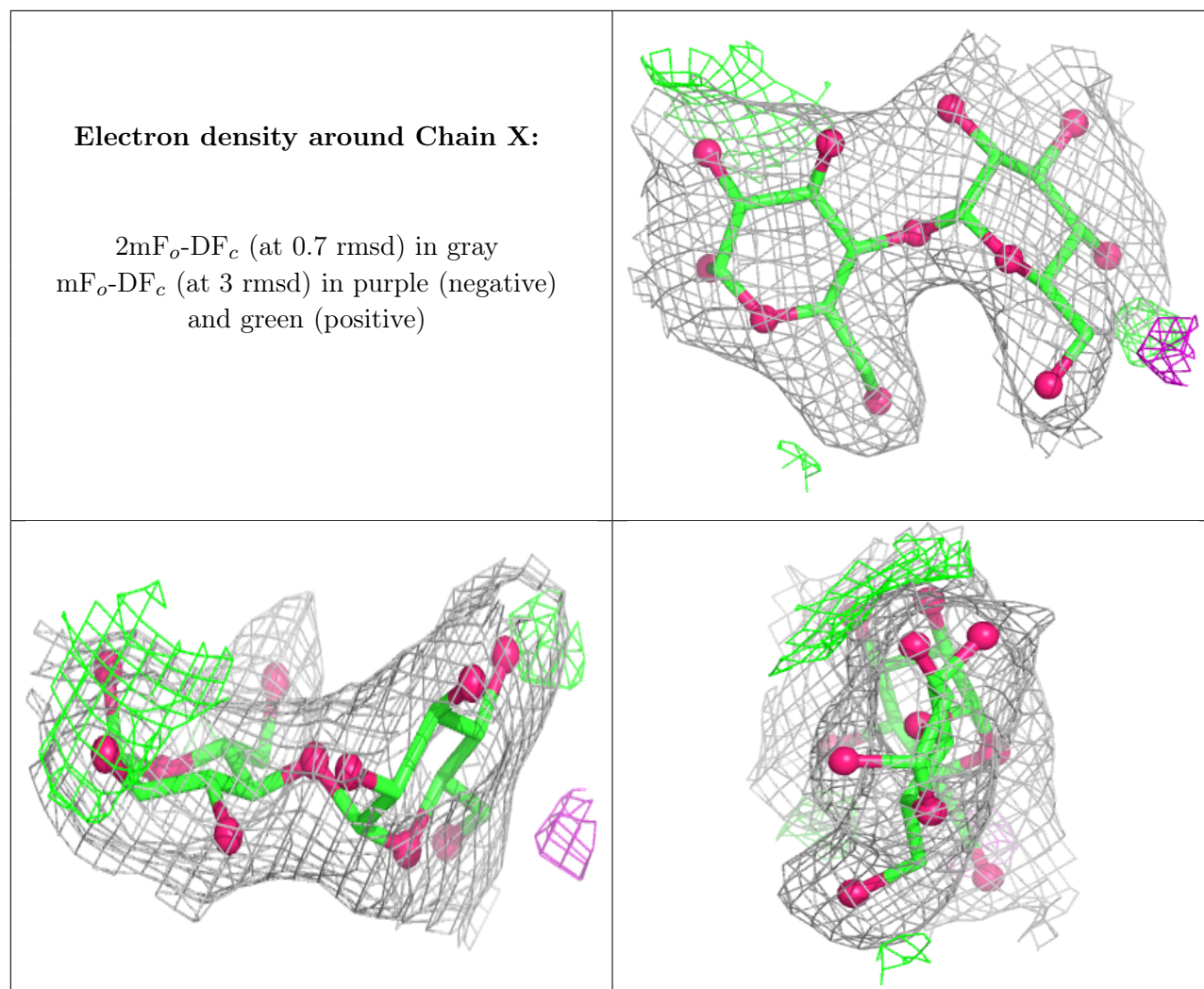
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	D	403	5/5	0.71	0.10	70,71,73,75	1
5	PO4	D	402	5/5	0.76	0.08	73,74,75,76	1
4	SO4	K	402	5/5	0.82	0.13	60,62,66,74	1
5	PO4	I	402	5/5	0.84	0.19	66,68,71,72	1
4	SO4	C	402	5/5	0.88	0.20	58,62,66,68	1
4	SO4	L	402	5/5	0.89	0.10	57,60,63,67	1
5	PO4	J	402	5/5	0.89	0.11	53,54,56,57	1
3	CU	B	401	1/1	0.90	0.08	83,83,83,83	0
3	CU	D	401	1/1	0.96	0.04	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	K	401	1/1	0.97	0.05	67,67,67,67	0
3	CU	A	401	1/1	0.98	0.03	74,74,74,74	0
3	CU	E	401	1/1	0.98	0.04	55,55,55,55	0
3	CU	I	401	1/1	0.98	0.04	80,80,80,80	0
3	CU	J	401	1/1	0.98	0.07	53,53,53,53	0
3	CU	L	401	1/1	0.99	0.02	71,71,71,71	0
3	CU	C	401	1/1	0.99	0.03	65,65,65,65	0
3	CU	G	401	1/1	0.99	0.03	64,64,64,64	0
3	CU	H	401	1/1	0.99	0.03	47,47,47,47	0
3	CU	F	401	1/1	1.00	0.04	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.