



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 11:10 PM BST

PDB ID : 4TZ1
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminaritriose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

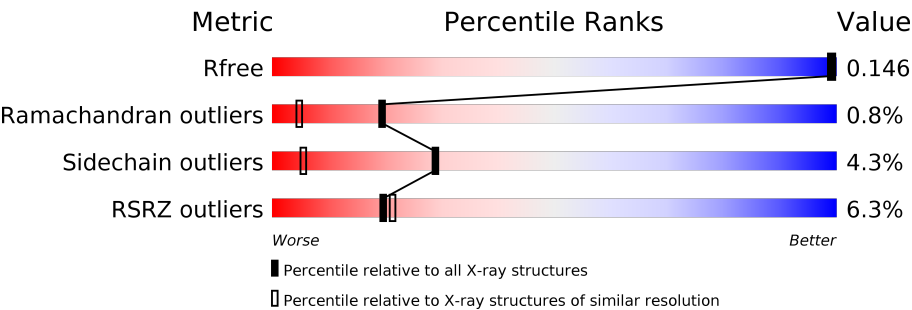
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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.



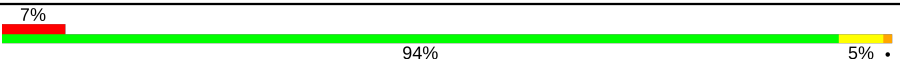
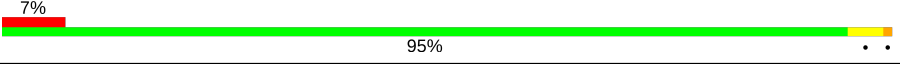
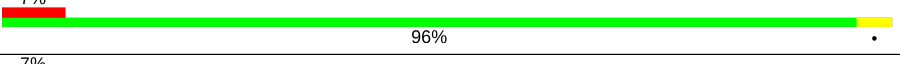
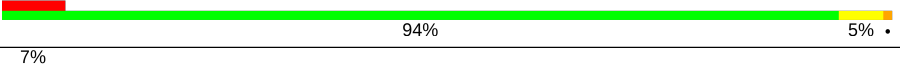
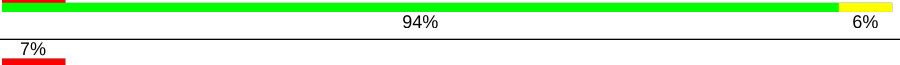
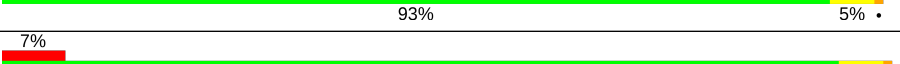
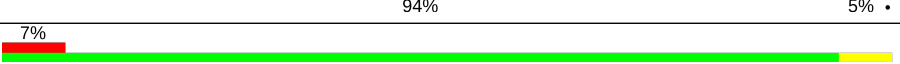
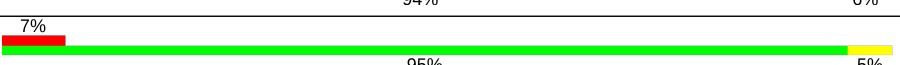
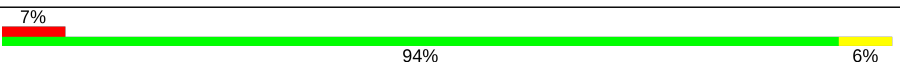
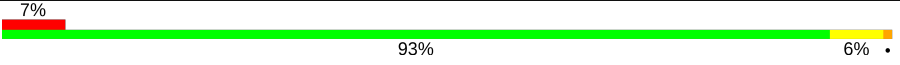
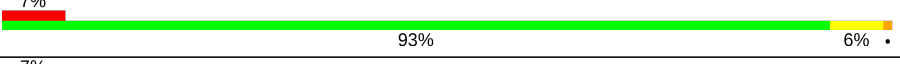
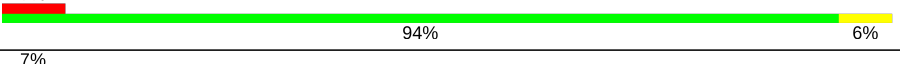
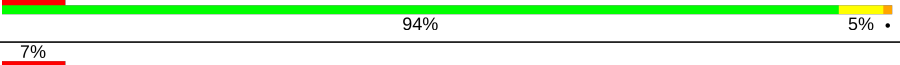
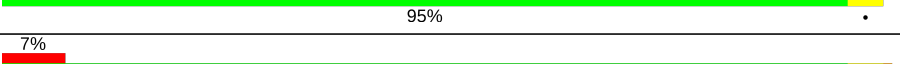
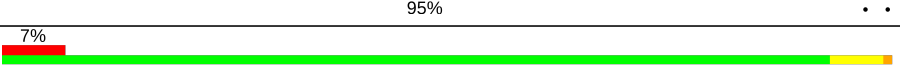
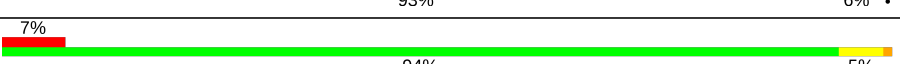
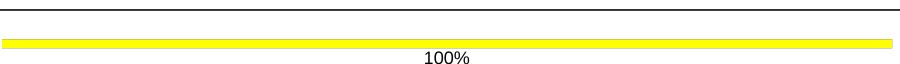
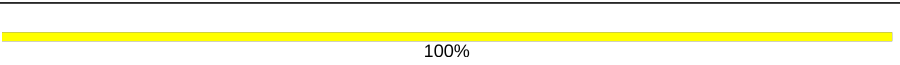
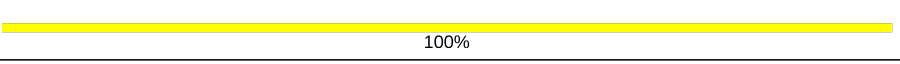
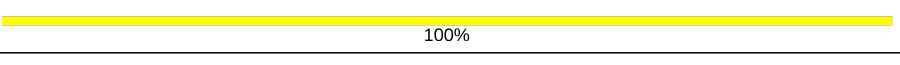
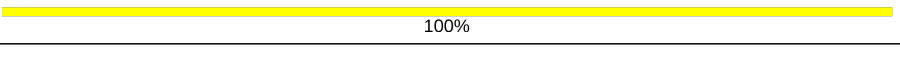
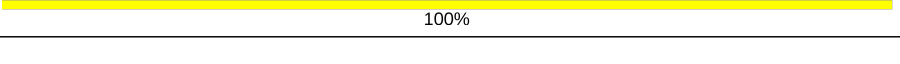
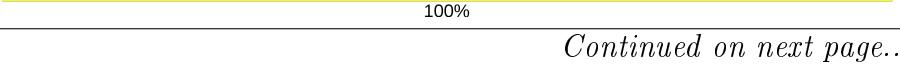


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	549	<div><div>7%</div><div>94%</div><div>6%</div></div>
1	10-A	549	<div><div>7%</div><div>96%</div><div>• •</div></div>
1	11-A	549	<div><div>7%</div><div>95%</div><div>5% •</div></div>
1	12-A	549	<div><div>7%</div><div>94%</div><div>5% •</div></div>
1	13-A	549	<div><div>7%</div><div>95%</div><div>5% •</div></div>
1	14-A	549	<div><div>7%</div><div>95%</div><div>5% •</div></div>
1	15-A	549	<div><div>7%</div><div>95%</div><div>5% •</div></div>

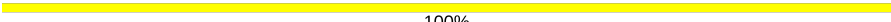
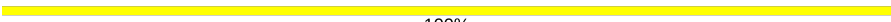
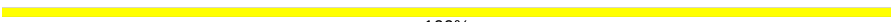
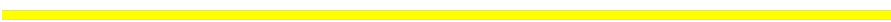











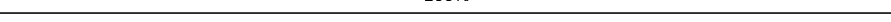
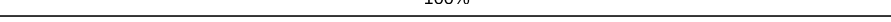
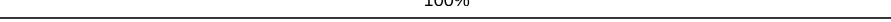
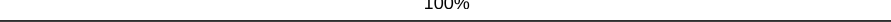
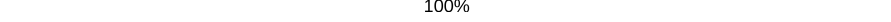
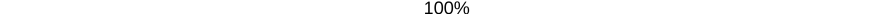
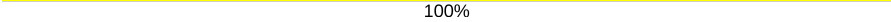
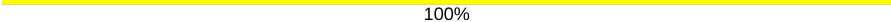
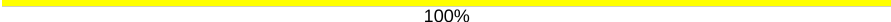
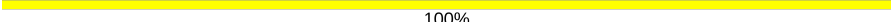
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Mol	Chain	Length	Quality of chain
1	16-A	549	
1	17-A	549	
1	18-A	549	
1	19-A	549	
1	2-A	549	
1	20-A	549	
1	21-A	549	
1	22-A	549	
1	23-A	549	
1	24-A	549	
1	25-A	549	
1	3-A	549	
1	4-A	549	
1	5-A	549	
1	6-A	549	
1	7-A	549	
1	8-A	549	
1	9-A	549	
2	1-B	3	
2	1-C	3	
2	10-B	3	
2	10-C	3	
2	11-B	3	
2	11-C	3	
2	12-B	3	

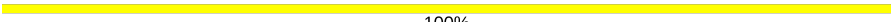
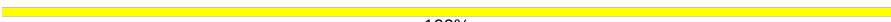
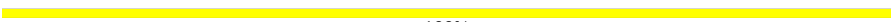
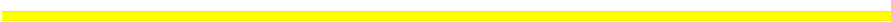








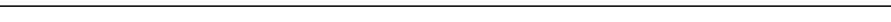


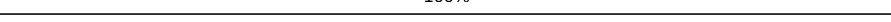
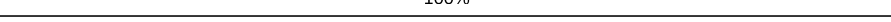
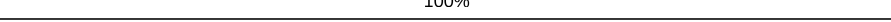
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Mol	Chain	Length	Quality of chain
2	12-C	3	 100%
2	13-B	3	 100%
2	13-C	3	 100%
2	14-B	3	 100%
2	14-C	3	 100%
2	15-B	3	 100%
2	15-C	3	 100%
2	16-B	3	 100%
2	16-C	3	 100%
2	17-B	3	 100%
2	17-C	3	 100%
2	18-B	3	 100%
2	18-C	3	 100%
2	19-B	3	 100%
2	19-C	3	 100%
2	2-B	3	 100%
2	2-C	3	 100%
2	20-B	3	 100%
2	20-C	3	 100%
2	21-B	3	 100%
2	21-C	3	 100%
2	22-B	3	 100%
2	22-C	3	 100%
2	23-B	3	 100%
2	23-C	3	 100%

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Mol	Chain	Length	Quality of chain
2	24-B	3	 100%
2	24-C	3	 100%
2	25-B	3	 100%
2	25-C	3	 100%
2	3-B	3	 100%
2	3-C	3	 100%
2	4-B	3	 100%
2	4-C	3	 100%
2	5-B	3	 100%
2	5-C	3	 100%
2	6-B	3	 100%
2	6-C	3	 100%
2	7-B	3	 100%
2	7-C	3	 100%
2	8-B	3	 100%
2	8-C	3	 100%
2	9-B	3	 100%
2	9-C	3	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 211855 atoms, of which 97675 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 Putative secreted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	2-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	3-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	4-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	5-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	6-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	7-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	8-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	9-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	10-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	11-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	12-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	13-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	14-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	15-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	16-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

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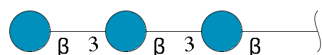
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	21-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	22-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	23-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	24-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	25-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ALA	GLU	engineered mutation	UNP G2NFJ9

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	1-B	3	Total	C	O	0	0	0
			34	18	16			
2	2-B	3	Total	C	O	0	0	0
			34	18	16			
2	3-B	3	Total	C	O	0	0	0
			34	18	16			
2	4-B	3	Total	C	O	0	0	0
			34	18	16			
2	5-B	3	Total	C	O	0	0	0
			34	18	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	6-B	3	Total	C	O	0	0	0
			34	18	16			
2	7-B	3	Total	C	O	0	0	0
			34	18	16			
2	8-B	3	Total	C	O	0	0	0
			34	18	16			
2	9-B	3	Total	C	O	0	0	0
			34	18	16			
2	10-B	3	Total	C	O	0	0	0
			34	18	16			
2	11-B	3	Total	C	O	0	0	0
			34	18	16			
2	12-B	3	Total	C	O	0	0	0
			34	18	16			
2	13-B	3	Total	C	O	0	0	0
			34	18	16			
2	14-B	3	Total	C	O	0	0	0
			34	18	16			
2	15-B	3	Total	C	O	0	0	0
			34	18	16			
2	16-B	3	Total	C	O	0	0	0
			34	18	16			
2	17-B	3	Total	C	O	0	0	0
			34	18	16			
2	18-B	3	Total	C	O	0	0	0
			34	18	16			
2	19-B	3	Total	C	O	0	0	0
			34	18	16			
2	20-B	3	Total	C	O	0	0	0
			34	18	16			
2	21-B	3	Total	C	O	0	0	0
			34	18	16			
2	22-B	3	Total	C	O	0	0	0
			34	18	16			
2	23-B	3	Total	C	O	0	0	0
			34	18	16			
2	24-B	3	Total	C	O	0	0	0
			34	18	16			
2	25-B	3	Total	C	O	0	0	0
			34	18	16			
2	1-C	3	Total	C	O	0	0	0
			34	18	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	2-C	3	Total	C	O	0	0	0
			34	18	16			
2	3-C	3	Total	C	O	0	0	0
			34	18	16			
2	4-C	3	Total	C	O	0	0	0
			34	18	16			
2	5-C	3	Total	C	O	0	0	0
			34	18	16			
2	6-C	3	Total	C	O	0	0	0
			34	18	16			
2	7-C	3	Total	C	O	0	0	0
			34	18	16			
2	8-C	3	Total	C	O	0	0	0
			34	18	16			
2	9-C	3	Total	C	O	0	0	0
			34	18	16			
2	10-C	3	Total	C	O	0	0	0
			34	18	16			
2	11-C	3	Total	C	O	0	0	0
			34	18	16			
2	12-C	3	Total	C	O	0	0	0
			34	18	16			
2	13-C	3	Total	C	O	0	0	0
			34	18	16			
2	14-C	3	Total	C	O	0	0	0
			34	18	16			
2	15-C	3	Total	C	O	0	0	0
			34	18	16			
2	16-C	3	Total	C	O	0	0	0
			34	18	16			
2	17-C	3	Total	C	O	0	0	0
			34	18	16			
2	18-C	3	Total	C	O	0	0	0
			34	18	16			
2	19-C	3	Total	C	O	0	0	0
			34	18	16			
2	20-C	3	Total	C	O	0	0	0
			34	18	16			
2	21-C	3	Total	C	O	0	0	0
			34	18	16			
2	22-C	3	Total	C	O	0	0	0
			34	18	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	23-C	3	Total	C	O	0	0	0
			34	18	16			
2	24-C	3	Total	C	O	0	0	0
			34	18	16			
2	25-C	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	339	Total	O	0	0
			339	339		
3	2-A	332	Total	O	0	0
			332	332		
3	3-A	343	Total	O	0	0
			343	343		
3	4-A	342	Total	O	0	0
			342	342		
3	5-A	340	Total	O	0	0
			340	340		
3	6-A	340	Total	O	0	0
			340	340		
3	7-A	327	Total	O	0	0
			327	327		
3	8-A	329	Total	O	0	0
			329	329		
3	9-A	329	Total	O	0	0
			329	329		
3	10-A	321	Total	O	0	0
			321	321		
3	11-A	342	Total	O	0	0
			342	342		
3	12-A	315	Total	O	0	0
			315	315		
3	13-A	340	Total	O	0	0
			340	340		
3	14-A	327	Total	O	0	0
			327	327		
3	15-A	354	Total	O	0	0
			354	354		
3	16-A	335	Total	O	0	0
			335	335		

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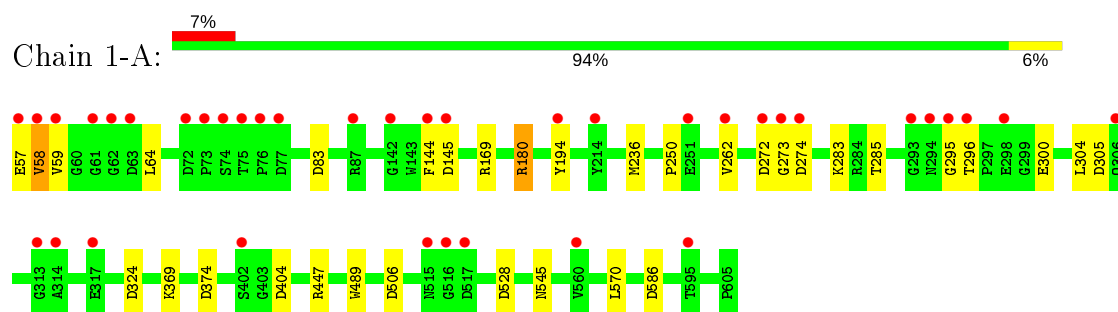
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	17-A	333	Total 333	O 333	0	0
3	18-A	328	Total 328	O 328	0	0
3	19-A	320	Total 320	O 320	0	0
3	20-A	341	Total 341	O 341	0	0
3	21-A	321	Total 321	O 321	0	0
3	22-A	304	Total 304	O 304	0	0
3	23-A	341	Total 341	O 341	0	0
3	24-A	326	Total 326	O 326	0	0
3	25-A	336	Total 336	O 336	0	0

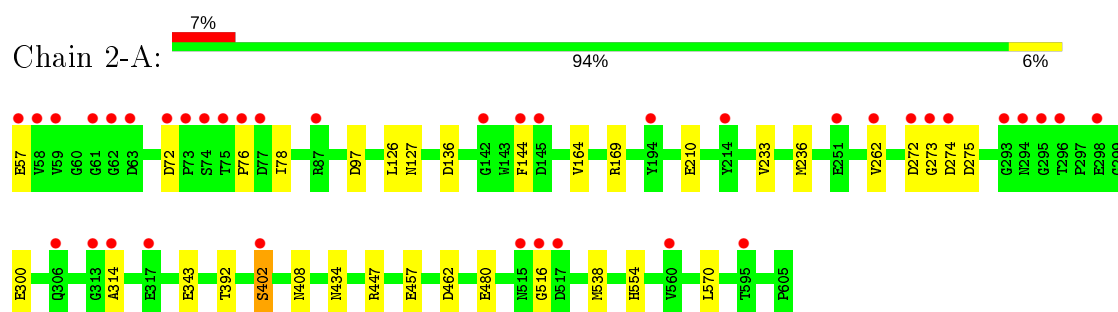
3 Residue-property plots [i](#)

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.

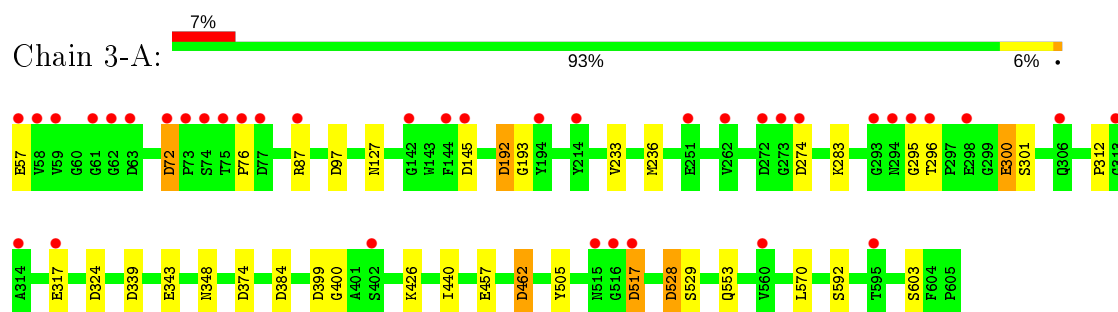
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

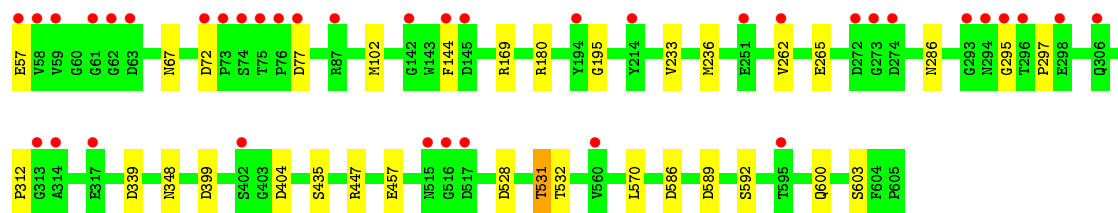


- Molecule 1: Putative secreted protein

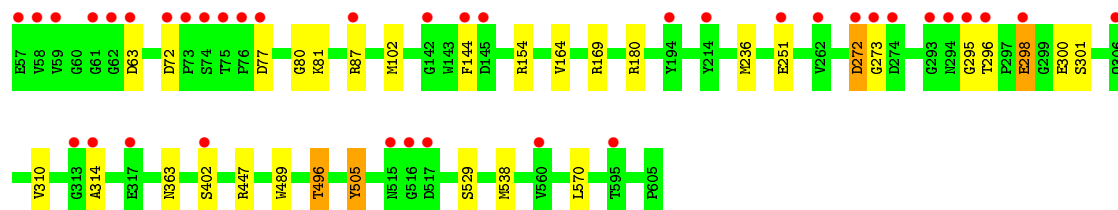


- Molecule 1: Putative secreted protein

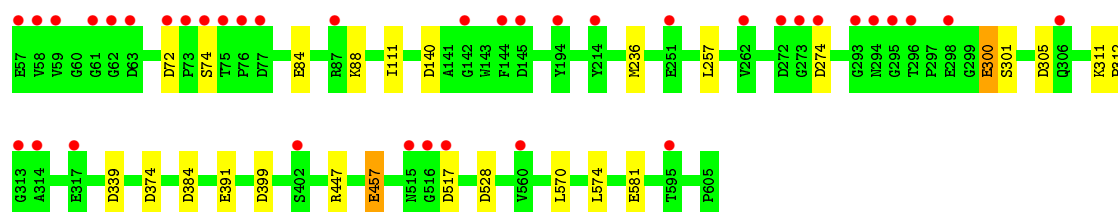




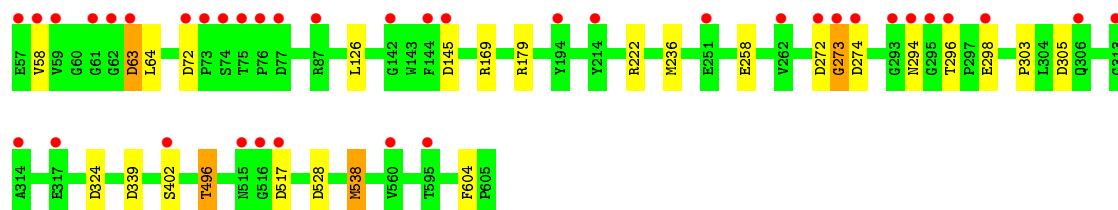
- Molecule 1: Putative secreted protein



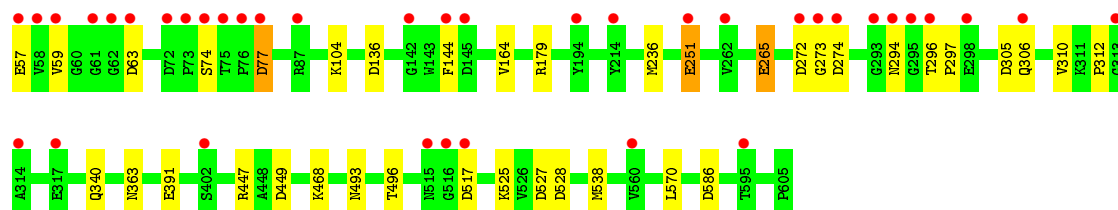
- Molecule 1: Putative secreted protein



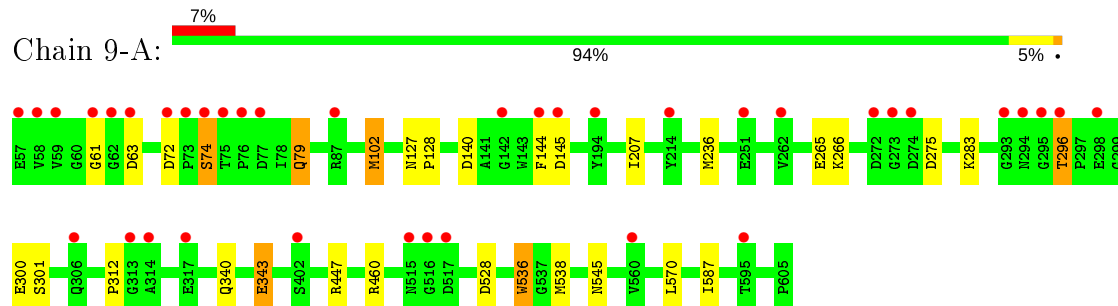
- Molecule 1: Putative secreted protein



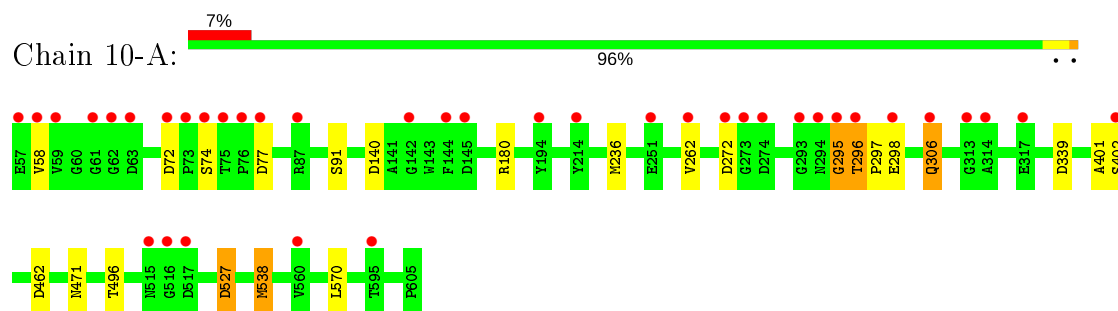
- Molecule 1: Putative secreted protein



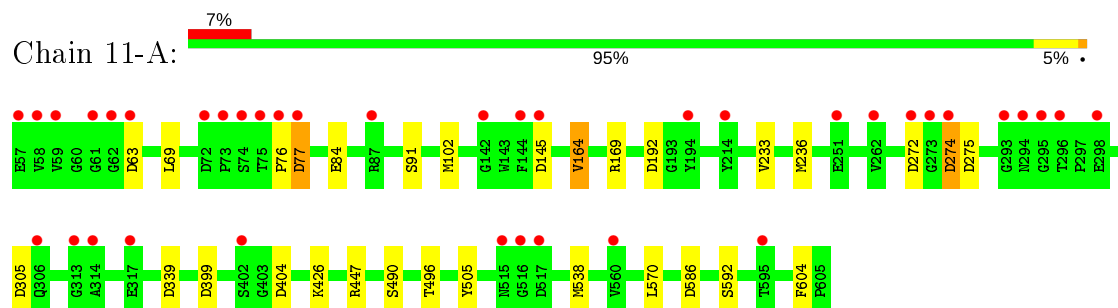
- Molecule 1: Putative secreted protein



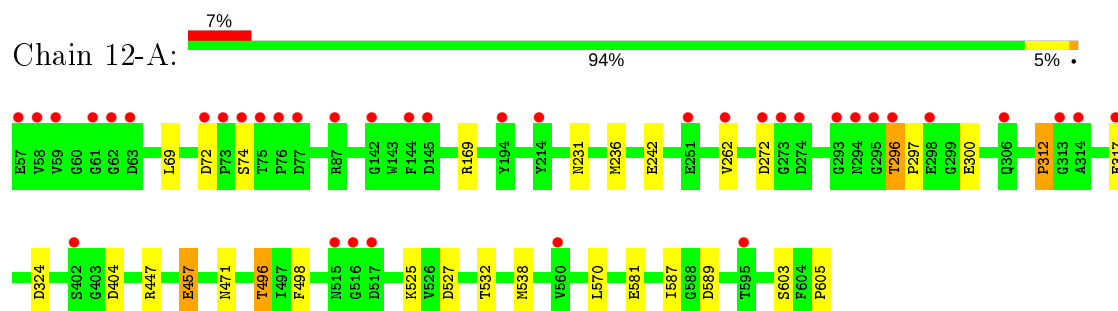
- Molecule 1: Putative secreted protein



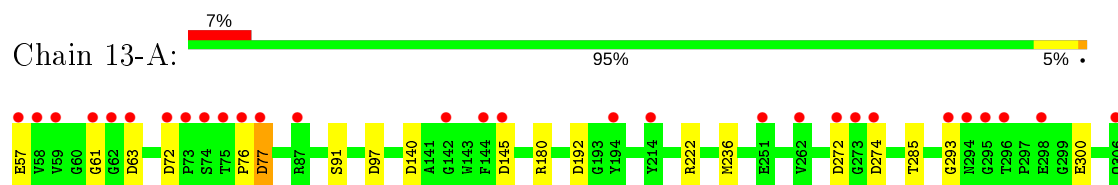
- Molecule 1: Putative secreted protein

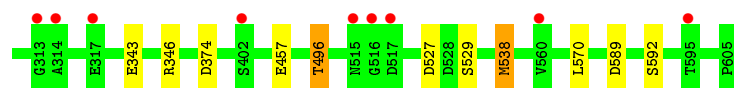


- Molecule 1: Putative secreted protein

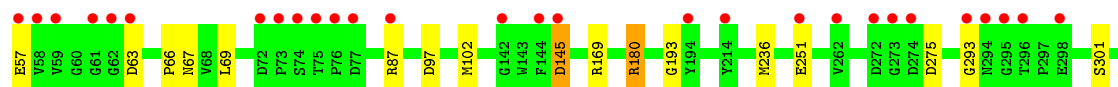


- Molecule 1: Putative secreted protein





- Molecule 1: Putative secreted protein



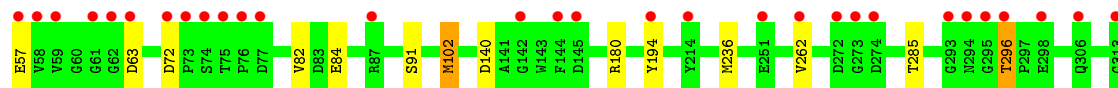
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

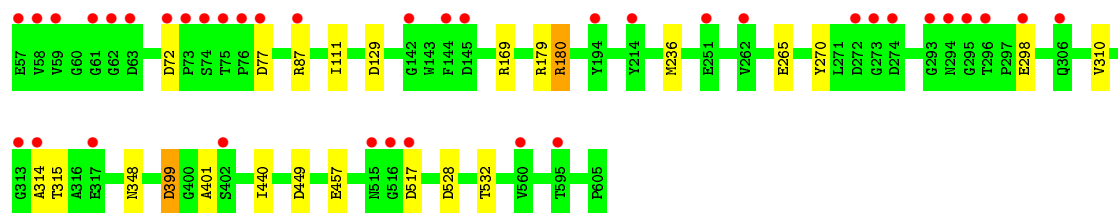


- Molecule 1: Putative secreted protein

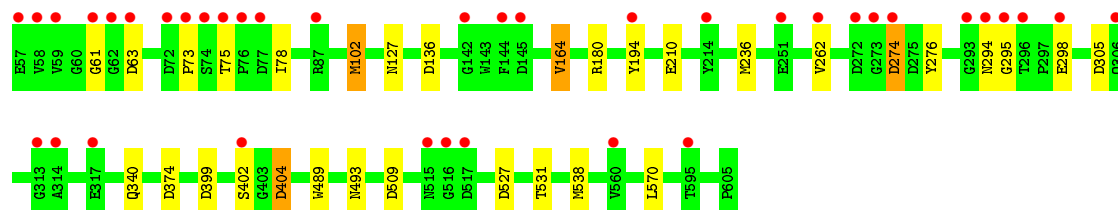


- Molecule 1: Putative secreted protein

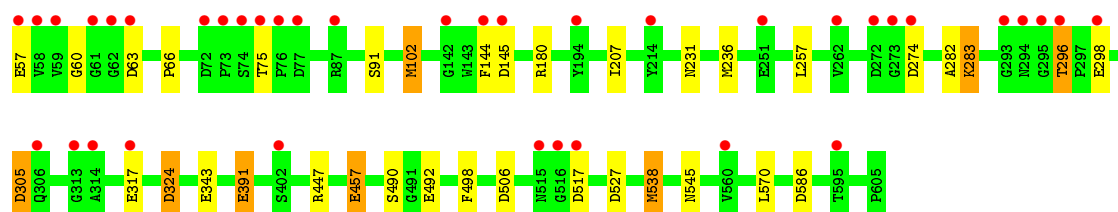




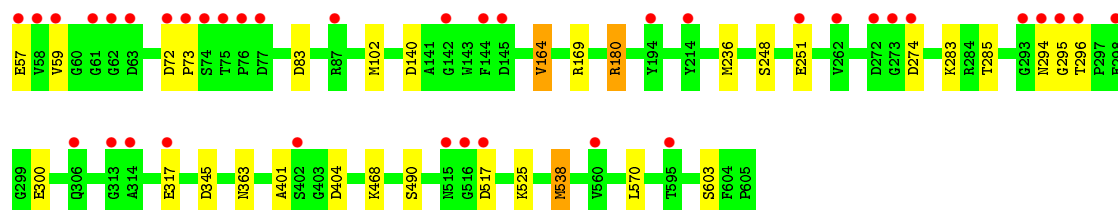
• Molecule 1: Putative secreted protein



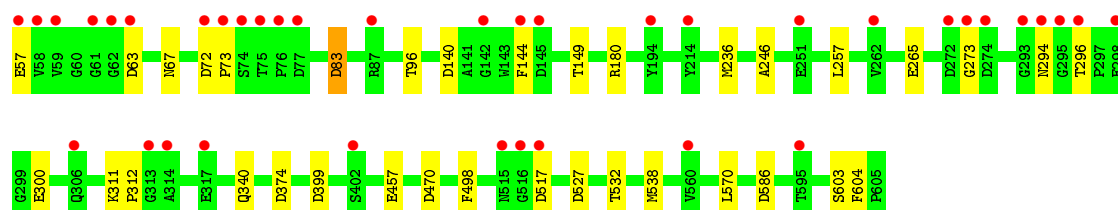
• Molecule 1: Putative secreted protein



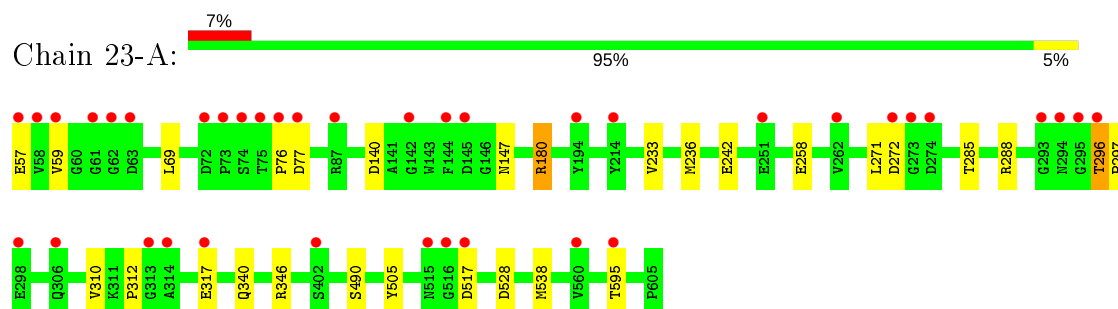
• Molecule 1: Putative secreted protein



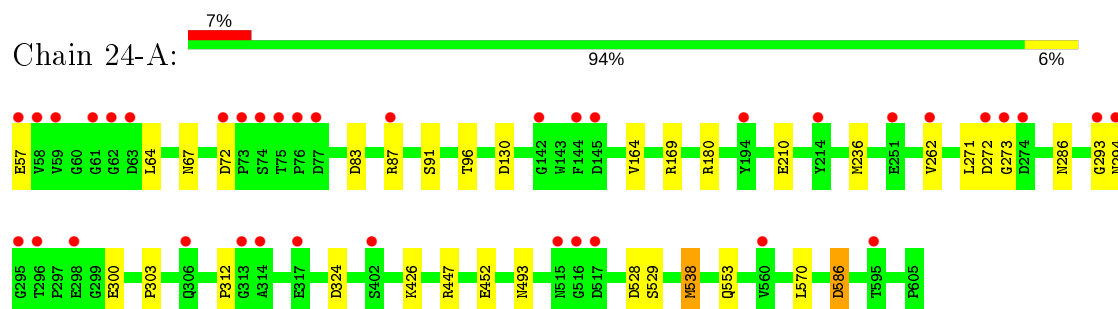
• Molecule 1: Putative secreted protein



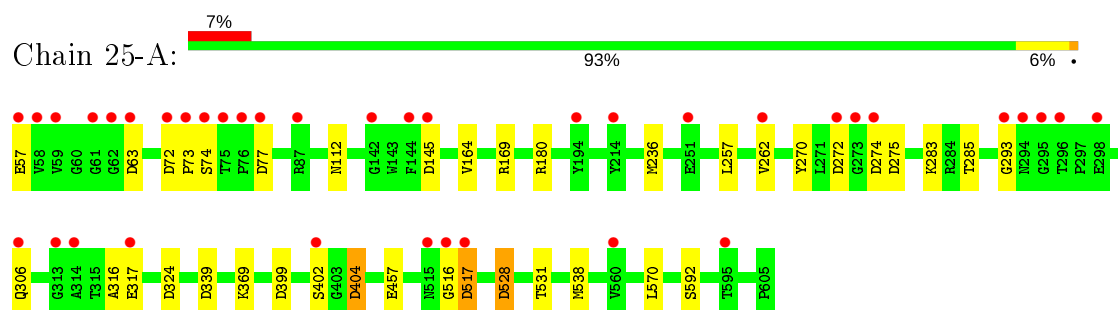
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-C:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-B:  100%

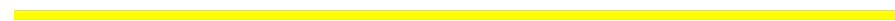
BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-C:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-B:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-C:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-C:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-C:  100%


BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-C:  100%

B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-B:  100%

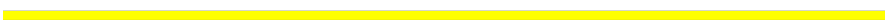
B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-C:  100%

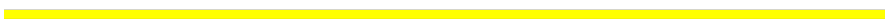
B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-B:  100%

B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-C:  100%

B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-B:  100%

B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-C:  100%

B0C1
B0C2
B0C3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-C:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-B:  100%

BGC1
BGC2
BGC3

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-C:  100%

BGC1
BGC2
BGC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.77 Å 100.19 Å 53.86 Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	24.23 – 1.50 24.23 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.23-1.50) 97.1 (24.23-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 1.50 Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.100 , 0.124 0.127 , 0.146	Depositor DCC
R_{free} test set	4085 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 168.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	211855	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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: BGC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1-A	0.78	5/4280 (0.1%)	0.94	11/5848 (0.2%)
1	2-A	0.74	3/4280 (0.1%)	0.92	6/5848 (0.1%)
1	3-A	0.79	5/4280 (0.1%)	0.94	8/5848 (0.1%)
1	4-A	0.72	2/4280 (0.0%)	0.92	6/5848 (0.1%)
1	5-A	0.77	1/4280 (0.0%)	0.99	14/5848 (0.2%)
1	6-A	0.77	5/4280 (0.1%)	0.95	6/5848 (0.1%)
1	7-A	0.75	1/4280 (0.0%)	0.94	10/5848 (0.2%)
1	8-A	0.77	3/4280 (0.1%)	0.95	14/5848 (0.2%)
1	9-A	0.78	4/4280 (0.1%)	0.97	12/5848 (0.2%)
1	10-A	0.76	3/4280 (0.1%)	0.98	11/5848 (0.2%)
1	11-A	0.75	3/4280 (0.1%)	0.95	12/5848 (0.2%)
1	12-A	0.78	8/4280 (0.2%)	0.94	11/5848 (0.2%)
1	13-A	0.77	4/4280 (0.1%)	0.99	15/5848 (0.3%)
1	14-A	0.75	1/4280 (0.0%)	0.93	7/5848 (0.1%)
1	15-A	0.76	5/4280 (0.1%)	0.97	9/5848 (0.2%)
1	16-A	0.74	3/4280 (0.1%)	0.98	16/5848 (0.3%)
1	17-A	0.75	3/4280 (0.1%)	0.92	8/5848 (0.1%)
1	18-A	0.77	6/4280 (0.1%)	0.94	8/5848 (0.1%)
1	19-A	0.75	3/4280 (0.1%)	0.95	12/5848 (0.2%)
1	20-A	0.78	7/4280 (0.2%)	0.95	12/5848 (0.2%)
1	21-A	0.74	4/4280 (0.1%)	0.98	10/5848 (0.2%)
1	22-A	0.77	4/4280 (0.1%)	0.98	10/5848 (0.2%)
1	23-A	0.74	2/4280 (0.0%)	0.97	10/5848 (0.2%)
1	24-A	0.76	5/4280 (0.1%)	0.93	9/5848 (0.2%)
1	25-A	0.75	4/4280 (0.1%)	0.95	10/5848 (0.2%)
All	All	0.76	94/107000 (0.1%)	0.95	257/146200 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	1
1	3-A	0	1
1	4-A	0	2
1	7-A	0	2
1	9-A	0	1
1	10-A	0	1
1	11-A	0	2
1	13-A	0	2
1	14-A	0	2
1	15-A	0	1
1	18-A	0	1
1	20-A	0	2
1	21-A	0	1
1	23-A	0	2
1	25-A	0	2
All	All	0	24

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-A	180	ARG	CB-CG	-10.28	1.24	1.52
1	20-A	538	MET	CB-CG	-10.08	1.19	1.51
1	3-A	462	ASP	CB-CG	-9.78	1.31	1.51
1	22-A	538	MET	CG-SD	9.54	2.06	1.81
1	1-A	300	GLU	CB-CG	9.27	1.69	1.52

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	538	MET	CG-SD-CE	-20.07	68.09	100.20
1	10-A	538	MET	CG-SD-CE	-19.51	68.99	100.20
1	21-A	538	MET	CG-SD-CE	-19.04	69.73	100.20
1	22-A	538	MET	CG-SD-CE	-18.99	69.81	100.20
1	23-A	538	MET	CG-SD-CE	-18.91	69.94	100.20

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	57	GLU	Peptide
1	2-A	126	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	3-A	295	GLY	Peptide
1	4-A	295	GLY	Peptide
1	4-A	57	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	4167	3907	3919	0	0
1	2-A	4167	3907	3919	0	0
1	3-A	4167	3907	3919	0	0
1	4-A	4167	3907	3919	0	0
1	5-A	4167	3907	3919	0	0
1	6-A	4167	3907	3919	0	0
1	7-A	4167	3907	3919	0	0
1	8-A	4167	3907	3919	0	0
1	9-A	4167	3907	3919	0	0
1	10-A	4167	3907	3919	0	0
1	11-A	4167	3907	3919	0	0
1	12-A	4167	3907	3919	0	0
1	13-A	4167	3907	3919	0	0
1	14-A	4167	3907	3919	0	0
1	15-A	4167	3907	3919	0	0
1	16-A	4167	3907	3919	0	0
1	17-A	4167	3907	3919	0	0
1	18-A	4167	3907	3919	0	0
1	19-A	4167	3907	3919	0	0
1	20-A	4167	3907	3919	0	0
1	21-A	4167	3907	3919	0	0
1	22-A	4167	3907	3919	0	0
1	23-A	4167	3907	3919	0	0
1	24-A	4167	3907	3919	0	0
1	25-A	4167	3907	3919	0	0
2	1-B	34	0	30	0	0
2	1-C	34	0	30	0	0
2	2-B	34	0	30	0	0
2	2-C	34	0	30	0	0
2	3-B	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-C	34	0	30	0	0
2	4-B	34	0	30	0	0
2	4-C	34	0	30	0	0
2	5-B	34	0	30	0	0
2	5-C	34	0	29	0	0
2	6-B	34	0	30	0	0
2	6-C	34	0	30	0	0
2	7-B	34	0	30	0	0
2	7-C	34	0	30	0	0
2	8-B	34	0	30	0	0
2	8-C	34	0	30	0	0
2	9-B	34	0	30	0	0
2	9-C	34	0	30	0	0
2	10-B	34	0	30	0	0
2	10-C	34	0	30	0	0
2	11-B	34	0	30	0	0
2	11-C	34	0	30	0	0
2	12-B	34	0	30	0	0
2	12-C	34	0	30	0	0
2	13-B	34	0	30	0	0
2	13-C	34	0	30	0	0
2	14-B	34	0	30	0	0
2	14-C	34	0	30	0	0
2	15-B	34	0	30	0	0
2	15-C	34	0	30	0	0
2	16-B	34	0	30	0	0
2	16-C	34	0	30	0	0
2	17-B	34	0	30	0	0
2	17-C	34	0	30	0	0
2	18-B	34	0	30	0	0
2	18-C	34	0	29	0	0
2	19-B	34	0	30	0	0
2	19-C	34	0	30	0	0
2	20-B	34	0	30	0	0
2	20-C	34	0	30	0	0
2	21-B	34	0	30	0	0
2	21-C	34	0	29	0	0
2	22-B	34	0	30	0	0
2	22-C	34	0	30	0	0
2	23-B	34	0	30	0	0
2	23-C	34	0	30	0	0
2	24-B	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	24-C	34	0	30	0	0
2	25-B	34	0	30	0	0
2	25-C	34	0	30	0	0
3	1-A	339	0	0	0	0
3	2-A	332	0	0	0	0
3	3-A	343	0	0	0	0
3	4-A	342	0	0	0	0
3	5-A	340	0	0	0	0
3	6-A	340	0	0	0	0
3	7-A	327	0	0	0	0
3	8-A	329	0	0	0	0
3	9-A	329	0	0	0	0
3	10-A	321	0	0	0	0
3	11-A	342	0	0	0	0
3	12-A	315	0	0	0	0
3	13-A	340	0	0	0	0
3	14-A	327	0	0	0	0
3	15-A	354	0	0	0	0
3	16-A	335	0	0	0	0
3	17-A	333	0	0	0	0
3	18-A	328	0	0	0	0
3	19-A	320	0	0	0	0
3	20-A	341	0	0	0	0
3	21-A	321	0	0	0	0
3	22-A	304	0	0	0	0
3	23-A	341	0	0	0	0
3	24-A	326	0	0	0	0
3	25-A	336	0	0	0	0
All	All	114180	97675	99472	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	14	2
1	2-A	547/549 (100%)	515 (94%)	28 (5%)	4 (1%)	22	6
1	3-A	547/549 (100%)	513 (94%)	27 (5%)	7 (1%)	12	2
1	4-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	14	2
1	5-A	547/549 (100%)	516 (94%)	26 (5%)	5 (1%)	17	3
1	6-A	547/549 (100%)	509 (93%)	37 (7%)	1 (0%)	47	23
1	7-A	547/549 (100%)	517 (94%)	28 (5%)	2 (0%)	34	13
1	8-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	29	9
1	9-A	547/549 (100%)	514 (94%)	28 (5%)	5 (1%)	17	3
1	10-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	17	3
1	11-A	547/549 (100%)	512 (94%)	32 (6%)	3 (0%)	29	9
1	12-A	547/549 (100%)	517 (94%)	25 (5%)	5 (1%)	17	3
1	13-A	547/549 (100%)	513 (94%)	32 (6%)	2 (0%)	34	13
1	14-A	547/549 (100%)	509 (93%)	31 (6%)	7 (1%)	12	2
1	15-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	29	9
1	16-A	547/549 (100%)	510 (93%)	33 (6%)	4 (1%)	22	6
1	17-A	547/549 (100%)	513 (94%)	32 (6%)	2 (0%)	34	13
1	18-A	547/549 (100%)	507 (93%)	36 (7%)	4 (1%)	22	6
1	19-A	547/549 (100%)	511 (93%)	29 (5%)	7 (1%)	12	2
1	20-A	547/549 (100%)	508 (93%)	32 (6%)	7 (1%)	12	2
1	21-A	547/549 (100%)	509 (93%)	33 (6%)	5 (1%)	17	3
1	22-A	547/549 (100%)	514 (94%)	27 (5%)	6 (1%)	14	2
1	23-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	14	2
1	24-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	17	3
1	25-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	14	2
All	All	13675/13725 (100%)	12797 (94%)	762 (6%)	116 (1%)	19	5

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	194	TYR
1	3-A	400	GLY
1	4-A	77	ASP
1	5-A	80	GLY

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	1-A	436/436 (100%)	418 (96%)	18 (4%)	30	6
1	2-A	436/436 (100%)	414 (95%)	22 (5%)	24	4
1	3-A	436/436 (100%)	409 (94%)	27 (6%)	18	2
1	4-A	436/436 (100%)	417 (96%)	19 (4%)	28	5
1	5-A	436/436 (100%)	417 (96%)	19 (4%)	28	5
1	6-A	436/436 (100%)	417 (96%)	19 (4%)	28	5
1	7-A	436/436 (100%)	419 (96%)	17 (4%)	32	7
1	8-A	436/436 (100%)	413 (95%)	23 (5%)	22	3
1	9-A	436/436 (100%)	417 (96%)	19 (4%)	28	5
1	10-A	436/436 (100%)	424 (97%)	12 (3%)	43	14
1	11-A	436/436 (100%)	421 (97%)	15 (3%)	37	9
1	12-A	436/436 (100%)	416 (95%)	20 (5%)	27	5
1	13-A	436/436 (100%)	421 (97%)	15 (3%)	37	9
1	14-A	436/436 (100%)	420 (96%)	16 (4%)	34	8
1	15-A	436/436 (100%)	416 (95%)	20 (5%)	27	5
1	16-A	436/436 (100%)	418 (96%)	18 (4%)	30	6
1	17-A	436/436 (100%)	419 (96%)	17 (4%)	32	7
1	18-A	436/436 (100%)	422 (97%)	14 (3%)	39	10
1	19-A	436/436 (100%)	416 (95%)	20 (5%)	27	5
1	20-A	436/436 (100%)	414 (95%)	22 (5%)	24	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	21-A	436/436 (100%)	416 (95%)	20 (5%)	27	5
1	22-A	436/436 (100%)	416 (95%)	20 (5%)	27	5
1	23-A	436/436 (100%)	422 (97%)	14 (3%)	39	10
1	24-A	436/436 (100%)	415 (95%)	21 (5%)	25	4
1	25-A	436/436 (100%)	415 (95%)	21 (5%)	25	4
All	All	10900/10900 (100%)	10432 (96%)	468 (4%)	29	5

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	72	ASP
1	15-A	57	GLU
1	24-A	96	THR
1	12-A	296	THR
1	13-A	300	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	11-A	514	GLN
1	14-A	231	ASN
1	23-A	493	ASN
1	13-A	114	GLN
1	14-A	600	GLN

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 ⓘ

150 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BGC	1-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	1-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	1-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	1-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	1-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	1-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	10-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	10-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	10-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	10-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	10-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	10-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	11-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	11-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	11-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	11-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	11-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	11-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	12-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	12-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	12-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	12-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	12-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	12-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	13-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	13-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	13-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	13-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	13-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	13-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	14-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	14-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	14-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	14-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	14-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	14-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	15-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	15-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	15-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	15-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	15-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	15-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	16-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	16-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	16-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	16-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	16-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	16-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	17-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	17-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	17-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	17-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	17-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	17-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	18-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	18-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	18-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	18-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	18-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	18-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	19-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	19-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	19-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	19-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	19-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	19-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	2-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	2-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	2-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	2-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	2-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	2-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	20-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	20-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	20-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	20-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	20-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	20-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	21-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	21-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	21-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	21-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	21-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	21-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	22-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	22-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	22-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	22-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	22-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	22-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	23-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	23-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	23-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	23-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	23-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	23-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	24-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	24-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	24-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	24-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	24-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	24-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	25-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	25-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	25-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	25-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	25-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	25-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	3-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	3-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	3-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	3-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	3-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	3-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	4-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	4-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	4-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	4-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	4-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	4-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	5-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	5-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	5-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	5-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	5-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	5-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	6-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	6-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	6-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	6-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	6-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	6-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	7-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	7-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	7-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	7-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	7-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	7-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	8-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	8-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	8-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	8-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	8-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	8-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)
2	BGC	9-B	1	2	12,12,12	2.08	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	9-B	2	2	11,11,12	2.59	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	9-B	3	2	11,11,12	2.48	5 (45%)	15,15,17	1.44	2 (13%)
2	BGC	9-C	1	2	12,12,12	2.56	6 (50%)	17,17,17	2.09	6 (35%)
2	BGC	9-C	2	2	11,11,12	3.07	6 (54%)	15,15,17	2.19	4 (26%)
2	BGC	9-C	3	2	11,11,12	2.99	4 (36%)	15,15,17	1.43	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	1-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	1-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	1-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	1-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	1-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	1-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	10-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	10-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	10-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	10-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	10-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	10-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	11-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	11-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	11-B	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	11-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	11-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	11-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	12-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	12-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	12-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	13-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	13-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	13-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	13-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	13-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	13-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	14-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	14-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	14-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	14-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	14-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	14-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	15-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	15-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	15-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	15-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	15-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	15-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	16-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	16-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	16-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	16-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	16-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	16-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	17-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	17-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	17-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	17-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	17-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	17-C	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	18-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	18-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	18-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	18-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	18-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	18-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	19-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	19-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	19-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	19-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	19-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	19-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	2-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	2-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	2-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	2-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	2-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	2-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	20-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	20-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	20-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	20-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	20-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	20-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	21-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	21-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	21-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	21-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	21-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	21-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	22-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	22-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	22-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	22-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	22-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	22-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	23-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	23-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	23-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	23-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	24-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	24-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	24-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	24-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	25-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	25-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	25-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	3-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	3-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	3-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	4-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	4-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	4-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	4-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	5-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	5-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	5-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	5-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	5-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	5-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	6-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	6-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	6-C	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	7-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	7-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	7-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	7-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	7-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	7-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	8-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	8-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	8-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	8-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	9-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	9-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	9-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	9-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	9-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	9-C	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 725 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	16-C	3	BGC	C2-C3	-6.87	1.42	1.52
2	8-C	3	BGC	C2-C3	-6.87	1.42	1.52
2	21-C	3	BGC	C2-C3	-6.87	1.42	1.52
2	1-C	3	BGC	C2-C3	-6.87	1.42	1.52
2	13-C	3	BGC	C2-C3	-6.87	1.42	1.52

The worst 5 of 500 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-C	2	BGC	C1-O5-C5	5.20	119.24	112.19
2	25-C	2	BGC	C1-O5-C5	5.20	119.24	112.19
2	9-C	2	BGC	C1-O5-C5	5.20	119.24	112.19
2	11-C	2	BGC	C1-O5-C5	5.20	119.24	112.19
2	21-C	2	BGC	C1-O5-C5	5.20	119.24	112.19

There are no chirality outliers.

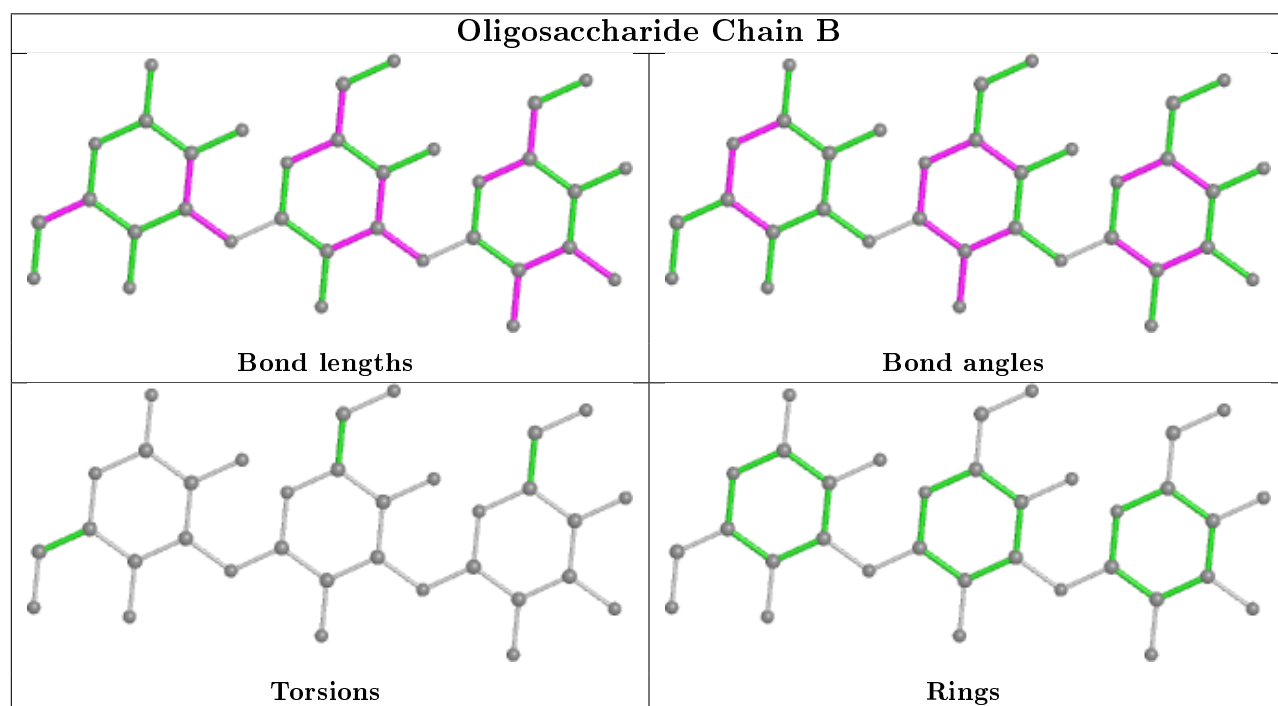
5 of 100 torsion outliers are listed below:

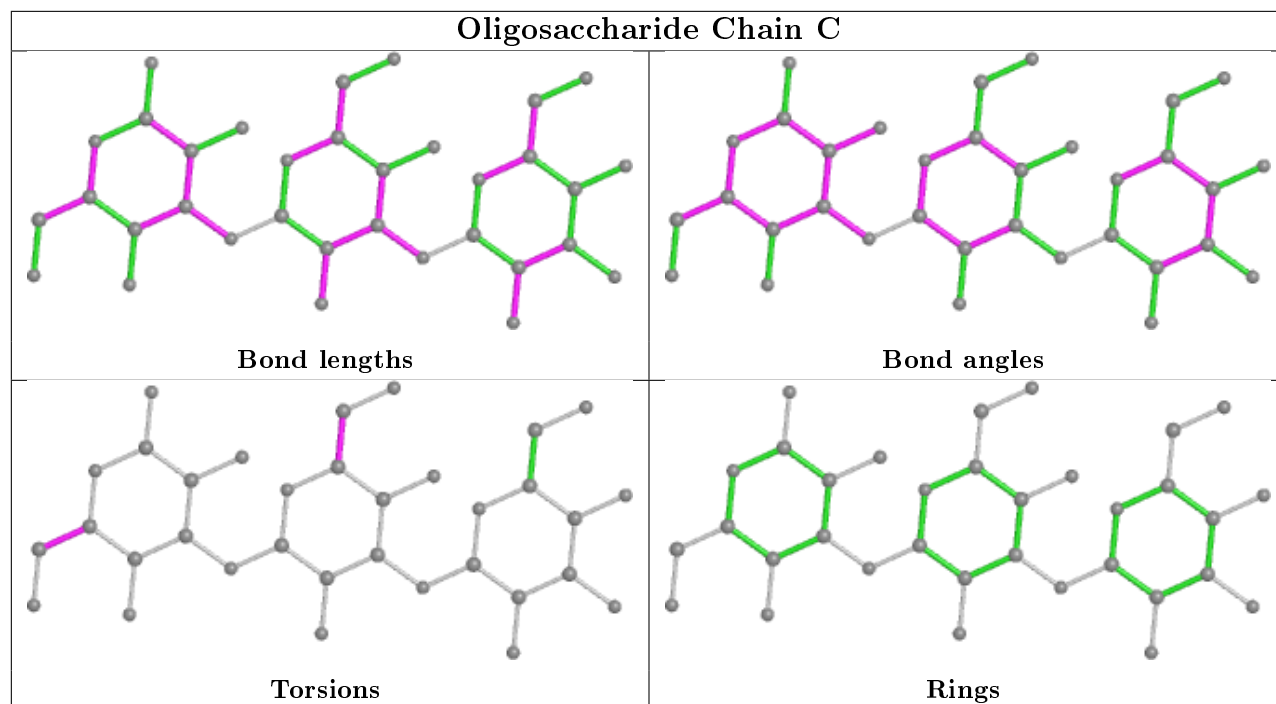
Mol	Chain	Res	Type	Atoms
2	14-C	2	BGC	O5-C5-C6-O6
2	25-C	2	BGC	O5-C5-C6-O6
2	9-C	2	BGC	O5-C5-C6-O6
2	11-C	2	BGC	O5-C5-C6-O6
2	21-C	2	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	2-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	3-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	4-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	5-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	6-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	7-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	8-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	9-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	10-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	11-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	12-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	13-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	14-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	15-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	16-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	17-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	18-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	19-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	20-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	21-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	22-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	23-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)
1	24-A	549/549 (100%)	0.01	38 (6%)	16	17	11, 14, 17, 21	549 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	25-A	549/549 (100%)	0.01	38 (6%) 16 17	11, 14, 17, 21	549 (100%)
All	All	13725/13725 (100%)	0.01	950 (6%) 20 17	11, 14, 17, 21	13725 (100%)

The worst 5 of 950 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	296	THR	10.6
1	2-A	296	THR	10.6
1	3-A	296	THR	10.6
1	4-A	296	THR	10.6
1	5-A	296	THR	10.6

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	12-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	1-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	7-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	25-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	23-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	20-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	10-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	19-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	16-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	15-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	24-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	8-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	18-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	21-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	2-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	14-C	1	12/12	0.78	0.38	21,21,21,21	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	5-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	3-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	17-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	4-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	6-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	11-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	9-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	22-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	13-C	1	12/12	0.78	0.38	21,21,21,21	12
2	BGC	4-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	6-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	15-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	25-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	21-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	24-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	16-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	18-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	1-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	3-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	11-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	22-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	19-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	7-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	13-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	10-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	8-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	9-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	17-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	20-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	14-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	23-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	12-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	2-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	5-C	3	11/12	0.90	0.23	23,27,32,34	11
2	BGC	13-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	7-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	22-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	16-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	18-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	23-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	14-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	6-C	2	11/12	0.91	0.28	25,27,31,47	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	12-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	3-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	17-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	10-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	2-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	20-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	11-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	24-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	8-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	25-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	21-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	4-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	5-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	19-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	1-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	9-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	15-C	2	11/12	0.91	0.28	25,27,31,47	11
2	BGC	23-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	15-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	13-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	11-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	9-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	17-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	8-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	19-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	6-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	14-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	18-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	4-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	16-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	25-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	22-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	3-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	2-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	7-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	24-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	5-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	10-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	1-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	21-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	12-B	3	11/12	0.93	0.10	14,15,20,26	11
2	BGC	20-B	3	11/12	0.93	0.10	14,15,20,26	11

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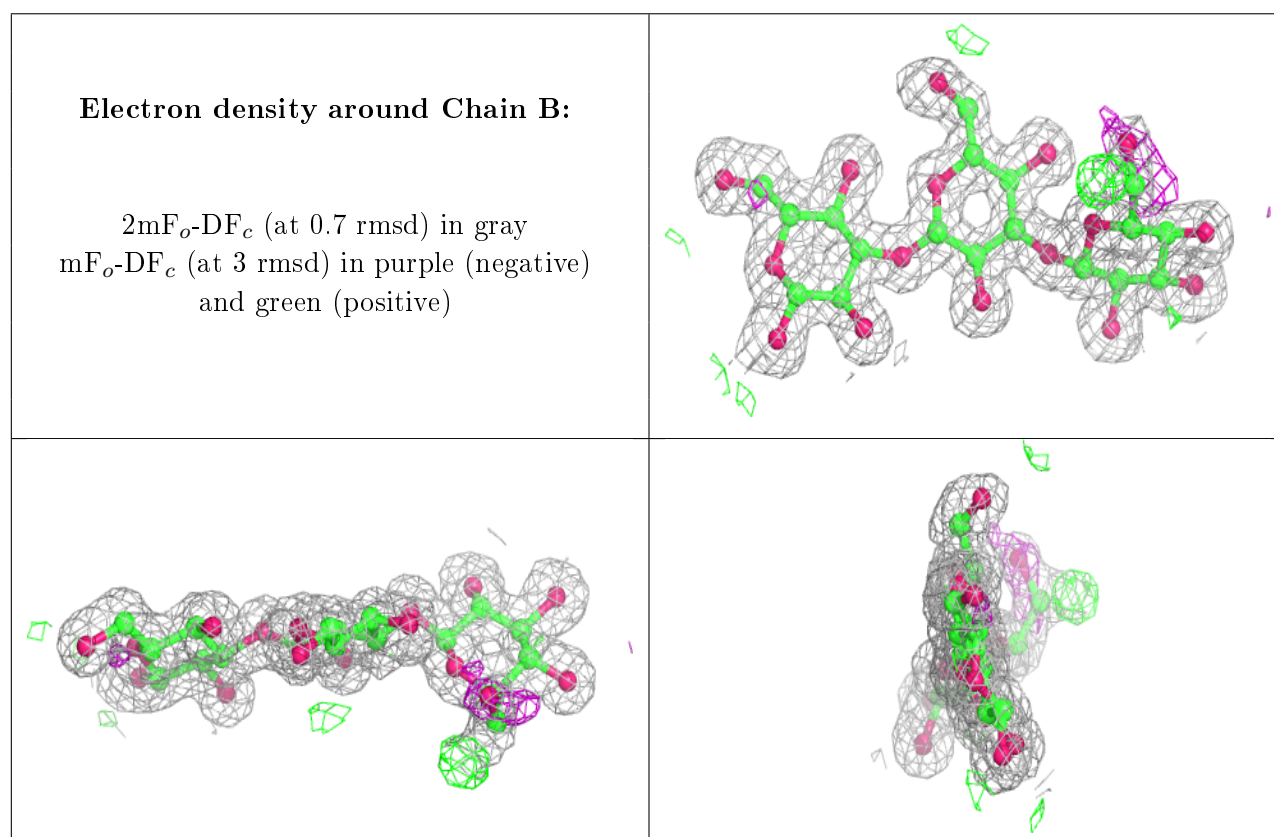
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	9-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	8-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	19-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	21-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	18-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	6-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	15-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	24-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	1-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	16-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	25-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	7-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	22-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	3-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	14-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	10-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	11-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	12-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	20-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	5-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	17-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	13-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	4-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	2-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	23-B	2	11/12	0.96	0.08	14,16,22,23	11
2	BGC	24-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	16-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	9-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	17-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	12-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	2-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	3-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	6-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	20-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	23-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	1-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	8-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	11-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	18-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	4-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	22-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	5-B	1	12/12	0.97	0.07	15,17,23,26	12

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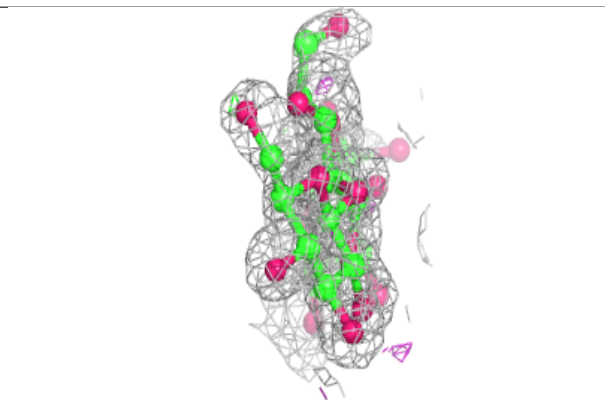
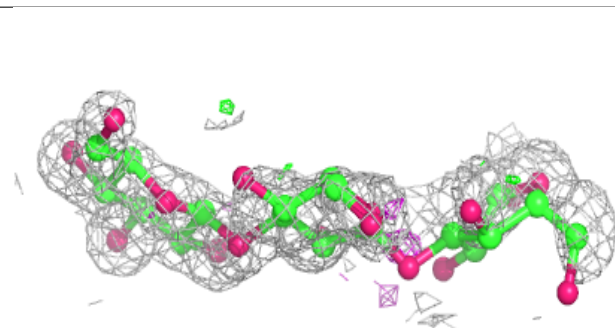
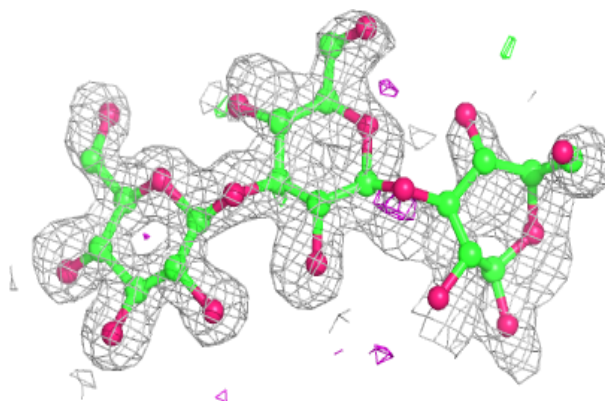
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	14-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	25-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	19-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	13-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	21-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	10-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	15-B	1	12/12	0.97	0.07	15,17,23,26	12
2	BGC	7-B	1	12/12	0.97	0.07	15,17,23,26	12

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

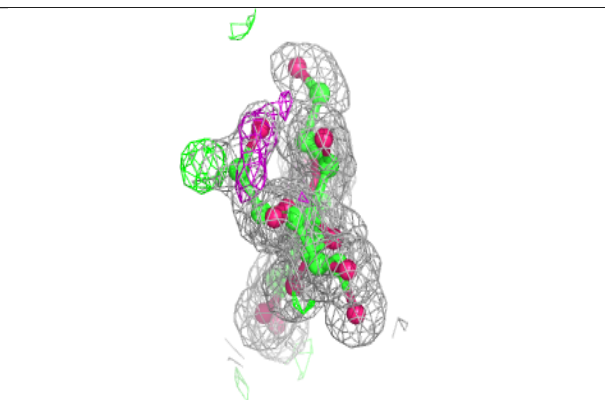
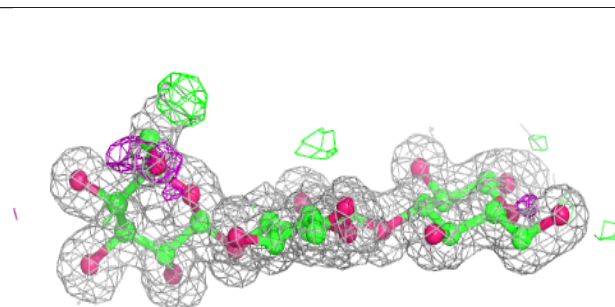
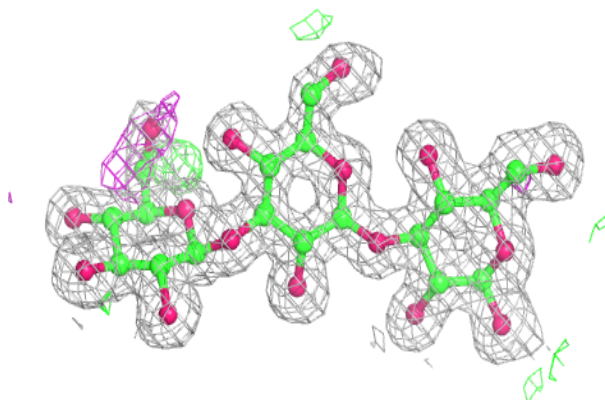


Electron density around Chain C:

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

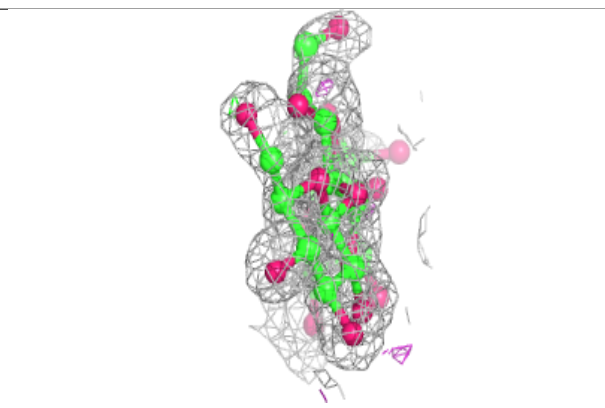
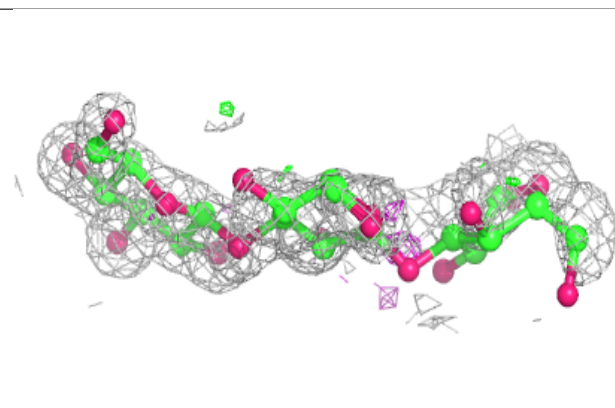
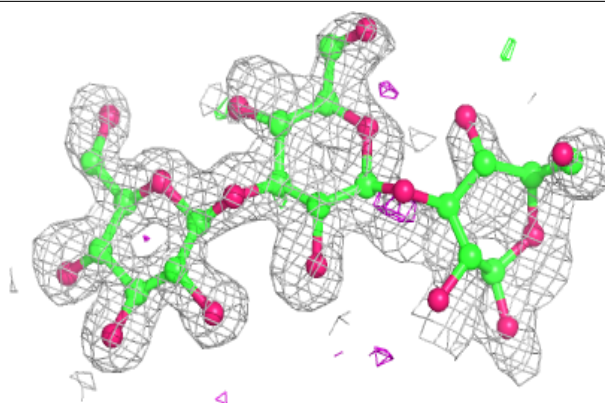
**Electron density around Chain B:**

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

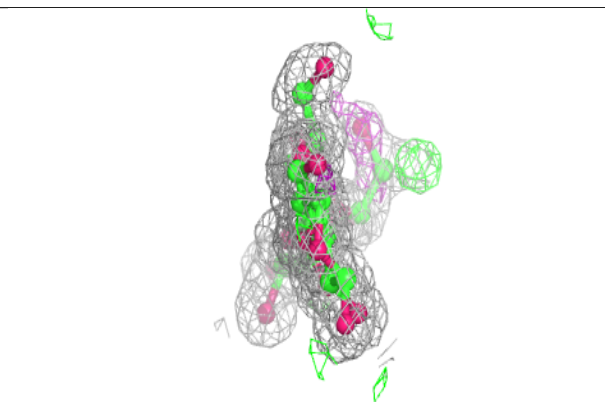
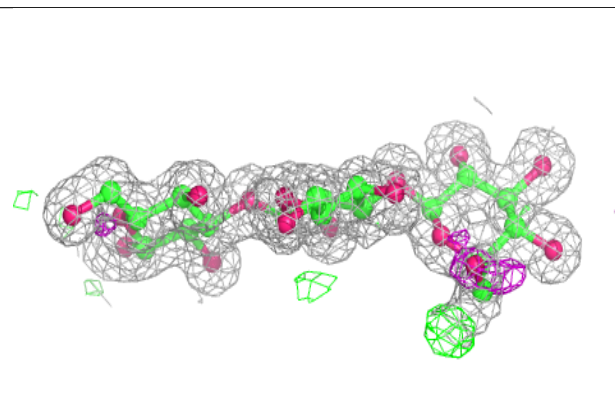
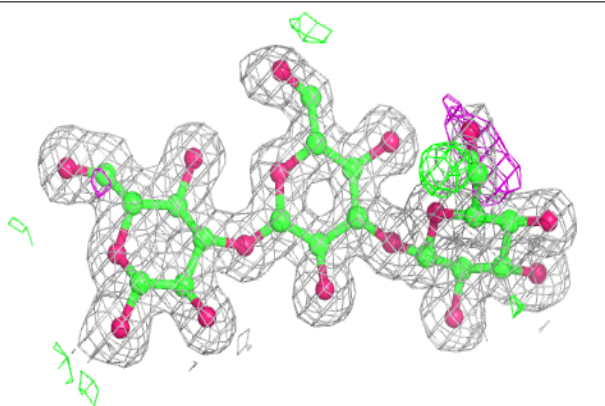


Electron density around Chain C:

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

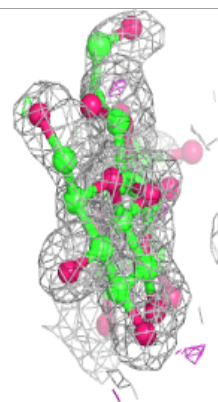
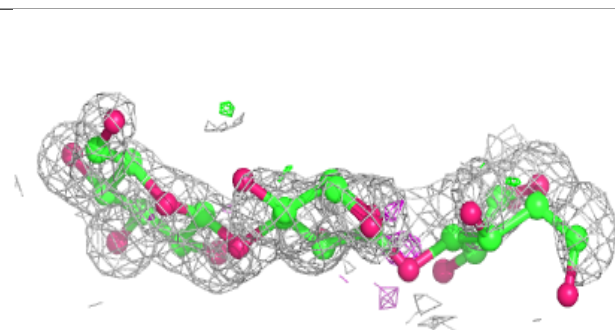
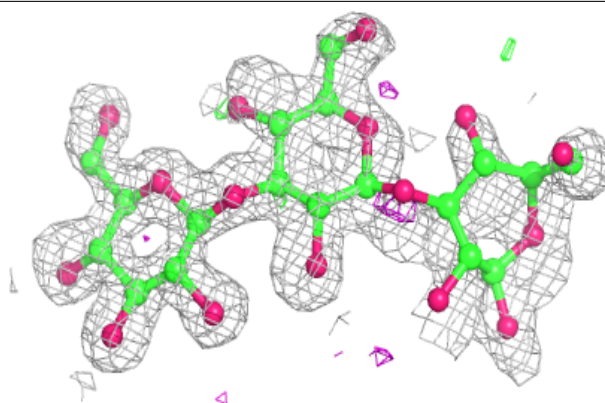
**Electron density around Chain B:**

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

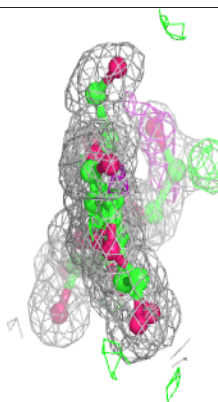
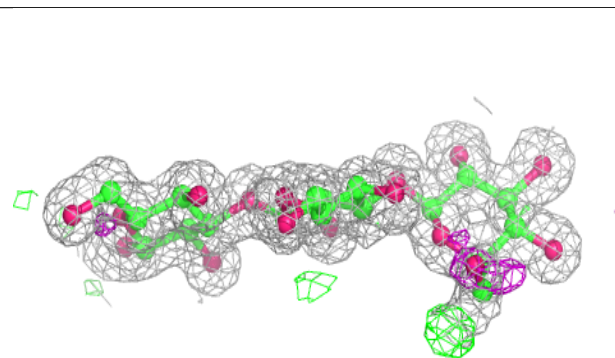
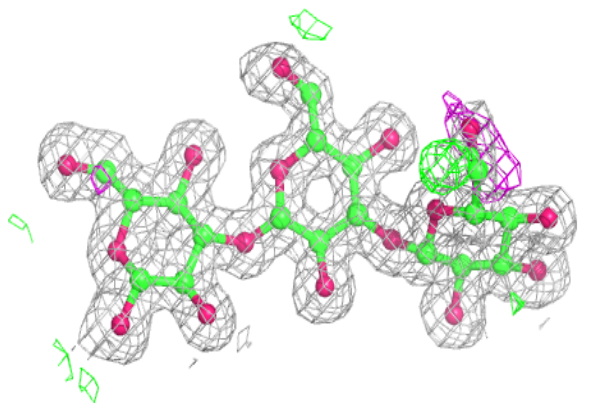


Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
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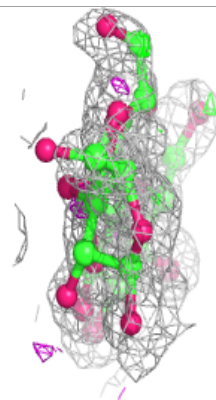
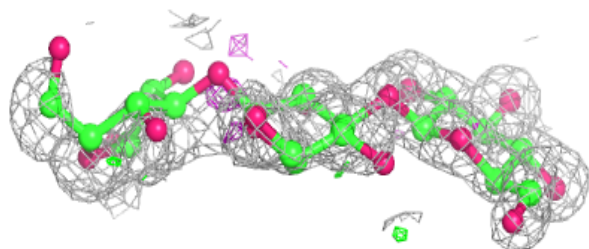
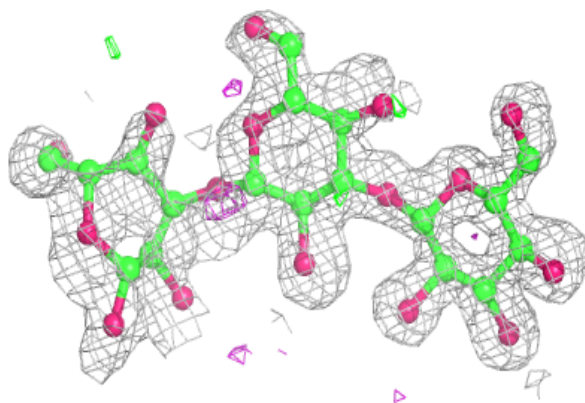
**Electron density around Chain B:**

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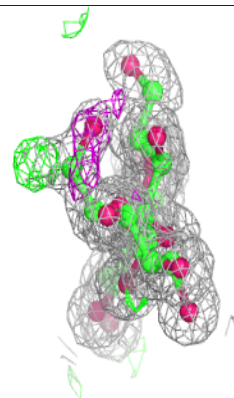
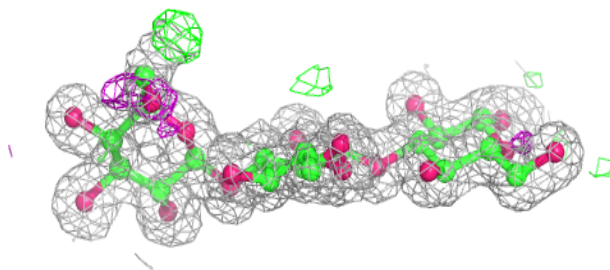
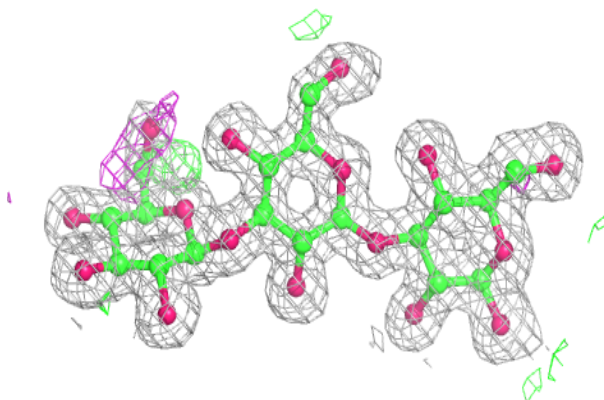


Electron density around Chain C:

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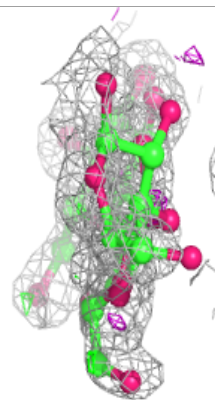
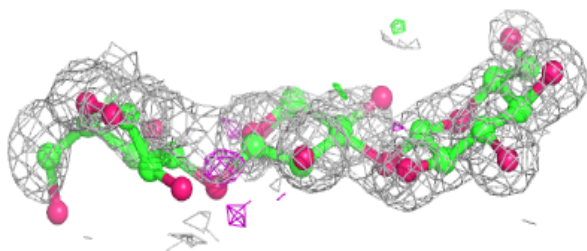
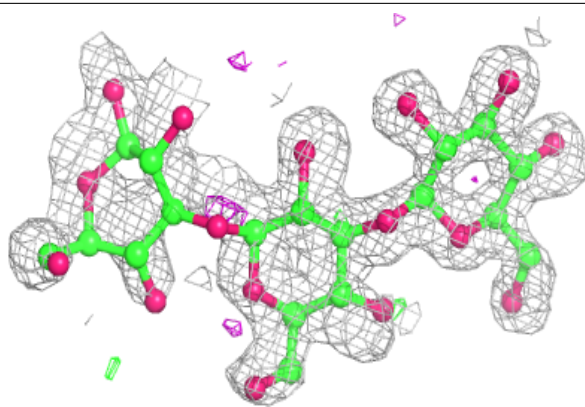
**Electron density around Chain B:**

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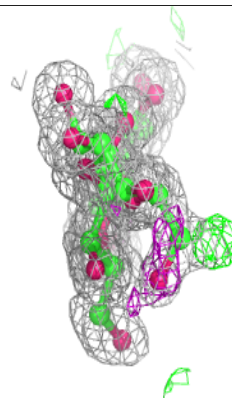
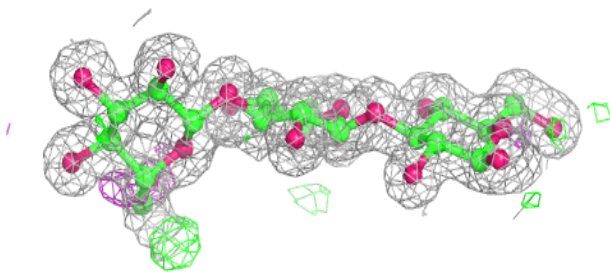
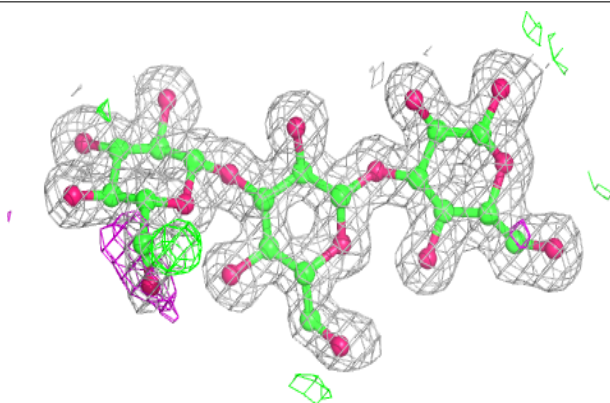


Electron density around Chain C:

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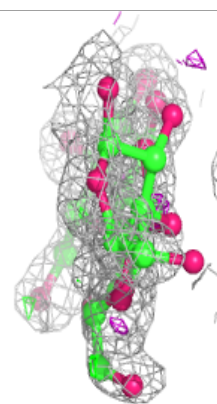
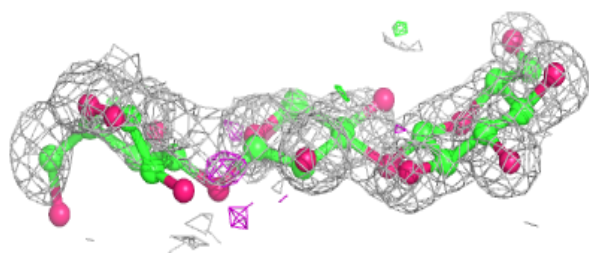
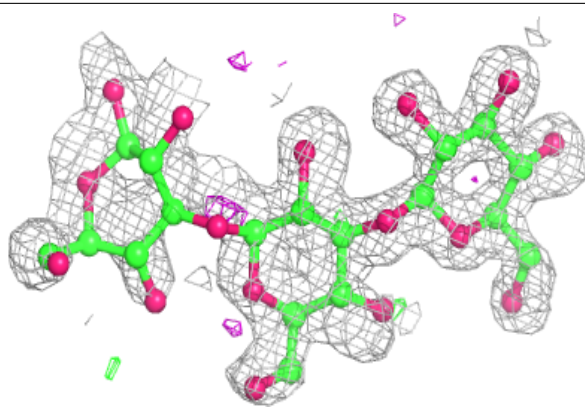
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and green (positive)

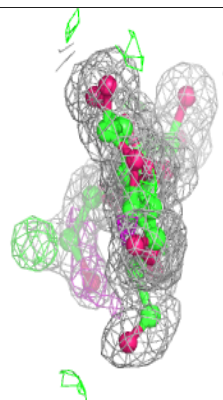
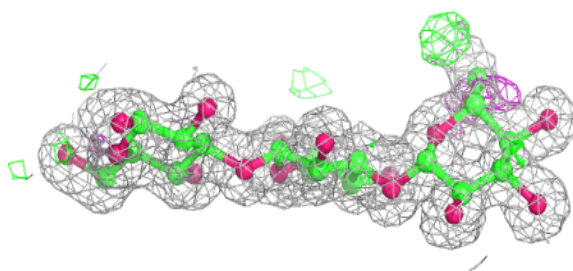
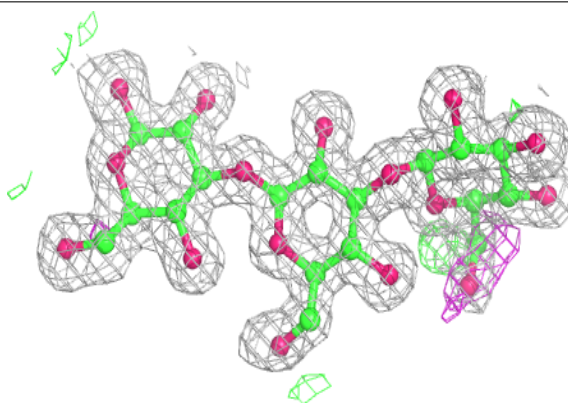


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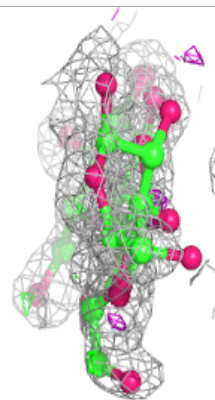
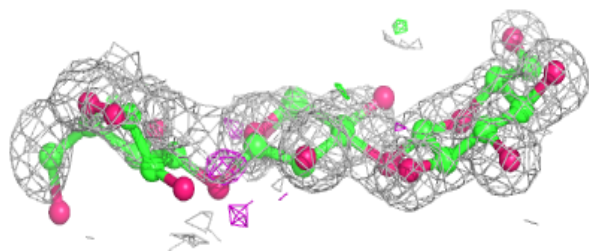
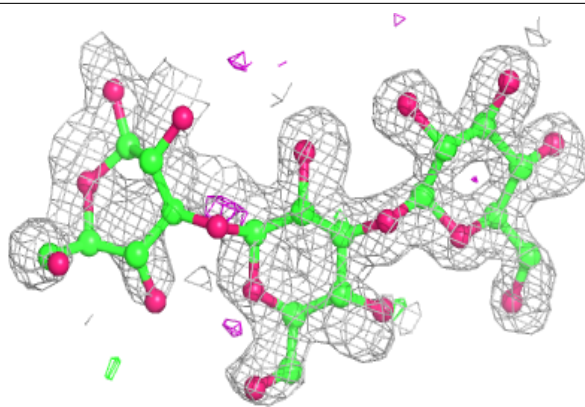
**Electron density around Chain B:**

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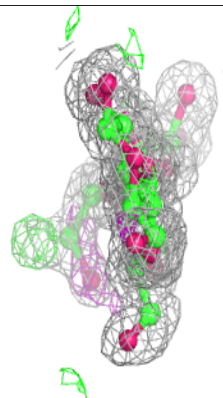
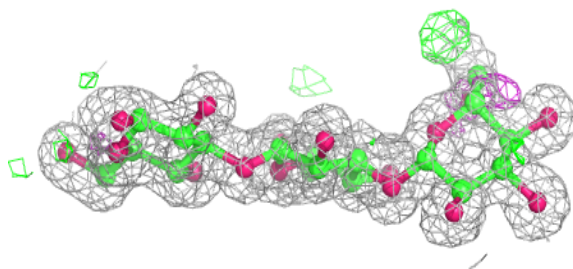
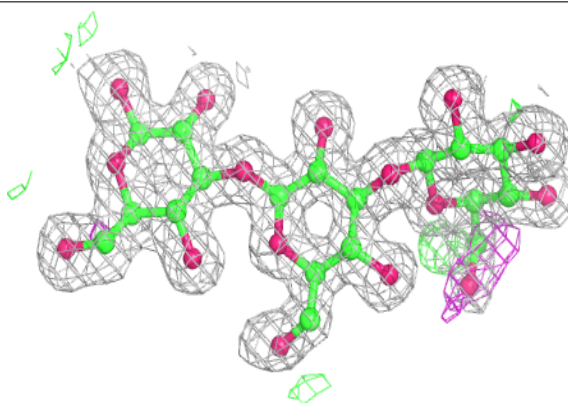


Electron density around Chain C:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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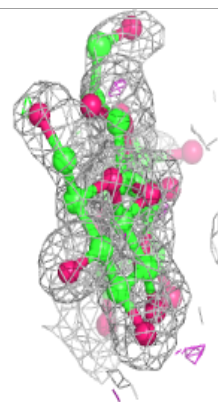
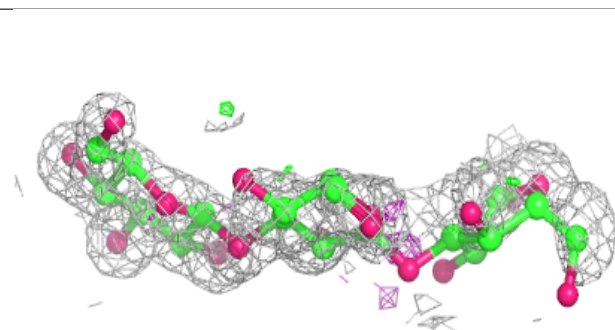
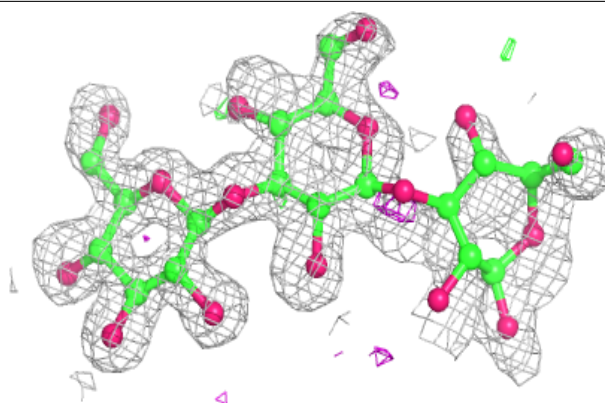
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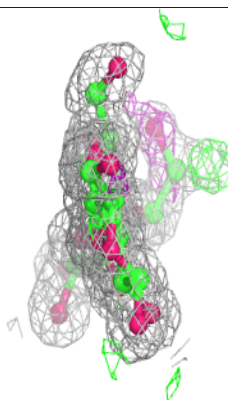
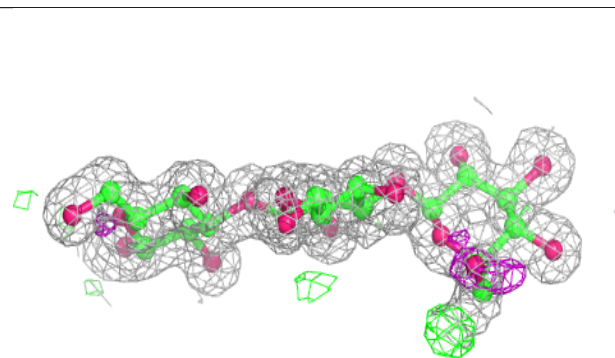
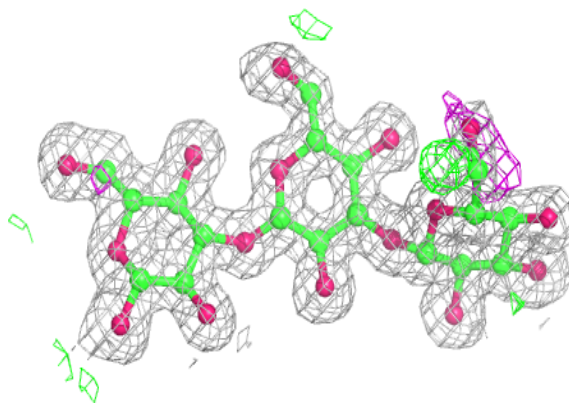


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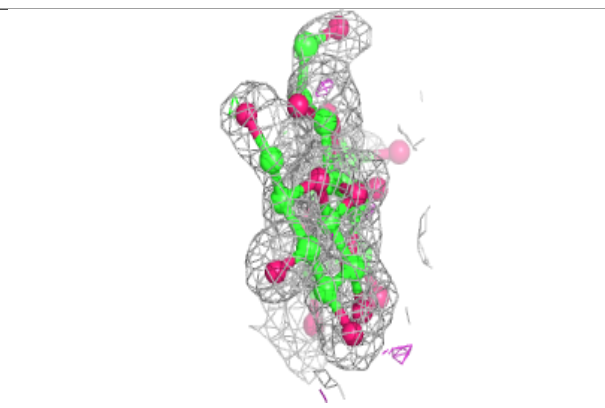
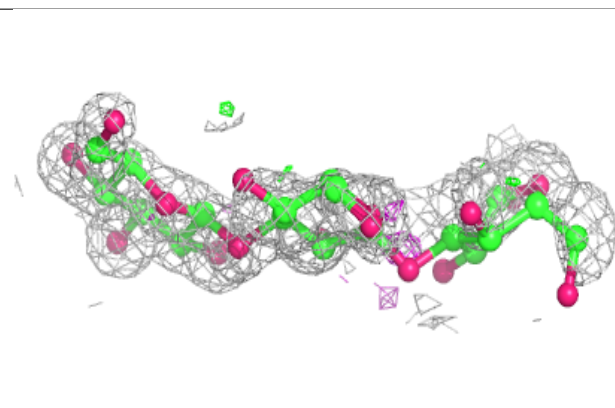
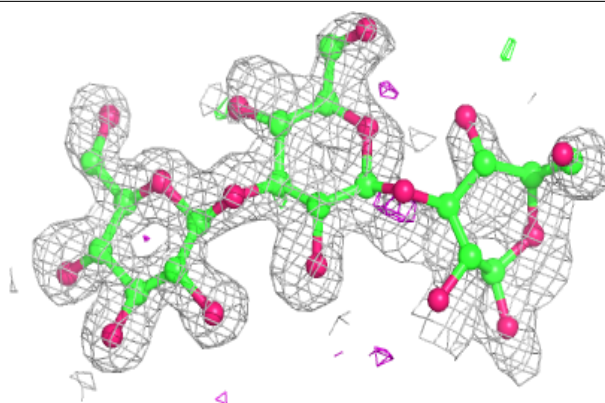
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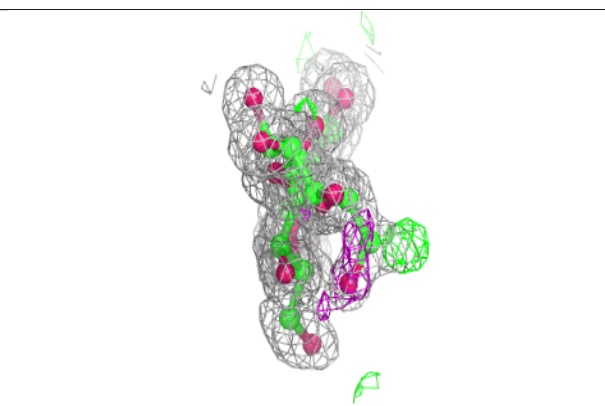
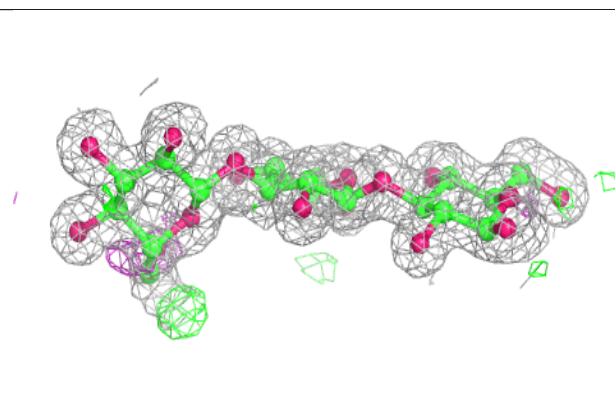
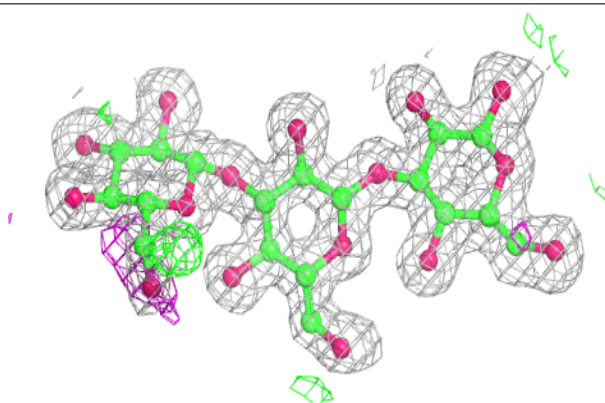


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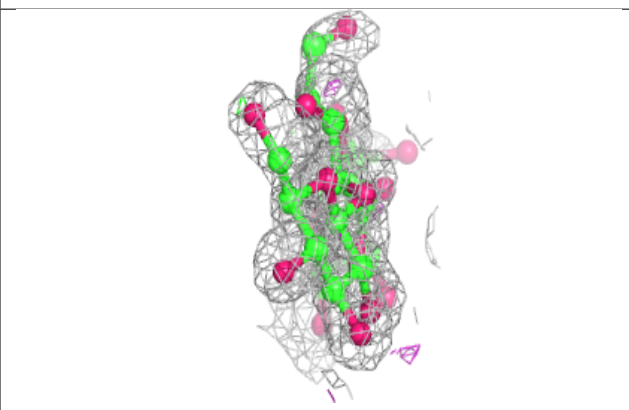
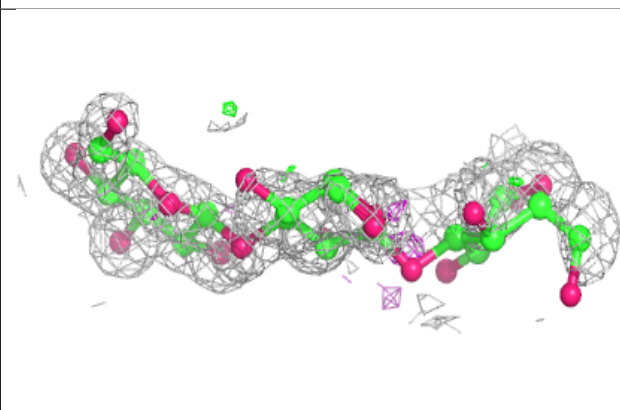
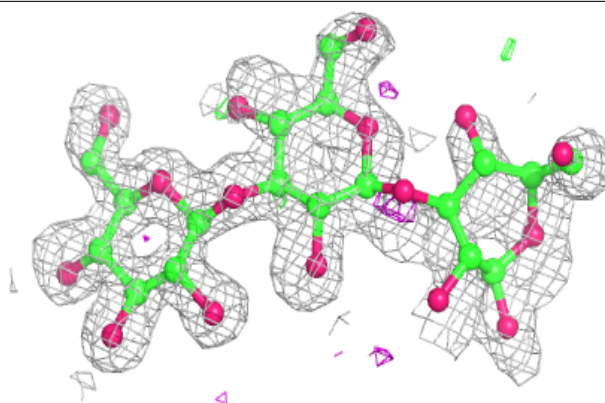
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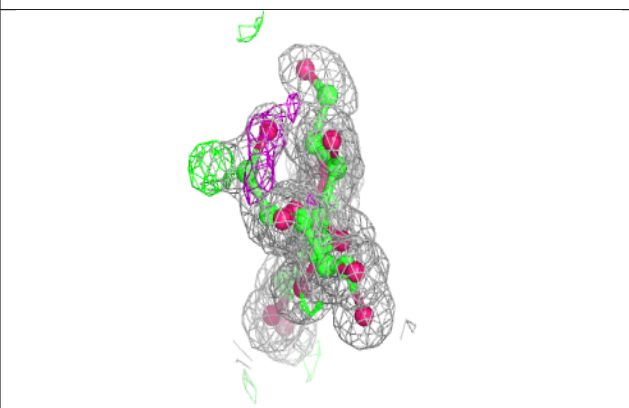
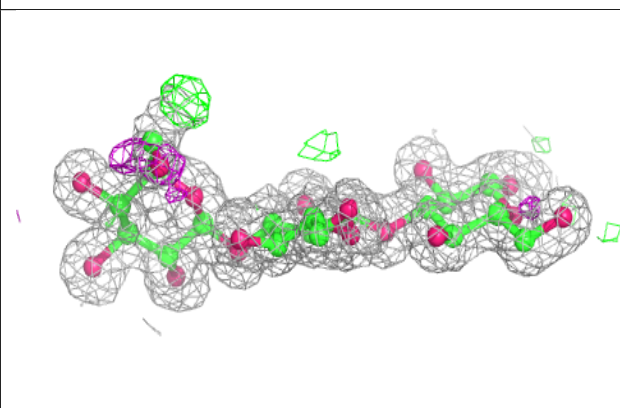
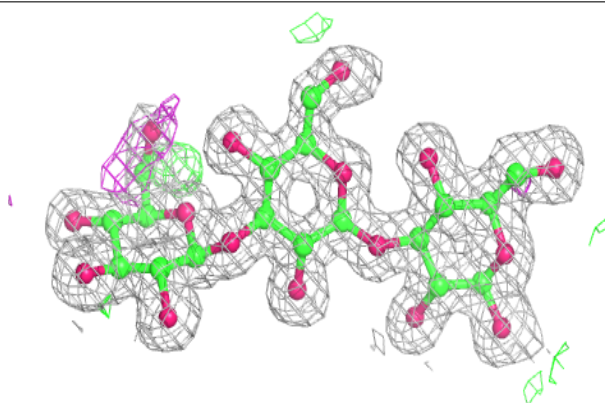


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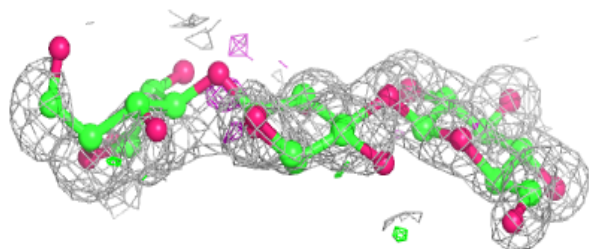
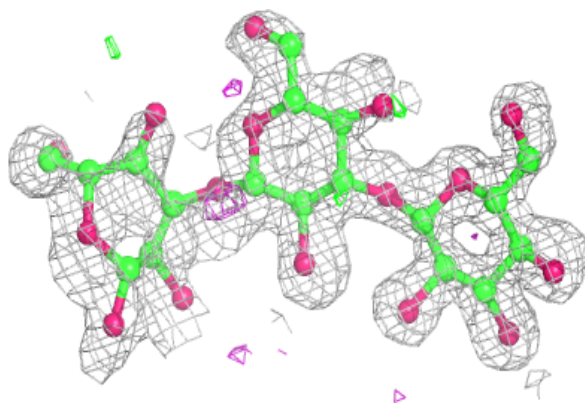
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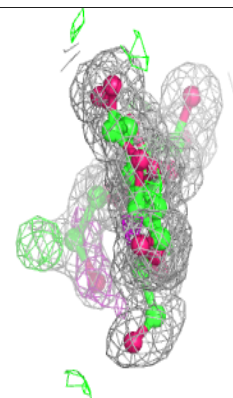
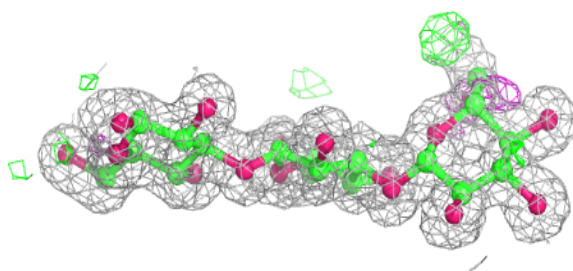
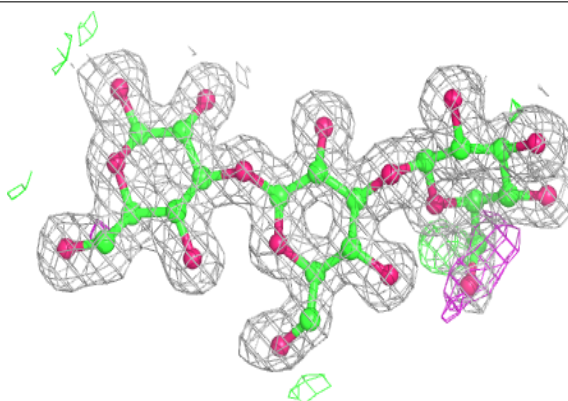


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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

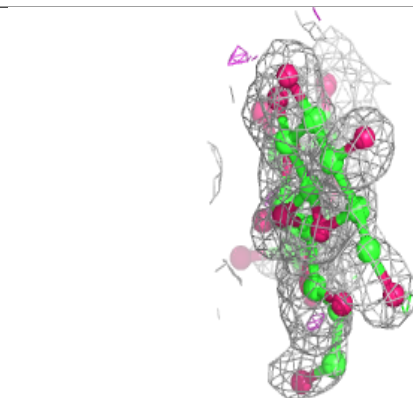
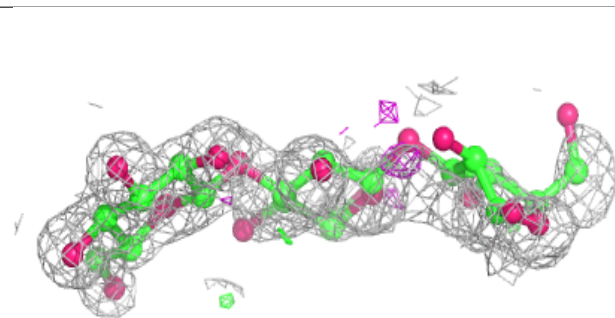
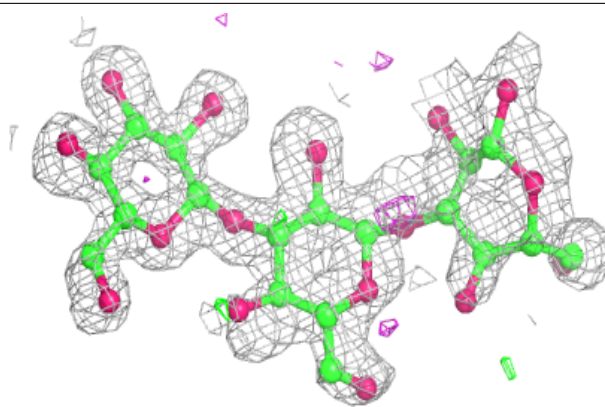
**Electron density around Chain B:**

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

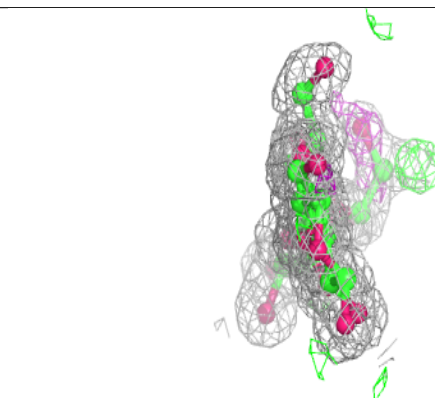
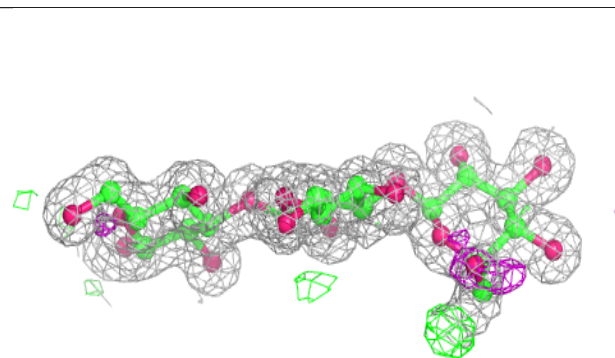
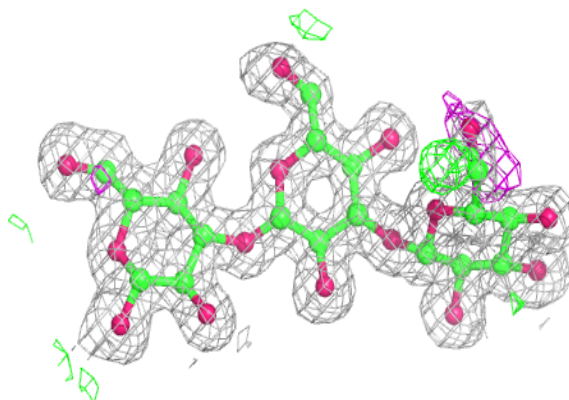


Electron density around Chain C:

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

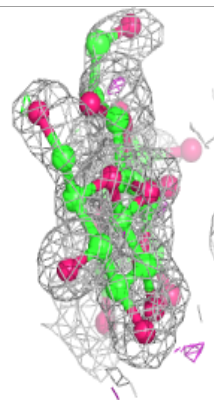
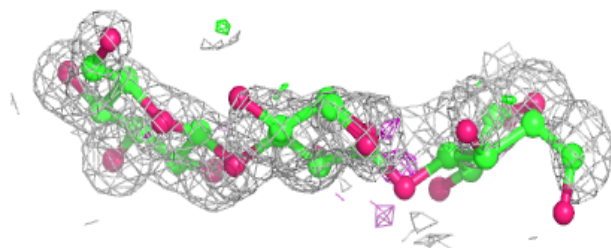
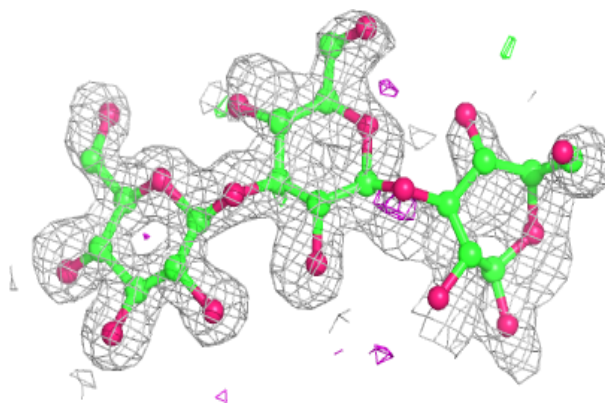
**Electron density around Chain B:**

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

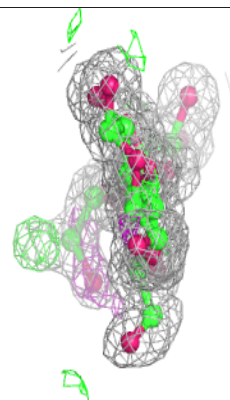
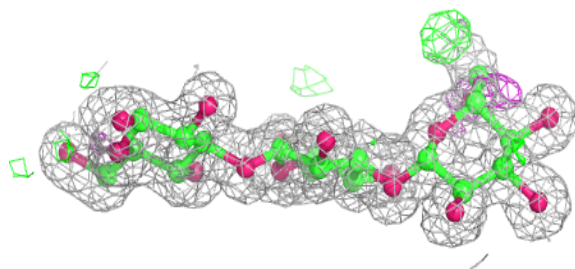
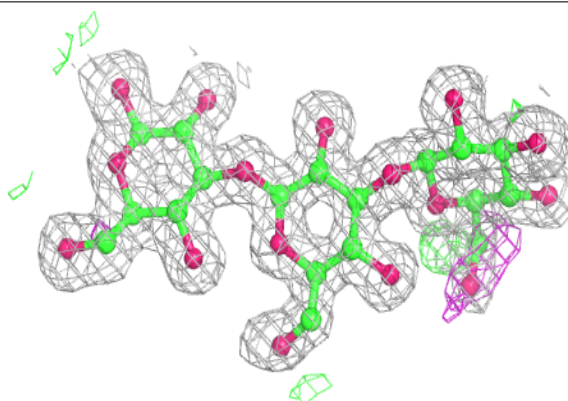


Electron density around Chain C:

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

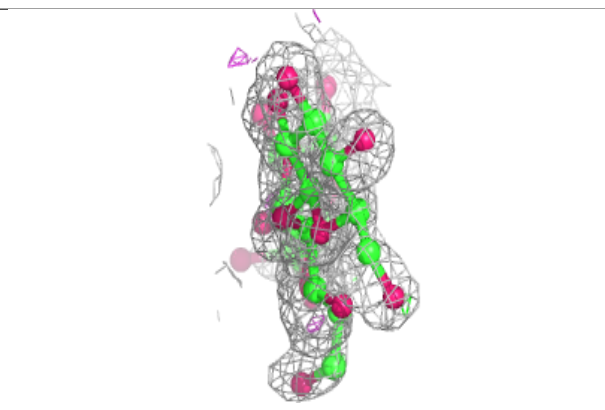
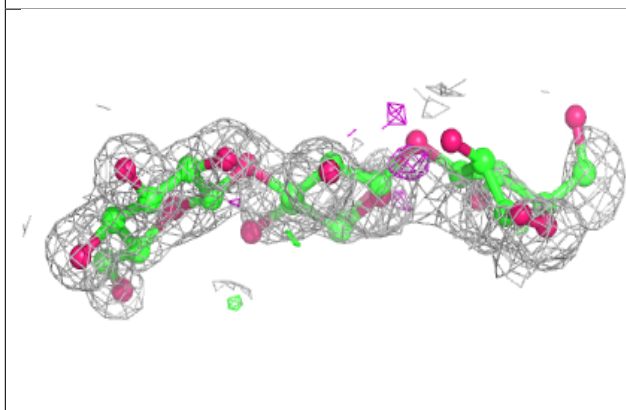
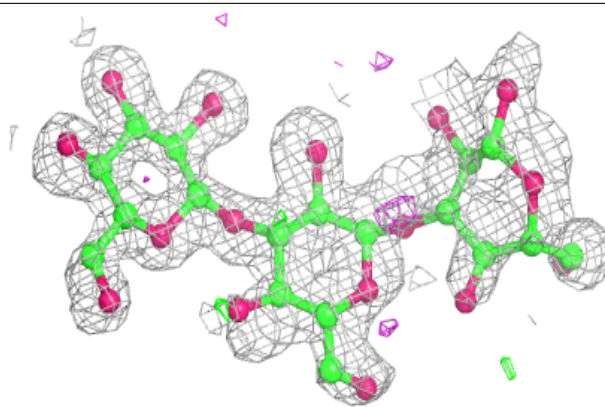
**Electron density around Chain B:**

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

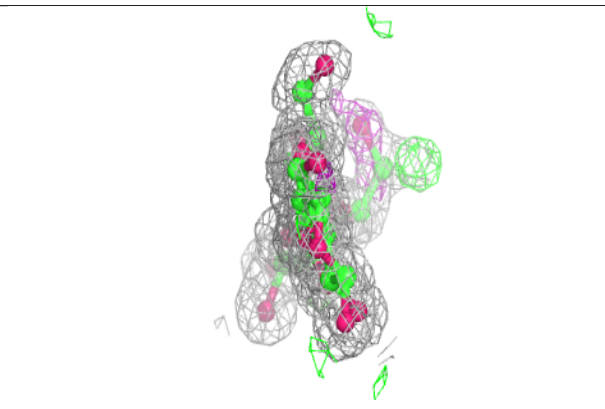
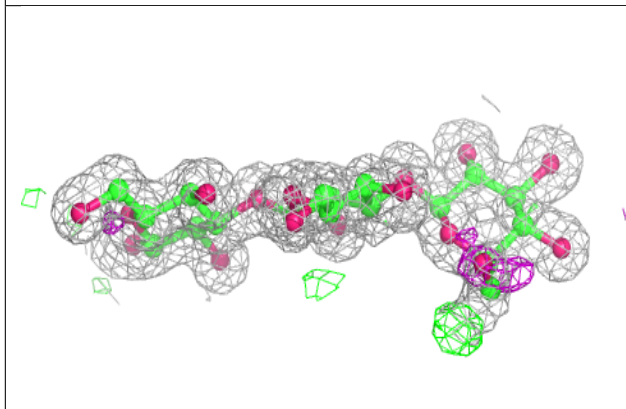
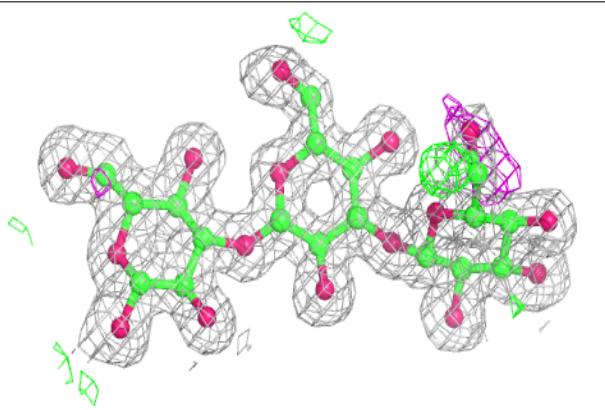


Electron density around Chain C:

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

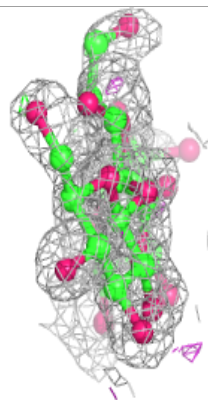
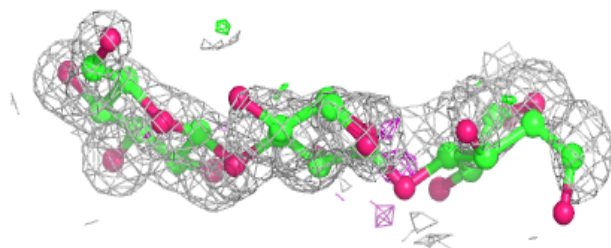
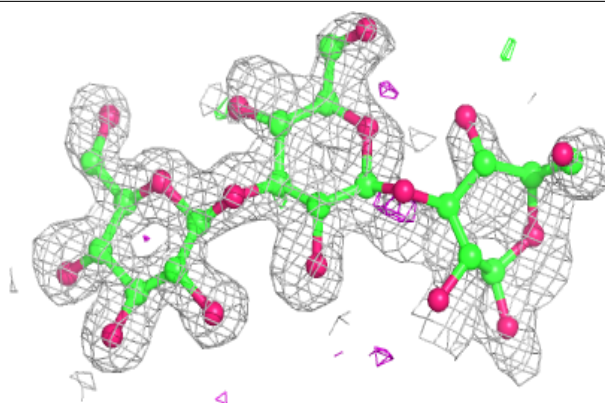
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$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

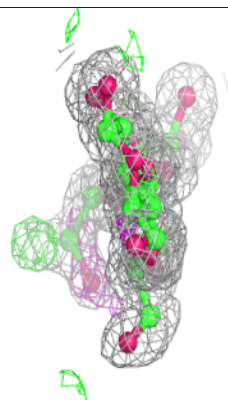
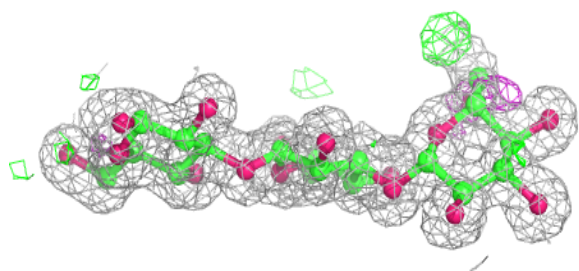
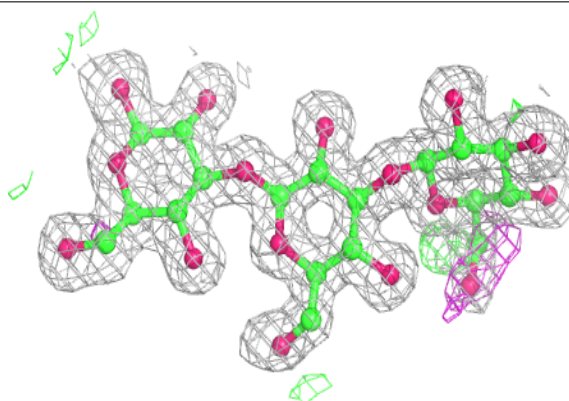


Electron density around Chain C:

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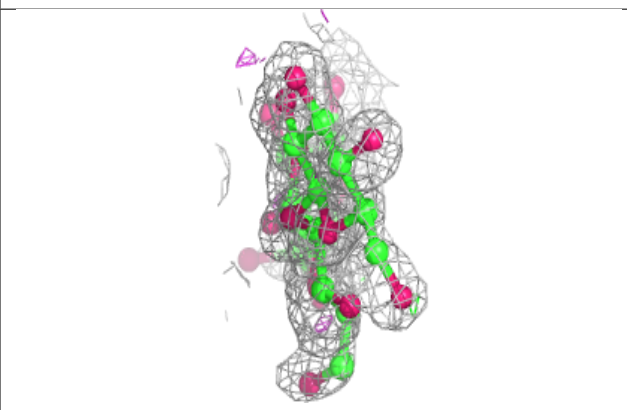
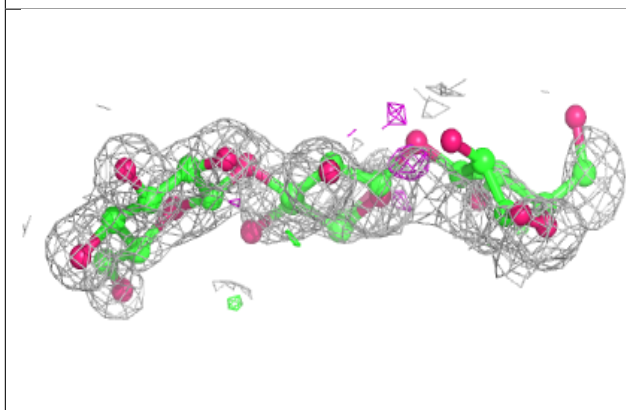
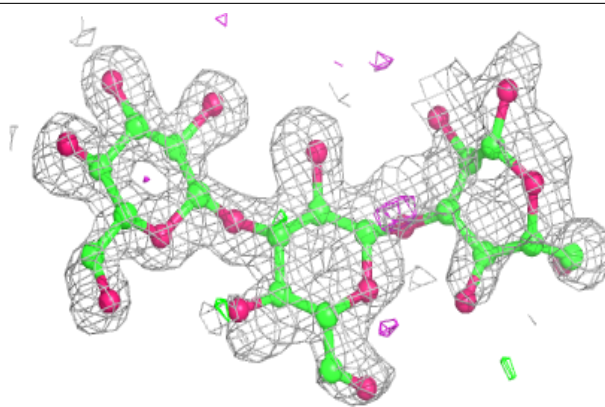
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$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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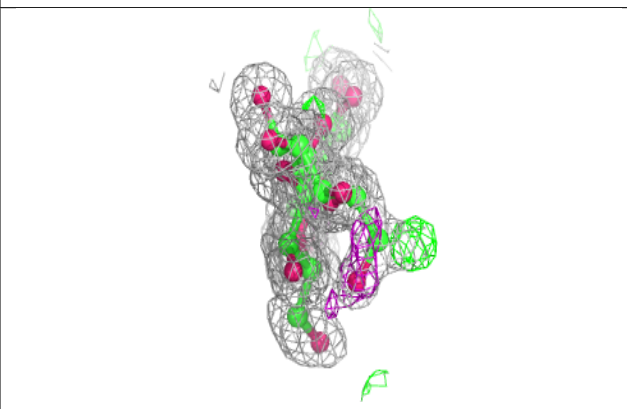
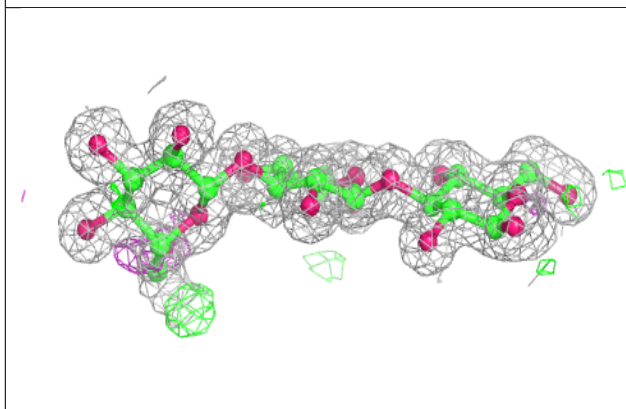
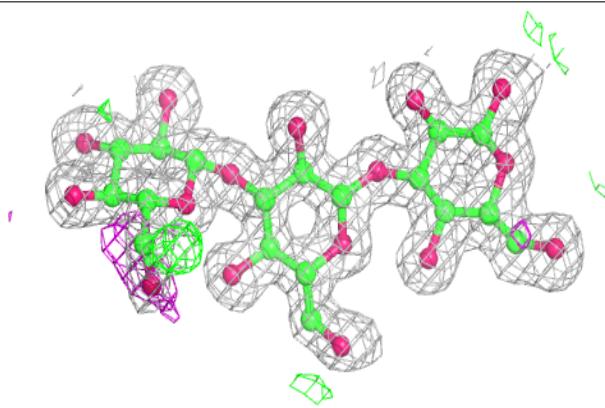


Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
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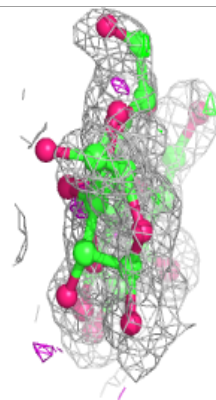
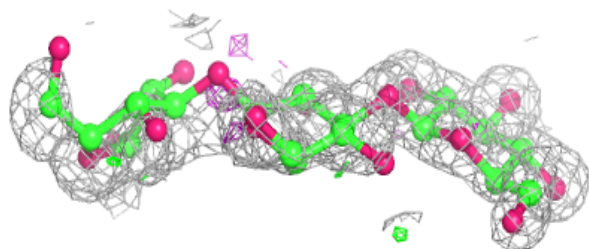
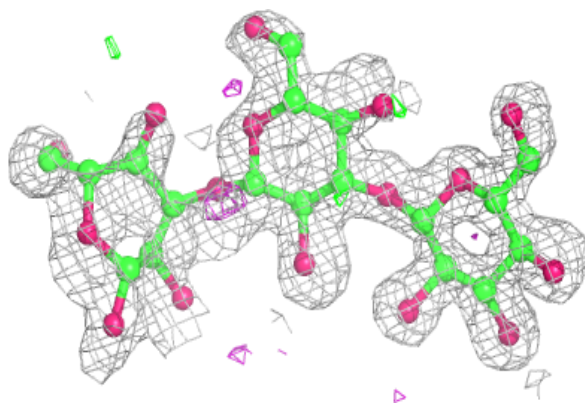
**Electron density around Chain B:**

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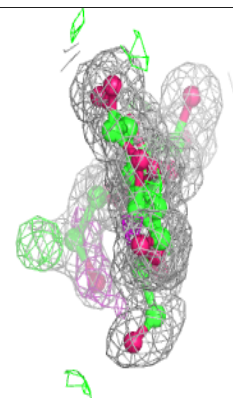
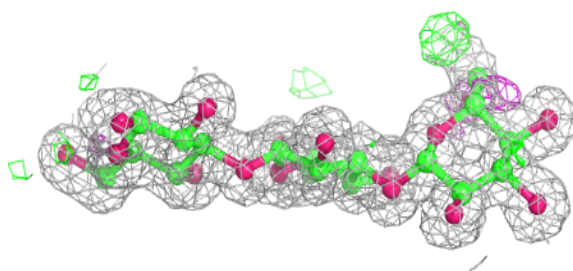
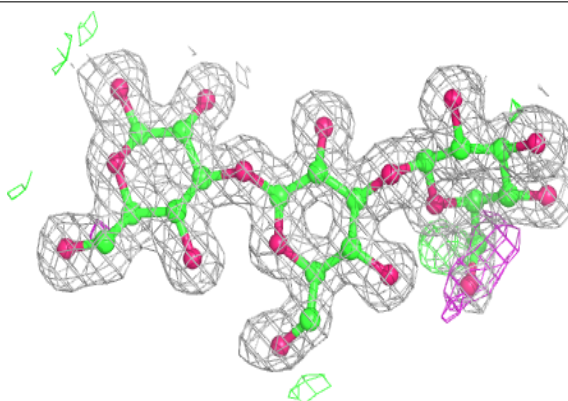


Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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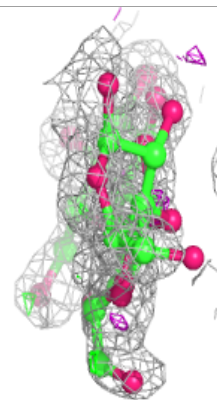
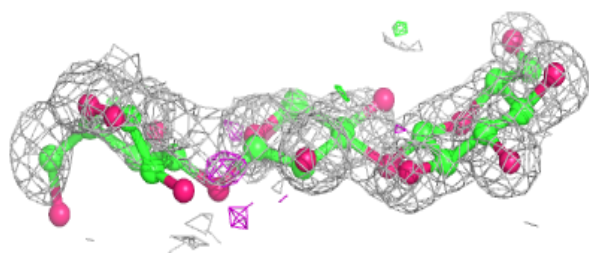
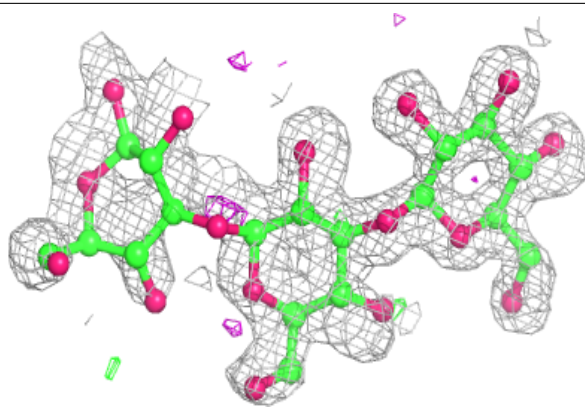
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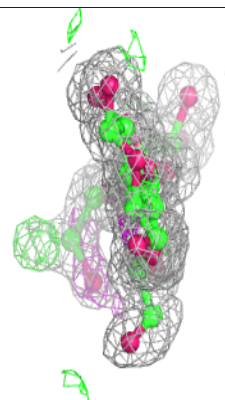
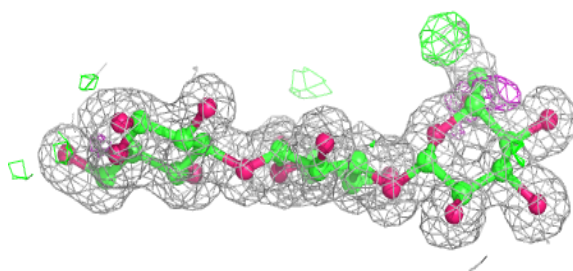
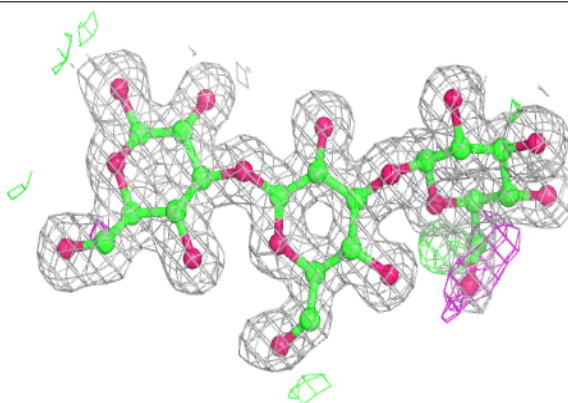


Electron density around Chain C:

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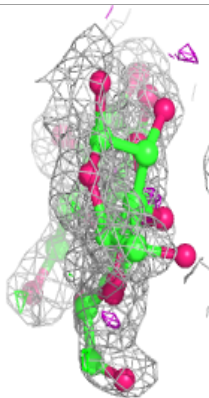
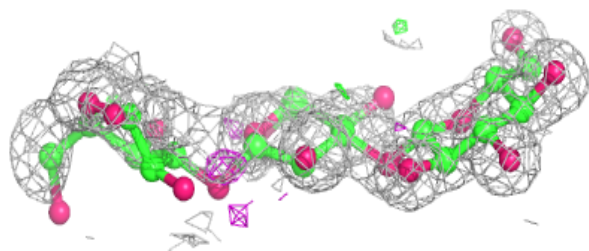
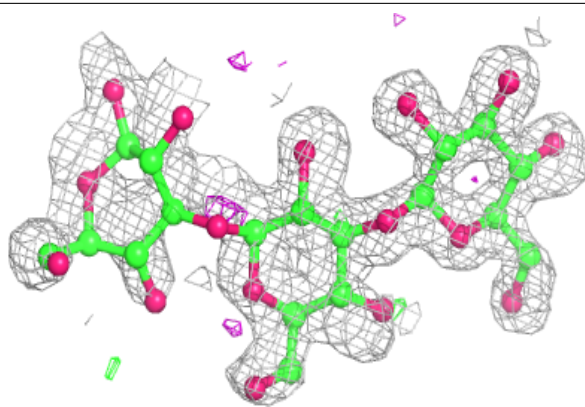
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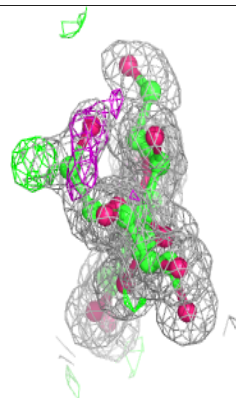
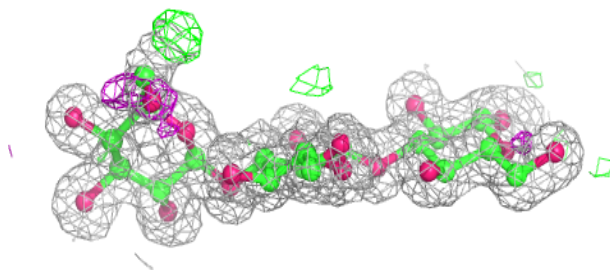
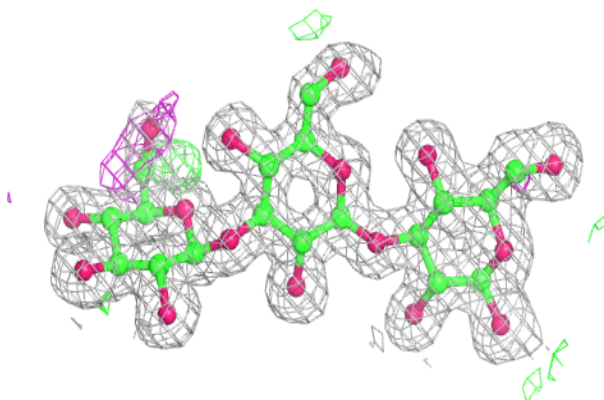


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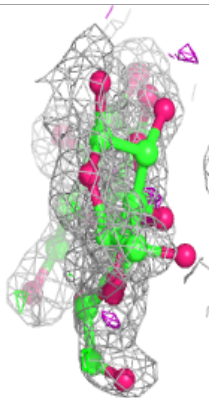
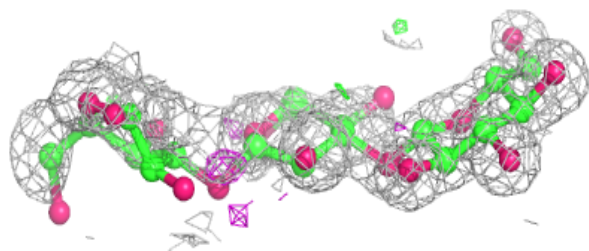
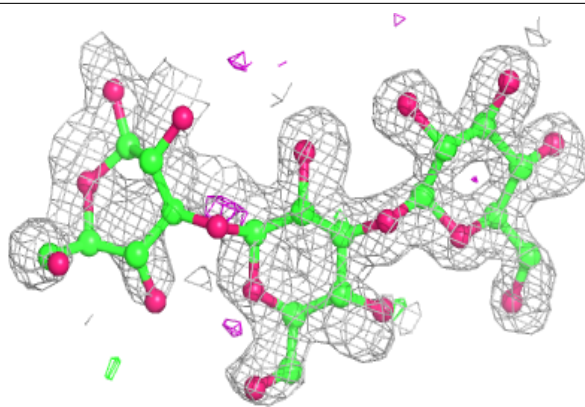
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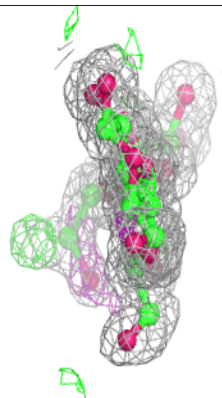
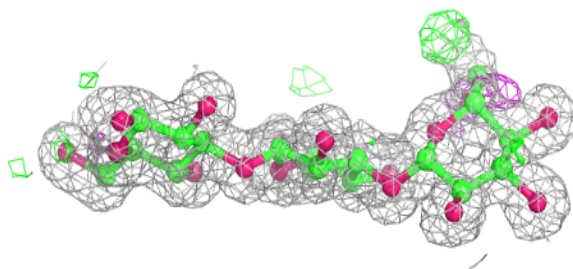
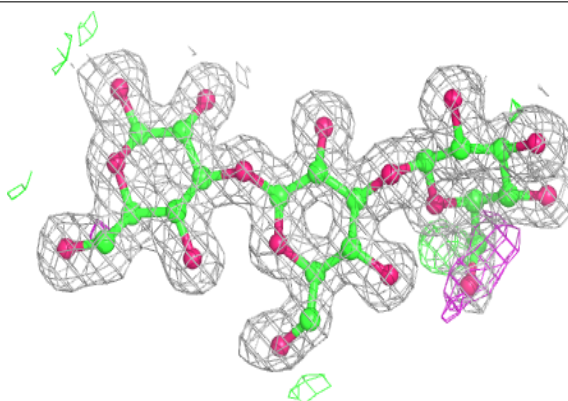


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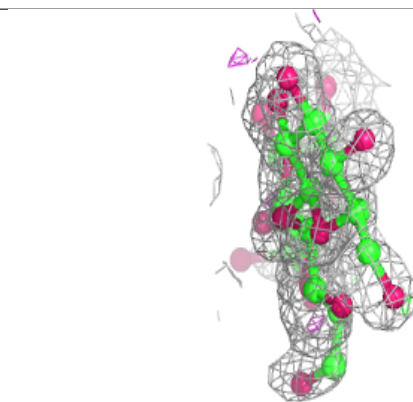
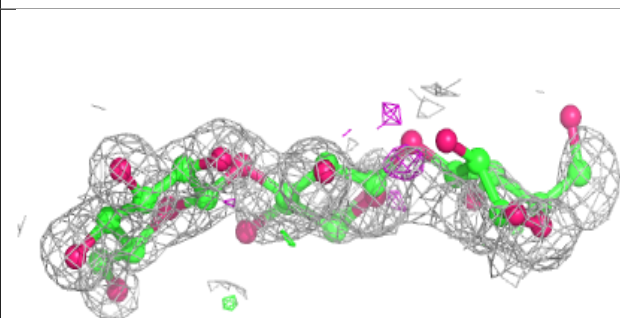
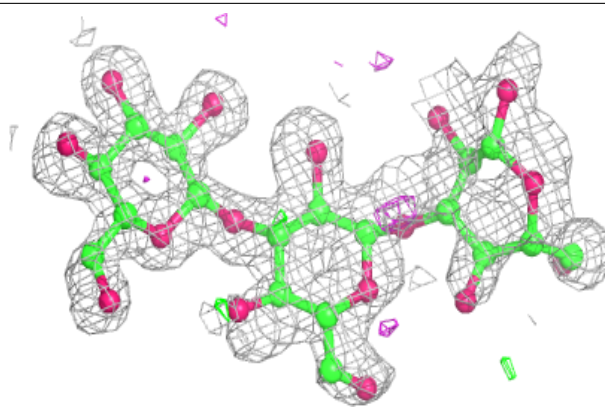
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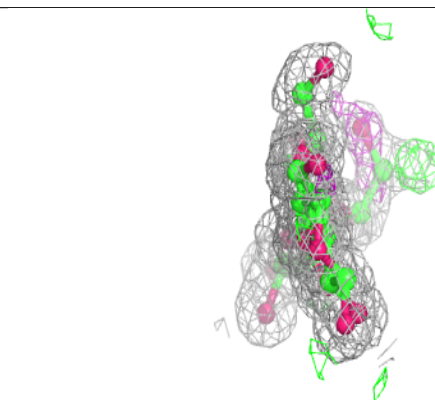
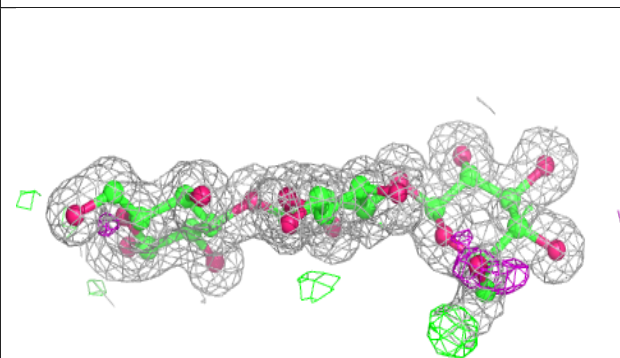
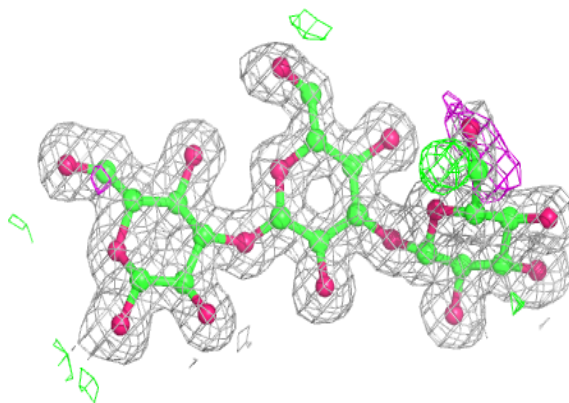


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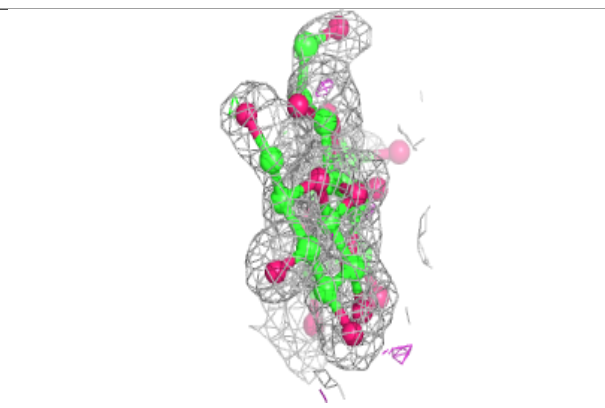
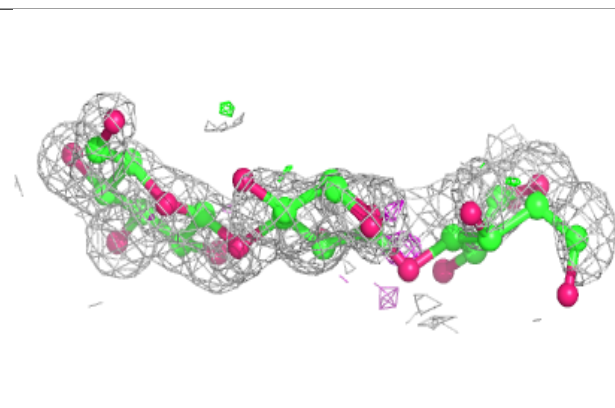
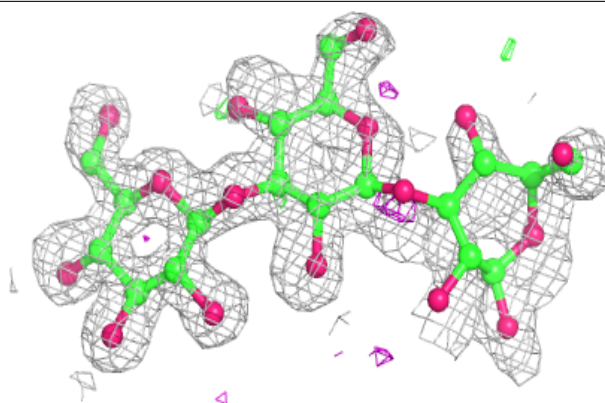
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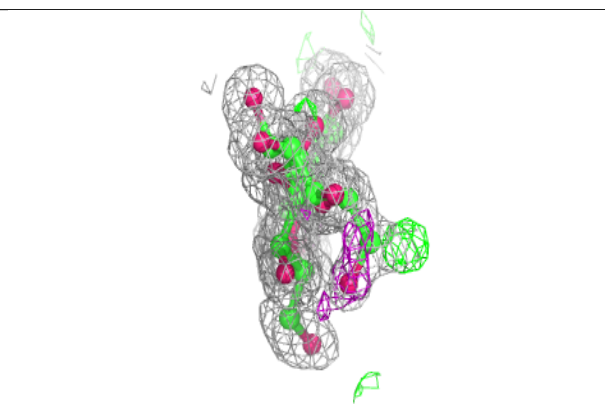
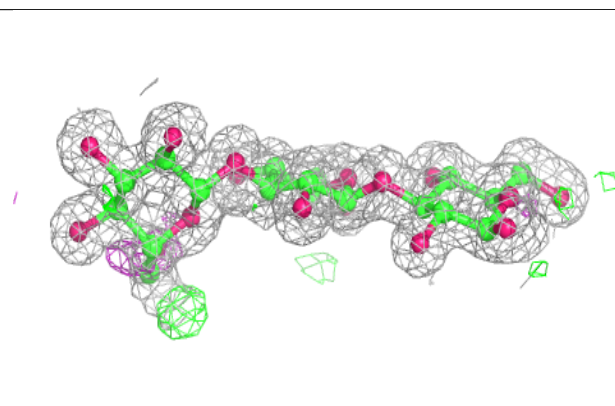
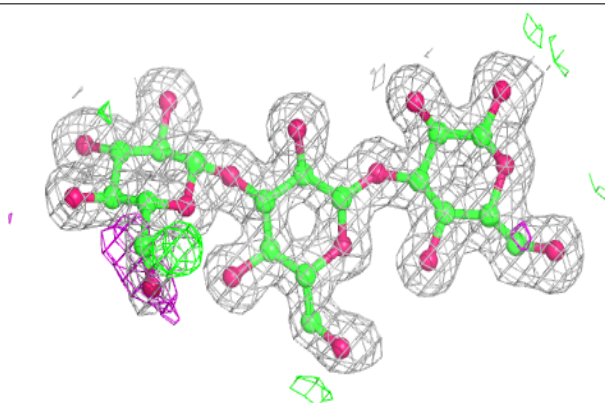


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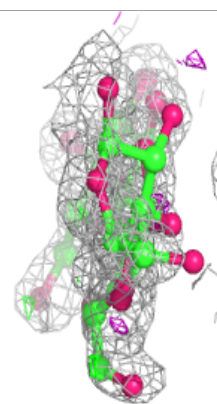
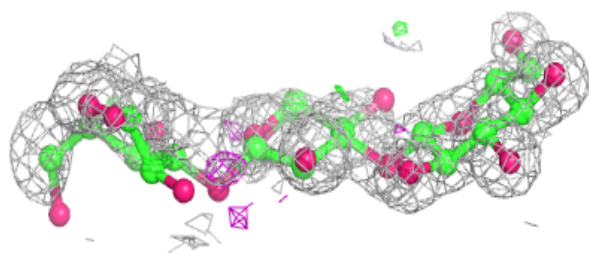
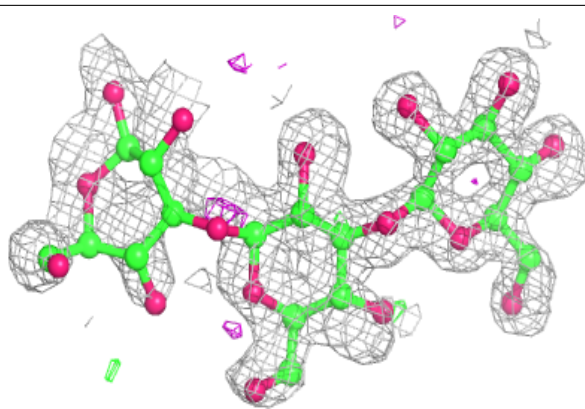
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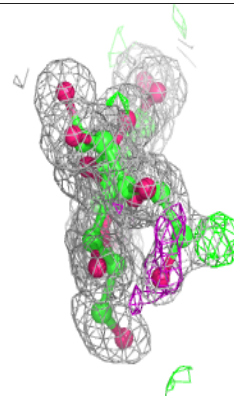
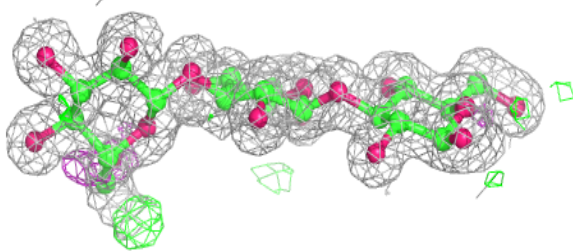
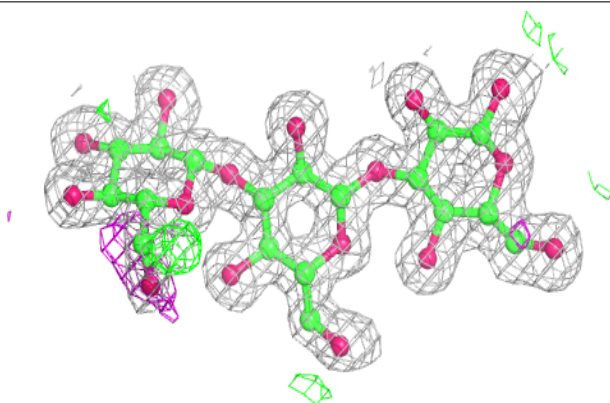


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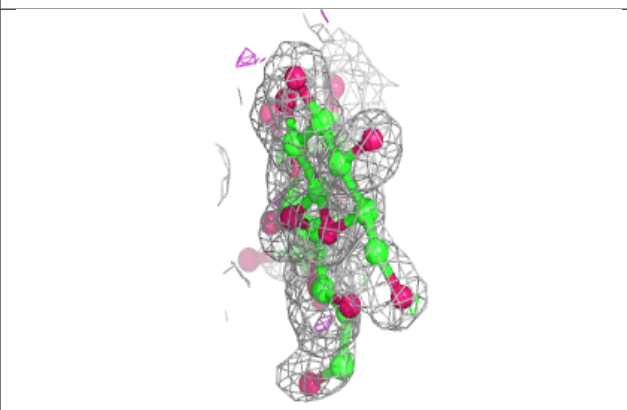
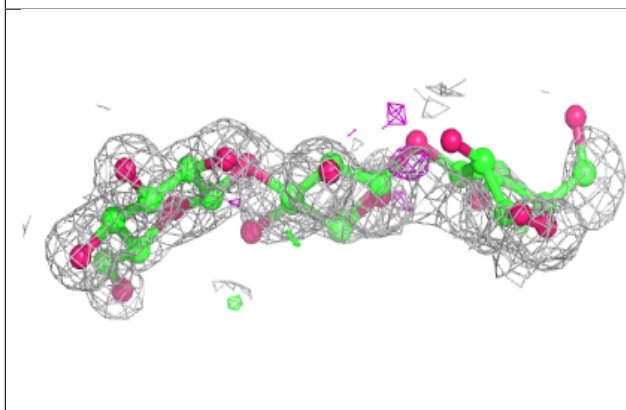
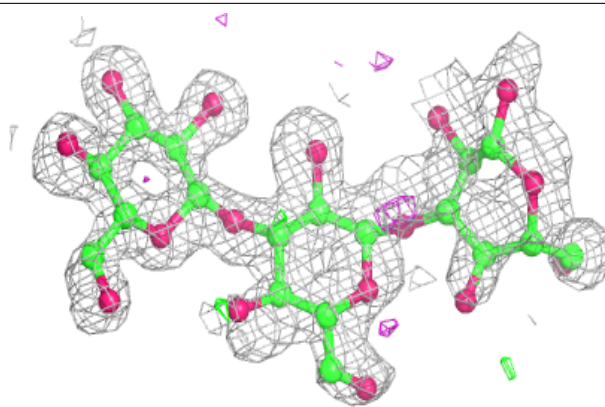
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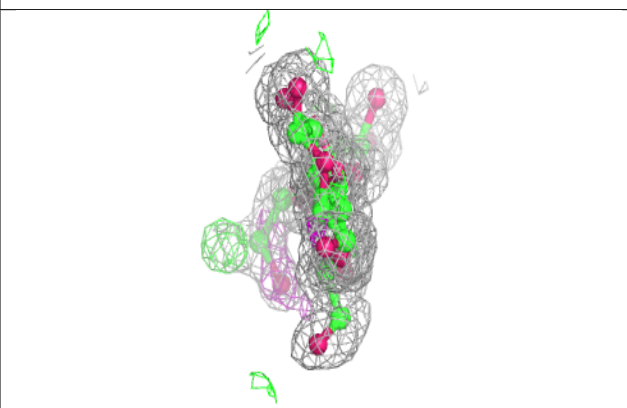
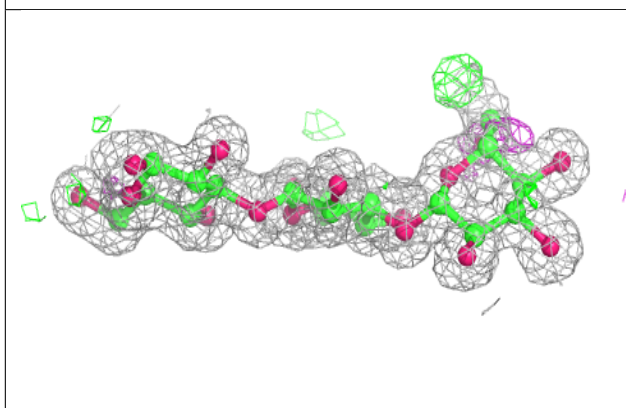
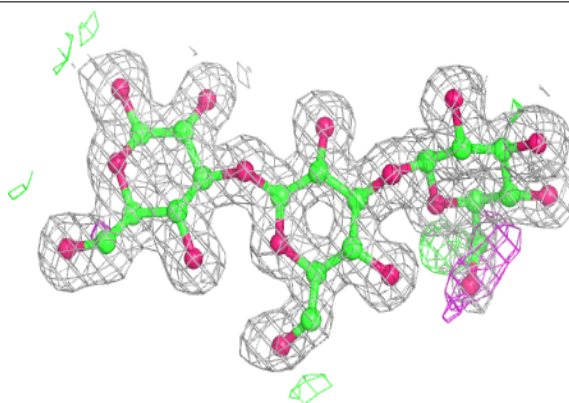


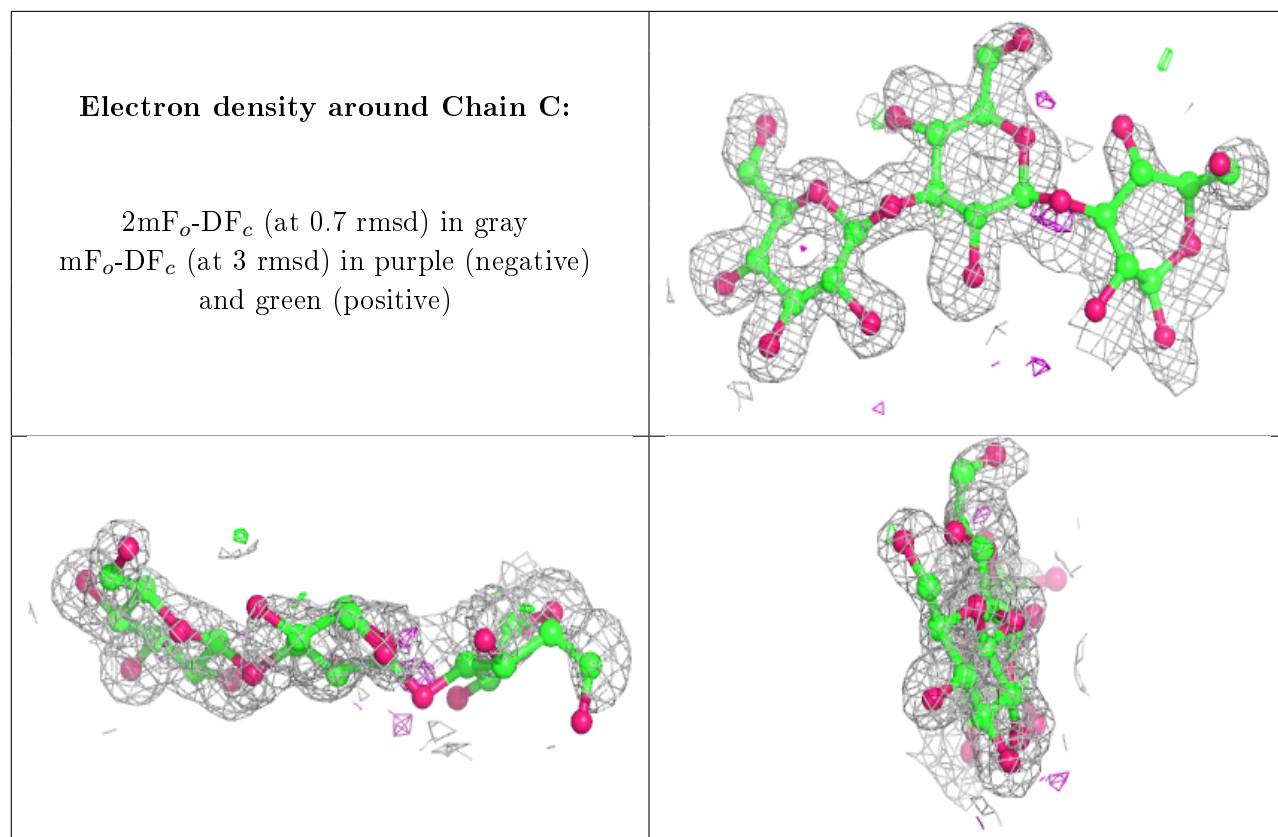
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6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.