



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 08:51 AM BST

PDB ID : 5XQJ  
Title : Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from *Penicillium chrysogenum* complexed with unsaturated galacturonosyl rhamnose substituted with galactose  
Authors : Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.  
Deposited on : 2017-06-07  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

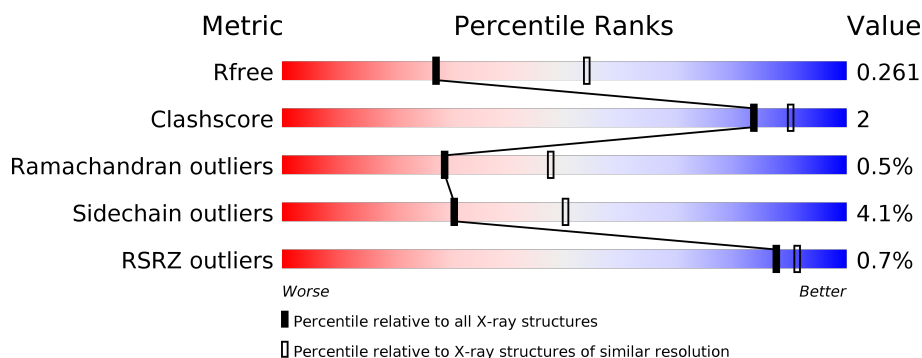
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div> <div>88% 10% ..</div>
1	B	906	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>90% 8% ..</div>
1	C	906	<div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> <div style="width: 2%;"></div> </div> <div>88% 9% ..</div>
1	D	906	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>89% 8% ..</div>
1	E	906	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>90% 8% ..</div>
1	F	906	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>

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Mol	Chain	Length	Quality of chain
1	G	906	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>88%</div><div>9%</div><div>..</div></div></div>
1	H	906	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>89%</div><div>8%</div><div>..</div></div></div>
2	I	3	<div><div><div></div><div></div><div></div></div><div>67%</div><div>33%</div></div>
2	K	3	<div><div><div></div><div></div><div></div></div><div>33%</div><div>67%</div></div>
2	M	3	<div><div><div></div><div></div><div></div></div><div>33%</div><div>67%</div></div>
2	N	3	<div><div><div></div><div></div><div></div></div><div>67%</div><div>33%</div></div>
2	O	3	<div><div><div></div><div></div><div></div></div><div>67%</div><div>33%</div></div>
3	J	2	<div><div><div></div><div></div><div></div></div><div>100%</div></div>
3	L	2	<div><div><div></div><div></div><div></div></div><div>100%</div></div>
3	P	2	<div><div><div></div><div></div><div></div></div><div>100%</div></div>

## 2 Entry composition [i](#)

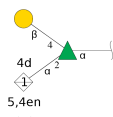
There are 5 unique types of molecules in this entry. The entry contains 57136 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Percglx protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	1	0
			7025	4479	1178	1362	6			
1	B	896	Total	C	N	O	S	0	2	0
			7052	4492	1182	1372	6			
1	C	885	Total	C	N	O	S	0	5	0
			7007	4473	1176	1352	6			
1	D	884	Total	C	N	O	S	0	6	0
			6992	4463	1174	1349	6			
1	E	900	Total	C	N	O	S	0	1	0
			7062	4497	1185	1374	6			
1	F	900	Total	C	N	O	S	0	0	0
			7040	4487	1183	1364	6			
1	G	886	Total	C	N	O	S	0	1	0
			6976	4452	1168	1351	5			
1	H	888	Total	C	N	O	S	0	1	0
			6997	4462	1174	1355	6			

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose.



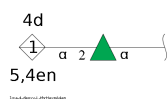
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	3	Total	C	O	0	0	0
			33	18	15			
2	K	3	Total	C	O	0	0	0
			33	18	15			
2	M	3	Total	C	O	0	0	0
			33	18	15			
2	N	3	Total	C	O	0	0	0
			33	18	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	O	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 3 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	J	2	Total	C	O	0	0	0
			22	12	10			
3	L	2	Total	C	O	0	0	0
			22	12	10			
3	P	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	H	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

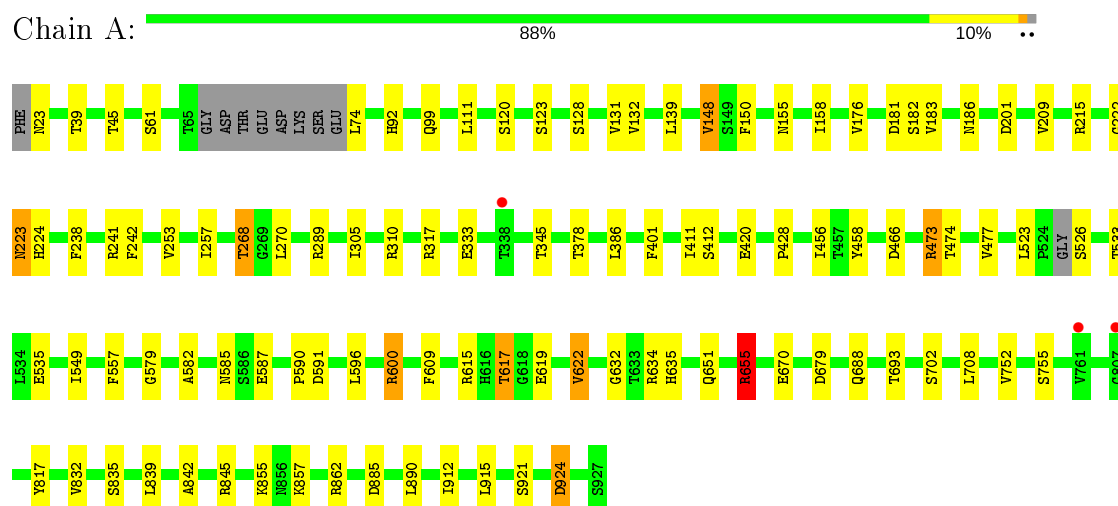
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total 119	O 119	0	0
5	B	108	Total 108	O 108	0	0
5	C	103	Total 103	O 103	0	0
5	D	92	Total 92	O 92	0	0
5	E	92	Total 92	O 92	0	0
5	F	98	Total 98	O 98	0	0
5	G	72	Total 72	O 72	0	0
5	H	62	Total 62	O 62	0	0

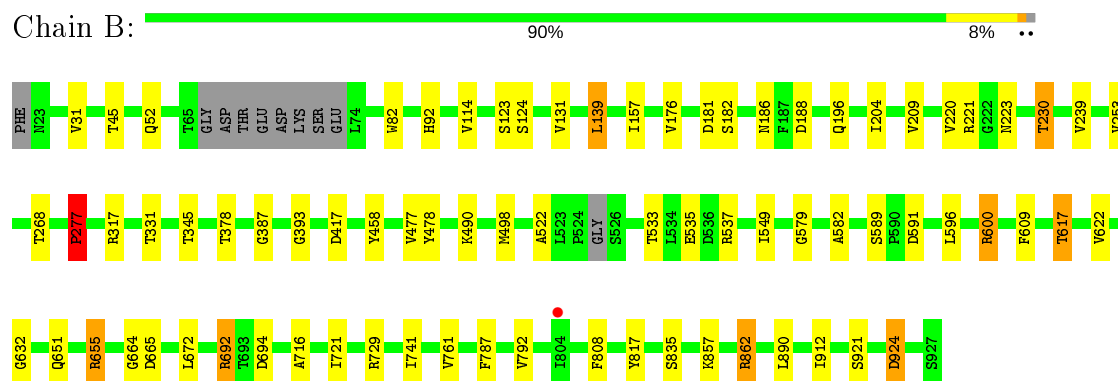
### 3 Residue-property plots

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.

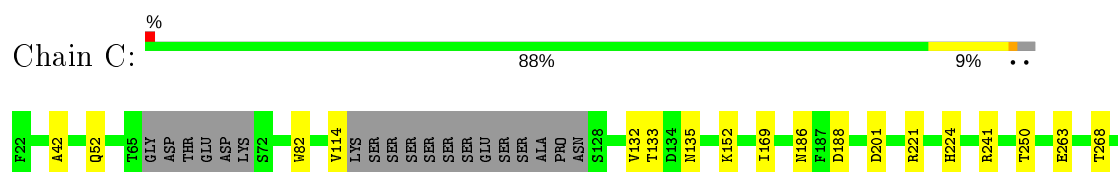
#### • Molecule 1: Pcrglx protein

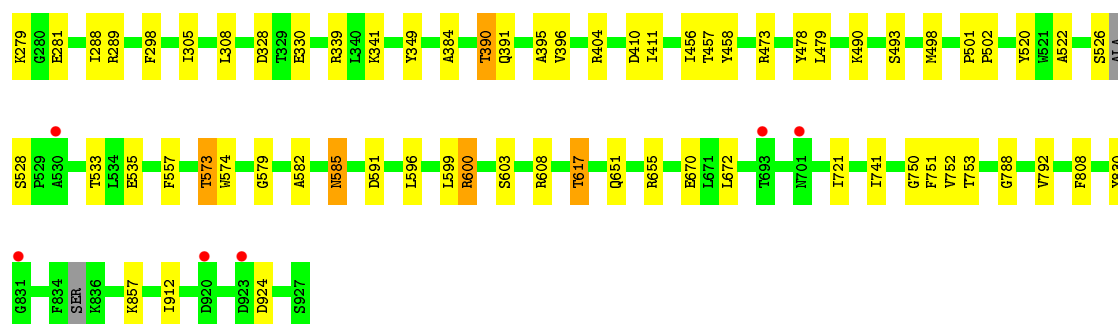


#### • Molecule 1: Pcrglx protein

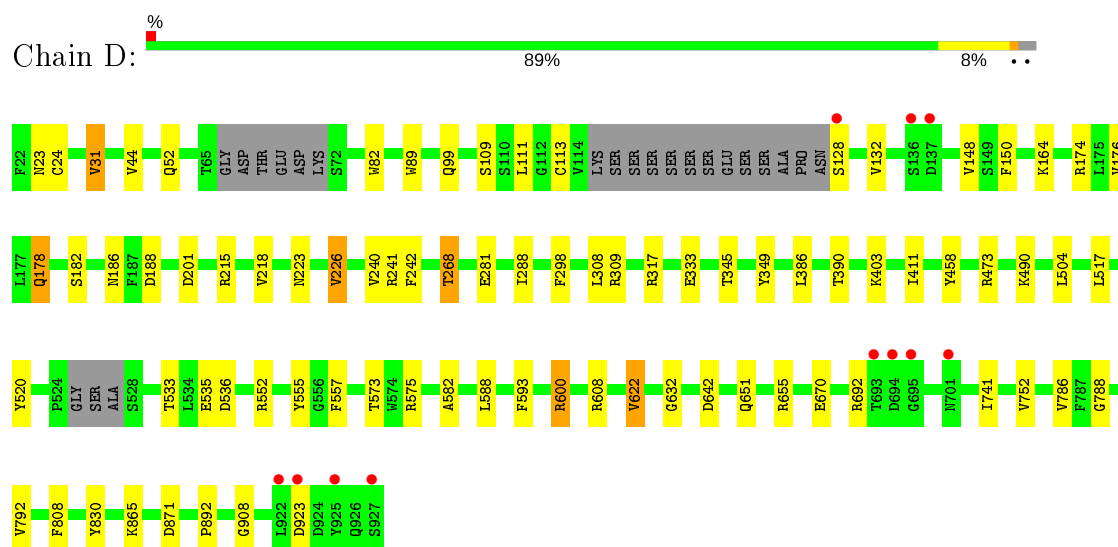


#### • Molecule 1: Pcrglx protein

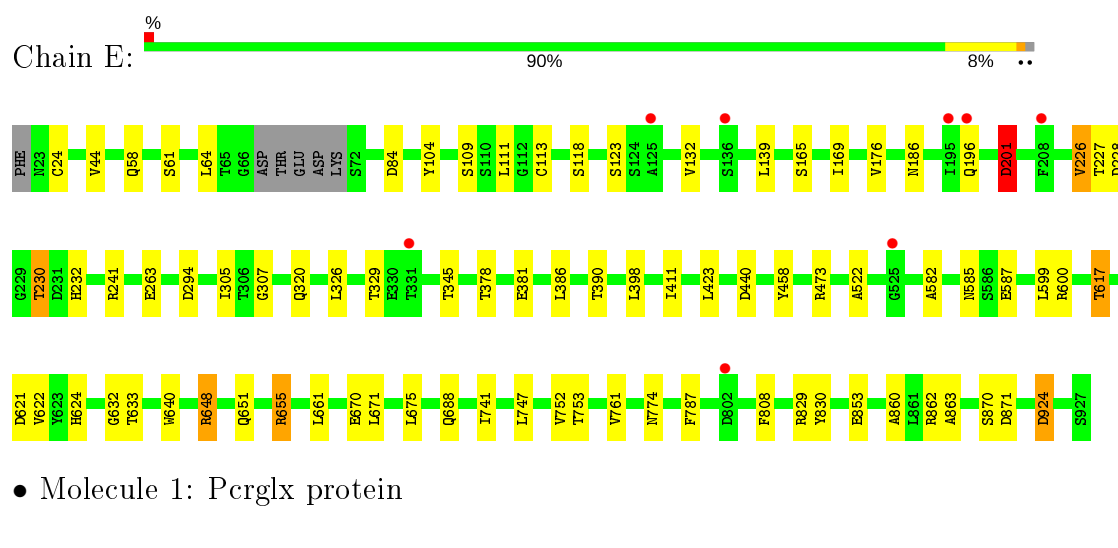




• Molecule 1: Pcrglx protein



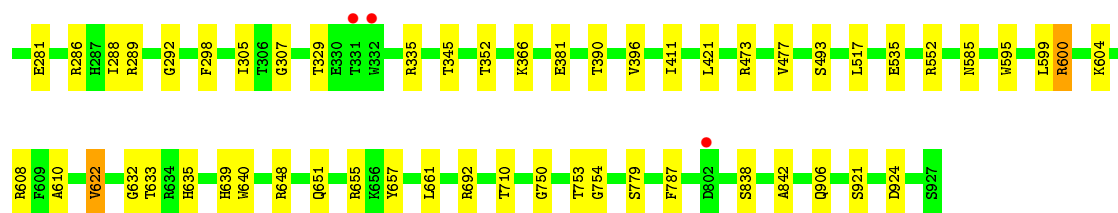
• Molecule 1: Pcrglx protein



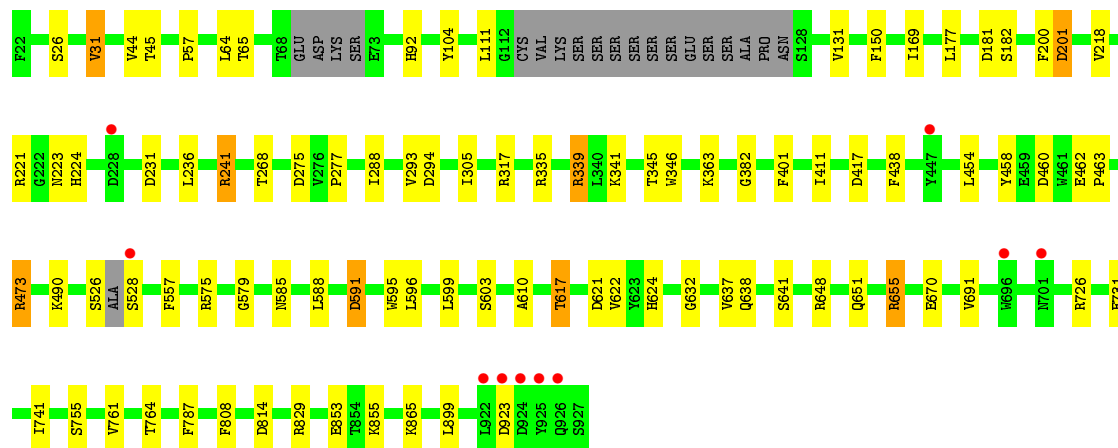
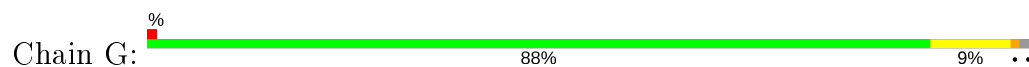
Chain F:



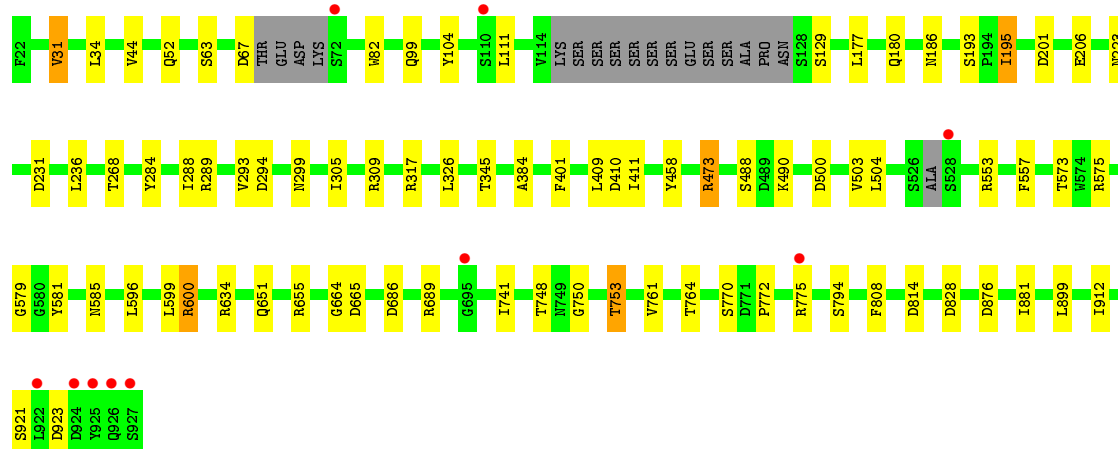
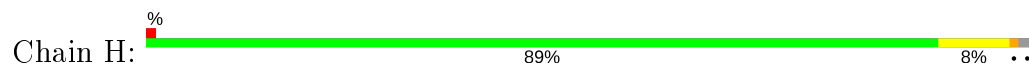




• Molecule 1: Pcrglx protein



• Molecule 1: Pcrglx protein



• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose



- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain K:  33% 67%

RAM1  
GAD2  
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain M:  33% 67%

RAM1  
GAD2  
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain N:  67% 33%

RAM1  
GAD2  
GAL3

- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-[beta-D-galactopyranose-(1-4)]alpha-L-rhamnopyranose

Chain O:  67% 33%

RAM1  
GAD2  
GAL3

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain J:  100%

RAM1  
GAD2

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain L:  100%

RAM1  
GAD2

- Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain P:  100%

RAM  
GAD2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.62Å 171.80Å 342.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.17 – 2.75 49.12 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (171.17-2.75) 99.9 (49.12-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.61 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.196 , 0.262 0.200 , 0.261	Depositor DCC
$R_{free}$ test set	12900 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 25.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	57136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4459e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: RAM, CA, GAD, GAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.73	0/7232	0.88	14/9878 (0.1%)
1	B	0.73	0/7256	0.87	11/9907 (0.1%)
1	C	0.70	0/7223	0.84	5/9857 (0.1%)
1	D	0.71	0/7218	0.86	16/9854 (0.2%)
1	E	0.71	0/7270	0.84	7/9925 (0.1%)
1	F	0.72	0/7245	0.88	10/9892 (0.1%)
1	G	0.69	0/7183	0.86	13/9804 (0.1%)
1	H	0.71	0/7204	0.87	15/9833 (0.2%)
All	All	0.71	0/57831	0.86	91/78950 (0.1%)

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	F	552	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	E	924	ASP	CB-CG-OD1	7.73	125.26	118.30
1	G	317	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	692	ARG	NE-CZ-NH1	7.42	124.01	120.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7025	0	6584	41	0
1	B	7052	0	6618	30	0
1	C	7007	0	6588	35	0
1	D	6992	0	6570	27	0
1	E	7062	0	6638	32	0
1	F	7040	0	6601	24	0
1	G	6976	0	6539	37	0
1	H	6997	0	6567	35	0
2	I	33	0	26	2	0
2	K	33	0	25	0	0
2	M	33	0	26	3	0
2	N	33	0	26	1	0
2	O	33	0	25	1	0
3	J	22	0	17	0	0
3	L	22	0	17	0	0
3	P	22	0	17	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	119	0	0	4	0
5	B	108	0	0	0	0
5	C	103	0	0	3	0
5	D	92	0	0	0	0
5	E	92	0	0	3	0
5	F	98	0	0	1	0
5	G	72	0	0	1	0
5	H	62	0	0	0	0
All	All	57136	0	52884	256	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 256 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:CYS:SG	1:D:113:CYS:CB	2.21	1.27
1:H:180:GLN:CD	1:H:195:ILE:CD1	2.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:CYS:CB	1:D:113:CYS:SG	2.67	0.83
1:C:526:SER:O	1:C:528:SER:N	2.17	0.78
1:F:73:GLU:CA	5:F:1191:HOH:O	2.32	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	891/906 (98%)	852 (96%)	35 (4%)	4 (0%)	34	53
1	B	892/906 (98%)	846 (95%)	42 (5%)	4 (0%)	34	53
1	C	880/906 (97%)	841 (96%)	35 (4%)	4 (0%)	29	47
1	D	882/906 (97%)	831 (94%)	49 (6%)	2 (0%)	47	69
1	E	897/906 (99%)	842 (94%)	48 (5%)	7 (1%)	19	34
1	F	896/906 (99%)	849 (95%)	42 (5%)	5 (1%)	25	42
1	G	879/906 (97%)	836 (95%)	40 (5%)	3 (0%)	41	60
1	H	881/906 (97%)	831 (94%)	47 (5%)	3 (0%)	41	60
All	All	7098/7248 (98%)	6728 (95%)	338 (5%)	32 (0%)	29	47

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	263	GLU
1	B	579	GLY
1	C	750	GLY
1	E	232	HIS
1	E	774	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	724/745 (97%)	687 (95%)	37 (5%)	24	41
1	B	731/745 (98%)	705 (96%)	26 (4%)	35	55
1	C	726/745 (97%)	703 (97%)	23 (3%)	39	59
1	D	724/745 (97%)	692 (96%)	32 (4%)	28	47
1	E	733/745 (98%)	701 (96%)	32 (4%)	28	47
1	F	724/745 (97%)	695 (96%)	29 (4%)	31	51
1	G	719/745 (96%)	691 (96%)	28 (4%)	32	52
1	H	724/745 (97%)	692 (96%)	32 (4%)	28	47
All	All	5805/5960 (97%)	5566 (96%)	239 (4%)	30	50

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	490	LYS
1	E	186	ASN
1	H	268	THR
1	D	573	THR
1	E	58[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	688	GLN
1	D	515	GLN
1	H	98	ASN
1	D	23	ASN
1	D	203	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

21 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	RAM	I	1	2	11,11,11	0.75	0	15,16,16	1.55	2 (13%)
2	GAD	I	2	2	7,11,11	2.32	2 (28%)	8,15,15	2.51	2 (25%)
2	GAL	I	3	2	11,11,12	1.21	1 (9%)	15,15,17	3.17	6 (40%)
3	RAM	J	1	3	11,11,11	0.66	0	15,16,16	1.62	2 (13%)
3	GAD	J	2	3	7,11,11	2.61	2 (28%)	8,15,15	2.73	2 (25%)
2	RAM	K	1	2	11,11,11	0.66	0	15,16,16	0.70	0
2	GAD	K	2	2	7,11,11	3.16	2 (28%)	8,15,15	2.91	3 (37%)
2	GAL	K	3	2	11,11,12	0.69	0	15,15,17	1.83	5 (33%)
3	RAM	L	1	3	11,11,11	0.95	0	15,16,16	1.21	1 (6%)
3	GAD	L	2	3	7,11,11	2.86	2 (28%)	8,15,15	2.52	3 (37%)
2	RAM	M	1	2	11,11,11	0.69	0	15,16,16	1.48	2 (13%)
2	GAD	M	2	2	7,11,11	2.89	2 (28%)	8,15,15	2.42	2 (25%)
2	GAL	M	3	2	11,11,12	0.88	0	15,15,17	2.86	5 (33%)
2	RAM	N	1	2	11,11,11	0.56	0	15,16,16	1.52	3 (20%)
2	GAD	N	2	2	7,11,11	3.18	3 (42%)	8,15,15	3.30	4 (50%)
2	GAL	N	3	2	11,11,12	0.96	0	15,15,17	1.70	2 (13%)
2	RAM	O	1	2	11,11,11	0.82	0	15,16,16	1.14	1 (6%)
2	GAD	O	2	2	7,11,11	2.59	2 (28%)	8,15,15	2.18	3 (37%)
2	GAL	O	3	1,2	11,11,12	1.80	2 (18%)	15,15,17	3.40	8 (53%)
3	RAM	P	1	3	11,11,11	0.94	0	15,16,16	1.83	3 (20%)
3	GAD	P	2	3	7,11,11	2.77	3 (42%)	8,15,15	3.14	3 (37%)

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	RAM	I	1	2	-	-	0/1/1/1
2	GAD	I	2	2	-	0/0/17/17	0/1/1/1
2	GAL	I	3	2	-	1/2/19/22	0/1/1/1
3	RAM	J	1	3	-	-	0/1/1/1
3	GAD	J	2	3	-	0/0/17/17	0/1/1/1
2	RAM	K	1	2	-	-	0/1/1/1
2	GAD	K	2	2	-	0/0/17/17	0/1/1/1
2	GAL	K	3	2	-	2/2/19/22	0/1/1/1
3	RAM	L	1	3	-	-	0/1/1/1
3	GAD	L	2	3	-	0/0/17/17	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	GAD	M	2	2	-	0/0/17/17	0/1/1/1
2	GAL	M	3	2	-	0/2/19/22	0/1/1/1
2	RAM	N	1	2	-	-	0/1/1/1
2	GAD	N	2	2	-	0/0/17/17	0/1/1/1
2	GAL	N	3	2	-	2/2/19/22	0/1/1/1
2	RAM	O	1	2	-	-	0/1/1/1
2	GAD	O	2	2	-	0/0/17/17	0/1/1/1
2	GAL	O	3	1,2	-	0/2/19/22	0/1/1/1
3	RAM	P	1	3	-	-	0/1/1/1
3	GAD	P	2	3	-	0/0/17/17	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	GAD	O5-C5	6.93	1.47	1.37
2	M	2	GAD	O5-C5	6.51	1.46	1.37
3	L	2	GAD	O5-C5	6.50	1.46	1.37
2	N	2	GAD	O5-C5	6.38	1.46	1.37
2	O	2	GAD	O5-C5	5.89	1.45	1.37

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	GAL	C1-O5-C5	7.42	122.25	112.19
2	O	3	GAL	C1-O5-C5	7.29	122.07	112.19
2	N	2	GAD	O5-C5-C4	-7.26	118.68	124.81
3	P	2	GAD	O5-C5-C4	-7.20	118.73	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	GAD	O5-C5-C4	-7.12	118.80	124.81

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	3	GAL	O5-C5-C6-O6
2	K	3	GAL	C4-C5-C6-O6
2	K	3	GAL	O5-C5-C6-O6
2	N	3	GAL	C4-C5-C6-O6
2	I	3	GAL	O5-C5-C6-O6

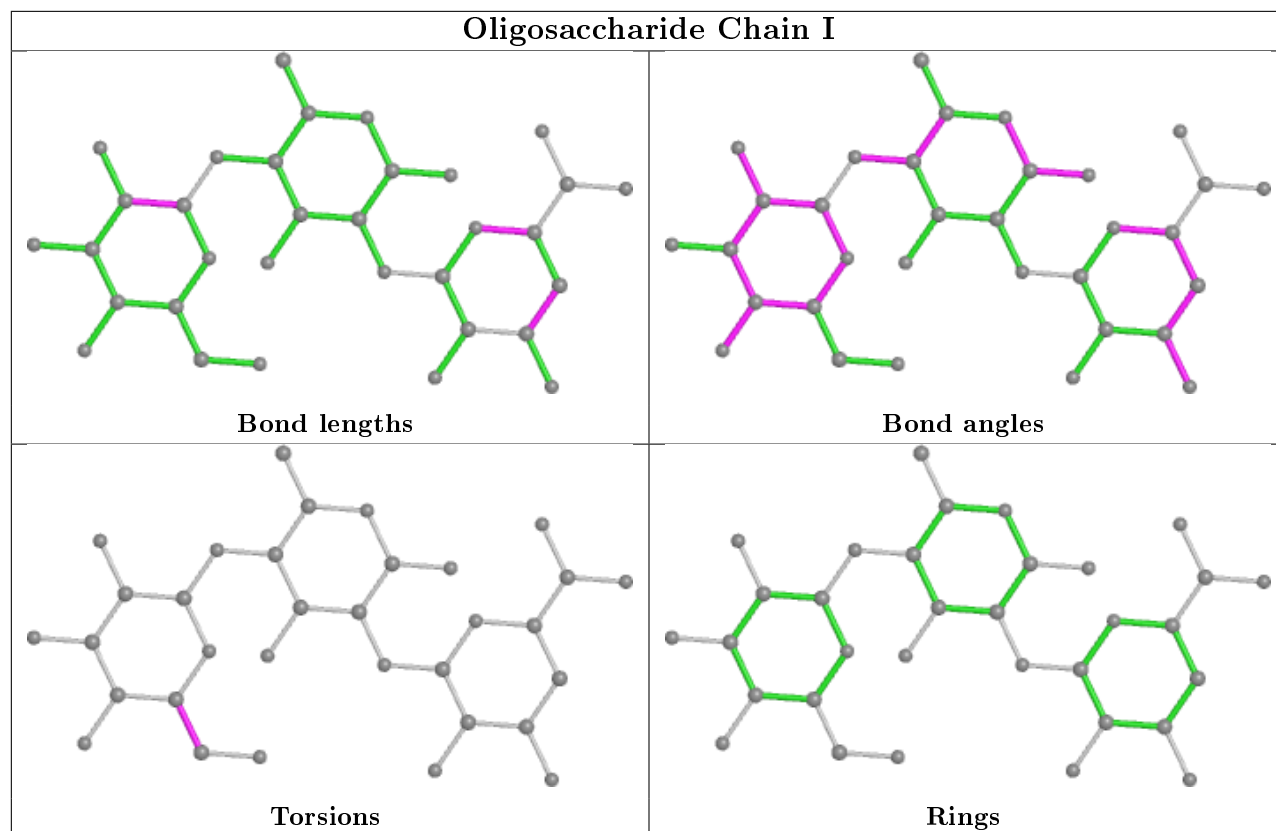
There are no ring outliers.

5 monomers are involved in 7 short contacts:

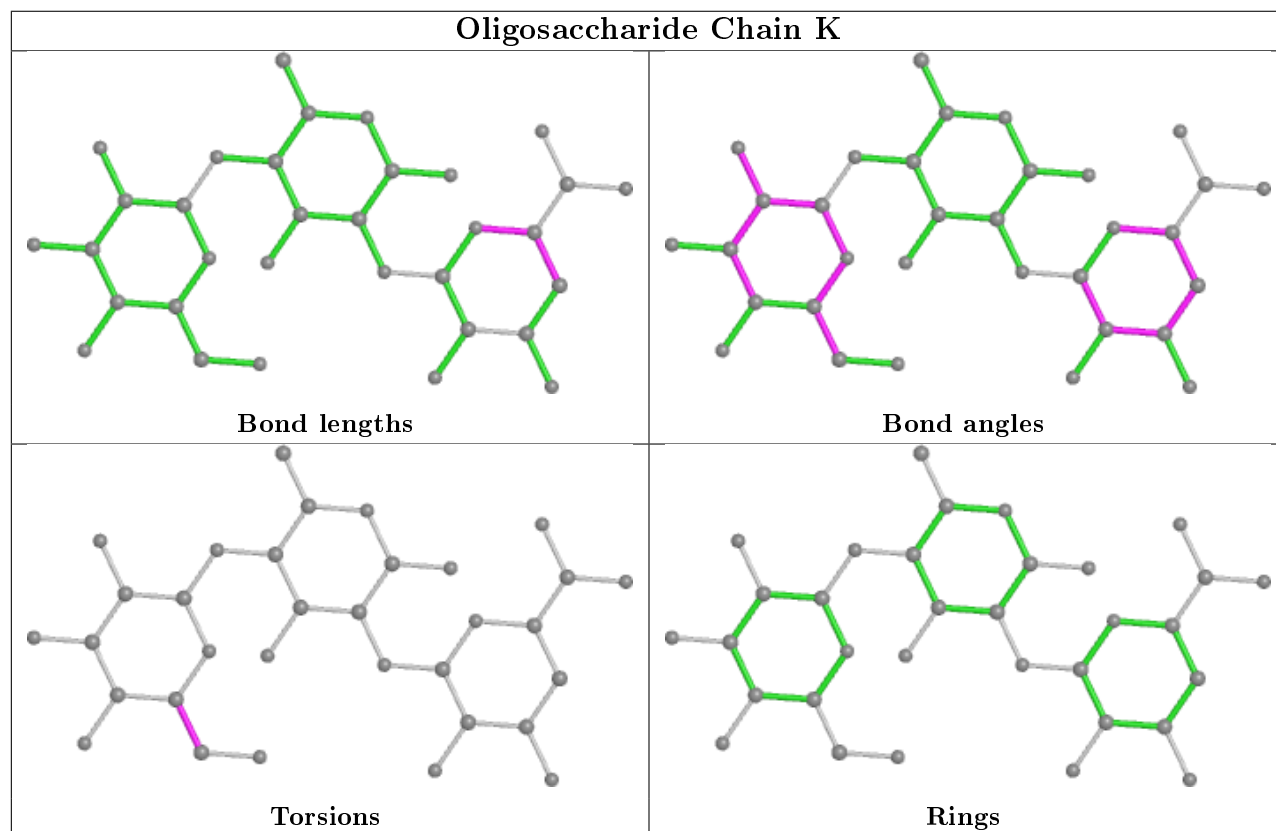
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	GAD	1	0
2	I	3	GAL	2	0
2	N	3	GAL	1	0
2	M	3	GAL	2	0
2	O	3	GAL	1	0

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

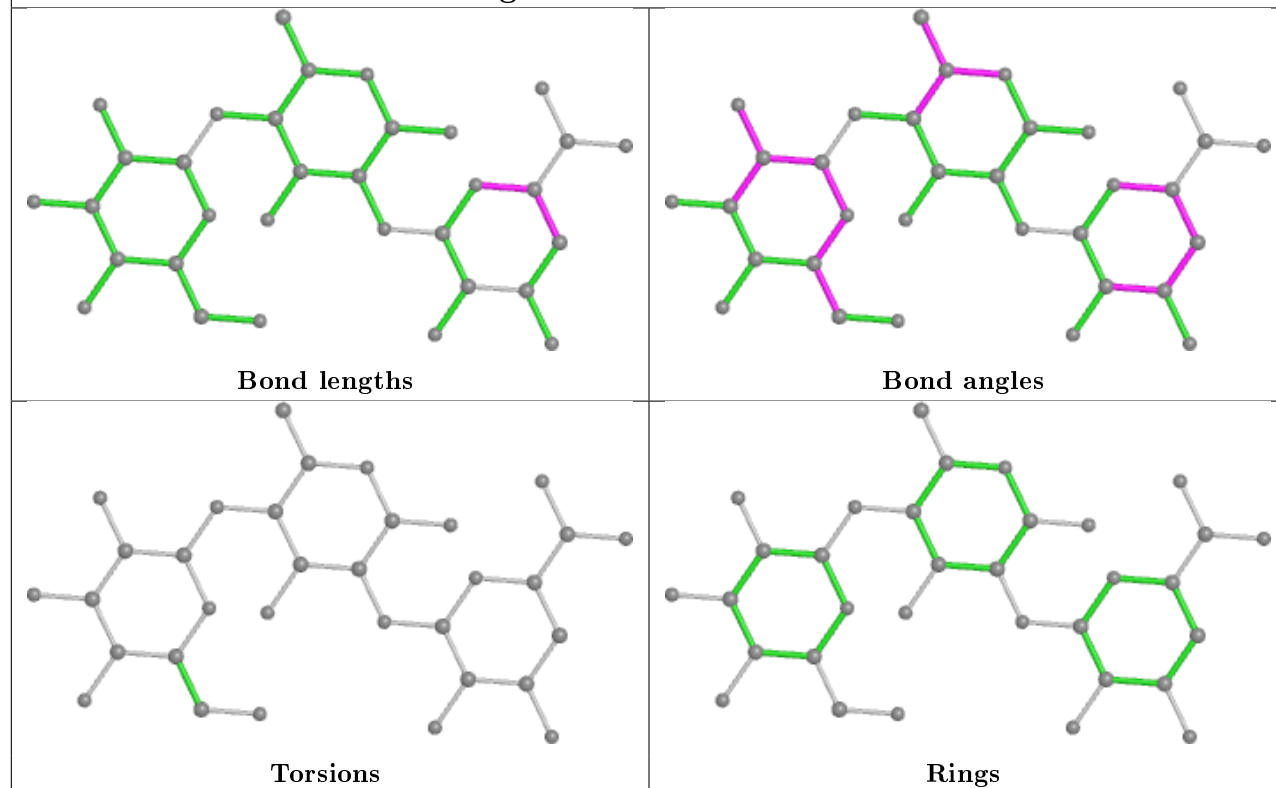
## Oligosaccharide Chain I



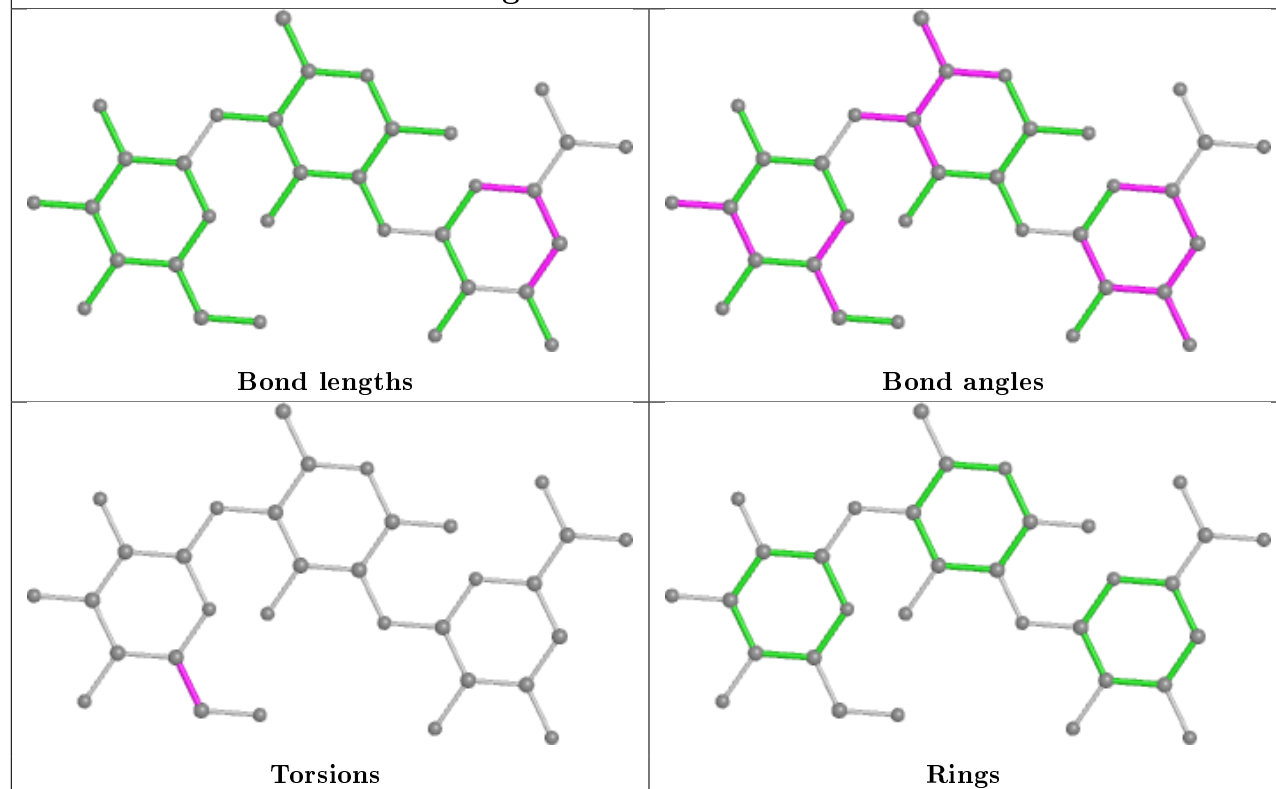
## Oligosaccharide Chain K

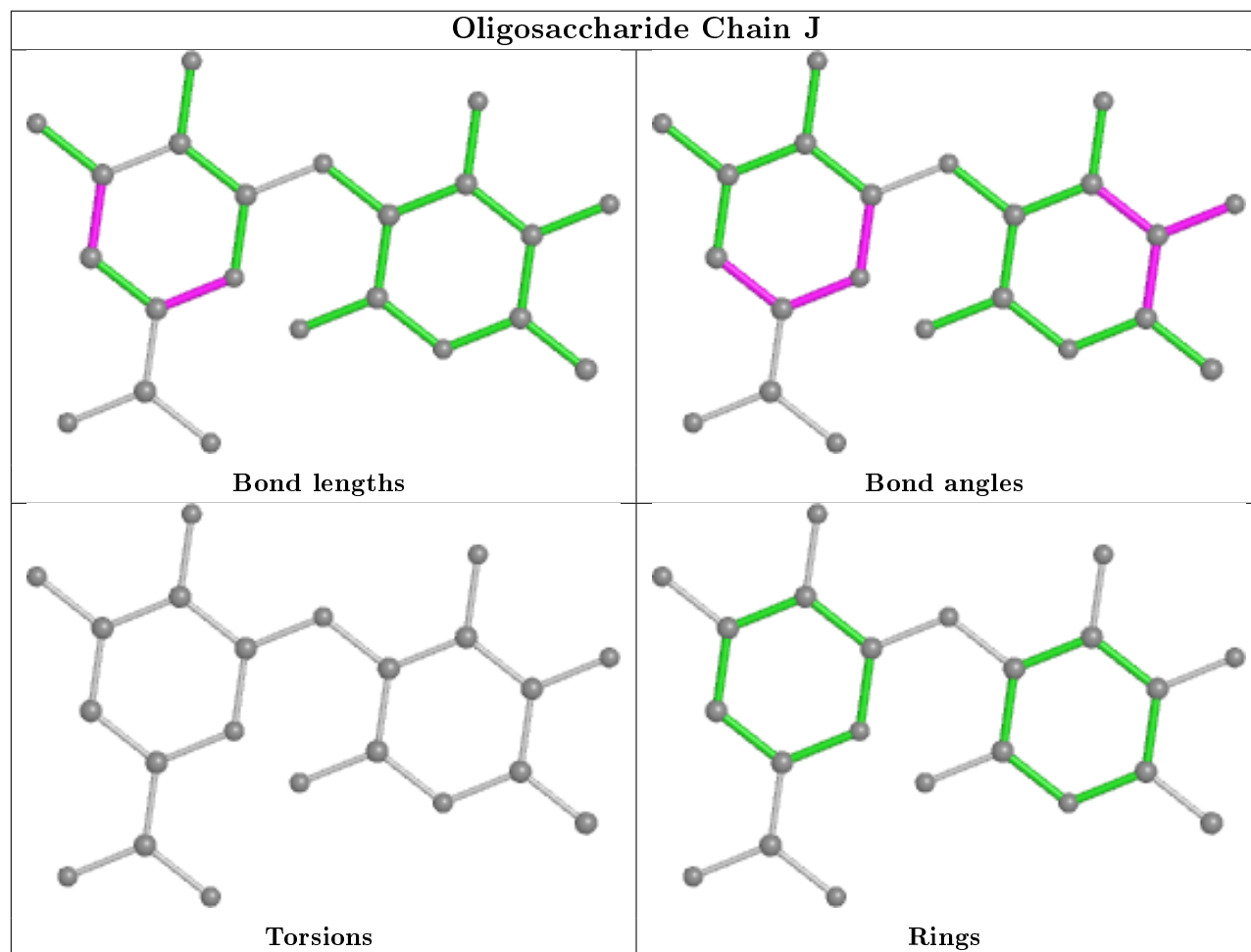
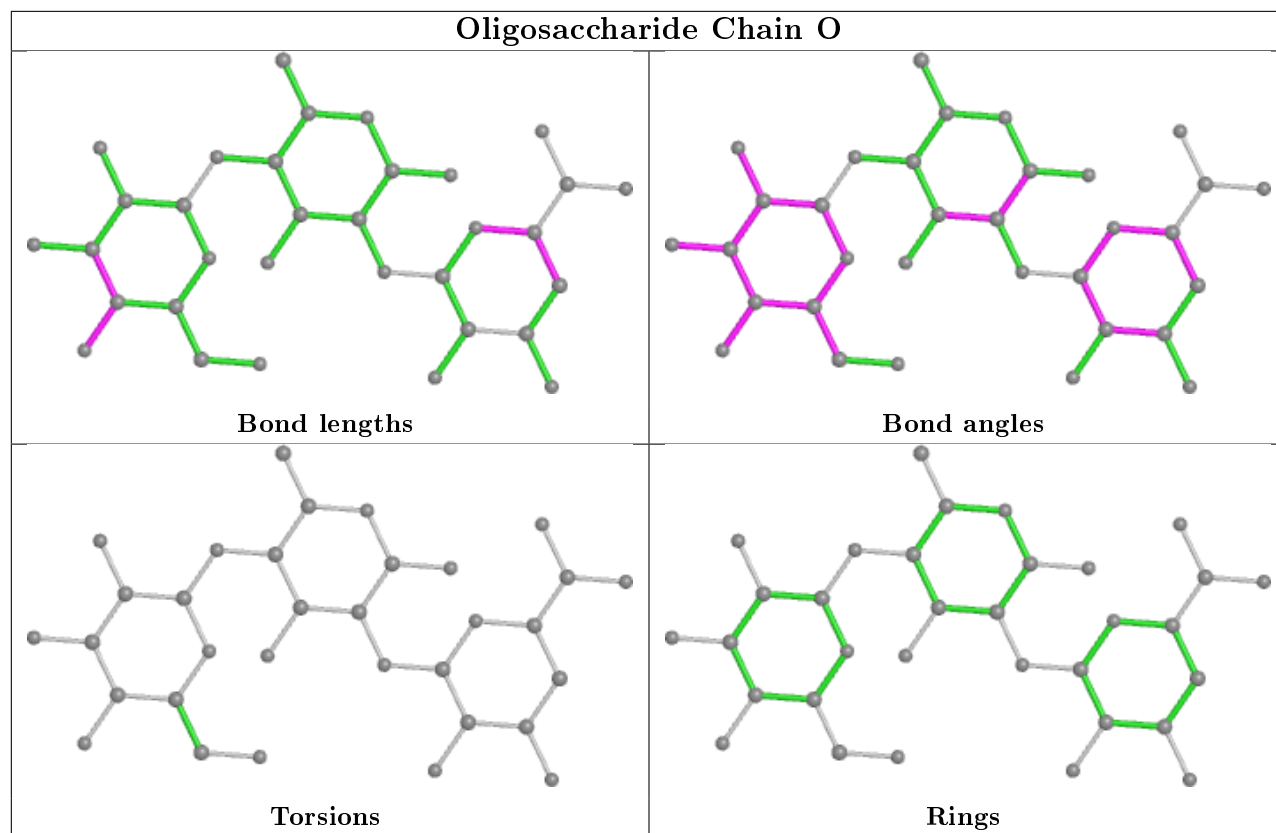


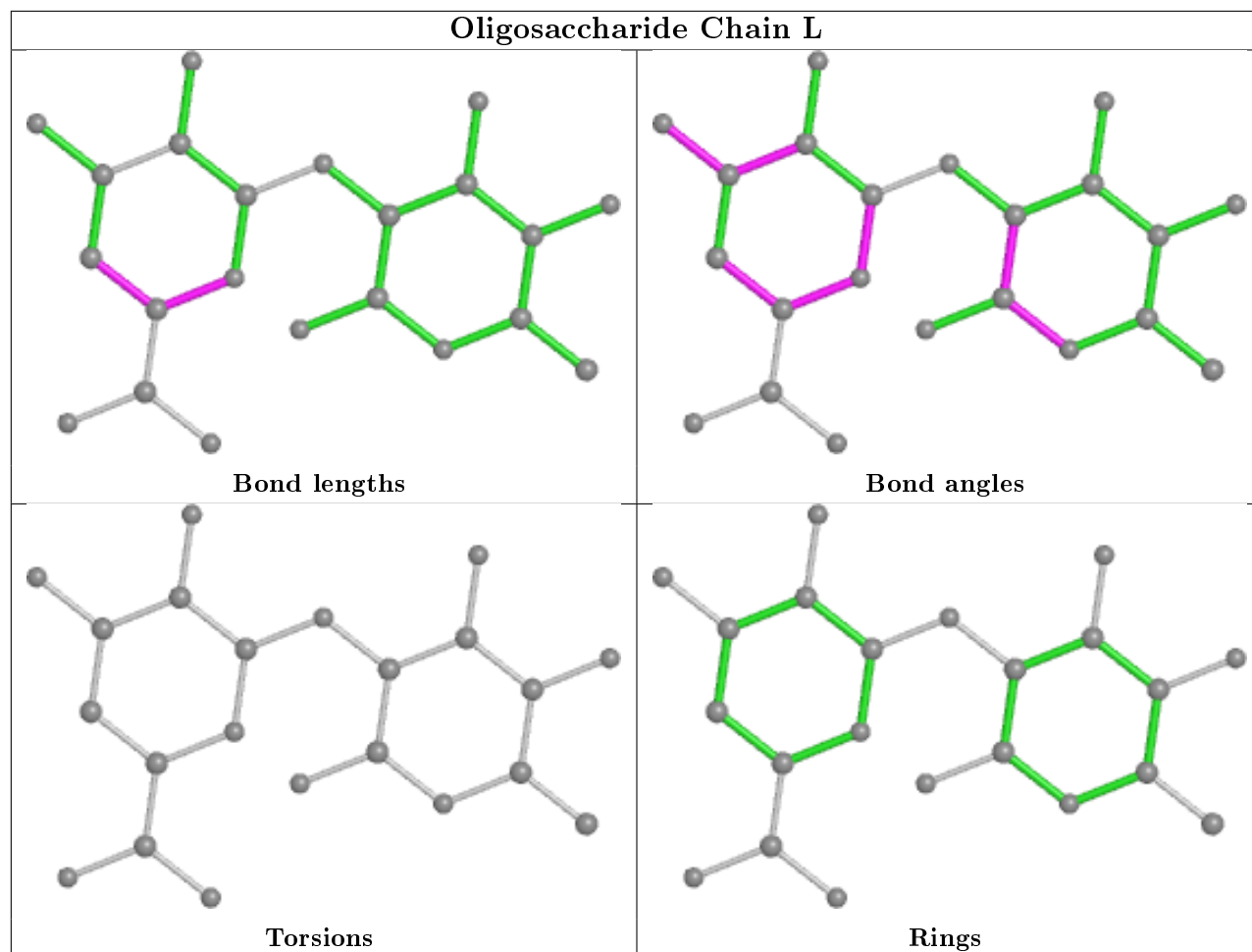
## Oligosaccharide Chain M

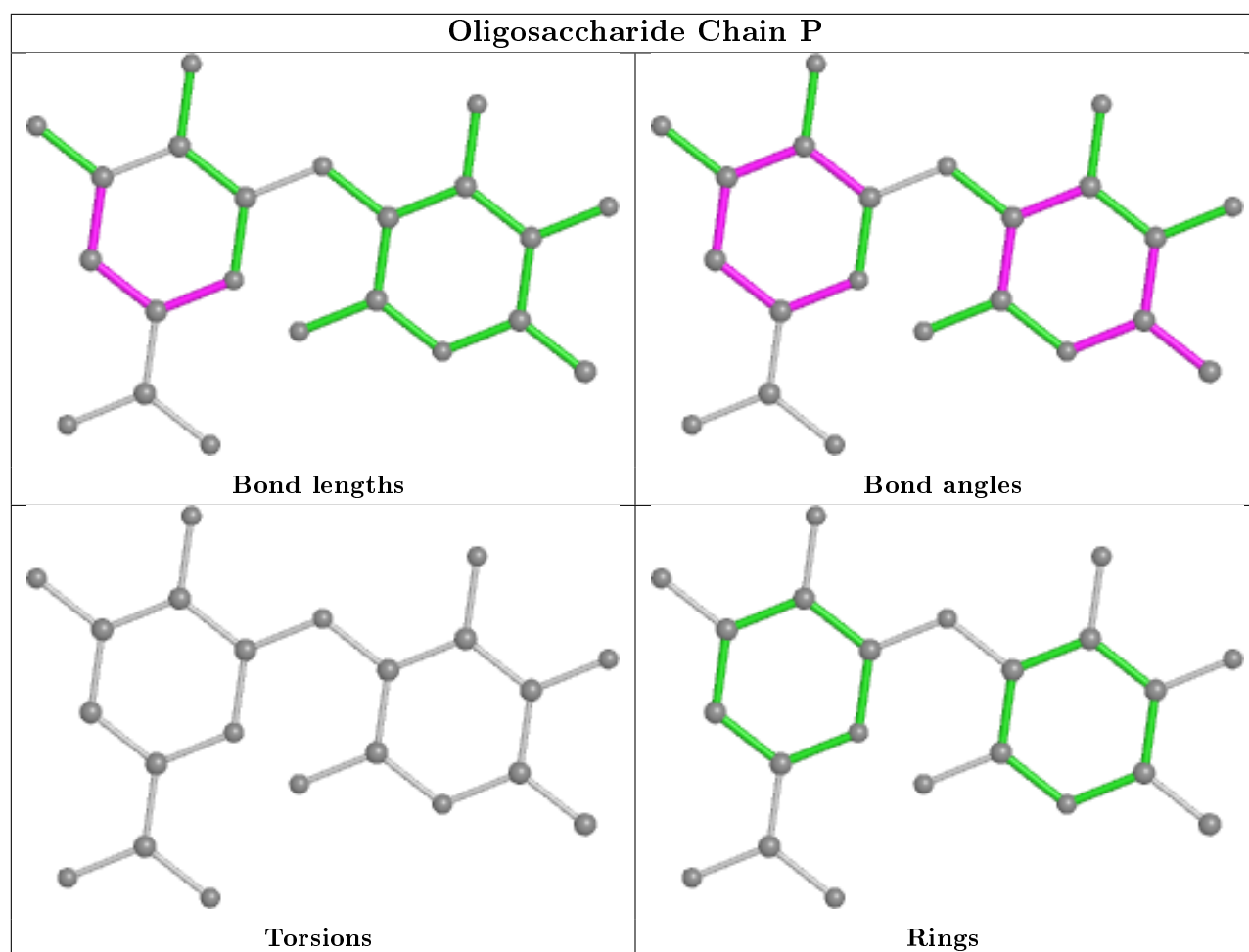


## Oligosaccharide Chain N









## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	896/906 (98%)	-0.35	3 (0%) 94 96	21, 33, 52, 76	0
1	B	896/906 (98%)	-0.34	1 (0%) 95 97	20, 32, 51, 78	0
1	C	885/906 (97%)	-0.31	6 (0%) 87 91	22, 35, 55, 81	0
1	D	884/906 (97%)	-0.28	11 (1%) 79 85	20, 37, 58, 81	0
1	E	900/906 (99%)	-0.26	8 (0%) 84 89	23, 36, 57, 84	0
1	F	900/906 (99%)	-0.33	4 (0%) 92 95	22, 34, 56, 79	0
1	G	886/906 (97%)	-0.19	10 (1%) 80 86	21, 39, 65, 86	0
1	H	888/906 (98%)	-0.17	10 (1%) 80 86	19, 39, 66, 90	0
All	All	7135/7248 (98%)	-0.28	53 (0%) 87 91	19, 35, 59, 90	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	923	ASP	3.7
1	F	23	ASN	3.6
1	G	926	GLN	3.5
1	A	761	VAL	3.4
1	D	693	THR	3.3

### 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,

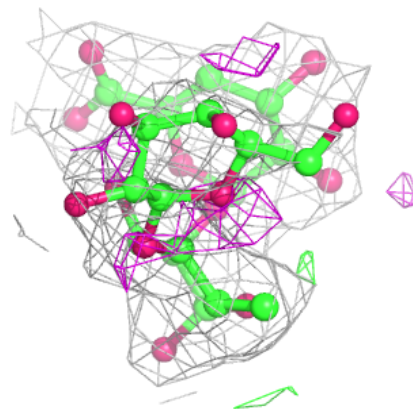
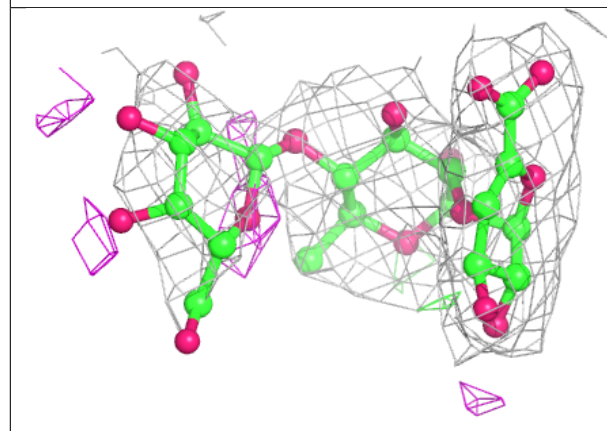
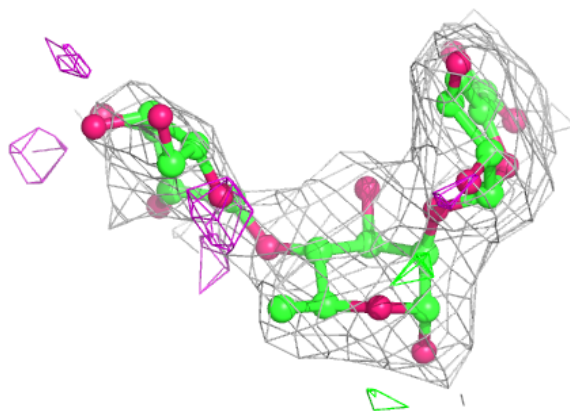
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GAL	O	3	11/12	0.79	0.38	71,79,95,96	0
2	GAL	N	3	11/12	0.80	0.43	70,78,88,89	0
2	GAL	K	3	11/12	0.88	0.41	82,94,105,107	0
2	GAL	M	3	11/12	0.89	0.28	52,60,76,77	0
2	GAL	I	3	11/12	0.90	0.42	59,63,68,68	0
2	GAD	K	2	11/11	0.93	0.14	49,53,55,58	0
2	GAD	O	2	11/11	0.94	0.17	46,57,62,64	0
3	GAD	L	2	11/11	0.94	0.13	47,57,62,65	0
3	GAD	P	2	11/11	0.94	0.18	46,52,55,56	0
2	RAM	K	1	11/11	0.95	0.18	63,67,73,78	0
2	RAM	O	1	11/11	0.95	0.16	49,61,68,69	0
3	RAM	P	1	11/11	0.95	0.14	45,55,60,64	0
2	GAD	N	2	11/11	0.95	0.15	37,47,51,51	0
2	RAM	M	1	11/11	0.95	0.14	37,41,51,51	0
2	GAD	M	2	11/11	0.95	0.14	43,48,49,50	0
3	RAM	L	1	11/11	0.96	0.14	48,52,57,65	0
2	RAM	N	1	11/11	0.96	0.13	43,47,52,58	0
3	RAM	J	1	11/11	0.96	0.12	30,32,35,36	0
2	RAM	I	1	11/11	0.96	0.14	34,35,39,46	0
3	GAD	J	2	11/11	0.97	0.11	29,37,42,44	0
2	GAD	I	2	11/11	0.97	0.13	33,37,38,46	0

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

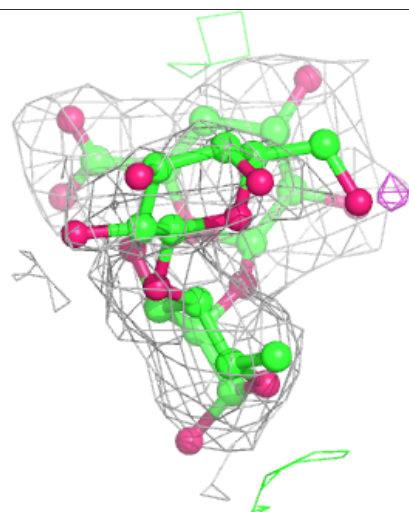
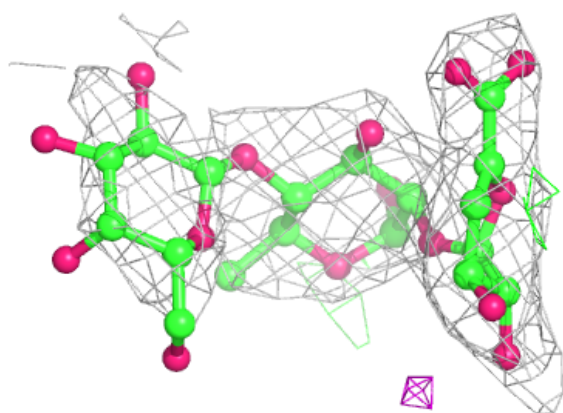
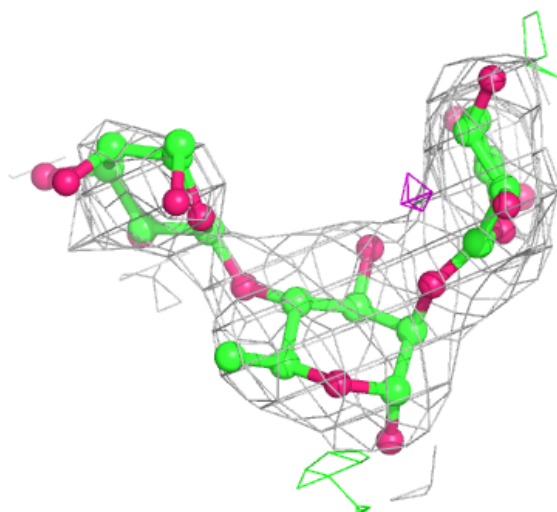
**Electron density around Chain I:**

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



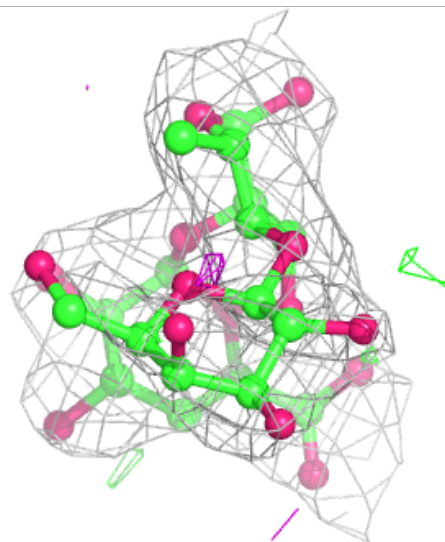
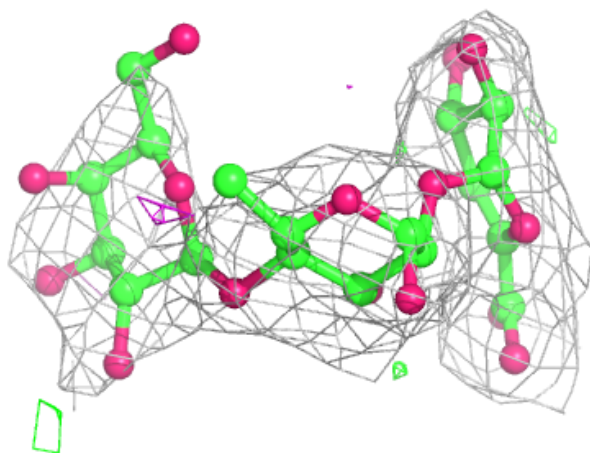
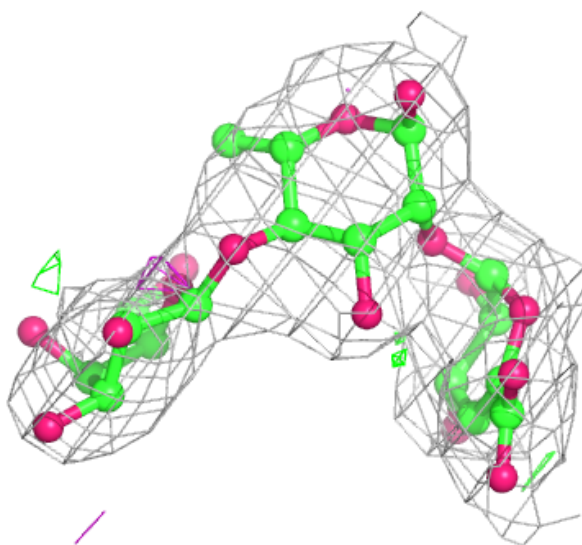
**Electron density around Chain K:**

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



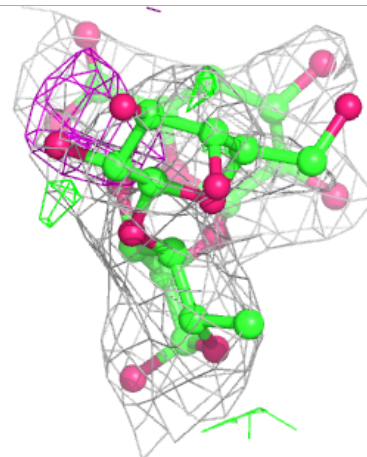
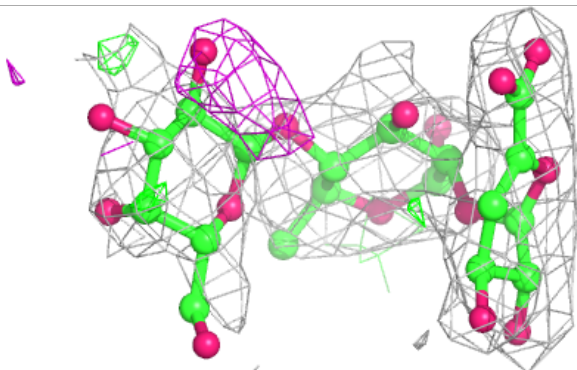
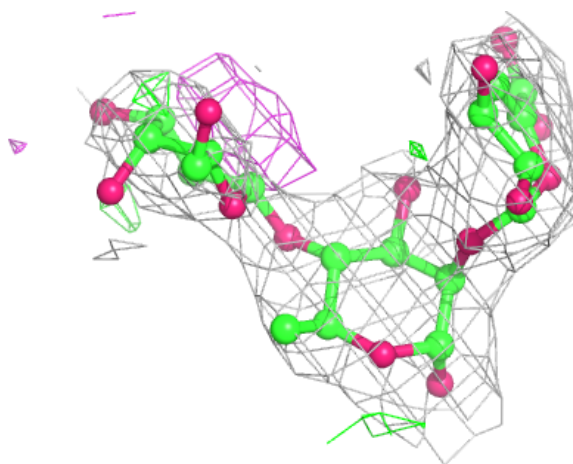
**Electron density around Chain M:**

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



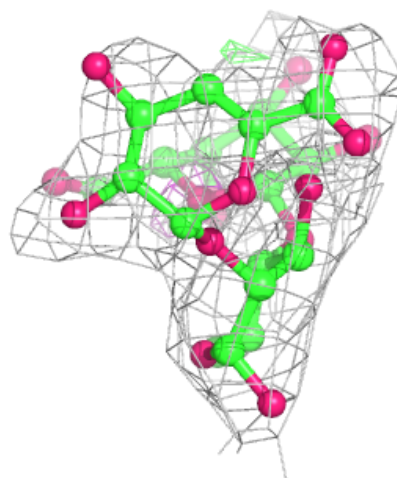
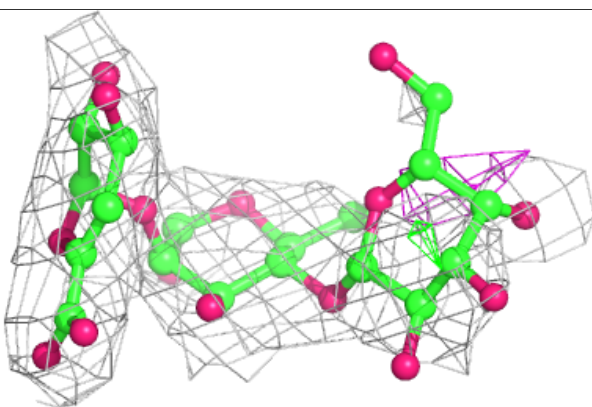
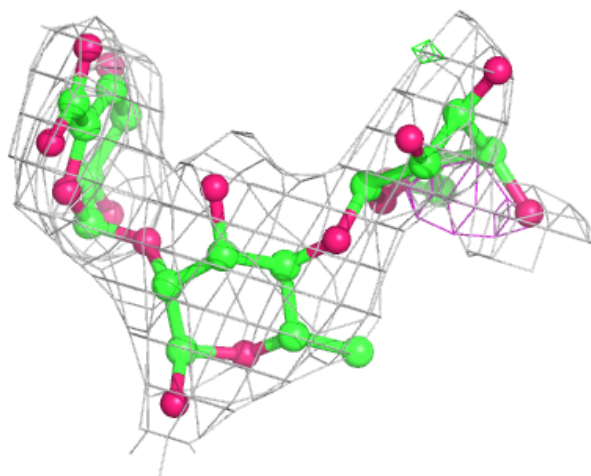
**Electron density around Chain N:**

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



**Electron density around Chain O:**

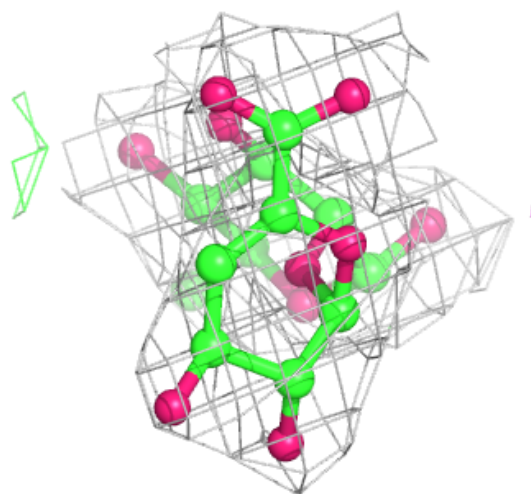
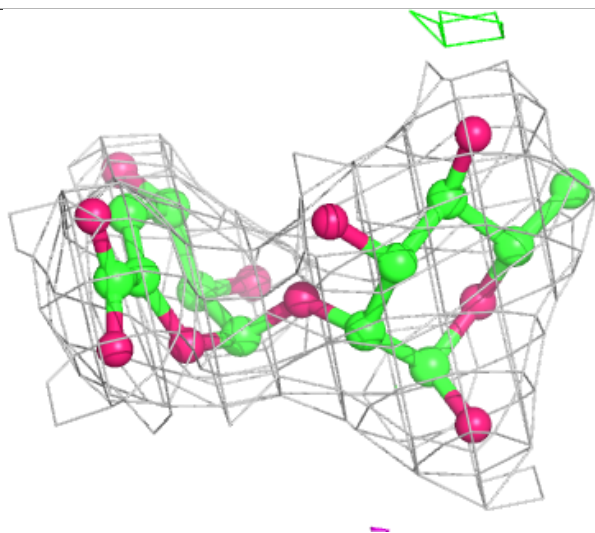
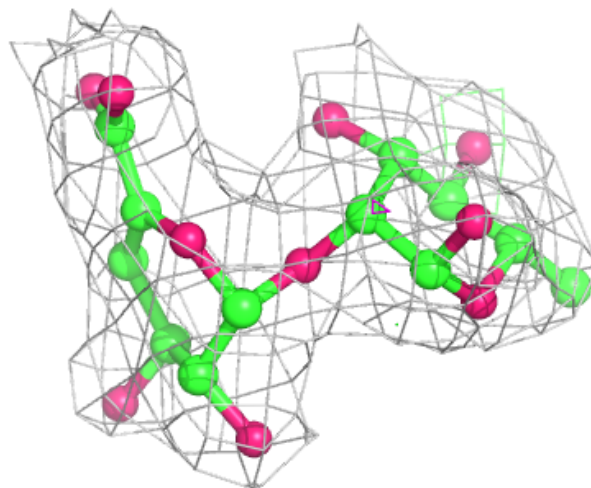
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





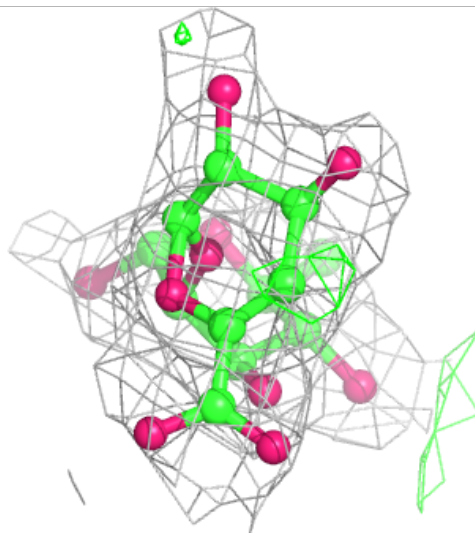
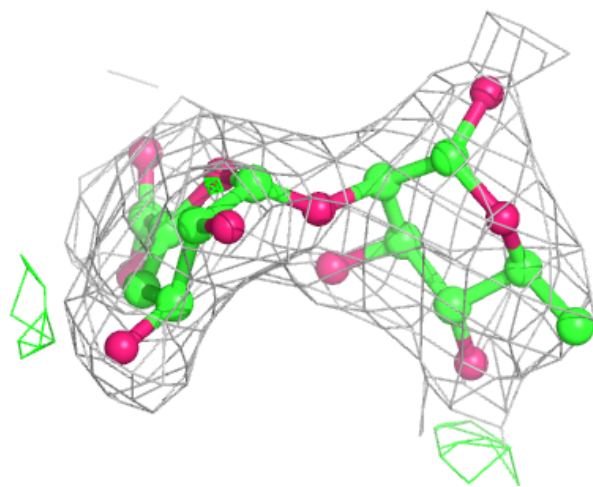
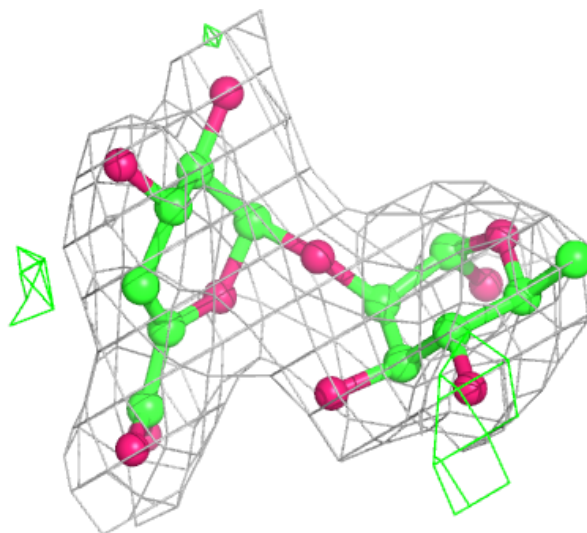
**Electron density around Chain J:**

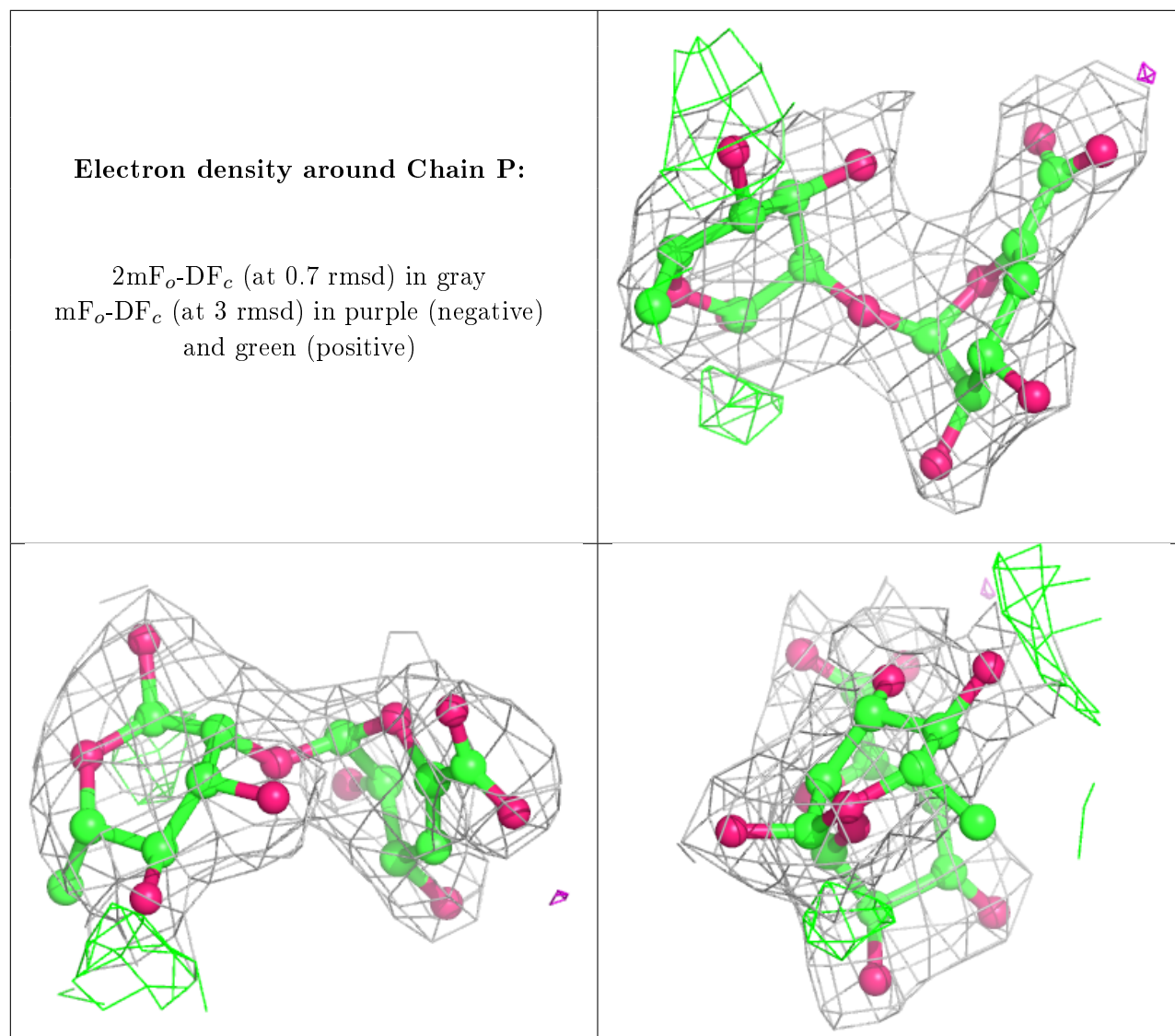
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

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





## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	E	1004	1/1	0.97	0.19	20,20,20,20	0
4	CA	F	1004	1/1	0.98	0.18	19,19,19,19	0
4	CA	A	1004	1/1	0.98	0.17	15,15,15,15	0
4	CA	H	1003	1/1	0.98	0.19	22,22,22,22	0
4	CA	G	1004	1/1	0.99	0.17	23,23,23,23	0
4	CA	B	1003	1/1	0.99	0.17	16,16,16,16	0
4	CA	C	1004	1/1	1.00	0.17	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	D	1003	1/1	1.00	0.18	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.