



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 08:46 PM BST

PDB ID : 6F7K  
Title : Crystal structure of Dettilon tailspike protein (gp208)  
Authors : Roske, Y.; Heinemann, U.  
Deposited on : 2017-12-11  
Resolution : 2.10 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

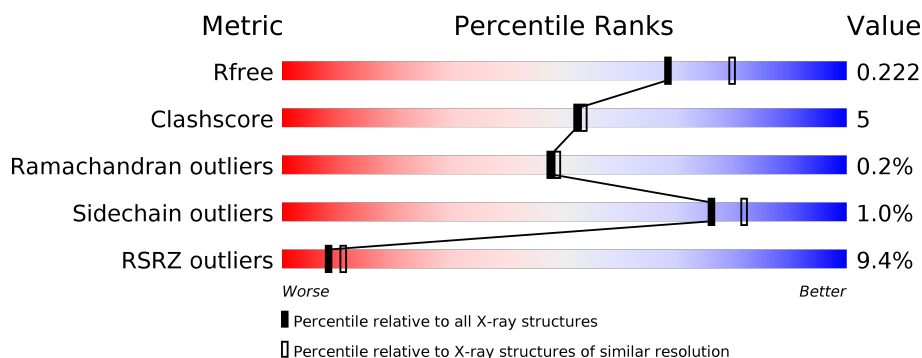
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	547	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
1	B	547	<div> <div>10%</div> <div>88%</div> <div>12%</div> </div>
1	C	547	<div> <div>10%</div> <div>89%</div> <div>11%</div> </div>
1	D	547	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
1	F	547	<div> <div>9%</div> <div>85%</div> <div>15%</div> </div>
1	G	547	<div> <div>11%</div> <div>89%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	6	 67%33%
2	H	6	 100%
2	K	6	 100%
2	L	6	 100%
2	M	6	 100%
3	I	4	 75%25%
4	J	2	 50%50%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26526 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.

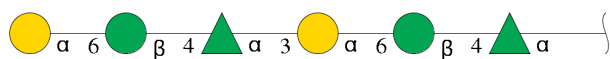
- Molecule 1 is a protein called Tailspike.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	2	0
			4086	2563	687	820	16			
1	B	547	Total	C	N	O	S	0	2	0
			4092	2565	688	822	17			
1	C	547	Total	C	N	O	S	0	1	0
			4089	2563	688	821	17			
1	D	547	Total	C	N	O	S	0	2	0
			4094	2568	688	821	17			
1	F	547	Total	C	N	O	S	0	2	0
			4090	2565	688	821	16			
1	G	547	Total	C	N	O	S	0	2	0
			4093	2567	688	821	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	MET	-	initiating methionine	UNP A0A0C5PVE3
B	252	MET	-	initiating methionine	UNP A0A0C5PVE3
C	252	MET	-	initiating methionine	UNP A0A0C5PVE3
D	252	MET	-	initiating methionine	UNP A0A0C5PVE3
F	252	MET	-	initiating methionine	UNP A0A0C5PVE3
G	252	MET	-	initiating methionine	UNP A0A0C5PVE3

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



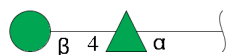
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	6	Total	C	O	0	0	0
			65	36	29			
2	H	6	Total	C	O	0	0	0
			65	36	29			
2	K	6	Total	C	O	0	0	0
			65	36	29			
2	L	6	Total	C	O	0	0	0
			65	36	29			
2	M	6	Total	C	O	0	0	0
			65	36	29			

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	I	4	Total	C	O	0	0	0
			43	24	19			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

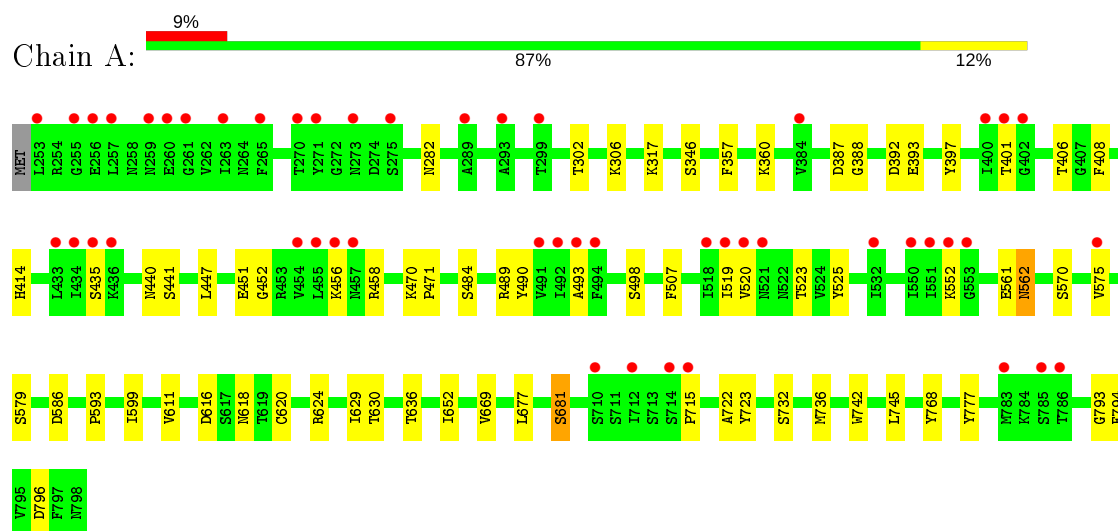
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	224	Total	O	0	0
			224	224		
6	C	295	Total	O	0	0
			295	295		
6	D	276	Total	O	0	0
			276	276		
6	F	255	Total	O	0	0
			255	255		
6	G	251	Total	O	0	0
			251	251		

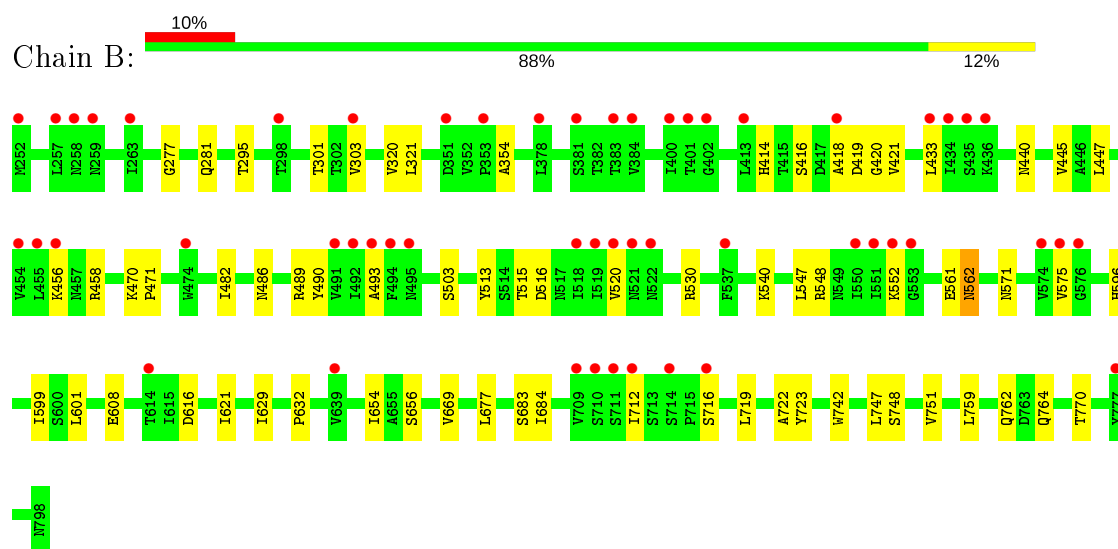
### 3 Residue-property plots [i](#)

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.

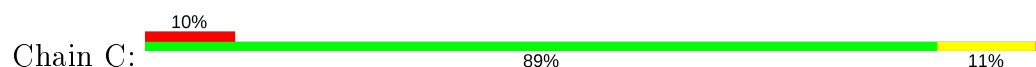
#### • Molecule 1: Tailspike

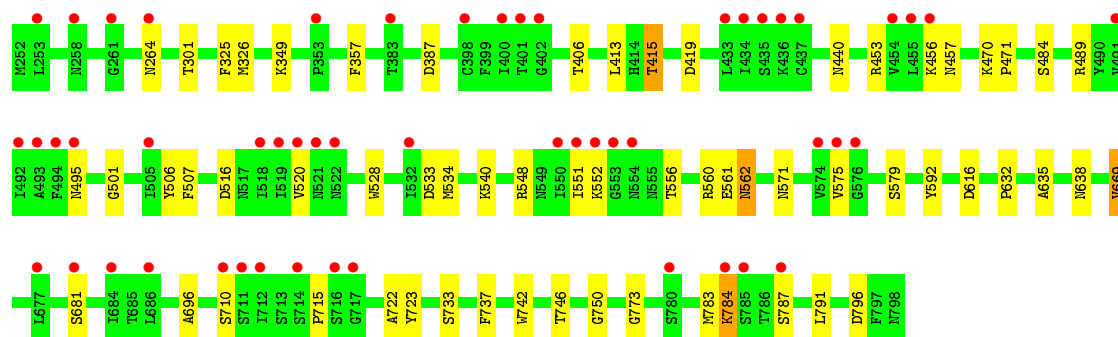


#### • Molecule 1: Tailspike

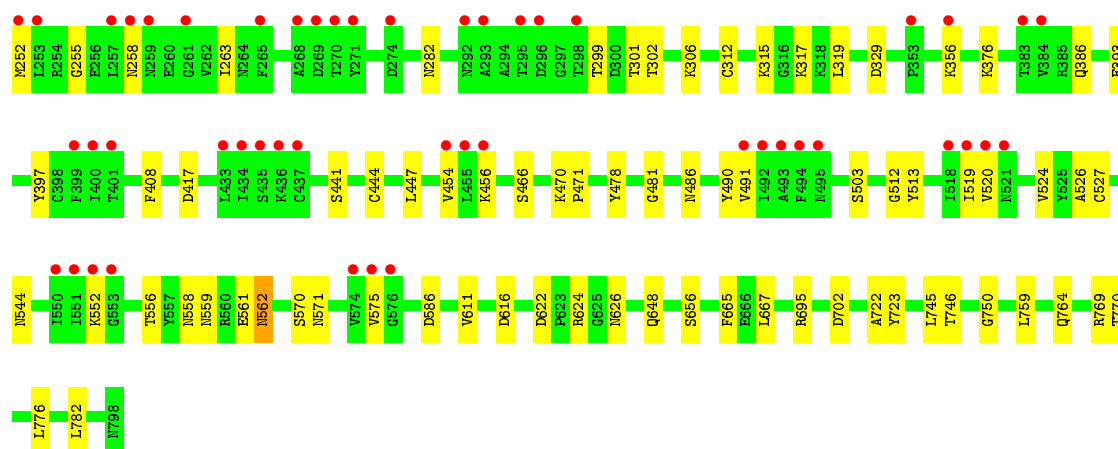
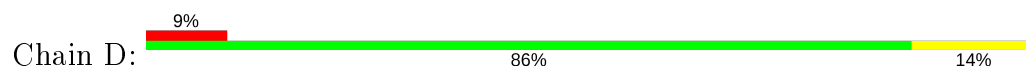


#### • Molecule 1: Tailspike

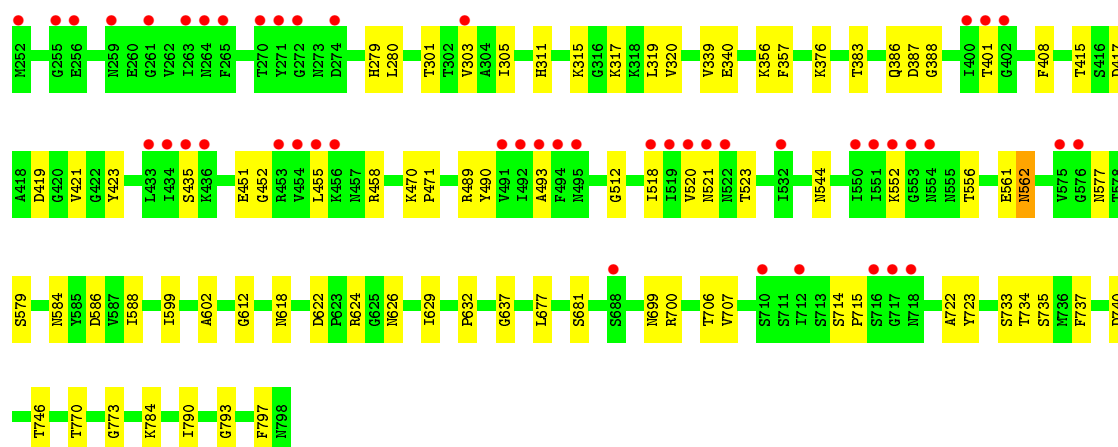
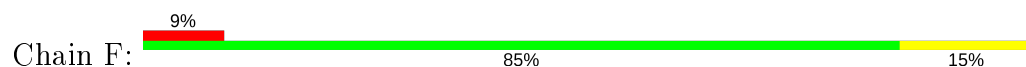




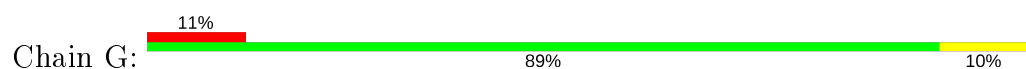
• Molecule 1: Tailspike



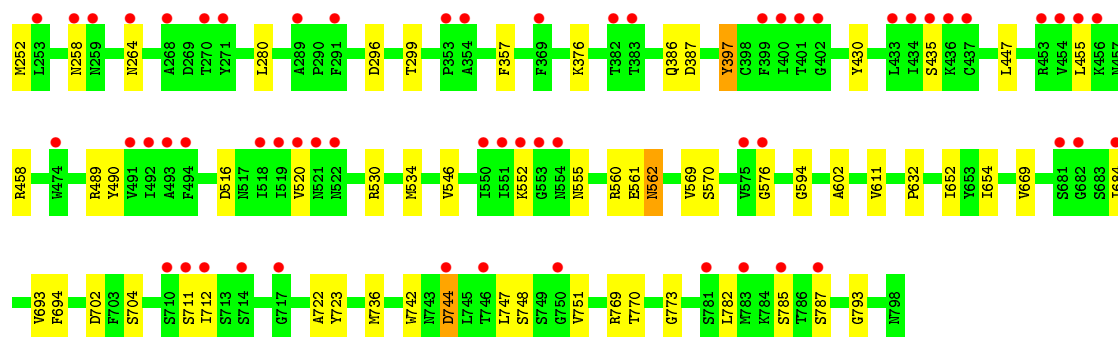
• Molecule 1: Tailspike



• Molecule 1: Tailspike







- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain E: 67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain H: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain K: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain L: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain M: 100%

RAM1  
BM2  
GLA3  
RAM4  
BM5  
GLA6

- Molecule 3: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose

Chain I:  75% 25%

GLA1  
RAM2  
BM3  
GLA4

- Molecule 4: beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain J:  50% 50%

RAM1  
BM2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.42Å 160.83Å 161.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.10 48.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.76-2.10) 99.5 (48.76-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.183 , 0.221 0.189 , 0.222	Depositor DCC
$R_{free}$ test set	2432 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	26526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, BMA, RAM, EDO

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	0.66	0/4175	0.66	0/5680
1	B	0.63	0/4181	0.64	0/5687
1	C	0.64	0/4175	0.64	1/5679 (0.0%)
1	D	0.63	0/4183	0.65	0/5690
1	F	0.64	0/4179	0.64	0/5686
1	G	0.62	0/4182	0.64	2/5689 (0.0%)
All	All	0.64	0/25075	0.65	3/34111 (0.0%)

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	A	0	2
1	D	0	1
1	G	0	3
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	453	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	458	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	G	458	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	618	ASN	Mainchain
1	A	630	THR	Mainchain
1	D	648	GLN	Mainchain
1	G	397	TYR	Sidechain
1	G	555	ASN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4086	0	3937	52	0
1	B	4092	0	3940	48	0
1	C	4089	0	3935	41	0
1	D	4094	0	3946	46	0
1	F	4090	0	3937	65	0
1	G	4093	0	3944	41	0
2	E	65	0	57	2	0
2	H	65	0	57	0	0
2	K	65	0	56	0	0
2	L	65	0	55	0	0
2	M	65	0	56	0	0
3	I	43	0	37	1	0
4	J	22	0	19	1	0
5	A	4	0	6	2	0
6	A	287	0	0	9	0
6	B	224	0	0	10	0
6	C	295	0	0	4	0
6	D	276	0	0	4	0
6	F	255	0	0	1	0
6	G	251	0	0	1	0
All	All	26526	0	23982	268	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 5.

The worst 5 of 268 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)
6:A:909:HOH:O	1:F:523:THR:HB	1.67	0.94
1:G:397:TYR:HH	1:G:430:TYR:HE1	1.01	0.92
1:D:456:LYS:HD3	1:D:456:LYS:O	1.69	0.92
1:B:456:LYS:HD3	1:B:456:LYS:O	1.71	0.90
1:F:520[A]:VAL:HG12	1:F:552:LYS:HB3	1.63	0.80

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	546/547 (100%)	528 (97%)	17 (3%)	1 (0%)	47	49
1	B	547/547 (100%)	525 (96%)	21 (4%)	1 (0%)	47	49
1	C	546/547 (100%)	523 (96%)	22 (4%)	1 (0%)	47	49
1	D	547/547 (100%)	527 (96%)	19 (4%)	1 (0%)	47	49
1	F	547/547 (100%)	525 (96%)	21 (4%)	1 (0%)	47	49
1	G	547/547 (100%)	526 (96%)	20 (4%)	1 (0%)	47	49
All	All	3280/3282 (100%)	3154 (96%)	120 (4%)	6 (0%)	47	49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	ASN
1	B	562	ASN
1	C	562	ASN
1	D	562	ASN
1	F	562	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	448/447 (100%)	446 (100%)	2 (0%)	91	94
1	B	449/447 (100%)	445 (99%)	4 (1%)	78	84
1	C	448/447 (100%)	441 (98%)	7 (2%)	62	69
1	D	449/447 (100%)	445 (99%)	4 (1%)	78	84
1	F	448/447 (100%)	443 (99%)	5 (1%)	73	79
1	G	449/447 (100%)	444 (99%)	5 (1%)	73	79
All	All	2691/2682 (100%)	2664 (99%)	27 (1%)	76	82

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	784	LYS
1	D	656	SER
1	G	534	MET
1	D	315	LYS
1	B	683	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	596	HIS
1	C	495	ASN
1	F	386	GLN
1	A	764	GLN
1	D	559	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 ⓘ

36 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	E	1	2	11,11,11	1.76	2 (18%)	15,16,16	2.22	3 (20%)
2	BMA	E	2	2	11,11,12	1.66	1 (9%)	15,15,17	1.36	2 (13%)
2	GLA	E	3	2	11,11,12	1.89	3 (27%)	15,15,17	0.71	0
2	RAM	E	4	2	10,10,11	2.17	3 (30%)	14,14,16	1.89	4 (28%)
2	BMA	E	5	2	11,11,12	1.84	2 (18%)	15,15,17	1.21	3 (20%)
2	GLA	E	6	2	11,11,12	1.83	3 (27%)	15,15,17	0.63	0
2	RAM	H	1	2	11,11,11	1.74	2 (18%)	15,16,16	1.35	3 (20%)
2	BMA	H	2	2	11,11,12	1.79	3 (27%)	15,15,17	1.47	3 (20%)
2	GLA	H	3	2	11,11,12	1.68	1 (9%)	15,15,17	0.72	0
2	RAM	H	4	2	10,10,11	2.19	4 (40%)	14,14,16	1.04	0
2	BMA	H	5	2	11,11,12	1.58	2 (18%)	15,15,17	1.14	2 (13%)
2	GLA	H	6	2	11,11,12	1.73	2 (18%)	15,15,17	0.89	0
3	GLA	I	1	3	11,11,12	1.50	2 (18%)	15,15,17	1.25	2 (13%)
3	RAM	I	2	3	10,10,11	2.22	3 (30%)	14,14,16	1.14	1 (7%)
3	BMA	I	3	3	11,11,12	1.82	2 (18%)	15,15,17	1.05	2 (13%)
3	GLA	I	4	3	11,11,12	1.81	3 (27%)	15,15,17	0.72	0
4	RAM	J	1	4	11,11,11	1.53	2 (18%)	15,16,16	1.95	3 (20%)
4	BMA	J	2	4	11,11,12	1.73	2 (18%)	15,15,17	1.26	2 (13%)
2	RAM	K	1	2	11,11,11	1.72	2 (18%)	15,16,16	1.16	0
2	BMA	K	2	2	11,11,12	1.43	2 (18%)	15,15,17	1.39	2 (13%)
2	GLA	K	3	2	11,11,12	1.62	2 (18%)	15,15,17	0.79	0
2	RAM	K	4	2	10,10,11	2.25	3 (30%)	14,14,16	1.71	4 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	K	5	2	11,11,12	1.79	3 (27%)	15,15,17	1.14	2 (13%)
2	GLA	K	6	2	11,11,12	1.88	3 (27%)	15,15,17	0.73	0
2	RAM	L	1	2	11,11,11	1.69	2 (18%)	15,16,16	2.84	4 (26%)
2	BMA	L	2	2	11,11,12	1.83	2 (18%)	15,15,17	2.03	4 (26%)
2	GLA	L	3	2	11,11,12	1.75	3 (27%)	15,15,17	0.81	0
2	RAM	L	4	2	10,10,11	2.40	4 (40%)	14,14,16	1.03	1 (7%)
2	BMA	L	5	2	11,11,12	1.70	3 (27%)	15,15,17	0.70	1 (6%)
2	GLA	L	6	2	11,11,12	1.69	3 (27%)	15,15,17	0.42	0
2	RAM	M	1	2	11,11,11	1.78	2 (18%)	15,16,16	2.03	3 (20%)
2	BMA	M	2	2	11,11,12	1.45	2 (18%)	15,15,17	1.56	3 (20%)
2	GLA	M	3	2	11,11,12	1.70	2 (18%)	15,15,17	0.41	0
2	RAM	M	4	2	10,10,11	2.19	4 (40%)	14,14,16	1.50	3 (21%)
2	BMA	M	5	2	11,11,12	1.78	3 (27%)	15,15,17	1.12	2 (13%)
2	GLA	M	6	2	11,11,12	1.76	2 (18%)	15,15,17	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RAM	E	1	2	-	-	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	0/1/1/1
2	GLA	E	3	2	-	0/2/19/22	0/1/1/1
2	RAM	E	4	2	-	-	0/1/1/1
2	BMA	E	5	2	-	0/2/19/22	0/1/1/1
2	GLA	E	6	2	-	0/2/19/22	0/1/1/1
2	RAM	H	1	2	-	-	0/1/1/1
2	BMA	H	2	2	-	1/2/19/22	0/1/1/1
2	GLA	H	3	2	-	1/2/19/22	0/1/1/1
2	RAM	H	4	2	-	-	0/1/1/1
2	BMA	H	5	2	-	0/2/19/22	0/1/1/1
2	GLA	H	6	2	-	0/2/19/22	0/1/1/1
3	GLA	I	1	3	-	0/2/19/22	0/1/1/1
3	RAM	I	2	3	-	-	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	GLA	I	4	3	-	0/2/19/22	0/1/1/1
4	RAM	J	1	4	-	-	0/1/1/1
4	BMA	J	2	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RAM	K	1	2	-	-	0/1/1/1
2	BMA	K	2	2	-	2/2/19/22	0/1/1/1
2	GLA	K	3	2	-	0/2/19/22	0/1/1/1
2	RAM	K	4	2	-	-	0/1/1/1
2	BMA	K	5	2	-	0/2/19/22	0/1/1/1
2	GLA	K	6	2	-	0/2/19/22	0/1/1/1
2	RAM	L	1	2	-	-	0/1/1/1
2	BMA	L	2	2	-	2/2/19/22	0/1/1/1
2	GLA	L	3	2	-	0/2/19/22	0/1/1/1
2	RAM	L	4	2	-	-	0/1/1/1
2	BMA	L	5	2	-	0/2/19/22	0/1/1/1
2	GLA	L	6	2	-	0/2/19/22	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	BMA	M	2	2	-	0/2/19/22	0/1/1/1
2	GLA	M	3	2	-	0/2/19/22	0/1/1/1
2	RAM	M	4	2	-	-	0/1/1/1
2	BMA	M	5	2	-	2/2/19/22	0/1/1/1
2	GLA	M	6	2	-	0/2/19/22	0/1/1/1

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	GLA	O5-C1	5.20	1.52	1.43
2	L	4	RAM	O5-C1	5.10	1.51	1.43
2	E	6	GLA	O5-C1	4.99	1.51	1.43
2	K	6	GLA	O5-C1	4.92	1.51	1.43
2	K	4	RAM	O5-C1	4.87	1.51	1.43

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	RAM	O4-C4-C5	9.49	130.69	109.67
2	E	1	RAM	O4-C4-C5	7.02	125.23	109.67
2	M	1	RAM	O4-C4-C5	6.31	123.65	109.67
2	L	2	BMA	C1-O5-C5	5.57	119.73	112.19
4	J	1	RAM	O4-C4-C5	4.78	120.26	109.67

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

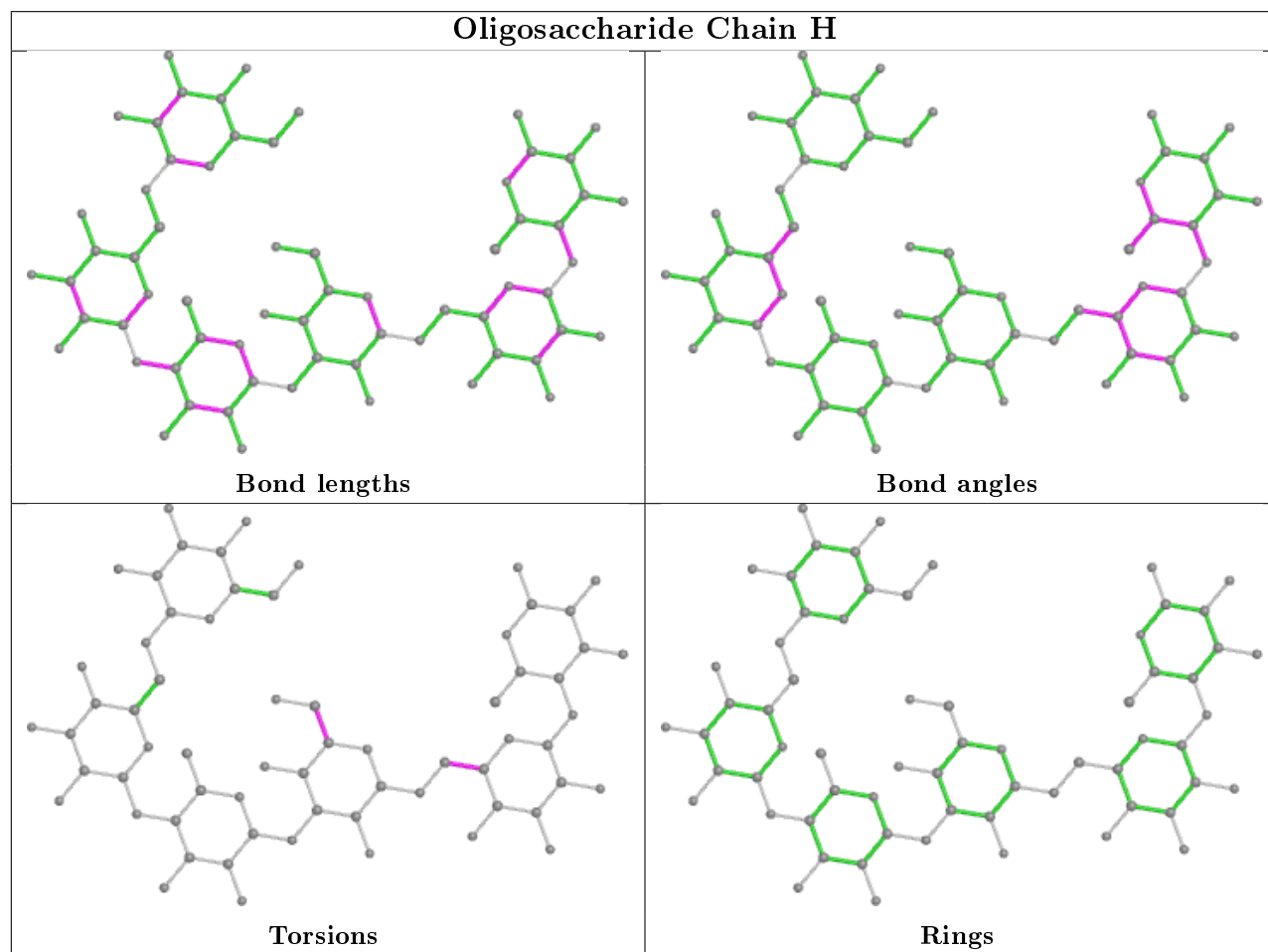
Mol	Chain	Res	Type	Atoms
2	L	2	BMA	O5-C5-C6-O6
2	L	2	BMA	C4-C5-C6-O6
2	K	2	BMA	C4-C5-C6-O6
2	K	2	BMA	O5-C5-C6-O6
4	J	2	BMA	C4-C5-C6-O6

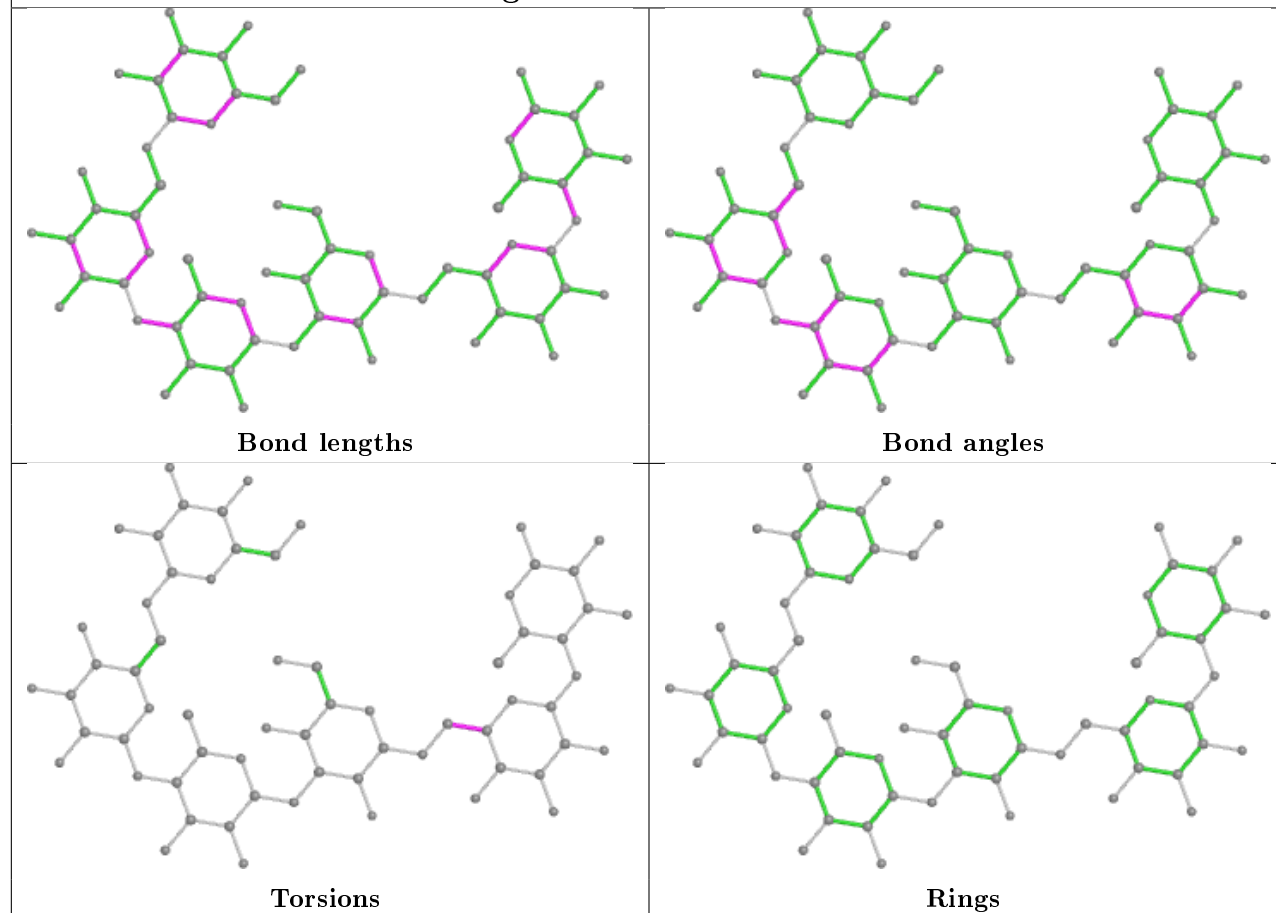
There are no ring outliers.

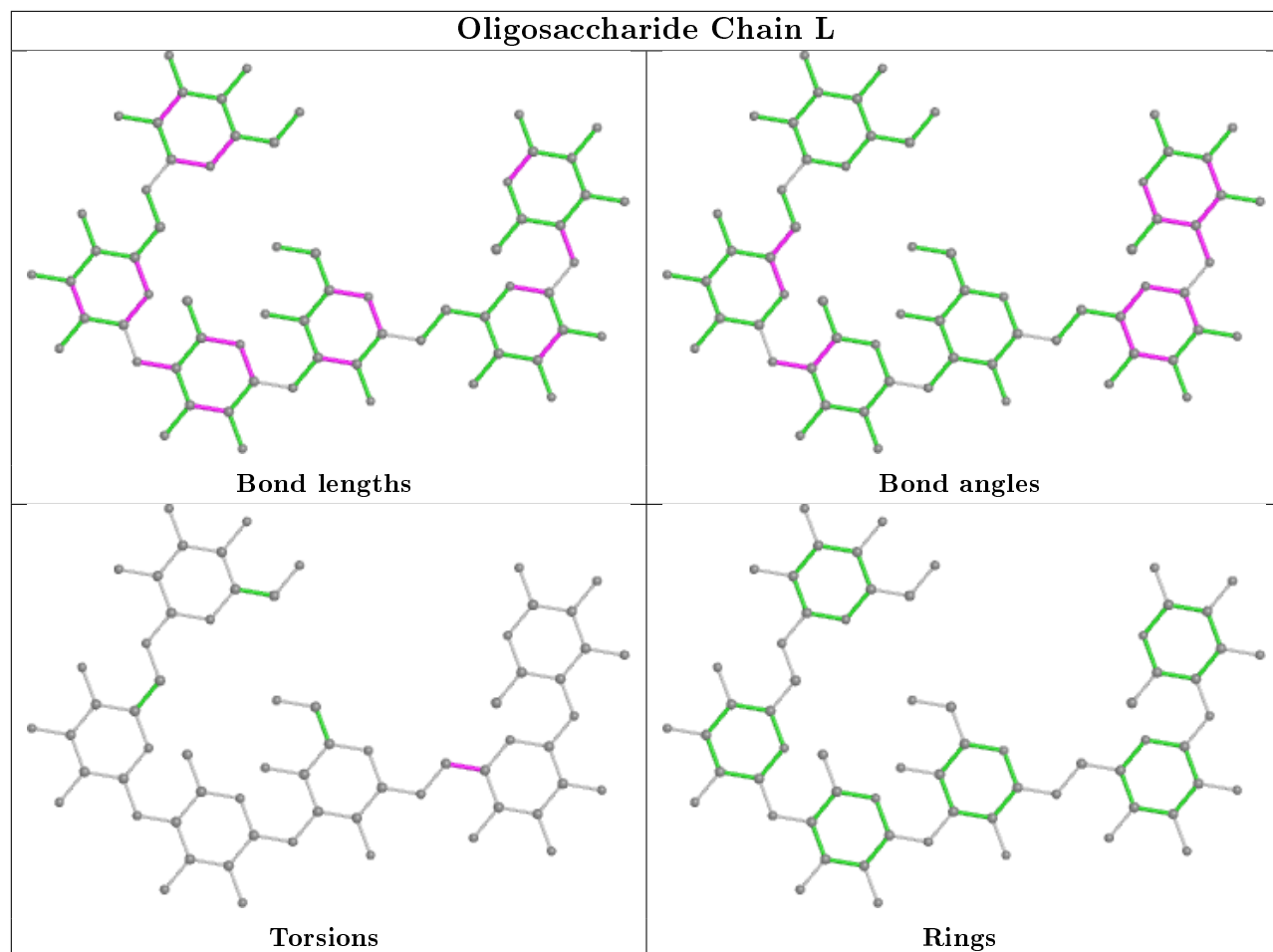
4 monomers are involved in 3 short contacts:

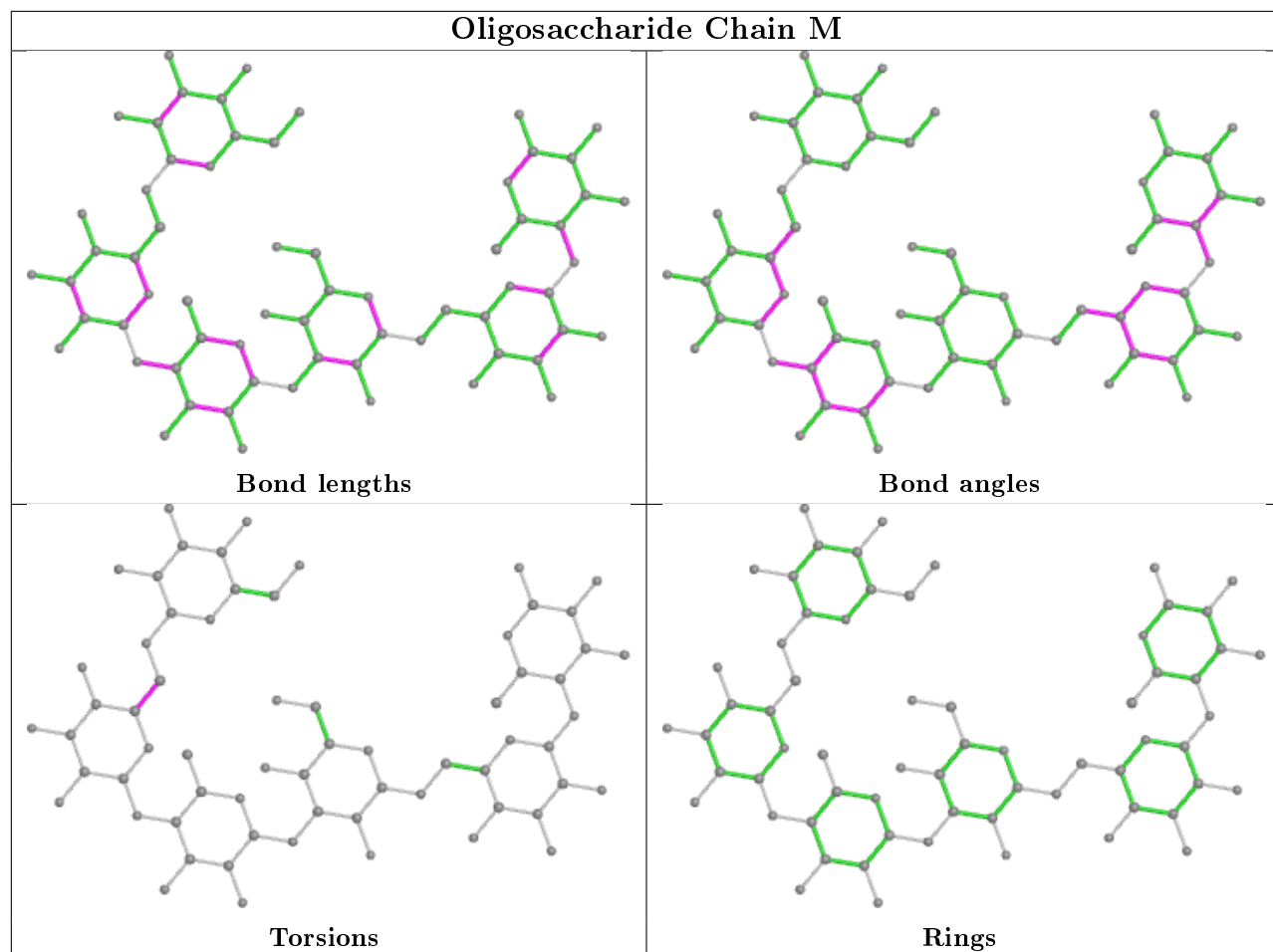
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	GLA	1	0
3	I	1	GLA	1	0
2	E	6	GLA	1	0
4	J	2	BMA	1	0

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

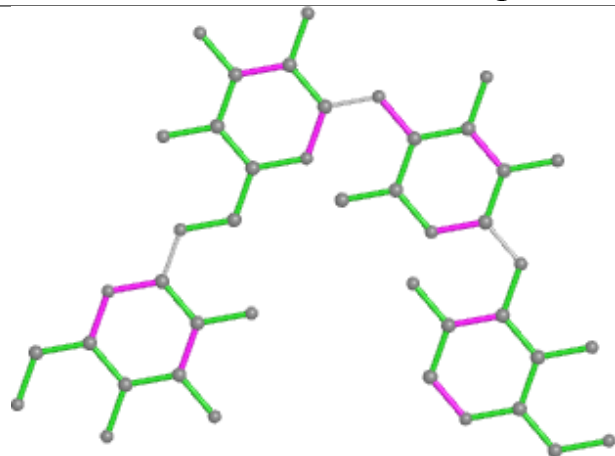


**Oligosaccharide Chain K**

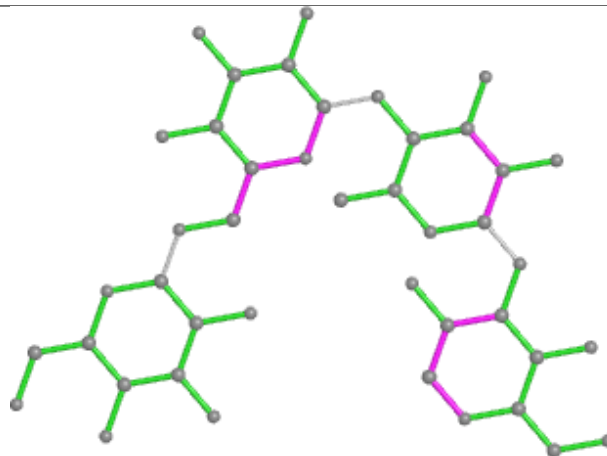


**Oligosaccharide Chain M**

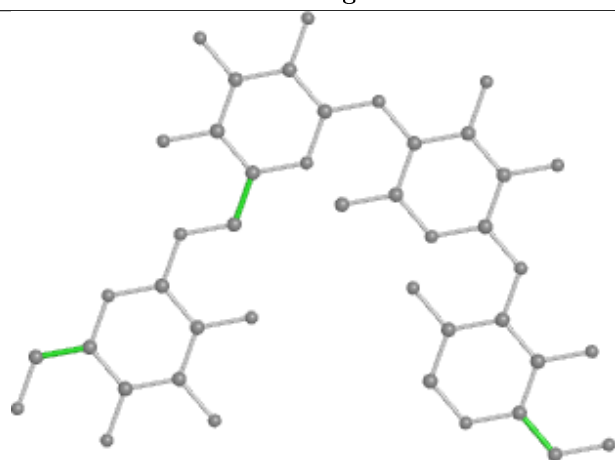
## Oligosaccharide Chain I



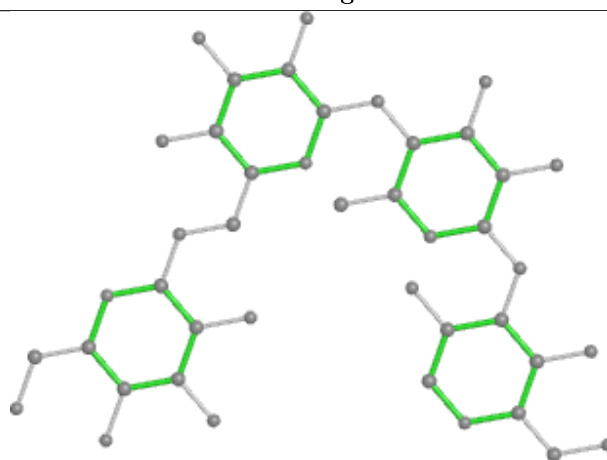
Bond lengths



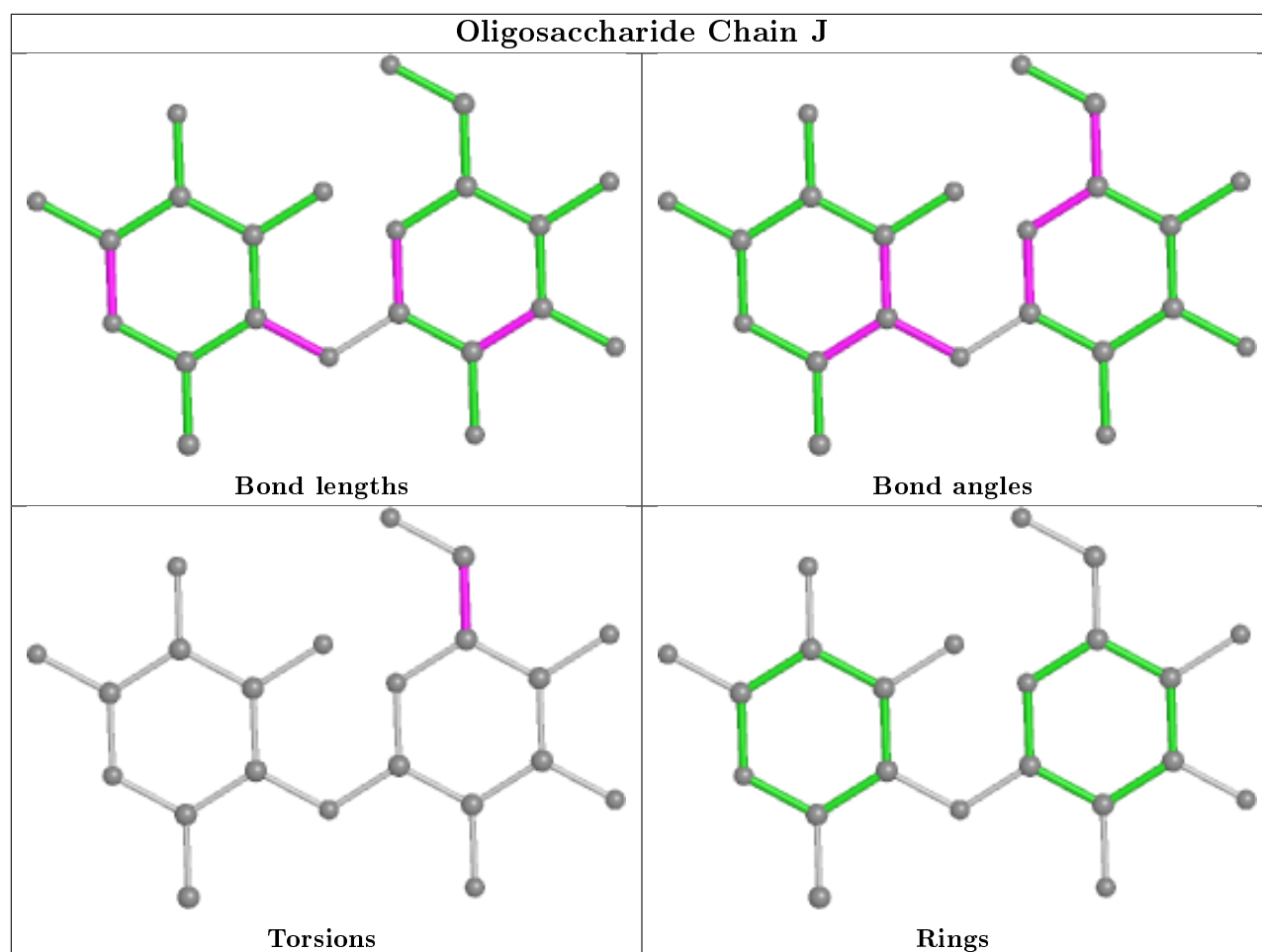
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
5	EDO	A	801	-	3,3,3	0.54	0	2,2,2	0.09	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	801	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	546/547 (99%)	0.38	49 (8%) 9 12	25, 47, 70, 88	0
1	B	547/547 (100%)	0.43	53 (9%) 7 10	27, 52, 75, 93	0
1	C	547/547 (100%)	0.41	52 (9%) 8 10	26, 46, 73, 93	0
1	D	547/547 (100%)	0.29	48 (8%) 10 12	25, 47, 68, 110	0
1	F	547/547 (100%)	0.32	48 (8%) 10 12	25, 47, 72, 97	0
1	G	547/547 (100%)	0.45	59 (10%) 5 7	28, 47, 72, 97	0
All	All	3281/3282 (99%)	0.38	309 (9%) 8 11	25, 48, 72, 110	0

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	252	MET	6.5
1	G	455	LEU	5.8
1	D	252	MET	5.8
1	A	455	LEU	5.2
1	D	455	LEU	5.2

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

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

### 6.3 Carbohydrates [i](#)

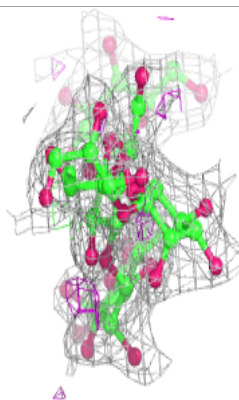
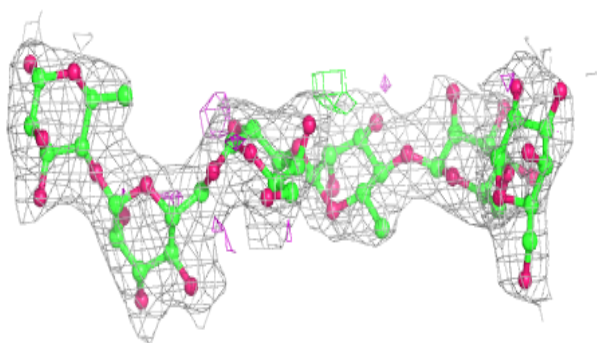
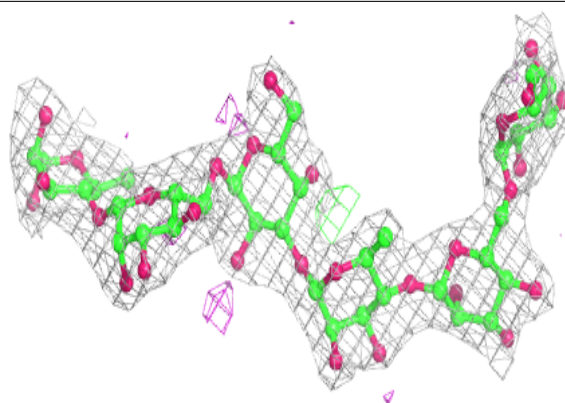
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLA	E	6	11/12	0.82	0.15	55,72,80,82	0
2	RAM	E	4	10/11	0.83	0.15	68,76,81,81	0
2	BMA	E	5	11/12	0.86	0.14	55,69,74,75	0
2	BMA	K	5	11/12	0.86	0.18	72,76,81,84	0
2	GLA	E	3	11/12	0.88	0.13	61,70,78,83	0
2	RAM	K	4	10/11	0.89	0.12	71,79,85,88	0
2	GLA	K	6	11/12	0.89	0.16	58,75,76,77	0
2	RAM	K	1	11/11	0.91	0.18	50,59,69,74	0
2	RAM	L	4	10/11	0.91	0.15	44,58,61,66	0
2	GLA	M	6	11/12	0.92	0.12	46,60,63,67	0
2	BMA	E	2	11/12	0.92	0.10	56,62,70,73	0
3	RAM	I	2	10/11	0.92	0.08	47,58,66,78	0
2	BMA	K	2	11/12	0.92	0.09	51,58,63,65	0
2	GLA	H	6	11/12	0.93	0.16	54,59,67,73	0
2	BMA	H	2	11/12	0.93	0.09	50,56,60,63	0
2	BMA	L	2	11/12	0.93	0.11	51,58,62,68	0
2	BMA	M	2	11/12	0.94	0.11	38,43,50,54	0
2	GLA	L	3	11/12	0.94	0.11	52,56,66,74	0
2	GLA	H	3	11/12	0.94	0.10	52,57,62,64	0
2	RAM	M	4	10/11	0.94	0.08	53,56,60,65	0
3	BMA	I	3	11/12	0.94	0.09	52,54,60,62	0
2	RAM	E	1	11/11	0.94	0.13	48,55,60,65	0
2	RAM	H	1	11/11	0.95	0.09	47,55,58,62	0
2	GLA	L	6	11/12	0.95	0.14	51,56,60,62	0
2	GLA	K	3	11/12	0.95	0.11	57,64,69,69	0
2	BMA	L	5	11/12	0.95	0.20	55,59,67,72	0
2	RAM	H	4	10/11	0.95	0.12	49,56,62,63	0
2	BMA	M	5	11/12	0.95	0.13	54,64,70,77	0
3	GLA	I	4	11/12	0.95	0.10	51,56,64,65	0
4	RAM	J	1	11/11	0.96	0.08	34,37,40,41	0
3	GLA	I	1	11/12	0.96	0.09	40,49,53,53	0
2	BMA	H	5	11/12	0.96	0.14	61,64,69,71	0
2	RAM	L	1	11/11	0.97	0.12	44,47,56,58	0
2	GLA	M	3	11/12	0.97	0.08	47,49,55,55	0
4	BMA	J	2	11/12	0.97	0.07	33,35,37,38	0
2	RAM	M	1	11/11	0.98	0.10	39,43,50,50	0

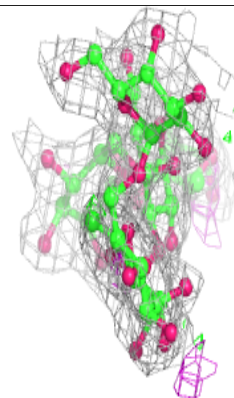
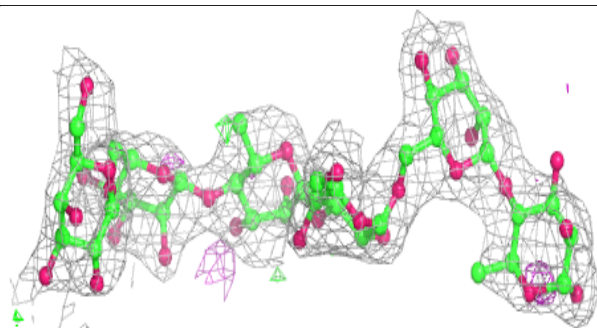
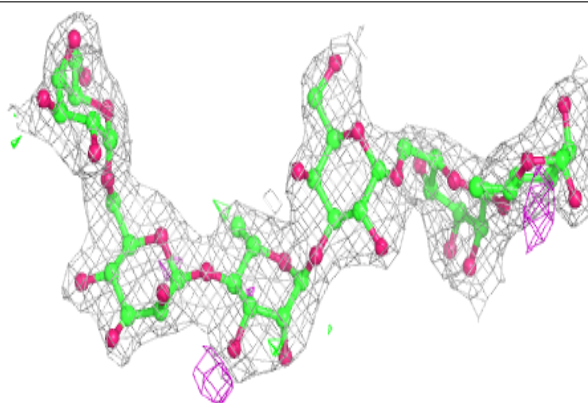
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain H:**

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

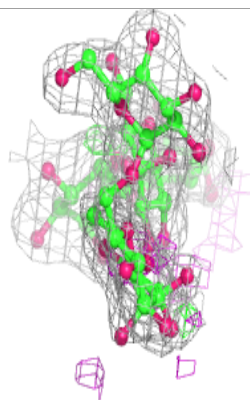
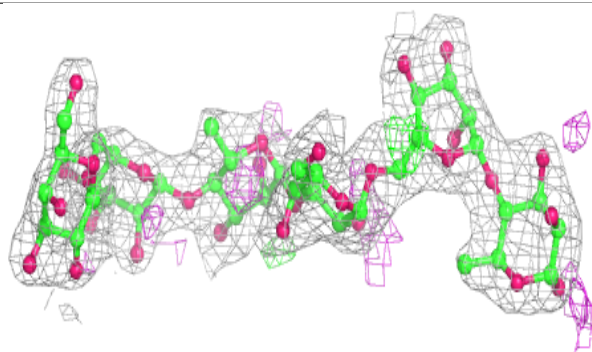
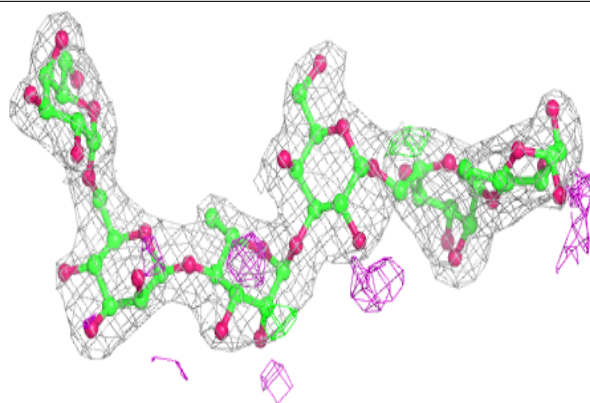
**Electron density around Chain K:**

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

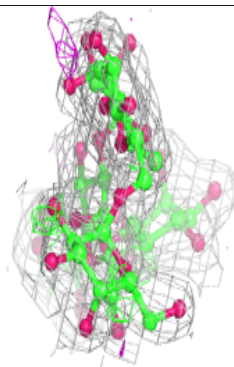
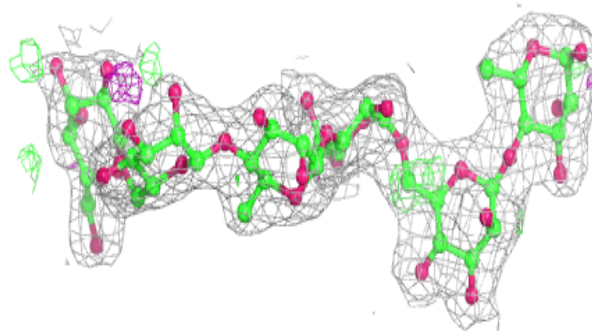
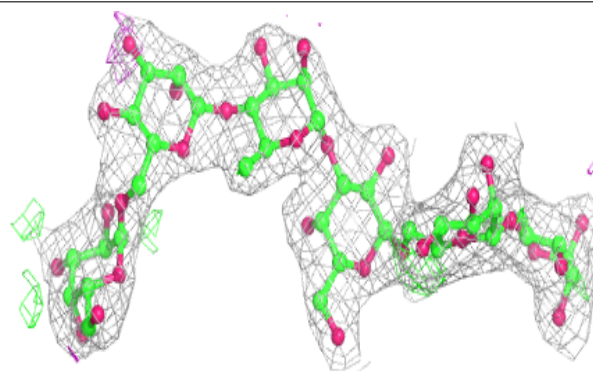


**Electron density around Chain L:**

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

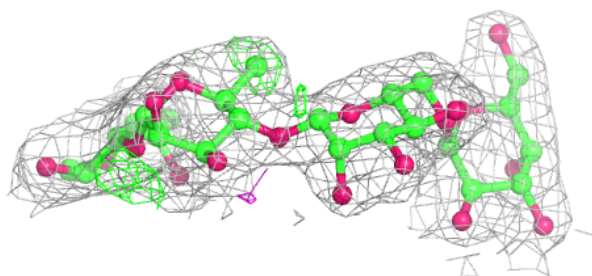
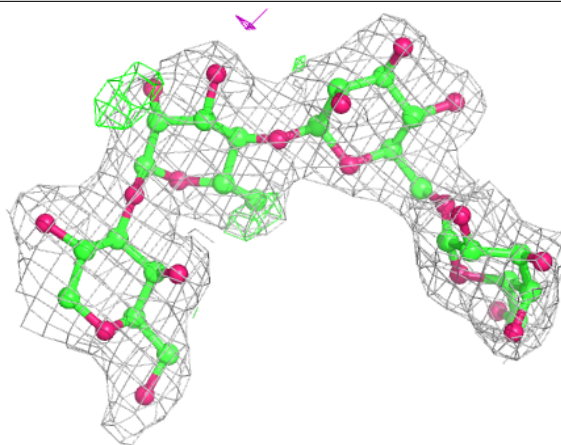
**Electron density around Chain M:**

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

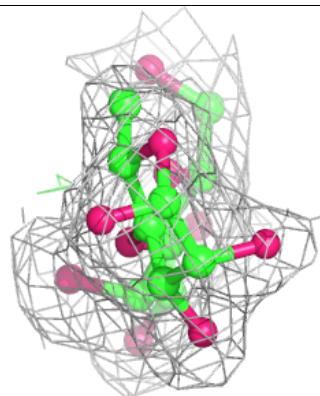
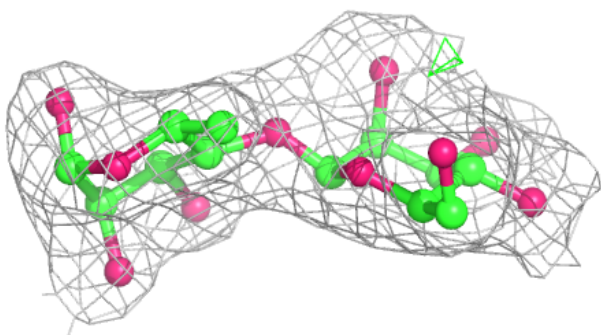
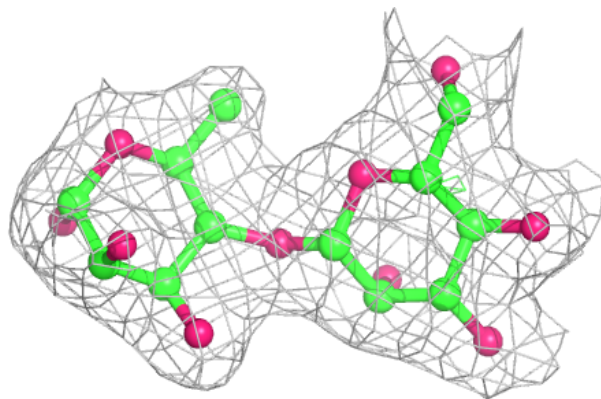


**Electron density around Chain I:**

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

**Electron density around Chain J:**

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



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	801	4/4	0.94	0.13	51,62,63,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.