



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 03:30 PM EDT

PDB ID : 3SLD  
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to A trisaccharide  
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.  
Deposited on : 2011-06-24  
Resolution : 2.68 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

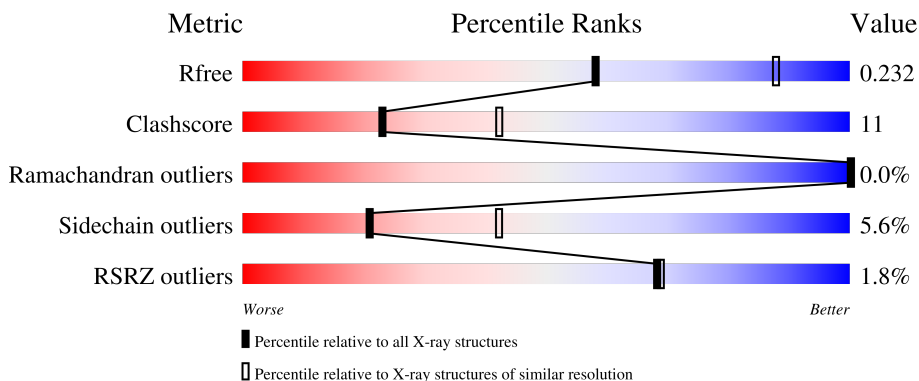
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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.



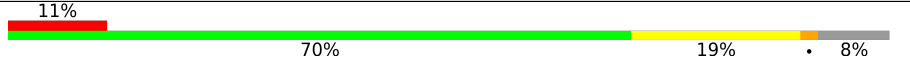
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	311	 81% 16% ..
1	B	311	 81% 15% ..
1	C	311	 84% 14% .
1	D	311	 77% 20% ..
1	E	311	 80% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	K	1	-	-	-	X
2	A2G	K	3	-	-	-	X
2	GAL	M	1	-	-	-	X
2	A2G	M	3	-	-	-	X
2	GAL	N	1	-	-	-	X
2	A2G	N	3	-	-	-	X
2	GAL	O	1	-	-	-	X
2	A2G	O	3	-	-	-	X
2	A2G	P	3	-	-	-	X
2	GAL	Q	1	-	-	-	X
2	A2G	Q	3	-	-	-	X
2	A2G	R	3	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24607 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 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2404	1517	415	462	10	0	0	0
1	B	308	2392	1510	411	461	10	0	0	0
1	C	311	2403	1514	413	466	10	0	0	0
1	D	307	2385	1507	410	458	10	0	0	0
1	E	309	2406	1518	415	463	10	0	0	0
1	F	308	2393	1511	411	461	10	0	0	0
1	G	308	2380	1505	407	458	10	0	0	0
1	H	293	2274	1445	386	434	9	0	0	0
1	I	286	2189	1391	376	414	8	0	0	0
1	J	307	2386	1507	410	459	10	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

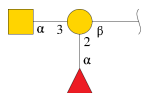
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
C	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	K	3	36	20	1	15	0	0	0
2	L	3	36	20	1	15	0	0	0
2	M	3	36	20	1	15	0	0	0
2	N	3	36	20	1	15	0	0	0
2	O	3	36	20	1	15	0	0	0
2	P	3	36	20	1	15	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	R	3	Total	C	N	O	0	0	0
			36	20	1	15			

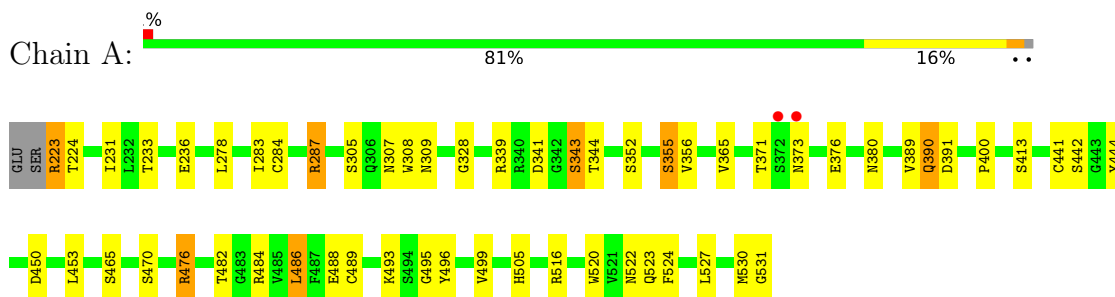
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	100	Total	O	0	0
			100	100		
3	C	93	Total	O	0	0
			93	93		
3	D	83	Total	O	0	0
			83	83		
3	E	80	Total	O	0	0
			80	80		
3	F	50	Total	O	0	0
			50	50		
3	G	50	Total	O	0	0
			50	50		
3	H	48	Total	O	0	0
			48	48		
3	I	30	Total	O	0	0
			30	30		
3	J	68	Total	O	0	0
			68	68		

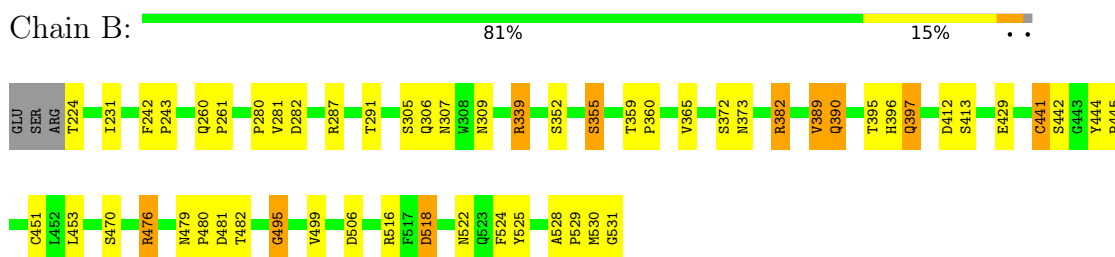
### 3 Residue-property plots

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.

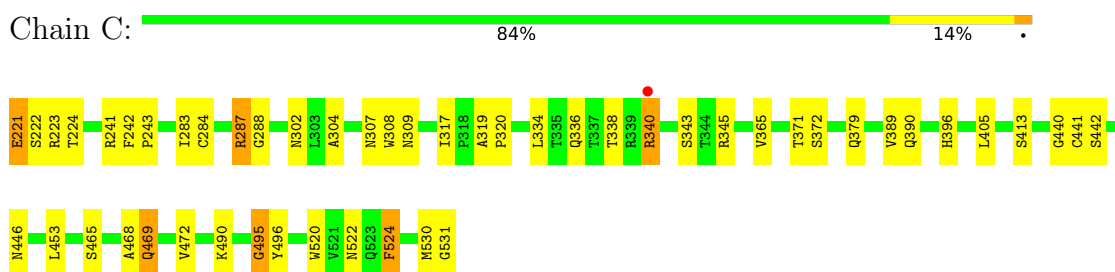
- Molecule 1: Capsid



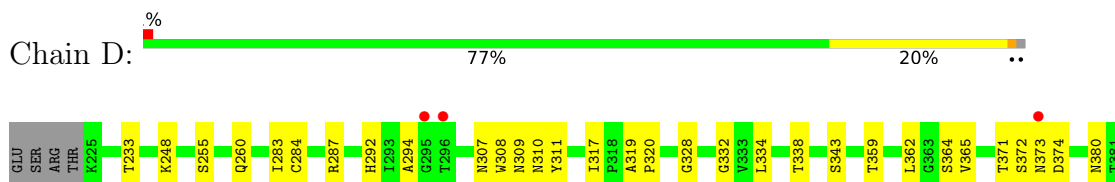
- Molecule 1: Capsid

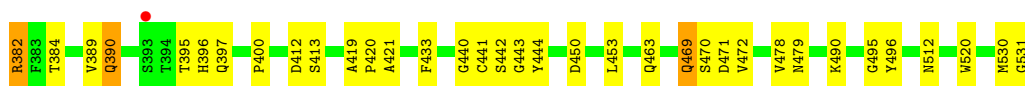


- Molecule 1: Capsid

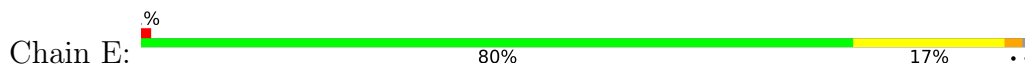


- Molecule 1: Capsid

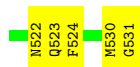
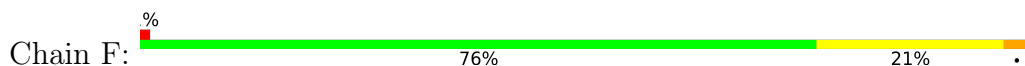




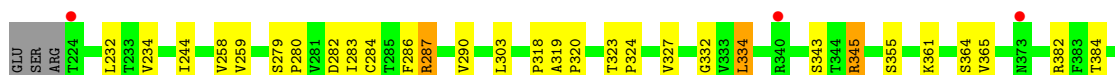
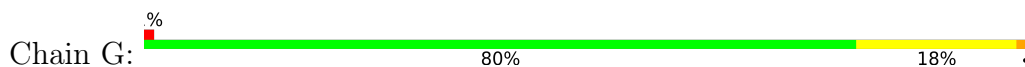
• Molecule 1: Capsid



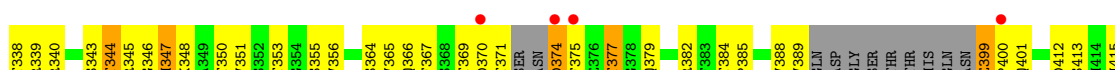
• Molecule 1: Capsid



• Molecule 1: Capsid



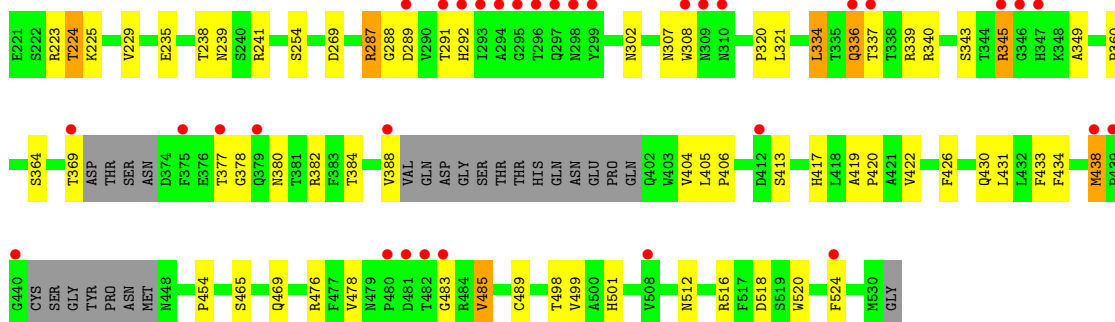
• Molecule 1: Capsid



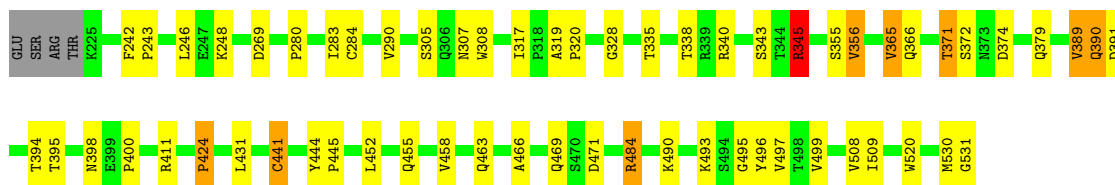
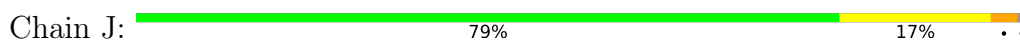




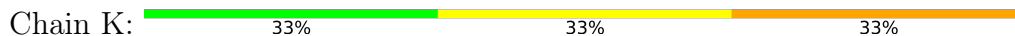
- Molecule 1: Capsid



- Molecule 1: Capsid



- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta ta-D-galactopyranose



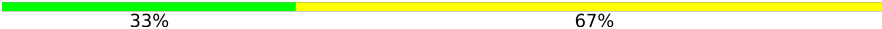
- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta ta-D-galactopyranose



- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta ta-D-galactopyranose

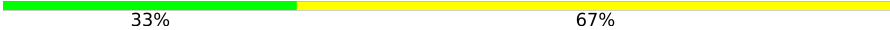


- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain N:  33% 67%

GAL1  
FUC2  
A2G3

- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain O:  33% 67%

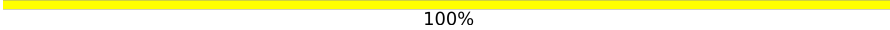
GAL1  
FUC2  
A2G3

- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain P:  33% 67%

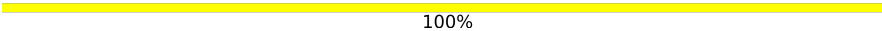
GAL1  
FUC2  
A2G3

- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain Q:  100%

GAL1  
FUC2  
A2G3

- Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain R:  100%

GAL1  
FUC2  
A2G3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	244.54Å 341.46Å 124.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.66 – 2.68 41.65 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.66-2.68) 98.2 (41.65-2.68)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.181 , 0.230 0.186 , 0.232	Depositor DCC
$R_{free}$ test set	7203 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, A2G, 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	1.14	3/2474 (0.1%)	0.97	5/3385 (0.1%)
1	B	1.09	8/2462 (0.3%)	0.93	1/3369 (0.0%)
1	C	1.01	2/2472 (0.1%)	0.94	4/3384 (0.1%)
1	D	0.99	1/2455 (0.0%)	0.98	3/3360 (0.1%)
1	E	1.03	2/2476 (0.1%)	0.97	6/3388 (0.2%)
1	F	0.93	1/2463 (0.0%)	0.93	3/3371 (0.1%)
1	G	0.93	0/2450	0.91	4/3355 (0.1%)
1	H	0.97	2/2338 (0.1%)	0.98	10/3197 (0.3%)
1	I	0.88	0/2251	0.88	2/3080 (0.1%)
1	J	1.01	4/2456 (0.2%)	0.94	3/3361 (0.1%)
All	All	1.00	23/24297 (0.1%)	0.94	41/33250 (0.1%)

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	E	0	1
1	I	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	CYS	CB-SG	-7.31	1.69	1.82
1	A	376	GLU	C-N	7.16	1.50	1.34
1	C	221	GLU	CG-CD	6.94	1.62	1.51
1	H	221	GLU	CG-CD	6.75	1.62	1.51
1	B	518	ASP	CB-CG	6.25	1.64	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	337	THR	O-C-N	11.56	141.20	122.70
1	H	223	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	I	337	THR	CA-C-N	-8.71	98.04	117.20
1	H	223	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	E	334	LEU	CA-CB-CG	7.21	131.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	223	ARG	Sidechain
1	I	223	ARG	Sidechain

## 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	2404	0	2295	53	0
1	B	2392	0	2278	57	0
1	C	2403	0	2282	45	0
1	D	2385	0	2272	43	0
1	E	2406	0	2297	52	1
1	F	2393	0	2282	62	0
1	G	2380	0	2263	49	0
1	H	2274	0	2173	81	0
1	I	2189	0	2066	61	1
1	J	2386	0	2275	52	0
2	K	36	0	32	2	0
2	L	36	0	32	0	0
2	M	36	0	32	1	0
2	N	36	0	32	1	0
2	O	36	0	32	2	0
2	P	36	0	32	0	0
2	Q	36	0	32	2	0
2	R	36	0	32	3	0
3	A	105	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	100	0	0	6	0
3	C	93	0	0	10	0
3	D	83	0	0	5	0
3	E	80	0	0	8	0
3	F	50	0	0	10	0
3	G	50	0	0	8	0
3	H	48	0	0	22	0
3	I	30	0	0	25	0
3	J	68	0	0	5	0
All	All	24607	0	22739	533	1

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 11.

The worst 5 of 533 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:C:453:LEU:HD21	1:C:495:GLY:O	1.33	1.27
1:D:310:ASN:HB3	3:D:555:HOH:O	1.48	1.14
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.01	1.10
1:A:223:ARG:HG2	1:A:224:THR:H	0.94	1.10
1:H:531:GLY:HA3	3:H:586:HOH:O	1.50	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ARG:NH1	1:I:321:LEU:CD2[4_555]	2.11	0.09

## 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	307/311 (99%)	299 (97%)	8 (3%)	0	100	100
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100	100
1	C	309/311 (99%)	301 (97%)	8 (3%)	0	100	100
1	D	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100	100
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	H	285/311 (92%)	264 (93%)	21 (7%)	0	100	100
1	I	278/311 (89%)	266 (96%)	11 (4%)	1 (0%)	34	58
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3014/3110 (97%)	2894 (96%)	119 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	483	GLY

### 5.3.2 Protein sidechains [i](#)

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	270/272 (99%)	256 (95%)	14 (5%)	23	46
1	B	269/272 (99%)	254 (94%)	15 (6%)	21	42
1	C	269/272 (99%)	258 (96%)	11 (4%)	30	56
1	D	267/272 (98%)	255 (96%)	12 (4%)	27	52
1	E	271/272 (100%)	259 (96%)	12 (4%)	28	53
1	F	269/272 (99%)	252 (94%)	17 (6%)	18	37
1	G	266/272 (98%)	253 (95%)	13 (5%)	25	49
1	H	254/272 (93%)	228 (90%)	26 (10%)	7	15
1	I	238/272 (88%)	225 (94%)	13 (6%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	268/272 (98%)	254 (95%)	14 (5%)	23	46
All	All	2641/2720 (97%)	2494 (94%)	147 (6%)	21	42

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	413	SER
1	J	390	GLN
1	H	523	GLN
1	I	438	MET
1	D	390	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	390	GLN
1	J	398	ASN
1	H	297	GLN
1	J	523	GLN
1	I	347	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GAL	K	1	2	12,12,12	0.46	0	17,17,17	0.80	1 (5%)
2	FUC	K	2	2	10,10,11	0.43	0	14,14,16	0.84	0
2	A2G	K	3	2	14,14,15	0.52	0	17,19,21	0.88	0
2	GAL	L	1	2	12,12,12	0.47	0	17,17,17	0.79	1 (5%)
2	FUC	L	2	2	10,10,11	0.43	0	14,14,16	0.84	0
2	A2G	L	3	2	14,14,15	0.54	0	17,19,21	0.89	0
2	GAL	M	1	2	12,12,12	0.47	0	17,17,17	0.79	1 (5%)
2	FUC	M	2	2	10,10,11	0.42	0	14,14,16	0.85	0
2	A2G	M	3	2	14,14,15	0.53	0	17,19,21	0.88	0
2	GAL	N	1	2	12,12,12	0.46	0	17,17,17	0.80	1 (5%)
2	FUC	N	2	2	10,10,11	0.43	0	14,14,16	0.83	0
2	A2G	N	3	2	14,14,15	0.53	0	17,19,21	0.89	0
2	GAL	O	1	2	12,12,12	0.48	0	17,17,17	0.80	1 (5%)
2	FUC	O	2	2	10,10,11	0.42	0	14,14,16	0.84	0
2	A2G	O	3	2	14,14,15	0.53	0	17,19,21	0.89	0
2	GAL	P	1	2	12,12,12	0.46	0	17,17,17	0.79	1 (5%)
2	FUC	P	2	2	10,10,11	0.41	0	14,14,16	0.83	0
2	A2G	P	3	2	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
2	GAL	Q	1	2	12,12,12	0.46	0	17,17,17	0.79	1 (5%)
2	FUC	Q	2	2	10,10,11	0.42	0	14,14,16	0.84	0
2	A2G	Q	3	2	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
2	GAL	R	1	2	12,12,12	0.46	0	17,17,17	0.79	1 (5%)
2	FUC	R	2	2	10,10,11	0.42	0	14,14,16	0.84	0
2	A2G	R	3	2	14,14,15	0.53	0	17,19,21	0.89	1 (5%)

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	GAL	K	1	2	-	2/2/22/22	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	A2G	K	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	1	2	-	2/2/22/22	0/1/1/1
2	FUC	L	2	2	-	-	0/1/1/1
2	A2G	L	3	2	-	1/6/23/26	0/1/1/1
2	GAL	M	1	2	-	2/2/22/22	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	M	3	2	-	2/6/23/26	0/1/1/1
2	GAL	N	1	2	-	2/2/22/22	0/1/1/1
2	FUC	N	2	2	-	-	0/1/1/1
2	A2G	N	3	2	-	1/6/23/26	0/1/1/1
2	GAL	O	1	2	-	2/2/22/22	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
2	A2G	O	3	2	-	1/6/23/26	0/1/1/1
2	GAL	P	1	2	-	1/2/22/22	0/1/1/1
2	FUC	P	2	2	-	-	0/1/1/1
2	A2G	P	3	2	-	2/6/23/26	0/1/1/1
2	GAL	Q	1	2	-	2/2/22/22	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1
2	A2G	Q	3	2	-	2/6/23/26	0/1/1/1
2	GAL	R	1	2	-	2/2/22/22	0/1/1/1
2	FUC	R	2	2	-	-	0/1/1/1
2	A2G	R	3	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GAL	C1-O5-C5	-2.24	109.43	113.66
2	O	1	GAL	C1-O5-C5	-2.23	109.46	113.66
2	L	1	GAL	C1-O5-C5	-2.23	109.46	113.66
2	M	1	GAL	C1-O5-C5	-2.22	109.48	113.66
2	N	1	GAL	C1-O5-C5	-2.20	109.51	113.66

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

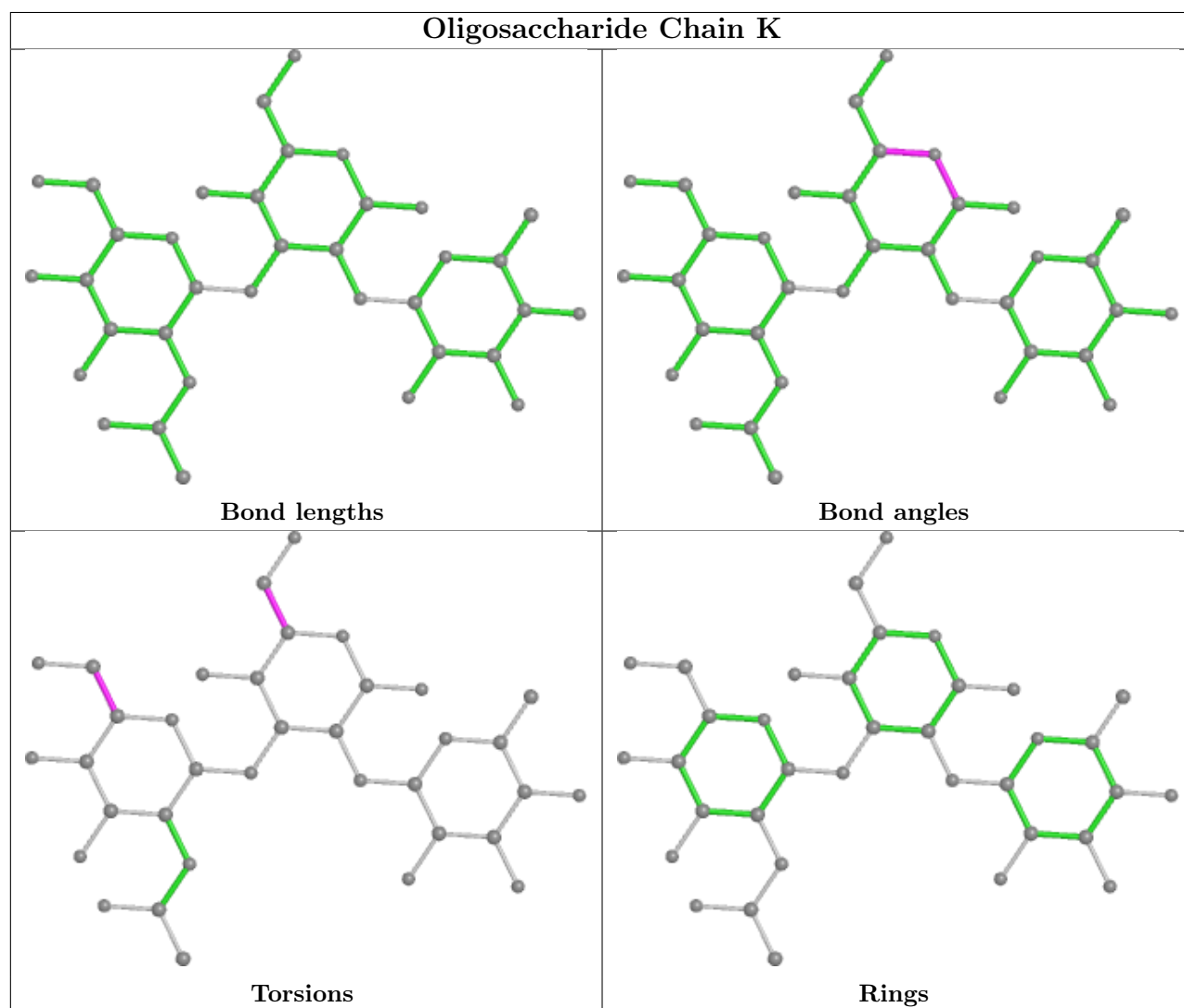
Mol	Chain	Res	Type	Atoms
2	L	1	GAL	O5-C5-C6-O6
2	P	3	A2G	O5-C5-C6-O6
2	M	1	GAL	O5-C5-C6-O6
2	O	1	GAL	O5-C5-C6-O6
2	M	1	GAL	C4-C5-C6-O6

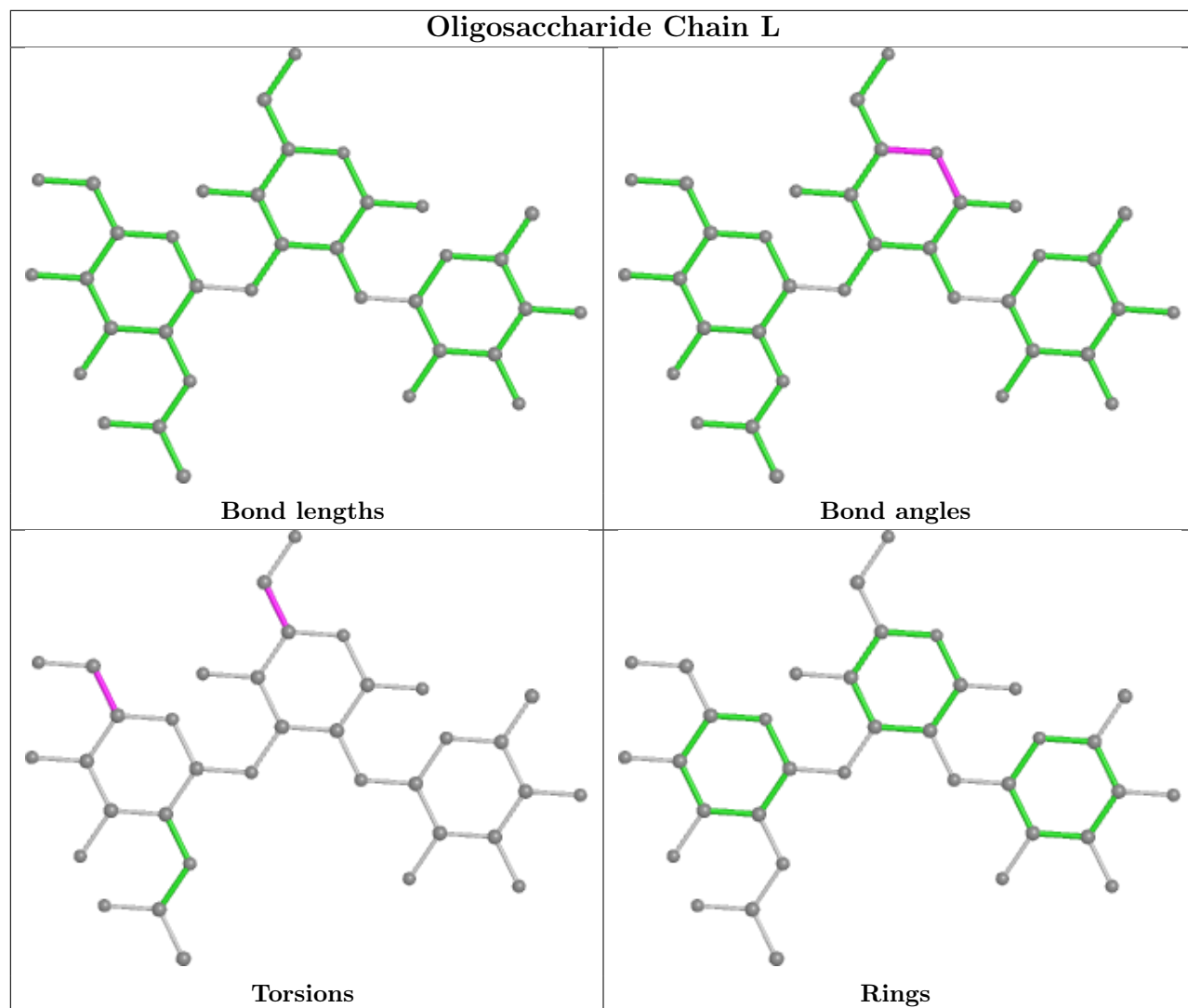
There are no ring outliers.

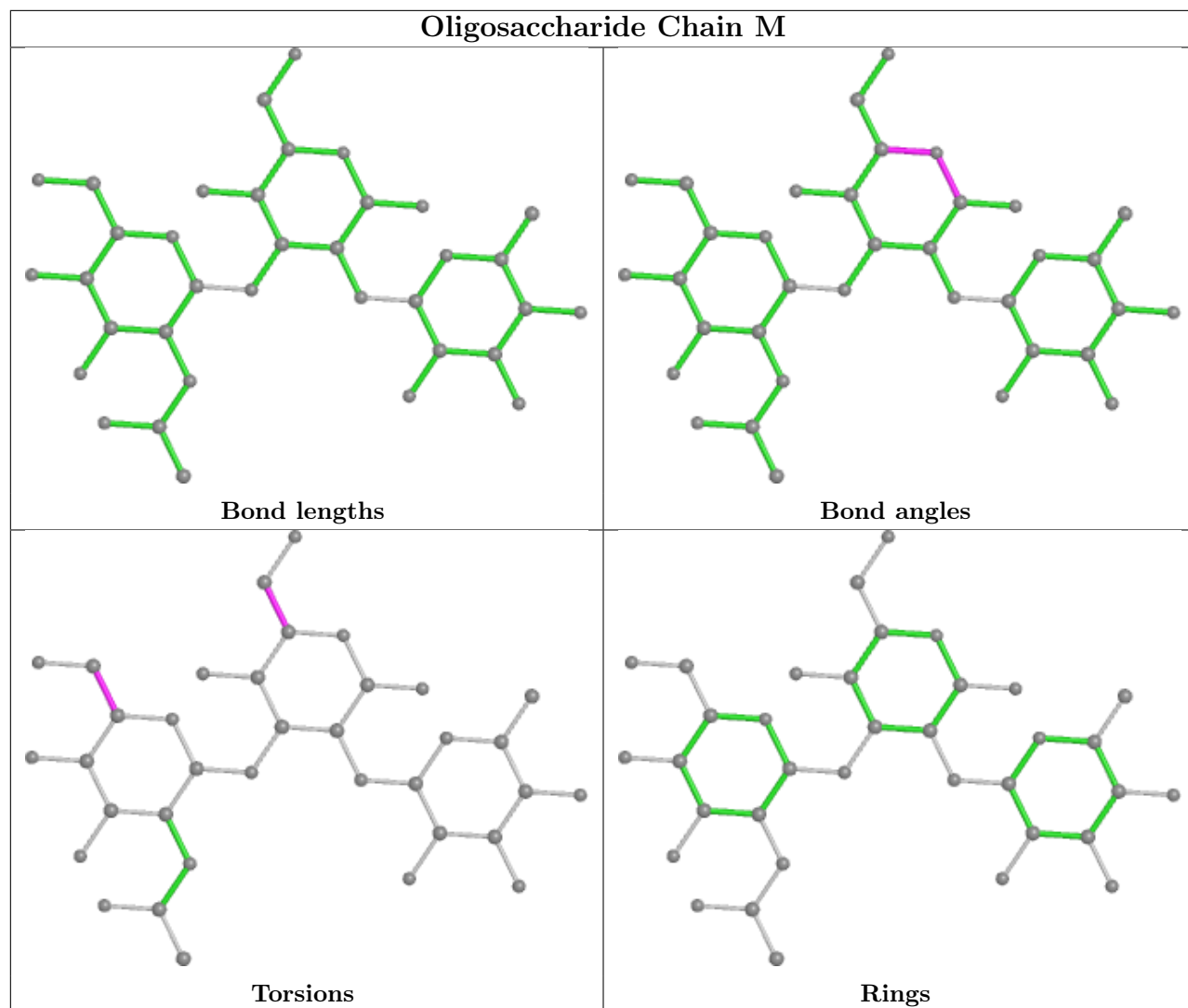
7 monomers are involved in 11 short contacts:

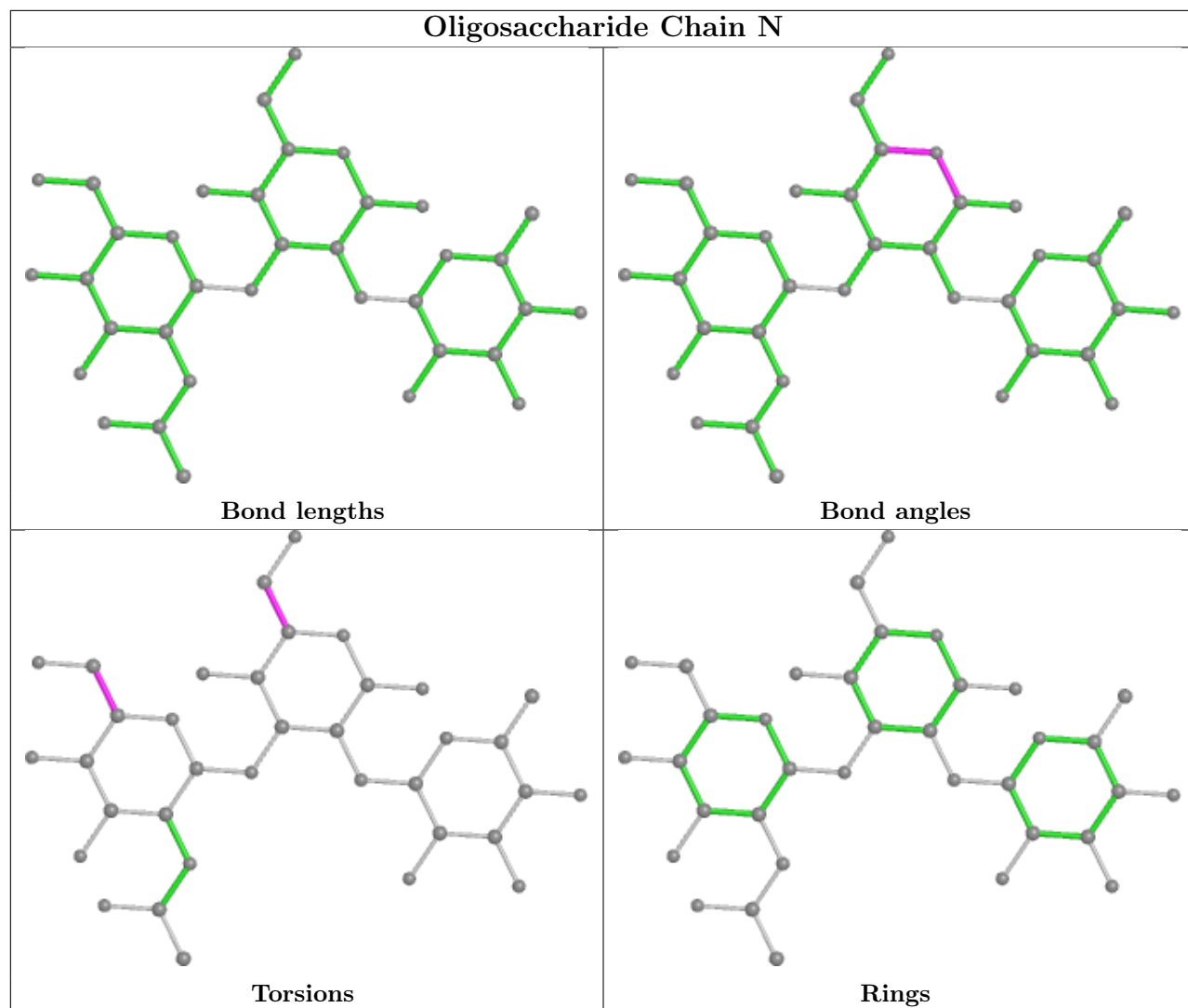
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	FUC	1	0
2	Q	2	FUC	2	0
2	M	2	FUC	1	0
2	O	2	FUC	2	0
2	K	1	GAL	1	0
2	R	2	FUC	3	0
2	N	2	FUC	1	0

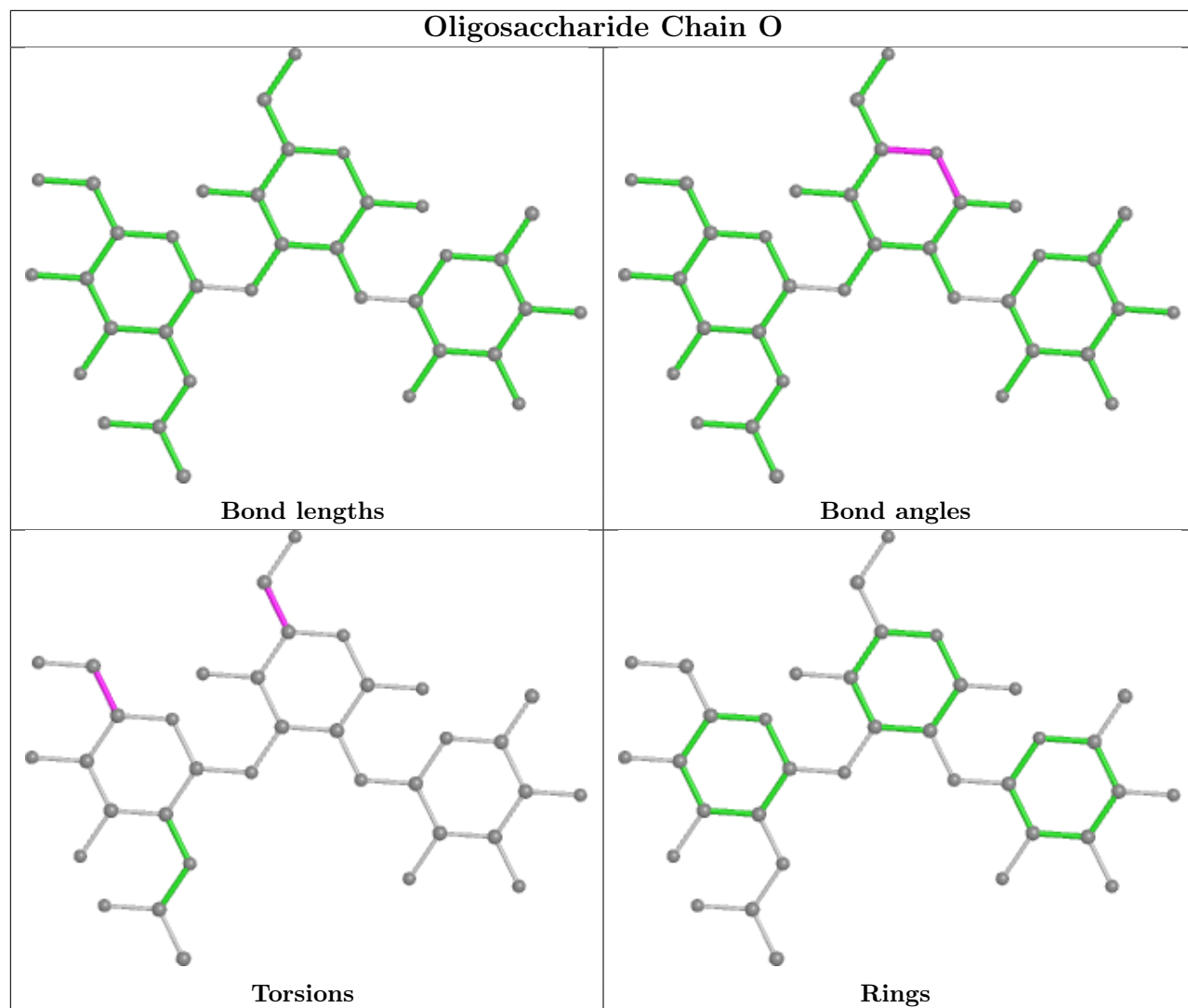
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



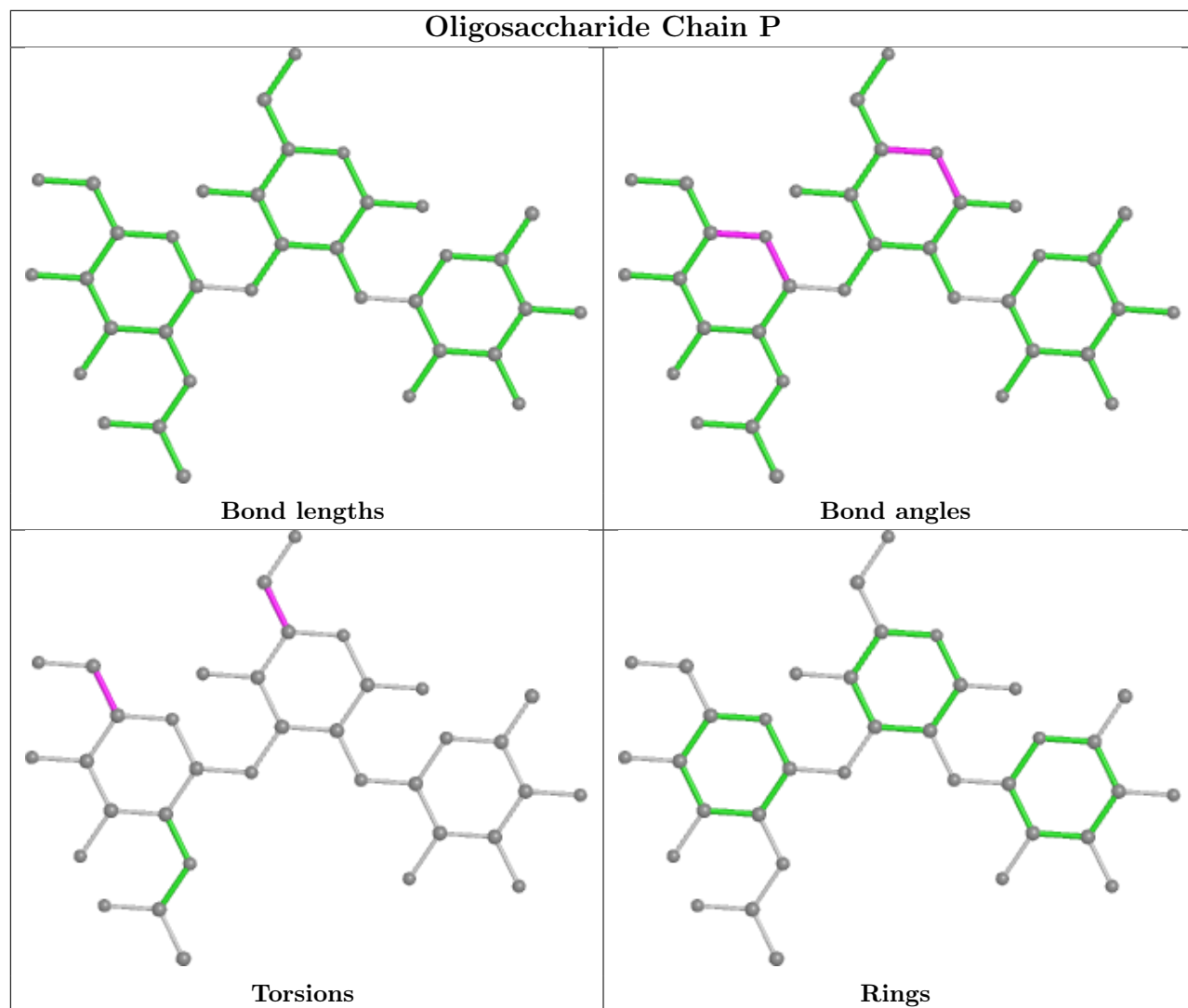


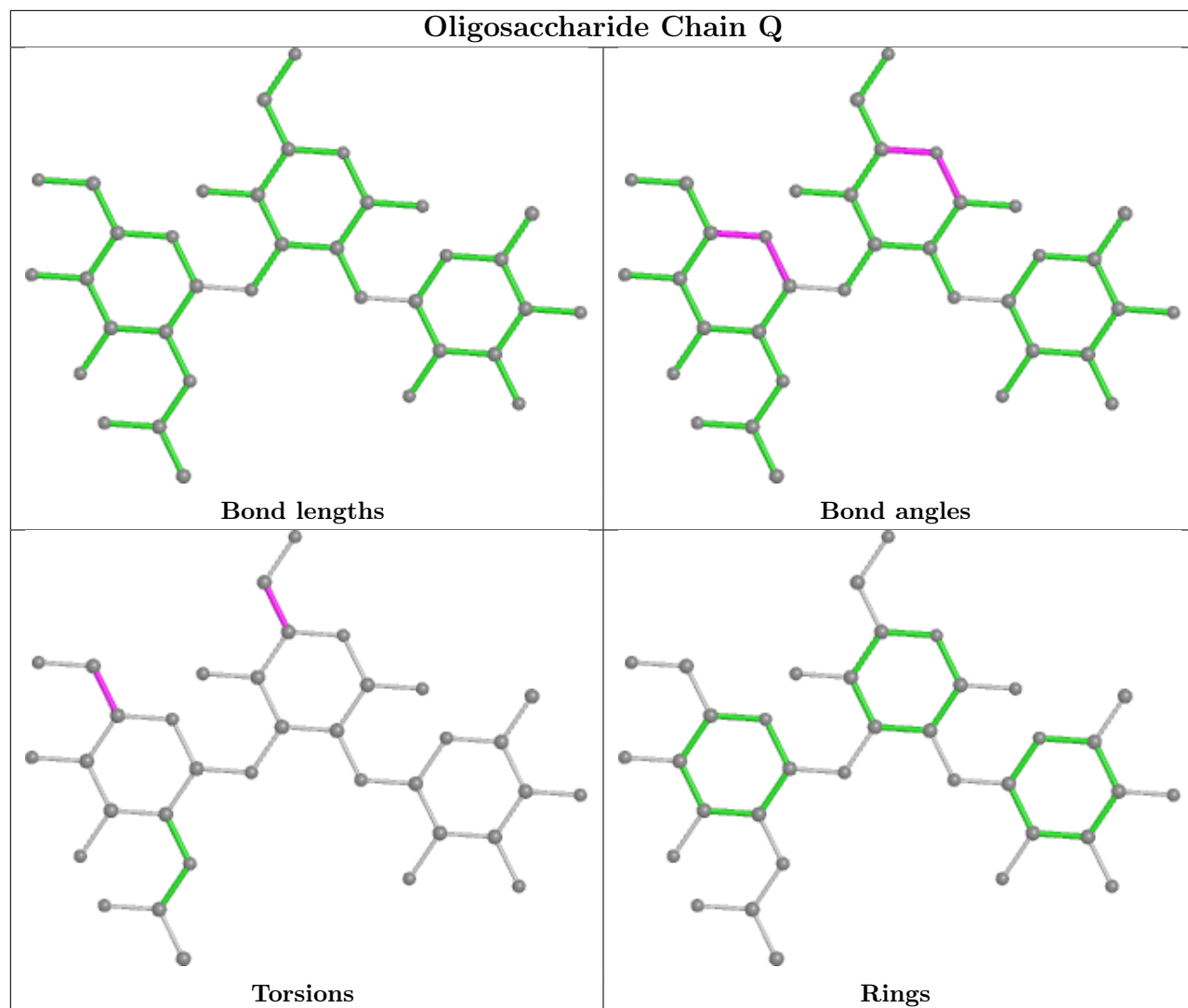


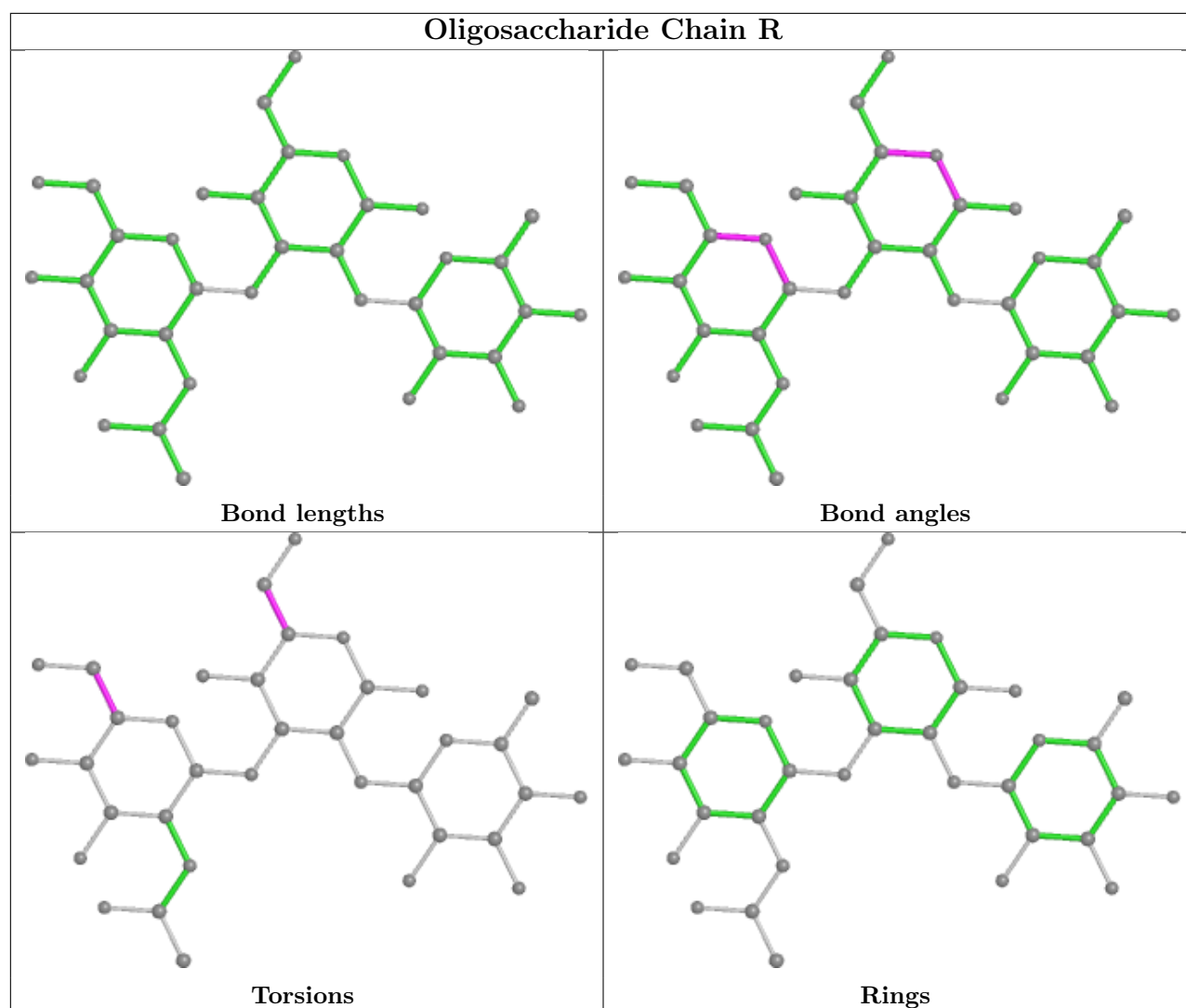












## 5.6 Ligand geometry [i](#)

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 [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	309/311 (99%)	-0.45	2 (0%) 89 90	16, 26, 50, 69	0
1	B	308/311 (99%)	-0.51	0 100 100	16, 28, 51, 74	0
1	C	311/311 (100%)	-0.36	1 (0%) 94 95	16, 30, 53, 79	0
1	D	307/311 (98%)	-0.37	4 (1%) 77 78	16, 29, 56, 75	0
1	E	309/311 (99%)	-0.36	2 (0%) 89 90	18, 29, 53, 72	0
1	F	308/311 (99%)	-0.27	3 (0%) 82 82	20, 37, 64, 86	0
1	G	308/311 (99%)	-0.47	3 (0%) 82 82	22, 35, 58, 85	0
1	H	293/311 (94%)	-0.36	6 (2%) 65 65	22, 41, 70, 81	0
1	I	286/311 (91%)	0.34	33 (11%) 4 3	34, 57, 81, 106	0
1	J	307/311 (98%)	-0.47	0 100 100	17, 29, 54, 69	0
All	All	3046/3110 (97%)	-0.33	54 (1%) 68 69	16, 33, 66, 106	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	336	GLN	7.4
1	I	524	PHE	5.4
1	I	375	PHE	5.4
1	I	295	GLY	4.6
1	I	296	THR	4.5

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

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

### 6.3 Carbohydrates [i](#)

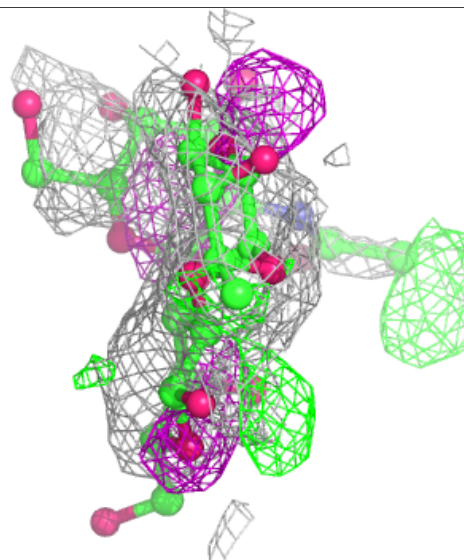
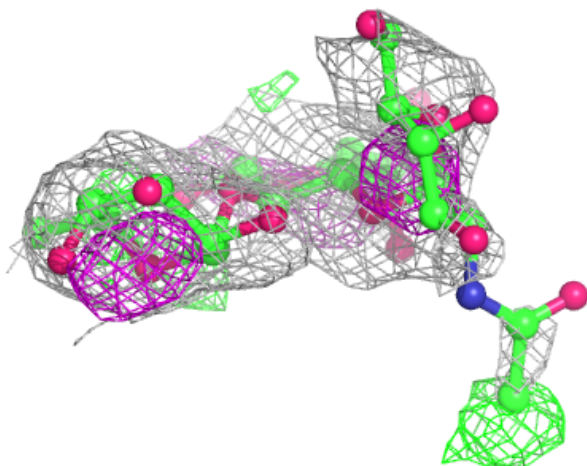
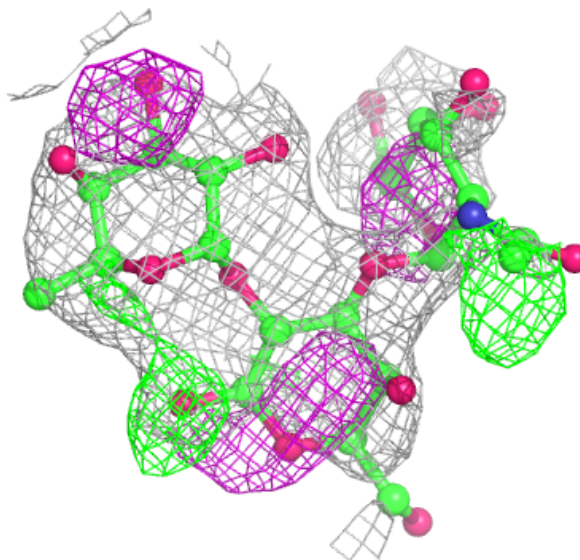
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GAL	K	1	12/12	0.58	0.47	83,93,95,99	0
2	A2G	K	3	14/15	0.62	0.50	102,104,105,105	0
2	A2G	N	3	14/15	0.65	0.60	112,114,118,118	0
2	GAL	M	1	12/12	0.68	0.41	87,98,98,102	0
2	A2G	M	3	14/15	0.69	0.59	105,109,110,110	0
2	A2G	O	3	14/15	0.69	0.72	110,111,112,112	0
2	GAL	O	1	12/12	0.70	0.42	89,101,102,105	0
2	A2G	R	3	14/15	0.70	0.45	91,97,100,101	0
2	A2G	P	3	14/15	0.71	0.50	108,115,120,121	0
2	A2G	Q	3	14/15	0.72	0.44	114,116,117,117	0
2	FUC	L	2	10/11	0.75	0.32	50,54,60,64	0
2	GAL	Q	1	12/12	0.75	0.42	102,109,110,114	0
2	GAL	N	1	12/12	0.77	0.54	93,103,105,110	0
2	GAL	P	1	12/12	0.78	0.40	100,108,110,113	0
2	FUC	O	2	10/11	0.79	0.34	65,73,77,81	0
2	A2G	L	3	14/15	0.80	0.42	93,95,96,96	0
2	FUC	R	2	10/11	0.81	0.26	65,69,72,74	0
2	GAL	R	1	12/12	0.81	0.33	81,91,92,93	0
2	FUC	M	2	10/11	0.82	0.29	67,71,76,79	0
2	FUC	P	2	10/11	0.82	0.31	83,89,91,93	0
2	GAL	L	1	12/12	0.83	0.42	75,87,89,90	0
2	FUC	Q	2	10/11	0.83	0.33	86,91,93,96	0
2	FUC	N	2	10/11	0.86	0.33	76,79,82,85	0
2	FUC	K	2	10/11	0.86	0.32	62,67,70,74	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.

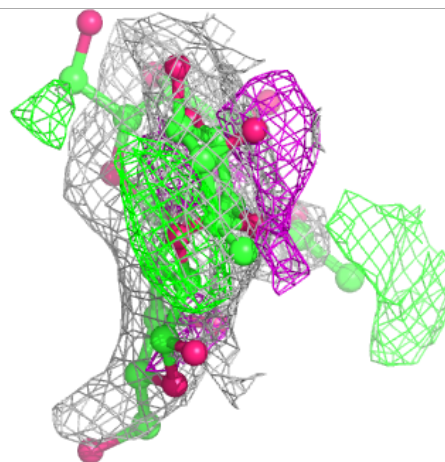
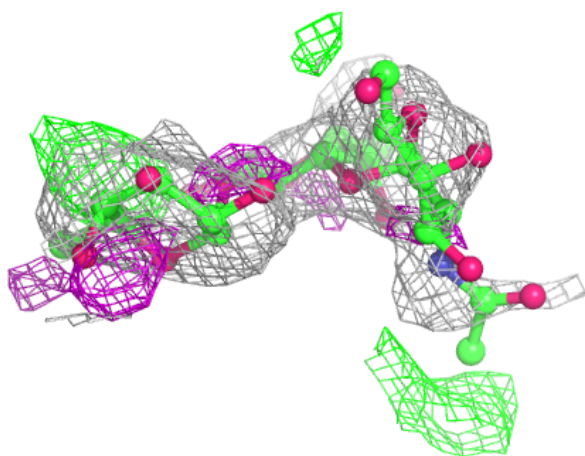
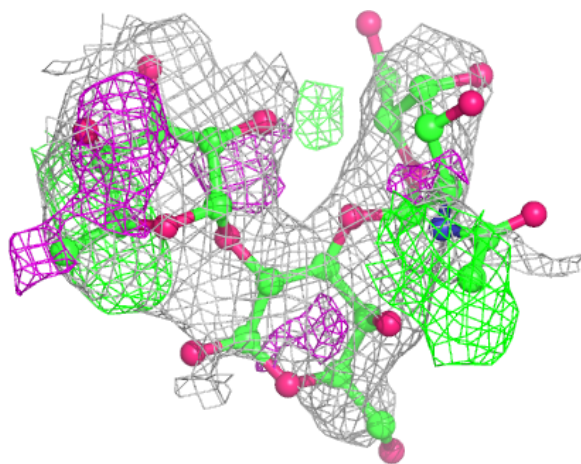
**Electron density around Chain K:**

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



**Electron density around Chain L:**

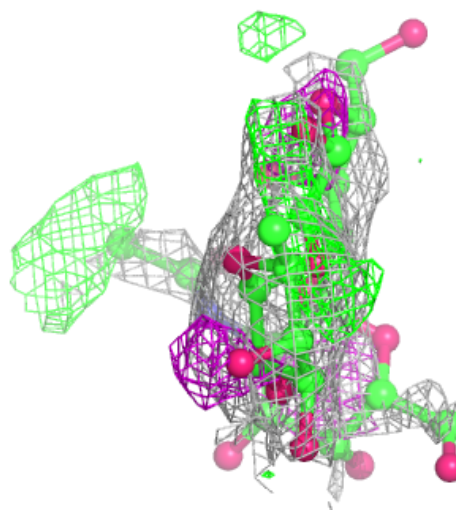
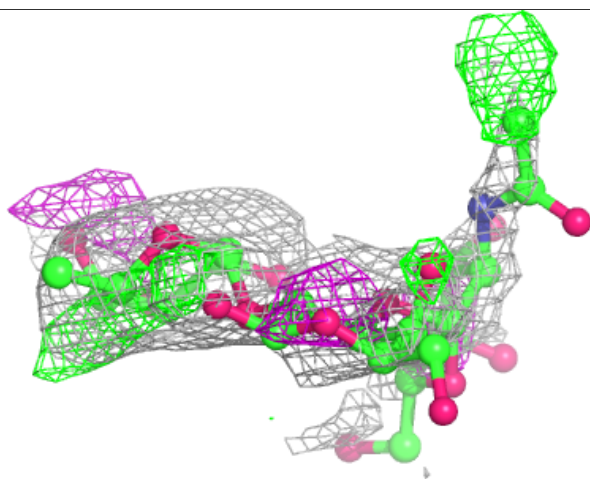
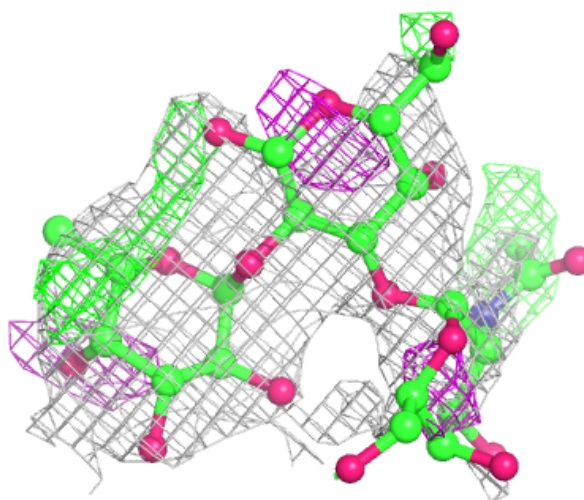
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain M:**

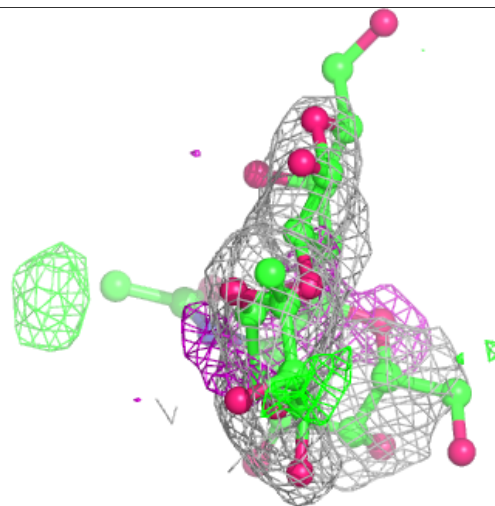
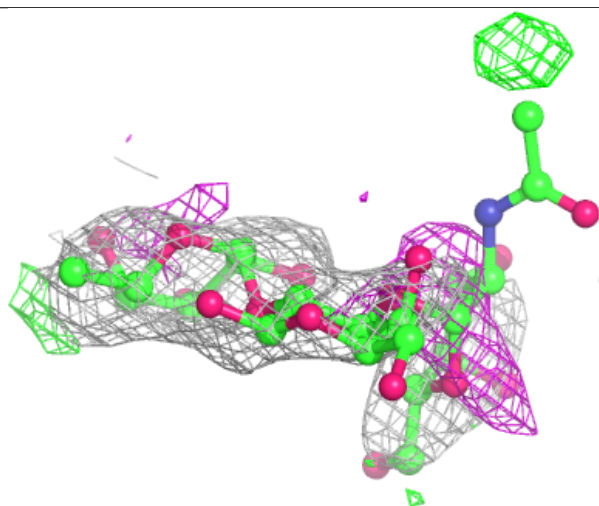
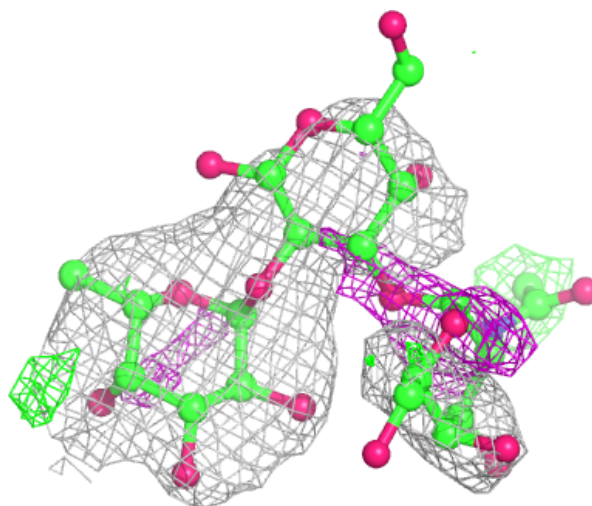
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





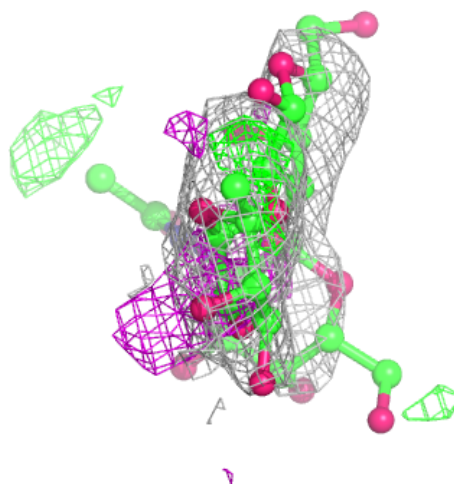
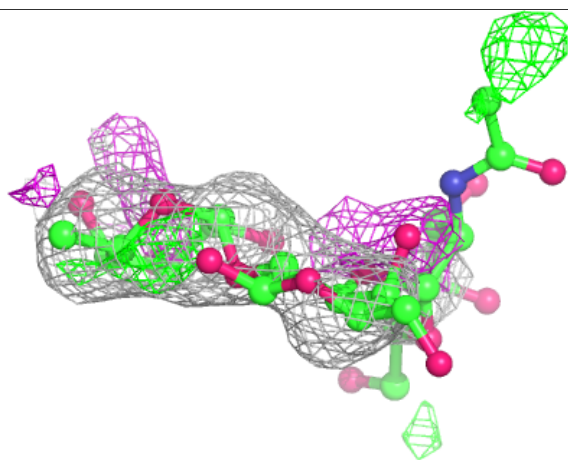
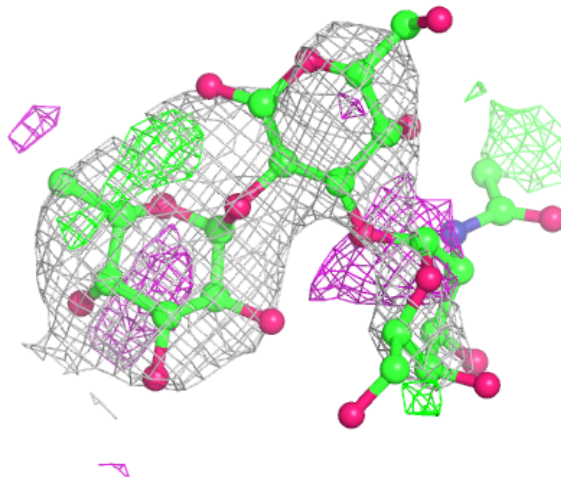
**Electron density around Chain N:**

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



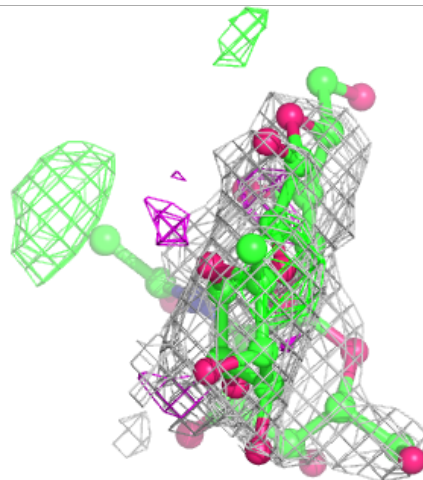
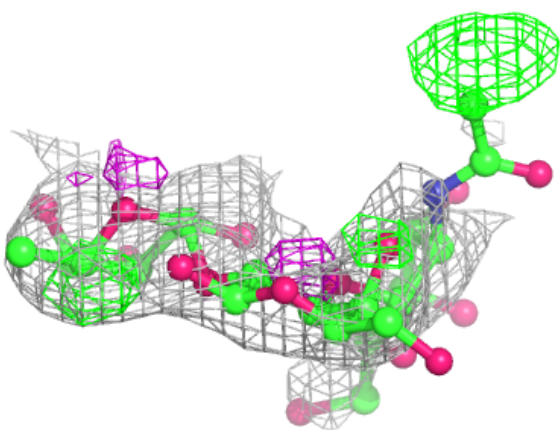
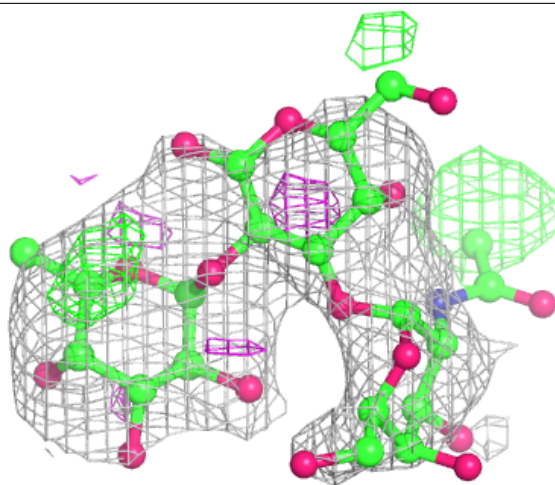
**Electron density around Chain O:**

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



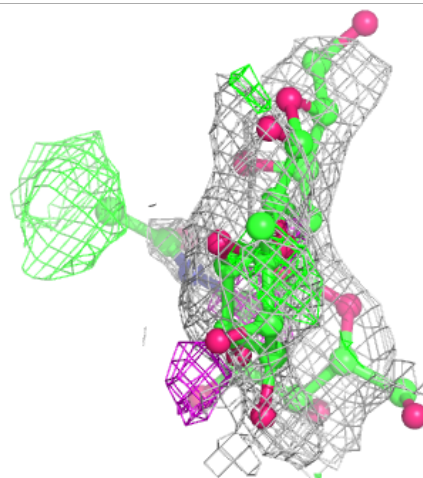
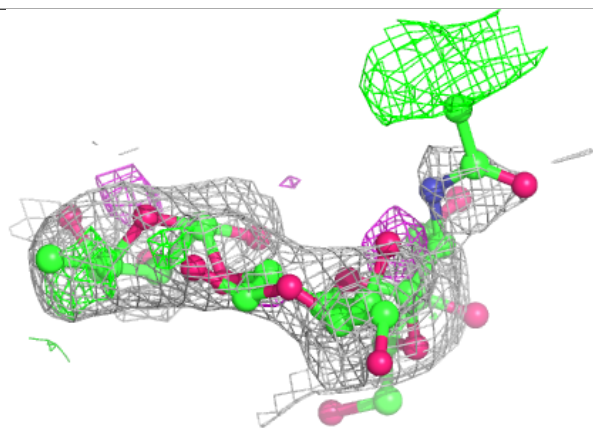
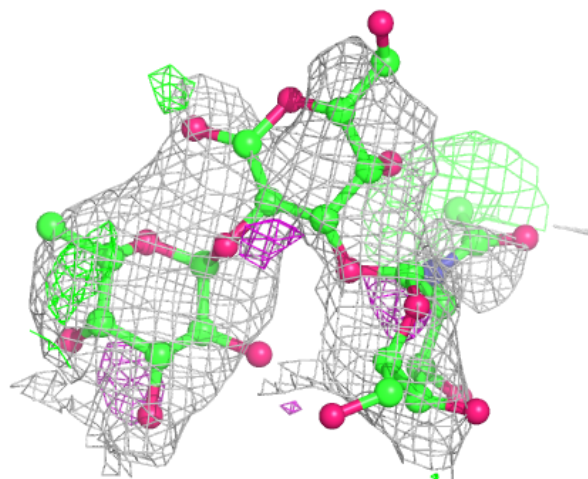
**Electron density around Chain P:**

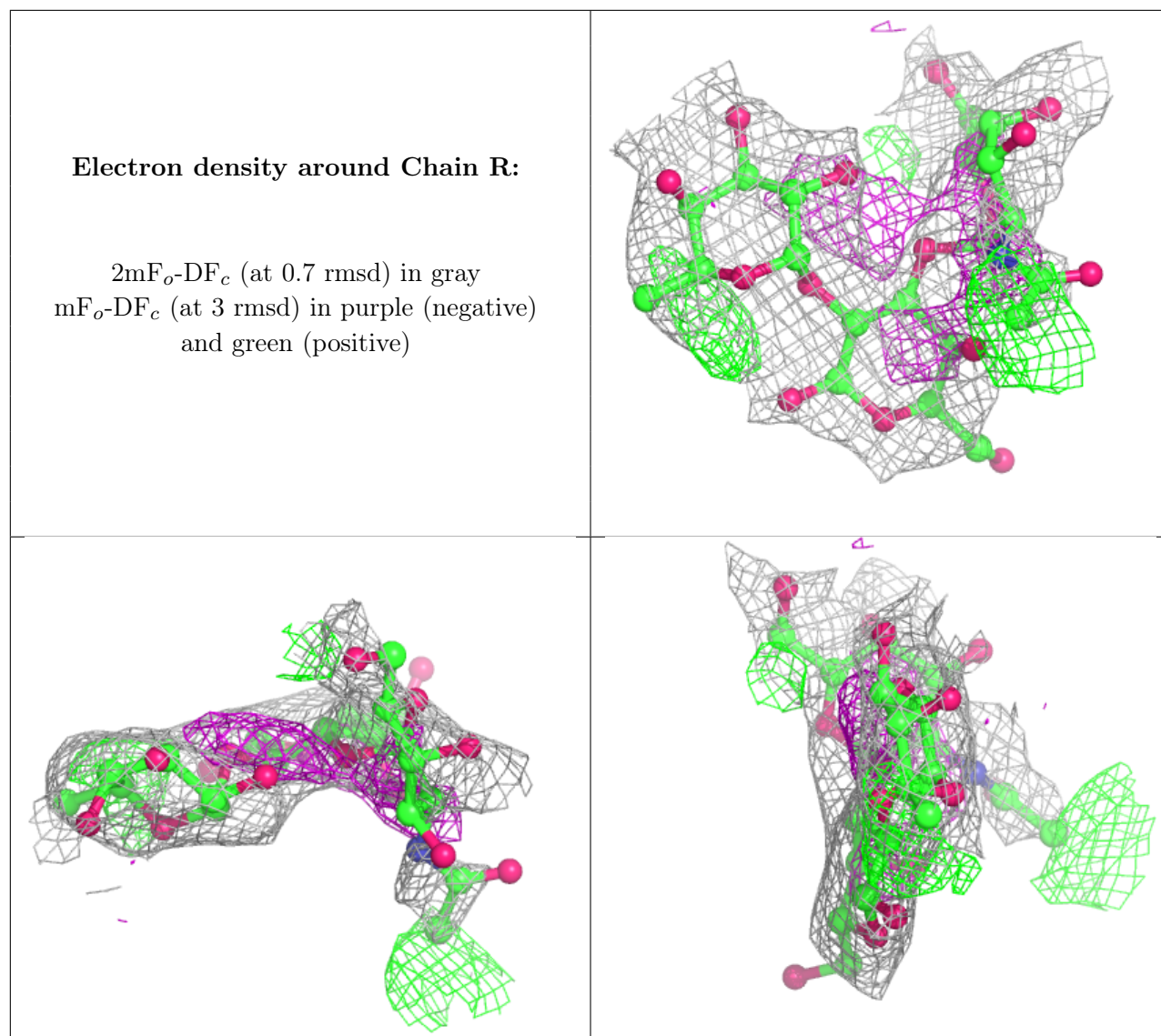
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain Q:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.