



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 02:18 PM BST

PDB ID : 3SLN  
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to H pentasaccharide  
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.  
Deposited on : 2011-06-24  
Resolution : 2.84 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

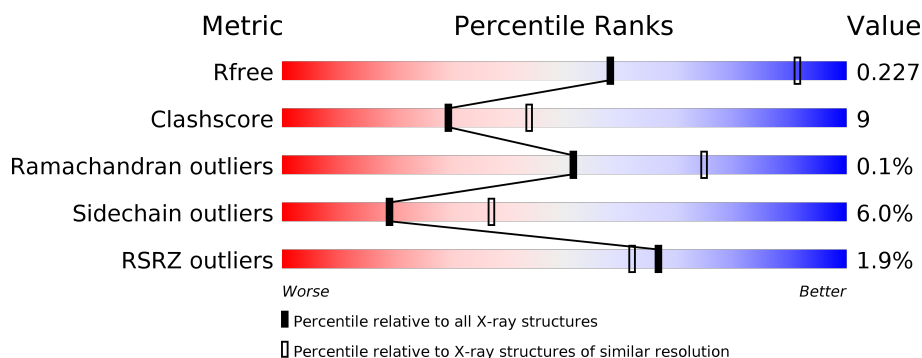
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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.



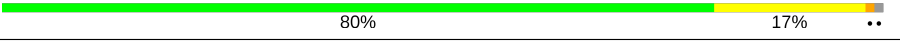





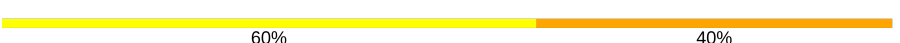

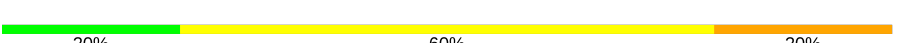
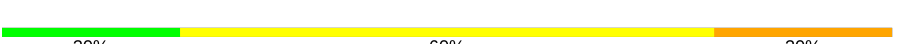
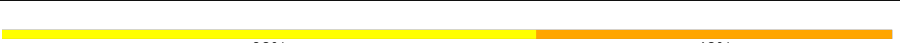
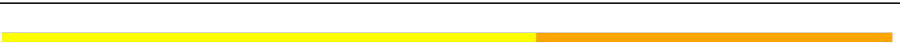
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	311	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	311	<div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	C	311	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	D	311	<div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	E	311	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	F	311	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	5	
2	L	5	
2	M	5	
2	N	5	
2	O	5	
2	P	5	
2	Q	5	
2	R	5	

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	BGC	K	1	-	-	X	-
2	GAL	K	2	-	-	X	X
2	NAG	K	3	-	-	-	X
2	BGC	L	1	-	-	-	X
2	GAL	L	2	-	-	-	X
2	NAG	L	3	-	-	-	X
2	GAL	L	4	-	-	-	X
2	BGC	M	1	-	-	-	X
2	GAL	M	2	-	-	-	X
2	NAG	M	3	-	-	-	X
2	BGC	N	1	-	-	X	X
2	GAL	N	2	-	-	X	X
2	NAG	N	3	-	-	-	X
2	GAL	N	4	-	-	-	X
2	BGC	O	1	-	-	-	X
2	GAL	O	2	-	-	-	X
2	NAG	O	3	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	O	4	-	-	-	X
2	FUC	O	5	-	-	X	-
2	BGC	P	1	-	-	-	X
2	GAL	P	2	-	-	X	X
2	NAG	P	3	-	-	-	X
2	BGC	Q	1	-	-	-	X
2	GAL	Q	2	-	-	-	X
2	BGC	R	1	-	-	X	X
2	GAL	R	2	-	-	X	X
2	NAG	R	3	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24066 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
1	A	309	Total	C	N	O	S	0	0	0
			2404	1517	415	462	10			
1	B	308	Total	C	N	O	S	0	0	0
			2392	1510	411	461	10			
1	C	311	Total	C	N	O	S	0	0	0
			2403	1514	413	466	10			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	410	458	10			
1	E	309	Total	C	N	O	S	0	0	0
			2406	1518	415	463	10			
1	F	308	Total	C	N	O	S	0	0	0
			2393	1511	411	461	10			
1	G	308	Total	C	N	O	S	0	0	0
			2383	1506	407	460	10			
1	H	292	Total	C	N	O	S	0	0	0
			2266	1441	385	431	9			
1	I	285	Total	C	N	O	S	0	0	0
			2184	1385	378	413	8			
1	J	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	10			

There are 30 discrepancies between the modelled and reference sequences:

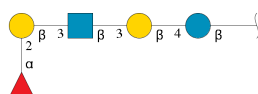
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	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)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	L	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	M	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	N	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	O	5	Total	C	N	O	0	0	0
			58	32	1	25			

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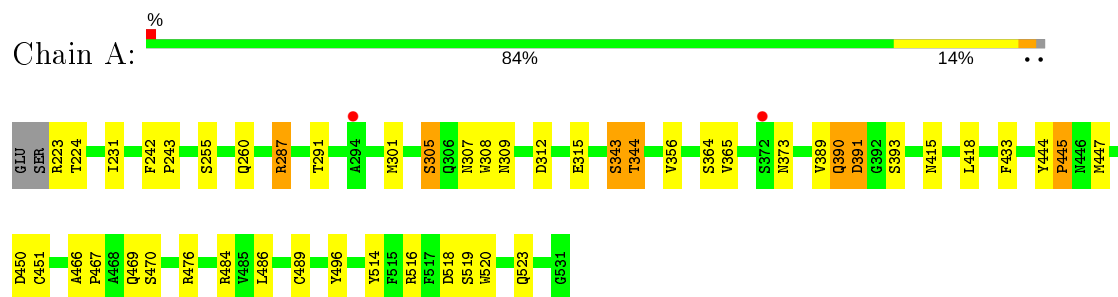
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	Q	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	R	5	Total	C	N	O	0	0	0
			58	32	1	25			

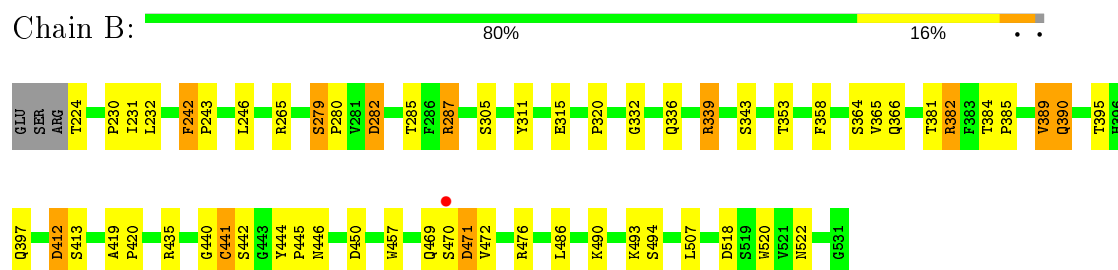
### 3 Residue-property plots

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.

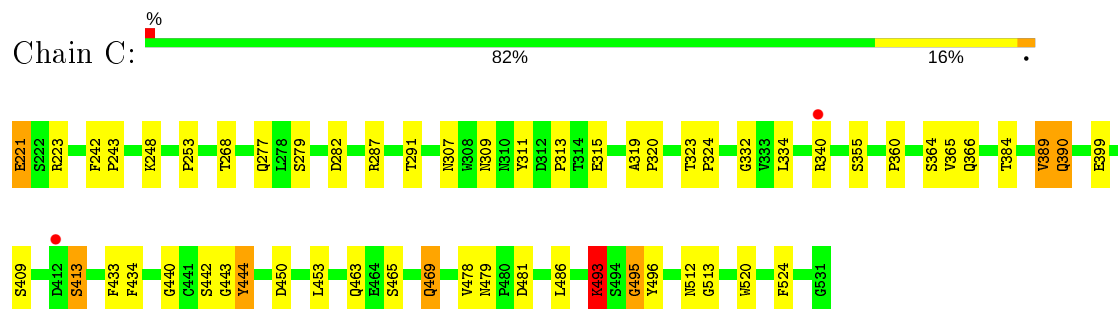
#### • Molecule 1: Capsid



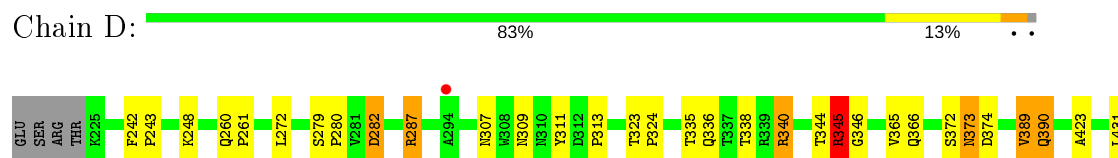
#### • Molecule 1: Capsid



#### • Molecule 1: Capsid



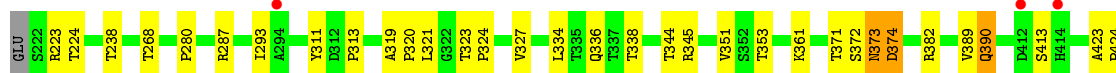
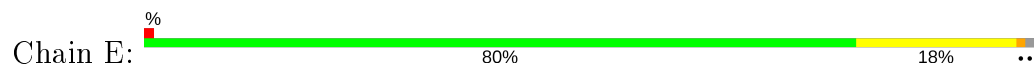
#### • Molecule 1: Capsid



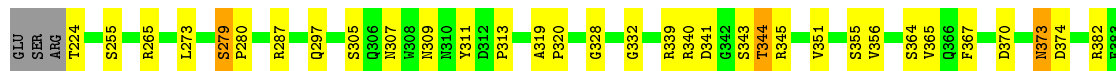
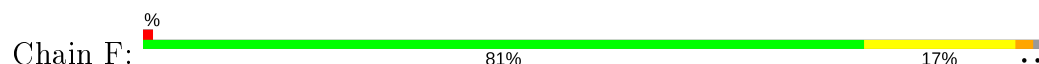




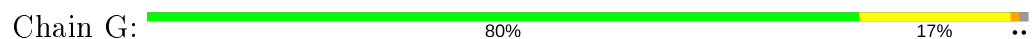
- Molecule 1: Capsid



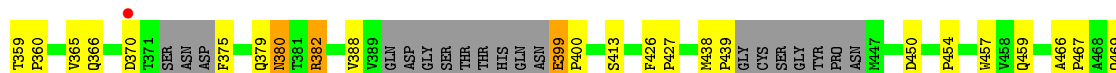
- Molecule 1: Capsid



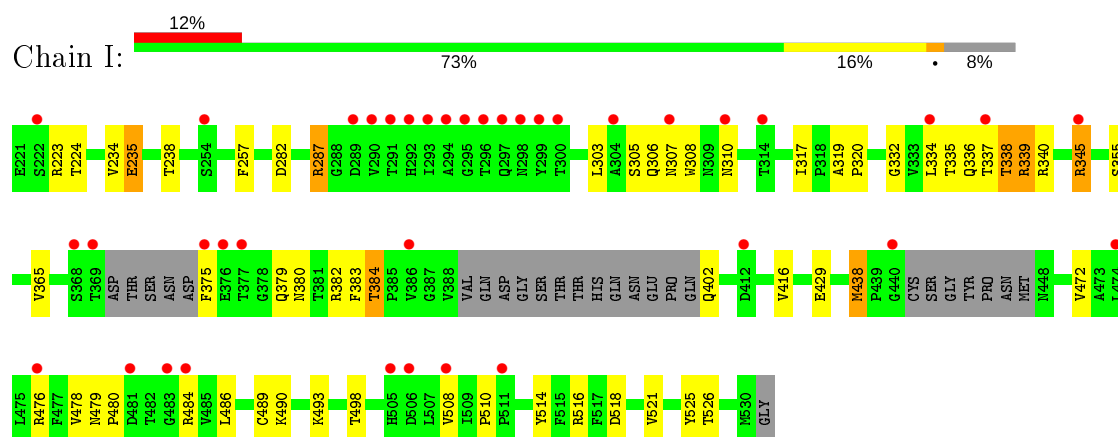
- Molecule 1: Capsid



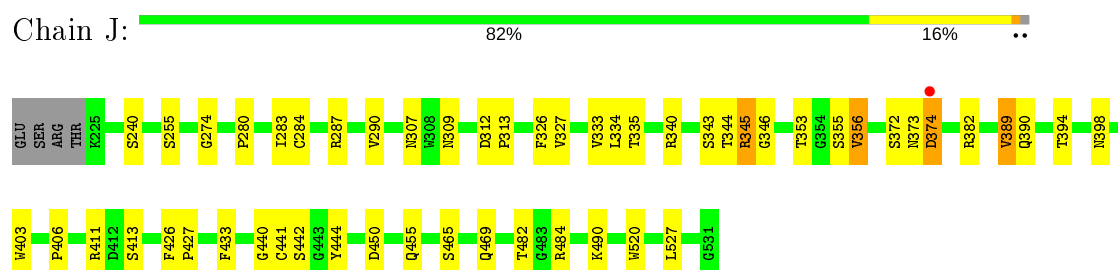
- Molecule 1: Capsid



- Molecule 1: Capsid



- Molecule 1: Capsid



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:  20% 80%

BGC1  
GAL2  
MAG3  
GAL4  
FUC5

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  20% 60% 20%

BGC1  
GAL2  
MAG3  
GAL4  
FUC5

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain P:  20% 60% 20%

BGC1  
GAL2  
MAG3  
GAL4  
FUC5

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Q:  60% 40%

BGC1  
GAL2  
MAG3  
GAL4  
FUC5

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R:  60% 40%

BGC1  
GAL2  
MAG3  
GAL4  
FUC5

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.22Å 339.03Å 124.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 2.84 39.52 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.85-2.84) 99.2 (39.52-2.84)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.187 , 0.231 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	6014 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 25.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: BGC, GAL, NAG, FUC

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	1.04	3/2474 (0.1%)	0.91	5/3385 (0.1%)
1	B	0.97	3/2462 (0.1%)	0.91	3/3369 (0.1%)
1	C	0.99	5/2472 (0.2%)	0.90	5/3384 (0.1%)
1	D	0.93	1/2455 (0.0%)	0.88	2/3360 (0.1%)
1	E	0.96	1/2476 (0.0%)	0.89	3/3388 (0.1%)
1	F	0.85	0/2463	0.91	5/3371 (0.1%)
1	G	0.87	0/2453	0.85	2/3359 (0.1%)
1	H	0.91	2/2330 (0.1%)	0.88	4/3186 (0.1%)
1	I	0.90	2/2245 (0.1%)	0.77	1/3071 (0.0%)
1	J	0.86	0/2456	0.83	0/3361
All	All	0.93	17/24286 (0.1%)	0.87	30/33234 (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	A	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	340	ARG	CB-CG	-8.15	1.30	1.52
1	H	340	ARG	CZ-NH1	-8.09	1.22	1.33
1	A	451	CYS	CB-SG	-6.12	1.71	1.82
1	B	518	ASP	CB-CG	6.02	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	GLU	CG-CD	6.00	1.60	1.51

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	241	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	496	TYR	N-CA-CB	-7.74	96.66	110.60
1	F	496	TYR	N-CA-CB	-7.01	97.99	110.60
1	A	496	TYR	N-CA-CB	-6.99	98.02	110.60
1	F	345	ARG	N-CA-CB	-6.95	98.08	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	SER	Peptide
1	D	345	ARG	Sidechain
1	E	223	ARG	Sidechain
1	H	336	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2404	0	2295	36	0
1	B	2392	0	2278	44	0
1	C	2403	0	2282	38	0
1	D	2385	0	2272	46	0
1	E	2406	0	2297	31	0
1	F	2393	0	2282	50	0
1	G	2383	0	2265	40	0
1	H	2266	0	2169	55	0
1	I	2184	0	2068	41	0
1	J	2386	0	2275	40	0
2	K	58	0	51	10	0
2	L	58	0	49	5	0
2	M	58	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	58	0	51	11	1
2	O	58	0	51	12	0
2	P	58	0	51	7	0
2	Q	58	0	51	5	0
2	R	58	0	51	14	0
All	All	24066	0	22889	445	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 9.

The worst 5 of 445 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:G:411:ARG:O	1:G:412:ASP:HB3	1.45	1.17
2:Q:3:NAG:O3	2:Q:5:FUC:H5	1.44	1.16
1:B:339:ARG:HH11	1:B:339:ARG:HG3	1.01	1.15
1:H:382:ARG:CG	1:H:382:ARG:HH11	1.60	1.12
1:H:382:ARG:HG2	1:H:382:ARG:NH1	1.54	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)
2:N:1:BGC:O2	2:N:2:GAL:O2[3_553]	1.29	0.91

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	295 (96%)	11 (4%)	1 (0%)	41 61
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	309/311 (99%)	296 (96%)	13 (4%)	0	100	100
1	D	305/311 (98%)	290 (95%)	15 (5%)	0	100	100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100	100
1	F	306/311 (98%)	294 (96%)	12 (4%)	0	100	100
1	G	306/311 (98%)	286 (94%)	18 (6%)	2 (1%)	22	42
1	H	284/311 (91%)	270 (95%)	14 (5%)	0	100	100
1	I	277/311 (89%)	258 (93%)	19 (7%)	0	100	100
1	J	305/311 (98%)	292 (96%)	13 (4%)	0	100	100
All	All	3012/3110 (97%)	2873 (95%)	136 (4%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	357	HIS
1	G	412	ASP
1	A	445	PRO

### 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	270/272 (99%)	255 (94%)	15 (6%)	21	40
1	B	269/272 (99%)	252 (94%)	17 (6%)	18	34
1	C	269/272 (99%)	254 (94%)	15 (6%)	21	40
1	D	267/272 (98%)	254 (95%)	13 (5%)	25	47
1	E	271/272 (100%)	256 (94%)	15 (6%)	21	41
1	F	269/272 (99%)	255 (95%)	14 (5%)	23	44
1	G	267/272 (98%)	253 (95%)	14 (5%)	23	44
1	H	253/272 (93%)	236 (93%)	17 (7%)	16	32
1	I	238/272 (88%)	213 (90%)	25 (10%)	7	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	268/272 (98%)	254 (95%)	14 (5%)	23	44
All	All	2641/2720 (97%)	2482 (94%)	159 (6%)	19	37

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	476	ARG
1	G	234	VAL
1	J	287	ARG
1	E	523	GLN
1	F	339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	523	GLN
1	F	390	GLN
1	J	390	GLN
1	F	297	GLN
1	F	373	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 ⓘ

40 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	K	1	2	12,12,12	0.90	1 (8%)	17,17,17	1.92	3 (17%)
2	GAL	K	2	2	11,11,12	0.62	0	15,15,17	2.77	7 (46%)
2	NAG	K	3	2	14,14,15	1.48	2 (14%)	17,19,21	2.80	2 (11%)
2	GAL	K	4	2	11,11,12	1.49	2 (18%)	15,15,17	2.97	6 (40%)
2	FUC	K	5	2	10,10,11	0.40	0	14,14,16	0.87	0
2	BGC	L	1	2	12,12,12	0.59	0	17,17,17	1.77	3 (17%)
2	GAL	L	2	2	11,11,12	0.62	0	15,15,17	4.91	4 (26%)
2	NAG	L	3	2	14,14,15	1.84	1 (7%)	17,19,21	3.94	10 (58%)
2	GAL	L	4	2	11,11,12	1.02	1 (9%)	15,15,17	2.22	5 (33%)
2	FUC	L	5	2	10,10,11	0.42	0	14,14,16	0.84	0
2	BGC	M	1	2	12,12,12	0.38	0	17,17,17	2.08	3 (17%)
2	GAL	M	2	2	11,11,12	0.44	0	15,15,17	2.48	4 (26%)
2	NAG	M	3	2	14,14,15	0.62	0	17,19,21	2.41	4 (23%)
2	GAL	M	4	2	11,11,12	0.84	0	15,15,17	2.59	4 (26%)
2	FUC	M	5	2	10,10,11	1.26	1 (10%)	14,14,16	2.70	3 (21%)
2	BGC	N	1	2	12,12,12	0.90	1 (8%)	17,17,17	1.91	3 (17%)
2	GAL	N	2	2	11,11,12	0.63	0	15,15,17	2.76	7 (46%)
2	NAG	N	3	2	14,14,15	1.49	2 (14%)	17,19,21	2.80	2 (11%)
2	GAL	N	4	2	11,11,12	1.49	2 (18%)	15,15,17	2.98	6 (40%)
2	FUC	N	5	2	10,10,11	0.41	0	14,14,16	0.87	0
2	BGC	O	1	2	12,12,12	0.49	0	17,17,17	0.78	1 (5%)
2	GAL	O	2	2	11,11,12	0.38	0	15,15,17	0.90	0
2	NAG	O	3	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
2	GAL	O	4	2	11,11,12	0.33	0	15,15,17	0.82	0
2	FUC	O	5	2	10,10,11	0.42	0	14,14,16	0.84	0
2	BGC	P	1	2	12,12,12	0.49	0	17,17,17	0.76	1 (5%)
2	GAL	P	2	2	11,11,12	0.37	0	15,15,17	0.89	0
2	NAG	P	3	2	14,14,15	0.54	0	17,19,21	0.91	0
2	GAL	P	4	2	11,11,12	0.33	0	15,15,17	0.82	0
2	FUC	P	5	2	10,10,11	0.42	0	14,14,16	0.83	0
2	BGC	Q	1	2	12,12,12	0.50	0	17,17,17	0.77	1 (5%)
2	GAL	Q	2	2	11,11,12	0.38	0	15,15,17	0.90	0
2	NAG	Q	3	2	14,14,15	0.54	0	17,19,21	0.91	0
2	GAL	Q	4	2	11,11,12	0.32	0	15,15,17	0.83	1 (6%)
2	FUC	Q	5	2	10,10,11	0.43	0	14,14,16	0.84	0
2	BGC	R	1	2	12,12,12	0.49	0	17,17,17	0.78	1 (5%)
2	GAL	R	2	2	11,11,12	0.37	0	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	R	3	2	14,14,15	0.54	0	17,19,21	1.03	0
2	GAL	R	4	2	11,11,12	0.33	0	15,15,17	0.83	0
2	FUC	R	5	2	10,10,11	0.42	0	14,14,16	0.83	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	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	2/2/19/22	0/1/1/1
2	NAG	K	3	2	-	0/6/23/26	0/1/1/1
2	GAL	K	4	2	-	2/2/19/22	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	GAL	L	2	2	-	1/2/19/22	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	4	2	-	2/2/19/22	0/1/1/1
2	FUC	L	5	2	-	-	0/1/1/1
2	BGC	M	1	2	-	2/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	NAG	M	3	2	-	0/6/23/26	0/1/1/1
2	GAL	M	4	2	-	1/2/19/22	0/1/1/1
2	FUC	M	5	2	-	-	0/1/1/1
2	BGC	N	1	2	-	2/2/22/22	0/1/1/1
2	GAL	N	2	2	-	2/2/19/22	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1
2	GAL	N	4	2	-	2/2/19/22	0/1/1/1
2	FUC	N	5	2	-	-	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1
2	NAG	O	3	2	-	1/6/23/26	0/1/1/1
2	GAL	O	4	2	-	2/2/19/22	0/1/1/1
2	FUC	O	5	2	-	-	0/1/1/1
2	BGC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	2/2/19/22	0/1/1/1
2	NAG	P	3	2	-	1/6/23/26	0/1/1/1
2	GAL	P	4	2	-	0/2/19/22	0/1/1/1
2	FUC	P	5	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	2/2/19/22	0/1/1/1
2	NAG	Q	3	2	-	0/6/23/26	0/1/1/1
2	GAL	Q	4	2	-	2/2/19/22	0/1/1/1
2	FUC	Q	5	2	-	-	0/1/1/1
2	BGC	R	1	2	-	0/2/22/22	0/1/1/1
2	GAL	R	2	2	-	2/2/19/22	0/1/1/1
2	NAG	R	3	2	-	2/6/23/26	0/1/1/1
2	GAL	R	4	2	-	1/2/19/22	0/1/1/1
2	FUC	R	5	2	-	-	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	NAG	O3-C3	6.11	1.57	1.43
2	N	3	NAG	C1-C2	4.05	1.58	1.52
2	K	3	NAG	C1-C2	4.00	1.58	1.52
2	N	4	GAL	O5-C1	-3.46	1.38	1.43
2	K	4	GAL	O5-C1	-3.44	1.38	1.43

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GAL	O3-C3-C2	-13.54	84.07	109.99
2	L	2	GAL	O3-C3-C4	10.15	133.81	110.35
2	L	3	NAG	O3-C3-C4	-9.68	87.98	110.35
2	N	3	NAG	C6-C5-C4	-9.39	91.00	113.00
2	K	3	NAG	C6-C5-C4	-9.38	91.04	113.00

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

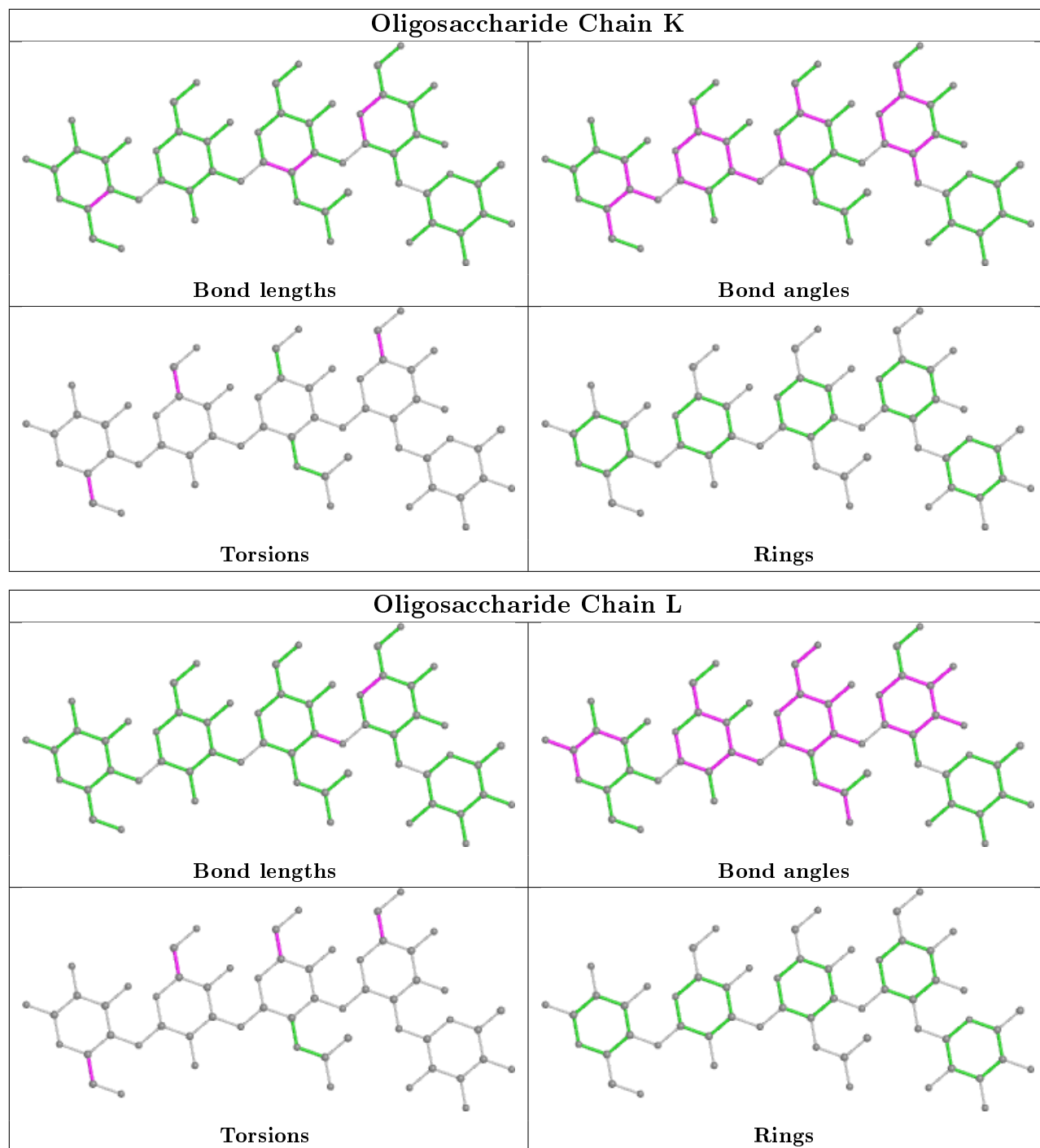
Mol	Chain	Res	Type	Atoms
2	R	2	GAL	O5-C5-C6-O6
2	Q	1	BGC	C4-C5-C6-O6
2	Q	2	GAL	O5-C5-C6-O6
2	R	2	GAL	C4-C5-C6-O6
2	M	1	BGC	O5-C5-C6-O6

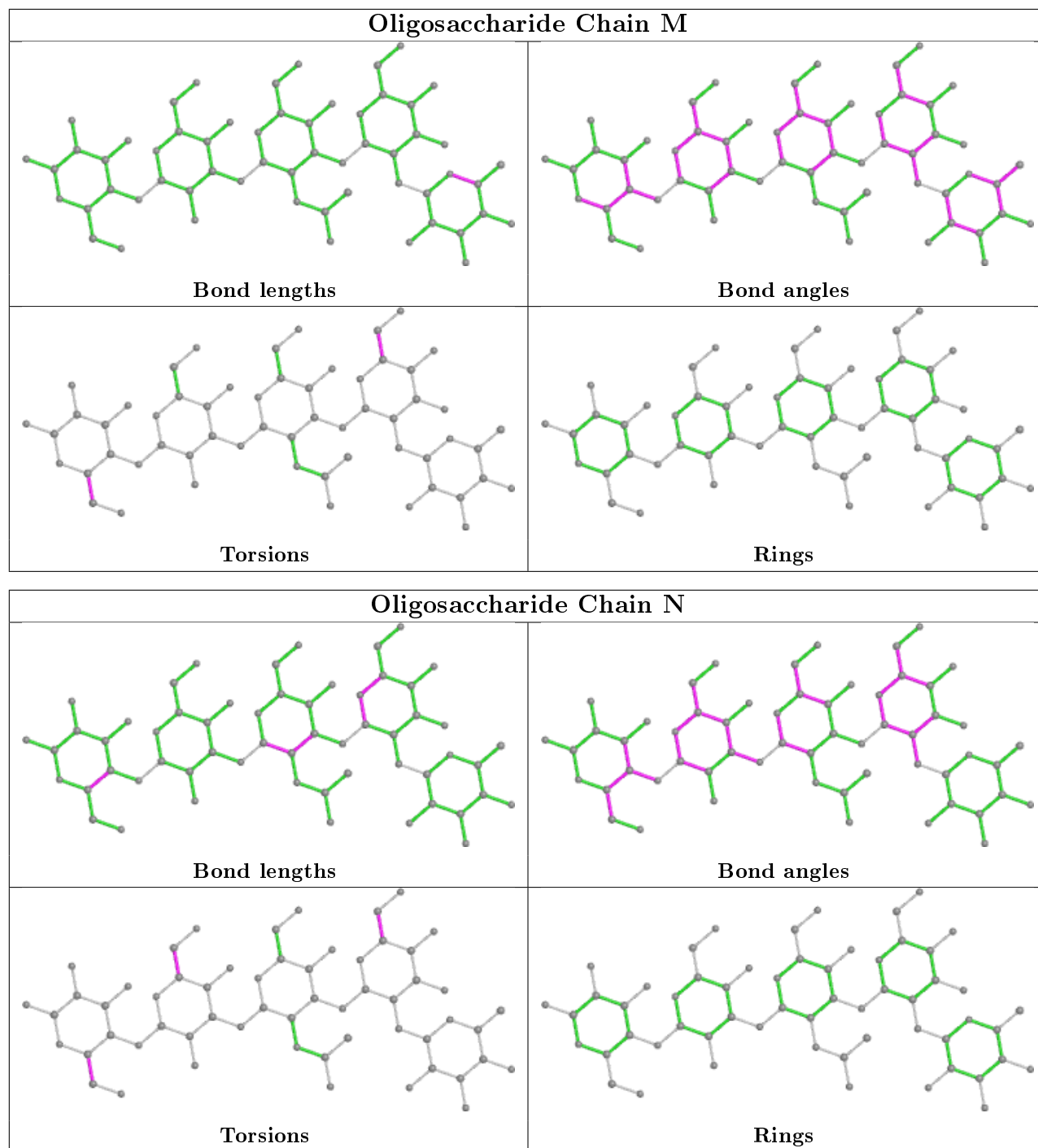
There are no ring outliers.

30 monomers are involved in 67 short contacts:

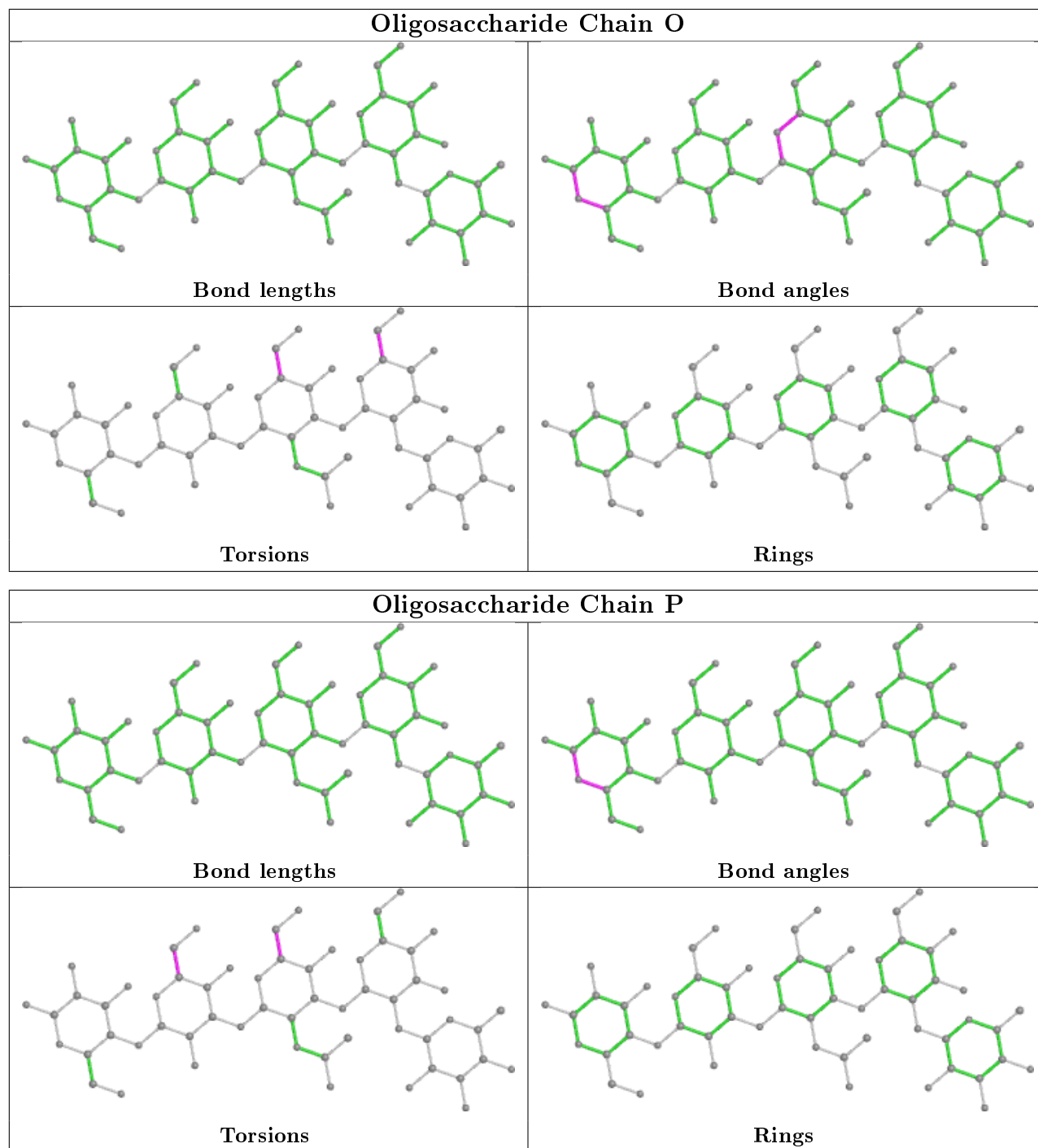
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	3	NAG	2	0
2	Q	5	FUC	4	0
2	Q	4	GAL	2	0
2	R	2	GAL	8	0
2	P	2	GAL	6	0
2	N	1	BGC	9	1
2	L	1	BGC	4	0
2	N	4	GAL	1	0
2	Q	2	GAL	1	0
2	R	4	GAL	1	0
2	R	3	NAG	5	0
2	R	1	BGC	6	0
2	Q	1	BGC	1	0
2	P	1	BGC	4	0
2	Q	3	NAG	2	0
2	K	2	GAL	9	0
2	N	2	GAL	10	1
2	K	1	BGC	8	0
2	R	5	FUC	5	0
2	M	2	GAL	2	0
2	O	2	GAL	2	0
2	O	3	NAG	3	0
2	K	3	NAG	2	0
2	K	4	GAL	1	0
2	P	3	NAG	2	0
2	P	4	GAL	1	0
2	O	5	FUC	10	0
2	L	2	GAL	3	0
2	L	5	FUC	1	0
2	M	3	NAG	2	0

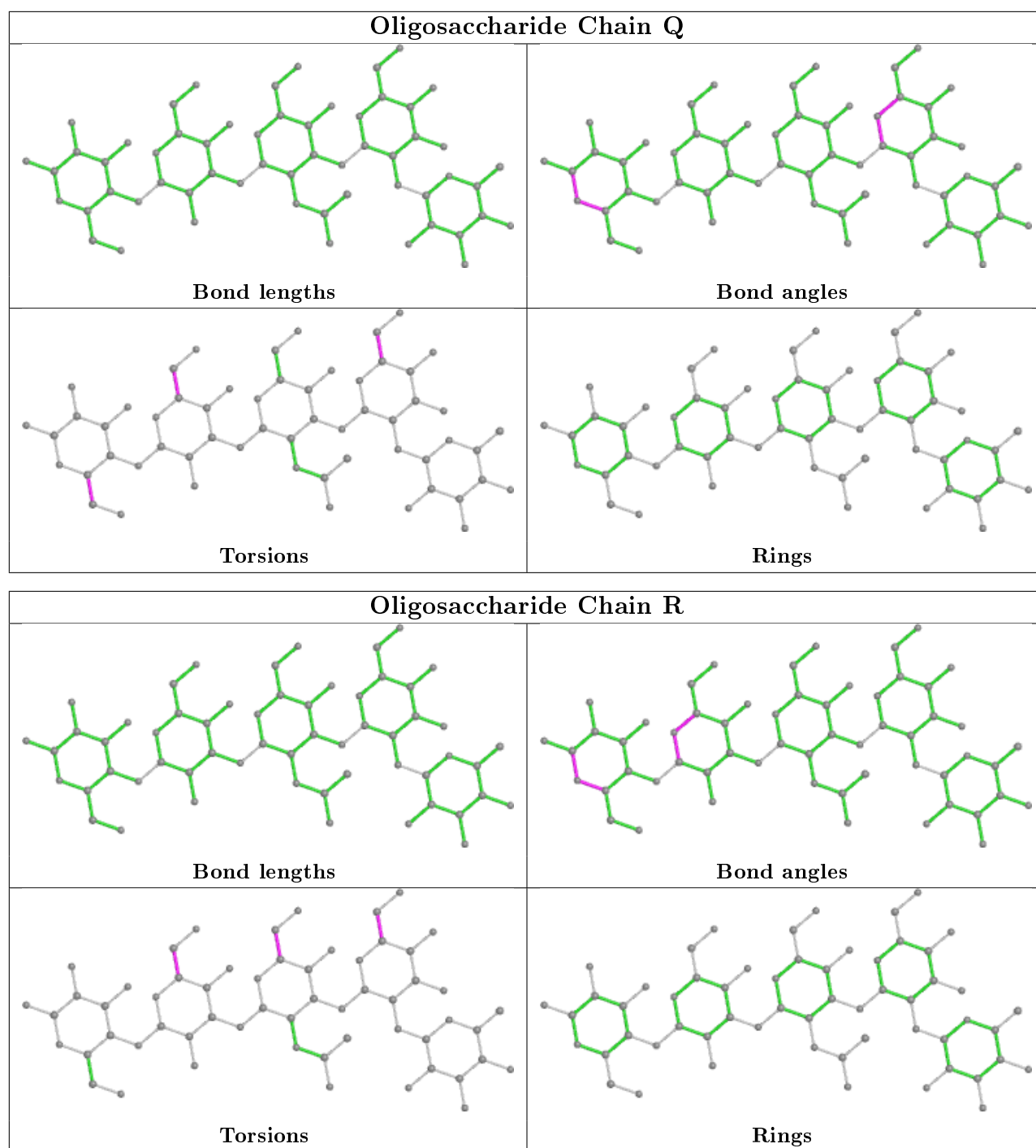
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 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 ⓘ

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	309/311 (99%)	-0.33	2 (0%) 89 88	29, 41, 66, 80	0
1	B	308/311 (99%)	-0.47	1 (0%) 94 93	32, 44, 67, 78	0
1	C	311/311 (100%)	-0.24	2 (0%) 89 88	30, 45, 68, 93	0
1	D	307/311 (98%)	-0.33	1 (0%) 94 93	29, 45, 77, 95	0
1	E	309/311 (99%)	-0.21	4 (1%) 77 74	32, 47, 76, 89	0
1	F	308/311 (99%)	-0.13	3 (0%) 82 79	38, 57, 87, 103	0
1	G	308/311 (99%)	-0.24	1 (0%) 94 93	41, 57, 82, 118	0
1	H	292/311 (93%)	-0.21	4 (1%) 75 71	34, 59, 93, 117	0
1	I	285/311 (91%)	0.57	38 (13%) 3 2	52, 83, 121, 146	0
1	J	307/311 (98%)	-0.18	1 (0%) 94 93	38, 53, 84, 105	0
All	All	3044/3110 (97%)	-0.18	57 (1%) 66 62	29, 52, 89, 146	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	377	THR	5.6
1	I	369	THR	4.3
1	I	296	THR	4.1
1	I	295	GLY	3.6
1	I	508	VAL	3.4

### 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.

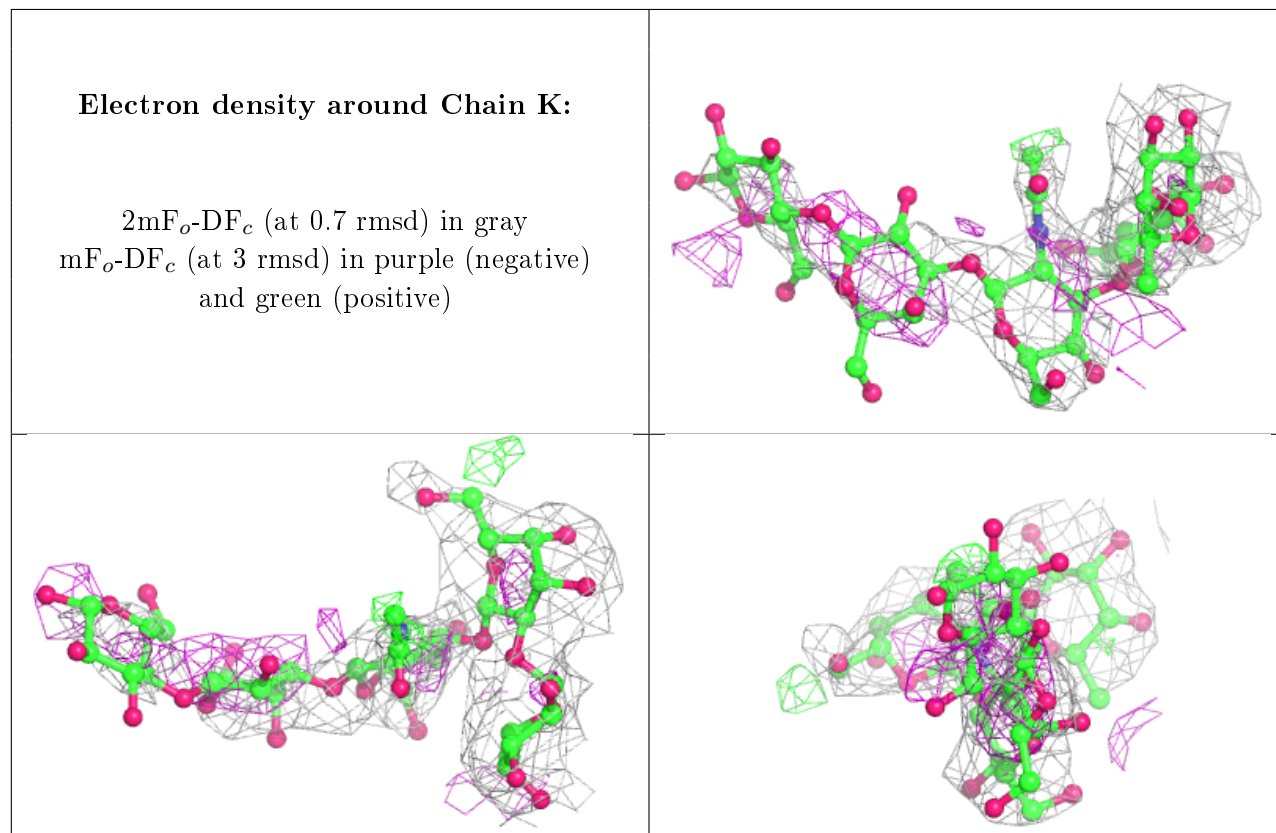
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	L	1	12/12	-0.09	1.72	178,181,181,182	0
2	BGC	N	1	12/12	0.31	0.56	139,141,141,141	0
2	NAG	L	3	14/15	0.32	0.79	155,162,164,166	0
2	GAL	M	2	11/12	0.33	0.72	147,151,153,153	0
2	BGC	Q	1	12/12	0.37	0.55	145,149,150,150	0
2	BGC	R	1	12/12	0.48	0.65	155,158,159,159	0
2	BGC	M	1	12/12	0.49	0.67	149,153,153,153	0
2	GAL	N	2	11/12	0.50	0.47	132,135,137,137	0
2	GAL	L	4	11/12	0.53	0.52	137,144,147,148	0
2	NAG	R	3	14/15	0.56	0.76	142,147,149,149	0
2	GAL	Q	2	11/12	0.58	0.50	145,146,147,148	0
2	BGC	P	1	12/12	0.58	0.84	162,163,164,164	0
2	GAL	R	2	11/12	0.58	0.57	151,152,154,154	0
2	GAL	L	2	11/12	0.58	0.96	169,174,175,176	0
2	GAL	R	4	11/12	0.63	0.40	134,136,138,139	0
2	GAL	N	4	11/12	0.66	0.44	115,119,122,122	0
2	BGC	O	1	12/12	0.69	0.60	145,146,147,147	0
2	GAL	K	2	11/12	0.69	0.73	132,135,137,137	0
2	NAG	P	3	14/15	0.70	0.79	147,153,156,156	0
2	GAL	K	4	11/12	0.70	0.38	115,119,122,122	0
2	FUC	R	5	10/11	0.73	0.36	129,131,131,132	0
2	GAL	O	4	11/12	0.74	0.44	124,129,131,131	0
2	FUC	L	5	10/11	0.74	0.35	123,126,129,131	0
2	NAG	O	3	14/15	0.76	0.58	132,135,138,139	0
2	NAG	M	3	14/15	0.76	0.50	137,140,142,144	0
2	GAL	O	2	11/12	0.77	0.60	142,146,147,147	0
2	NAG	K	3	14/15	0.77	0.51	124,127,129,130	0
2	FUC	O	5	10/11	0.78	0.35	112,116,117,119	0
2	NAG	N	3	14/15	0.78	0.52	124,127,129,130	0
2	GAL	P	4	11/12	0.79	0.36	136,138,141,142	0
2	FUC	P	5	10/11	0.79	0.40	129,130,132,133	0
2	GAL	P	2	11/12	0.79	0.77	158,161,163,163	0
2	GAL	Q	4	11/12	0.80	0.42	129,132,135,135	0
2	NAG	Q	3	14/15	0.81	0.55	138,142,143,143	0
2	BGC	K	1	12/12	0.81	0.80	139,141,141,141	0
2	FUC	K	5	10/11	0.82	0.26	101,104,107,109	0

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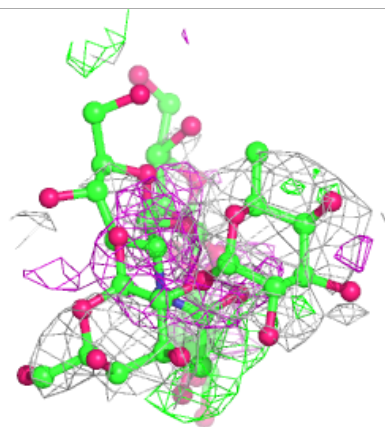
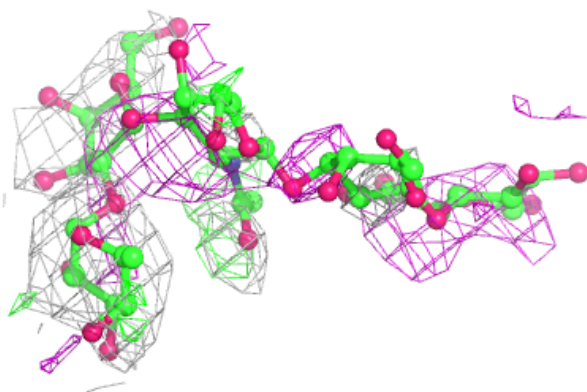
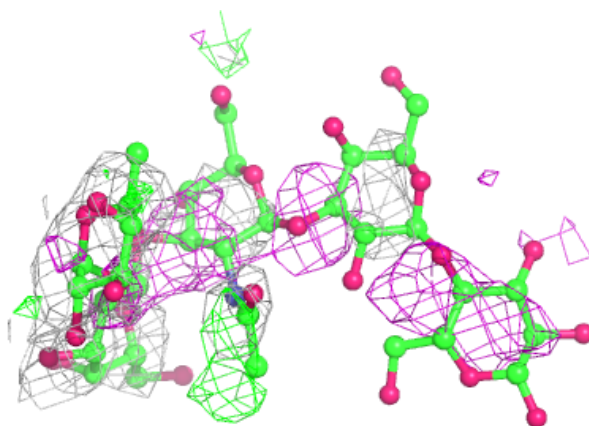
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FUC	N	5	10/11	0.83	0.39	101,104,107,109	0
2	FUC	M	5	10/11	0.84	0.26	121,123,124,126	0
2	GAL	M	4	11/12	0.84	0.40	130,133,135,135	0
2	FUC	Q	5	10/11	0.86	0.31	122,123,124,125	0

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.



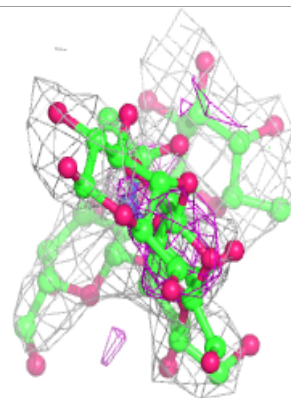
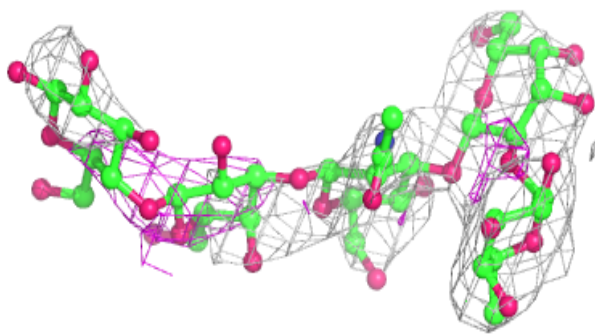
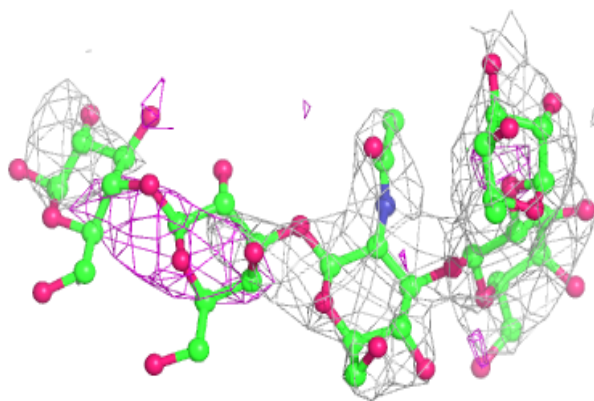
**Electron density around Chain L:**

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

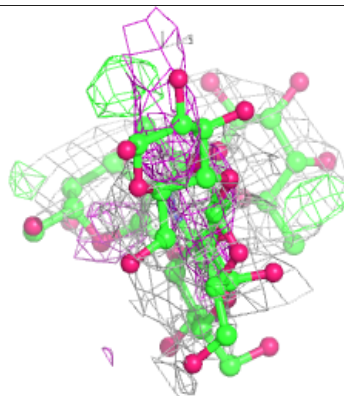
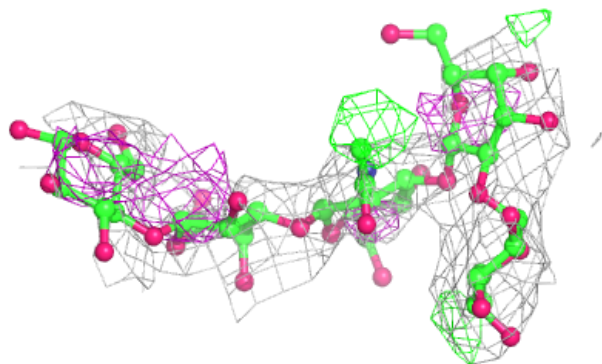
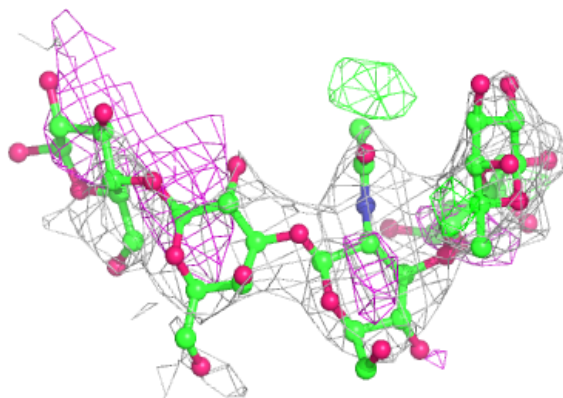


**Electron density around Chain M:**

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

**Electron density around Chain N:**

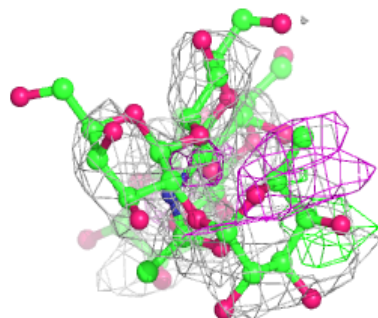
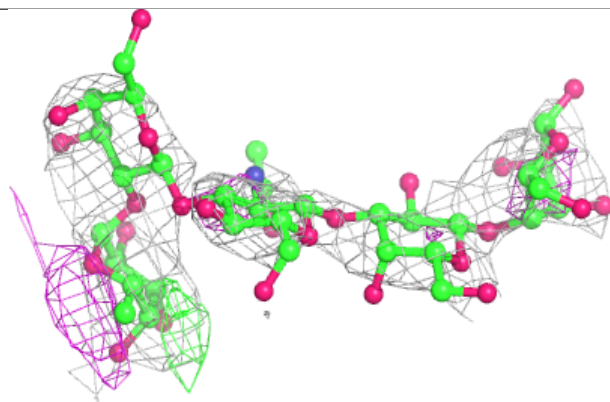
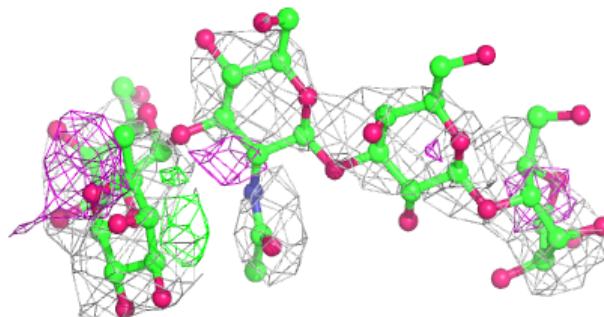
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



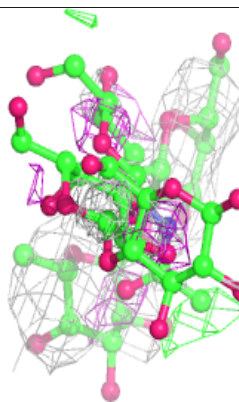
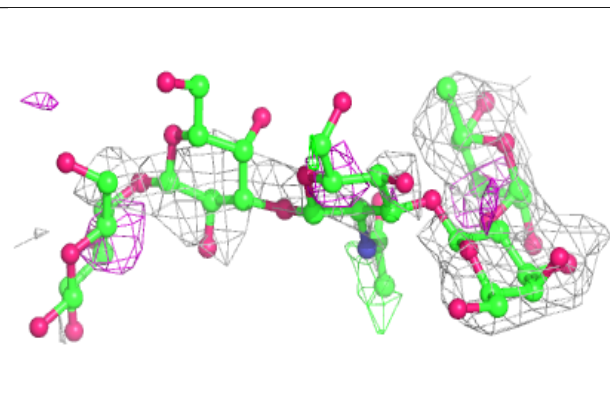
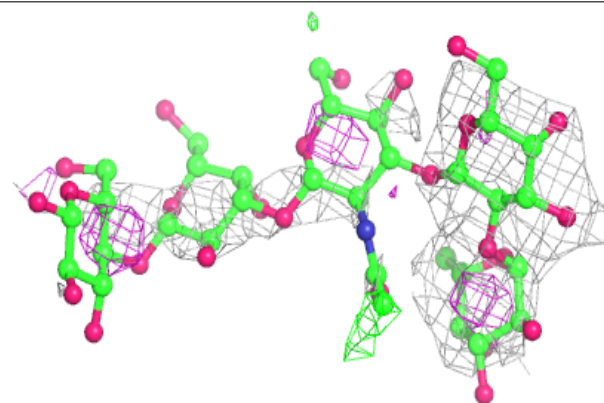


**Electron density around Chain O:**

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

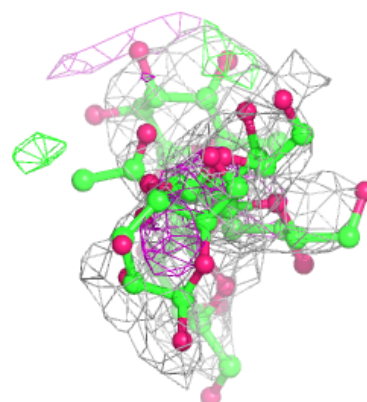
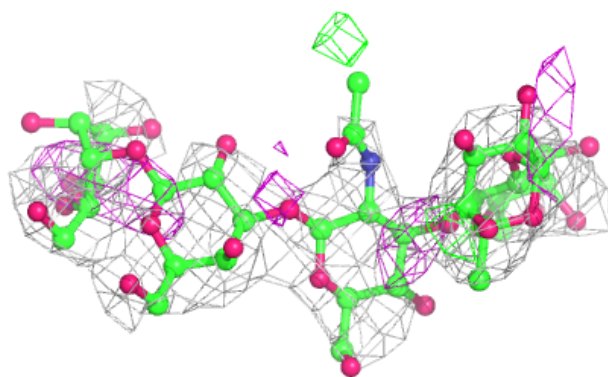
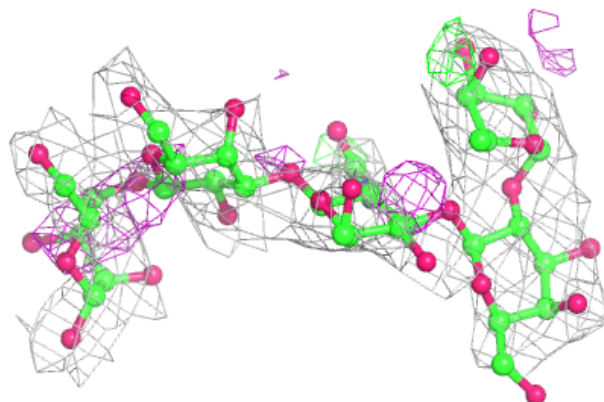
**Electron density around Chain P:**

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

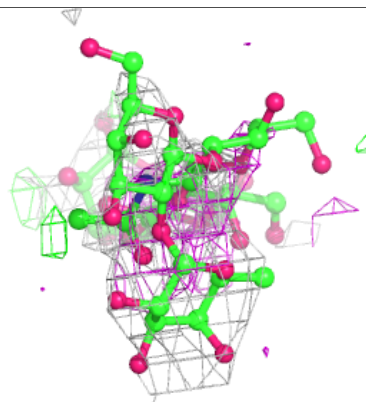
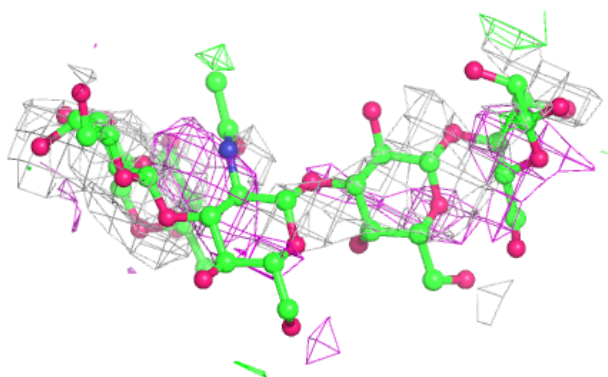
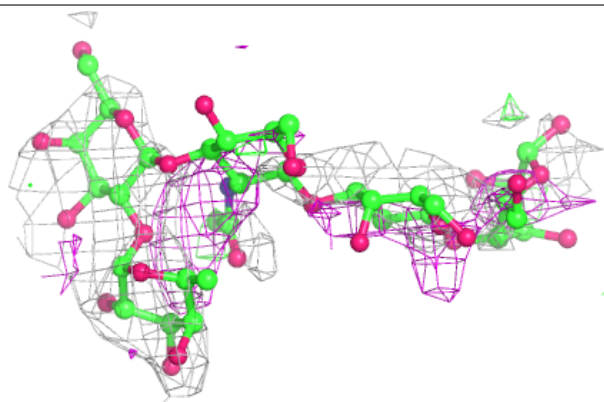


**Electron density around Chain Q:**

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

**Electron density around Chain R:**

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



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.