



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:16 PM BST

PDB ID : 6IS5  
Title : P domain of GII.3-TV24 with A-tetrasaccharide complex  
Authors : Yang, Y.  
Deposited on : 2018-11-15  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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

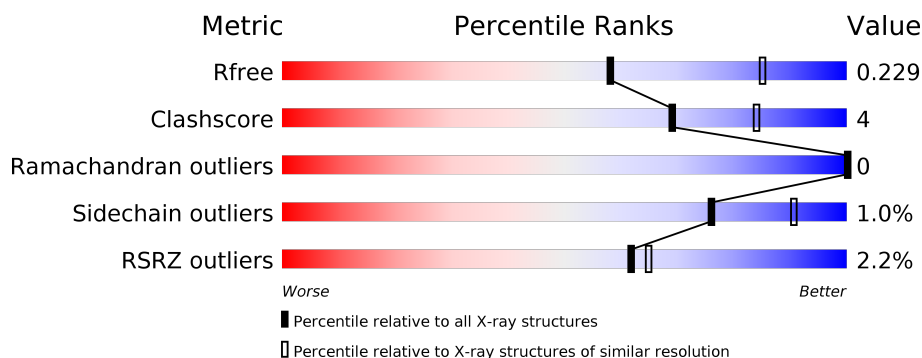
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




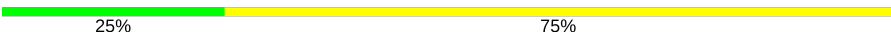
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	327	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	327	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	327	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	327	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
2	E	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	G	4	 25%75%
2	H	4	 25%75%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10344 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.

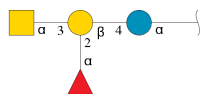
- Molecule 1 is a protein called VP1 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2346	1495	393	450	8			
1	B	304	Total	C	N	O	S	0	0	0
			2380	1514	403	455	8			
1	C	301	Total	C	N	O	S	0	0	0
			2352	1498	396	450	8			
1	D	303	Total	C	N	O	S	0	0	0
			2374	1511	402	453	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q66296
A	218	PRO	-	expression tag	UNP Q66296
A	219	LEU	-	expression tag	UNP Q66296
A	220	GLY	-	expression tag	UNP Q66296
A	221	SER	-	expression tag	UNP Q66296
B	217	GLY	-	expression tag	UNP Q66296
B	218	PRO	-	expression tag	UNP Q66296
B	219	LEU	-	expression tag	UNP Q66296
B	220	GLY	-	expression tag	UNP Q66296
B	221	SER	-	expression tag	UNP Q66296
C	217	GLY	-	expression tag	UNP Q66296
C	218	PRO	-	expression tag	UNP Q66296
C	219	LEU	-	expression tag	UNP Q66296
C	220	GLY	-	expression tag	UNP Q66296
C	221	SER	-	expression tag	UNP Q66296
D	217	GLY	-	expression tag	UNP Q66296
D	218	PRO	-	expression tag	UNP Q66296
D	219	LEU	-	expression tag	UNP Q66296
D	220	GLY	-	expression tag	UNP Q66296
D	221	SER	-	expression tag	UNP Q66296

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	F	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	G	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	H	4	Total	C	N	O	0	0	0
			47	26	1	20			

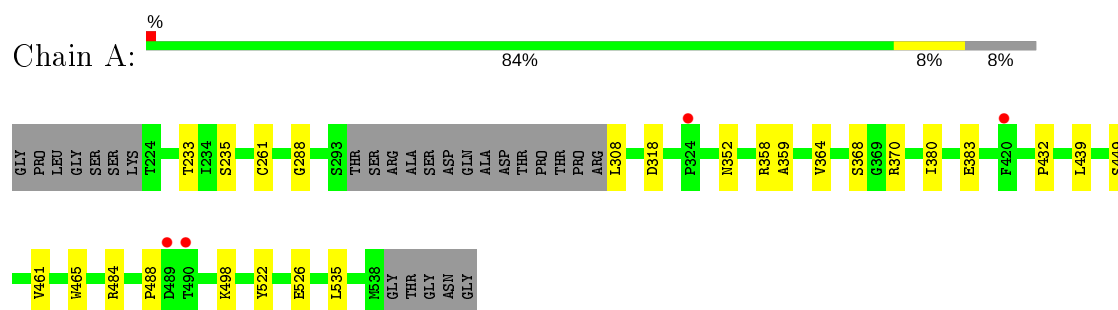
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total	O	0	0
			210	210		
3	B	169	Total	O	0	0
			169	169		
3	C	178	Total	O	0	0
			178	178		
3	D	147	Total	O	0	0
			147	147		

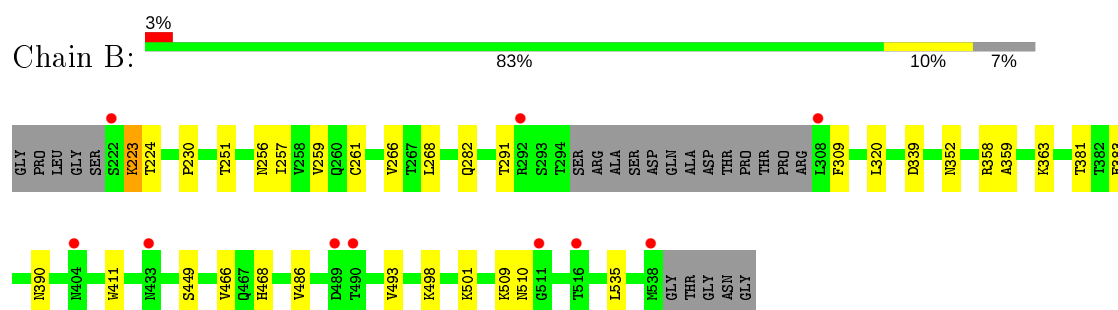
### 3 Residue-property plots [i](#)

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.

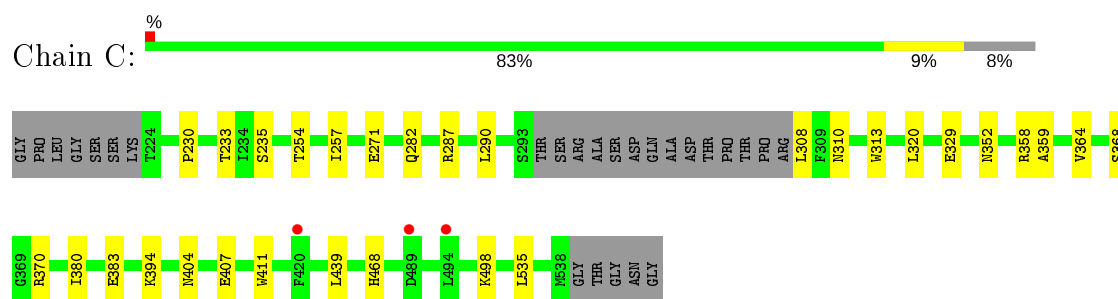
- Molecule 1: VP1 Capsid protein



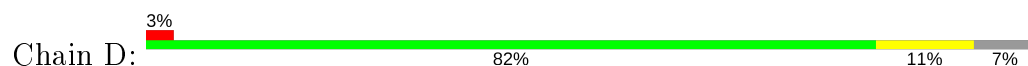
- Molecule 1: VP1 Capsid protein

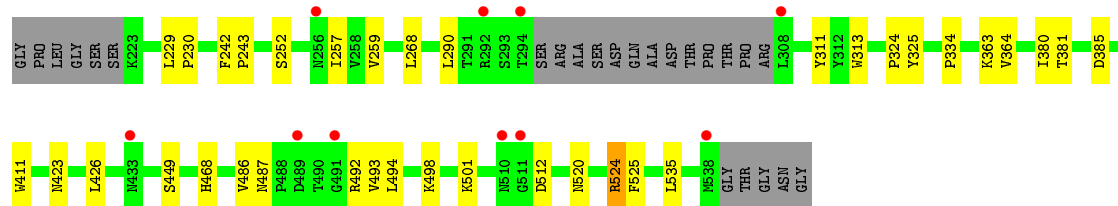


- Molecule 1: VP1 Capsid protein



- Molecule 1: VP1 Capsid protein





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

Chain E:  50% 50%



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

Chain F:  50% 50%



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

Chain G:  25% 75%



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

Chain H:  25% 75%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.37Å 122.37Å 215.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.50 49.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.25-2.50) 99.7 (49.25-2.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.187 , 0.230 0.186 , 0.229	Depositor DCC
$R_{free}$ test set	2889 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.8	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	0.95	EDS
Total number of atoms	10344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2515e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GAL, FUC, A2G

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	0.29	0/2415	0.48	0/3304
1	B	0.28	0/2449	0.47	0/3347
1	C	0.29	0/2421	0.48	0/3311
1	D	0.35	0/2443	0.48	0/3339
All	All	0.30	0/9728	0.48	0/13301

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2346	0	2247	15	0
1	B	2380	0	2294	19	0
1	C	2352	0	2258	16	0
1	D	2374	0	2289	24	0
2	E	47	0	41	0	0
2	F	47	0	41	2	0
2	G	47	0	41	1	0
2	H	47	0	41	0	0
3	A	210	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	169	0	0	0	0
3	C	178	0	0	1	0
3	D	147	0	0	1	0
All	All	10344	0	9252	70	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 4.

All (70) 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:A:233:THR:HG22	1:A:235:SER:H	1.55	0.71
1:C:233:THR:HG22	1:C:235:SER:H	1.60	0.66
1:D:524:ARG:NH2	1:D:525:PHE:H	1.97	0.63
1:B:363:LYS:HB2	1:B:381:THR:HG22	1.83	0.61
1:C:352:ASN:OD1	1:C:358:ARG:NH1	2.33	0.61
1:A:352:ASN:OD1	1:A:358:ARG:NH1	2.36	0.58
1:D:363:LYS:HB2	1:D:381:THR:HG22	1.85	0.58
1:B:390:ASN:HB2	1:D:324:PRO:HG3	1.86	0.58
2:G:1:GLC:O6	2:G:2:GAL:C1	2.52	0.58
1:C:498:LYS:HG3	1:C:535:LEU:HD11	1.86	0.56
1:D:524:ARG:HA	1:D:524:ARG:HH21	1.70	0.56
1:B:352:ASN:OD1	1:B:358:ARG:NH2	2.40	0.54
1:B:223:LYS:HD3	1:B:224:THR:H	1.72	0.54
1:D:486:VAL:HG12	1:D:493:VAL:HG22	1.91	0.52
1:A:233:THR:HG22	1:A:235:SER:N	2.25	0.52
1:B:486:VAL:HG12	1:B:493:VAL:HG22	1.91	0.52
1:B:259:VAL:HG13	1:B:411:TRP:CZ3	2.46	0.51
1:A:449:SER:HA	1:B:359:ALA:HB3	1.91	0.51
1:C:359:ALA:HB3	1:D:449:SER:HA	1.95	0.48
1:C:233:THR:HG22	1:C:235:SER:N	2.26	0.48
1:B:261:CYS:HB2	1:B:339:ASP:OD2	2.14	0.48
1:D:364:VAL:HG22	1:D:380:ILE:HG22	1.95	0.48
1:C:254:THR:HG21	1:C:439:LEU:HD12	1.96	0.47
1:C:282:GLN:HB3	1:C:320:LEU:HD13	1.96	0.47
1:A:359:ALA:HB3	1:B:449:SER:HA	1.95	0.47
1:A:358:ARG:HD3	2:F:3:FUC:O3	2.15	0.47
1:A:358:ARG:NH2	2:F:3:FUC:O4	2.48	0.47
1:A:364:VAL:HG22	1:A:380:ILE:HG22	1.96	0.47
1:B:309:PHE:HB3	1:B:381:THR:HG23	1.97	0.47
1:C:404:ASN:N	1:C:407:GLU:OE2	2.40	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:H	1:D:524:ARG:HH12	1.63	0.46
1:B:282:GLN:HB3	1:B:320:LEU:HD13	1.98	0.46
1:B:268:LEU:HG	1:B:501:LYS:HA	1.97	0.46
1:D:230:PRO:HD3	1:D:468:HIS:CD2	2.51	0.46
1:D:259:VAL:HG13	1:D:411:TRP:CZ3	2.51	0.46
1:C:287:ARG:HG3	1:C:394:LYS:HD3	1.99	0.45
1:A:432:PRO:HD3	1:A:439:LEU:HG	1.99	0.45
1:B:230:PRO:HD3	1:B:468:HIS:CD2	2.50	0.45
1:D:487:ASN:HB2	1:D:494:LEU:HD11	1.98	0.44
1:A:461:VAL:HG13	1:A:465:TRP:HB2	1.99	0.44
1:A:484:ARG:HG3	1:A:526:GLU:HG3	1.99	0.44
1:B:257:ILE:HD13	1:B:411:TRP:CD1	2.52	0.44
1:D:498:LYS:HG3	1:D:535:LEU:HD21	1.98	0.44
1:B:509:LYS:HG3	1:B:510:ASN:N	2.32	0.44
1:D:229:LEU:HB2	1:D:524:ARG:NH2	2.33	0.44
1:D:423:ASN:HB3	1:D:426:LEU:HD21	1.98	0.44
1:B:291:THR:HG23	1:D:324:PRO:HB2	1.99	0.44
1:B:251:THR:HG21	1:B:509:LYS:HG2	2.00	0.44
1:A:488:PRO:HG3	1:A:522:TYR:HE1	1.83	0.43
1:A:288:GLY:HA2	1:A:318:ASP:OD2	2.18	0.43
1:D:229:LEU:HB2	1:D:524:ARG:HH22	1.83	0.43
1:B:498:LYS:HG3	1:B:535:LEU:HD11	1.99	0.43
1:C:308:LEU:O	1:C:383:GLU:HG2	2.18	0.43
1:D:252:SER:HB3	1:D:512:ASP:OD2	2.18	0.43
1:A:498:LYS:HG3	1:A:535:LEU:HD11	2.00	0.43
1:C:271:GLU:OE1	3:C:701:HOH:O	2.21	0.43
1:D:268:LEU:HG	1:D:501:LYS:HA	2.02	0.42
1:C:230:PRO:HD3	1:C:468:HIS:CD2	2.54	0.42
1:C:308:LEU:HB3	1:C:310:ASN:OD1	2.19	0.41
1:D:325:TYR:CE1	1:D:334:PRO:HG3	2.56	0.41
1:B:266:VAL:HG11	1:B:466:VAL:HA	2.01	0.41
1:C:257:ILE:HD12	1:C:411:TRP:CD1	2.55	0.41
1:D:242:PHE:HA	1:D:243:PRO:HD3	1.92	0.41
1:D:257:ILE:HD12	1:D:411:TRP:CD1	2.55	0.41
1:D:520:ASN:HB2	3:D:659:HOH:O	2.19	0.41
1:D:311:TYR:CZ	1:D:385:ASP:HB3	2.56	0.41
1:C:364:VAL:HG22	1:C:380:ILE:HG22	2.03	0.41
1:C:290:LEU:HD21	1:C:313:TRP:CE3	2.57	0.41
1:D:290:LEU:HD21	1:D:313:TRP:CE3	2.57	0.40
1:A:308:LEU:O	1:A:383:GLU:OE2	2.39	0.40

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	297/327 (91%)	291 (98%)	6 (2%)	0	100	100
1	B	300/327 (92%)	293 (98%)	7 (2%)	0	100	100
1	C	297/327 (91%)	290 (98%)	7 (2%)	0	100	100
1	D	299/327 (91%)	294 (98%)	5 (2%)	0	100	100
All	All	1193/1308 (91%)	1168 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/283 (93%)	259 (99%)	3 (1%)	73	89
1	B	267/283 (94%)	264 (99%)	3 (1%)	73	89
1	C	263/283 (93%)	260 (99%)	3 (1%)	73	89
1	D	266/283 (94%)	264 (99%)	2 (1%)	81	93
All	All	1058/1132 (94%)	1047 (99%)	11 (1%)	76	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	CYS
1	A	368	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	370	ARG
1	B	223	LYS
1	B	256	ASN
1	B	383	GLU
1	C	329	GLU
1	C	368	SER
1	C	370	ARG
1	D	492	ARG
1	D	524	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

16 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	GLC	E	1	2	12,12,12	0.45	0	17,17,17	0.49	0
2	GAL	E	2	2	11,11,12	0.74	0	15,15,17	0.92	1 (6%)
2	FUC	E	3	2	10,10,11	0.85	0	14,14,16	0.91	0
2	A2G	E	4	2	14,14,15	0.36	0	17,19,21	1.18	1 (5%)
2	GLC	F	1	2	12,12,12	0.45	0	17,17,17	0.50	0
2	GAL	F	2	2	11,11,12	0.23	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FUC	F	3	2	10,10,11	0.26	0	14,14,16	0.62	0
2	A2G	F	4	2	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
2	GLC	G	1	2	12,12,12	0.45	0	17,17,17	0.49	0
2	GAL	G	2	2	11,11,12	0.67	0	15,15,17	0.75	0
2	FUC	G	3	2	10,10,11	0.78	0	14,14,16	0.79	0
2	A2G	G	4	2	14,14,15	0.34	0	17,19,21	0.79	1 (5%)
2	GLC	H	1	2	12,12,12	0.45	0	17,17,17	0.49	0
2	GAL	H	2	2	11,11,12	0.62	0	15,15,17	1.04	1 (6%)
2	FUC	H	3	2	10,10,11	0.90	1 (10%)	14,14,16	1.11	1 (7%)
2	A2G	H	4	2	14,14,15	0.38	0	17,19,21	1.50	2 (11%)

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	GLC	E	1	2	-	1/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	A2G	E	4	2	-	0/6/23/26	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	A2G	F	4	2	-	2/6/23/26	0/1/1/1
2	GLC	G	1	2	-	1/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1
2	A2G	G	4	2	-	0/6/23/26	0/1/1/1
2	GLC	H	1	2	-	1/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	FUC	H	3	2	-	-	0/1/1/1
2	A2G	H	4	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	FUC	O5-C1	-2.07	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	A2G	C1-O5-C5	4.73	118.61	112.19
2	E	4	A2G	C1-O5-C5	4.25	117.96	112.19
2	H	4	A2G	O5-C1-C2	-2.54	107.27	111.29
2	F	4	A2G	C1-O5-C5	2.53	115.62	112.19
2	H	2	GAL	C1-C2-C3	2.45	112.67	109.67
2	H	3	FUC	O2-C2-C1	2.43	114.12	109.15
2	G	4	A2G	C1-O5-C5	2.33	115.35	112.19
2	E	2	GAL	C1-C2-C3	2.21	112.38	109.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

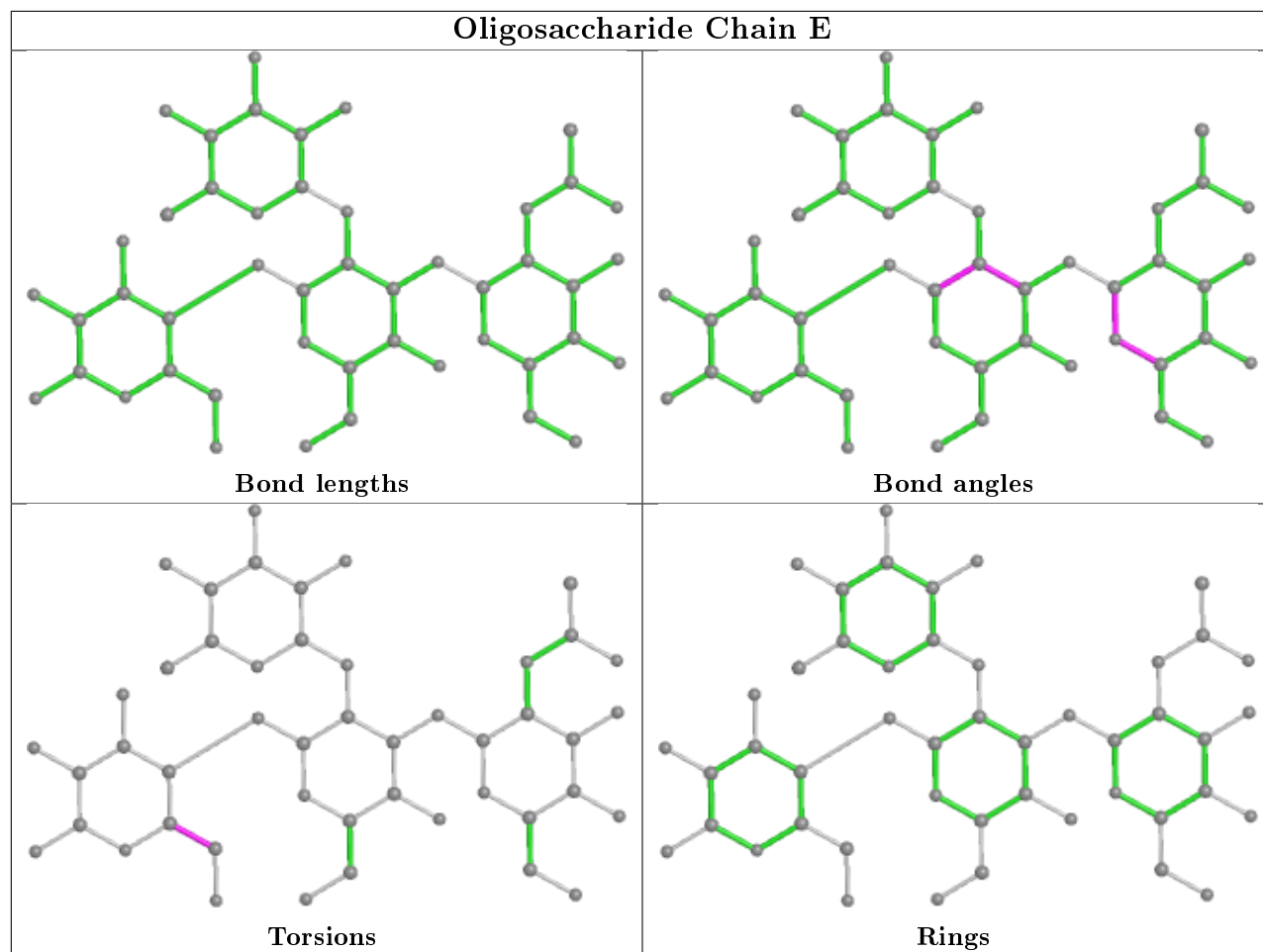
Mol	Chain	Res	Type	Atoms
2	F	4	A2G	O5-C5-C6-O6
2	F	4	A2G	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	H	4	A2G	C4-C5-C6-O6

There are no ring outliers.

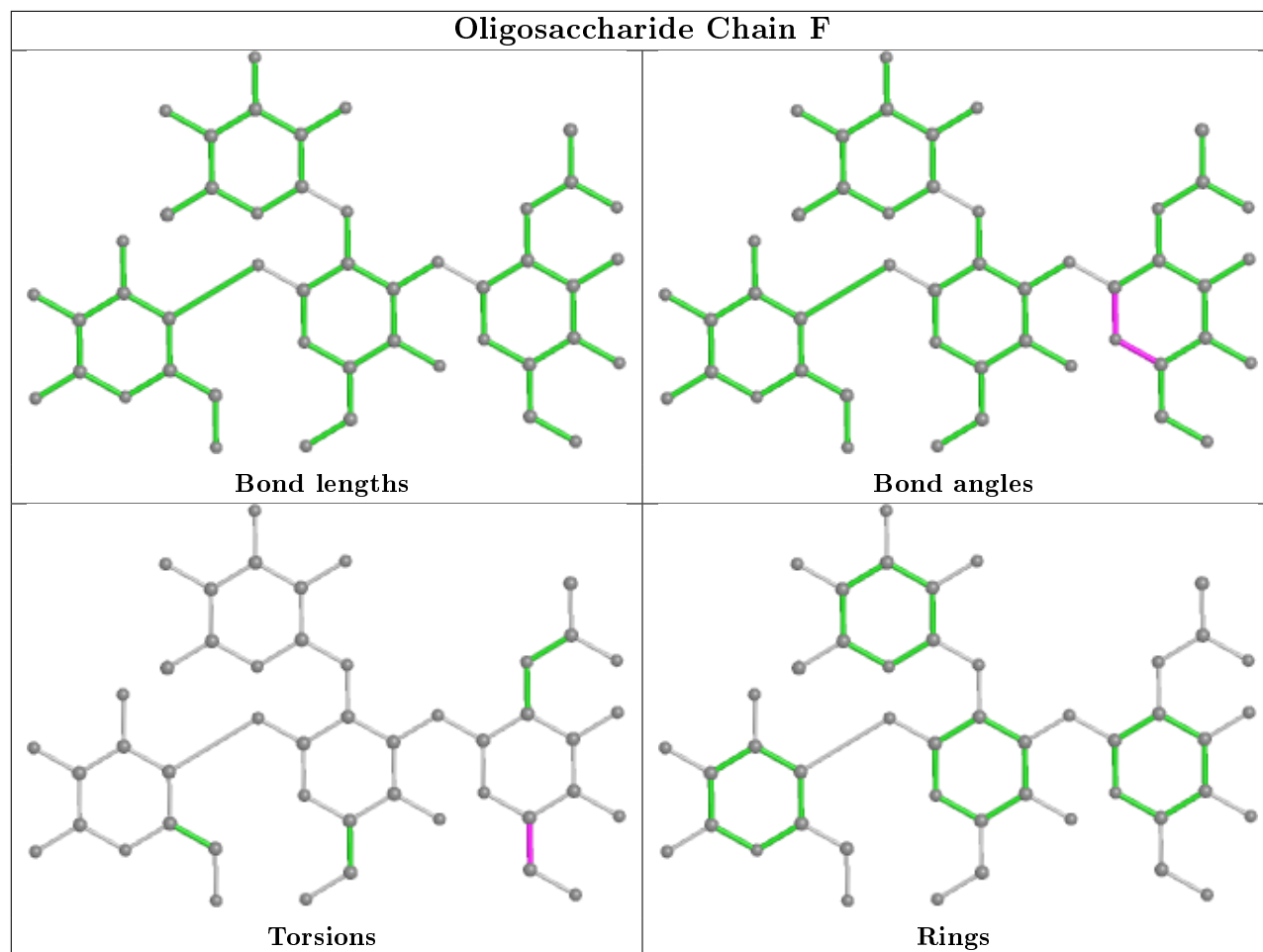
3 monomers are involved in 3 short contacts:

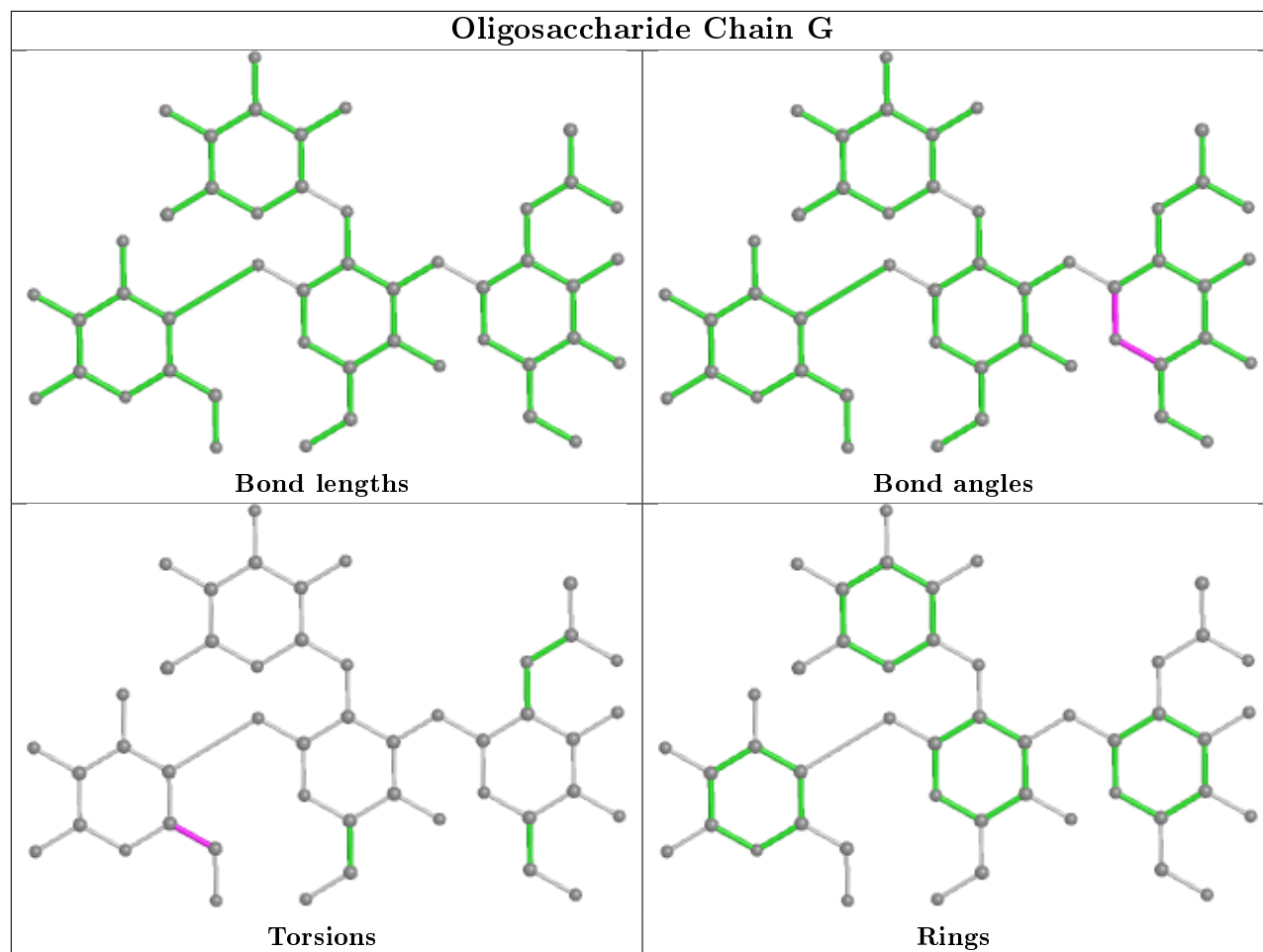
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	GAL	1	0
2	F	3	FUC	2	0
2	G	1	GLC	1	0

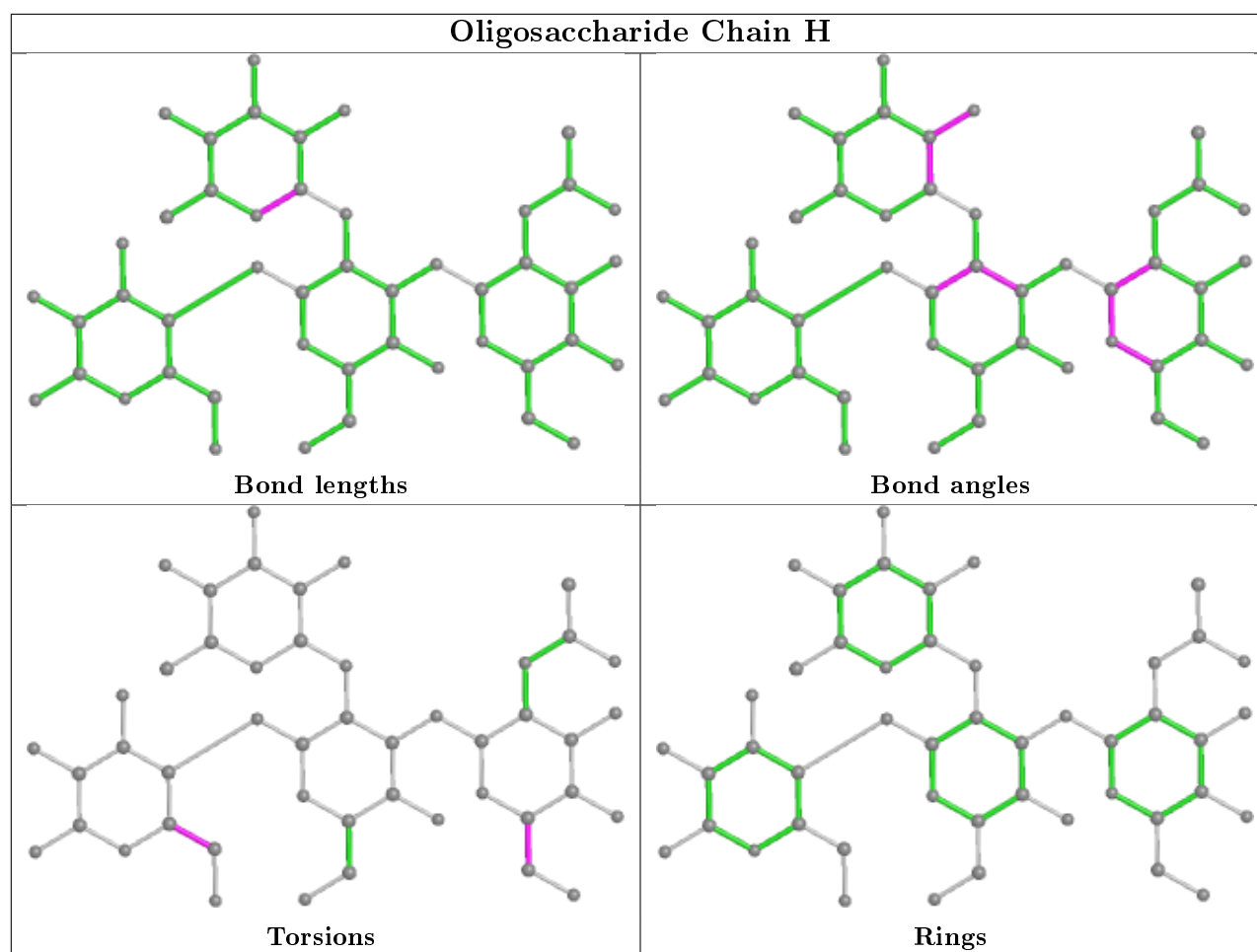
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 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 ⓘ

### 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	301/327 (92%)	-0.34	4 (1%) 77 79	12, 20, 39, 50	0
1	B	304/327 (92%)	-0.25	10 (3%) 46 50	13, 21, 48, 64	0
1	C	301/327 (92%)	-0.32	3 (0%) 82 84	12, 20, 39, 53	0
1	D	303/327 (92%)	-0.15	10 (3%) 46 50	13, 23, 48, 64	0
All	All	1209/1308 (92%)	-0.27	27 (2%) 62 65	12, 21, 44, 64	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	PHE	4.9
1	D	308	LEU	4.4
1	D	489	ASP	4.0
1	B	222	SER	3.9
1	C	420	PHE	3.9
1	A	489	ASP	3.3
1	D	491	GLY	3.1
1	D	294	THR	3.0
1	D	256	ASN	2.9
1	D	538	MET	2.7
1	C	494	LEU	2.6
1	C	489	ASP	2.6
1	D	292	ARG	2.6
1	B	489	ASP	2.5
1	B	490	THR	2.5
1	B	511	GLY	2.5
1	B	433	ASN	2.4
1	B	404	ASN	2.3
1	D	433	ASN	2.3
1	B	292	ARG	2.3
1	B	538	MET	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	324	PRO	2.2
1	D	511	GLY	2.2
1	D	510	ASN	2.2
1	B	308	LEU	2.1
1	A	490	THR	2.1
1	B	516	THR	2.0

## 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](#)

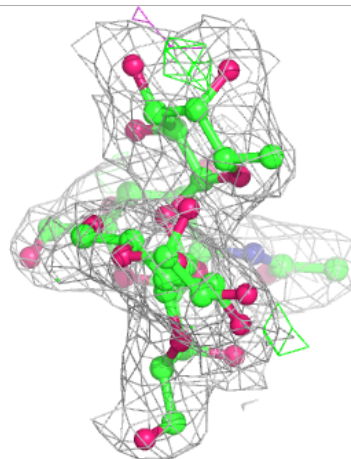
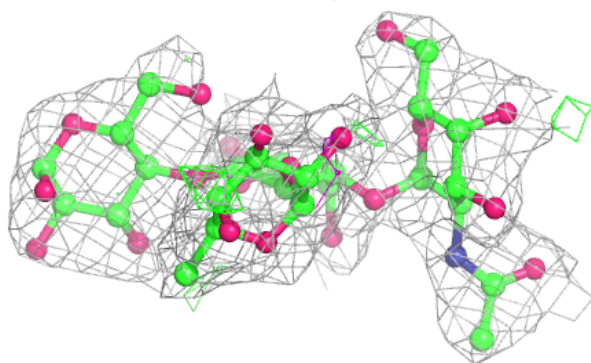
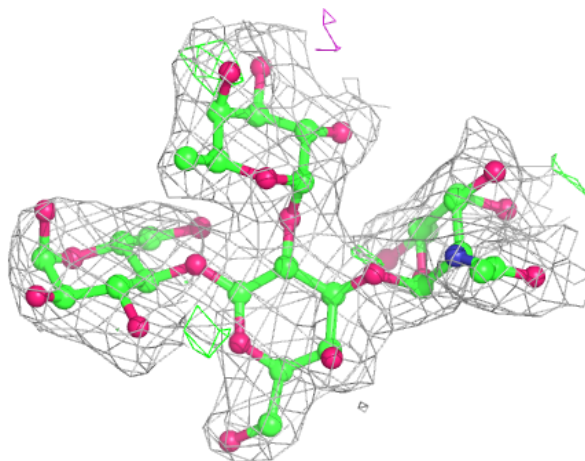
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	GAL	F	2	11/12	0.89	0.13	30,35,41,44	0
2	GLC	F	1	12/12	0.89	0.27	36,44,59,68	0
2	GLC	G	1	12/12	0.89	0.23	34,43,48,67	0
2	GLC	H	1	12/12	0.93	0.24	33,39,48,62	0
2	GAL	H	2	11/12	0.93	0.20	30,32,35,42	0
2	GAL	E	2	11/12	0.94	0.19	28,30,35,37	0
2	FUC	E	3	10/11	0.94	0.13	19,25,26,26	0
2	GLC	E	1	12/12	0.95	0.21	30,37,52,58	0
2	FUC	G	3	10/11	0.95	0.11	25,26,27,28	0
2	A2G	H	4	14/15	0.95	0.16	23,26,29,36	0
2	A2G	E	4	14/15	0.96	0.16	22,23,29,36	0
2	FUC	F	3	10/11	0.96	0.14	21,25,27,28	0
2	A2G	F	4	14/15	0.96	0.15	22,30,36,42	0
2	A2G	G	4	14/15	0.96	0.16	24,27,33,39	0
2	GAL	G	2	11/12	0.96	0.12	31,32,37,39	0
2	FUC	H	3	10/11	0.97	0.12	23,26,27,27	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.

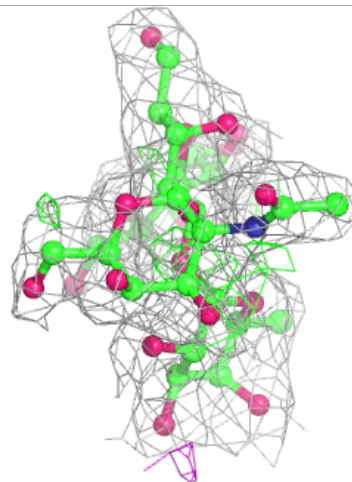
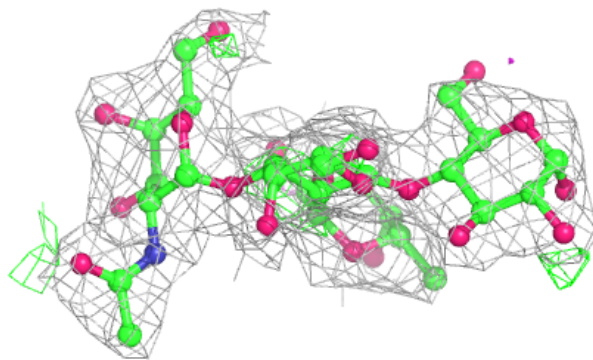
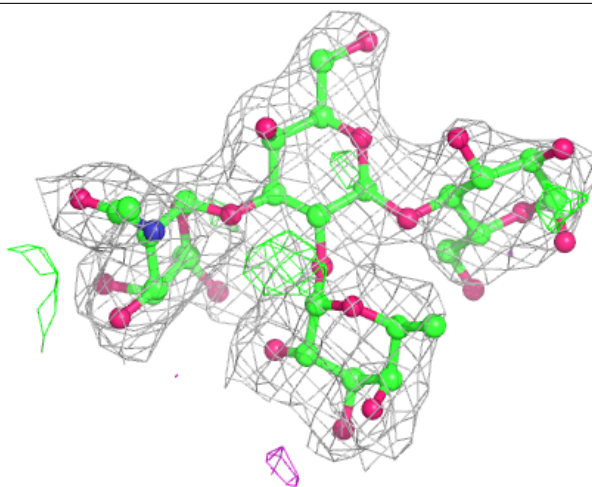
**Electron density around Chain E:**

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



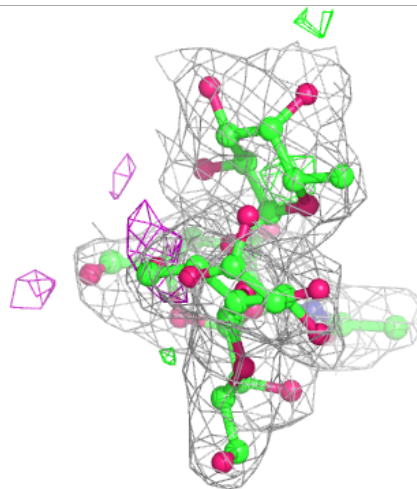
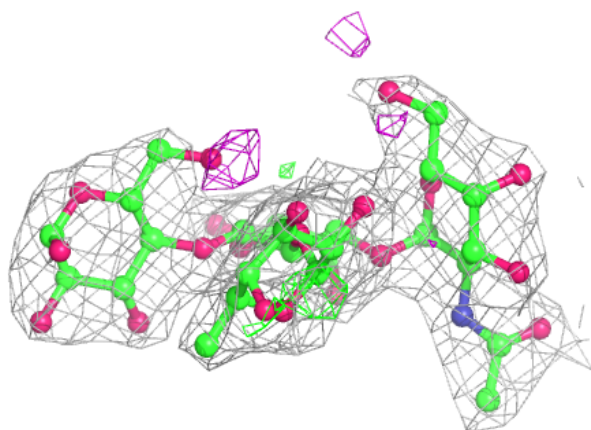
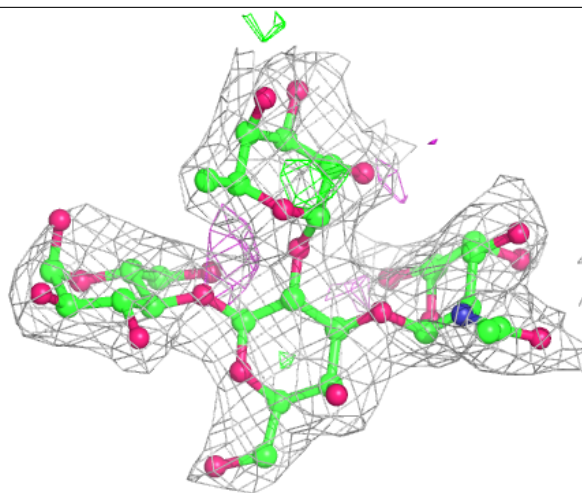
**Electron density around Chain F:**

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

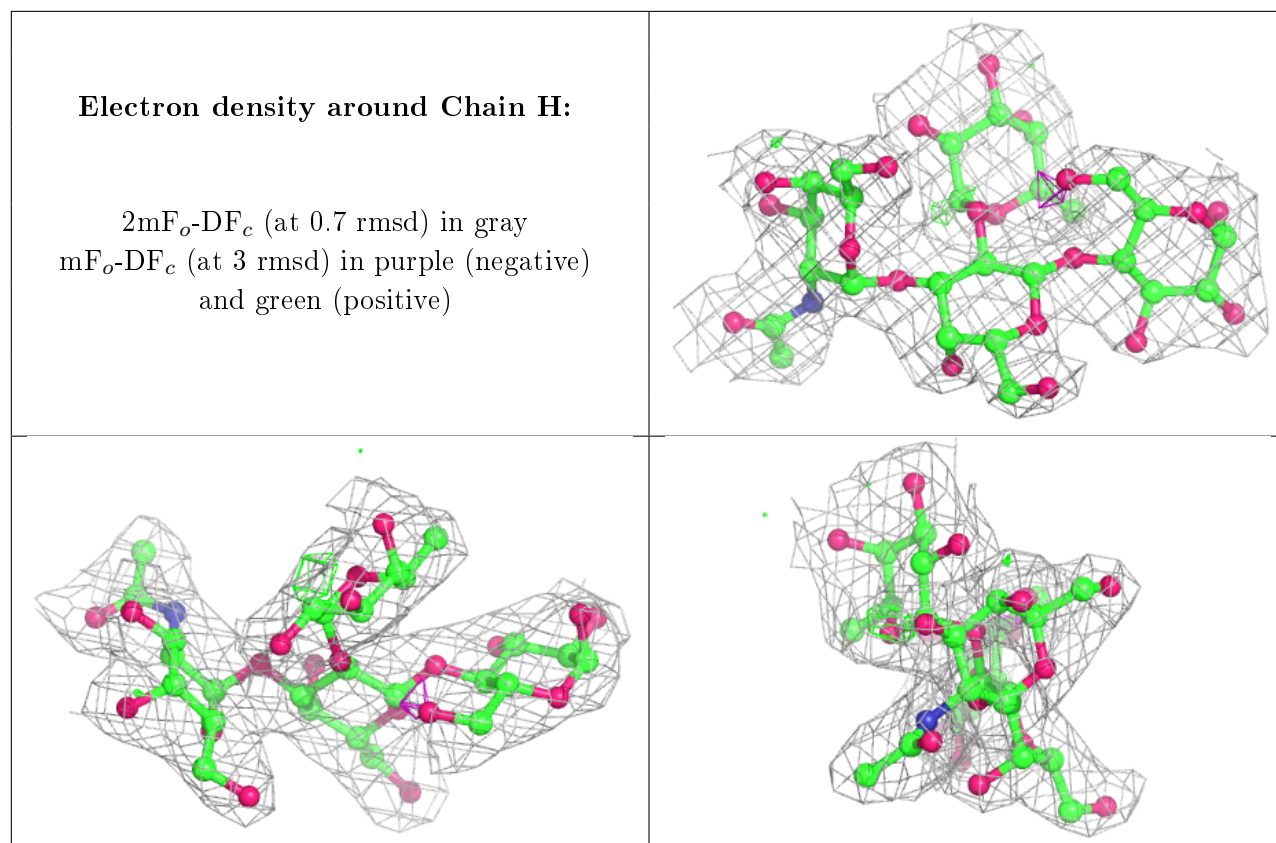


**Electron density around Chain G:**

$2mF_o-DF_c$  (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.