



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 09:27 pm GMT

PDB ID : 5CPW  
Title : Crystal structure of murine polyomavirus PTA strain VP1 in complex with the GT1a glycan  
Authors : Liaci, A.M.; Buch, M.H.C.; Neu, U.; Stehle, T.  
Deposited on : 2015-07-21  
Resolution : 1.75 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 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

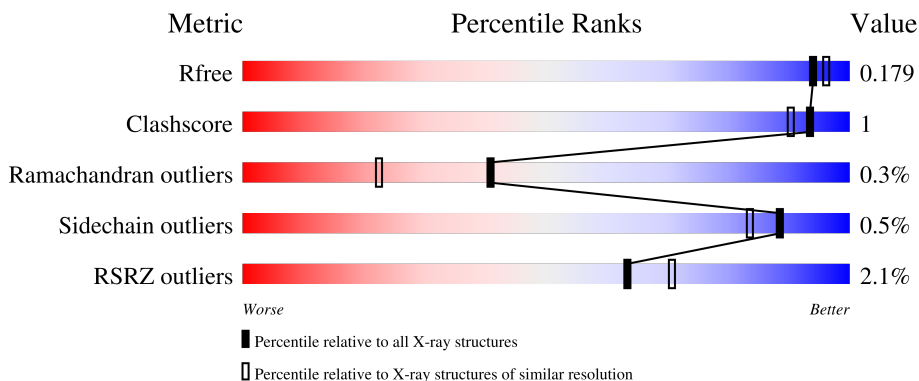
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	284	 95%
1	B	284	 94%
1	C	284	 95%
1	D	284	 95%
1	E	284	 95%

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Mol	Chain	Length	Quality of chain
2	F	5	 60% 40%
2	G	5	 20% 80%
2	H	5	 40% 60%
3	I	6	 33% 67%
3	J	6	 100%

## 2 Entry composition [i](#)

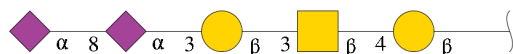
There are 5 unique types of molecules in this entry. The entry contains 13340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

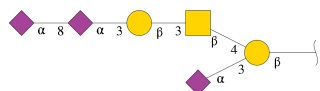
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	Total 2225	C 1421	N 373	O 422	S 9	0	11	0
1	B	278	Total 2212	C 1408	N 374	O 422	S 8	0	7	0
1	C	278	Total 2195	C 1400	N 369	O 418	S 8	0	5	0
1	D	283	Total 2249	C 1429	N 375	O 432	S 13	0	7	0
1	E	278	Total 2207	C 1408	N 372	O 419	S 8	0	8	0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.



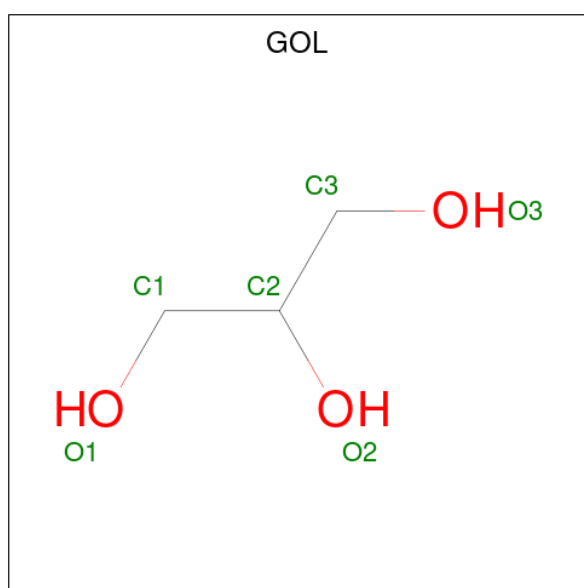
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	5	Total 77	C 42	N 3	O 32	0	0	0
2	G	5	Total 77	C 42	N 3	O 32	0	0	0
2	H	5	Total 77	C 42	N 3	O 32	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	6	Total	C	N	O	0	0	0
			97	53	4	40			
3	J	6	Total	C	N	O	0	0	0
			97	53	4	40			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

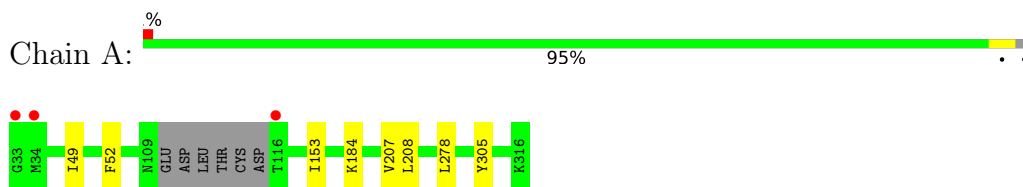
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	347	Total	O	0	0
			347	347		
5	B	329	Total	O	0	0
			329	329		
5	C	348	Total	O	0	0
			348	348		
5	D	401	Total	O	0	0
			401	401		
5	E	370	Total	O	0	0
			370	370		

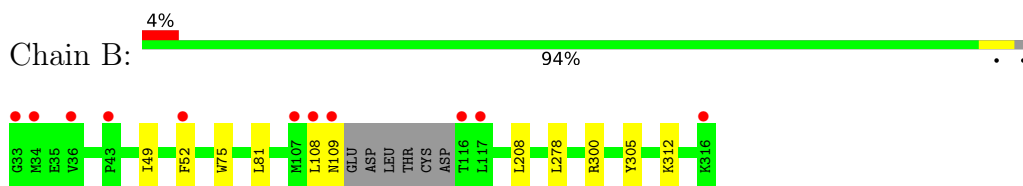
### 3 Residue-property plots [i](#)

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.

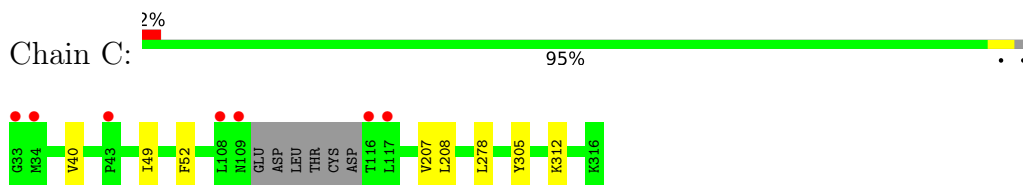
- Molecule 1: VP1



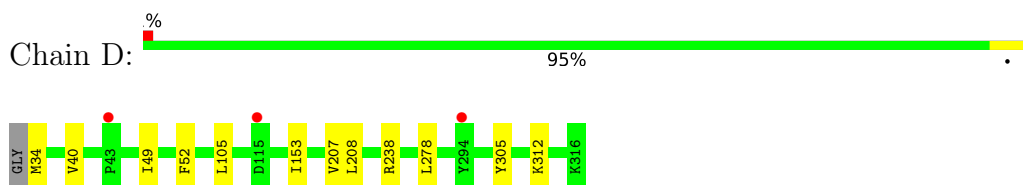
- Molecule 1: VP1



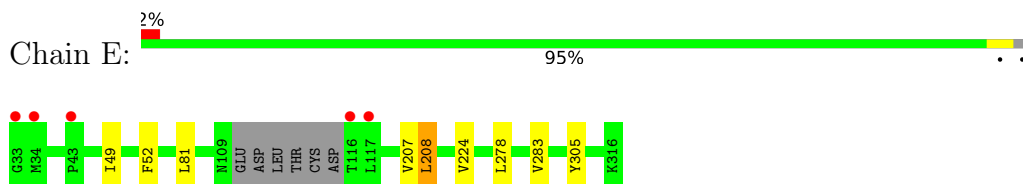
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1



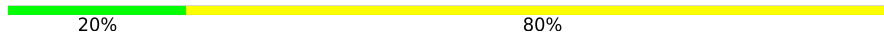
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranos

e

Chain F: 

GAL1
NGA2
GAL3
SIA4
SIA5

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranos e

Chain G: 

GAL1
NGA2
GAL3
SIA4
SIA5

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranos e

Chain H: 

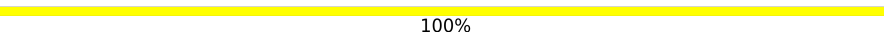
GAL1
NGA2
GAL3
SIA4
SIA5

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

Chain I: 

GAL1
NGA2
GAL3
SIA4
SIA5
SIA6

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

Chain J: 

GAL1
NGA2
GAL3
SIA4
SIA5
SIA6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.60Å 219.60Å 99.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.59 – 1.75 47.54 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.59-1.75) 97.6 (47.54-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.160 , 0.181 0.159 , 0.179	Depositor DCC
$R_{free}$ test set	8140 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: NGA, GOL, SIA, GAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/2306	0.56	0/3141
1	B	0.38	0/2277	0.55	0/3100
1	C	0.38	0/2266	0.56	0/3089
1	D	0.39	0/2324	0.58	0/3165
1	E	0.41	0/2279	0.58	0/3106
All	All	0.39	0/11452	0.57	0/15601

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	2225	0	2219	5	0
1	B	2212	0	2188	9	0
1	C	2195	0	2179	5	0
1	D	2249	0	2230	11	0
1	E	2207	0	2188	7	0
2	F	77	0	65	0	0
2	G	77	0	65	0	0
2	H	77	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	97	0	81	0	0
3	J	97	0	81	0	0
4	A	8	0	8	1	0
4	B	8	0	8	0	0
4	C	4	0	4	0	0
4	D	8	0	8	1	0
4	E	4	0	4	0	0
5	A	347	0	0	0	0
5	B	329	0	0	0	0
5	C	348	0	0	1	0
5	D	401	0	0	0	0
5	E	370	0	0	0	0
All	All	13340	0	11393	33	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 1.

All (33) 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:E:49:ILE:HD11	1:E:278:LEU:HD23	1.71	0.71
1:D:52[A]:PHE:CD1	1:E:208:LEU:HD13	2.27	0.69
1:A:49:ILE:HD11	1:A:278:LEU:HD23	1.78	0.66
1:B:49:ILE:HD11	1:B:278:LEU:HD23	1.78	0.66
1:C:49:ILE:HD11	1:C:278:LEU:CD2	2.32	0.59
1:E:49:ILE:HD11	1:E:278:LEU:CD2	2.33	0.59
1:D:49:ILE:HD11	1:D:278:LEU:CD2	2.33	0.58
1:D:49:ILE:HD13	1:D:105:LEU:HD21	1.86	0.58
1:D:52[A]:PHE:CE1	1:D:305:TYR:HB2	2.40	0.57
1:A:49:ILE:HD11	1:A:278:LEU:CD2	2.36	0.55
1:D:52[A]:PHE:CE1	1:E:208:LEU:HD13	2.43	0.53
1:C:49:ILE:HD11	1:C:278:LEU:HD23	1.90	0.53
1:A:184:LYS:HG2	4:A:401:GOL:H11	1.92	0.52
1:B:52[B]:PHE:CE1	1:B:305:TYR:HB2	2.44	0.52
1:B:108[B]:LEU:O	1:B:109[B]:ASN:HB2	2.10	0.52
1:B:49:ILE:HD11	1:B:278:LEU:CD2	2.41	0.50
1:A:52[B]:PHE:CE1	1:A:305:TYR:HB2	2.48	0.49
1:D:49:ILE:HD11	1:D:278:LEU:HD23	1.94	0.48
1:D:49:ILE:HD13	1:D:105:LEU:CD2	2.45	0.47
1:E:52[A]:PHE:CE1	1:E:305:TYR:HB2	2.51	0.46
1:D:40:VAL:HB	1:D:312:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52[A]:PHE:HZ	5:C:839:HOH:O	1.98	0.46
1:B:108[B]:LEU:O	1:B:109[B]:ASN:CB	2.62	0.46
1:C:52[A]:PHE:CE1	1:C:305:TYR:HB2	2.51	0.45
1:B:75:TRP:CZ3	1:B:300:ARG:HB2	2.52	0.44
1:D:49:ILE:CD1	1:D:105:LEU:HD21	2.47	0.44
1:C:49:ILE:HD11	1:C:278:LEU:HD22	2.00	0.43
1:D:238:ARG:HH22	4:D:402:GOL:C2	2.30	0.43
1:D:153:ILE:HA	1:E:81:LEU:HD21	2.00	0.43
1:C:40:VAL:HB	1:C:312:LYS:HB2	2.01	0.42
1:E:224:VAL:HG11	1:E:283:VAL:HG21	2.02	0.42
1:B:108[B]:LEU:HD21	1:B:312:LYS:HE2	2.03	0.41
1:A:153:ILE:HA	1:B:81:LEU:HD21	2.02	0.41

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	284/284 (100%)	276 (97%)	7 (2%)	1 (0%)	34	17
1	B	280/284 (99%)	273 (98%)	7 (2%)	0	100	100
1	C	280/284 (99%)	271 (97%)	8 (3%)	1 (0%)	34	17
1	D	288/284 (101%)	278 (96%)	9 (3%)	1 (0%)	41	22
1	E	281/284 (99%)	273 (97%)	7 (2%)	1 (0%)	34	17
All	All	1413/1420 (100%)	1371 (97%)	38 (3%)	4 (0%)	41	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	VAL
1	D	207	VAL

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Mol	Chain	Res	Type
1	C	207	VAL
1	E	207	VAL

### 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	250/250 (100%)	249 (100%)	1 (0%)	91	87
1	B	246/250 (98%)	245 (100%)	1 (0%)	91	87
1	C	245/250 (98%)	244 (100%)	1 (0%)	91	87
1	D	254/250 (102%)	252 (99%)	2 (1%)	81	72
1	E	246/250 (98%)	245 (100%)	1 (0%)	91	87
All	All	1241/1250 (99%)	1235 (100%)	6 (0%)	88	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	B	208	LEU
1	C	208	LEU
1	D	34	MET
1	D	208	LEU
1	E	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	293	ASN

### 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](#)

27 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	F	1	2	12,12,12	0.52	0	17,17,17	0.65	0
2	NGA	F	2	2	14,14,15	0.39	0	17,19,21	0.69	0
2	GAL	F	3	2	11,11,12	0.45	0	15,15,17	0.59	0
2	SIA	F	4	2	20,20,21	0.59	0	24,28,31	1.03	2 (8%)
2	SIA	F	5	2	20,20,21	0.57	0	24,28,31	1.02	2 (8%)
2	GAL	G	1	2	12,12,12	0.54	0	17,17,17	0.81	1 (5%)
2	NGA	G	2	2	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
2	GAL	G	3	2	11,11,12	0.55	0	15,15,17	0.63	0
2	SIA	G	4	2	20,20,21	0.59	0	24,28,31	0.99	1 (4%)
2	SIA	G	5	2	20,20,21	0.59	0	24,28,31	0.98	2 (8%)
2	GAL	H	1	2	12,12,12	0.51	0	17,17,17	0.81	1 (5%)
2	NGA	H	2	2	14,14,15	0.48	0	17,19,21	0.63	0
2	GAL	H	3	2	11,11,12	0.71	0	15,15,17	0.70	0
2	SIA	H	4	2	20,20,21	0.67	0	24,28,31	1.10	2 (8%)
2	SIA	H	5	2	20,20,21	0.60	0	24,28,31	0.97	2 (8%)
3	GAL	I	1	3	12,12,12	0.50	0	17,17,17	0.97	2 (11%)
3	NGA	I	2	3	14,14,15	0.48	0	17,19,21	0.79	1 (5%)
3	GAL	I	3	3	11,11,12	0.52	0	15,15,17	0.70	0
3	SIA	I	4	3	20,20,21	0.58	0	24,28,31	0.87	0
3	SIA	I	5	3	20,20,21	0.66	0	24,28,31	1.05	2 (8%)
3	SIA	I	6	3	20,20,21	0.63	0	24,28,31	1.15	1 (4%)
3	GAL	J	1	3	12,12,12	0.51	0	17,17,17	0.98	1 (5%)
3	NGA	J	2	3	14,14,15	0.42	0	17,19,21	0.84	1 (5%)
3	GAL	J	3	3	11,11,12	0.59	0	15,15,17	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SIA	J	4	3	20,20,21	0.59	0	24,28,31	0.97	1 (4%)
3	SIA	J	5	3	20,20,21	0.60	0	24,28,31	0.96	1 (4%)
3	SIA	J	6	3	20,20,21	0.62	0	24,28,31	1.03	2 (8%)

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	F	1	2	-	2/2/22/22	0/1/1/1
2	NGA	F	2	2	-	0/6/23/26	0/1/1/1
2	GAL	F	3	2	-	0/2/19/22	0/1/1/1
2	SIA	F	4	2	-	4/18/34/38	0/1/1/1
2	SIA	F	5	2	-	0/18/34/38	0/1/1/1
2	GAL	G	1	2	-	2/2/22/22	0/1/1/1
2	NGA	G	2	2	-	0/6/23/26	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	SIA	G	4	2	-	6/18/34/38	0/1/1/1
2	SIA	G	5	2	-	0/18/34/38	0/1/1/1
2	GAL	H	1	2	-	1/2/22/22	0/1/1/1
2	NGA	H	2	2	-	0/6/23/26	0/1/1/1
2	GAL	H	3	2	-	0/2/19/22	0/1/1/1
2	SIA	H	4	2	-	5/18/34/38	0/1/1/1
2	SIA	H	5	2	-	0/18/34/38	0/1/1/1
3	GAL	I	1	3	-	2/2/22/22	0/1/1/1
3	NGA	I	2	3	-	0/6/23/26	0/1/1/1
3	GAL	I	3	3	-	0/2/19/22	0/1/1/1
3	SIA	I	4	3	-	2/18/34/38	0/1/1/1
3	SIA	I	5	3	-	0/18/34/38	0/1/1/1
3	SIA	I	6	3	-	4/18/34/38	0/1/1/1
3	GAL	J	1	3	-	1/2/22/22	0/1/1/1
3	NGA	J	2	3	-	0/6/23/26	0/1/1/1
3	GAL	J	3	3	-	0/2/19/22	0/1/1/1
3	SIA	J	4	3	-	4/18/34/38	0/1/1/1
3	SIA	J	5	3	-	0/18/34/38	0/1/1/1
3	SIA	J	6	3	-	5/18/34/38	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5	SIA	C6-O6-C2	2.86	117.47	111.34
2	F	5	SIA	C6-O6-C2	2.67	117.05	111.34
3	I	2	NGA	C1-O5-C5	2.50	115.58	112.19
3	J	2	NGA	C1-O5-C5	2.49	115.57	112.19
2	G	2	NGA	C1-O5-C5	2.48	115.56	112.19
3	I	1	GAL	C3-C4-C5	-2.47	105.83	110.24
2	H	4	SIA	O6-C2-C1	2.45	112.50	107.70
3	I	6	SIA	C6-O6-C2	2.44	116.55	111.34
2	F	5	SIA	O1B-C1-C2	2.38	119.81	113.03
2	H	5	SIA	C6-O6-C2	2.35	116.37	111.34
2	F	4	SIA	O1B-C1-C2	2.34	119.70	113.03
3	I	5	SIA	O1B-C1-C2	2.33	119.67	113.03
3	J	3	GAL	C1-O5-C5	2.28	115.28	112.19
3	J	5	SIA	C6-O6-C2	2.26	116.17	111.34
2	F	4	SIA	C6-O6-C2	2.23	116.12	111.34
3	J	6	SIA	C6-O6-C2	2.22	116.10	111.34
2	H	5	SIA	O1B-C1-C2	2.22	119.36	113.03
3	I	1	GAL	O5-C5-C6	2.12	111.72	106.44
3	J	1	GAL	O5-C5-C6	2.11	111.68	106.44
3	J	6	SIA	O1B-C1-C2	2.10	119.04	113.03
2	G	5	SIA	C6-O6-C2	2.10	115.84	111.34
2	G	1	GAL	O5-C5-C6	2.08	111.61	106.44
3	J	4	SIA	C6-O6-C2	2.07	115.77	111.34
2	G	4	SIA	O1B-C1-C2	2.04	118.86	113.03
2	G	5	SIA	O1B-C1-C2	2.04	118.85	113.03
2	H	4	SIA	O1B-C1-C2	2.02	118.80	113.03
2	H	1	GAL	O5-C5-C6	2.02	111.45	106.44

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	6	SIA	O7-C7-C8-O8
3	I	6	SIA	C6-C7-C8-O8
3	I	6	SIA	C6-C7-C8-C9
3	J	6	SIA	O8-C8-C9-O9
2	F	1	GAL	O5-C5-C6-O6
3	J	6	SIA	C7-C8-C9-O9
2	G	1	GAL	O5-C5-C6-O6
3	I	1	GAL	O5-C5-C6-O6
3	I	6	SIA	O7-C7-C8-C9

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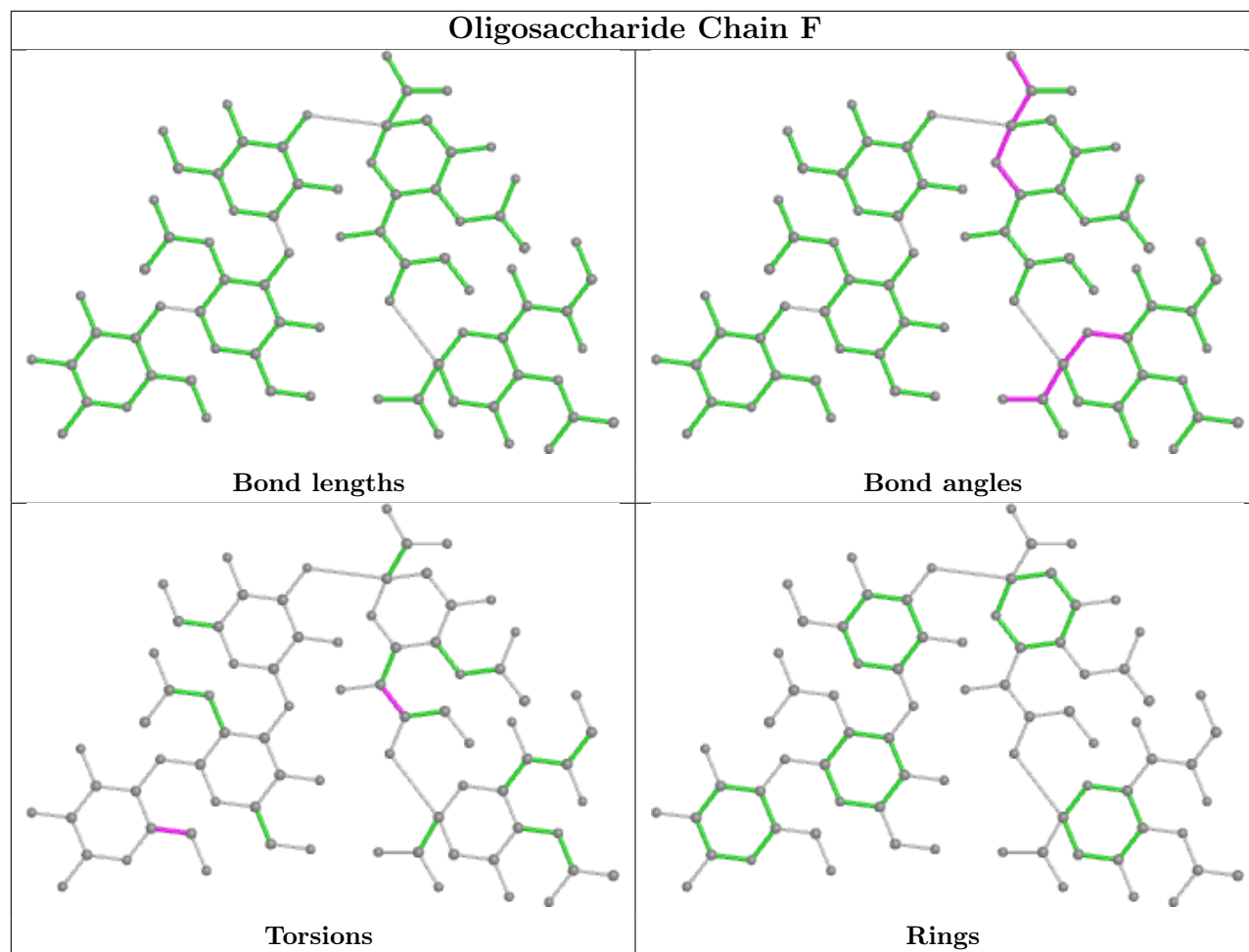
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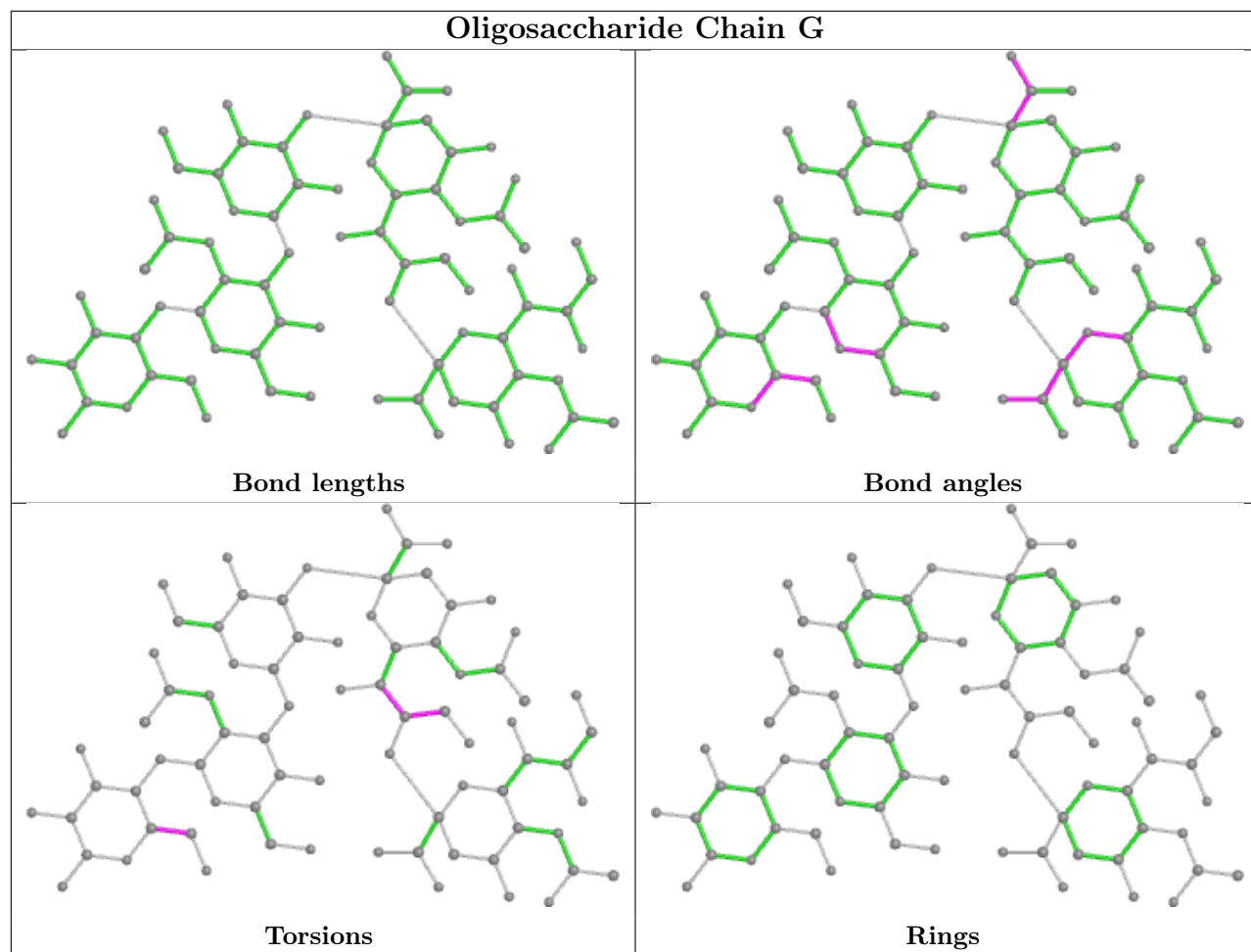
Mol	Chain	Res	Type	Atoms
3	I	1	GAL	C4-C5-C6-O6
2	H	4	SIA	O8-C8-C9-O9
2	F	4	SIA	C6-C7-C8-O8
2	H	4	SIA	C6-C7-C8-O8
3	J	4	SIA	C6-C7-C8-O8
2	G	1	GAL	C4-C5-C6-O6
2	H	1	GAL	O5-C5-C6-O6
2	G	4	SIA	C6-C7-C8-O8
2	H	4	SIA	C7-C8-C9-O9
2	F	1	GAL	C4-C5-C6-O6
2	F	4	SIA	C6-C7-C8-C9
2	H	4	SIA	C6-C7-C8-C9
3	J	4	SIA	C6-C7-C8-C9
2	G	4	SIA	O8-C8-C9-O9
3	I	4	SIA	C6-C7-C8-O8
3	J	6	SIA	C6-C7-C8-O8
3	J	1	GAL	O5-C5-C6-O6
2	G	4	SIA	C6-C7-C8-C9
2	F	4	SIA	O7-C7-C8-O8
3	J	4	SIA	O7-C7-C8-O8
2	H	4	SIA	O7-C7-C8-O8
2	G	4	SIA	O7-C7-C8-O8
3	I	4	SIA	C6-C7-C8-C9
2	G	4	SIA	C7-C8-C9-O9
2	F	4	SIA	O7-C7-C8-C9
3	J	4	SIA	O7-C7-C8-C9
3	J	6	SIA	C6-C7-C8-C9
2	G	4	SIA	O7-C7-C8-C9
3	J	6	SIA	O7-C7-C8-C9

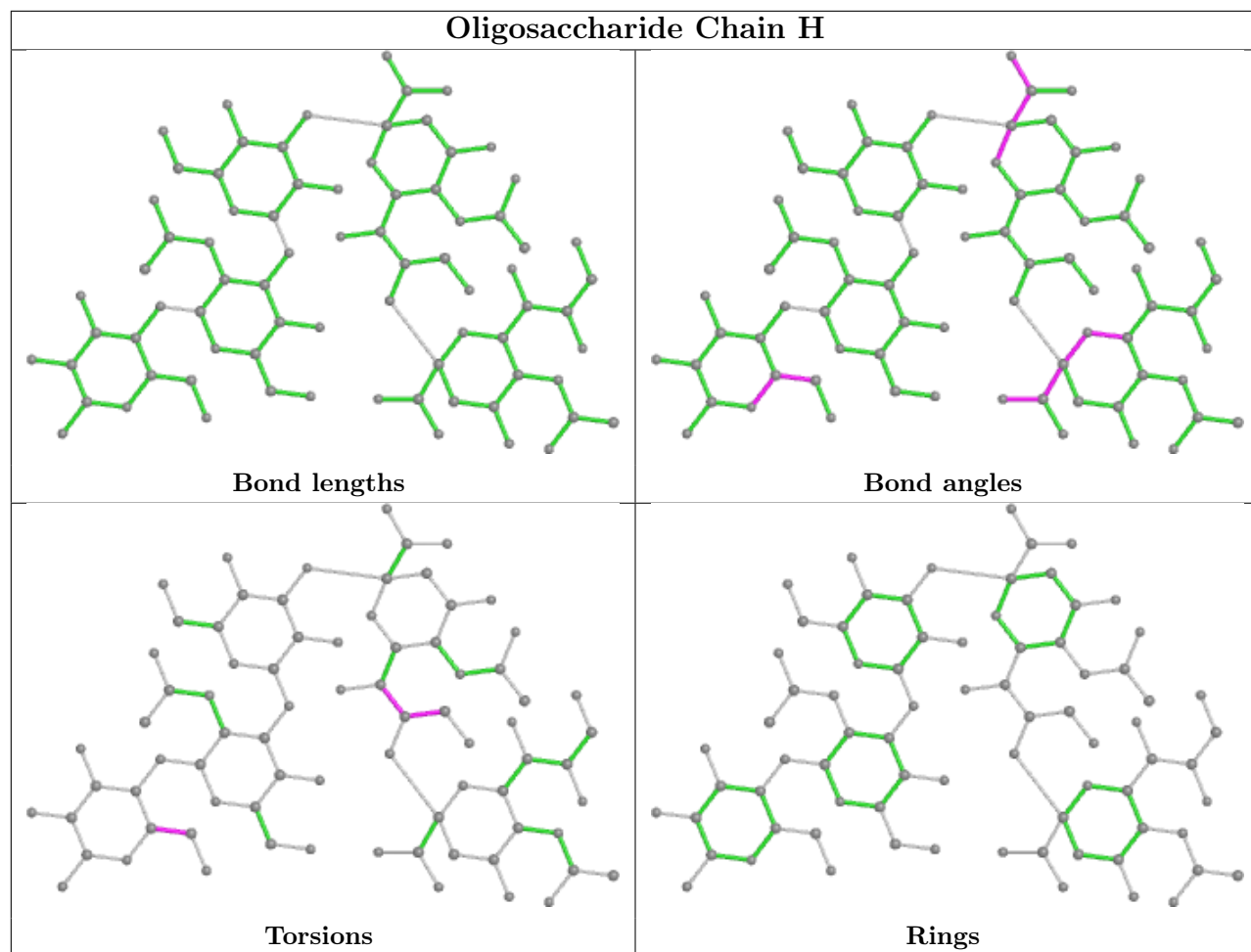
There are no ring outliers.

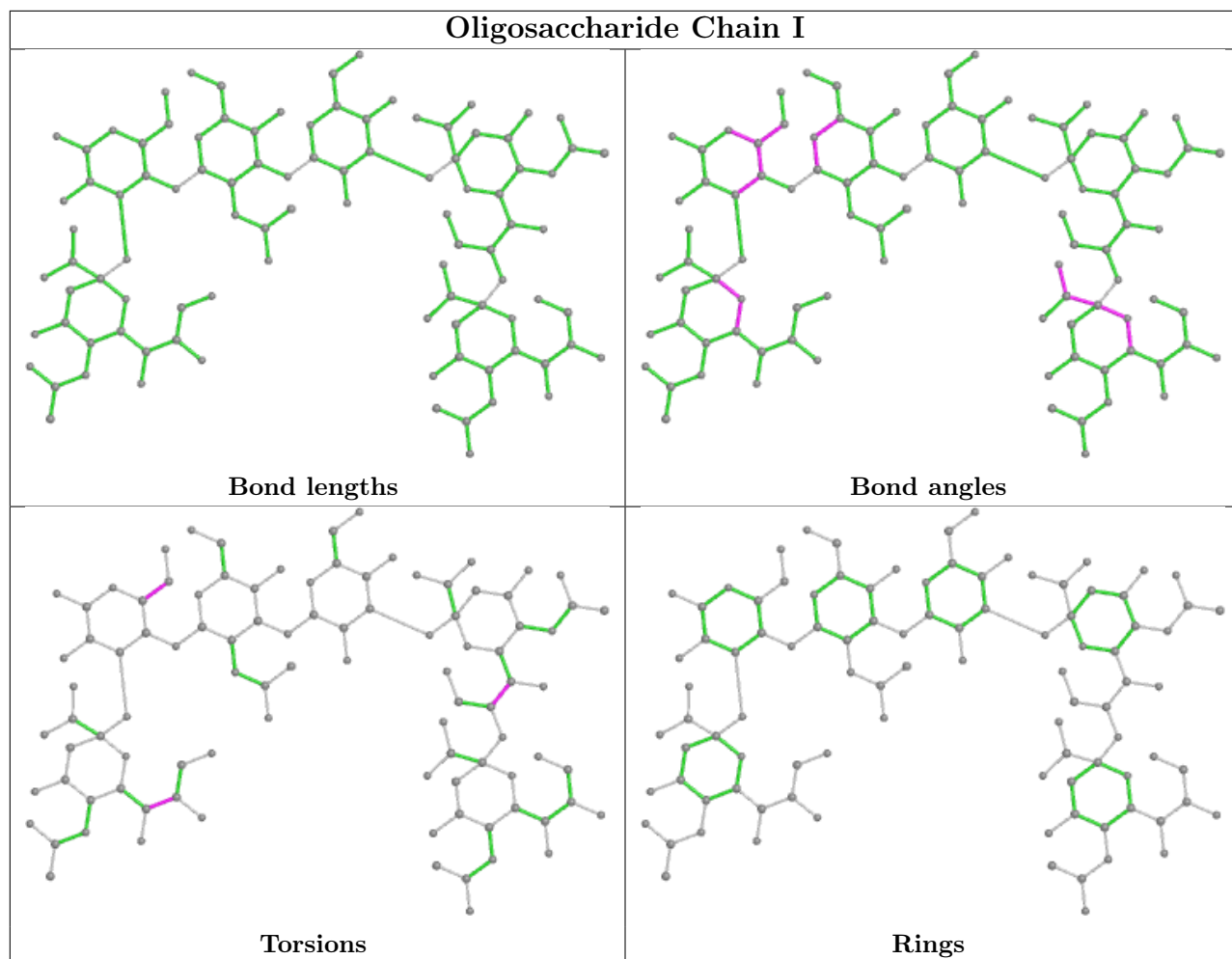
No monomer is involved in short contacts.

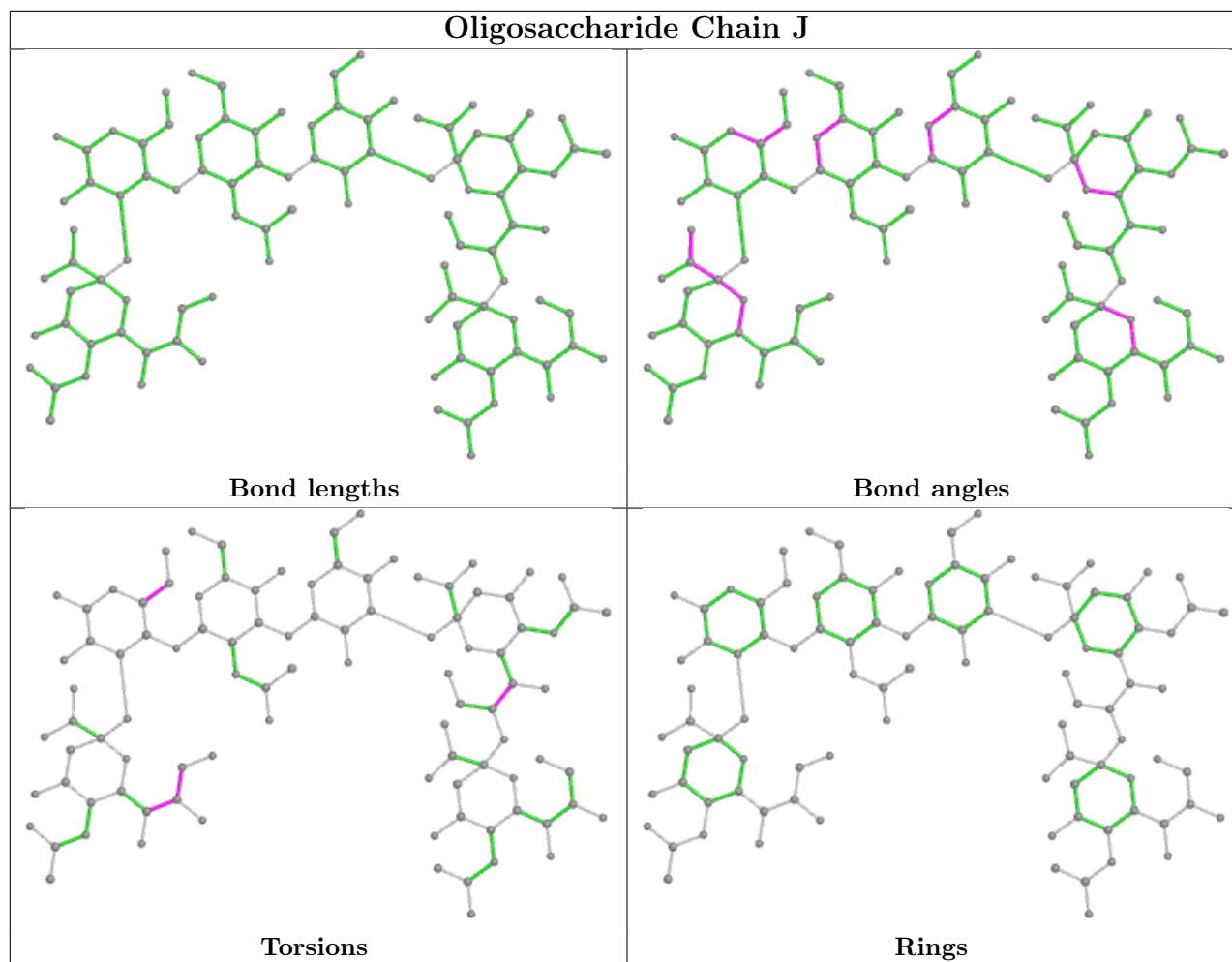
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

8 ligands 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	$\# Z  > 2$
4	GOL	A	401	-	3,3,5	0.48	0	2,2,5	0.36	0
4	GOL	E	401	-	3,3,5	0.43	0	2,2,5	0.44	0
4	GOL	B	402	-	3,3,5	0.47	0	2,2,5	0.29	0
4	GOL	A	402	-	3,3,5	0.44	0	2,2,5	0.44	0
4	GOL	C	401	-	3,3,5	0.45	0	2,2,5	0.34	0
4	GOL	D	401	-	3,3,5	0.46	0	2,2,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	D	402	-	3,3,5	0.50	0	2,2,5	0.32	0
4	GOL	B	401	-	3,3,5	0.44	0	2,2,5	0.33	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
4	GOL	A	401	-	-	0/1/1/4	-
4	GOL	E	401	-	-	0/1/1/4	-
4	GOL	B	402	-	-	1/1/1/4	-
4	GOL	A	402	-	-	0/1/1/4	-
4	GOL	C	401	-	-	1/1/1/4	-
4	GOL	D	401	-	-	1/1/1/4	-
4	GOL	D	402	-	-	1/1/1/4	-
4	GOL	B	401	-	-	1/1/1/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	GOL	O1-C1-C2-O2
4	D	402	GOL	O1-C1-C2-O2
4	B	402	GOL	O1-C1-C2-O2
4	B	401	GOL	O1-C1-C2-O2
4	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	GOL	1	0
4	D	402	GOL	1	0

## 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	278/284 (97%)	-0.41	3 (1%) 80 86	11, 16, 37, 70	0
1	B	278/284 (97%)	-0.23	11 (3%) 38 45	14, 20, 40, 70	0
1	C	278/284 (97%)	-0.21	7 (2%) 57 63	13, 20, 43, 70	0
1	D	283/284 (99%)	-0.43	3 (1%) 80 86	11, 17, 33, 63	0
1	E	278/284 (97%)	-0.39	5 (1%) 68 76	11, 16, 39, 69	0
All	All	1395/1420 (98%)	-0.33	29 (2%) 63 71	11, 18, 39, 70	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	GLY	5.3
1	B	34	MET	5.1
1	E	34	MET	4.7
1	C	34	MET	4.6
1	C	116	THR	4.5
1	C	33	GLY	4.3
1	C	117	LEU	4.3
1	E	33	GLY	3.9
1	B	117	LEU	3.9
1	B	316	LYS	3.8
1	B	108[A]	LEU	3.6
1	E	117	LEU	3.4
1	C	108	LEU	3.3
1	C	43	PRO	3.3
1	B	116	THR	3.2
1	B	107	MET	3.1
1	A	34	MET	3.1
1	A	116	THR	3.1
1	E	116	THR	2.9
1	A	33	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	36	VAL	2.8
1	D	43	PRO	2.8
1	D	115[A]	ASP	2.7
1	E	43	PRO	2.6
1	D	294	TYR	2.6
1	C	109	ASN	2.5
1	B	43	PRO	2.4
1	B	52[A]	PHE	2.3
1	B	109[A]	ASN	2.2

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

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

## 6.3 Carbohydrates [i](#)

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

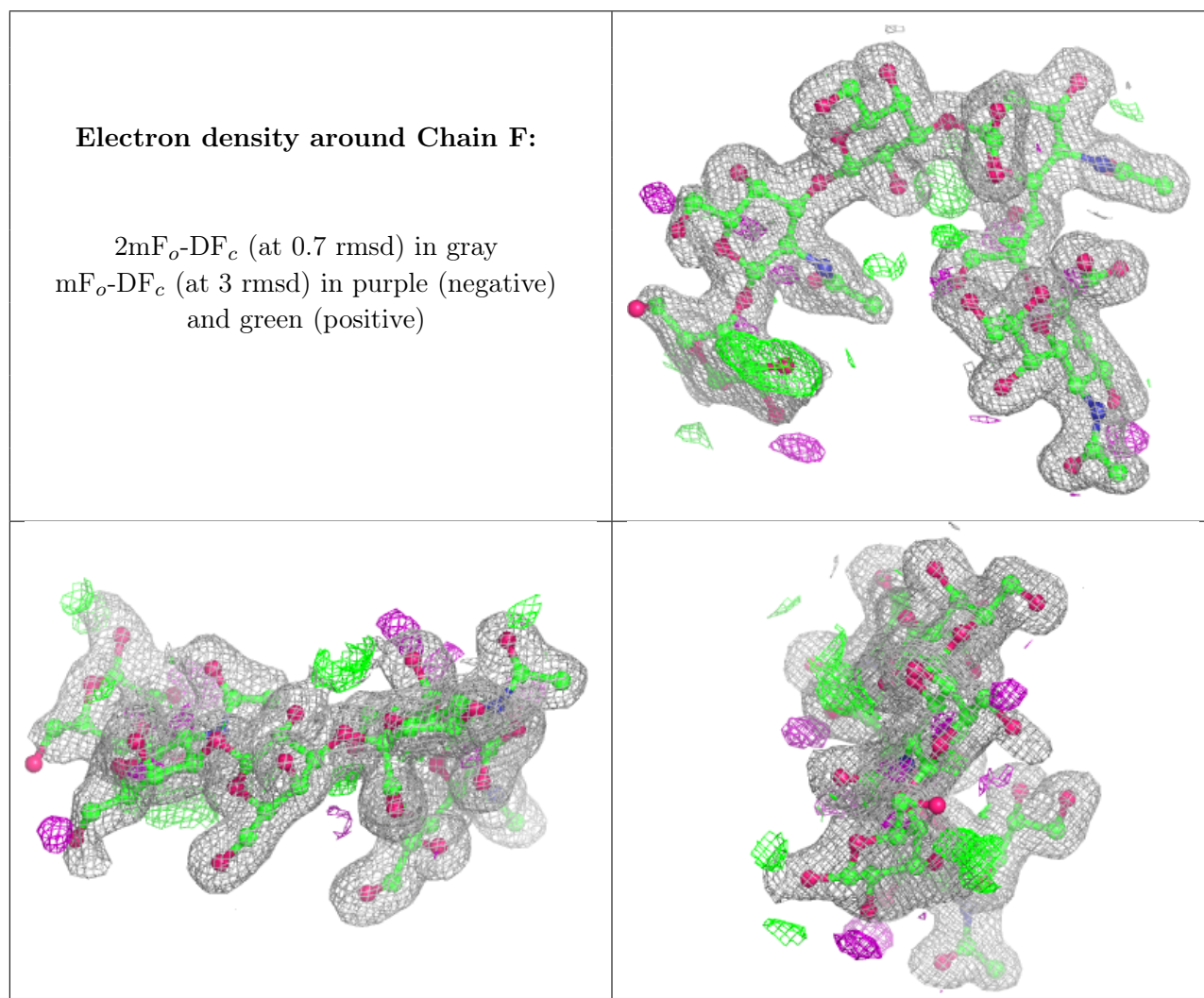
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GAL	G	1	12/12	0.80	0.22	35,48,58,62	0
2	GAL	H	1	12/12	0.86	0.23	42,48,52,58	0
3	GAL	I	1	12/12	0.87	0.20	36,45,48,55	0
3	GAL	J	1	12/12	0.88	0.17	31,42,47,62	0
3	SIA	J	6	20/21	0.89	0.28	42,52,77,80	0
2	GAL	F	1	12/12	0.90	0.19	32,47,58,75	0
3	SIA	I	6	20/21	0.90	0.23	44,55,79,88	0
2	NGA	G	2	14/15	0.92	0.22	24,31,42,43	0
2	NGA	H	2	14/15	0.92	0.20	24,35,44,45	0
3	NGA	I	2	14/15	0.95	0.12	18,27,33,37	0
2	NGA	F	2	14/15	0.95	0.12	19,30,40,62	0
2	SIA	F	5	20/21	0.95	0.09	20,23,30,31	0
2	SIA	G	5	20/21	0.95	0.14	22,28,32,35	0
2	SIA	G	4	20/21	0.96	0.08	18,21,31,39	0
2	GAL	G	3	11/12	0.96	0.10	18,20,26,28	0
3	SIA	I	5	20/21	0.96	0.08	18,23,30,33	0
2	GAL	H	3	11/12	0.96	0.09	18,20,22,23	0
2	SIA	H	4	20/21	0.96	0.09	15,20,28,32	0
3	NGA	J	2	14/15	0.96	0.12	19,31,35,36	0

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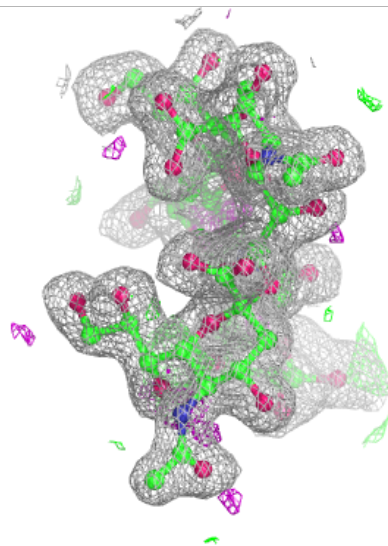
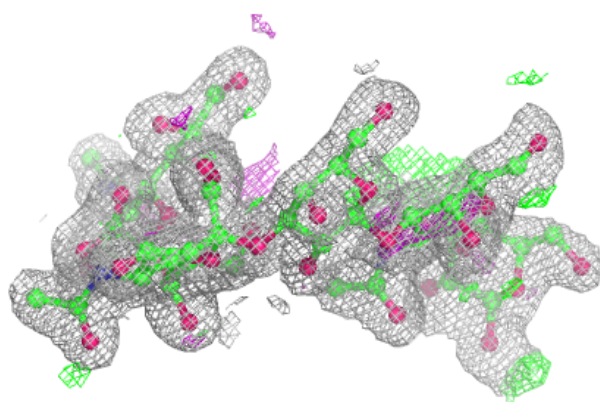
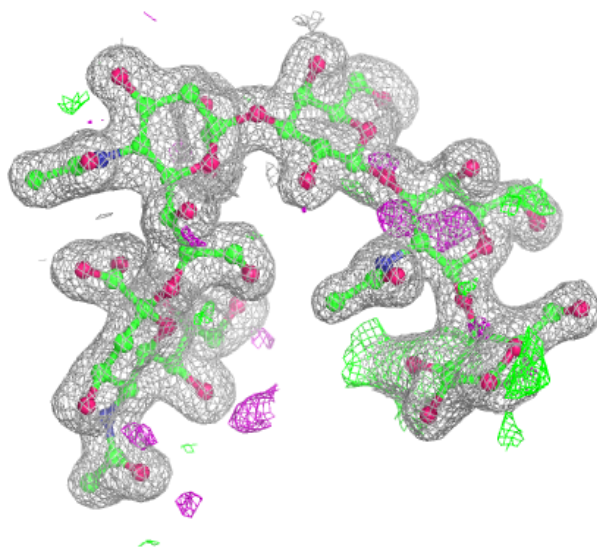
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SIA	H	5	20/21	0.96	0.14	21,27,33,37	0
3	SIA	I	4	20/21	0.97	0.06	13,16,22,28	0
3	GAL	J	3	11/12	0.97	0.06	14,16,20,21	0
3	SIA	J	4	20/21	0.97	0.06	13,16,23,27	0
3	SIA	J	5	20/21	0.97	0.06	17,21,25,30	0
2	SIA	F	4	20/21	0.97	0.06	12,16,24,32	0
3	GAL	I	3	11/12	0.98	0.05	14,16,18,19	0
2	GAL	F	3	11/12	0.98	0.05	15,17,21,22	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.



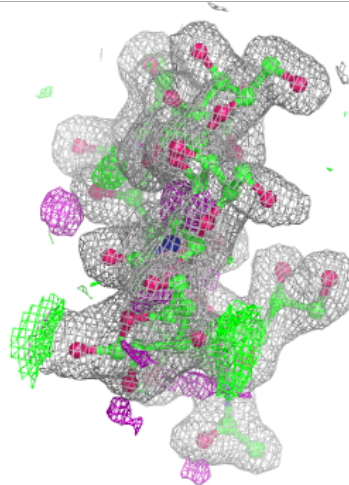
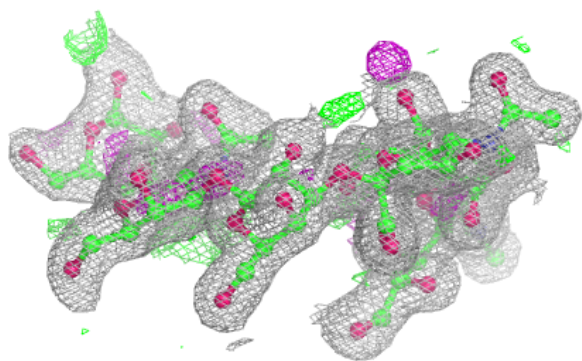
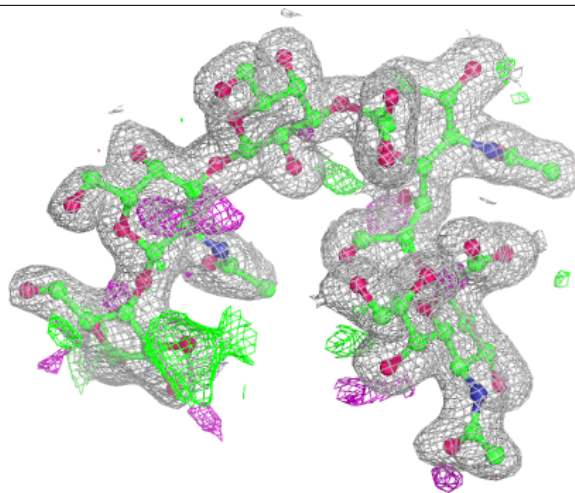
**Electron density around Chain G:**

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



**Electron density around Chain H:**

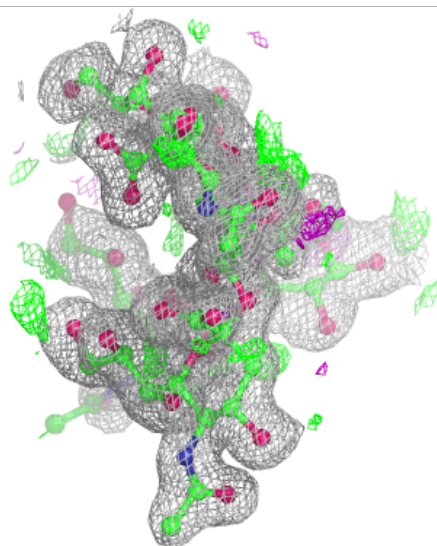
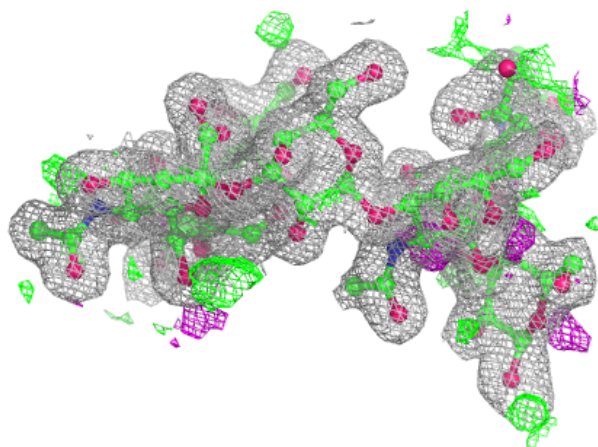
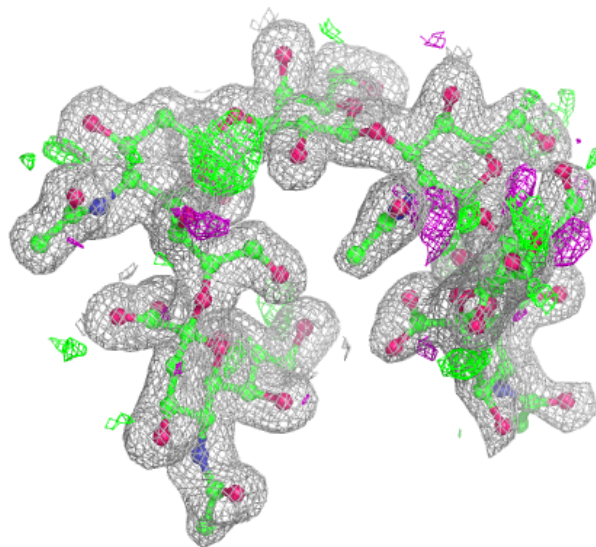
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

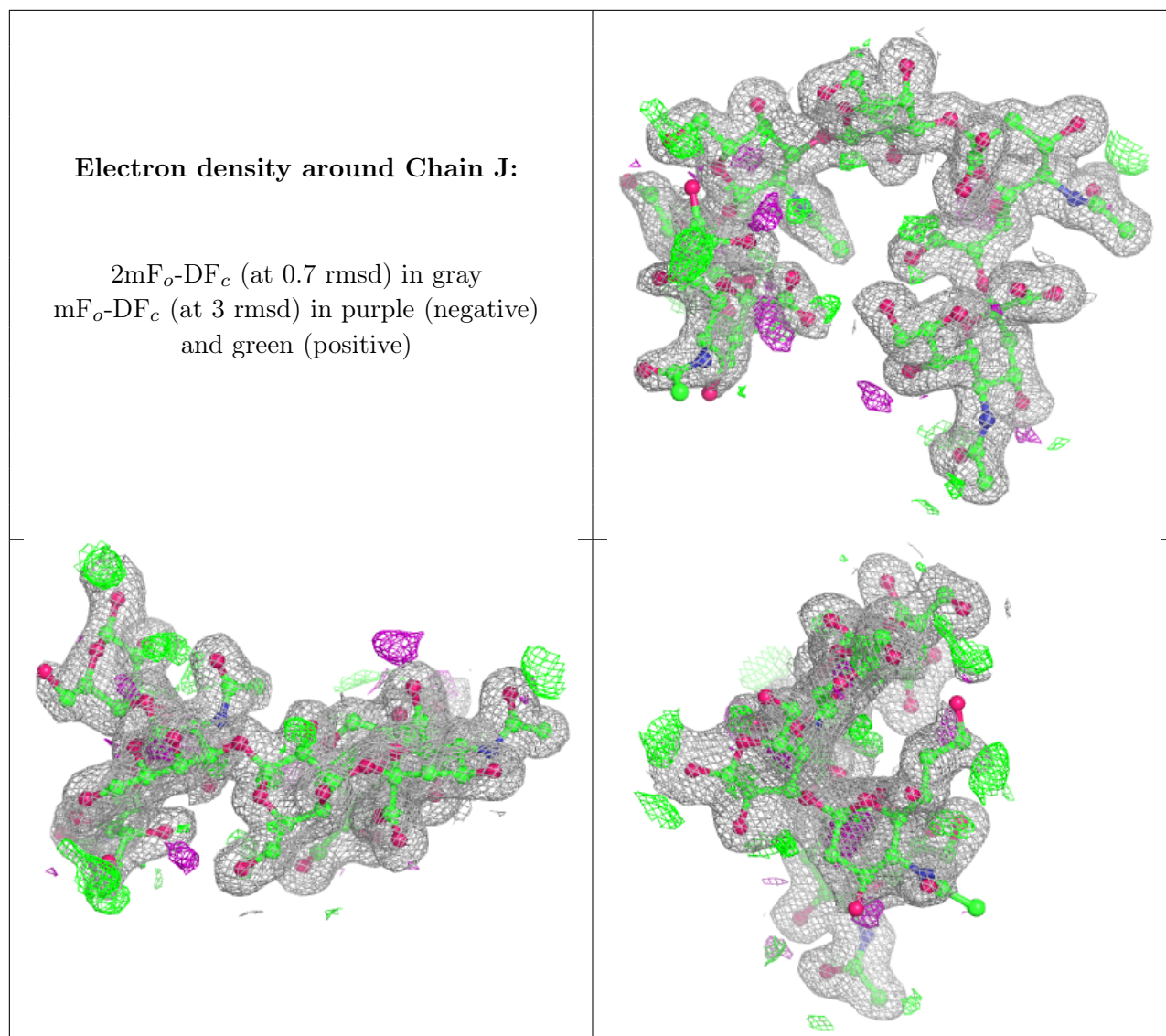




**Electron density around Chain I:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	402	4/6	0.74	0.14	39,40,47,48	0
4	GOL	C	401	4/6	0.80	0.14	45,48,55,61	0
4	GOL	B	402	4/6	0.82	0.17	37,44,46,55	0
4	GOL	A	402	4/6	0.84	0.12	39,41,49,51	0
4	GOL	A	401	4/6	0.85	0.13	39,40,43,43	0
4	GOL	E	401	4/6	0.89	0.20	35,46,47,49	0
4	GOL	D	401	4/6	0.93	0.27	29,38,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	401	4/6	0.96	0.27	34,39,50,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.