



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 08:57 am BST

PDB ID : 6RUS  
Title : Structure of a functional properdin monomer  
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Deposited on : 2019-05-29  
Resolution : 2.80 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)

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<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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

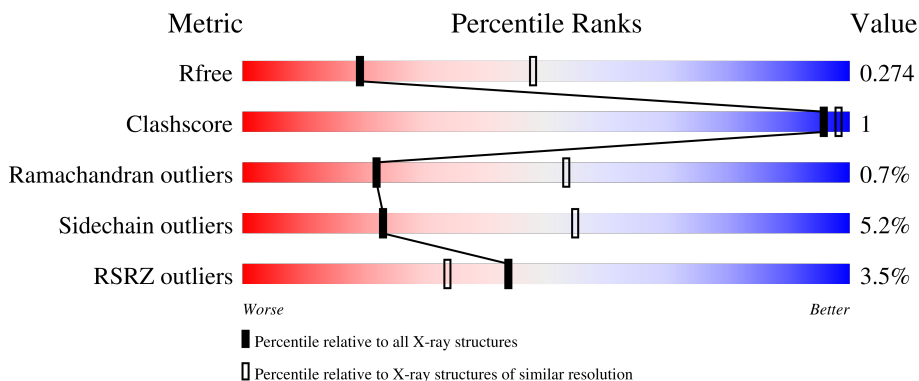
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.




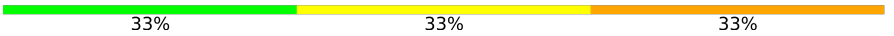
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	234	 94% 6%
2	B	221	 91% 8%
3	C	2	 50% 50%
3	D	2	 100%
3	E	2	 100%

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Mol	Chain	Length	Quality of chain
3	F	2	 50% 50%
4	G	3	 33% 33% 33%

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
4	FUC	G	3	X	-	-	-
5	MAN	A	304	-	-	-	X
5	MAN	A	314	-	-	-	X
5	MAN	B	511	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3782 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1771	1086	327	331	27	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	GLU	-	expression tag	UNP P27918
A	257	ASN	-	expression tag	UNP P27918
A	258	LEU	-	expression tag	UNP P27918
A	259	TYR	-	expression tag	UNP P27918
A	260	PHE	-	expression tag	UNP P27918
A	261	GLN	-	expression tag	UNP P27918

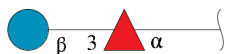
- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	220	1714	1063	319	310	22	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

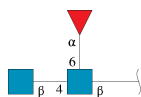
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	expression tag	UNP P27918
B	470	GLU	-	expression tag	UNP P27918
B	471	ASN	-	expression tag	UNP P27918
B	472	LEU	-	expression tag	UNP P27918
B	473	TYR	-	expression tag	UNP P27918
B	474	PHE	-	expression tag	UNP P27918
B	475	GLN	-	expression tag	UNP P27918

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



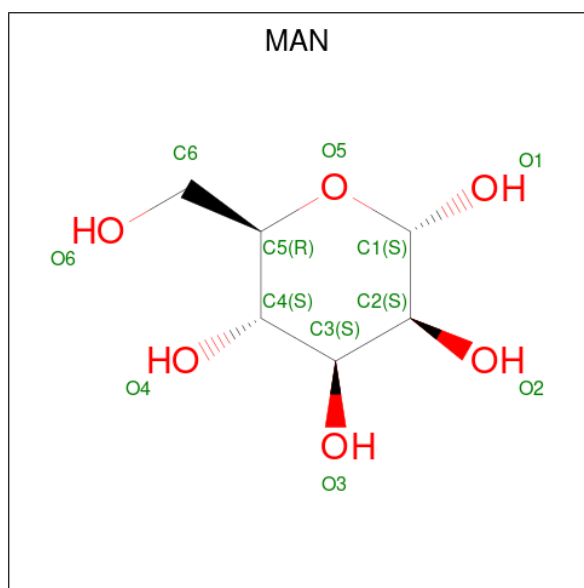
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	12	9			
3	D	2	Total	C	O	0	0	0
			21	12	9			
3	E	2	Total	C	O	0	0	0
			21	12	9			
3	F	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



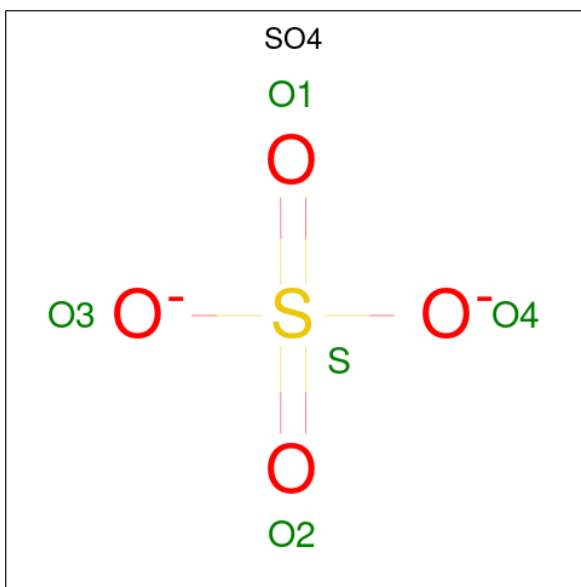
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

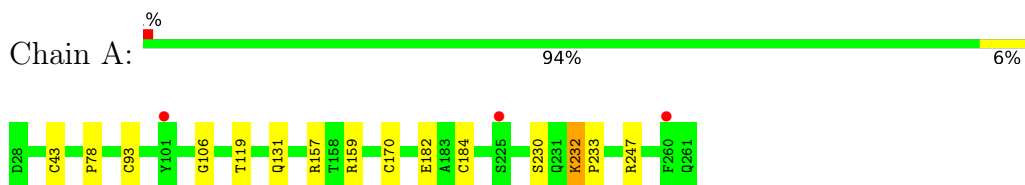


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

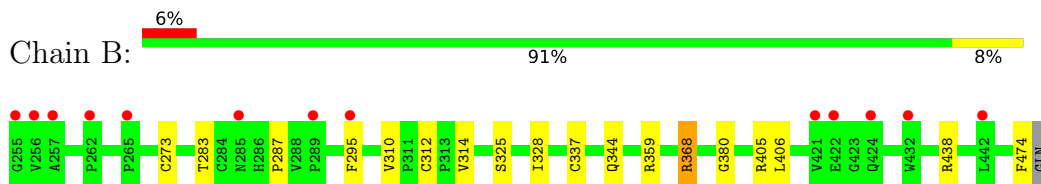
### 3 Residue-property plots [i](#)

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: Properdin



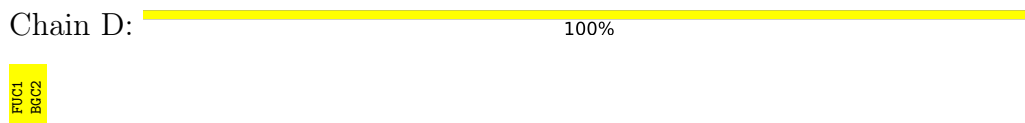
- Molecule 2: Properdin



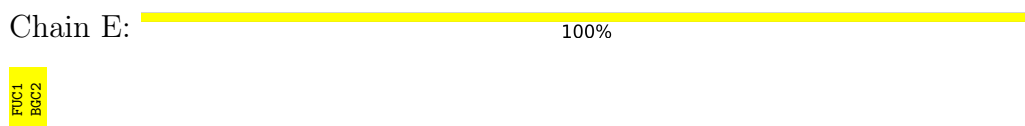
- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose





FUC1  
BGC2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-[alpha-L-fucofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucofuranose

Chain G:  33% 33% 33%

MAG1  
MAG2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.97Å 47.11Å 122.93Å 90.00° 119.41° 90.00°	Depositor
Resolution (Å)	45.58 – 2.80 45.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (45.58-2.80) 96.3 (45.58-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.238 , 0.274 0.238 , 0.274	Depositor DCC
$R_{free}$ test set	2000 reflections (8.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.5	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: FUC, BGC, SO4, MAN, NAG

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	0/1830	0.54	0/2492
2	B	0.33	0/1770	0.55	0/2410
All	All	0.31	0/3600	0.55	0/4902

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

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	1771	0	1624	4	0
2	B	1714	0	1614	3	0
3	C	21	0	19	0	0
3	D	21	0	19	0	0
3	E	21	0	19	0	0
3	F	21	0	19	0	0
4	G	38	0	34	1	0
5	A	88	0	80	0	0
5	B	77	0	70	0	0
6	A	10	0	0	1	0
All	All	3782	0	3498	8	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 (8) 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)
2:B:344:GLN:OE1	2:B:368:ARG:NH1	2.23	0.71
1:A:157:ARG:NH2	1:A:182:GLU:OE2	2.26	0.66
1:A:247:ARG:NH2	6:A:315:SO4:O4	2.30	0.65
4:G:2:NAG:H3	4:G:2:NAG:H83	1.84	0.60
2:B:325:SER:O	2:B:344:GLN:NE2	2.43	0.51
2:B:380:GLY:N	2:B:438:ARG:O	2.48	0.47
1:A:232:LYS:HB2	1:A:233:PRO:HD3	1.98	0.44
1:A:78:PRO:HA	1:A:106:GLY:HA3	2.03	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	232/234 (99%)	212 (91%)	18 (8%)	2 (1%)	17	46
2	B	218/221 (99%)	202 (93%)	15 (7%)	1 (0%)	29	61
All	All	450/455 (99%)	414 (92%)	33 (7%)	3 (1%)	22	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	232	LYS
2	B	287	PRO

### 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	193/193 (100%)	186 (96%)	7 (4%)	35	69
2	B	189/190 (100%)	176 (93%)	13 (7%)	15	41
All	All	382/383 (100%)	362 (95%)	20 (5%)	23	55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	CYS
1	A	93	CYS
1	A	119	THR
1	A	131	GLN
1	A	159	ARG
1	A	170	CYS
1	A	184	CYS
2	B	273	CYS
2	B	283	THR
2	B	295	PHE
2	B	310	VAL
2	B	312	CYS
2	B	314	VAL
2	B	328	ILE
2	B	337	CYS
2	B	359	ARG
2	B	368	ARG
2	B	405	ARG
2	B	406	LEU
2	B	474	PHE

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

### 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](#)

11 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
3	FUC	C	1	1,3	10,10,11	0.74	0	14,14,16	1.03	0
3	BGC	C	2	3	11,11,12	1.77	3 (27%)	15,15,17	1.45	2 (13%)
3	FUC	D	1	1,3	10,10,11	0.90	0	14,14,16	1.02	1 (7%)
3	BGC	D	2	3	11,11,12	1.79	2 (18%)	15,15,17	0.86	1 (6%)
3	FUC	E	1	1,3	10,10,11	0.92	1 (10%)	14,14,16	0.72	0
3	BGC	E	2	3	11,11,12	1.72	3 (27%)	15,15,17	1.55	3 (20%)
3	FUC	F	1	3,2	10,10,11	1.00	0	14,14,16	1.00	0
3	BGC	F	2	3	11,11,12	1.84	3 (27%)	15,15,17	1.44	4 (26%)
4	NAG	G	1	4,2	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	G	2	4	14,14,15	0.82	1 (7%)	17,19,21	1.21	2 (11%)
4	FUC	G	3	4	10,10,11	0.72	0	14,14,16	1.26	3 (21%)

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
3	FUC	C	1	1,3	-	-	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	FUC	D	1	1,3	-	-	0/1/1/1
3	BGC	D	2	3	-	2/2/19/22	0/1/1/1
3	FUC	E	1	1,3	-	-	0/1/1/1
3	BGC	E	2	3	-	0/2/19/22	0/1/1/1

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	BGC	O5-C1	4.74	1.51	1.43
3	F	2	BGC	O5-C1	4.65	1.51	1.43
3	E	2	BGC	O5-C1	4.47	1.50	1.43
3	C	2	BGC	O5-C1	4.42	1.50	1.43
3	C	2	BGC	C2-C3	-2.82	1.48	1.52
3	F	2	BGC	C2-C3	-2.50	1.48	1.52
3	F	2	BGC	O5-C5	2.43	1.48	1.43
3	D	2	BGC	C2-C3	-2.41	1.49	1.52
3	E	2	BGC	C2-C3	-2.36	1.49	1.52
4	G	2	NAG	O5-C1	2.21	1.47	1.43
3	E	1	FUC	O5-C1	-2.12	1.40	1.43
3	C	2	BGC	O5-C5	2.12	1.47	1.43
3	E	2	BGC	O5-C5	2.07	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	C1-O5-C5	-3.98	106.80	112.19
4	G	2	NAG	C2-N2-C7	3.85	128.39	122.90
3	C	2	BGC	O5-C5-C6	3.48	112.66	107.20
3	E	2	BGC	C1-C2-C3	3.36	113.79	109.67
3	F	2	BGC	C6-C5-C4	-2.96	106.07	113.00
4	G	3	FUC	C1-O5-C5	2.96	119.48	112.78
3	E	2	BGC	O5-C5-C6	2.96	111.84	107.20
3	F	2	BGC	C3-C4-C5	2.78	115.19	110.24
3	E	2	BGC	C1-O5-C5	-2.66	108.59	112.19
3	F	2	BGC	C1-O5-C5	2.20	115.17	112.19
3	F	2	BGC	O5-C5-C4	2.14	116.05	110.83
3	D	1	FUC	O5-C5-C4	2.10	113.30	109.52
3	D	2	BGC	O5-C5-C6	2.09	110.48	107.20
4	G	3	FUC	O5-C5-C4	2.04	113.18	109.52
4	G	3	FUC	C1-C2-C3	2.04	112.17	109.67
4	G	2	NAG	C1-C2-N2	2.03	113.95	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	3	FUC	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6
3	D	2	BGC	C4-C5-C6-O6
3	D	2	BGC	O5-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
3	F	2	BGC	O5-C5-C6-O6
4	G	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7

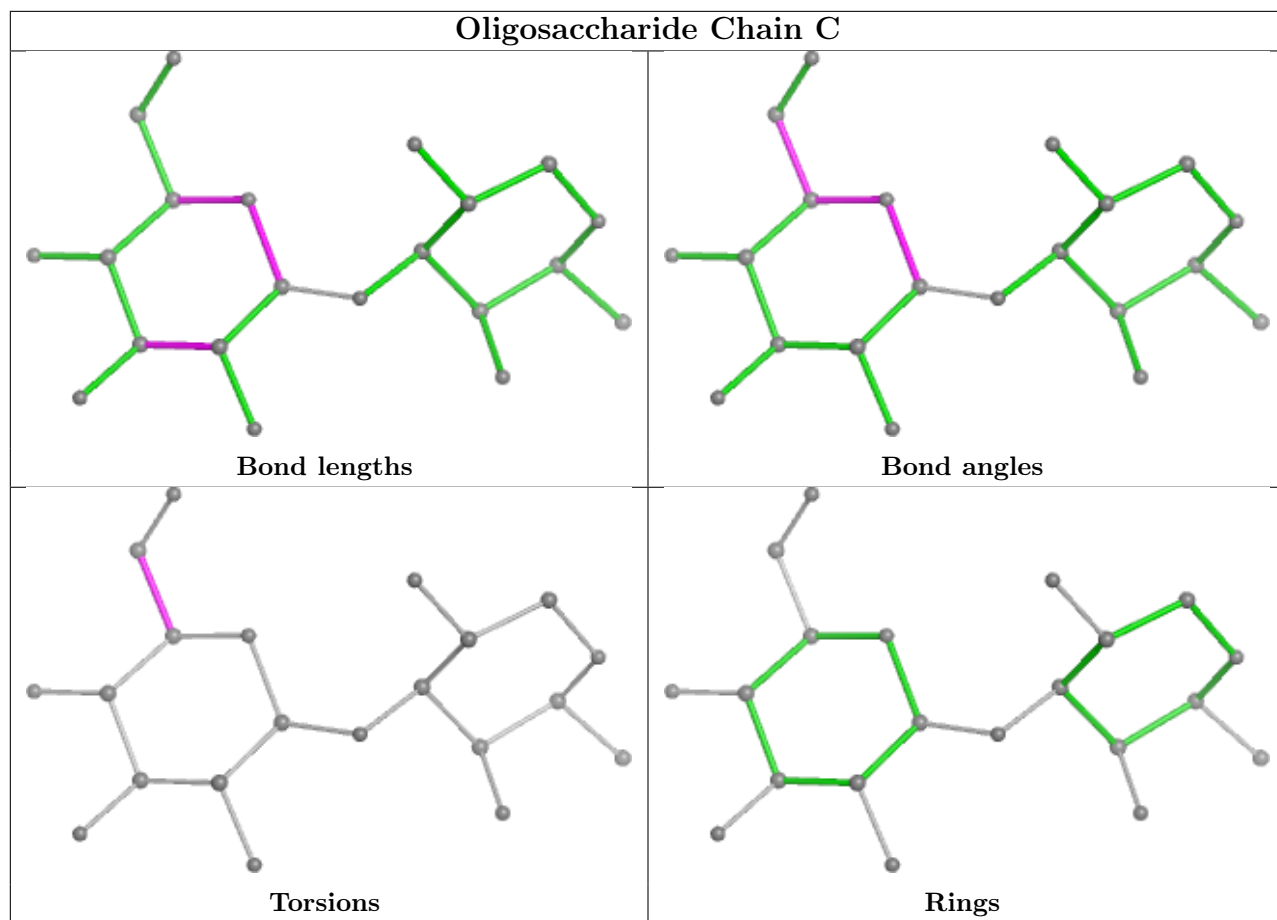
There are no ring outliers.

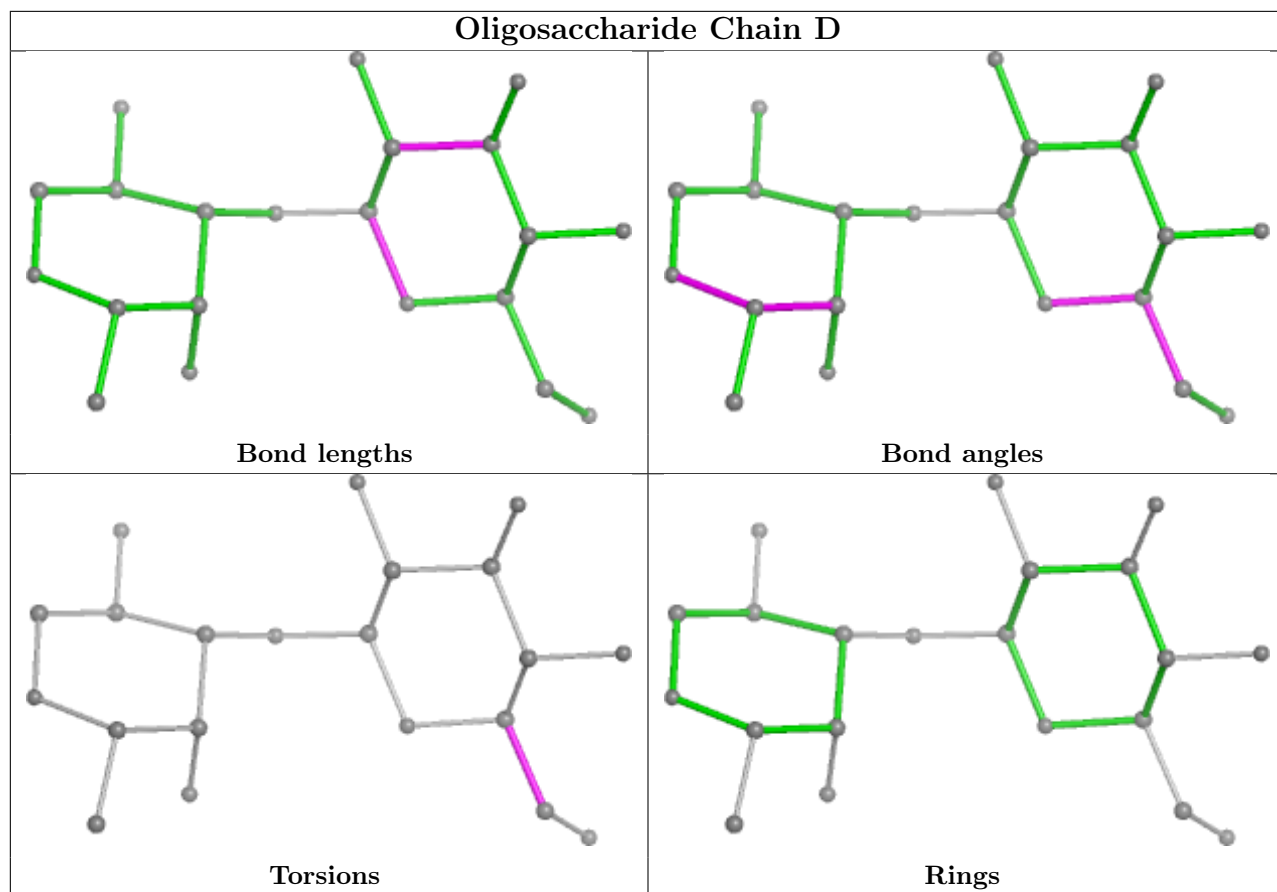
1 monomer is involved in 1 short contact:

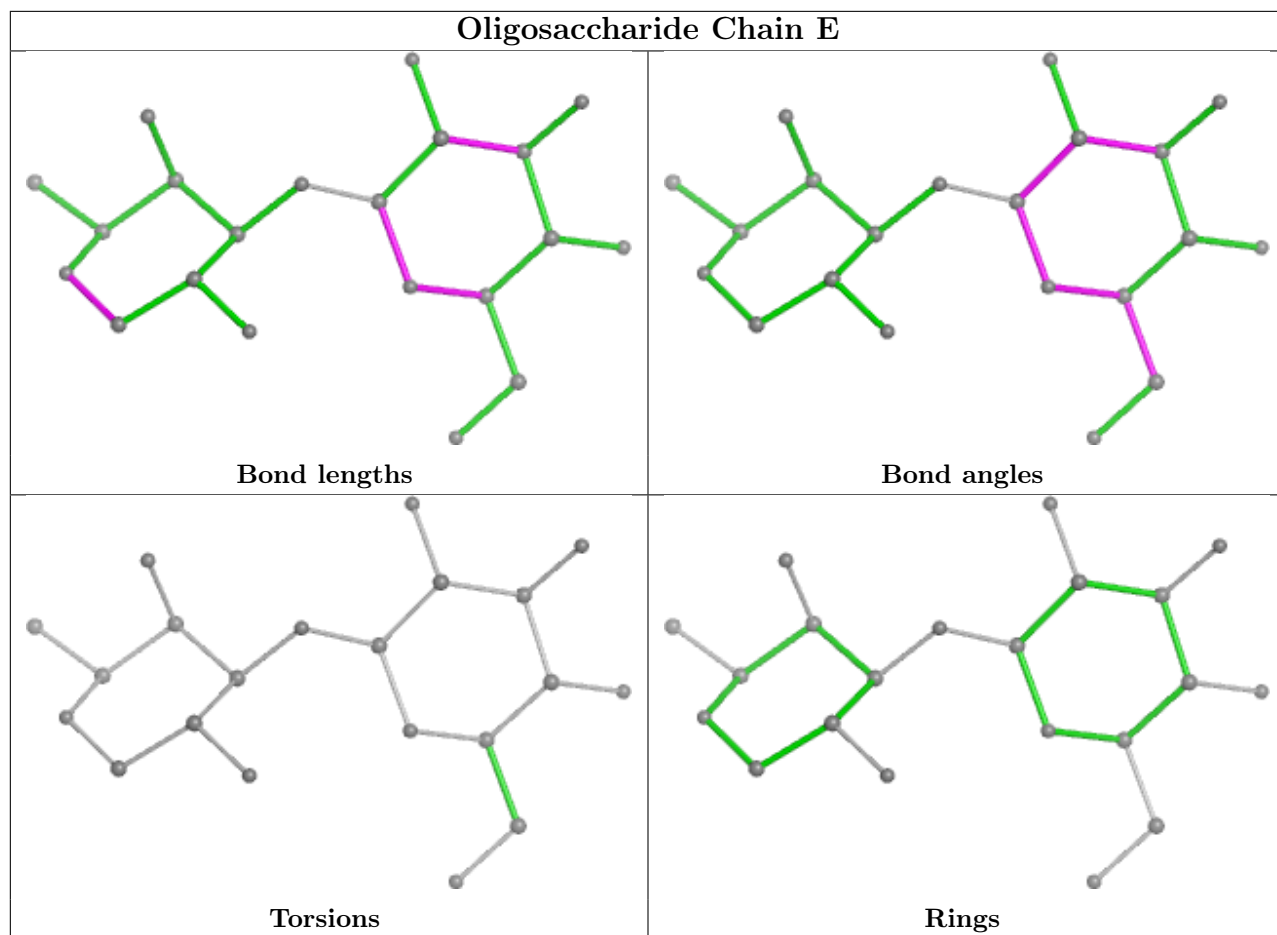
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0

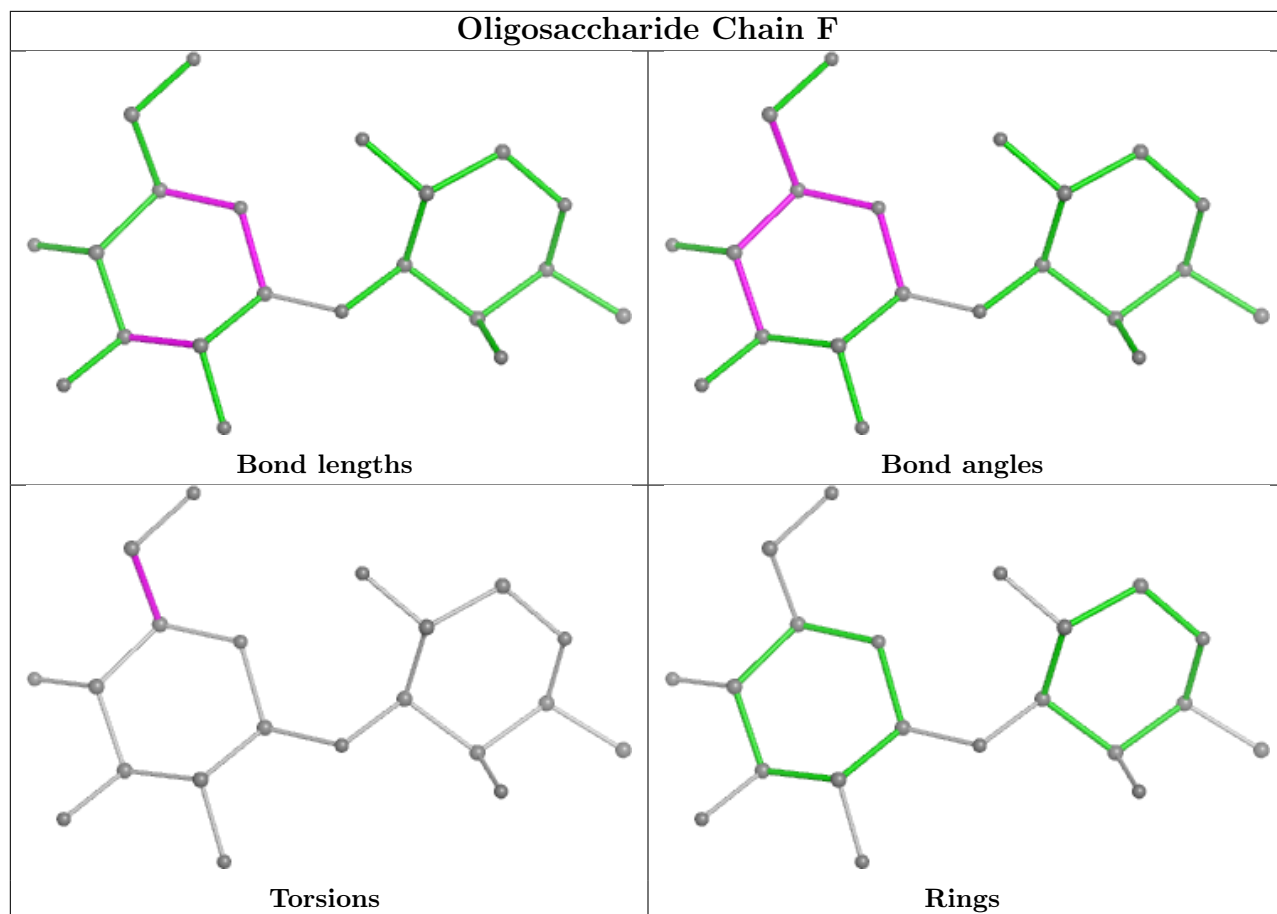
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

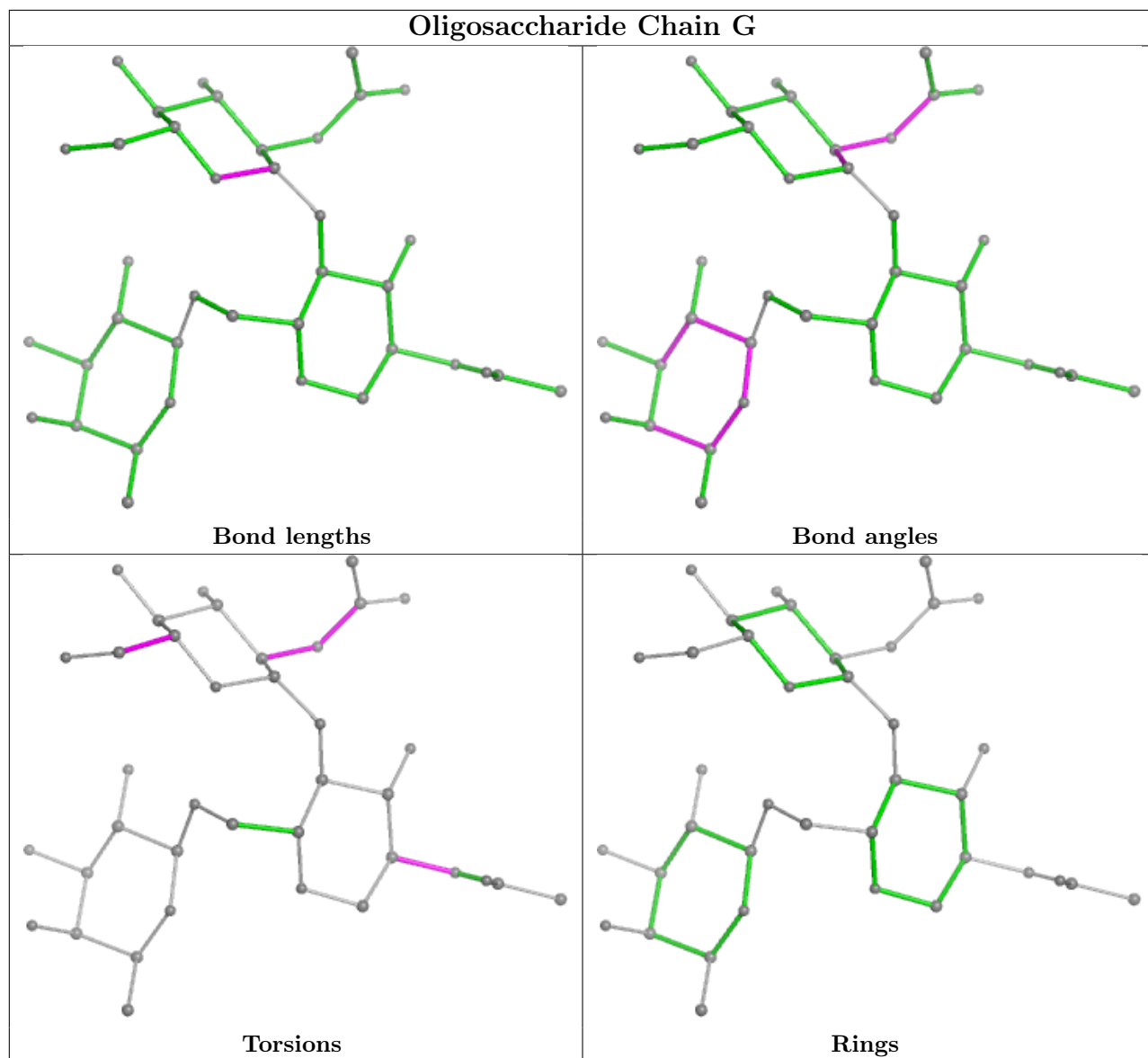












## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
5	MAN	A	307	1	11,11,12	0.96	0	15,15,17	1.85	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	B	510	2	11,11,12	0.97	0	15,15,17	1.92	3 (20%)
5	MAN	B	503	2	11,11,12	1.05	1 (9%)	15,15,17	1.86	4 (26%)
5	MAN	A	310	1	11,11,12	1.09	0	15,15,17	1.97	3 (20%)
5	MAN	A	308	1	11,11,12	1.05	0	15,15,17	1.83	3 (20%)
5	MAN	B	505	2	11,11,12	1.32	1 (9%)	15,15,17	2.53	3 (20%)
5	MAN	A	314	1	11,11,12	1.27	2 (18%)	15,15,17	1.78	2 (13%)
5	MAN	B	509	2	11,11,12	1.19	1 (9%)	15,15,17	1.97	3 (20%)
5	MAN	B	511	2	11,11,12	1.45	2 (18%)	15,15,17	2.42	3 (20%)
5	MAN	B	512	2	11,11,12	1.28	1 (9%)	15,15,17	2.83	4 (26%)
5	MAN	A	304	1	11,11,12	1.22	1 (9%)	15,15,17	2.15	4 (26%)
6	SO4	A	316	-	4,4,4	0.16	0	6,6,6	0.06	0
5	MAN	A	311	1	11,11,12	1.28	1 (9%)	15,15,17	2.22	3 (20%)
5	MAN	A	309	1	11,11,12	0.98	0	15,15,17	1.90	2 (13%)
5	MAN	B	504	2	11,11,12	1.14	1 (9%)	15,15,17	1.91	4 (26%)
6	SO4	A	315	-	4,4,4	0.14	0	6,6,6	0.05	0
5	MAN	A	303	1	11,11,12	1.42	1 (9%)	15,15,17	2.49	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	307	1	-	0/2/19/22	0/1/1/1
5	MAN	B	510	2	-	0/2/19/22	0/1/1/1
5	MAN	B	503	2	-	0/2/19/22	0/1/1/1
5	MAN	A	310	1	-	0/2/19/22	0/1/1/1
5	MAN	A	308	1	-	1/2/19/22	0/1/1/1
5	MAN	B	505	2	-	1/2/19/22	0/1/1/1
5	MAN	A	314	1	-	2/2/19/22	0/1/1/1
5	MAN	B	509	2	-	1/2/19/22	0/1/1/1
5	MAN	B	511	2	-	1/2/19/22	0/1/1/1
5	MAN	B	512	2	-	2/2/19/22	0/1/1/1
5	MAN	A	304	1	-	1/2/19/22	0/1/1/1
5	MAN	A	311	1	-	0/2/19/22	0/1/1/1
5	MAN	A	309	1	-	0/2/19/22	0/1/1/1
5	MAN	B	504	2	-	0/2/19/22	0/1/1/1
5	MAN	A	303	1	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	MAN	O5-C5	3.44	1.50	1.43
5	B	511	MAN	C1-C2	3.10	1.59	1.52
5	A	311	MAN	O5-C5	3.00	1.49	1.43
5	B	505	MAN	O5-C5	2.78	1.49	1.43
5	B	511	MAN	O5-C5	2.66	1.48	1.43
5	A	314	MAN	O5-C5	2.58	1.48	1.43
5	A	304	MAN	O5-C5	2.23	1.48	1.43
5	B	504	MAN	O5-C5	2.23	1.48	1.43
5	B	512	MAN	C4-C3	2.13	1.57	1.52
5	B	509	MAN	O5-C5	2.05	1.47	1.43
5	B	503	MAN	O5-C5	2.04	1.47	1.43
5	A	314	MAN	C4-C5	2.01	1.57	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	303	MAN	C1-O5-C5	7.48	122.33	112.19
5	B	512	MAN	C1-O5-C5	7.40	122.22	112.19
5	B	511	MAN	C1-O5-C5	7.25	122.01	112.19
5	B	505	MAN	C1-O5-C5	6.99	121.67	112.19
5	A	311	MAN	C1-O5-C5	6.39	120.86	112.19
5	A	310	MAN	C1-O5-C5	5.86	120.13	112.19
5	A	304	MAN	C1-O5-C5	5.86	120.13	112.19
5	B	512	MAN	O5-C1-C2	5.71	119.58	110.77
5	A	309	MAN	C1-O5-C5	5.69	119.91	112.19
5	B	510	MAN	C1-O5-C5	5.61	119.79	112.19
5	B	509	MAN	C1-O5-C5	5.47	119.61	112.19
5	B	504	MAN	C1-O5-C5	5.38	119.49	112.19
5	B	503	MAN	C1-O5-C5	5.12	119.13	112.19
5	A	308	MAN	C1-O5-C5	5.10	119.10	112.19
5	A	314	MAN	C1-O5-C5	5.10	119.10	112.19
5	A	307	MAN	C1-O5-C5	4.81	118.71	112.19
5	B	505	MAN	O5-C1-C2	4.65	117.95	110.77
5	B	511	MAN	O2-C2-C3	-3.85	102.42	110.14
5	A	303	MAN	O5-C1-C2	3.83	116.68	110.77
5	A	311	MAN	O5-C1-C2	3.74	116.54	110.77
5	A	303	MAN	O2-C2-C3	-3.42	103.28	110.14
5	B	505	MAN	O2-C2-C3	-3.29	103.55	110.14
5	A	304	MAN	O2-C2-C3	-3.28	103.57	110.14
5	A	307	MAN	O2-C2-C3	-3.23	103.67	110.14
5	B	509	MAN	O5-C1-C2	3.04	115.46	110.77
5	A	304	MAN	O5-C1-C2	3.01	115.42	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	314	MAN	O2-C2-C3	-2.86	104.41	110.14
5	B	512	MAN	C1-C2-C3	2.83	113.14	109.67
5	A	307	MAN	O5-C1-C2	2.77	115.04	110.77
5	B	510	MAN	O2-C2-C3	-2.75	104.63	110.14
5	B	510	MAN	O5-C1-C2	2.71	114.95	110.77
5	A	311	MAN	O2-C2-C3	-2.56	105.02	110.14
5	A	309	MAN	O2-C2-C3	-2.54	105.04	110.14
5	B	503	MAN	O2-C2-C3	-2.54	105.06	110.14
5	B	504	MAN	O2-C2-C3	-2.53	105.06	110.14
5	B	511	MAN	O5-C1-C2	2.48	114.60	110.77
5	A	310	MAN	O5-C1-C2	2.48	114.60	110.77
5	A	304	MAN	C1-C2-C3	2.40	112.62	109.67
5	B	509	MAN	O2-C2-C3	-2.39	105.34	110.14
5	B	512	MAN	O3-C3-C2	2.31	114.42	109.99
5	B	504	MAN	O5-C1-C2	2.31	114.33	110.77
5	A	308	MAN	O5-C1-C2	2.28	114.30	110.77
5	A	308	MAN	O2-C2-C3	-2.23	105.68	110.14
5	B	504	MAN	C1-C2-C3	2.21	112.38	109.67
5	A	310	MAN	O2-C2-C3	-2.19	105.74	110.14
5	B	503	MAN	C1-C2-C3	2.18	112.35	109.67
5	B	503	MAN	O5-C1-C2	2.13	114.05	110.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	512	MAN	C4-C5-C6-O6
5	B	512	MAN	O5-C5-C6-O6
5	A	303	MAN	C4-C5-C6-O6
5	A	304	MAN	O5-C5-C6-O6
5	A	314	MAN	C4-C5-C6-O6
5	A	303	MAN	O5-C5-C6-O6
5	B	511	MAN	C4-C5-C6-O6
5	B	509	MAN	O5-C5-C6-O6
5	B	505	MAN	C4-C5-C6-O6
5	A	314	MAN	O5-C5-C6-O6
5	A	308	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	315	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	234/234 (100%)	0.33	3 (1%) 77 72	47, 77, 110, 136	0
2	B	220/221 (99%)	0.50	13 (5%) 22 14	48, 76, 159, 177	0
All	All	454/455 (99%)	0.41	16 (3%) 44 34	47, 76, 146, 177	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	PHE	5.0
2	B	257	ALA	4.5
2	B	255	GLY	3.9
2	B	285	ASN	3.8
2	B	265	PRO	3.6
2	B	262	PRO	3.0
2	B	442	LEU	2.7
1	A	260	PHE	2.6
2	B	421	VAL	2.5
2	B	424	GLN	2.4
2	B	289	PRO	2.4
1	A	101	TYR	2.3
2	B	256	VAL	2.2
1	A	225	SER	2.2
2	B	432	TRP	2.2
2	B	422	GLU	2.2

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

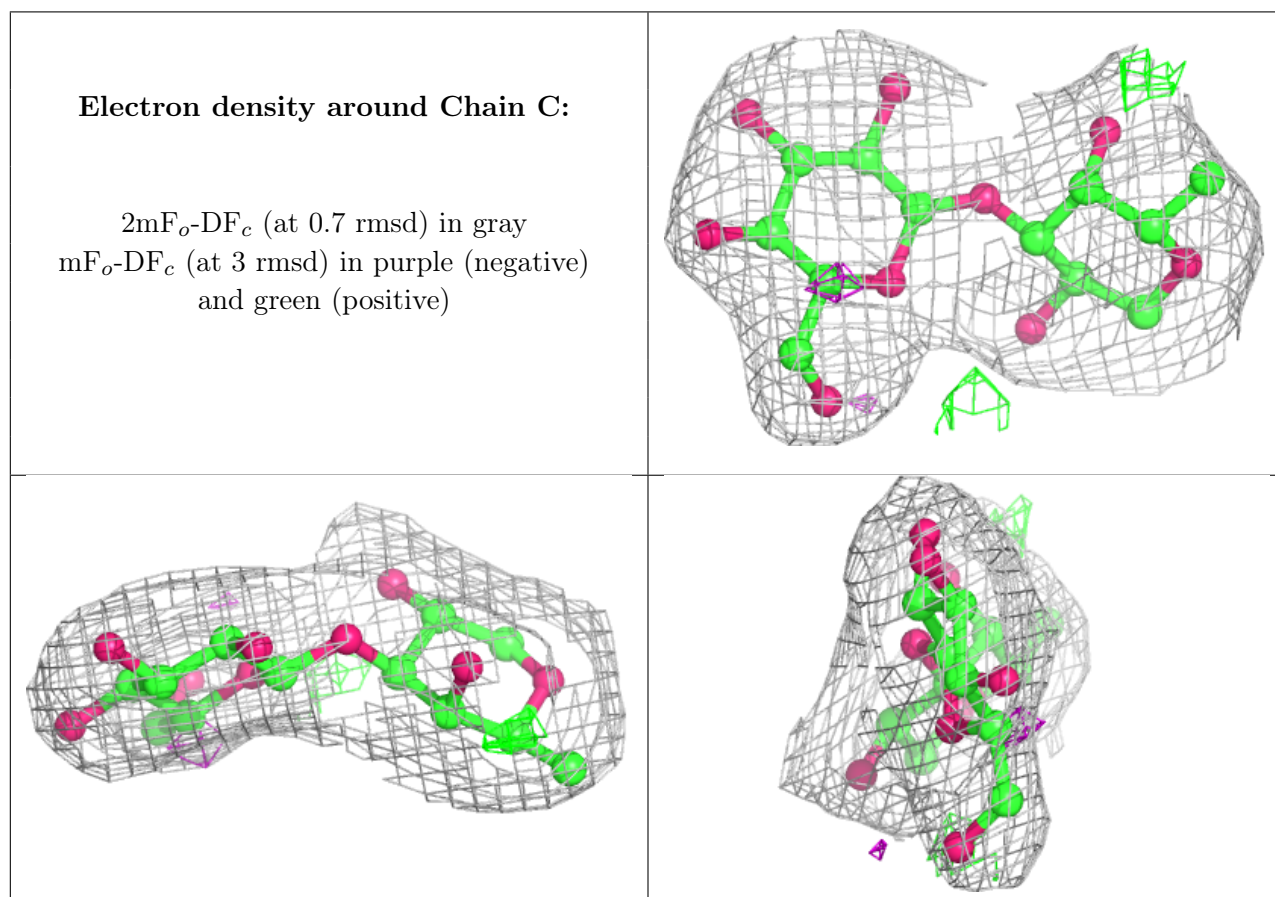
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

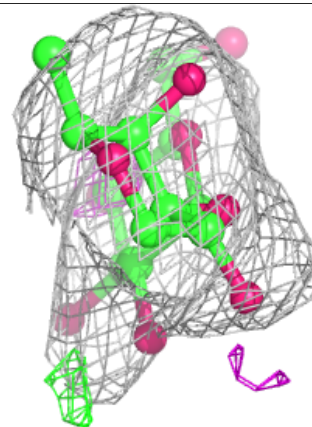
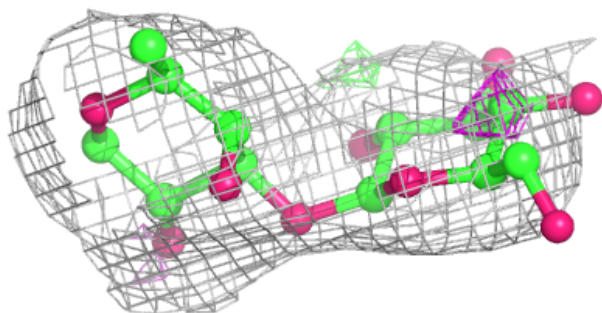
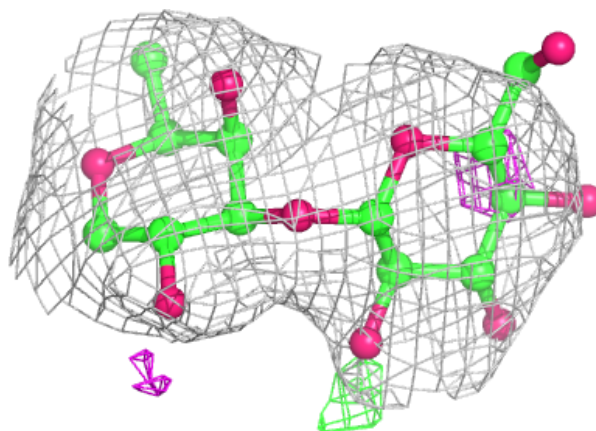
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	F	2	11/12	0.70	0.35	106,110,124,125	0
4	NAG	G	1	14/15	0.77	0.21	136,141,149,154	0
4	NAG	G	2	14/15	0.82	0.34	146,157,164,167	0
3	BGC	D	2	11/12	0.86	0.35	95,102,115,123	0
4	FUC	G	3	10/11	0.89	0.37	120,120,120,120	0
3	BGC	E	2	11/12	0.94	0.22	74,74,74,74	0
3	FUC	F	1	10/11	0.94	0.23	57,69,76,104	0
3	FUC	D	1	10/11	0.94	0.15	78,91,102,106	0
3	BGC	C	2	11/12	0.95	0.19	57,63,68,72	0
3	FUC	E	1	10/11	0.96	0.22	53,59,71,75	0
3	FUC	C	1	10/11	0.97	0.13	56,65,74,90	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.



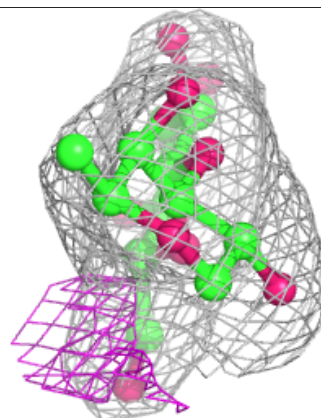
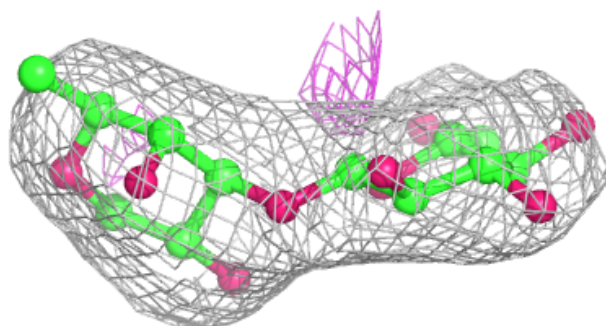
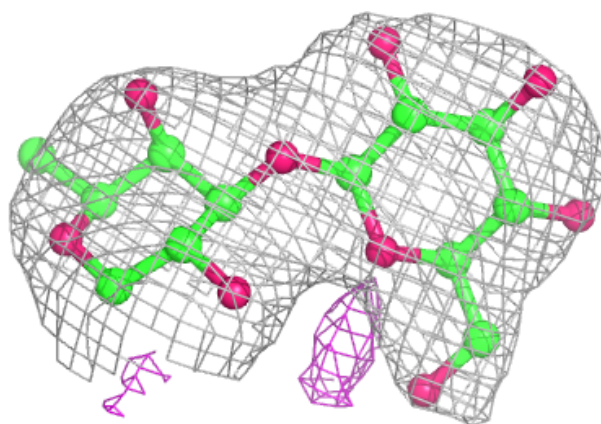
**Electron density around Chain D:**

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

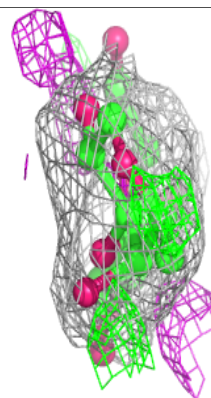
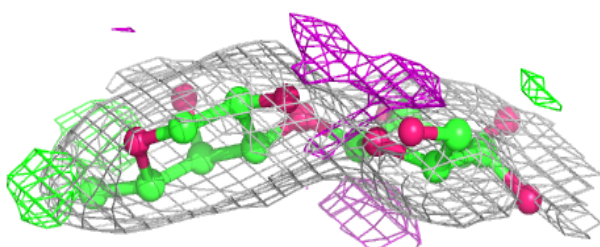
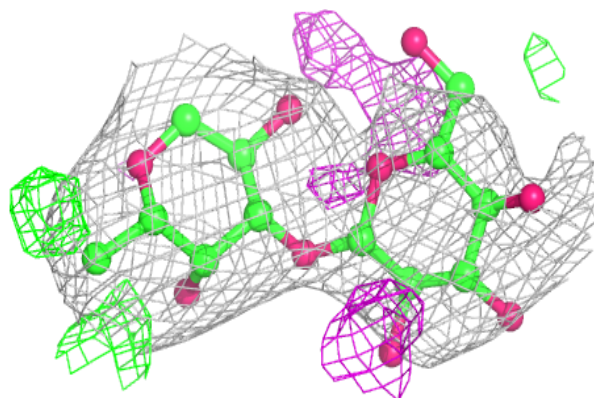


**Electron density around Chain E:**

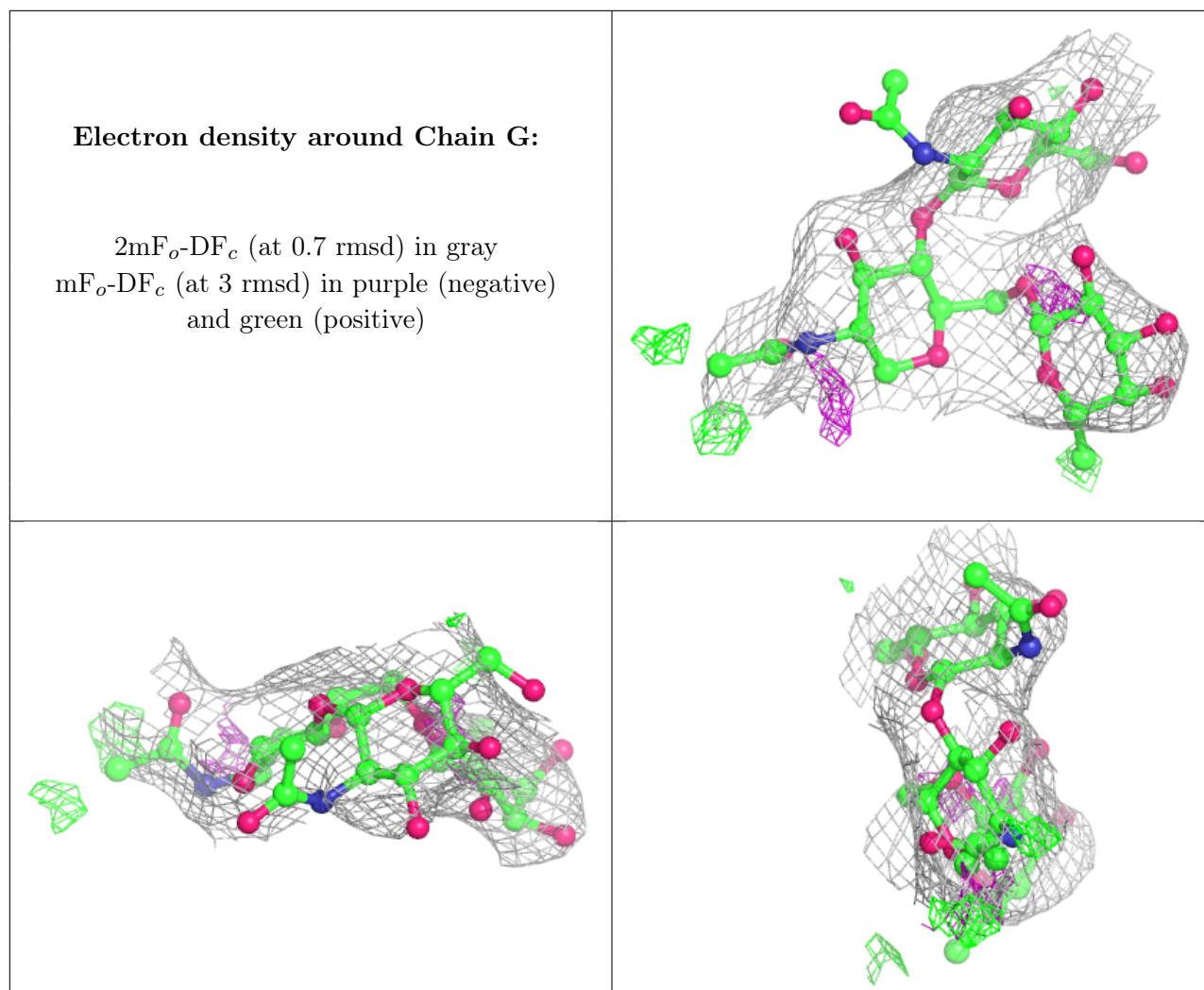
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 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
5	MAN	A	314	11/12	0.58	0.69	87,87,87,87	0
5	MAN	B	512	11/12	0.68	0.35	87,87,87,87	0
5	MAN	B	505	11/12	0.76	0.23	87,87,87,87	0
5	MAN	B	511	11/12	0.77	0.41	87,87,87,87	0
5	MAN	A	304	11/12	0.80	0.50	87,87,87,87	0
5	MAN	B	510	11/12	0.82	0.21	87,87,87,87	0
5	MAN	B	509	11/12	0.85	0.24	87,87,87,87	0
5	MAN	A	307	11/12	0.86	0.28	87,87,87,87	0
5	MAN	A	309	11/12	0.86	0.23	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	310	11/12	0.86	0.20	87,87,87,87	0
5	MAN	A	303	11/12	0.89	0.27	87,87,87,87	0
5	MAN	B	503	11/12	0.90	0.26	87,87,87,87	0
6	SO4	A	316	5/5	0.91	0.15	80,90,100,101	0
5	MAN	B	504	11/12	0.92	0.29	87,87,87,87	0
5	MAN	A	311	11/12	0.94	0.25	87,87,87,87	0
5	MAN	A	308	11/12	0.94	0.25	87,87,87,87	0
6	SO4	A	315	5/5	0.96	0.13	88,88,91,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.