



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:30 AM BST

PDB ID : 4WRN  
Title : Crystal structure of the polymerization region of human uromodulin/Tamm-Horsfall protein  
Authors : Bokhove, M.; De Sanctis, D.; Jovine, L.  
Deposited on : 2014-10-24  
Resolution : 3.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

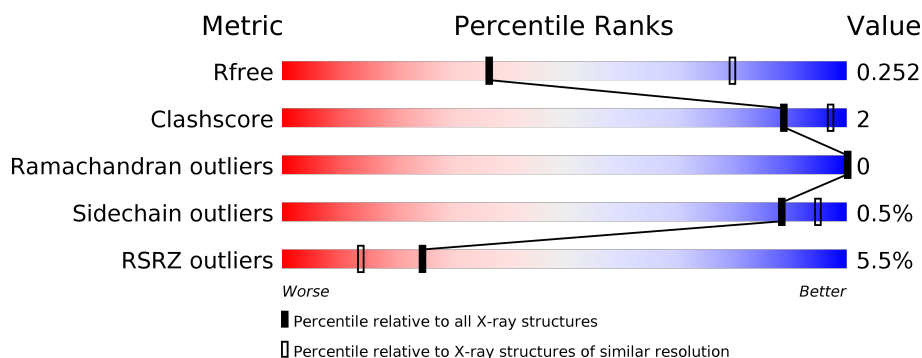
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	695	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	695	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	D	2	-	-	-	X
3	NAG	A	803	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20898 atoms, of which 10325 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 Maltose-binding periplasmic protein,Uromodulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	693	Total	C	H	N	O	S	0	0	0
			10579	3394	5219	906	1028	32			
1	B	663	Total	C	H	N	O	S	0	0	0
			10147	3258	5024	862	976	27			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLU	-	expression tag	UNP P0AEY0
A	17	THR	-	expression tag	UNP P0AEY0
A	18	GLY	-	expression tag	UNP P0AEY0
A	19	HIS	-	expression tag	UNP P0AEY0
A	20	HIS	-	expression tag	UNP P0AEY0
A	21	HIS	-	expression tag	UNP P0AEY0
A	22	HIS	-	expression tag	UNP P0AEY0
A	23	HIS	-	expression tag	UNP P0AEY0
A	24	HIS	-	expression tag	UNP P0AEY0
A	26	THR	ILE	engineered mutation	UNP P0AEY0
A	106	ALA	ASP	engineered mutation	UNP P0AEY0
A	107	ALA	LYS	engineered mutation	UNP P0AEY0
A	196	ALA	GLU	engineered mutation	UNP P0AEY0
A	197	ALA	ASN	engineered mutation	UNP P0AEY0
A	239	HIS	ALA	engineered mutation	UNP P0AEY0
A	243	HIS	LYS	engineered mutation	UNP P0AEY0
A	263	ALA	LYS	engineered mutation	UNP P0AEY0
A	336	VAL	ALA	engineered mutation	UNP P0AEY0
A	341	VAL	ILE	engineered mutation	UNP P0AEY0
A	383	ALA	GLU	engineered mutation	UNP P0AEY0
A	386	ALA	LYS	engineered mutation	UNP P0AEY0
A	387	ALA	ASP	engineered mutation	UNP P0AEY0
A	391	ASN	ARG	engineered mutation	UNP P0AEY0
A	392	ALA	-	linker	UNP P0AEY0
A	393	ALA	-	linker	UNP P0AEY0

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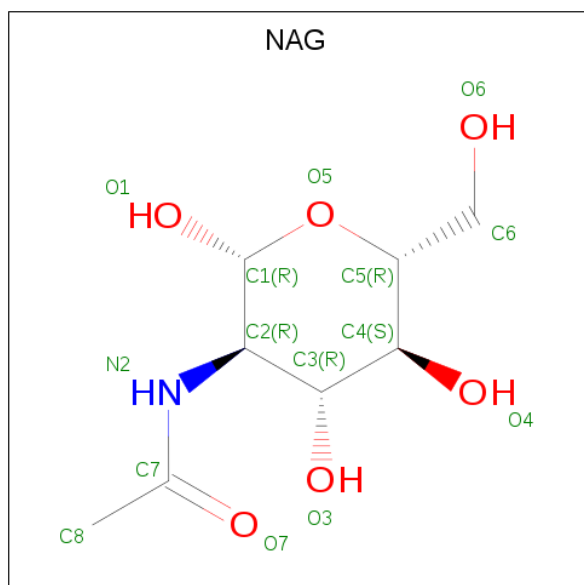
Chain	Residue	Modelled	Actual	Comment	Reference
A	394	ALA	-	linker	UNP P0AEY0
A	613	GLN	ASN	engineered mutation	UNP P07911
A	686	ALA	ARG	engineered mutation	UNP P07911
A	688	ALA	ARG	engineered mutation	UNP P07911
B	16	GLU	-	expression tag	UNP P0AEY0
B	17	THR	-	expression tag	UNP P0AEY0
B	18	GLY	-	expression tag	UNP P0AEY0
B	19	HIS	-	expression tag	UNP P0AEY0
B	20	HIS	-	expression tag	UNP P0AEY0
B	21	HIS	-	expression tag	UNP P0AEY0
B	22	HIS	-	expression tag	UNP P0AEY0
B	23	HIS	-	expression tag	UNP P0AEY0
B	24	HIS	-	expression tag	UNP P0AEY0
B	26	THR	ILE	engineered mutation	UNP P0AEY0
B	106	ALA	ASP	engineered mutation	UNP P0AEY0
B	107	ALA	LYS	engineered mutation	UNP P0AEY0
B	196	ALA	GLU	engineered mutation	UNP P0AEY0
B	197	ALA	ASN	engineered mutation	UNP P0AEY0
B	239	HIS	ALA	engineered mutation	UNP P0AEY0
B	243	HIS	LYS	engineered mutation	UNP P0AEY0
B	263	ALA	LYS	engineered mutation	UNP P0AEY0
B	336	VAL	ALA	engineered mutation	UNP P0AEY0
B	341	VAL	ILE	engineered mutation	UNP P0AEY0
B	383	ALA	GLU	engineered mutation	UNP P0AEY0
B	386	ALA	LYS	engineered mutation	UNP P0AEY0
B	387	ALA	ASP	engineered mutation	UNP P0AEY0
B	391	ASN	ARG	engineered mutation	UNP P0AEY0
B	392	ALA	-	linker	UNP P0AEY0
B	393	ALA	-	linker	UNP P0AEY0
B	394	ALA	-	linker	UNP P0AEY0
B	613	GLN	ASN	engineered mutation	UNP P07911
B	686	ALA	ARG	engineered mutation	UNP P07911
B	688	ALA	ARG	engineered mutation	UNP P07911

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			44	12	21	11			
2	D	2	Total	C	H	O	0	0	0
			44	12	21	11			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

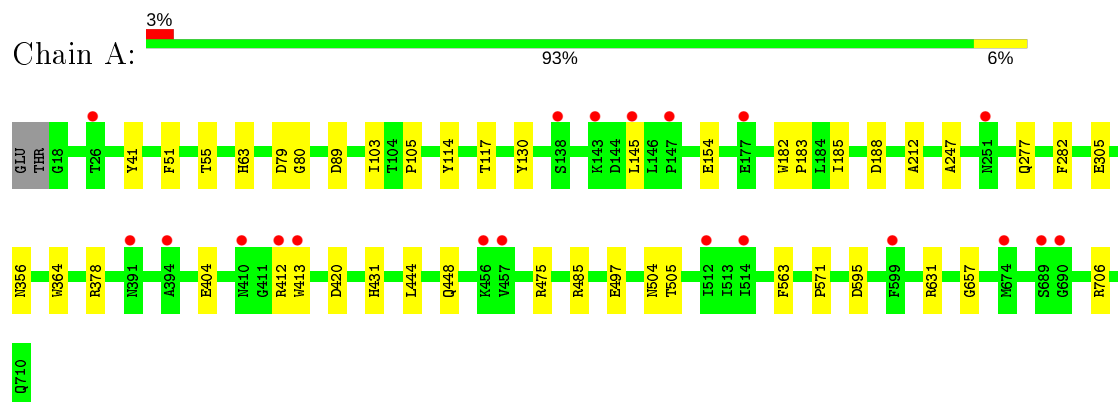
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

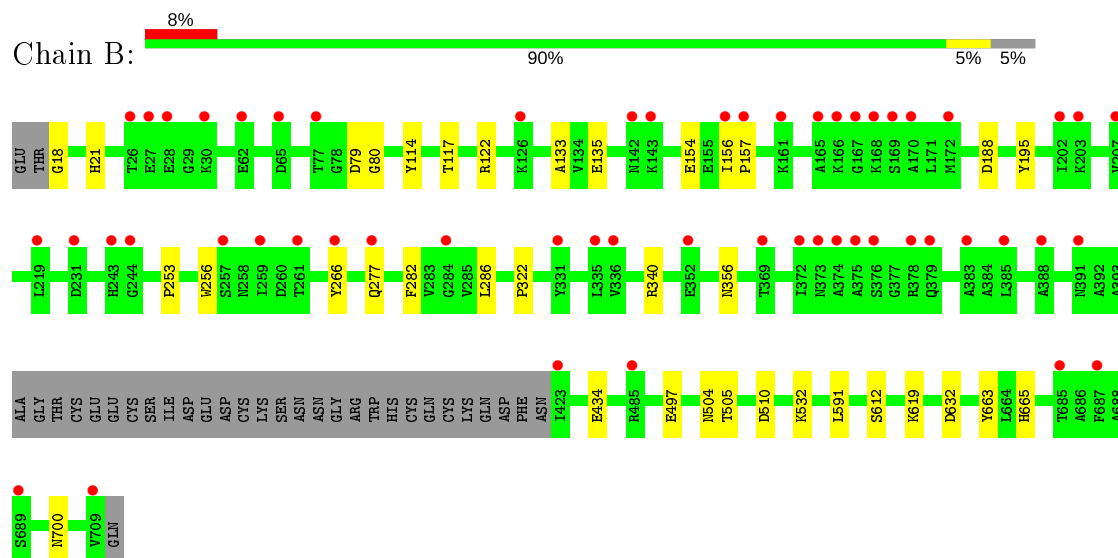
### 3 Residue-property plots [i](#)

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: Maltose-binding periplasmic protein,Uromodulin



- Molecule 1: Maltose-binding periplasmic protein,Uromodulin



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  50% 50%

GLC1  
GLC2



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.32Å 242.32Å 258.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.98 – 3.20 34.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.98-3.20) 90.0 (34.98-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.88 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.221 , 0.246 0.227 , 0.252	Depositor DCC
$R_{free}$ test set	2432 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.7	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 87.8	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	0.93	EDS
Total number of atoms	20898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: ZN, GLC, 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	0.27	0/5483	0.46	0/7441
1	B	0.26	0/5241	0.44	0/7116
All	All	0.27	0/10724	0.45	0/14557

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	5360	5219	5221	22	1
1	B	5123	5024	5026	19	1
2	C	23	21	21	1	0
2	D	23	21	21	1	0
3	A	28	26	26	1	0
3	B	14	14	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	10573	10325	10328	40	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (40) 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:B:188:ASP:OD1	1:B:277:GLN:NE2	2.20	0.74
1:A:188:ASP:OD2	1:A:277:GLN:NE2	2.21	0.72
1:B:532:LYS:NZ	1:B:591:LEU:O	2.30	0.63
1:B:504:ASN:OD1	1:B:505:THR:N	2.34	0.61
3:A:802:NAG:O4	1:B:434:GLU:OE1	2.21	0.59
1:A:154:GLU:N	1:A:154:GLU:OE1	2.36	0.58
1:B:154:GLU:N	1:B:154:GLU:OE1	2.36	0.57
1:B:122:ARG:O	1:B:356:ASN:ND2	2.39	0.56
1:A:504:ASN:OD1	1:A:505:THR:N	2.40	0.54
1:A:114:TYR:O	1:A:117:THR:OG1	2.24	0.54
1:A:448:GLN:OE1	1:A:448:GLN:N	2.38	0.53
1:A:657:GLY:O	1:A:706:ARG:NH2	2.41	0.53
1:B:18:GLY:O	1:B:21:HIS:ND1	2.41	0.53
1:A:404:GLU:OE1	1:A:475:ARG:NH1	2.42	0.53
1:A:79:ASP:OD1	1:A:80:GLY:N	2.43	0.52
1:B:665:HIS:ND1	1:B:700:ASN:OD1	2.43	0.52
1:A:631:ARG:O	1:B:195:TYR:OH	2.28	0.49
1:A:51:PHE:O	1:A:55:THR:OG1	2.28	0.48
1:B:266:TYR:OH	1:B:340:ARG:NH1	2.45	0.47
1:B:79:ASP:OD1	1:B:80:GLY:N	2.47	0.46
1:B:135:GLU:OE2	2:D:1:GLC:O2	2.32	0.46
1:B:133:ALA:O	1:B:286:LEU:N	2.51	0.44
1:B:114:TYR:O	1:B:117:THR:OG1	2.29	0.43
1:A:130:TYR:OH	1:A:305:GLU:OE1	2.33	0.43
1:B:253:PRO:HA	1:B:256:TRP:CD2	2.53	0.43
1:B:612:SER:HA	1:B:663:TYR:CD1	2.54	0.42
1:A:41:TYR:HB3	1:A:63:HIS:HE1	1.84	0.42
1:B:510:ASP:OD1	1:B:510:ASP:N	2.51	0.42
1:A:364:TRP:CD1	2:C:2:GLC:H4	2.55	0.41
1:A:378:ARG:NH2	1:A:420:ASP:O	2.44	0.41
1:A:103:ILE:HG22	1:A:105:PRO:HD3	2.01	0.41
1:A:145:LEU:HD23	1:A:247:ALA:HA	2.02	0.41
1:B:156:ILE:HB	1:B:157:PRO:HD3	2.02	0.41
1:A:89:ASP:HA	1:A:356:ASN:HA	2.02	0.41
1:A:431:HIS:HB3	1:A:444:LEU:HD21	2.02	0.41
1:B:256:TRP:HB2	1:B:322:PRO:HG2	2.03	0.41
1:A:185:ILE:HG23	1:A:212:ALA:HA	2.04	0.40
1:A:412:ARG:CG	1:A:413:TRP:N	2.84	0.40
1:A:182:TRP:N	1:A:183:PRO:CD	2.85	0.40
1:A:563:PHE:HA	1:A:571:PRO:HA	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:NH1	1:B:619:LYS:O[6_555]	2.17	0.03

## 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	691/695 (99%)	683 (99%)	8 (1%)	0	100	100
1	B	659/695 (95%)	652 (99%)	7 (1%)	0	100	100
All	All	1350/1390 (97%)	1335 (99%)	15 (1%)	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	573/575 (100%)	570 (100%)	3 (0%)	88	95
1	B	546/575 (95%)	543 (100%)	3 (0%)	88	95
All	All	1119/1150 (97%)	1113 (100%)	6 (0%)	88	95

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

Mol	Chain	Res	Type
1	A	282	PHE
1	A	497	GLU
1	A	595	ASP
1	B	282	PHE
1	B	497	GLU
1	B	632	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	349	GLN
1	A	419	GLN
1	A	613	GLN
1	B	277	GLN

### 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 ⓘ

4 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	C	1	2	12,12,12	1.05	1 (8%)	17,17,17	1.29	3 (17%)
2	GLC	C	2	2	11,11,12	1.49	3 (27%)	15,15,17	0.90	1 (6%)
2	GLC	D	1	2	12,12,12	1.07	1 (8%)	17,17,17	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	D	2	2	11,11,12	1.53	3 (27%)	15,15,17	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C2-C3	-3.02	1.48	1.52
2	C	2	GLC	C2-C3	-2.81	1.48	1.52
2	C	2	GLC	O3-C3	2.38	1.48	1.43
2	D	2	GLC	O5-C5	2.32	1.48	1.43
2	C	2	GLC	O5-C5	2.19	1.47	1.43
2	D	2	GLC	O3-C3	2.18	1.48	1.43
2	D	1	GLC	O5-C1	2.17	1.48	1.42
2	C	1	GLC	O5-C1	2.11	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-C2-C3	3.00	116.54	110.31
2	C	1	GLC	C4-C3-C2	2.26	114.76	110.82
2	C	1	GLC	O5-C1-C2	2.06	113.96	110.28
2	C	2	GLC	C6-C5-C4	-2.00	108.31	113.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

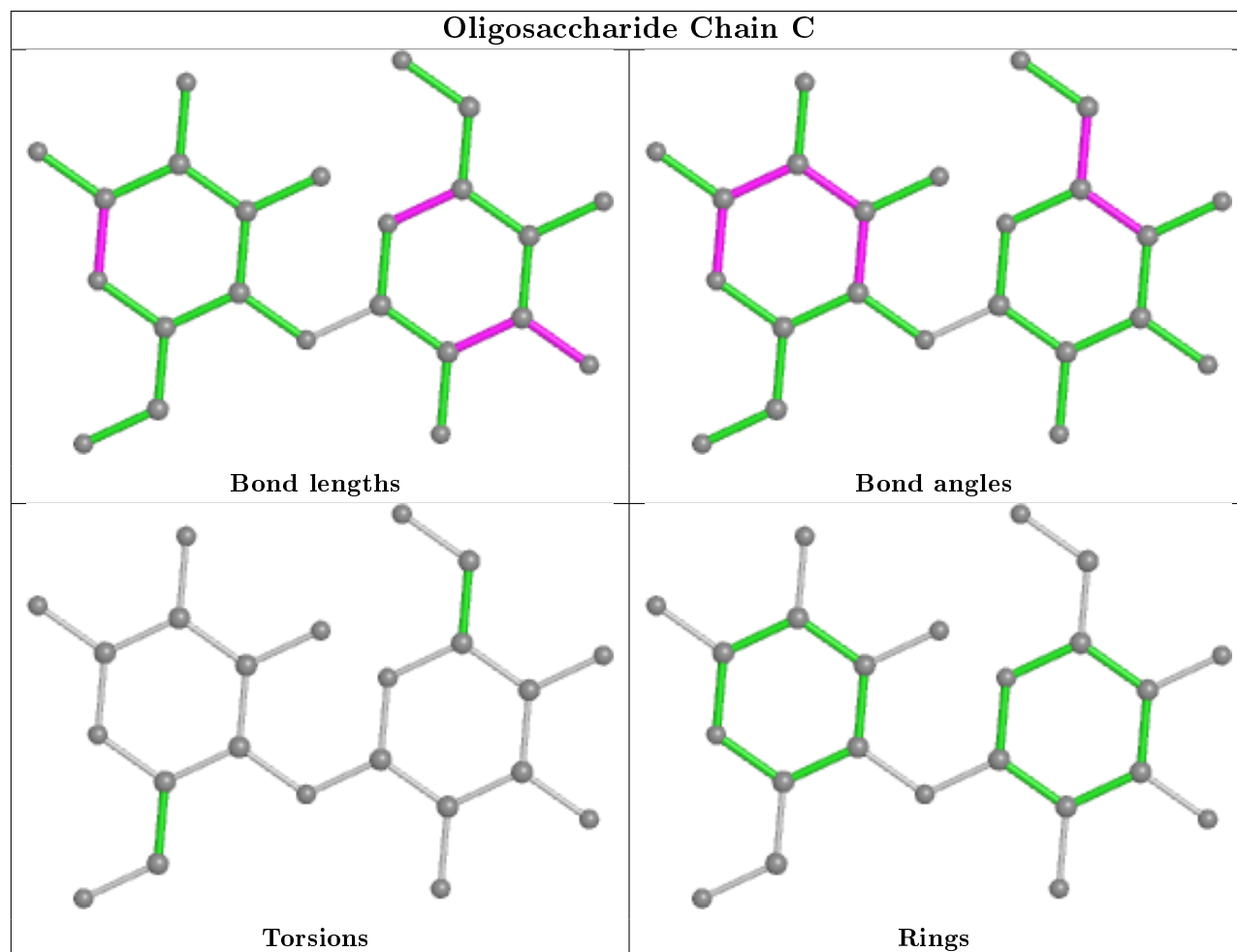
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6

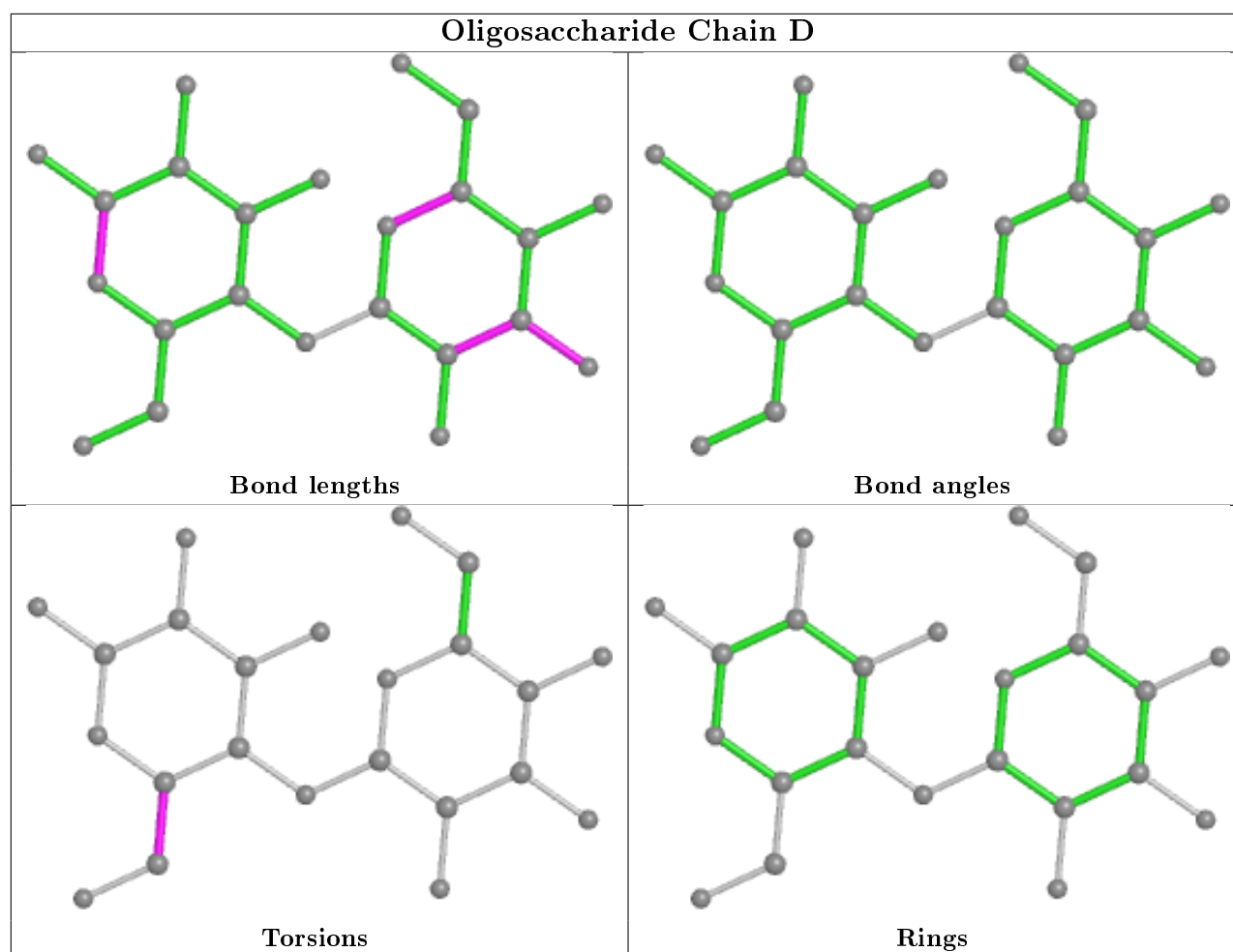
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	1	0
2	D	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	NAG	A	803	1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	B	803	1	14,14,15	0.24	0	17,19,21	0.35	0
3	NAG	A	802	1	14,14,15	0.31	0	17,19,21	0.45	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
3	NAG	A	803	1	-	2/6/23/26	0/1/1/1
3	NAG	B	803	1	-	2/6/23/26	0/1/1/1
3	NAG	A	802	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	NAG	C4-C5-C6-O6
3	B	803	NAG	O5-C5-C6-O6
3	A	803	NAG	C1-C2-N2-C7
3	A	802	NAG	O5-C5-C6-O6
3	A	803	NAG	C3-C2-N2-C7
3	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	NAG	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

### 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	693/695 (99%)	0.15	20 (2%) 51 36	82, 118, 177, 300	0
1	B	663/695 (95%)	0.48	55 (8%) 11 6	77, 160, 249, 309	0
All	All	1356/1390 (97%)	0.31	75 (5%) 25 14	77, 128, 235, 309	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ALA	5.6
1	B	244	GLY	5.1
1	B	156	ILE	5.0
1	B	685	THR	4.5
1	B	385	LEU	4.3
1	B	243	HIS	4.3
1	B	709	VAL	4.2
1	B	168	LYS	4.1
1	B	167	GLY	4.1
1	A	26	THR	4.0
1	B	157	PRO	4.0
1	B	202	ILE	3.9
1	B	231	ASP	3.8
1	B	259	ILE	3.6
1	A	251	ASN	3.6
1	A	391	ASN	3.4
1	B	27	GLU	3.4
1	A	456	LYS	3.3
1	B	372	ILE	3.3
1	A	512	ILE	3.3
1	A	514	ILE	3.2
1	B	383	ALA	3.2
1	B	379	GLN	3.1
1	B	143	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	335	LEU	3.0
1	B	203	LYS	3.0
1	B	166	LYS	2.8
1	A	599	PHE	2.8
1	A	147	PRO	2.8
1	B	352	GLU	2.8
1	B	375	ALA	2.7
1	B	169	SER	2.7
1	B	388	ALA	2.7
1	B	30	LYS	2.7
1	B	161	LYS	2.6
1	B	373	ASN	2.6
1	B	26	THR	2.6
1	B	369	THR	2.6
1	B	170	ALA	2.6
1	B	62	GLU	2.6
1	B	336	VAL	2.6
1	B	689	SER	2.6
1	B	77	THR	2.6
1	B	126	LYS	2.6
1	B	257	SER	2.5
1	A	457	VAL	2.5
1	B	266	TYR	2.5
1	B	28	GLU	2.5
1	B	485	ARG	2.5
1	A	394	ALA	2.5
1	B	378	ARG	2.5
1	A	177	GLU	2.4
1	B	219	LEU	2.4
1	A	412	ARG	2.4
1	B	331	TYR	2.4
1	A	138	SER	2.4
1	A	413	TRP	2.4
1	B	277	GLN	2.3
1	B	391	ASN	2.3
1	B	376	SER	2.3
1	A	674	MET	2.3
1	B	374	ALA	2.2
1	B	207	VAL	2.2
1	B	142	ASN	2.2
1	A	689	SER	2.2
1	B	284	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	410	ASN	2.1
1	A	143	LYS	2.1
1	A	690	GLY	2.1
1	B	65	ASP	2.1
1	B	423	ILE	2.0
1	B	172	MET	2.0
1	B	261	THR	2.0
1	B	687	PHE	2.0
1	A	145	LEU	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](#)

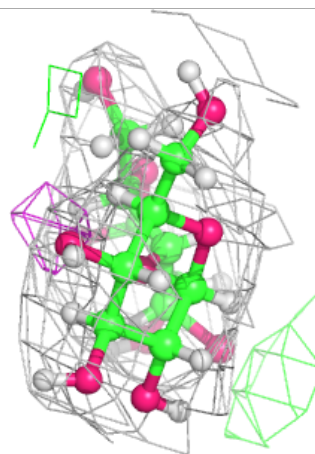
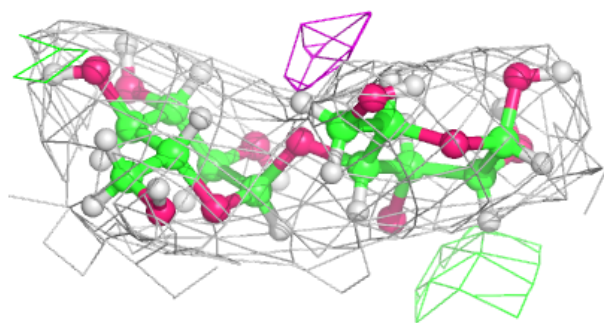
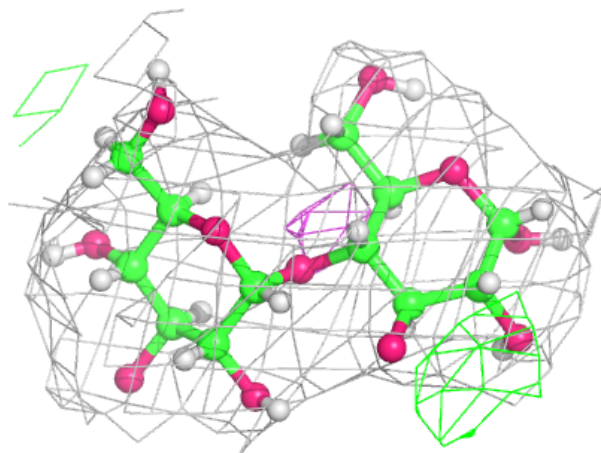
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

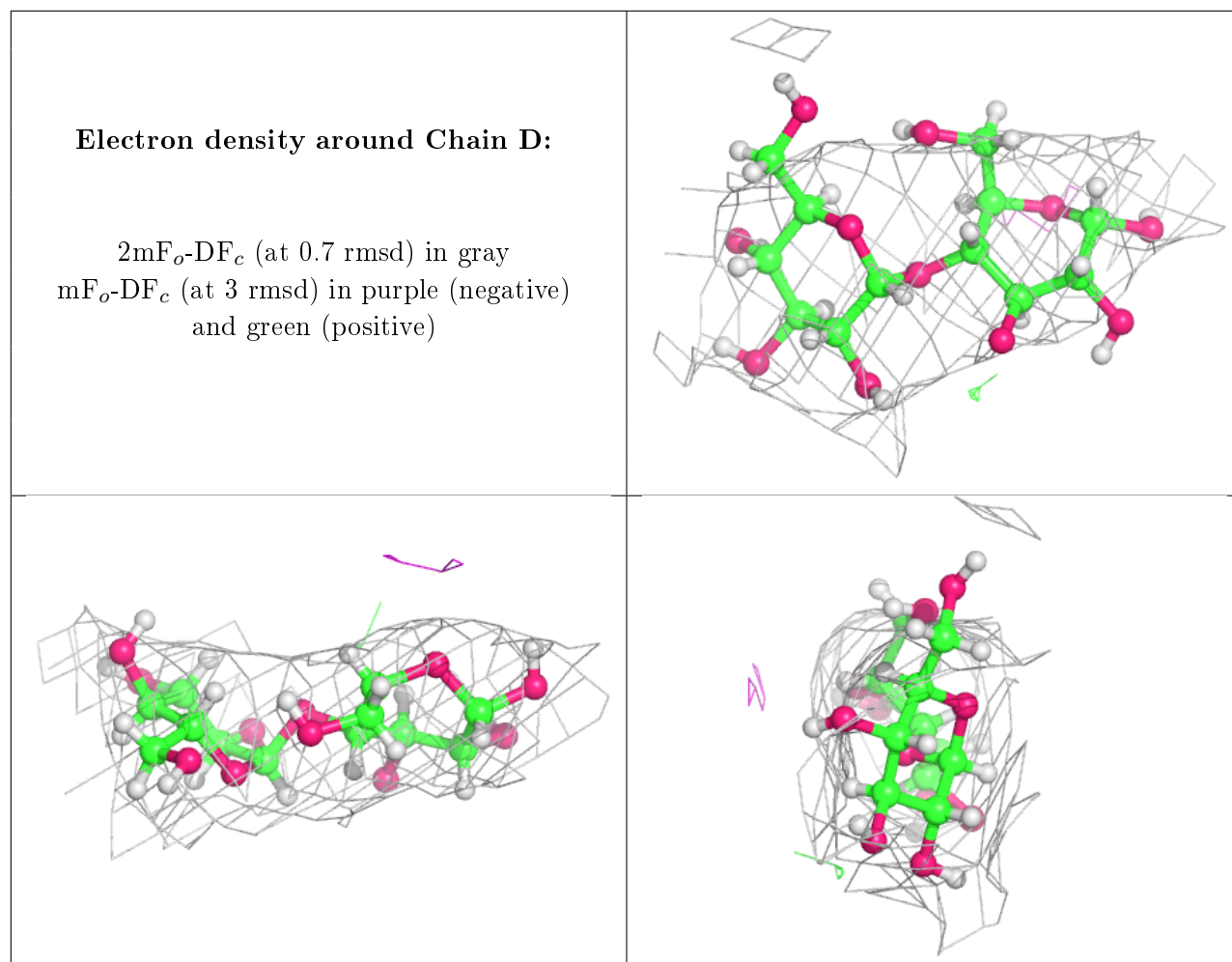
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	D	2	11/12	0.79	0.44	114,114,195,196	0
2	GLC	D	1	12/12	0.87	0.48	114,180,190,193	0
2	GLC	C	1	12/12	0.95	0.51	99,101,114,114	0
2	GLC	C	2	11/12	0.95	0.44	98,103,114,114	0

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 C:**

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





## 6.4 Ligands ⓘ

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	NAG	A	803	14/15	0.72	0.45	114,213,226,231	0
3	NAG	B	803	14/15	0.87	0.23	114,114,119,119	0
3	NAG	A	802	14/15	0.89	0.17	114,114,150,151	0
4	ZN	B	801	1/1	0.93	0.09	114,114,114,114	0
4	ZN	A	804	1/1	0.95	0.13	114,114,114,114	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.