



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 06:14 PM JST

PDB ID : 7EAP  
Title : Crystal structure of IpeA-XXXG complex  
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Deposited on : 2021-03-08  
Resolution : 1.42 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 : 2.27  
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) : 2.27

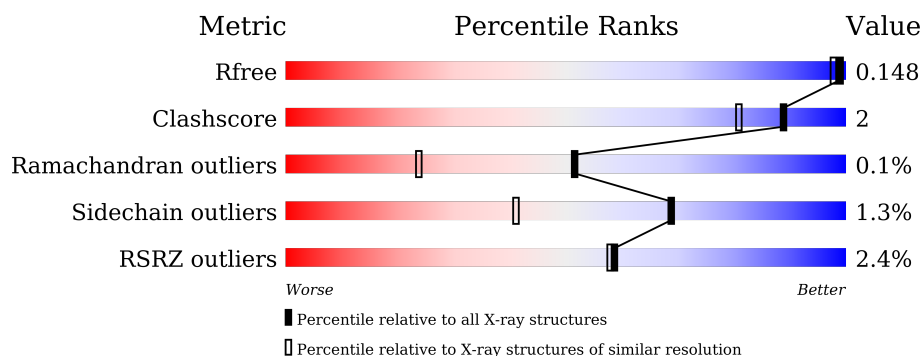
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.42 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	765	<div> <div>2%</div> <div>93%</div> <div>5% ..</div> </div>
2	B	7	<div> <div>86%</div> <div>14%</div> </div>
3	C	2	<div> <div>100%</div> </div>
4	D	2	<div> <div>100%</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	BGC	B	1	-	-	-	X
2	XYS	B	7	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6646 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.

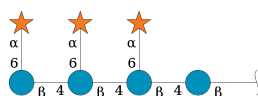
- Molecule 1 is a protein called Fn3\_like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	755	5837	3720	973	1126	18	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	ALA	GLU	conflict	UNP Q2U8V9
A	780	VAL	-	expression tag	UNP Q2U8V9
A	781	ASP	-	expression tag	UNP Q2U8V9
A	782	HIS	-	expression tag	UNP Q2U8V9
A	783	HIS	-	expression tag	UNP Q2U8V9
A	784	HIS	-	expression tag	UNP Q2U8V9
A	785	HIS	-	expression tag	UNP Q2U8V9
A	786	HIS	-	expression tag	UNP Q2U8V9
A	787	HIS	-	expression tag	UNP Q2U8V9

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	7	72	39	33	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	11	10			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

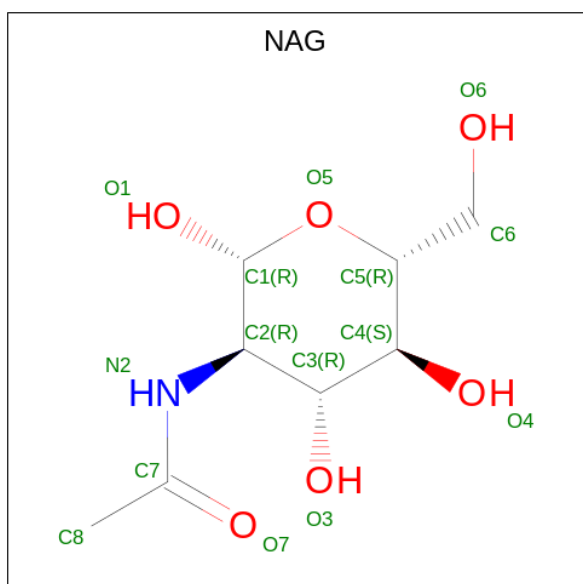


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	1	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

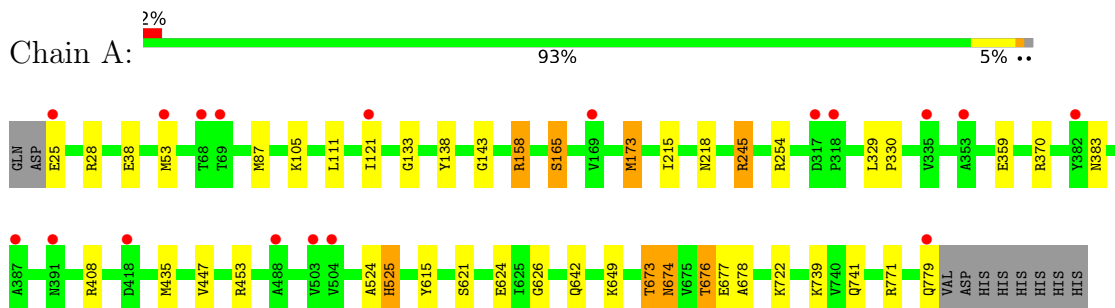
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	603	Total	O	0	0
			603	603		

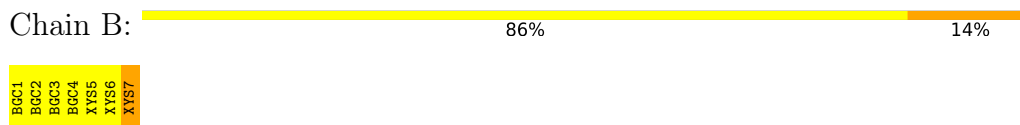
### 3 Residue-property plots [i](#)

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.

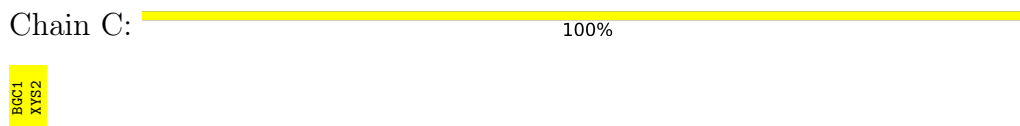
- Molecule 1: Fn3\_like domain-containing protein



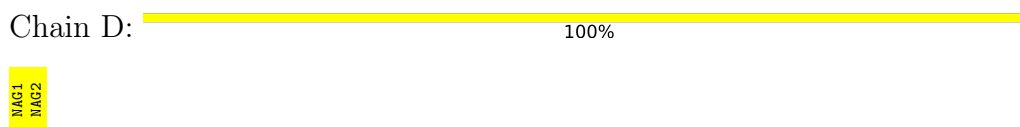
- Molecule 2: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.20Å 94.20Å 189.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.48 – 1.42 29.48 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.48-1.42) 99.7 (29.48-1.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.118 , 0.147 0.119 , 0.148	Depositor DCC
$R_{free}$ test set	9099 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: YYS, CA, BGC, 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	0.88	7/5981 (0.1%)	1.01	17/8144 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CZ-NH2	8.66	1.44	1.33
1	A	38	GLU	CD-OE1	8.31	1.34	1.25
1	A	38	GLU	CD-OE2	8.04	1.34	1.25
1	A	383	ASN	CG-OD1	6.75	1.38	1.24
1	A	624	GLU	CD-OE2	-5.90	1.19	1.25
1	A	359	GLU	CD-OE1	5.44	1.31	1.25
1	A	165	SER	CB-OG	-5.33	1.35	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	MET	CG-SD-CE	-9.70	84.68	100.20
1	A	254	ARG	CG-CD-NE	-9.53	91.78	111.80
1	A	158	ARG	NE-CZ-NH1	-9.21	115.69	120.30
1	A	453	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	A	53	MET	CA-CB-CG	7.92	126.76	113.30
1	A	673	THR	CA-CB-OG1	-7.65	92.93	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	53	MET	CG-SD-CE	-6.94	89.10	100.20
1	A	370	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	676	THR	CA-CB-CG2	6.78	121.89	112.40
1	A	28	ARG	CG-CD-NE	-6.74	97.65	111.80
1	A	771	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	245	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	453	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	677	GLU	CB-CG-CD	-5.59	99.10	114.20
1	A	138	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	245	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ARG	Sidechain

## 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	5837	0	5690	22	0
2	B	72	0	60	1	0
3	C	21	0	18	0	0
4	D	28	0	25	0	0
5	A	1	0	0	0	0
6	A	84	0	78	0	0
7	A	603	0	0	5	0
All	All	6646	0	5871	23	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 2.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:HG22	1:A:678:ALA:H	1.26	1.01
1:A:674:ASN:HD21	1:A:779:GLN:HG3	1.48	0.77
1:A:674:ASN:HD21	1:A:779:GLN:CG	1.99	0.76
1:A:105:LYS:NZ	7:A:901:HOH:O	2.19	0.75
1:A:158:ARG:HH21	1:A:158:ARG:CG	2.07	0.67
1:A:674:ASN:ND2	1:A:779:GLN:CG	2.60	0.65
1:A:158:ARG:HH21	1:A:158:ARG:HG2	1.61	0.65
1:A:524:ALA:O	1:A:525:HIS:HD2	1.81	0.64
1:A:158:ARG:CG	1:A:158:ARG:NH2	2.64	0.61
1:A:165:SER:HB3	1:A:215:ILE:HD11	1.81	0.61
1:A:143:GLY:HA3	7:A:1245:HOH:O	2.01	0.60
1:A:525:HIS:HE1	7:A:1429:HOH:O	1.84	0.59
1:A:649:LYS:HG3	7:A:1273:HOH:O	2.04	0.57
1:A:676:THR:HG22	1:A:678:ALA:N	2.10	0.55
1:A:739:LYS:HE2	1:A:741:GLN:HE21	1.74	0.52
1:A:524:ALA:O	1:A:525:HIS:CD2	2.65	0.50
1:A:674:ASN:ND2	1:A:779:GLN:HG3	2.21	0.49
7:A:1160:HOH:O	2:B:7:XYS:H2	2.15	0.46
1:A:133:GLY:HA2	1:A:447:VAL:HG21	1.99	0.44
1:A:329:LEU:HB3	1:A:330:PRO:HD3	2.00	0.43
1:A:87:MET:HA	1:A:121:ILE:O	2.19	0.43
1:A:173:MET:HA	1:A:218:ASN:HB3	2.02	0.42
1:A:626:GLY:HA3	1:A:642:GLN:OE1	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	754/765 (99%)	741 (98%)	12 (2%)	1 (0%)	51 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	621	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	621/630 (99%)	613 (99%)	8 (1%)	69 41

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	111	LEU
1	A	435	MET
1	A	525	HIS
1	A	615	TYR
1	A	673	THR
1	A	674	ASN
1	A	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	238	HIS
1	A	525	HIS
1	A	575	GLN
1	A	674	ASN
1	A	741	GLN
1	A	773	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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
2	BGC	B	1	2	12,12,12	1.07	1 (8%)	17,17,17	1.77	4 (23%)
2	BGC	B	2	2	11,11,12	1.49	1 (9%)	15,15,17	2.23	5 (33%)
2	BGC	B	3	2	11,11,12	1.31	1 (9%)	15,15,17	3.51	10 (66%)
2	BGC	B	4	2	11,11,12	1.46	1 (9%)	15,15,17	1.61	2 (13%)
2	XYS	B	5	2	9,9,10	1.18	0	10,12,14	1.93	2 (20%)
2	XYS	B	6	2	9,9,10	1.00	0	10,12,14	1.95	3 (30%)
2	XYS	B	7	2	9,9,10	1.33	1 (11%)	10,12,14	2.28	2 (20%)
3	BGC	C	1	3	12,12,12	1.14	1 (8%)	17,17,17	2.12	6 (35%)
3	XYS	C	2	3	9,9,10	1.47	2 (22%)	10,12,14	1.67	3 (30%)
4	NAG	D	1	1,4	14,14,15	1.31	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	D	2	4	14,14,15	1.36	2 (14%)	17,19,21	1.95	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4	2	-	0/2/19/22	0/1/1/1
2	XYS	B	5	2	-	-	0/1/1/1
2	XYS	B	6	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYS	B	7	2	-	-	0/1/1/1
3	BGC	C	1	3	-	0/2/22/22	0/1/1/1
3	XYS	C	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BGC	O4-C4	-3.92	1.33	1.43
4	D	1	NAG	C1-C2	3.49	1.57	1.52
2	B	3	BGC	C2-C3	3.26	1.57	1.52
4	D	2	NAG	O5-C1	3.23	1.48	1.43
3	C	2	XYS	O4-C4	-3.19	1.36	1.43
2	B	1	BGC	O4-C4	-3.06	1.35	1.43
3	C	1	BGC	C4-C5	2.61	1.58	1.53
2	B	4	BGC	O5-C5	-2.52	1.38	1.43
2	B	7	XYS	C2-C3	2.44	1.56	1.52
3	C	2	XYS	C4-C3	2.23	1.55	1.52
4	D	2	NAG	O5-C5	2.20	1.47	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BGC	O4-C4-C3	9.83	133.07	110.35
2	B	2	BGC	C1-O5-C5	5.80	120.06	112.19
2	B	7	XYS	C1-C2-C3	5.56	116.50	109.67
2	B	3	BGC	C3-C4-C5	-5.46	100.50	110.24
4	D	2	NAG	O5-C1-C2	-5.19	103.09	111.29
2	B	5	XYS	C1-C2-C3	5.06	115.88	109.67
4	D	2	NAG	C1-O5-C5	4.27	117.97	112.19
2	B	2	BGC	C1-C2-C3	4.23	114.87	109.67
3	C	1	BGC	O4-C4-C5	4.05	119.34	109.30
2	B	4	BGC	O5-C5-C6	-3.70	101.40	107.20
3	C	1	BGC	C1-O5-C5	-3.46	107.13	113.66
2	B	4	BGC	O5-C1-C2	3.46	116.11	110.77
2	B	1	BGC	O4-C4-C3	3.42	118.26	110.35
3	C	1	BGC	O5-C5-C4	3.33	115.74	109.69
2	B	6	XYS	C4-C3-C2	-3.28	107.02	110.92
2	B	1	BGC	O3-C3-C2	-3.28	102.76	110.35
2	B	3	BGC	O2-C2-C1	3.23	115.77	109.15
3	C	1	BGC	O4-C4-C3	-3.21	102.94	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	XYS	O3-C3-C2	3.01	115.75	109.99
2	B	6	XYS	C1-C2-C3	2.97	113.32	109.67
2	B	1	BGC	C4-C3-C2	2.95	115.97	110.82
3	C	1	BGC	O1-C1-C2	-2.93	100.78	109.03
2	B	7	XYS	C5-O5-C1	2.92	116.02	111.52
2	B	3	BGC	O5-C5-C6	-2.78	102.85	107.20
2	B	3	BGC	O5-C5-C4	2.66	117.31	110.83
3	C	2	XYS	C5-C4-C3	2.64	112.91	109.67
4	D	1	NAG	O5-C1-C2	-2.64	107.12	111.29
2	B	3	BGC	C1-O5-C5	-2.61	108.66	112.19
2	B	2	BGC	O5-C5-C6	2.54	111.19	107.20
2	B	6	XYS	C5-C4-C3	-2.54	106.55	109.67
2	B	3	BGC	O3-C3-C4	2.53	116.19	110.35
3	C	1	BGC	O5-C1-C2	-2.49	105.84	110.28
2	B	5	XYS	C4-C3-C2	-2.47	107.99	110.92
2	B	3	BGC	O5-C1-C2	-2.46	106.98	110.77
2	B	1	BGC	O4-C4-C5	2.43	115.32	109.30
2	B	2	BGC	O2-C2-C1	2.34	113.94	109.15
2	B	3	BGC	O6-C6-C5	-2.25	103.56	111.29
4	D	1	NAG	C8-C7-N2	-2.23	112.32	116.10
4	D	2	NAG	C1-C2-N2	2.14	114.14	110.49
2	B	2	BGC	O4-C4-C3	2.13	115.27	110.35
3	C	2	XYS	O4-C4-C3	2.08	114.31	110.14
2	B	3	BGC	O4-C4-C5	-2.04	104.24	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

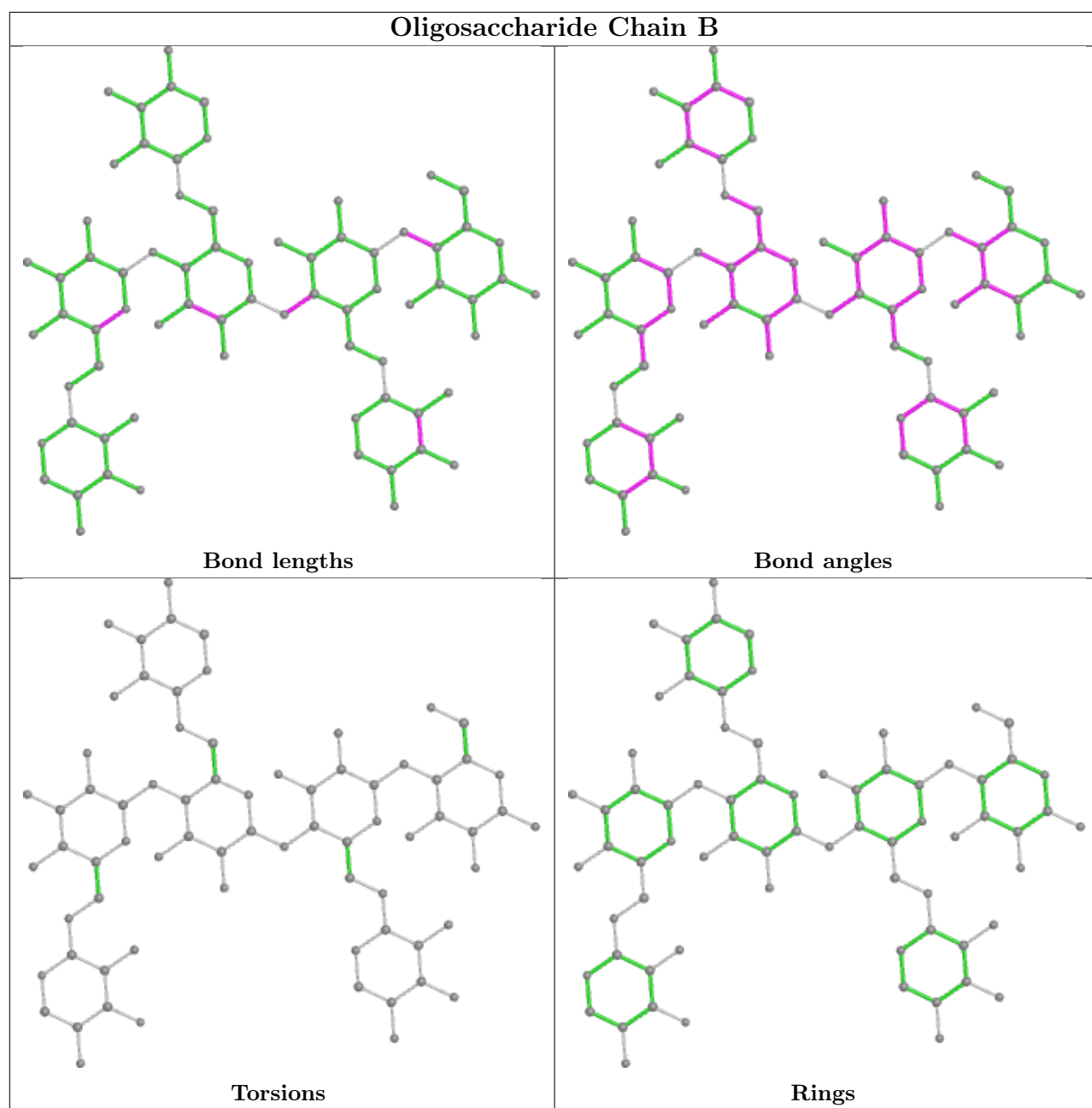
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

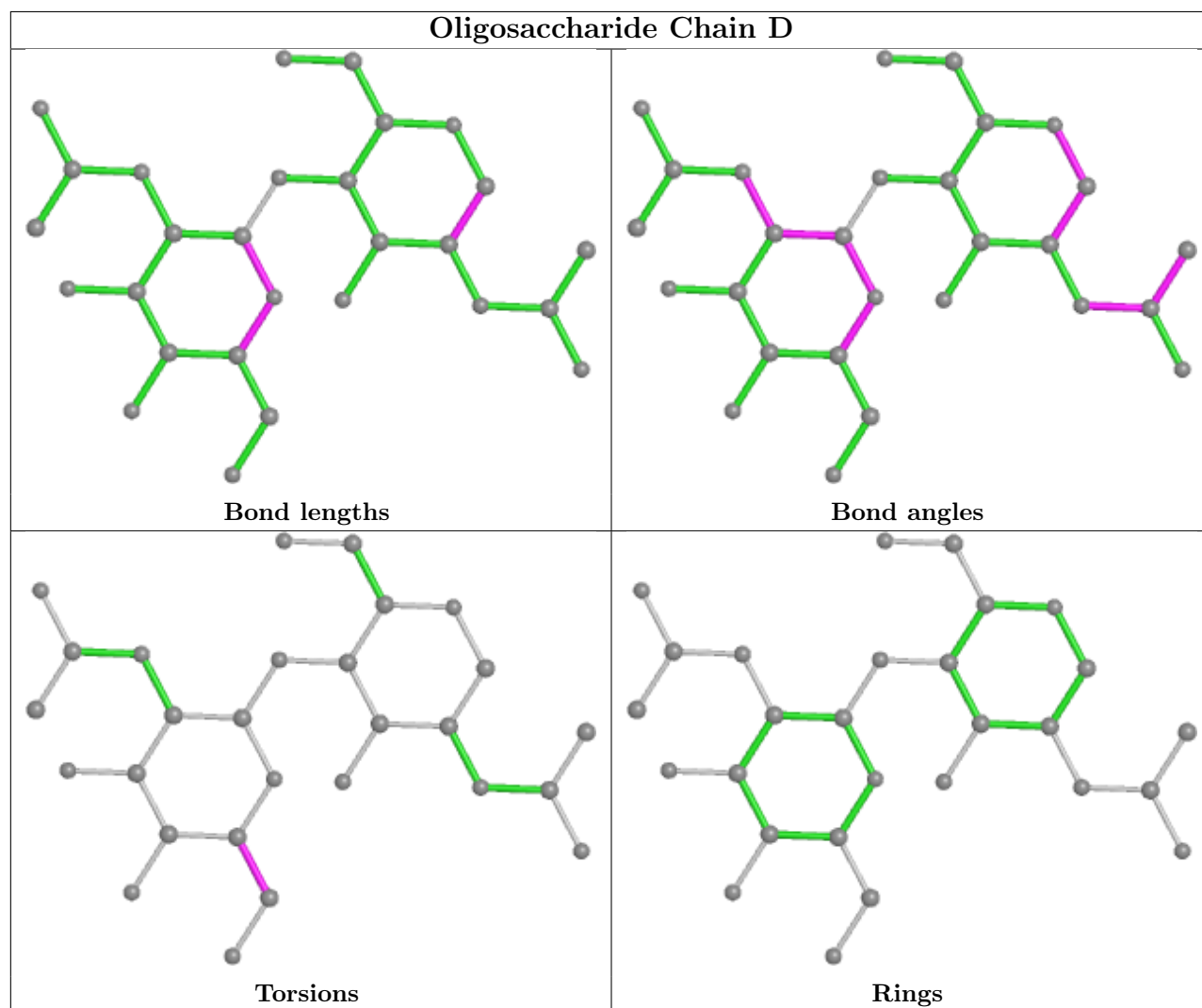
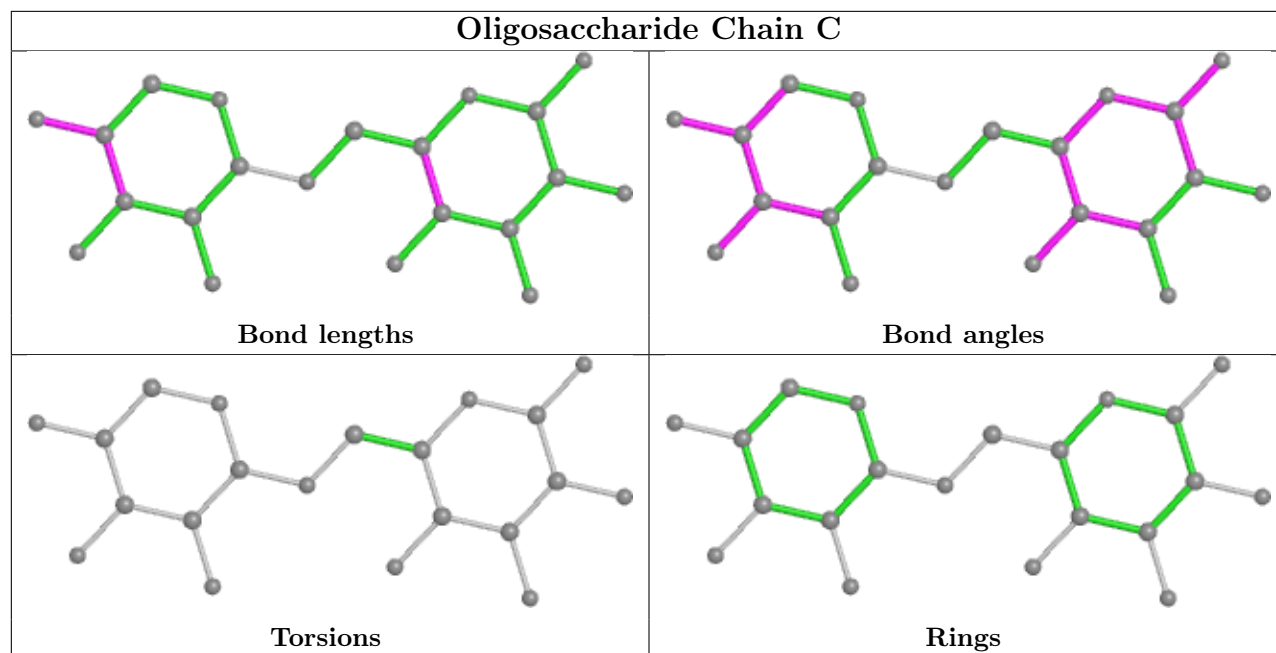
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7	XYS	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

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
6	NAG	A	804	1	14,14,15	1.10	2 (14%)	17,19,21	1.07	2 (11%)
6	NAG	A	803	1	14,14,15	1.16	1 (7%)	17,19,21	1.99	7 (41%)
6	NAG	A	802	1	14,14,15	1.02	1 (7%)	17,19,21	1.90	5 (29%)
6	NAG	A	805	1	14,14,15	0.86	0	17,19,21	1.35	3 (17%)
6	NAG	A	807	1	14,14,15	1.72	4 (28%)	17,19,21	1.78	5 (29%)
6	NAG	A	806	1	14,14,15	1.06	0	17,19,21	2.47	4 (23%)

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
6	NAG	A	804	1	-	0/6/23/26	0/1/1/1
6	NAG	A	803	1	-	0/6/23/26	0/1/1/1
6	NAG	A	802	1	-	2/6/23/26	0/1/1/1
6	NAG	A	805	1	-	0/6/23/26	0/1/1/1
6	NAG	A	807	1	-	0/6/23/26	0/1/1/1
6	NAG	A	806	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	807	NAG	O5-C1	-3.89	1.37	1.43
6	A	803	NAG	O5-C1	2.69	1.48	1.43
6	A	807	NAG	C1-C2	-2.57	1.48	1.52
6	A	807	NAG	O3-C3	-2.28	1.37	1.43
6	A	807	NAG	C4-C5	-2.15	1.48	1.53
6	A	804	NAG	C2-N2	2.15	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	804	NAG	C4-C5	-2.12	1.48	1.53
6	A	802	NAG	C4-C3	-2.08	1.47	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	NAG	C1-O5-C5	7.42	122.25	112.19
6	A	802	NAG	C6-C5-C4	-4.70	102.00	113.00
6	A	806	NAG	O5-C5-C6	-4.69	99.85	107.20
6	A	803	NAG	O5-C5-C6	4.23	113.83	107.20
6	A	802	NAG	C3-C4-C5	4.00	117.38	110.24
6	A	803	NAG	O5-C1-C2	-3.29	106.09	111.29
6	A	807	NAG	C1-C2-N2	-3.28	104.89	110.49
6	A	805	NAG	C1-O5-C5	3.28	116.63	112.19
6	A	803	NAG	O3-C3-C4	-3.17	103.01	110.35
6	A	807	NAG	O3-C3-C4	-3.04	103.33	110.35
6	A	803	NAG	O5-C5-C4	-2.79	104.04	110.83
6	A	805	NAG	O5-C1-C2	-2.73	106.98	111.29
6	A	804	NAG	C6-C5-C4	-2.69	106.71	113.00
6	A	807	NAG	C3-C4-C5	-2.66	105.50	110.24
6	A	802	NAG	O3-C3-C4	-2.65	104.23	110.35
6	A	803	NAG	C1-O5-C5	2.45	115.52	112.19
6	A	807	NAG	C1-O5-C5	-2.44	108.88	112.19
6	A	806	NAG	O5-C5-C4	2.35	116.56	110.83
6	A	803	NAG	O7-C7-N2	2.33	126.24	121.95
6	A	806	NAG	O3-C3-C4	-2.24	105.16	110.35
6	A	804	NAG	O5-C1-C2	-2.24	107.76	111.29
6	A	802	NAG	C4-C3-C2	-2.15	107.86	111.02
6	A	805	NAG	O7-C7-N2	2.13	125.87	121.95
6	A	803	NAG	C8-C7-N2	-2.04	112.64	116.10
6	A	802	NAG	O5-C5-C4	2.03	115.75	110.83
6	A	807	NAG	O7-C7-C8	2.01	125.79	122.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	806	NAG	O5-C5-C6-O6
6	A	806	NAG	C4-C5-C6-O6
6	A	802	NAG	C4-C5-C6-O6
6	A	802	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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 [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	755/765 (98%)	-0.06	18 (2%) 59 58	13, 18, 34, 60	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	ASP	4.3
1	A	68	THR	3.8
1	A	382	TYR	3.8
1	A	318	PRO	3.5
1	A	69	THR	2.9
1	A	779	GLN	2.8
1	A	25	GLU	2.7
1	A	418	ASP	2.6
1	A	353	ALA	2.5
1	A	391	ASN	2.4
1	A	488	ALA	2.4
1	A	53	MET	2.3
1	A	169	VAL	2.2
1	A	504	VAL	2.1
1	A	387	ALA	2.1
1	A	335	VAL	2.0
1	A	503	VAL	2.0
1	A	121	ILE	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 ⓘ

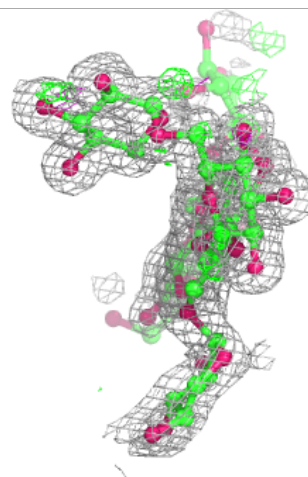
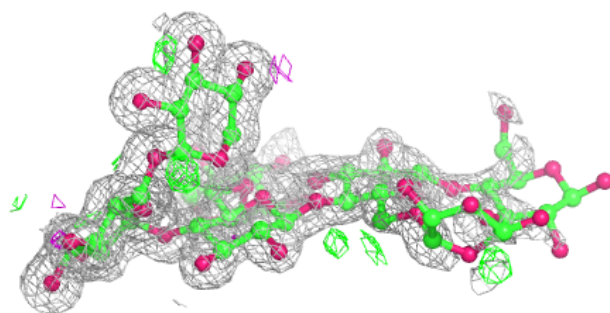
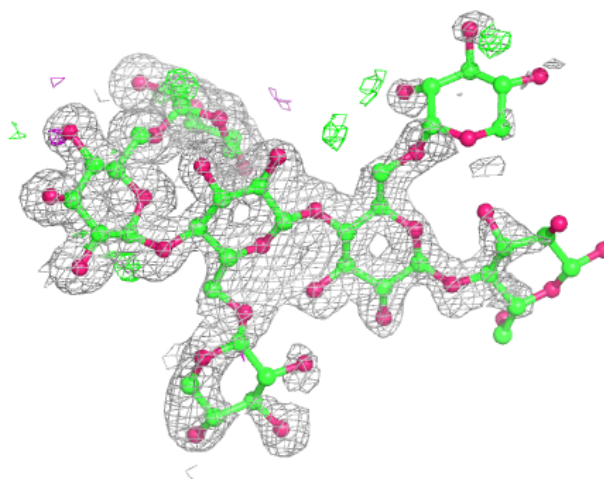
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	XYS	B	7	9/10	0.54	0.50	70,98,106,110	0
2	XYS	B	6	9/10	0.67	0.29	35,50,53,57	0
2	BGC	B	1	12/12	0.75	0.60	58,82,101,103	0
2	BGC	B	2	11/12	0.81	0.30	35,45,55,57	0
4	NAG	D	2	14/15	0.86	0.28	34,51,71,72	0
3	BGC	C	1	12/12	0.88	0.27	23,35,49,49	0
3	XYS	C	2	9/10	0.91	0.29	22,31,37,37	0
2	BGC	B	3	11/12	0.94	0.16	27,34,44,50	0
4	NAG	D	1	14/15	0.96	0.10	22,24,29,33	0
2	BGC	B	4	11/12	0.97	0.10	15,16,18,19	0
2	XYS	B	5	9/10	0.98	0.10	15,15,18,19	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.

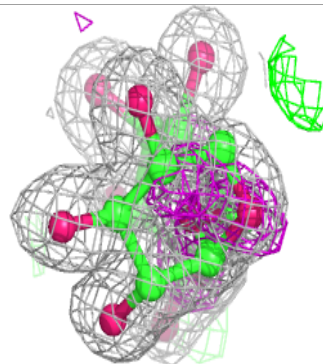
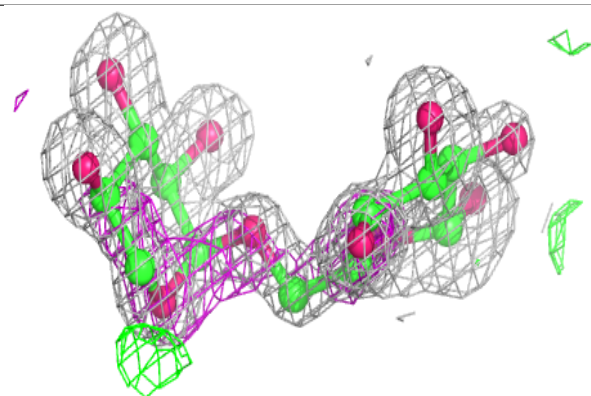
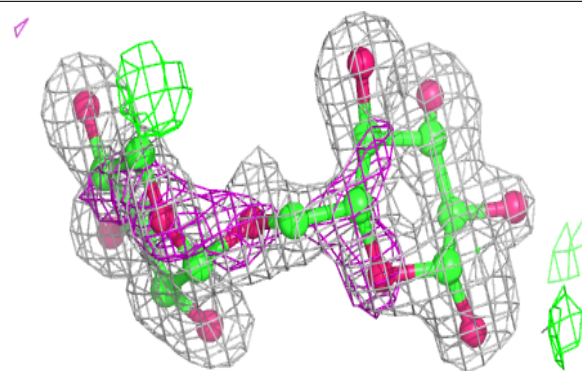
**Electron density around Chain B:**

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

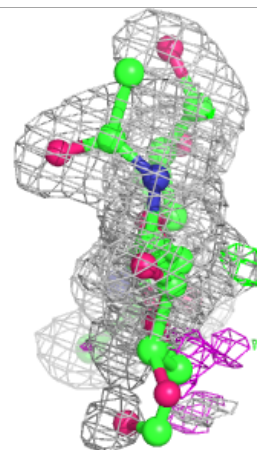
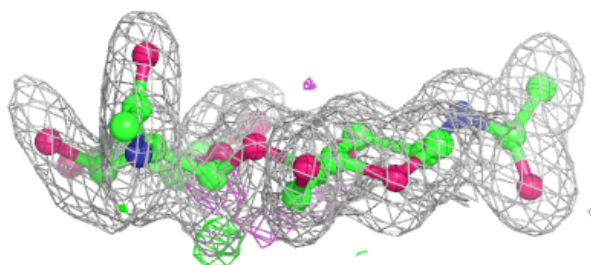
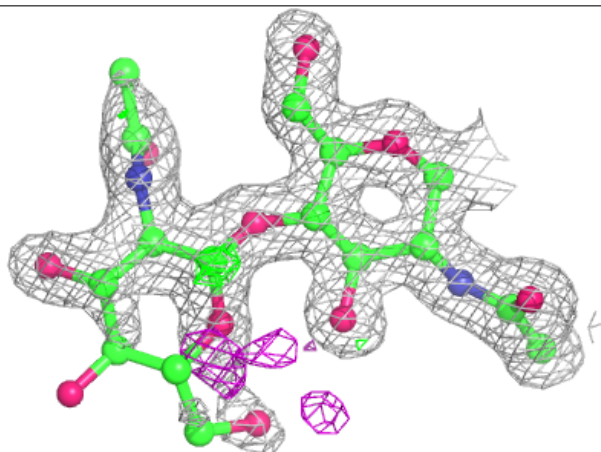


**Electron density around Chain C:**

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

**Electron density around Chain D:**

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



## 6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

## 6.5 Other polymers [i](#)

There are no such residues in this entry.