



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 08:06 AM EDT

PDB ID : 4AX7  
Title : Hypocrea jecorina Cel6A D221A mutant soaked with 4-Methylumbelliferyl-beta-D-cellobioside  
Authors : Wu, M.; Nerinckx, W.; Piens, K.; Ishida, T.; Hansson, H.; Stahlberg, J.; Sandgren, M.  
Deposited on : 2012-06-11  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

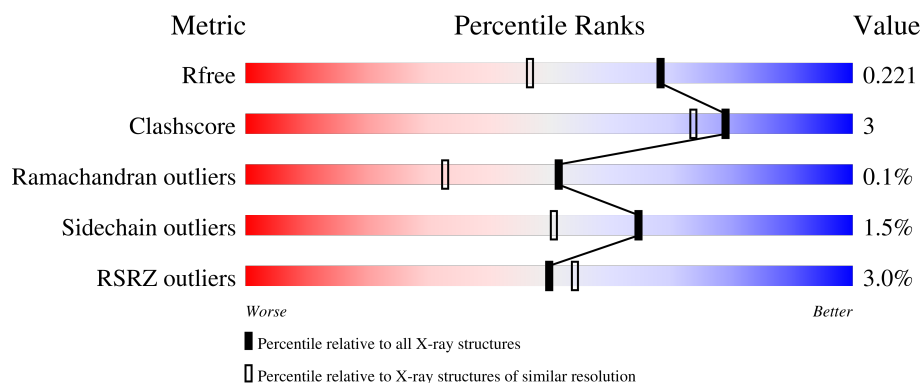
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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.




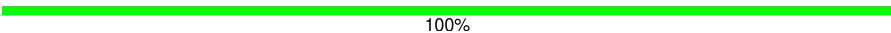
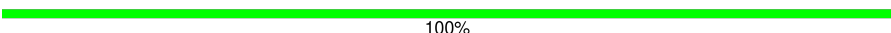
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	363	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
1	B	363	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	C	363	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	D	363	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
2	E	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	4	 50%25%25%
3	F	2	 100%
3	H	2	 100%

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
2	BGC	G	3	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12750 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 EXOGLUCANASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	2	0
			2758	1750	466	532	10			
1	B	360	Total	C	N	O	S	0	3	0
			2740	1740	462	528	10			
1	C	363	Total	C	N	O	S	0	3	0
			2764	1755	466	533	10			
1	D	360	Total	C	N	O	S	0	3	0
			2737	1738	461	528	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	ALA	ASP	engineered mutation	UNP P07987
B	221	ALA	ASP	engineered mutation	UNP P07987
C	221	ALA	ASP	engineered mutation	UNP P07987
D	221	ALA	ASP	engineered mutation	UNP P07987

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	4	Total	C	O	0	0	0
			44	24	20			
2	G	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			22	12	10			
3	H	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



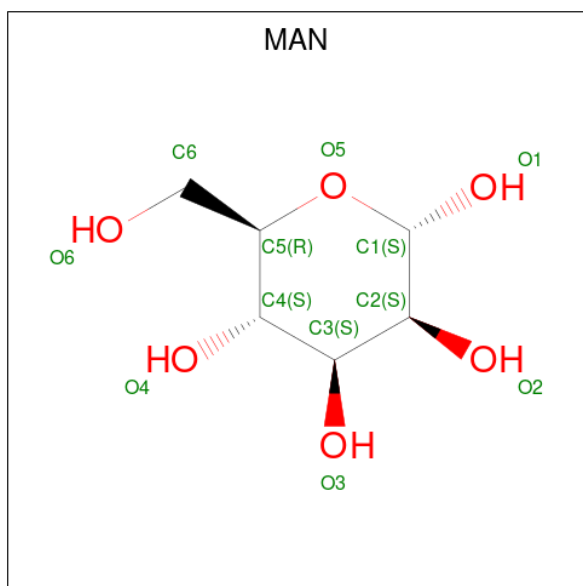
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



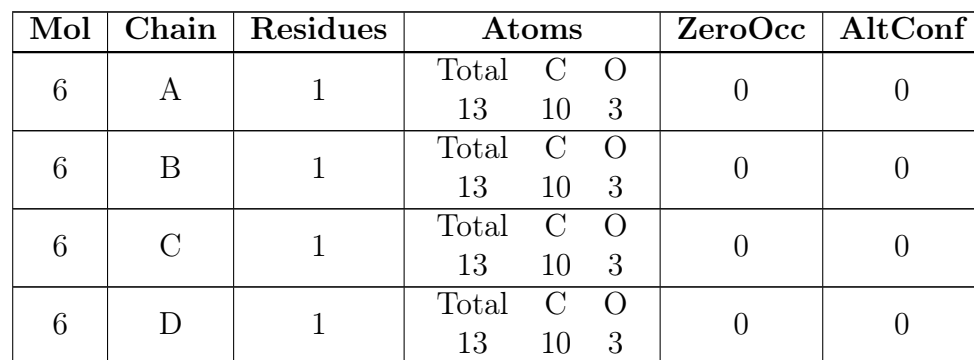
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5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

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

- Molecule 6 is 7-hydroxy-4-methyl-2H-chromen-2-one (three-letter code: 4MU) (formula: C<sub>10</sub>H<sub>8</sub>O<sub>3</sub>).



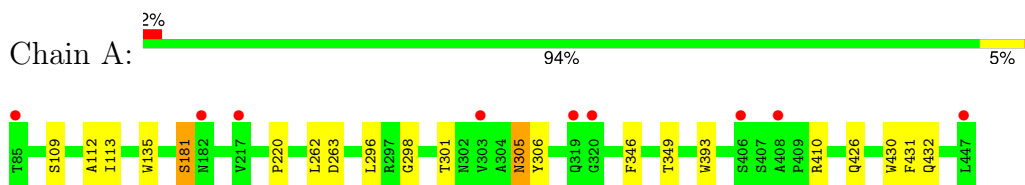
- | Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 7   | A     | 329      | Total O<br>329 329 | 0       | 0       |
| 7   | B     | 287      | Total O<br>287 287 | 0       | 0       |
| 7   | C     | 285      | Total O<br>285 285 | 0       | 0       |
| 7   | D     | 257      | Total O<br>257 257 | 0       | 0       |



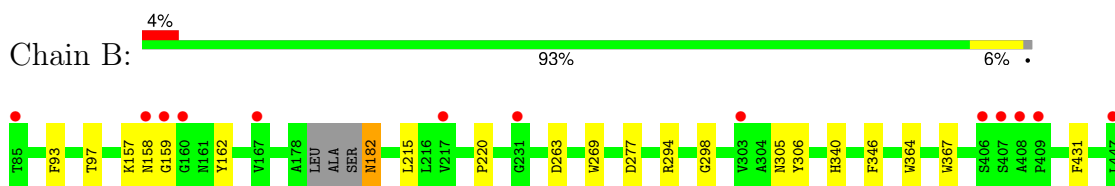
### 3 Residue-property plots [i](#)

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.

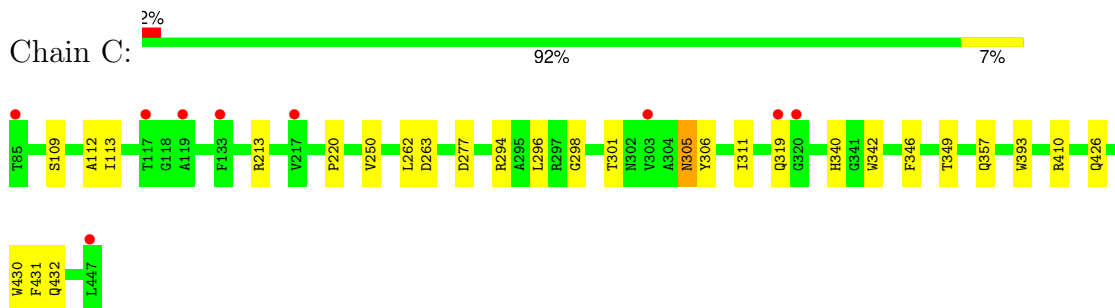
- Molecule 1: EXOGLUCANASE 2



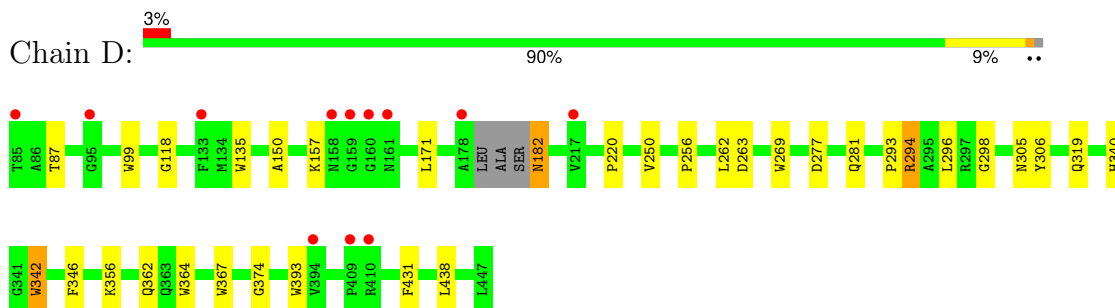
- Molecule 1: EXOGLUCANASE 2




- Molecule 1: EXOGLUCANASE 2



- Molecule 1: EXOGLUCANASE 2



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

Chain E:  25% 25% 50%



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

Chain G:  50% 25% 25%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:  100%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.82Å 74.68Å 93.30Å 103.97° 103.43° 90.00°	Depositor
Resolution (Å)	87.90 – 1.70 29.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (87.90-1.70) 96.4 (29.86-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.189 , 0.221 0.188 , 0.221	Depositor DCC
$R_{free}$ test set	6627 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4432e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, MAN, 4MU, 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	0.53	1/2834 (0.0%)	0.55	0/3887
1	B	0.52	3/2821 (0.1%)	0.54	0/3866
1	C	0.52	2/2840 (0.1%)	0.54	0/3894
1	D	0.53	7/2818 (0.2%)	0.54	0/3862
All	All	0.52	13/11313 (0.1%)	0.55	0/15509

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	TRP	CD2-CE2	5.24	1.47	1.41
1	B	269	TRP	CD2-CE2	5.22	1.47	1.41
1	D	269	TRP	CD2-CE2	5.17	1.47	1.41
1	D	364	TRP	CD2-CE2	5.16	1.47	1.41
1	D	135	TRP	CD2-CE2	5.11	1.47	1.41

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	2758	0	2618	14	0
1	B	2740	0	2604	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2764	0	2628	15	0
1	D	2737	0	2601	19	0
2	E	44	0	37	3	0
2	G	44	0	37	1	0
3	F	22	0	19	0	0
3	H	22	0	19	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	77	0	70	1	0
5	B	77	0	70	0	0
5	C	66	0	60	0	0
5	D	77	0	70	1	0
6	A	13	0	7	1	0
6	B	13	0	7	1	0
6	C	13	0	7	0	0
6	D	13	0	7	0	0
7	A	329	0	0	1	0
7	B	287	0	0	1	0
7	C	285	0	0	1	0
7	D	257	0	0	4	0
All	All	12750	0	10965	62	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 3.

The worst 5 of 62 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:305:ASN:HD22	1:A:306:TYR:H	1.21	0.87
1:B:305:ASN:HD22	1:B:306:TYR:H	1.25	0.83
1:D:305:ASN:HD22	1:D:306:TYR:H	1.25	0.81
1:C:305:ASN:HD22	1:C:306:TYR:H	1.29	0.81
1:B:305:ASN:ND2	1:B:306:TYR:H	1.84	0.76

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	363/363 (100%)	353 (97%)	10 (3%)	0	100	100
1	B	359/363 (99%)	343 (96%)	15 (4%)	1 (0%)	41	24
1	C	364/363 (100%)	351 (96%)	13 (4%)	0	100	100
1	D	359/363 (99%)	345 (96%)	14 (4%)	0	100	100
All	All	1445/1452 (100%)	1392 (96%)	52 (4%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ASN

### 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	285/283 (101%)	282 (99%)	3 (1%)	73	63
1	B	283/283 (100%)	280 (99%)	3 (1%)	73	63
1	C	285/283 (101%)	280 (98%)	5 (2%)	59	43
1	D	283/283 (100%)	277 (98%)	6 (2%)	53	36
All	All	1136/1132 (100%)	1119 (98%)	17 (2%)	65	51

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	319	GLN
1	D	431	PHE
1	C	294	ARG
1	C	305	ASN
1	C	319	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	285	ASN
1	D	441	ASN
1	C	363	GLN
1	D	319	GLN
1	C	319	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 ⓘ

12 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	E	1	2,6	11,11,12	0.60	0	15,15,17	0.66	0
2	BGC	E	2	2	11,11,12	1.14	1 (9%)	15,15,17	0.62	0
2	BGC	E	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.57	2 (13%)
2	BGC	E	4	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	F	1	3,6	11,11,12	0.42	0	15,15,17	0.83	0
3	BGC	F	2	3	11,11,12	0.63	0	15,15,17	0.46	0
2	BGC	G	1	2,6	11,11,12	0.61	0	15,15,17	0.73	0
2	BGC	G	2	2	11,11,12	1.34	2 (18%)	15,15,17	0.70	0
2	BGC	G	3	2	11,11,12	0.81	0	15,15,17	1.69	4 (26%)
2	BGC	G	4	2	11,11,12	0.53	0	15,15,17	0.78	0
3	BGC	H	1	3,6	11,11,12	0.61	0	15,15,17	0.63	0
3	BGC	H	2	3	11,11,12	0.69	0	15,15,17	0.62	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	BGC	E	1	2,6	-	0/2/19/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
3	BGC	F	1	3,6	-	0/2/19/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2,6	-	0/2/19/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	1/2/19/22	0/1/1/1
2	BGC	G	4	2	-	0/2/19/22	0/1/1/1
3	BGC	H	1	3,6	-	0/2/19/22	0/1/1/1
3	BGC	H	2	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BGC	O4-C4	2.46	1.49	1.43
2	G	2	BGC	O4-C4	2.34	1.48	1.43
2	E	4	BGC	O5-C5	2.23	1.47	1.43
2	G	2	BGC	C2-C3	2.10	1.55	1.52
2	E	3	BGC	O5-C5	2.07	1.47	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	BGC	C1-O5-C5	4.76	118.57	112.19
2	E	3	BGC	C1-O5-C5	4.13	117.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	BGC	O4-C4-C3	-2.48	104.53	110.38
2	E	3	BGC	O2-C2-C3	-2.18	105.64	110.15
2	G	3	BGC	O5-C5-C6	2.08	111.71	107.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

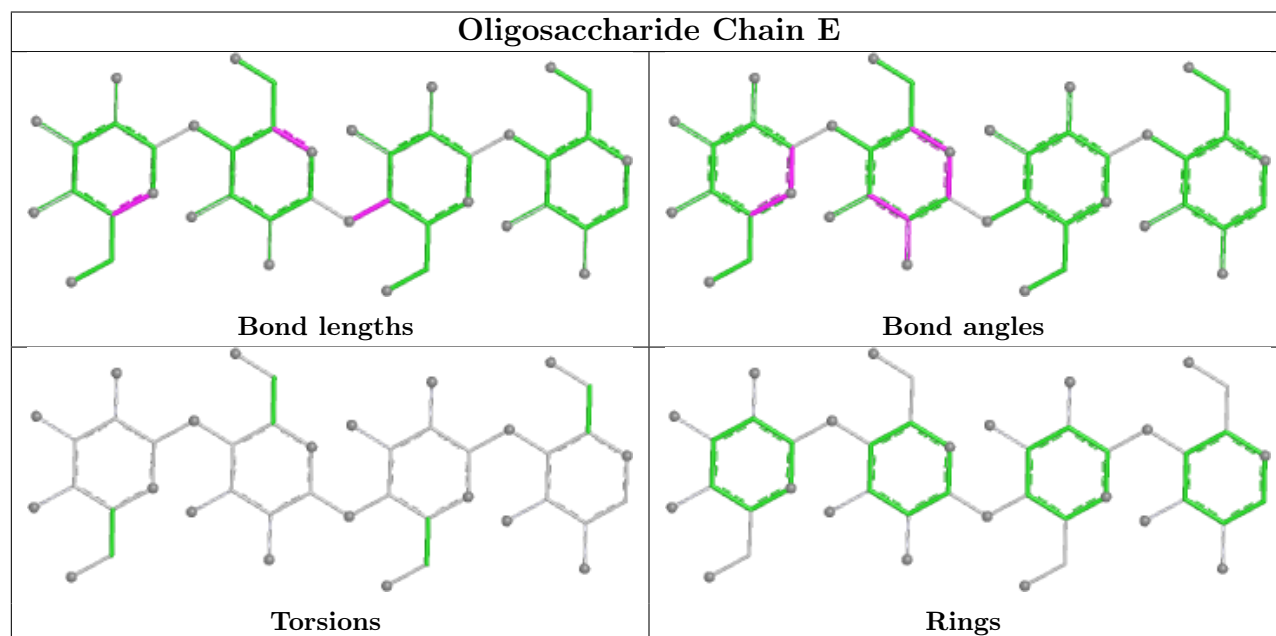
Mol	Chain	Res	Type	Atoms
2	G	3	BGC	O5-C5-C6-O6

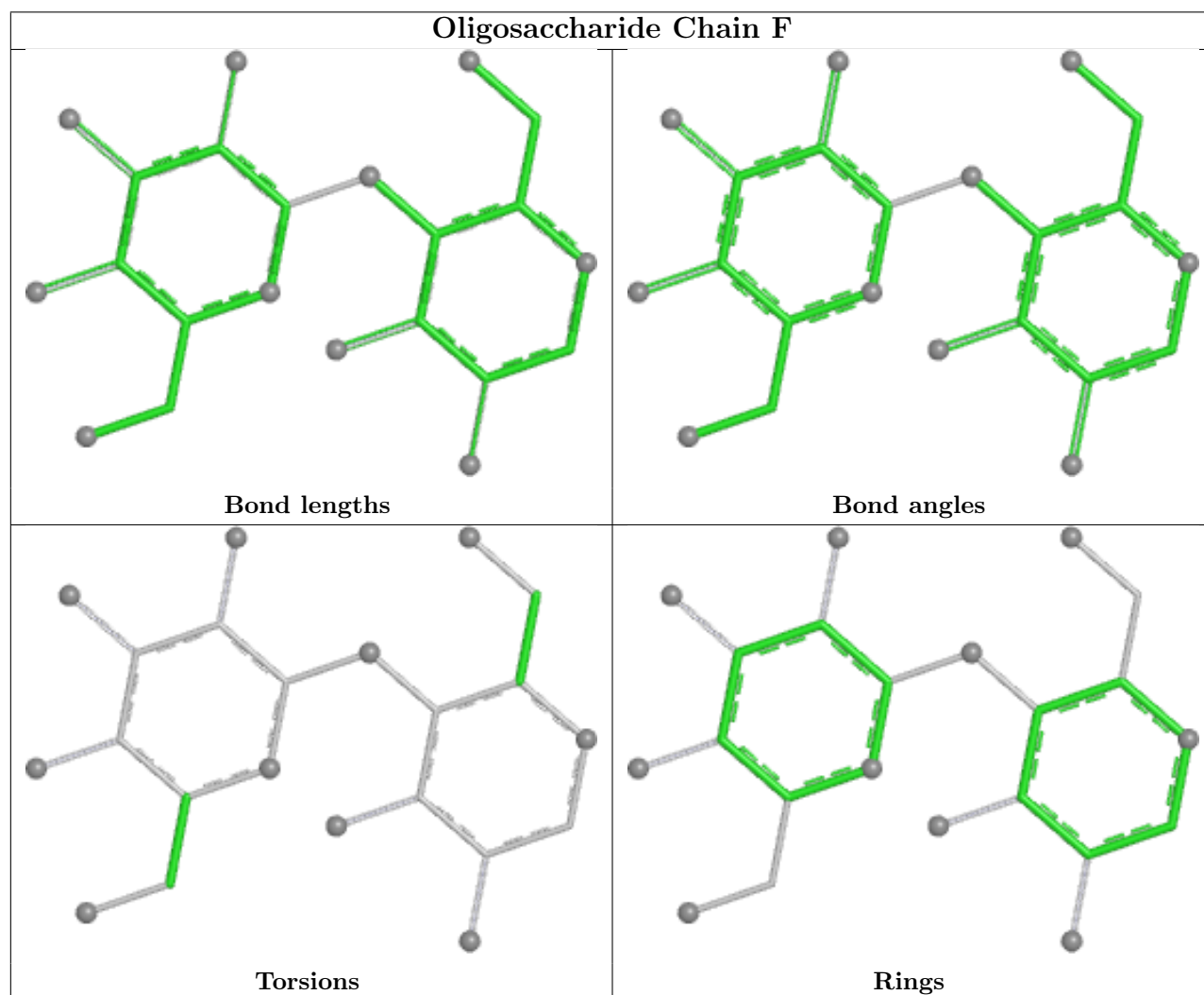
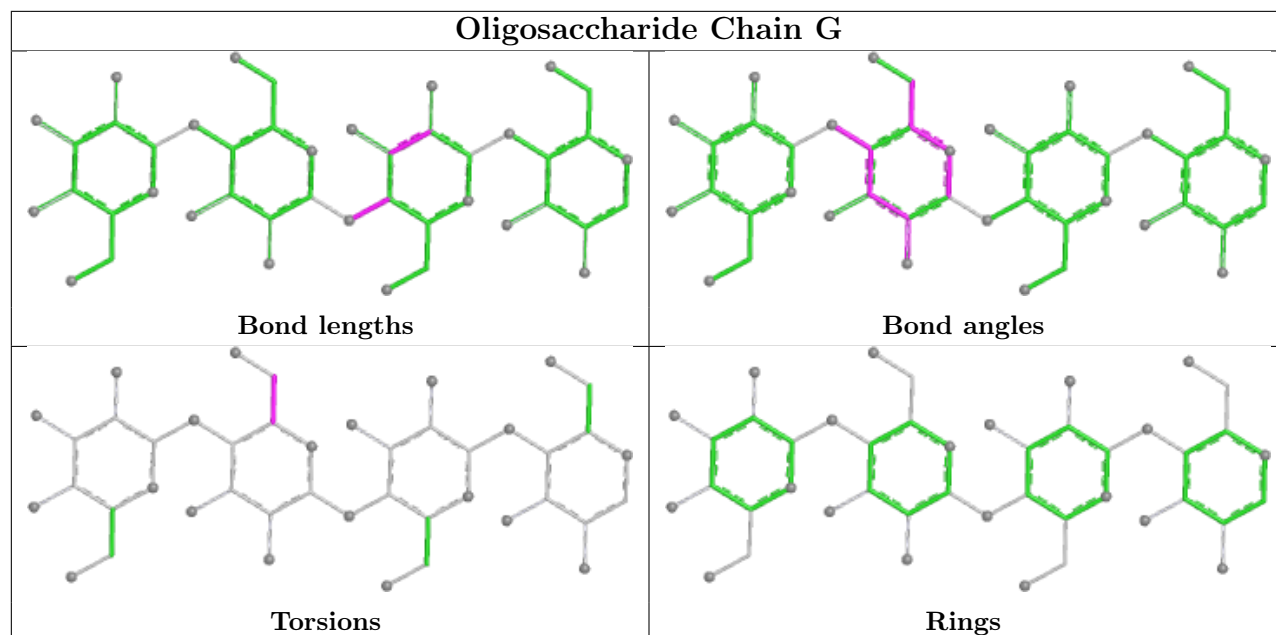
There are no ring outliers.

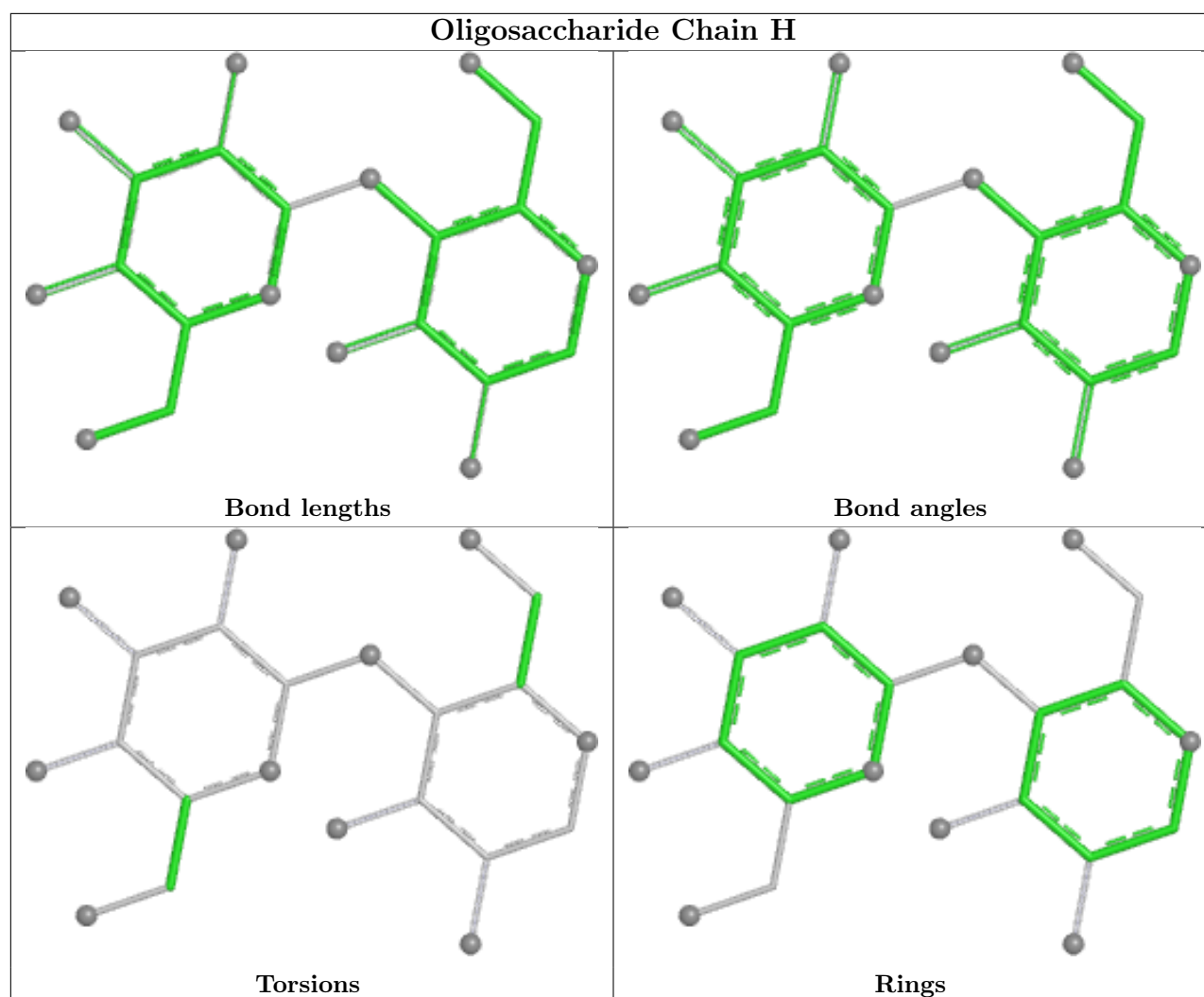
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	BGC	1	0
2	E	4	BGC	2	0
2	G	3	BGC	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](#)

39 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	B	504	1	11,11,12	0.61	0	15,15,17	0.94	1 (6%)
5	MAN	C	509	1	11,11,12	0.61	0	15,15,17	0.92	1 (6%)
4	NAG	C	501	1	14,14,15	0.62	0	17,19,21	1.41	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	4MU	D	600	3	14,14,14	1.50	3 (21%)	20,20,20	2.00	6 (30%)
5	MAN	B	505	1	11,11,12	0.66	0	15,15,17	1.08	1 (6%)
5	MAN	C	508	1	11,11,12	0.65	0	15,15,17	1.19	2 (13%)
5	MAN	D	504	1	11,11,12	0.54	0	15,15,17	0.73	1 (6%)
4	NAG	D	501	1	14,14,15	0.53	0	17,19,21	0.61	0
5	MAN	D	508	1	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
5	MAN	C	504	1	11,11,12	0.60	0	15,15,17	0.81	0
4	NAG	A	502	1	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
4	NAG	B	502	1	14,14,15	0.53	0	17,19,21	0.96	2 (11%)
5	MAN	D	503	1	11,11,12	0.58	0	15,15,17	0.68	0
6	4MU	B	600	3	14,14,14	1.55	3 (21%)	20,20,20	1.88	5 (25%)
5	MAN	A	505	1	11,11,12	0.61	0	15,15,17	0.86	1 (6%)
5	MAN	A	507	1	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
5	MAN	B	508	1	11,11,12	0.54	0	15,15,17	1.04	1 (6%)
4	NAG	A	501	1	14,14,15	0.55	0	17,19,21	0.80	0
6	4MU	A	600	2	14,14,14	1.98	4 (28%)	20,20,20	1.98	6 (30%)
4	NAG	B	501	1	14,14,15	0.51	0	17,19,21	0.88	0
5	MAN	A	504	1	11,11,12	0.58	0	15,15,17	1.05	2 (13%)
5	MAN	A	509	1	11,11,12	0.67	0	15,15,17	1.28	2 (13%)
5	MAN	B	503	1	11,11,12	0.52	0	15,15,17	0.92	1 (6%)
5	MAN	B	509	1	11,11,12	0.48	0	15,15,17	0.95	1 (6%)
5	MAN	C	505	1	11,11,12	0.62	0	15,15,17	1.04	1 (6%)
5	MAN	A	508	1	11,11,12	0.53	0	15,15,17	0.73	1 (6%)
5	MAN	C	506	1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
5	MAN	D	507	1	11,11,12	0.58	0	15,15,17	1.14	1 (6%)
5	MAN	A	503	1	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
5	MAN	D	506	1	11,11,12	0.60	0	15,15,17	0.83	1 (6%)
6	4MU	C	600	2	14,14,14	1.98	4 (28%)	20,20,20	2.25	9 (45%)
5	MAN	B	507	1	11,11,12	0.54	0	15,15,17	0.86	1 (6%)
5	MAN	B	506	1	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
4	NAG	C	502	1	14,14,15	0.55	0	17,19,21	0.80	0
5	MAN	C	507	1	11,11,12	0.56	0	15,15,17	1.02	1 (6%)
4	NAG	D	502	1	14,14,15	1.08	1 (7%)	17,19,21	2.45	2 (11%)
5	MAN	D	505	1	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
5	MAN	D	509	1	11,11,12	0.53	0	15,15,17	0.91	0
5	MAN	A	506	1	11,11,12	0.62	0	15,15,17	0.63	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
5	MAN	B	504	1	-	2/2/19/22	0/1/1/1
5	MAN	C	509	1	-	1/2/19/22	0/1/1/1
4	NAG	C	501	1	-	0/6/23/26	0/1/1/1
6	4MU	D	600	3	-	-	0/2/2/2
5	MAN	B	505	1	-	0/2/19/22	0/1/1/1
5	MAN	C	508	1	-	0/2/19/22	0/1/1/1
5	MAN	D	504	1	-	2/2/19/22	0/1/1/1
4	NAG	D	501	1	-	1/6/23/26	0/1/1/1
5	MAN	D	508	1	-	0/2/19/22	0/1/1/1
5	MAN	C	504	1	-	2/2/19/22	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	502	1	-	0/6/23/26	0/1/1/1
5	MAN	D	503	1	-	2/2/19/22	0/1/1/1
6	4MU	B	600	3	-	-	0/2/2/2
5	MAN	A	505	1	-	0/2/19/22	0/1/1/1
5	MAN	A	507	1	-	0/2/19/22	0/1/1/1
5	MAN	B	508	1	-	0/2/19/22	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	4MU	A	600	2	-	-	0/2/2/2
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	MAN	A	504	1	-	2/2/19/22	0/1/1/1
5	MAN	A	509	1	-	2/2/19/22	0/1/1/1
5	MAN	B	503	1	-	0/2/19/22	0/1/1/1
5	MAN	B	509	1	-	0/2/19/22	0/1/1/1
5	MAN	C	505	1	-	0/2/19/22	0/1/1/1
5	MAN	A	508	1	-	0/2/19/22	0/1/1/1
5	MAN	C	506	1	-	0/2/19/22	0/1/1/1
5	MAN	D	507	1	-	0/2/19/22	0/1/1/1
5	MAN	A	503	1	-	2/2/19/22	0/1/1/1
5	MAN	D	506	1	-	0/2/19/22	0/1/1/1
6	4MU	C	600	2	-	-	0/2/2/2
5	MAN	B	507	1	-	2/2/19/22	0/1/1/1
5	MAN	B	506	1	-	0/2/19/22	0/1/1/1
4	NAG	C	502	1	-	1/6/23/26	0/1/1/1
5	MAN	C	507	1	-	0/2/19/22	0/1/1/1
4	NAG	D	502	1	-	0/6/23/26	0/1/1/1
5	MAN	D	505	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	D	509	1	-	2/2/19/22	0/1/1/1
5	MAN	A	506	1	-	0/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	4MU	CM4-C4	-5.27	1.40	1.50
6	A	600	4MU	CM4-C4	-5.17	1.40	1.50
4	D	502	NAG	C1-C2	3.67	1.57	1.52
6	B	600	4MU	C3-C4	3.49	1.39	1.35
6	A	600	4MU	C3-C4	3.21	1.39	1.35

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	502	NAG	C1-O5-C5	7.23	121.88	112.19
4	D	502	NAG	O5-C1-C2	-6.04	101.94	111.29
6	D	600	4MU	O1-C2-C3	4.64	122.80	117.16
6	C	600	4MU	O2-C2-C3	-4.51	116.84	125.92
6	C	600	4MU	O1-C2-O2	4.50	122.24	116.40

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	MAN	O5-C5-C6-O6
5	A	509	MAN	O5-C5-C6-O6
5	D	509	MAN	O5-C5-C6-O6
5	D	504	MAN	O5-C5-C6-O6
5	D	504	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	4MU	1	0
6	A	600	4MU	1	0
5	A	509	MAN	1	0
5	D	509	MAN	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	363/363 (100%)	-0.06	9 (2%) 57 61	7, 14, 23, 29	1 (0%)
1	B	360/363 (99%)	0.05	13 (3%) 42 47	7, 15, 27, 43	0
1	C	363/363 (100%)	0.01	9 (2%) 57 61	9, 16, 24, 37	0
1	D	360/363 (99%)	0.14	12 (3%) 46 51	10, 18, 27, 44	1 (0%)
All	All	1446/1452 (99%)	0.04	43 (2%) 50 54	7, 15, 26, 44	2 (0%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	159	GLY	7.2
1	C	85	THR	5.6
1	D	160	GLY	5.0
1	D	158	ASN	4.8
1	B	447	LEU	4.8

### 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	BGC	E	3	11/12	0.69	0.35	17,18,19,21	10
2	BGC	G	3	11/12	0.74	0.41	18,19,20,20	10

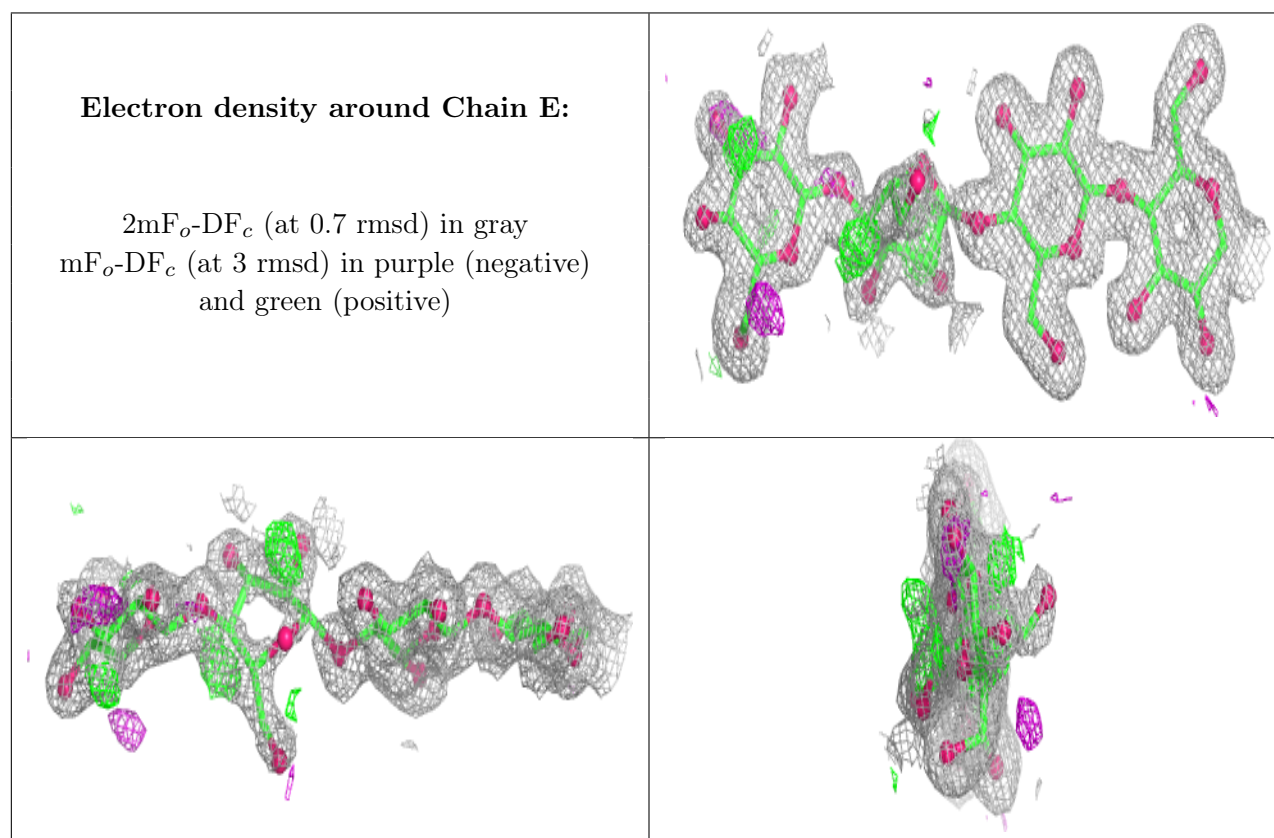
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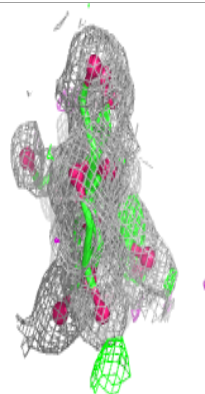
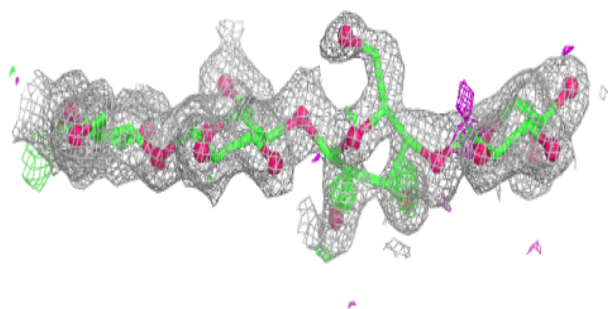
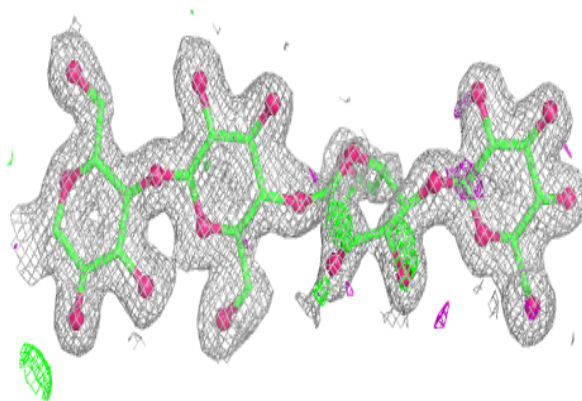
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	4	11/12	0.77	0.15	17,21,22,22	0
2	BGC	G	4	11/12	0.88	0.13	16,20,21,21	0
2	BGC	G	2	11/12	0.90	0.12	19,20,21,21	0
3	BGC	H	2	11/12	0.93	0.08	13,15,15,15	0
3	BGC	F	1	11/12	0.94	0.08	14,14,16,16	0
3	BGC	H	1	11/12	0.94	0.08	15,16,18,20	0
2	BGC	G	1	11/12	0.94	0.08	17,19,20,21	0
2	BGC	E	2	11/12	0.95	0.12	14,15,16,17	0
2	BGC	E	1	11/12	0.96	0.08	14,15,16,17	0
3	BGC	F	2	11/12	0.97	0.08	12,13,13,13	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.

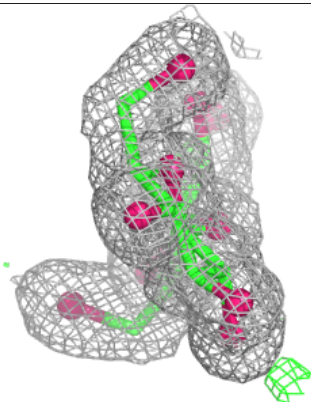
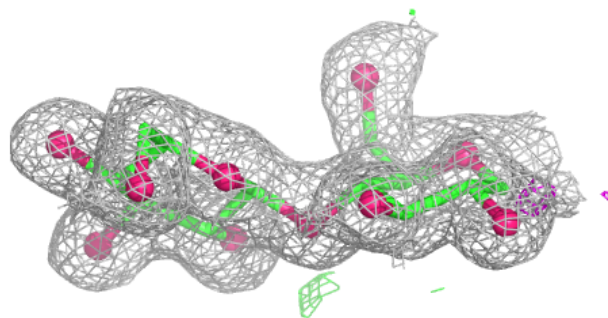
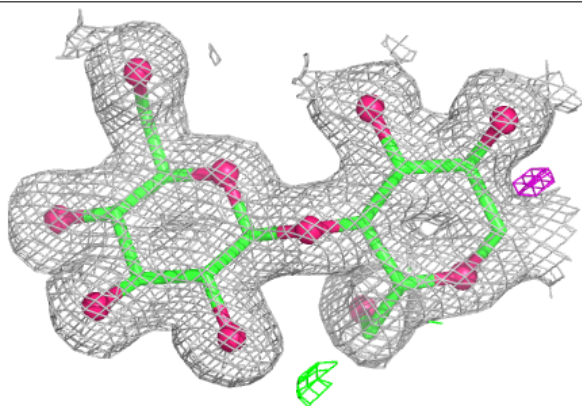


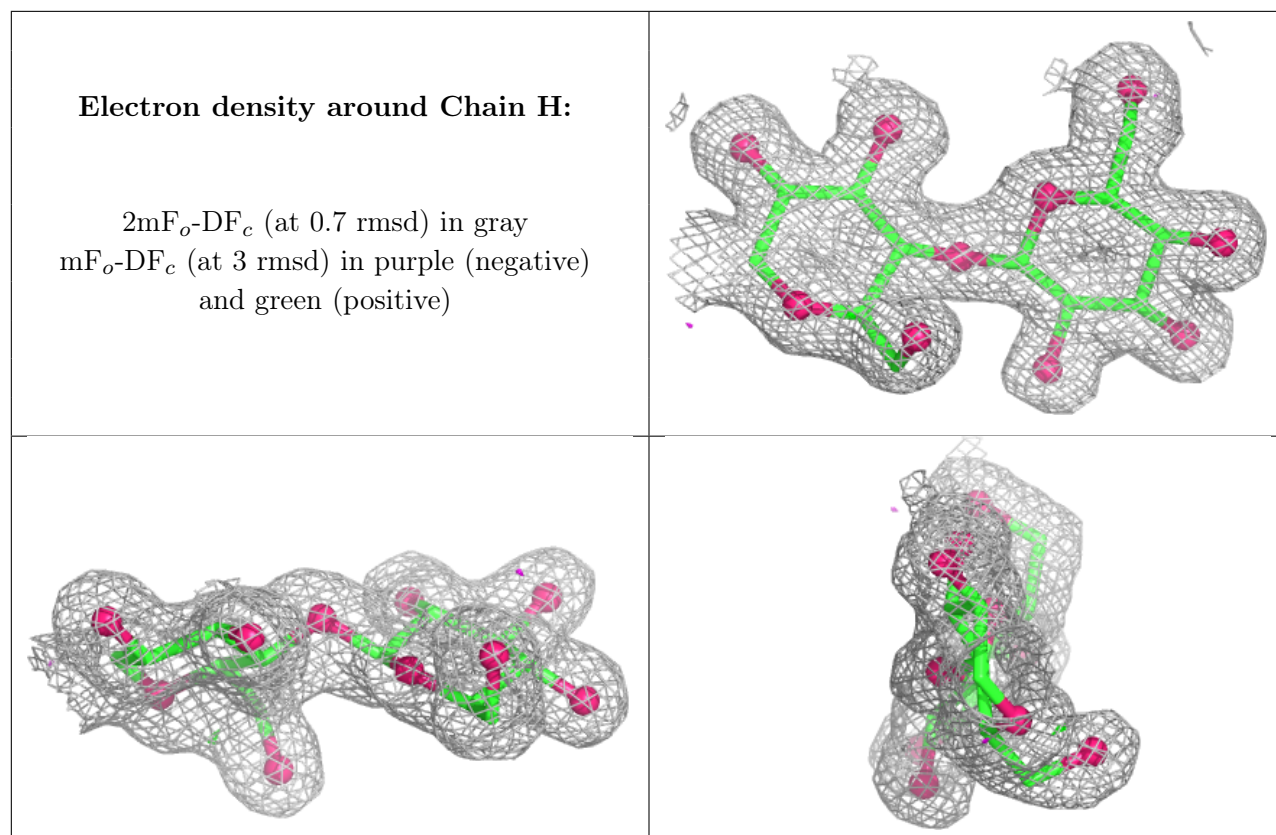
**Electron density around Chain G:**

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

**Electron density around Chain 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	501	14/15	0.60	0.31	33,36,41,41	0
4	NAG	B	501	14/15	0.63	0.30	39,42,43,44	0
5	MAN	B	503	11/12	0.70	0.28	33,38,39,41	0
5	MAN	A	503	11/12	0.72	0.25	31,35,38,39	0
5	MAN	B	509	11/12	0.73	0.29	37,39,41,42	0
4	NAG	D	501	14/15	0.74	0.24	38,40,41,43	0
5	MAN	A	509	11/12	0.74	0.24	30,32,33,33	0
5	MAN	D	503	11/12	0.75	0.27	36,39,40,41	0
5	MAN	C	509	11/12	0.76	0.18	33,34,36,36	0
5	MAN	D	504	11/12	0.78	0.24	32,35,37,37	0
5	MAN	D	507	11/12	0.80	0.18	26,30,31,32	0
5	MAN	D	509	11/12	0.81	0.21	26,30,32,33	0
5	MAN	B	504	11/12	0.82	0.22	26,29,32,32	0
5	MAN	C	506	11/12	0.83	0.12	22,23,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	4MU	B	600	13/13	0.83	0.17	18,22,25,26	0
5	MAN	B	508	11/12	0.84	0.10	29,31,32,32	0
6	4MU	C	600	13/13	0.84	0.24	24,29,31,32	0
5	MAN	C	507	11/12	0.85	0.12	25,27,29,29	0
5	MAN	A	505	11/12	0.85	0.14	22,24,27,27	0
5	MAN	B	507	11/12	0.86	0.17	27,29,30,32	0
5	MAN	A	504	11/12	0.86	0.16	22,26,29,30	0
5	MAN	A	507	11/12	0.87	0.14	25,28,30,30	0
5	MAN	D	505	11/12	0.87	0.12	23,26,27,28	0
5	MAN	C	504	11/12	0.87	0.21	28,31,32,34	0
5	MAN	A	506	11/12	0.88	0.12	20,22,24,24	0
5	MAN	C	505	11/12	0.88	0.11	21,23,24,25	0
4	NAG	D	502	14/15	0.88	0.10	18,20,22,24	0
5	MAN	A	508	11/12	0.88	0.10	24,25,27,28	0
4	NAG	C	502	14/15	0.89	0.10	19,21,22,24	0
4	NAG	A	501	14/15	0.89	0.12	28,29,32,33	0
5	MAN	B	505	11/12	0.89	0.12	22,23,24,25	0
6	4MU	D	600	13/13	0.89	0.13	19,22,24,24	0
5	MAN	B	506	11/12	0.90	0.11	21,22,23,25	0
4	NAG	A	502	14/15	0.91	0.11	18,19,21,21	0
6	4MU	A	600	13/13	0.92	0.15	17,21,22,23	0
4	NAG	B	502	14/15	0.93	0.09	16,18,19,20	0
5	MAN	C	508	11/12	0.93	0.08	21,21,22,23	0
5	MAN	D	508	11/12	0.94	0.07	18,19,20,20	0
5	MAN	D	506	11/12	0.94	0.09	18,20,21,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.