WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 11:41 AM EDT

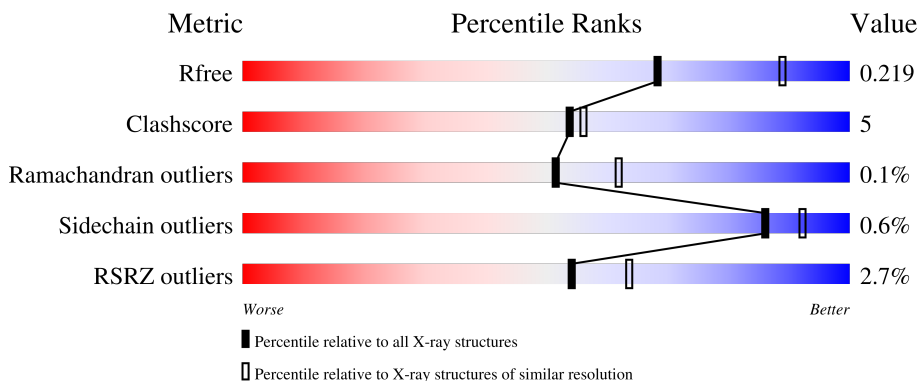|		
PDB ID	:	7JHK
Title	:	Structure of human beta 1,3-N-acetylglucosaminyltransferase 2 in unliganded form
Authors	:	Hao, Y.; Huang, X.
Deposited on	:	2020-07-20
Resolution	:	2.34 Å(reported)

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 2.34 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.
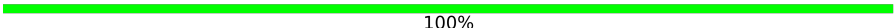
Metric	Percentile Ranks	Value
Rfree		0.219
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		0.6%
RSRZ outliers		2.7%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 >=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 <=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	370	5% / 72% 15% · 13%
1	B	370	.% / 78% 11% 11%
1	C	370	3% / 75% 14% · 11%
1	D	370	.% / 79% 10% 11%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	2	100%
3	I	2	100%
4	G	4	50% 50%
5	H	4	50% 50%
6	J	5	40% 60%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11700 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 N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	3	0
			2674	1721	459	482	12			
1	B	331	Total	C	N	O	S	0	2	0
			2742	1761	473	495	13			
1	C	331	Total	C	N	O	S	0	4	0
			2746	1763	474	496	13			
1	D	330	Total	C	N	O	S	0	0	0
			2717	1746	467	491	13			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP Q9NY97
A	29	HIS	-	expression tag	UNP Q9NY97
A	30	HIS	-	expression tag	UNP Q9NY97
A	31	HIS	-	expression tag	UNP Q9NY97
A	32	HIS	-	expression tag	UNP Q9NY97
A	33	HIS	-	expression tag	UNP Q9NY97
A	34	HIS	-	expression tag	UNP Q9NY97
A	35	HIS	-	expression tag	UNP Q9NY97
A	36	HIS	-	expression tag	UNP Q9NY97
A	37	GLU	-	expression tag	UNP Q9NY97
A	38	ASN	-	expression tag	UNP Q9NY97
A	39	LEU	-	expression tag	UNP Q9NY97
A	40	TYR	-	expression tag	UNP Q9NY97
A	41	PHE	-	expression tag	UNP Q9NY97
A	42	GLN	-	expression tag	UNP Q9NY97
A	43	GLY	-	expression tag	UNP Q9NY97
A	44	SER	-	expression tag	UNP Q9NY97
B	28	MET	-	initiating methionine	UNP Q9NY97
B	29	HIS	-	expression tag	UNP Q9NY97
B	30	HIS	-	expression tag	UNP Q9NY97

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	HIS	-	expression tag	UNP Q9NY97
B	32	HIS	-	expression tag	UNP Q9NY97
B	33	HIS	-	expression tag	UNP Q9NY97
B	34	HIS	-	expression tag	UNP Q9NY97
B	35	HIS	-	expression tag	UNP Q9NY97
B	36	HIS	-	expression tag	UNP Q9NY97
B	37	GLU	-	expression tag	UNP Q9NY97
B	38	ASN	-	expression tag	UNP Q9NY97
B	39	LEU	-	expression tag	UNP Q9NY97
B	40	TYR	-	expression tag	UNP Q9NY97
B	41	PHE	-	expression tag	UNP Q9NY97
B	42	GLN	-	expression tag	UNP Q9NY97
B	43	GLY	-	expression tag	UNP Q9NY97
B	44	SER	-	expression tag	UNP Q9NY97
C	28	MET	-	initiating methionine	UNP Q9NY97
C	29	HIS	-	expression tag	UNP Q9NY97
C	30	HIS	-	expression tag	UNP Q9NY97
C	31	HIS	-	expression tag	UNP Q9NY97
C	32	HIS	-	expression tag	UNP Q9NY97
C	33	HIS	-	expression tag	UNP Q9NY97
C	34	HIS	-	expression tag	UNP Q9NY97
C	35	HIS	-	expression tag	UNP Q9NY97
C	36	HIS	-	expression tag	UNP Q9NY97
C	37	GLU	-	expression tag	UNP Q9NY97
C	38	ASN	-	expression tag	UNP Q9NY97
C	39	LEU	-	expression tag	UNP Q9NY97
C	40	TYR	-	expression tag	UNP Q9NY97
C	41	PHE	-	expression tag	UNP Q9NY97
C	42	GLN	-	expression tag	UNP Q9NY97
C	43	GLY	-	expression tag	UNP Q9NY97
C	44	SER	-	expression tag	UNP Q9NY97
D	28	MET	-	initiating methionine	UNP Q9NY97
D	29	HIS	-	expression tag	UNP Q9NY97
D	30	HIS	-	expression tag	UNP Q9NY97
D	31	HIS	-	expression tag	UNP Q9NY97
D	32	HIS	-	expression tag	UNP Q9NY97
D	33	HIS	-	expression tag	UNP Q9NY97
D	34	HIS	-	expression tag	UNP Q9NY97
D	35	HIS	-	expression tag	UNP Q9NY97
D	36	HIS	-	expression tag	UNP Q9NY97
D	37	GLU	-	expression tag	UNP Q9NY97
D	38	ASN	-	expression tag	UNP Q9NY97

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Chain	Residue	Modelled	Actual	Comment	Reference
D	39	LEU	-	expression tag	UNP Q9NY97
D	40	TYR	-	expression tag	UNP Q9NY97
D	41	PHE	-	expression tag	UNP Q9NY97
D	42	GLN	-	expression tag	UNP Q9NY97
D	43	GLY	-	expression tag	UNP Q9NY97
D	44	SER	-	expression tag	UNP Q9NY97

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
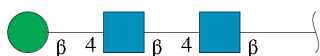
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	39	22	2	15	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
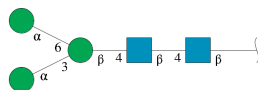
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
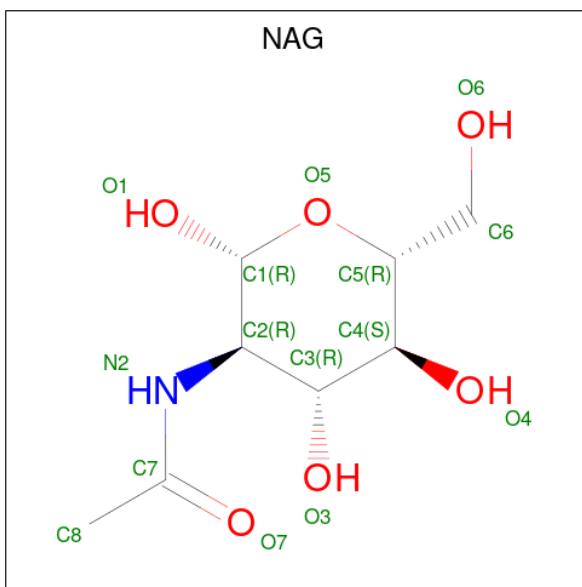
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total 2	Cl 2	0	0
8	B	1	Total 1	Cl 1	0	0
8	C	1	Total 1	Cl 1	0	0
8	D	2	Total 2	Cl 2	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Na 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	119	Total 119	O 119	0	0
10	B	148	Total 148	O 148	0	0
10	C	125	Total 125	O 125	0	0
10	D	124	Total 124	O 124	0	0

3 Residue-property plots ⓘ

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: N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase 2

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- Molecule 1: N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase 2

K351 R354 T355 F356 D357 I358 E359 N362 Y369 V370 D371 L372 H376 S377 R378 K379 E382 A393 C397

• Molecule 1: N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase 2

Chain D:

%

79% 10% 11%

MET HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY SER LYS GLU LYS PHE TRP LYS ILE SER THR PRO PRO E56 R68 S75 M76 LEU THR ASN GLN THR GLY GLU ALA GLY ARG LEU SER N89 H92 C96 V102 V105 F109 L112

L120 R124 C125 Y128 P142 A147 Q174 T175 Q184 N212 L222 L228 R229 T233 K243 N260 S261 L262 K266 P281 D284 K285 K286 Y290 I291 L319 Y320 H321 I322 T323 E348 H376 S377 C397

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

Chain E:

33% 67%

NAG1 NAG2 BMA3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

100%

NAG1 NAG2

• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

50% 50%

NAG1 NAG2 BMA3 MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

50% 50%

NAG1 NAG2 BMA3 MAN4

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain J:

40%   60%

NAG1 NAG2 BMA3 MAN4 MAN5

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.42Å 80.07Å 157.61Å 90.00° 98.82° 90.00°	Depositor
Resolution (Å)	47.18 – 2.34 47.18 – 2.34	Depositor EDS
% Data completeness (in resolution range)	84.9 (47.18-2.34) 84.9 (47.18-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.179 , 0.217 0.180 , 0.219	Depositor DCC
R_{free} test set	2818 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, NAG, CL, BMA, MAN

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	0/2746	0.46	0/3718
1	B	0.28	0/2817	0.44	0/3816
1	C	0.32	0/2821	0.46	0/3820
1	D	0.26	0/2790	0.44	0/3779
All	All	0.29	0/11174	0.45	0/15133

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2674	0	2614	35	0
1	B	2742	0	2682	26	0
1	C	2746	0	2685	37	0
1	D	2717	0	2662	21	0
2	E	39	0	34	1	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
4	G	50	0	43	0	0
5	H	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	61	0	52	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	2	0	0	1	0
8	B	1	0	0	0	0
8	C	1	0	0	1	0
8	D	2	0	0	0	0
9	C	1	0	0	0	0
10	A	119	0	0	0	0
10	B	148	0	0	1	0
10	C	125	0	0	2	0
10	D	124	0	0	0	0
All	All	11700	0	10904	117	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 5.

The worst 5 of 117 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:C:64:GLU:OE1	1:C:67:ASN:ND2	2.11	0.83
1:D:266:LYS:NZ	1:D:348:GLU:OE1	2.19	0.76
1:D:184:GLN:OE1	1:D:212:ASN:ND2	2.20	0.74
1:A:100:LEU:O	1:A:103:THR:OG1	2.06	0.73
1:A:140:LYS:HE3	1:A:175:THR:OG1	1.89	0.73

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	318/370 (86%)	306 (96%)	11 (4%)	1 (0%)	41	47
1	B	329/370 (89%)	323 (98%)	6 (2%)	0	100	100
1	C	331/370 (90%)	325 (98%)	6 (2%)	0	100	100
1	D	326/370 (88%)	320 (98%)	6 (2%)	0	100	100
All	All	1304/1480 (88%)	1274 (98%)	29 (2%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	LYS

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	297/339 (88%)	295 (99%)	2 (1%)	84	90
1	B	306/339 (90%)	305 (100%)	1 (0%)	92	96
1	C	305/339 (90%)	301 (99%)	4 (1%)	69	79
1	D	303/339 (89%)	303 (100%)	0	100	100
All	All	1211/1356 (89%)	1204 (99%)	7 (1%)	86	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	LYS
1	C	351	LYS
1	C	371	ASP
1	C	354	ARG
1	B	184	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	C	260	ASN
1	D	391	GLN
1	D	212	ASN
1	C	94	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 ⓘ

20 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	NAG	E	1	2,1	14,14,15	0.38	0	17,19,21	0.41	0
2	NAG	E	2	2	14,14,15	0.68	1 (7%)	17,19,21	0.48	0
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	0.77	0
3	NAG	F	1	3,1	14,14,15	0.34	0	17,19,21	0.38	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	G	1	4,1	14,14,15	0.62	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.61	0
4	BMA	G	3	4	11,11,12	0.67	0	15,15,17	0.67	0
4	MAN	G	4	4	11,11,12	0.73	0	15,15,17	1.01	2 (13%)
5	NAG	H	1	5,1	14,14,15	0.50	0	17,19,21	0.44	0
5	NAG	H	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.53	0
5	BMA	H	3	5	11,11,12	0.49	0	15,15,17	0.75	0
5	MAN	H	4	5	11,11,12	0.81	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	I	1	3,1	14,14,15	0.37	0	17,19,21	0.40	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	J	1	1,6	14,14,15	0.56	0	17,19,21	0.46	0
6	NAG	J	2	6	14,14,15	0.59	0	17,19,21	0.47	0
6	BMA	J	3	6	11,11,12	1.16	2 (18%)	15,15,17	0.99	1 (6%)
6	MAN	J	4	6	11,11,12	0.95	0	15,15,17	1.04	1 (6%)
6	MAN	J	5	6	11,11,12	1.05	1 (9%)	15,15,17	1.19	2 (13%)

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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	1/2/19/22	0/1/1/1
6	MAN	J	4	6	-	1/2/19/22	0/1/1/1
6	MAN	J	5	6	-	2/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5	MAN	C1-C2	2.80	1.58	1.52
4	G	2	NAG	O5-C1	-2.72	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	O5-C1	-2.35	1.40	1.43
2	E	2	NAG	O5-C1	-2.23	1.40	1.43
6	J	3	BMA	C4-C5	2.16	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	5	MAN	O2-C2-C3	-2.56	105.01	110.14
6	J	5	MAN	C1-C2-C3	2.45	112.68	109.67
4	G	4	MAN	C1-O5-C5	2.30	115.31	112.19
6	J	3	BMA	C3-C4-C5	2.25	114.25	110.24
5	H	4	MAN	O2-C2-C3	-2.11	105.91	110.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

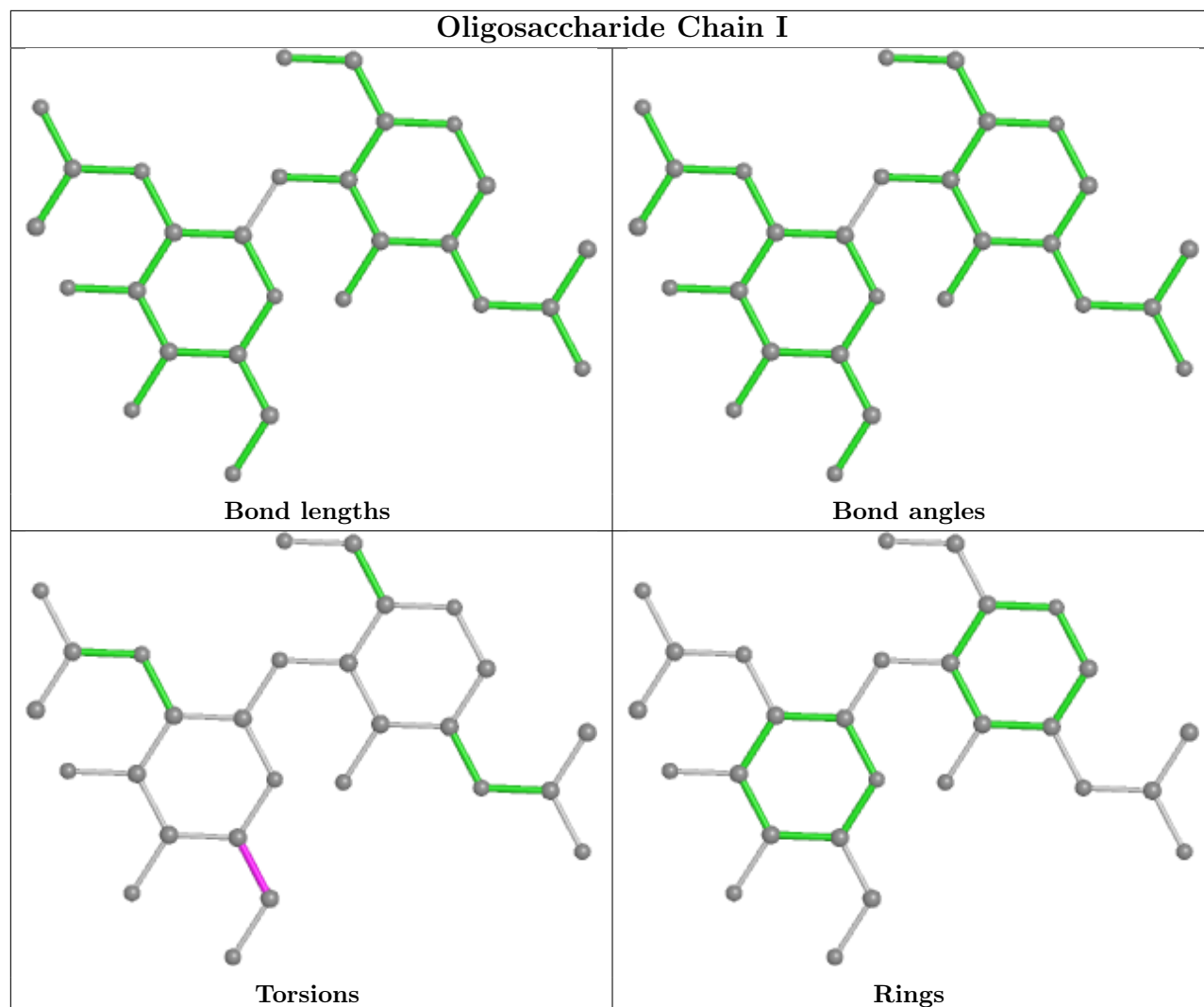| Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

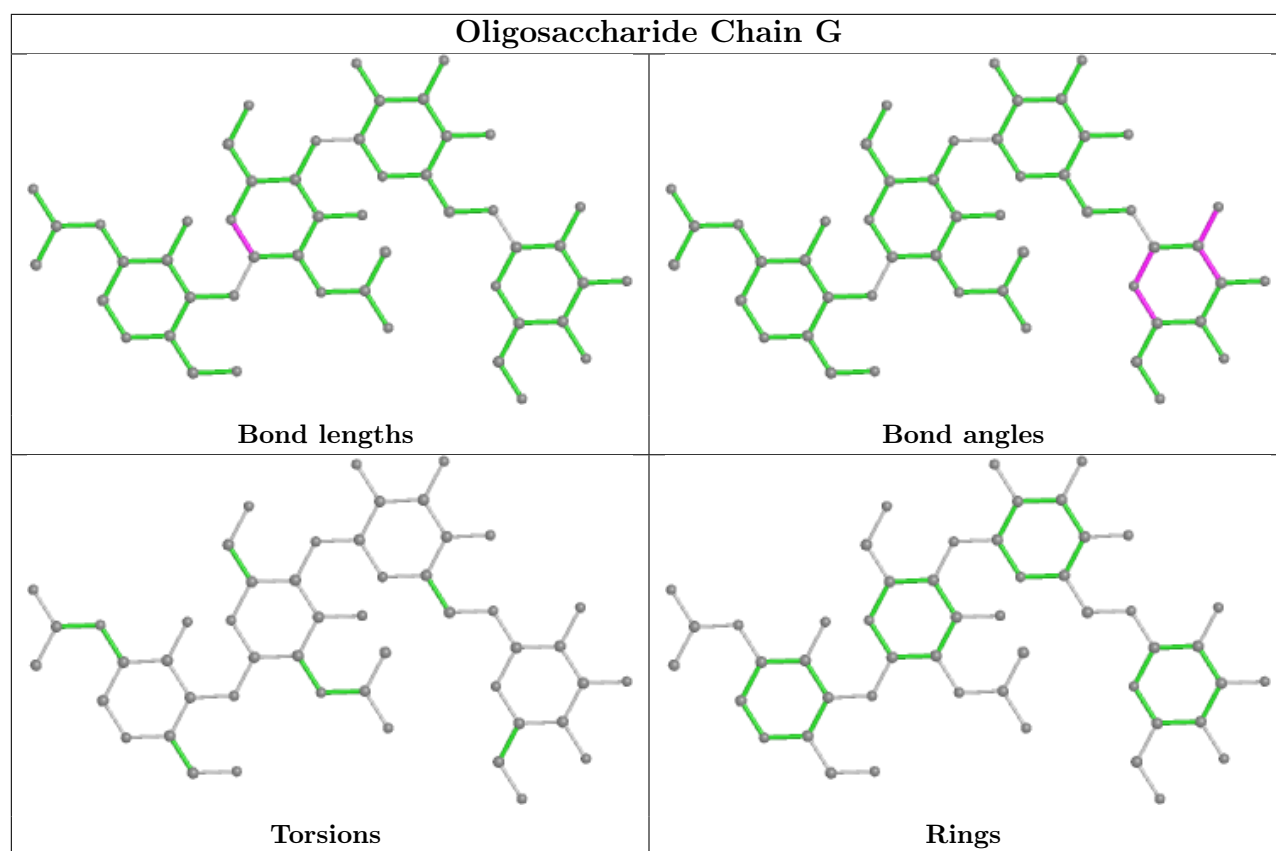1 monomer is involved in 1 short contact:

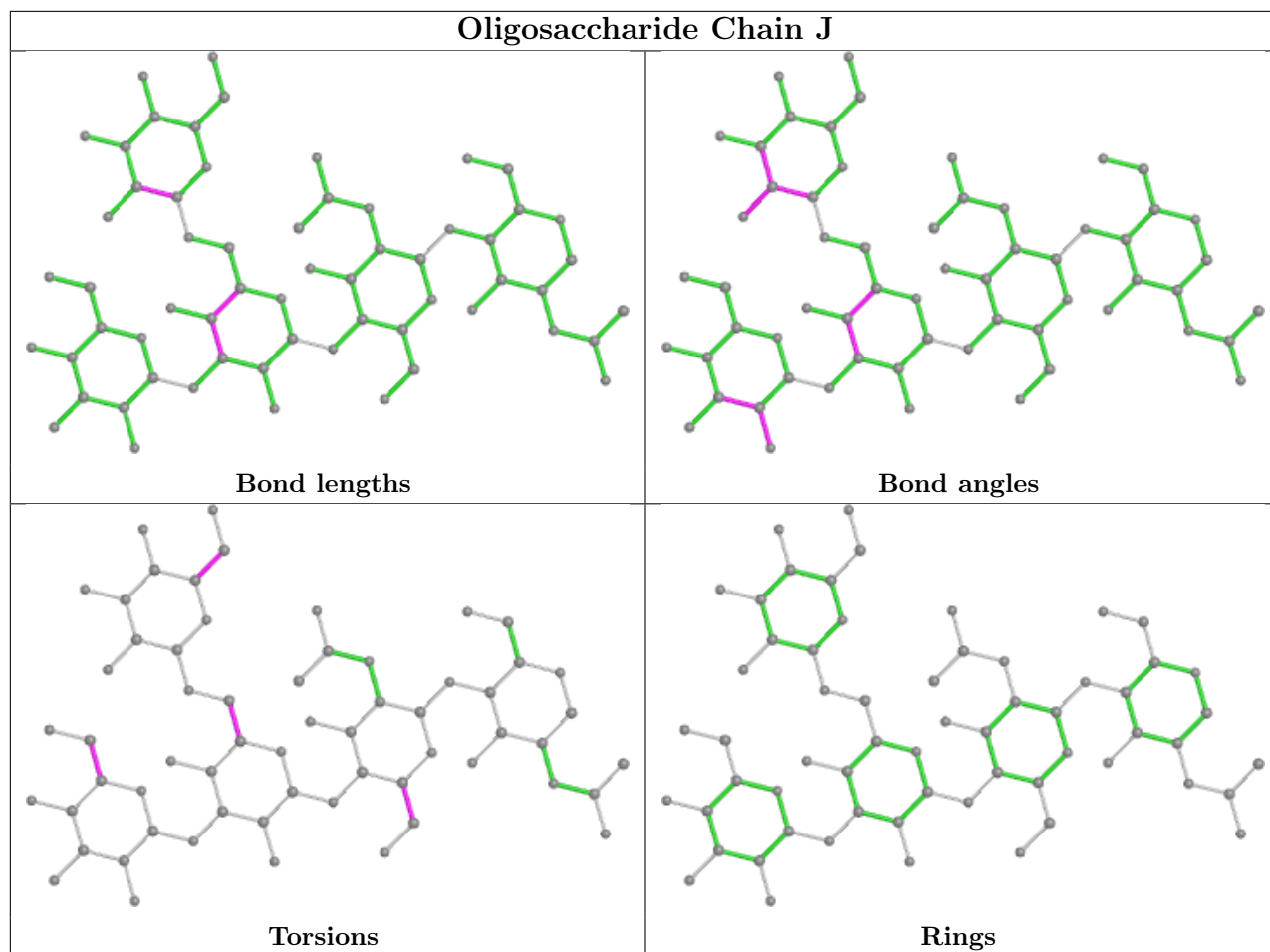| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

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

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 7 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	#$\|Z\| > 2$
7	NAG	C	401	1	14,14,15	0.48	0	17,19,21	0.45	0
7	NAG	D	401	1	14,14,15	0.44	0	17,19,21	0.47	0
7	NAG	A	401	1	14,14,15	0.48	0	17,19,21	0.53	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
7	NAG	C	401	1	-	0/6/23/26	0/1/1/1
7	NAG	D	401	1	-	2/6/23/26	0/1/1/1
7	NAG	A	401	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 (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	401	NAG	O5-C5-C6-O6
7	D	401	NAG	C4-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	A	401	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 ⓘ

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, 95th 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(Å²)	Q<0.9
1	A	323/370 (87%)	0.32	20 (6%)	20	28	19, 37, 70, 109	0
1	B	331/370 (89%)	-0.00	4 (1%)	79	85	19, 32, 53, 82	0
1	C	331/370 (89%)	0.17	10 (3%)	50	60	19, 34, 63, 88	0
1	D	330/370 (89%)	0.07	2 (0%)	89	93	19, 33, 59, 77	0
All	All	1315/1480 (88%)	0.14	36 (2%)	54	64	19, 34, 63, 109	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	THR	7.7
1	A	356	PHE	5.2
1	C	55	PRO	5.0
1	A	396	LYS	4.8
1	A	397	CYS	4.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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.
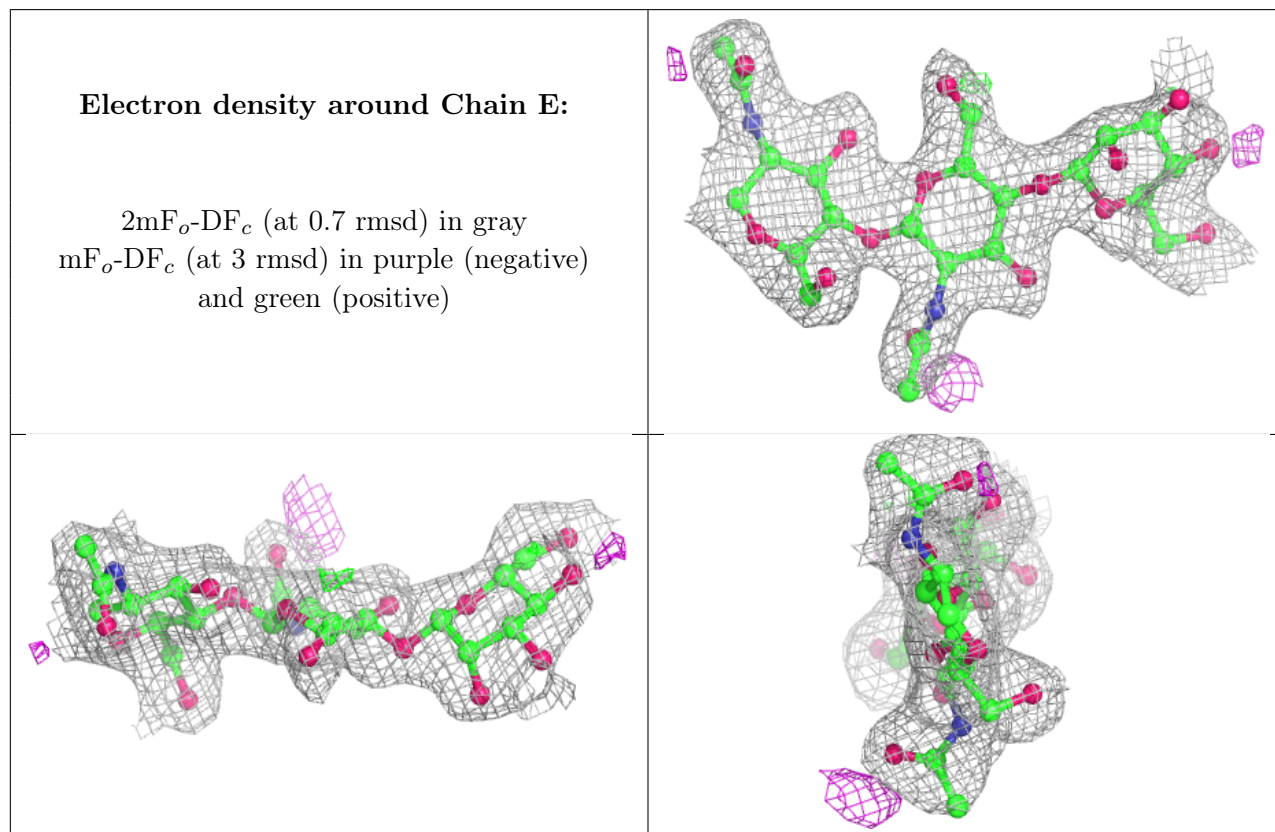
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	MAN	H	4	11/12	0.59	0.32	72,106,114,114	0
4	MAN	G	4	11/12	0.64	0.26	84,87,97,99	0

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| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	J	4	11/12	0.67	0.17	60,87,89,91	0
5	BMA	H	3	11/12	0.78	0.21	75,84,96,100	0
6	MAN	J	5	11/12	0.80	0.23	85,89,101,107	0
3	NAG	F	2	14/15	0.85	0.36	63,79,82,83	0
6	BMA	J	3	11/12	0.85	0.14	53,65,72,82	0
2	BMA	E	3	11/12	0.87	0.14	48,58,70,70	0
4	BMA	G	3	11/12	0.87	0.12	55,59,68,73	0
3	NAG	I	2	14/15	0.90	0.18	73,83,90,97	0
3	NAG	F	1	14/15	0.91	0.22	48,56,58,68	0
3	NAG	I	1	14/15	0.92	0.12	59,70,77,78	0
4	NAG	G	2	14/15	0.94	0.12	29,39,47,49	0
2	NAG	E	2	14/15	0.96	0.12	38,44,51,54	0
6	NAG	J	2	14/15	0.97	0.11	27,37,42,44	0
2	NAG	E	1	14/15	0.97	0.14	22,31,35,40	0
5	NAG	H	2	14/15	0.97	0.13	35,42,52,70	0
6	NAG	J	1	14/15	0.97	0.15	18,24,30,32	0
4	NAG	G	1	14/15	0.98	0.13	24,28,35,40	0
5	NAG	H	1	14/15	0.98	0.14	23,28,33,41	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.
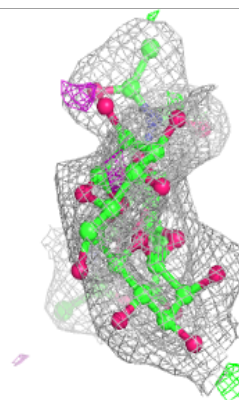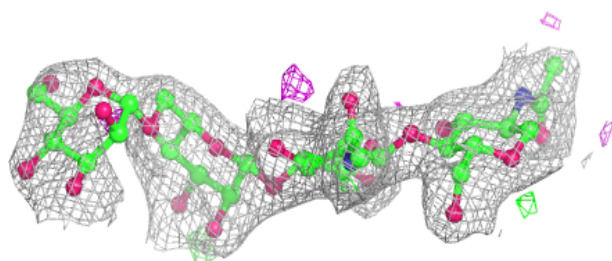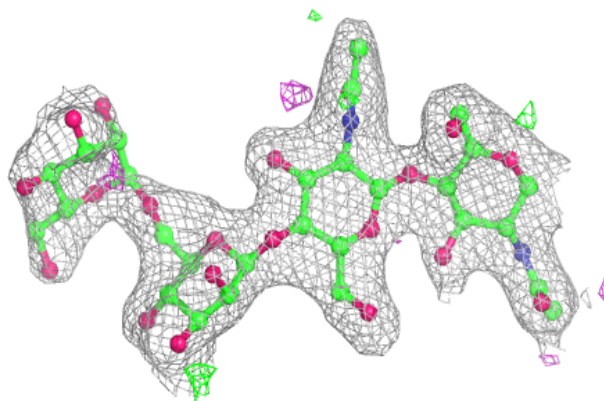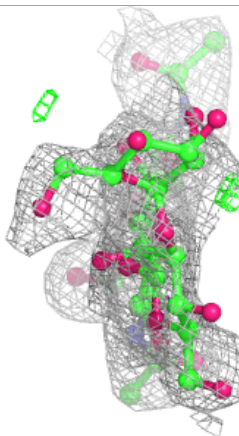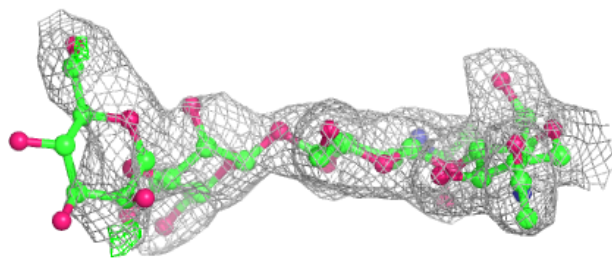

Electron density around Chain E:

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)
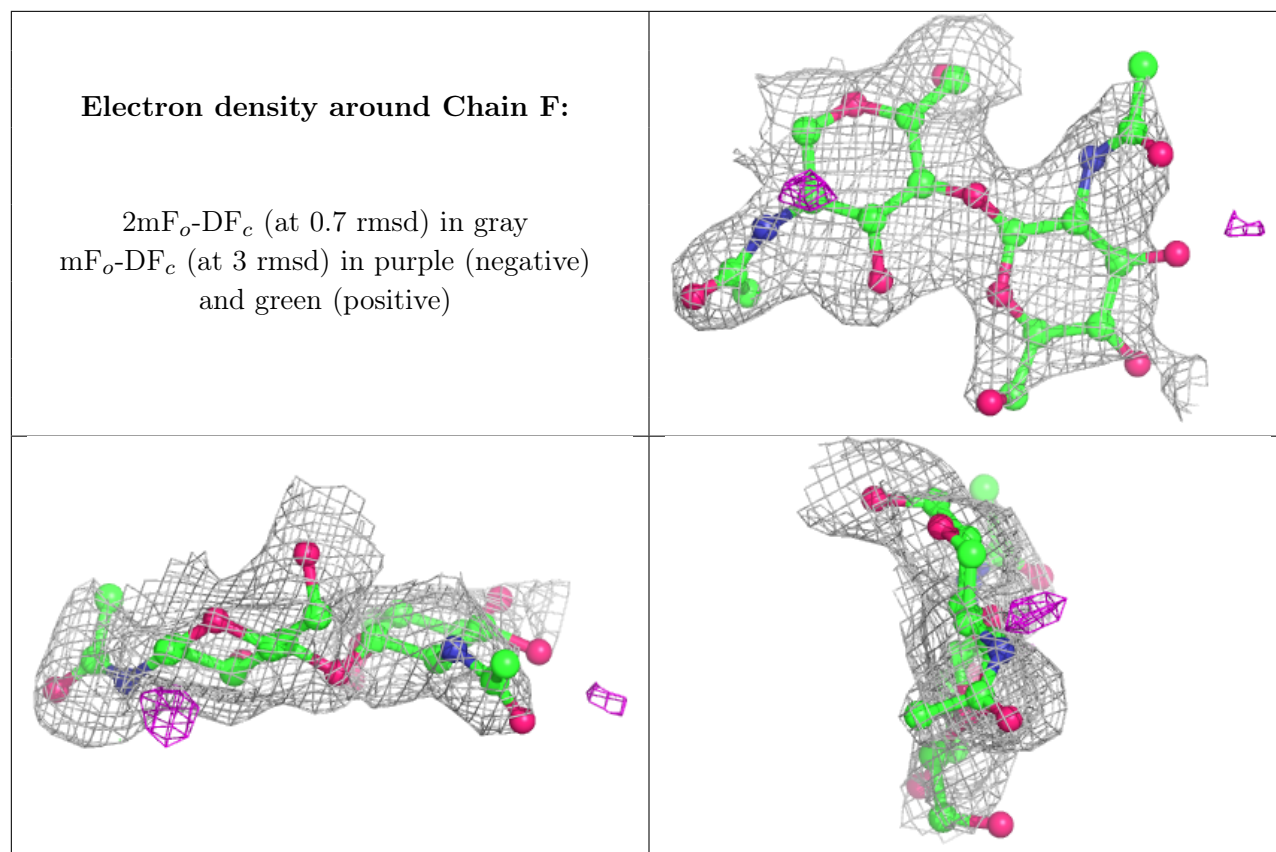
Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
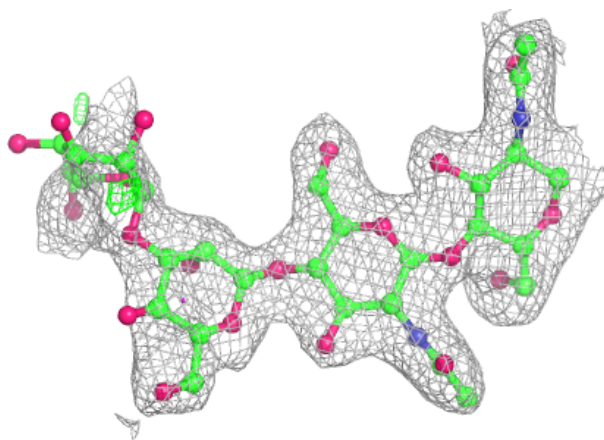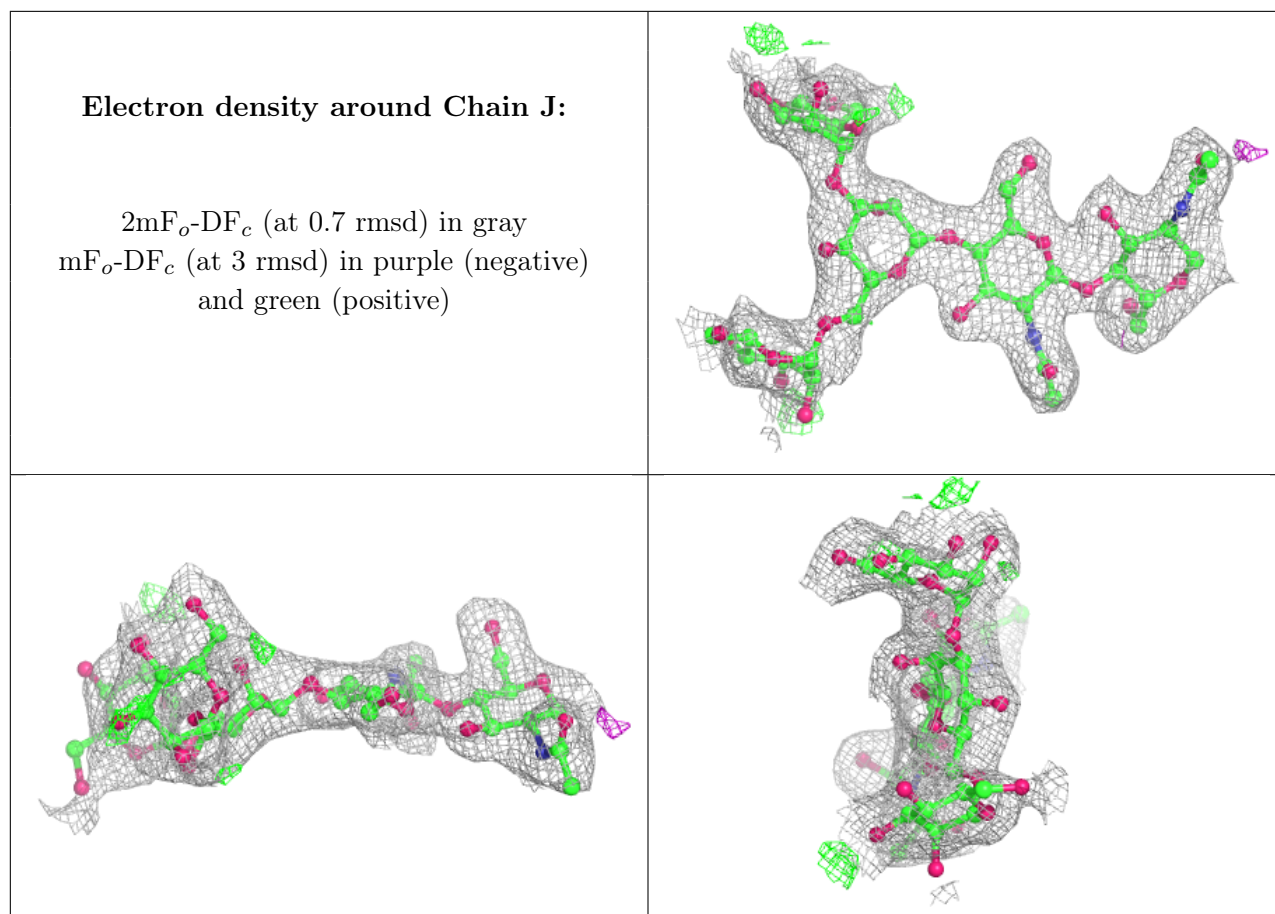and green (positive)
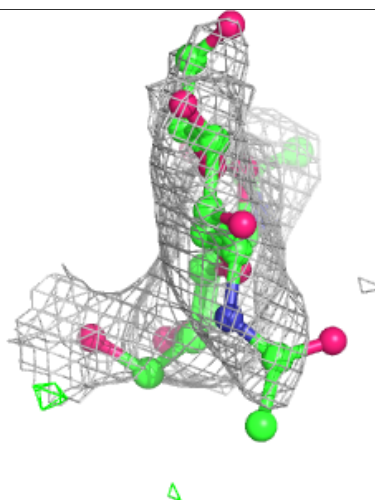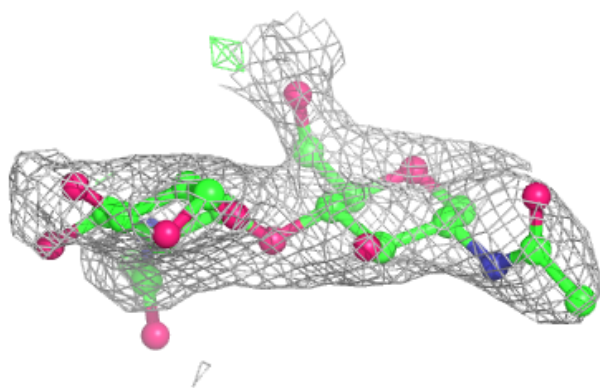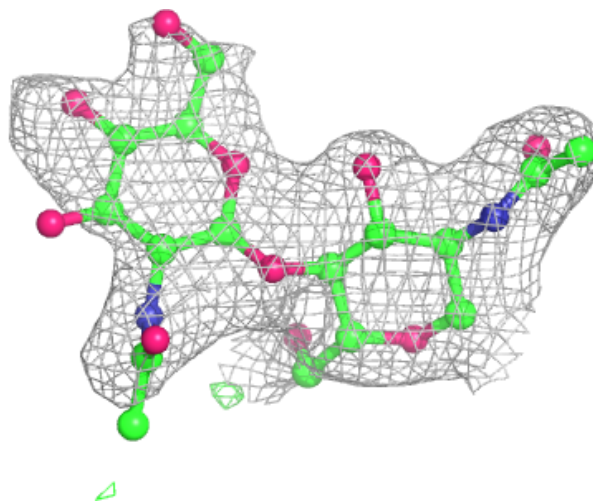
Electron density around Chain G:

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

Electron density around Chain H:

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

Electron density around Chain J:

$2mF_o$-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, 95th 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^2)	Q<0.9
7	NAG	C	401	14/15	0.88	0.15	48,57,66,67	0
7	NAG	D	401	14/15	0.90	0.16	37,46,55,56	0
9	NA	C	403	1/1	0.91	0.12	52,52,52,52	0
8	CL	A	403	1/1	0.92	0.14	69,69,69,69	0
7	NAG	A	401	14/15	0.93	0.16	46,54,62,63	0
8	CL	B	401	1/1	0.99	0.11	46,46,46,46	0
8	CL	C	402	1/1	0.99	0.10	39,39,39,39	0
8	CL	D	402	1/1	0.99	0.07	36,36,36,36	0
8	CL	D	403	1/1	0.99	0.13	38,38,38,38	0
8	CL	A	402	1/1	0.99	0.07	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.