



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 06:37 AM EDT

PDB ID : 3HN3
Title : Human beta-glucuronidase at 1.7 Å resolution
Authors : Klei, H.E.; Ghosh, K.; Anumula, R.
Deposited on : 2009-05-29
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

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>.

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

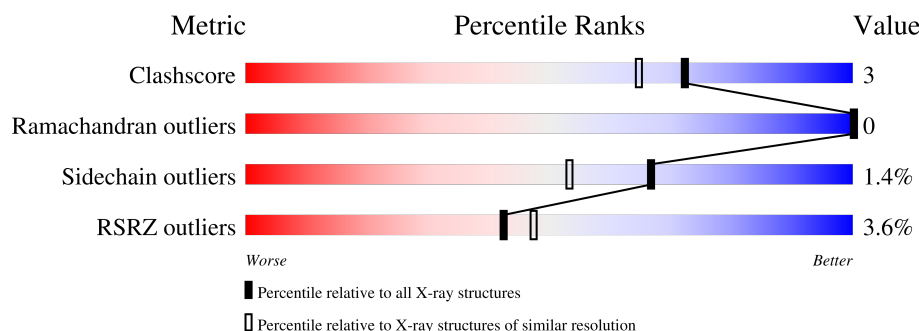
1 Overall quality at a glance

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))
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 ≥ 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	613	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	613	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	D	613	<div> <div>4%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	E	613	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
2	C	10	<div> <div>40%</div> <div>60%</div> </div>
3	F	10	<div> <div>60%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	10	 <div>40% 60%</div>
5	H	10	 <div>50% 30% 20%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	650	X	-	-	-

2 Entry composition [i](#)

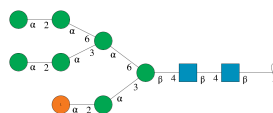
There are 10 unique types of molecules in this entry. The entry contains 23390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-glucuronidase.

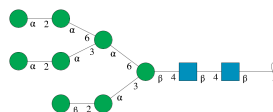
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	7	10	0
			5014	3227	855	917	15			
1	B	609	Total	C	N	O	S	10	8	0
			5007	3225	847	920	15			
1	D	607	Total	C	N	O	S	4	10	0
			5013	3223	856	918	16			
1	E	606	Total	C	N	O	S	10	7	0
			4977	3208	844	910	15			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-L-gulopyranose-(1-2)-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.



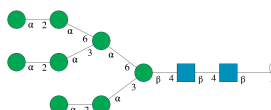
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-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.



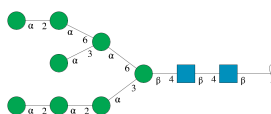
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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
4	G	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



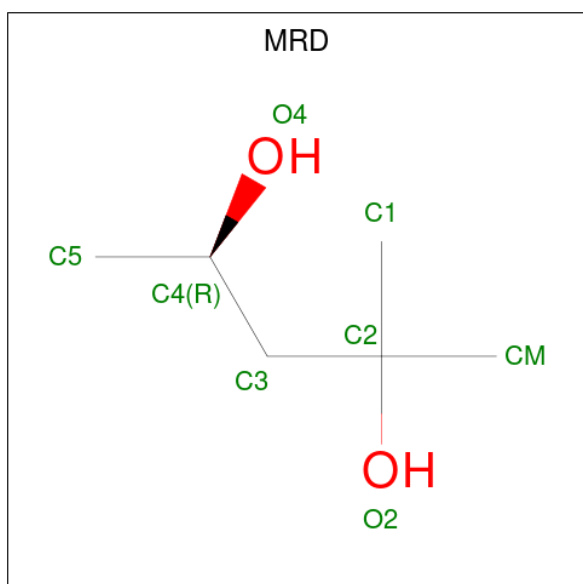
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



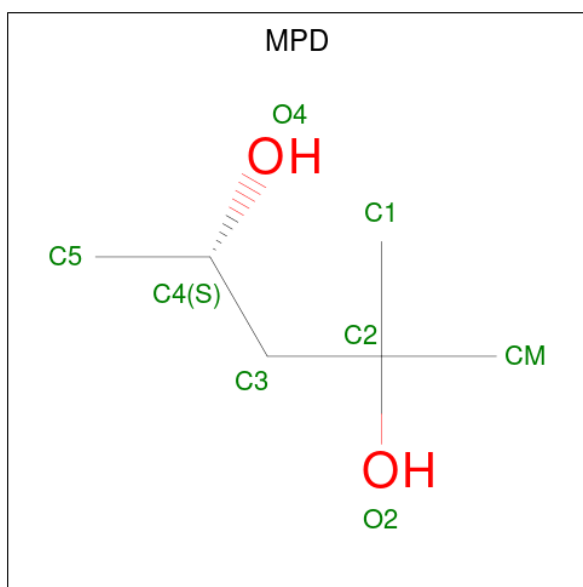
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



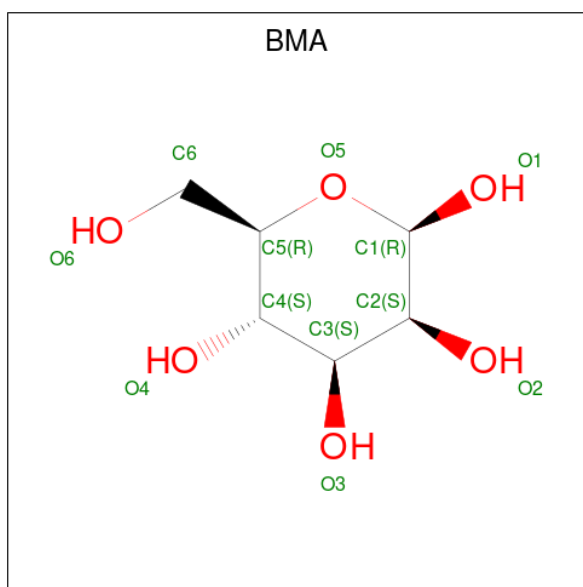
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	D	1	Total	C	O	0	0
			8	6	2		
7	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			8	6	2		
8	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			12	6	6		

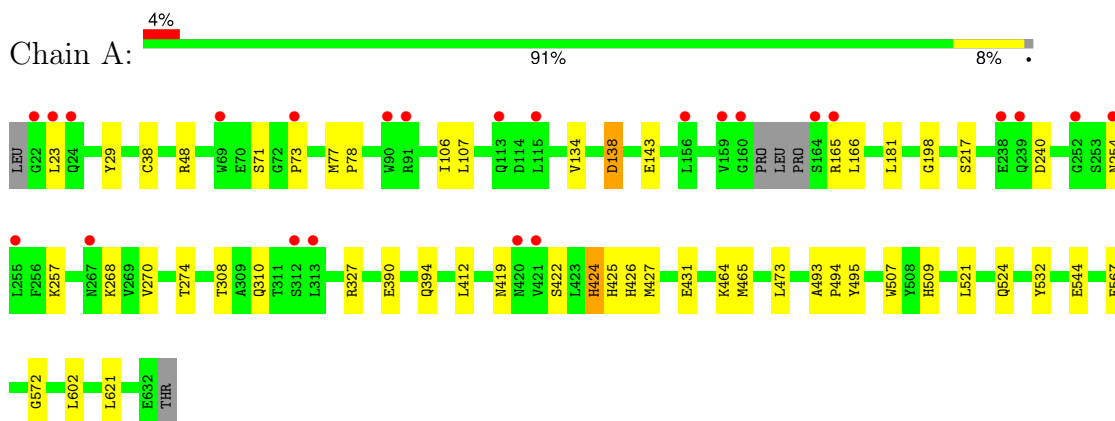
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	691	Total	O	0	0
			691	691		
10	B	706	Total	O	0	0
			706	706		
10	D	646	Total	O	0	0
			646	646		
10	E	764	Total	O	0	0
			764	764		

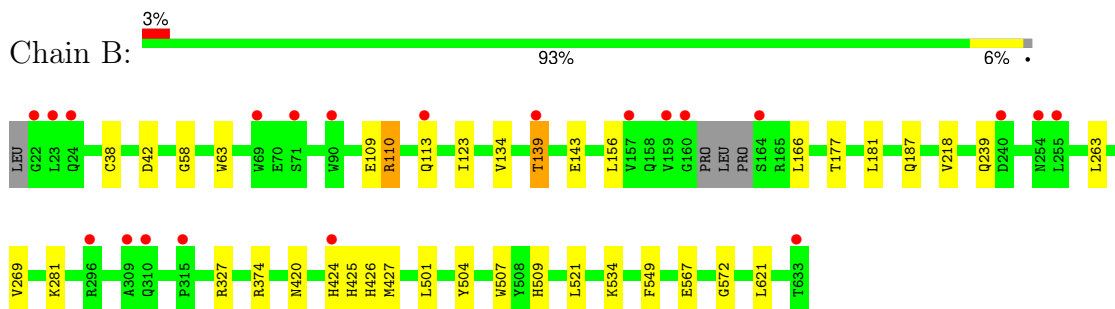
3 Residue-property plots [i](#)

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.

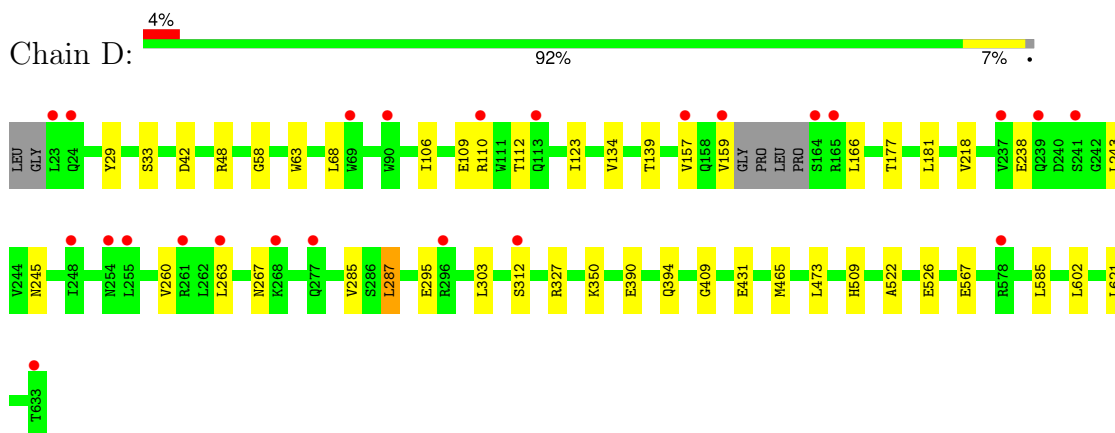
- Molecule 1: Beta-glucuronidase



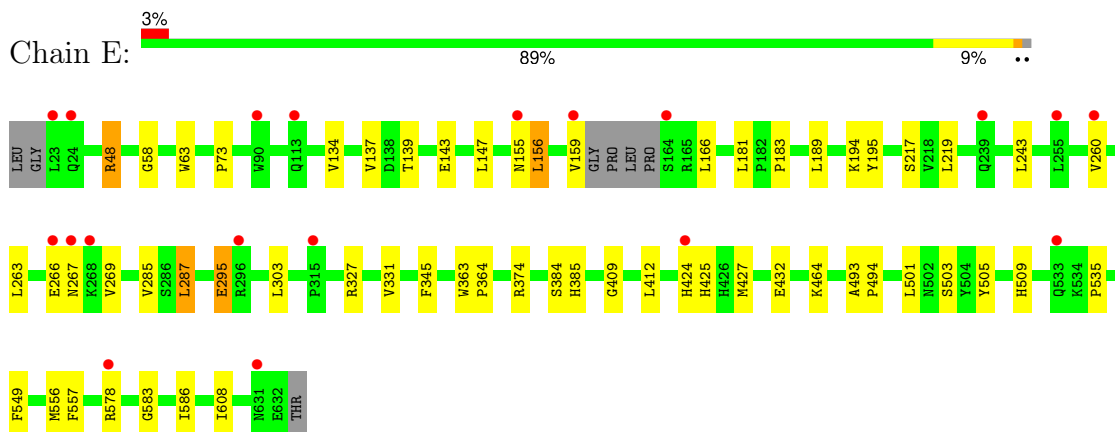
- Molecule 1: Beta-glucuronidase



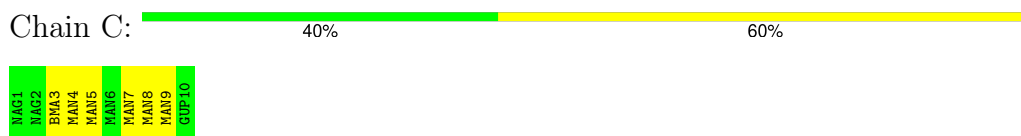
- Molecule 1: Beta-glucuronidase



- Molecule 1: Beta-glucuronidase



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-L-gulopyranose-(1-2)-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



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-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



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.58Å 123.11Å 266.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.70 19.92 – 1.66	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.90-1.70) 84.5 (19.92-1.66)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.240 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23390	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 32.11 % 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 9.9123e-04.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MAN, MPD, GUP, BMA, NAG, MRD

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	0.48	2/5203 (0.0%)	0.63	1/7080 (0.0%)
1	B	0.49	4/5188 (0.1%)	0.65	3/7063 (0.0%)
1	D	0.44	0/5199	0.63	1/7076 (0.0%)
1	E	0.70	5/5150 (0.1%)	0.66	5/7012 (0.1%)
All	All	0.54	11/20740 (0.1%)	0.64	10/28231 (0.0%)

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	E	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	266	GLU	CD-OE1	27.08	1.55	1.25
1	E	266	GLU	CD-OE2	-23.65	0.99	1.25
1	E	194	LYS	CD-CE	-12.30	1.20	1.51
1	A	424	HIS	CB-CG	-11.31	1.29	1.50
1	B	239	GLN	CD-OE1	-9.06	1.04	1.24

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ARG	CB-CG-CD	10.21	138.13	111.60
1	E	295	GLU	OE1-CD-OE2	-10.02	111.28	123.30
1	E	194	LYS	CG-CD-CE	8.36	136.97	111.90
1	E	266	GLU	CG-CD-OE2	7.32	132.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	HIS	CA-CB-CG	5.85	123.54	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	295	GLU	Sidechain

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	5014	0	4876	35	0
1	B	5007	0	4864	28	0
1	D	5013	0	4860	34	0
1	E	4977	0	4833	37	0
2	C	116	0	97	1	0
3	F	116	0	97	0	0
4	G	116	0	97	1	0
5	H	116	0	97	3	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
6	D	14	0	13	1	0
6	E	14	0	13	0	0
7	A	8	0	14	1	0
7	D	8	0	14	3	0
7	E	8	0	14	0	0
8	B	8	0	14	1	0
8	E	8	0	14	1	0
9	E	12	0	12	3	0
10	A	691	0	0	7	0
10	B	706	0	0	5	0
10	D	646	0	0	7	0
10	E	764	0	0	5	0
All	All	23390	0	19955	137	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 137 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:D:465:MET:HA	1:D:465:MET:HE2	1.52	0.90
1:D:390[B]:GLU:OE1	10:D:2481:HOH:O	1.91	0.86
1:E:183:PRO:HG3	1:E:412:LEU:HD23	1.57	0.86
1:B:143[B]:GLU:OE1	1:B:425:HIS:NE2	2.10	0.85
1:E:134:VAL:HG13	1:E:166:LEU:HD11	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/613 (100%)	592 (96%)	22 (4%)	0	100	100
1	B	614/613 (100%)	593 (97%)	21 (3%)	0	100	100
1	D	613/613 (100%)	594 (97%)	19 (3%)	0	100	100
1	E	609/613 (99%)	586 (96%)	23 (4%)	0	100	100
All	All	2450/2452 (100%)	2365 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/542 (101%)	538 (98%)	9 (2%)	62	48
1	B	546/542 (101%)	540 (99%)	6 (1%)	73	63
1	D	548/542 (101%)	542 (99%)	6 (1%)	73	63
1	E	542/542 (100%)	533 (98%)	9 (2%)	60	46
All	All	2183/2168 (101%)	2153 (99%)	30 (1%)	67	53

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	534	LYS
1	E	327	ARG
1	D	287	LEU
1	E	578	ARG
1	E	219	LEU

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

Mol	Chain	Res	Type
1	A	245	ASN
1	A	279	GLN
1	B	575	GLN
1	D	245	ASN
1	D	279	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

40 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	C	1	2,1	14,14,15	0.39	0	17,19,21	0.80	0
2	GUP	C	10	2	11,11,12	0.56	0	15,15,17	0.54	0
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.96	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	0.84	1 (6%)
2	MAN	C	4	2	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
2	MAN	C	5	2	11,11,12	0.52	0	15,15,17	1.28	2 (13%)
2	MAN	C	6	2	11,11,12	0.63	0	15,15,17	0.65	0
2	MAN	C	7	2	11,11,12	0.57	0	15,15,17	0.91	1 (6%)
2	MAN	C	8	2	11,11,12	0.55	0	15,15,17	0.56	0
2	MAN	C	9	2	11,11,12	0.52	0	15,15,17	1.30	3 (20%)
3	NAG	F	1	3,1	14,14,15	0.44	0	17,19,21	0.88	0
3	BMA	F	10	3	11,11,12	0.77	0	15,15,17	1.97	4 (26%)
3	NAG	F	2	3	14,14,15	0.62	0	17,19,21	1.17	0
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.92	0
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	0.89	0
3	MAN	F	5	3	11,11,12	0.58	0	15,15,17	1.12	1 (6%)
3	MAN	F	6	3	11,11,12	0.66	0	15,15,17	0.54	0
3	MAN	F	7	3	11,11,12	0.42	0	15,15,17	0.86	1 (6%)
3	MAN	F	8	3	11,11,12	0.57	0	15,15,17	0.71	0
3	MAN	F	9	3	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.51	0	17,19,21	0.98	0
4	MAN	G	10	4	11,11,12	0.74	0	15,15,17	1.24	2 (13%)
4	NAG	G	2	4	14,14,15	0.55	0	17,19,21	0.90	0
4	BMA	G	3	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	G	4	4	11,11,12	0.48	0	15,15,17	0.96	1 (6%)
4	MAN	G	5	4	11,11,12	0.53	0	15,15,17	0.92	2 (13%)
4	MAN	G	6	4	11,11,12	0.69	0	15,15,17	0.86	0
4	MAN	G	7	4	11,11,12	0.54	0	15,15,17	0.99	1 (6%)
4	MAN	G	8	4	11,11,12	0.59	0	15,15,17	0.53	0
4	MAN	G	9	4	11,11,12	0.74	0	15,15,17	0.79	0
5	NAG	H	1	5,1	14,14,15	0.76	1 (7%)	17,19,21	0.81	0
5	MAN	H	10	5	11,11,12	0.58	0	15,15,17	0.92	1 (6%)
5	NAG	H	2	5	14,14,15	0.44	0	17,19,21	1.07	0
5	BMA	H	3	5	11,11,12	0.42	0	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	H	4	5	11,11,12	0.57	0	15,15,17	1.17	2 (13%)
5	MAN	H	5	5	11,11,12	0.58	0	15,15,17	1.14	2 (13%)
5	MAN	H	6	5	11,11,12	0.53	0	15,15,17	0.71	0
5	MAN	H	7	5	11,11,12	0.64	0	15,15,17	1.28	1 (6%)
5	MAN	H	8	5	11,11,12	0.52	0	15,15,17	0.84	0
5	MAN	H	9	5	11,11,12	0.61	0	15,15,17	0.68	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	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	GUP	C	10	2	-	0/2/19/22	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	F	10	3	-	0/2/19/22	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	2/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	MAN	F	8	3	-	0/2/19/22	0/1/1/1
3	MAN	F	9	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	MAN	G	10	4	-	2/2/19/22	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
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	8	4	-	1/2/19/22	0/1/1/1
4	MAN	G	9	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	MAN	H	10	5	-	1/2/19/22	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
5	MAN	H	9	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-2.24	1.39	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	10	BMA	C1-O5-C5	4.71	118.50	112.19
5	H	7	MAN	C1-O5-C5	3.71	117.16	112.19
3	F	10	BMA	C1-C2-C3	3.43	114.64	109.64
2	C	5	MAN	C1-O5-C5	3.37	116.70	112.19
2	C	9	MAN	O2-C2-C1	-3.32	101.61	109.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

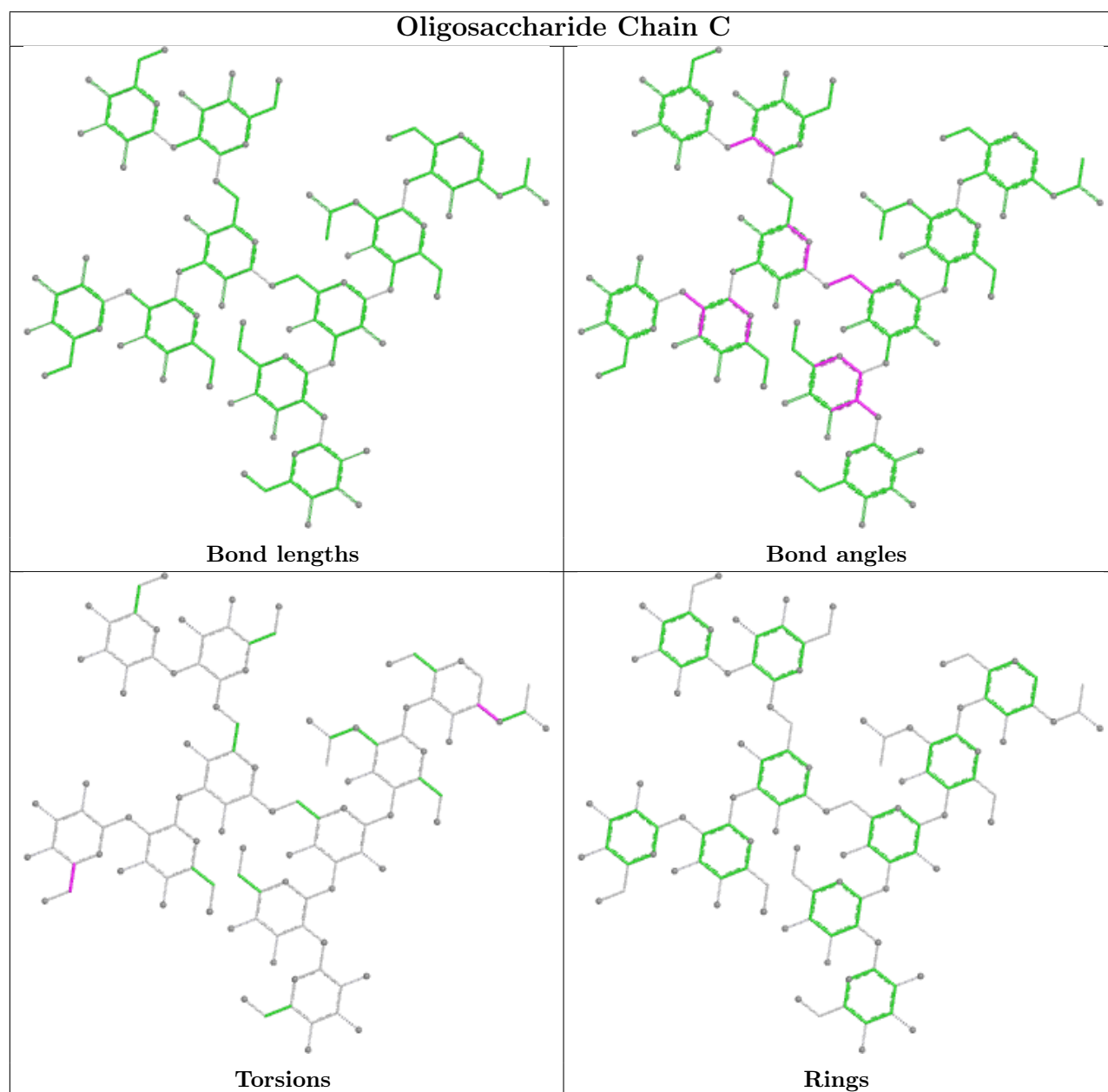
Mol	Chain	Res	Type	Atoms
4	G	10	MAN	O5-C5-C6-O6
4	G	10	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
3	F	6	MAN	C4-C5-C6-O6
4	G	6	MAN	C4-C5-C6-O6

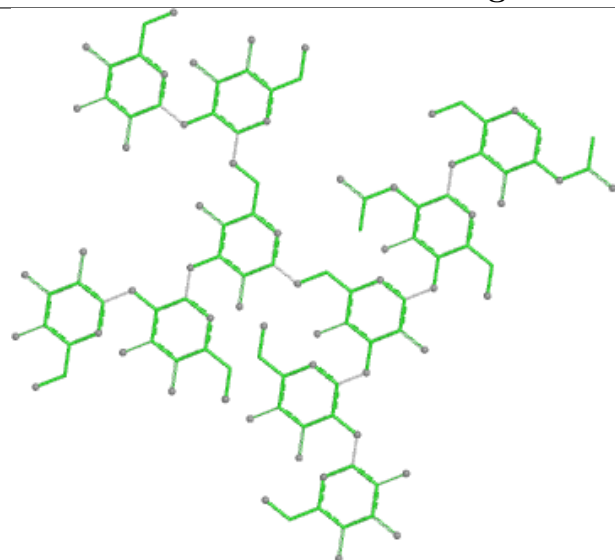
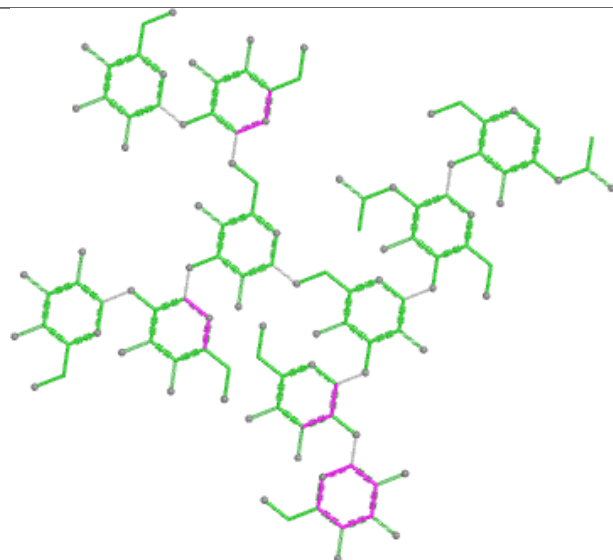
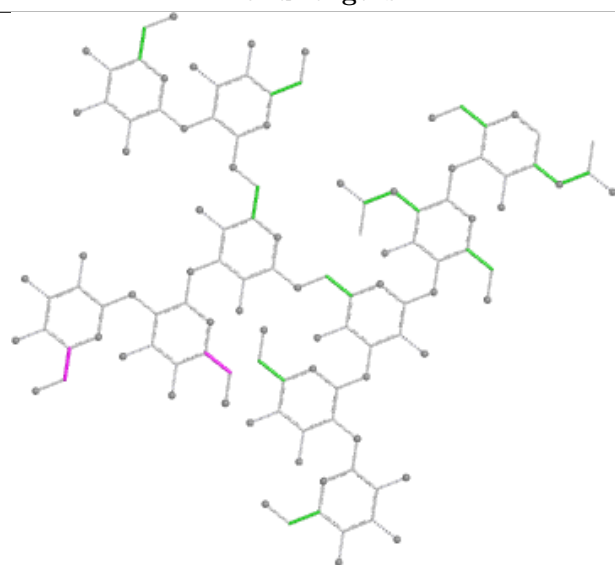
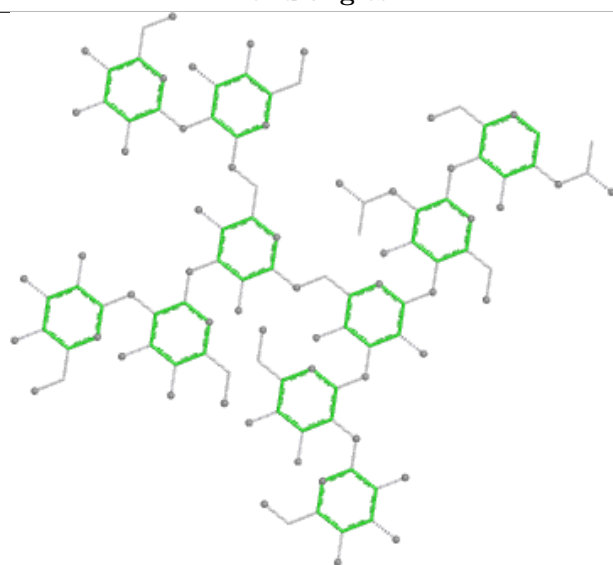
There are no ring outliers.

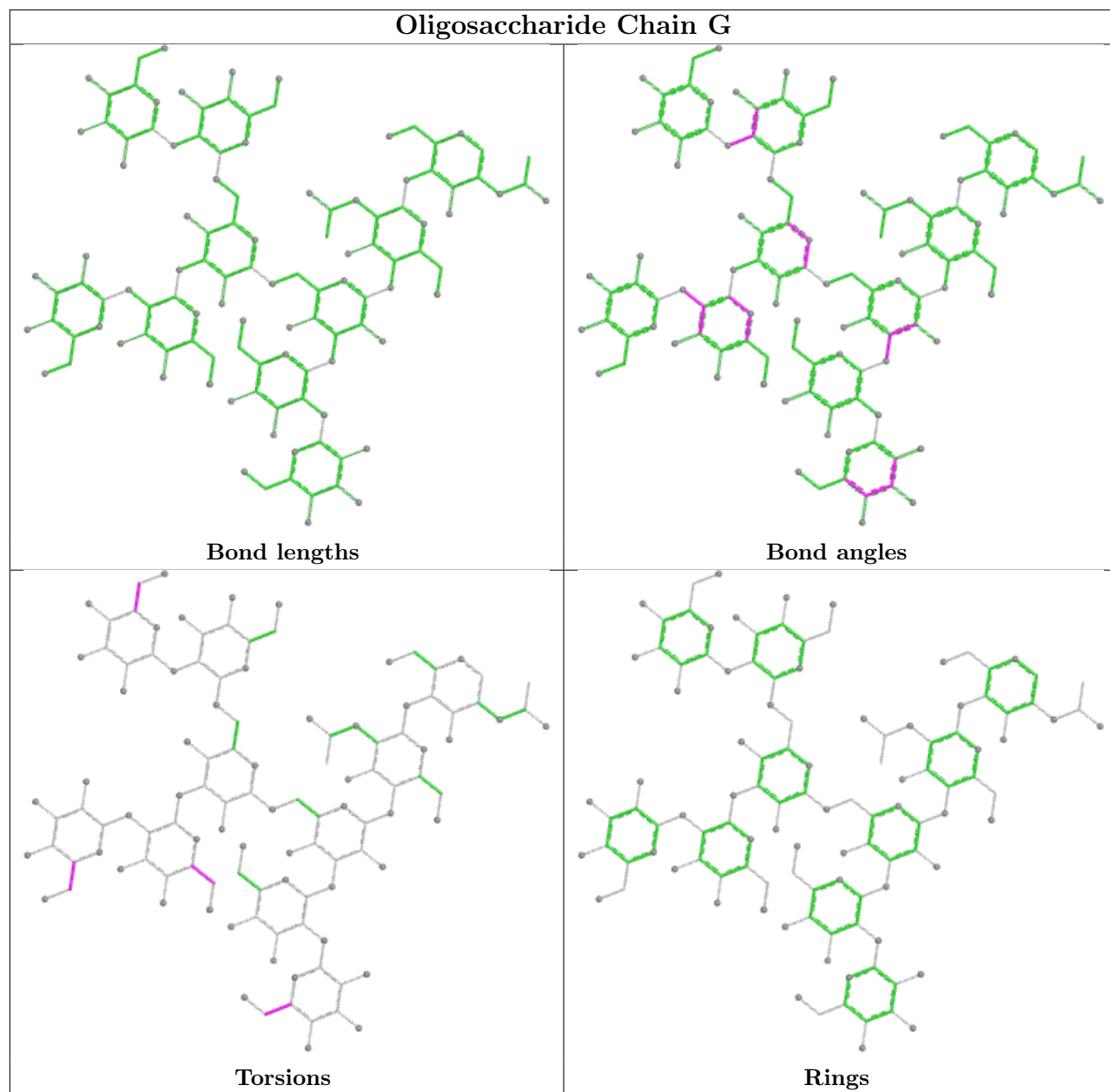
4 monomers are involved in 5 short contacts:

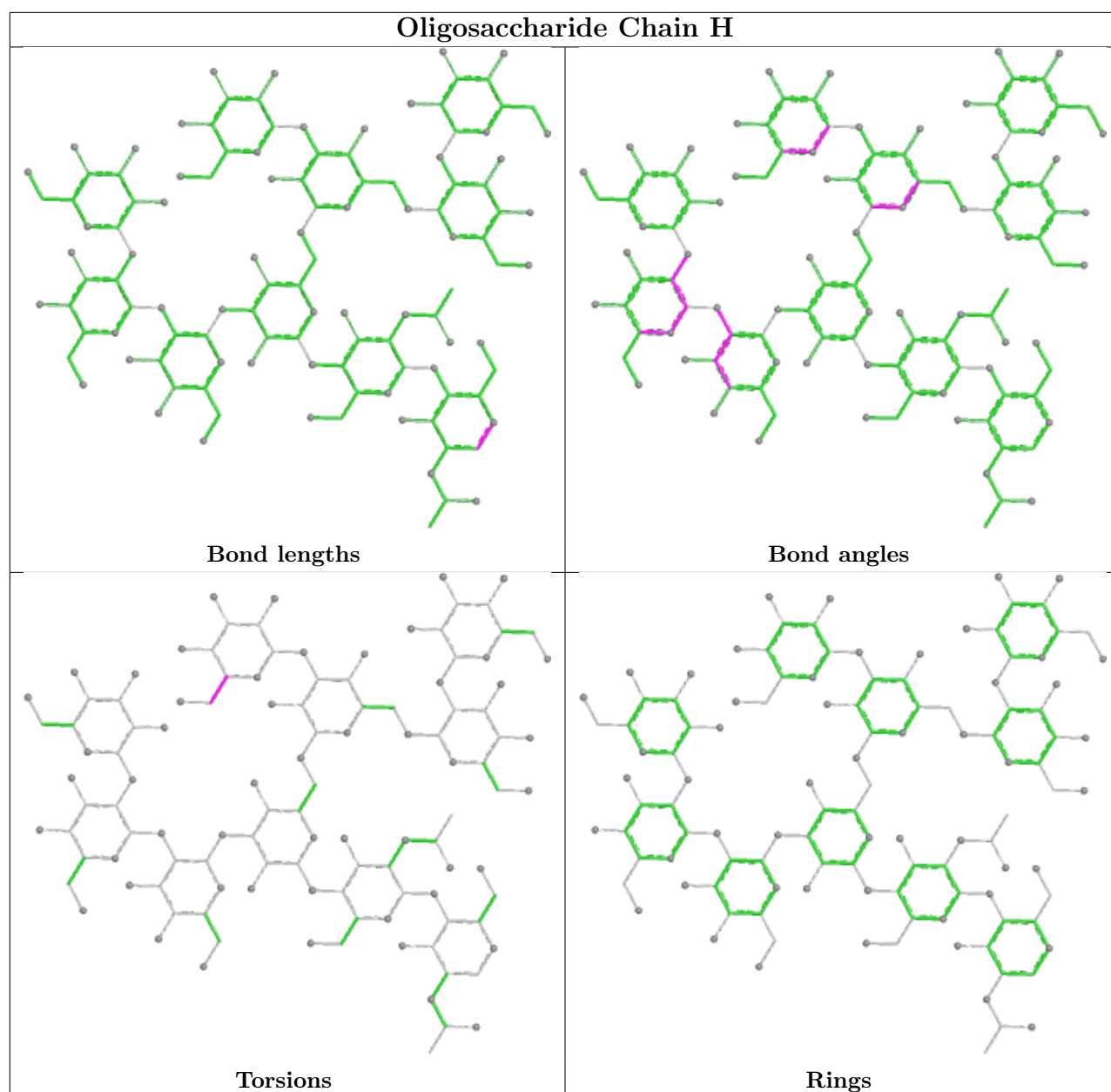
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
2	C	8	MAN	1	0
5	H	1	NAG	1	0
5	H	10	MAN	2	0

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 F**Bond lengths****Bond angles****Torsions****Rings**





5.6 Ligand geometry [i](#)

10 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
8	MPD	B	2	-	7,7,7	0.37	0	9,10,10	0.72	0
9	BMA	E	661	-	12,12,12	0.57	0	17,17,17	1.85	4 (23%)
6	NAG	A	650	1	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
8	MPD	E	4	-	7,7,7	0.26	0	9,10,10	0.54	0
6	NAG	B	650	1	14,14,15	0.54	0	17,19,21	0.84	0
7	MRD	E	5	-	7,7,7	0.27	0	9,10,10	0.19	0
7	MRD	D	3	-	7,7,7	0.32	0	9,10,10	0.75	0
7	MRD	A	1	-	7,7,7	0.31	0	9,10,10	0.53	0
6	NAG	D	650	1	14,14,15	0.51	0	17,19,21	0.74	0
6	NAG	E	650	1	14,14,15	0.50	0	17,19,21	0.91	1 (5%)

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
8	MPD	B	2	-	-	2/5/5/5	-
9	BMA	E	661	-	-	0/2/22/22	0/1/1/1
6	NAG	A	650	1	1/1/5/7	4/6/23/26	0/1/1/1
8	MPD	E	4	-	-	3/5/5/5	-
6	NAG	B	650	1	-	2/6/23/26	0/1/1/1
7	MRD	E	5	-	-	0/5/5/5	-
7	MRD	D	3	-	-	5/5/5/5	-
7	MRD	A	1	-	-	2/5/5/5	-
6	NAG	D	650	1	-	2/6/23/26	0/1/1/1
6	NAG	E	650	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	661	BMA	O5-C1-C2	4.25	117.78	110.30
9	E	661	BMA	C1-O5-C5	3.93	121.26	113.65
6	A	650	NAG	C1-O5-C5	2.73	115.85	112.19
9	E	661	BMA	C3-C4-C5	-2.72	105.30	110.23
6	A	650	NAG	C8-C7-N2	2.50	120.27	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	650	NAG	C1

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	650	NAG	C8-C7-N2-C2
7	A	1	MRD	C2-C3-C4-C5
7	D	3	MRD	C2-C3-C4-C5
6	A	650	NAG	O7-C7-N2-C2
6	B	650	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2	MPD	1	0
9	E	661	BMA	3	0
6	A	650	NAG	1	0
8	E	4	MPD	1	0
7	D	3	MRD	3	0
7	A	1	MRD	1	0
6	D	650	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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(Å ²)	Q < 0.9
1	A	608/613 (99%)	0.31	24 (3%)	39 44	6, 13, 27, 36	2 (0%)
1	B	609/613 (99%)	0.21	21 (3%)	45 50	5, 12, 24, 34	3 (0%)
1	D	607/613 (99%)	0.24	24 (3%)	38 42	6, 13, 27, 33	1 (0%)
1	E	606/613 (98%)	0.17	19 (3%)	49 53	6, 12, 23, 30	6 (0%)
All	All	2430/2452 (99%)	0.23	88 (3%)	42 47	5, 12, 26, 36	12 (0%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	9.2
1	E	23	LEU	8.0
1	D	633	THR	7.7
1	D	23	LEU	7.5
1	A	23	LEU	7.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	MAN	G	10	11/12	0.47	0.34	40,42,43,44	0
2	GUP	C	10	11/12	0.62	0.31	34,36,38,39	0

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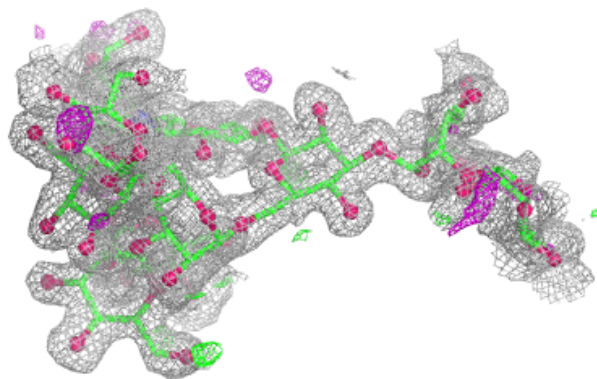
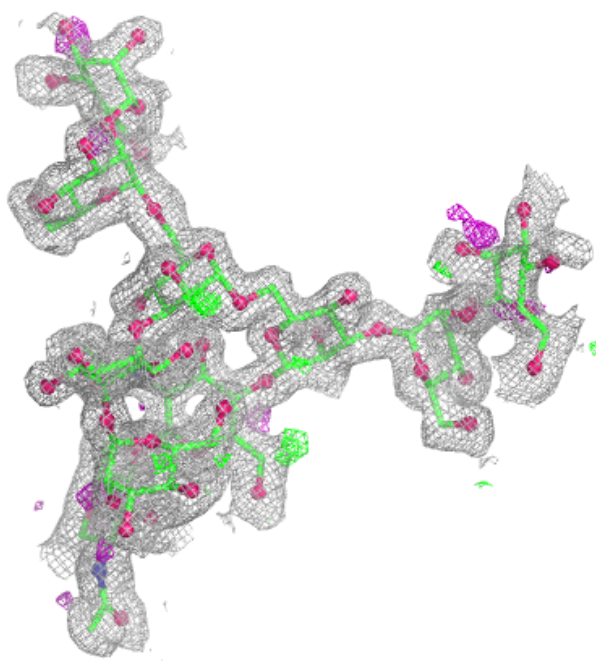
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	F	10	11/12	0.63	0.17	34,36,37,37	0
3	MAN	F	6	11/12	0.67	0.24	37,40,41,41	0
2	MAN	C	8	11/12	0.69	0.23	26,28,29,31	0
4	MAN	G	8	11/12	0.72	0.21	31,32,34,34	0
4	MAN	G	9	11/12	0.76	0.14	29,32,34,36	0
3	MAN	F	5	11/12	0.79	0.14	28,31,33,34	0
3	MAN	F	9	11/12	0.80	0.13	23,27,30,30	0
4	MAN	G	6	11/12	0.80	0.19	32,34,36,36	0
4	MAN	G	7	11/12	0.80	0.16	27,28,29,29	0
3	MAN	F	8	11/12	0.82	0.15	26,26,28,29	0
2	MAN	C	9	11/12	0.83	0.18	22,23,26,29	0
2	MAN	C	6	11/12	0.83	0.16	28,30,32,33	0
2	MAN	C	7	11/12	0.84	0.11	22,23,25,26	0
3	NAG	F	2	14/15	0.86	0.12	11,13,18,19	0
4	MAN	G	5	11/12	0.87	0.10	24,26,29,29	0
3	MAN	F	7	11/12	0.87	0.13	18,20,21,23	0
2	MAN	C	5	11/12	0.88	0.17	20,21,23,26	0
3	MAN	F	4	11/12	0.89	0.10	15,17,20,23	0
4	MAN	G	4	11/12	0.89	0.09	19,21,23,24	0
5	MAN	H	9	11/12	0.89	0.12	15,18,20,20	0
2	MAN	C	4	11/12	0.90	0.09	18,19,20,21	0
3	NAG	F	1	14/15	0.91	0.11	11,13,19,19	0
5	MAN	H	6	11/12	0.91	0.12	15,16,18,19	0
4	NAG	G	2	14/15	0.91	0.12	12,14,17,21	0
4	BMA	G	3	11/12	0.92	0.08	13,16,18,23	0
3	BMA	F	3	11/12	0.92	0.09	12,13,15,19	0
2	NAG	C	1	14/15	0.93	0.09	10,12,15,15	0
2	NAG	C	2	14/15	0.93	0.10	12,14,18,19	0
2	BMA	C	3	11/12	0.94	0.10	12,14,16,19	0
5	MAN	H	8	11/12	0.94	0.08	15,17,21,21	0
5	MAN	H	4	11/12	0.94	0.08	9,11,14,15	0
5	NAG	H	2	14/15	0.95	0.08	7,9,13,13	0
4	NAG	G	1	14/15	0.95	0.08	9,12,14,15	0
5	MAN	H	5	11/12	0.95	0.08	12,13,14,15	0
5	MAN	H	10	11/12	0.95	0.07	11,14,16,17	0
5	MAN	H	7	11/12	0.96	0.07	8,11,13,14	0
5	BMA	H	3	11/12	0.96	0.07	7,9,10,11	0
5	NAG	H	1	14/15	0.97	0.06	7,9,10,10	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

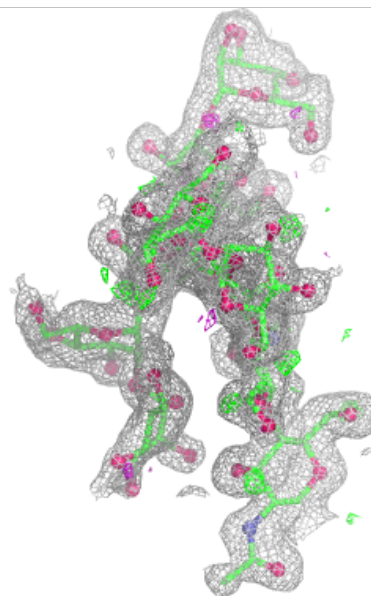
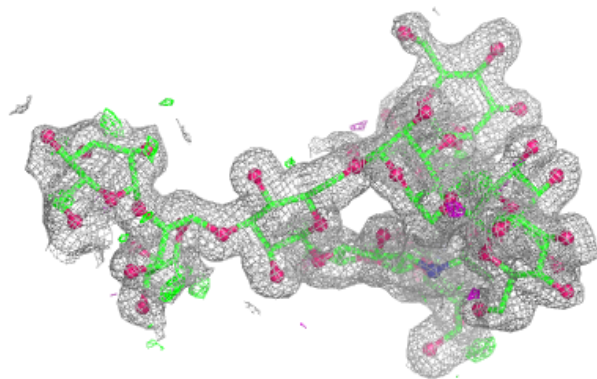
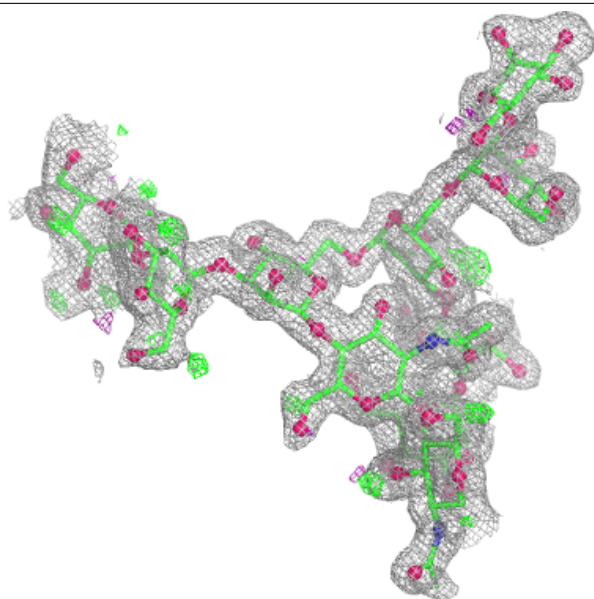
Electron density around Chain C:

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



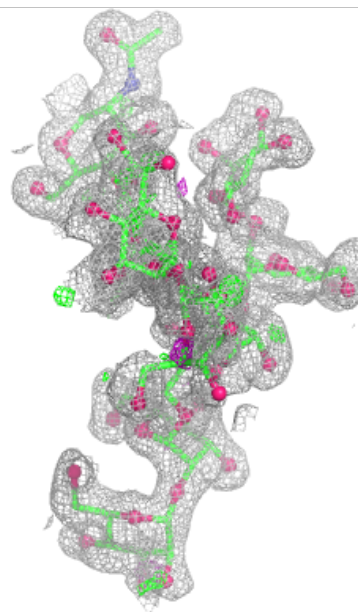
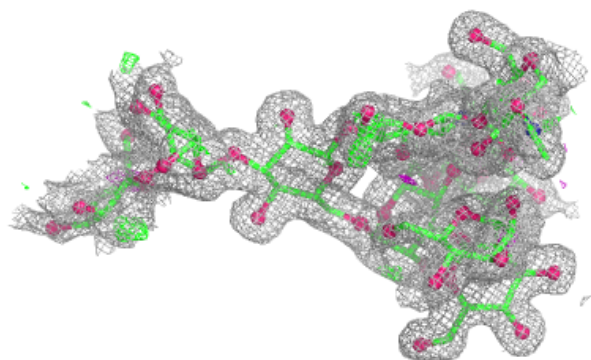
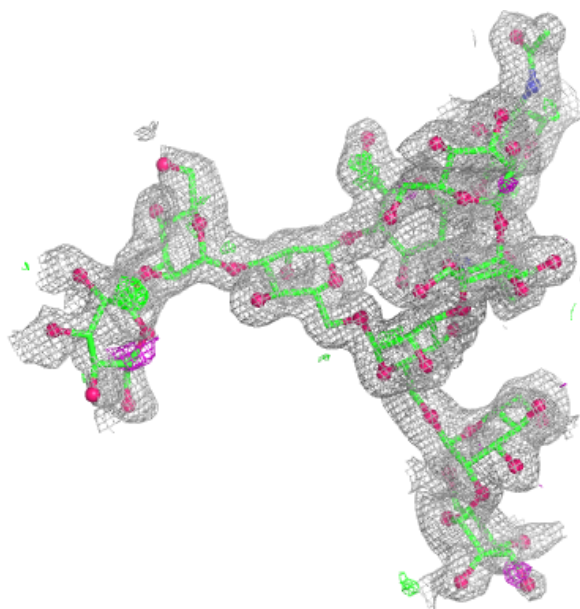
Electron density around Chain F:

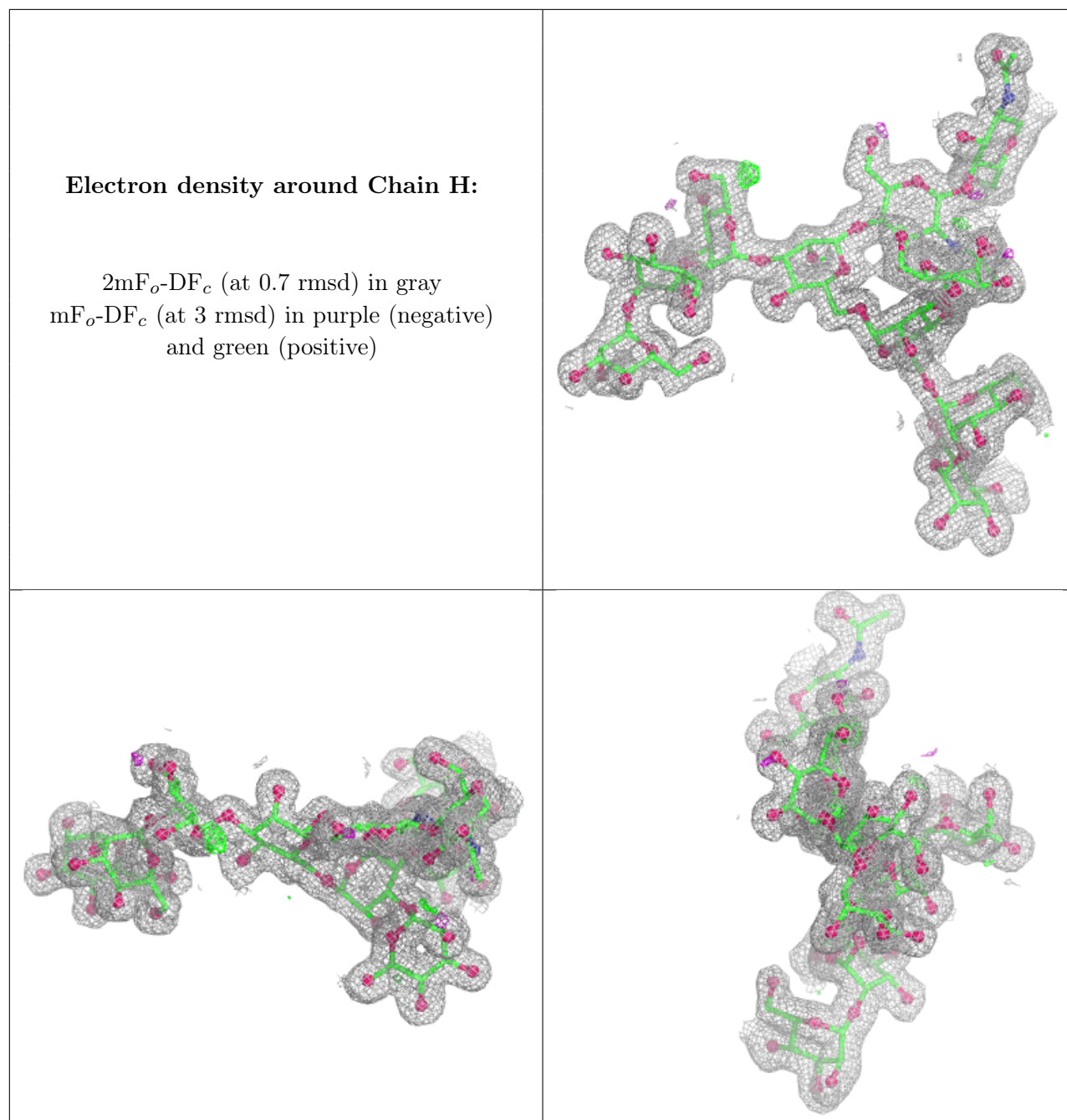
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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, 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
6	NAG	A	650	14/15	0.62	0.23	37,40,41,41	0
9	BMA	E	661	12/12	0.62	0.23	33,36,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MRD	E	5	8/8	0.72	0.20	36,36,37,38	0
6	NAG	D	650	14/15	0.75	0.24	31,33,35,36	0
6	NAG	E	650	14/15	0.78	0.19	24,30,34,34	0
6	NAG	B	650	14/15	0.81	0.16	20,22,24,25	0
7	MRD	A	1	8/8	0.82	0.17	23,26,27,28	0
8	MPD	E	4	8/8	0.86	0.16	24,26,28,29	0
8	MPD	B	2	8/8	0.86	0.13	20,23,25,27	0
7	MRD	D	3	8/8	0.87	0.16	25,27,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.