



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 02:05 PM EDT

PDB ID : 7LR6
Title : Crystal structure of GH5_18-E140A from Bifidobacterium longum subsp. longum ATCC 55813 in complex with Manb1-4GlcNAc
Authors : Higgins, M.A.; Ryan, K.S.
Deposited on : 2021-02-16
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

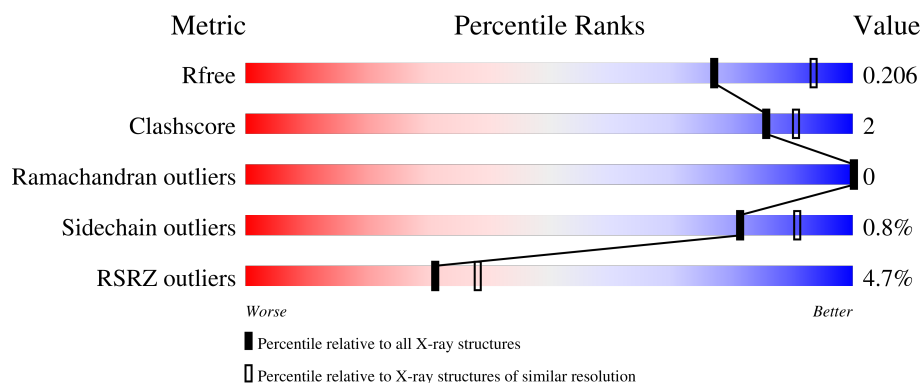
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.





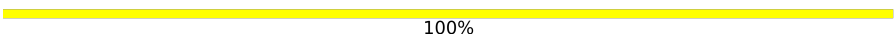
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	446	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	B	446	<div> <div>6%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	C	446	<div> <div>4%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	446	<div> <div>4%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 50% 50%
2	H	2	 50% 50%
2	I	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
3	PO4	A	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14124 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 Glycosyl hydrolase BlGH5_18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	1	0
			3320	2116	566	623	15			
1	B	424	Total	C	N	O	S	0	2	0
			3313	2111	565	622	15			
1	C	423	Total	C	N	O	S	0	1	0
			3309	2109	563	622	15			
1	D	423	Total	C	N	O	S	0	2	0
			3318	2114	566	623	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP C2GY91
A	-18	GLY	-	expression tag	UNP C2GY91
A	-17	SER	-	expression tag	UNP C2GY91
A	-16	SER	-	expression tag	UNP C2GY91
A	-15	HIS	-	expression tag	UNP C2GY91
A	-14	HIS	-	expression tag	UNP C2GY91
A	-13	HIS	-	expression tag	UNP C2GY91
A	-12	HIS	-	expression tag	UNP C2GY91
A	-11	HIS	-	expression tag	UNP C2GY91
A	-10	HIS	-	expression tag	UNP C2GY91
A	-9	SER	-	expression tag	UNP C2GY91
A	-8	SER	-	expression tag	UNP C2GY91
A	-7	GLY	-	expression tag	UNP C2GY91
A	-6	LEU	-	expression tag	UNP C2GY91
A	-5	VAL	-	expression tag	UNP C2GY91
A	-4	PRO	-	expression tag	UNP C2GY91
A	-3	ARG	-	expression tag	UNP C2GY91
A	-2	GLY	-	expression tag	UNP C2GY91
A	-1	SER	-	expression tag	UNP C2GY91
A	0	HIS	-	expression tag	UNP C2GY91
A	140	ALA	GLU	engineered mutation	UNP C2GY91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP C2GY91
B	-18	GLY	-	expression tag	UNP C2GY91
B	-17	SER	-	expression tag	UNP C2GY91
B	-16	SER	-	expression tag	UNP C2GY91
B	-15	HIS	-	expression tag	UNP C2GY91
B	-14	HIS	-	expression tag	UNP C2GY91
B	-13	HIS	-	expression tag	UNP C2GY91
B	-12	HIS	-	expression tag	UNP C2GY91
B	-11	HIS	-	expression tag	UNP C2GY91
B	-10	HIS	-	expression tag	UNP C2GY91
B	-9	SER	-	expression tag	UNP C2GY91
B	-8	SER	-	expression tag	UNP C2GY91
B	-7	GLY	-	expression tag	UNP C2GY91
B	-6	LEU	-	expression tag	UNP C2GY91
B	-5	VAL	-	expression tag	UNP C2GY91
B	-4	PRO	-	expression tag	UNP C2GY91
B	-3	ARG	-	expression tag	UNP C2GY91
B	-2	GLY	-	expression tag	UNP C2GY91
B	-1	SER	-	expression tag	UNP C2GY91
B	0	HIS	-	expression tag	UNP C2GY91
B	140	ALA	GLU	engineered mutation	UNP C2GY91
C	-19	MET	-	initiating methionine	UNP C2GY91
C	-18	GLY	-	expression tag	UNP C2GY91
C	-17	SER	-	expression tag	UNP C2GY91
C	-16	SER	-	expression tag	UNP C2GY91
C	-15	HIS	-	expression tag	UNP C2GY91
C	-14	HIS	-	expression tag	UNP C2GY91
C	-13	HIS	-	expression tag	UNP C2GY91
C	-12	HIS	-	expression tag	UNP C2GY91
C	-11	HIS	-	expression tag	UNP C2GY91
C	-10	HIS	-	expression tag	UNP C2GY91
C	-9	SER	-	expression tag	UNP C2GY91
C	-8	SER	-	expression tag	UNP C2GY91
C	-7	GLY	-	expression tag	UNP C2GY91
C	-6	LEU	-	expression tag	UNP C2GY91
C	-5	VAL	-	expression tag	UNP C2GY91
C	-4	PRO	-	expression tag	UNP C2GY91
C	-3	ARG	-	expression tag	UNP C2GY91
C	-2	GLY	-	expression tag	UNP C2GY91
C	-1	SER	-	expression tag	UNP C2GY91
C	0	HIS	-	expression tag	UNP C2GY91
C	140	ALA	GLU	engineered mutation	UNP C2GY91

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP C2GY91
D	-18	GLY	-	expression tag	UNP C2GY91
D	-17	SER	-	expression tag	UNP C2GY91
D	-16	SER	-	expression tag	UNP C2GY91
D	-15	HIS	-	expression tag	UNP C2GY91
D	-14	HIS	-	expression tag	UNP C2GY91
D	-13	HIS	-	expression tag	UNP C2GY91
D	-12	HIS	-	expression tag	UNP C2GY91
D	-11	HIS	-	expression tag	UNP C2GY91
D	-10	HIS	-	expression tag	UNP C2GY91
D	-9	SER	-	expression tag	UNP C2GY91
D	-8	SER	-	expression tag	UNP C2GY91
D	-7	GLY	-	expression tag	UNP C2GY91
D	-6	LEU	-	expression tag	UNP C2GY91
D	-5	VAL	-	expression tag	UNP C2GY91
D	-4	PRO	-	expression tag	UNP C2GY91
D	-3	ARG	-	expression tag	UNP C2GY91
D	-2	GLY	-	expression tag	UNP C2GY91
D	-1	SER	-	expression tag	UNP C2GY91
D	0	HIS	-	expression tag	UNP C2GY91
D	140	ALA	GLU	engineered mutation	UNP C2GY91

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	G	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	H	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	I	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		

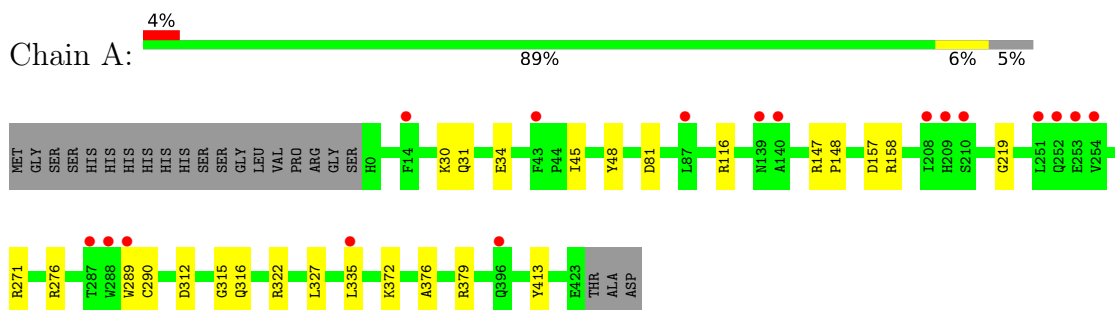
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		
4	B	146	Total	O	0	0
			146	146		
4	C	180	Total	O	0	0
			180	180		
4	D	161	Total	O	0	0
			161	161		

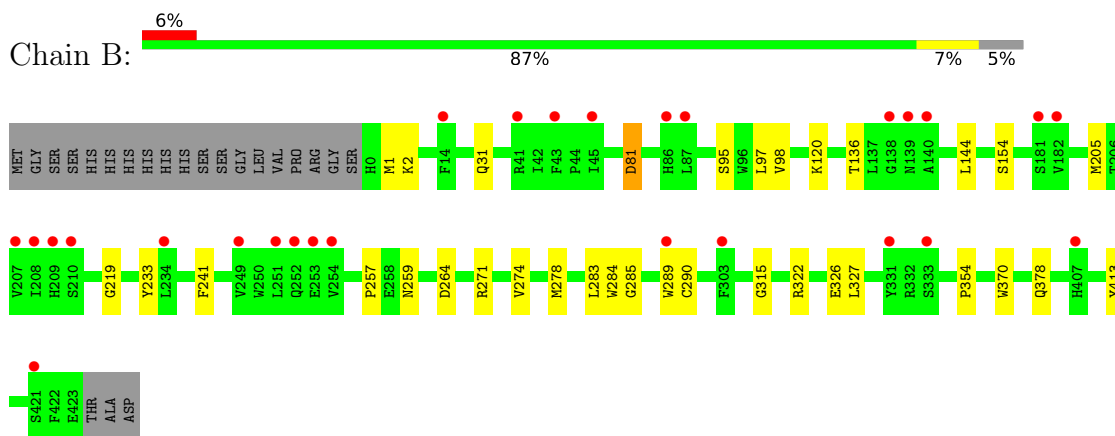
3 Residue-property plots [i](#)

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.

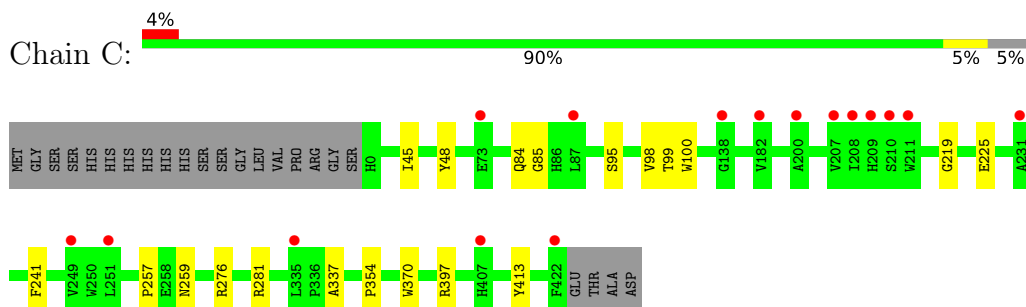
- Molecule 1: Glycosyl hydrolase BIGH5_18




- Molecule 1: Glycosyl hydrolase BIGH5_18

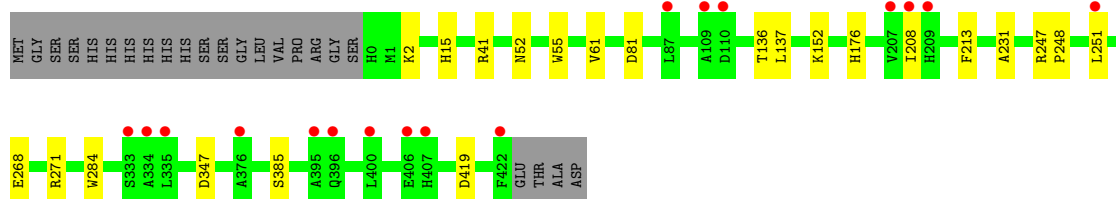


- Molecule 1: Glycosyl hydrolase BIGH5_18



- Molecule 1: Glycosyl hydrolase BIGH5_18

Chain D:  4% 90% 5% 5%



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

Chain E:  100%

MAG1
BMA2

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

Chain G:  50% 50%

MAG1
BMA2

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

Chain H:  50% 50%

MAG1
BMA2

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

Chain I:  100%

MAG1
BMA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.26Å 142.99Å 157.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.30 39.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.36-2.30) 99.1 (39.36-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.161 , 0.206 0.161 , 0.206	Depositor DCC
R_{free} test set	5139 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14124	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PO4, BMA, 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	0.44	1/3424 (0.0%)	0.56	1/4675 (0.0%)
1	B	0.40	0/3417	0.56	0/4669
1	C	0.42	0/3413	0.55	0/4662
1	D	0.42	0/3422	0.55	0/4674
All	All	0.42	1/13676 (0.0%)	0.56	1/18680 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	LYS	CE-NZ	5.25	1.62	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LYS	CD-CE-NZ	-5.21	99.71	111.70

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	3320	0	3143	13	0
1	B	3313	0	3118	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3309	0	3123	11	0
1	D	3318	0	3132	16	0
2	E	26	0	24	0	0
2	G	26	0	24	0	0
2	H	26	0	24	0	0
2	I	26	0	24	2	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	A	198	0	0	2	0
4	B	146	0	0	0	0
4	C	180	0	0	1	0
4	D	161	0	0	7	0
All	All	14124	0	12612	58	0

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

All (58) 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:147:ARG:HG2	1:A:148:PRO:HA	1.70	0.73
1:B:322:ARG:O	1:B:326:GLU:HG3	1.93	0.68
1:D:419:ASP:OD2	4:D:601:HOH:O	2.11	0.68
1:B:274:VAL:O	1:B:278:MET:HG3	2.00	0.61
1:A:376:ALA:HB2	4:A:625:HOH:O	2.00	0.61
4:D:700:HOH:O	2:I:1:NAG:H1	2.01	0.59
1:D:61:VAL:HG11	4:D:718:HOH:O	2.04	0.57
1:A:271:ARG:HA	1:A:327:LEU:HD11	1.87	0.56
1:C:397:ARG:NH1	4:C:602:HOH:O	2.37	0.56
1:A:322:ARG:NE	1:B:378:GLN:OE1	2.38	0.51
4:D:711:HOH:O	2:I:1:NAG:O6	2.19	0.51
1:C:95:SER:HA	1:C:98:VAL:HG22	1.93	0.50
1:D:15:HIS:ND1	4:D:604:HOH:O	2.35	0.50
1:D:268:GLU:OE2	1:D:271:ARG:NH2	2.40	0.50
1:D:81:ASP:OD2	1:D:136:THR:HB	2.13	0.49
1:B:271:ARG:HA	1:B:327:LEU:HD11	1.95	0.49
1:B:257:PRO:HB2	1:B:259:ASN:OD1	2.13	0.49
1:B:95:SER:HA	1:B:98:VAL:HG22	1.95	0.48
1:A:31:GLN:NE2	1:A:315:GLY:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLY:HA3	1:C:413:TYR:CD2	2.49	0.47
1:A:276:ARG:NH1	4:A:609:HOH:O	2.48	0.47
1:C:281:ARG:HG3	1:C:337:ALA:O	2.15	0.46
1:D:208:ILE:HD11	1:D:251:LEU:HD13	1.98	0.46
1:B:1:MET:HE1	1:B:283:LEU:O	2.16	0.45
1:B:31:GLN:NE2	1:B:315:GLY:O	2.49	0.45
1:B:2:LYS:HD2	1:B:284:TRP:CZ2	2.51	0.45
1:D:231:ALA:HB1	1:D:251:LEU:HD21	1.99	0.45
1:B:289:TRP:CD1	1:B:290:CYS:HB3	2.52	0.45
1:D:41:ARG:NH2	1:D:81:ASP:OD1	2.50	0.44
1:B:219:GLY:HA3	1:B:413:TYR:CD1	2.53	0.44
1:B:1:MET:SD	1:B:285:GLY:HA2	2.57	0.44
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.83	0.44
1:C:99:THR:OG1	1:C:100:TRP:N	2.50	0.44
1:D:347:ASP:HA	1:D:385:SER:HB3	1.99	0.43
1:D:268:GLU:HG2	4:D:739:HOH:O	2.18	0.43
1:D:208:ILE:CD1	1:D:251:LEU:HD13	2.49	0.43
1:D:176:HIS:ND1	4:D:605:HOH:O	2.37	0.43
1:A:219:GLY:HA3	1:A:413:TYR:CD2	2.54	0.43
1:A:45:ILE:HB	1:A:48:TYR:CD2	2.53	0.43
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.81	0.42
1:B:233:TYR:HB2	1:B:370:TRP:CZ3	2.55	0.42
1:A:312:ASP:OD2	1:A:316:GLN:HB2	2.20	0.42
1:B:241:PHE:CE1	1:B:354:PRO:HG3	2.55	0.42
1:D:52:ASN:HB3	1:D:55:TRP:HB3	2.01	0.42
1:B:97:LEU:HD23	1:B:97:LEU:HA	1.91	0.41
1:C:225:GLU:HG3	1:C:276:ARG:HH21	1.85	0.41
1:A:289:TRP:CD1	1:A:290:CYS:HB3	2.55	0.41
1:C:84:GLN:HA	1:C:85:GLY:HA3	1.82	0.41
1:B:289:TRP:HA	1:B:290:CYS:HA	1.80	0.41
1:C:233:TYR:HB2	1:C:370:TRP:CZ3	2.56	0.41
1:C:241:PHE:CZ	1:C:354:PRO:HG3	2.56	0.41
1:D:247:ARG:HA	1:D:248:PRO:HD3	1.98	0.41
1:B:81:ASP:HA	1:B:136:THR:O	2.21	0.40
1:A:157:ASP:OD1	1:A:158:ARG:N	2.54	0.40
1:A:30:LYS:HE3	1:A:34:GLU:OE2	2.21	0.40
1:C:257:PRO:HB2	1:C:259:ASN:OD1	2.21	0.40
1:C:45:ILE:HB	1:C:48:TYR:CD2	2.56	0.40
1:D:2:LYS:HE3	1:D:284:TRP:CZ2	2.56	0.40

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	423/446 (95%)	414 (98%)	9 (2%)	0	100	100
1	B	424/446 (95%)	416 (98%)	8 (2%)	0	100	100
1	C	422/446 (95%)	415 (98%)	7 (2%)	0	100	100
1	D	423/446 (95%)	415 (98%)	8 (2%)	0	100	100
All	All	1692/1784 (95%)	1660 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	346/367 (94%)	343 (99%)	3 (1%)	78	89
1	B	343/367 (94%)	337 (98%)	6 (2%)	60	76
1	C	344/367 (94%)	344 (100%)	0	100	100
1	D	345/367 (94%)	343 (99%)	2 (1%)	86	94
All	All	1378/1468 (94%)	1367 (99%)	11 (1%)	81	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	116	ARG

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Mol	Chain	Res	Type
1	A	379	ARG
1	B	81	ASP
1	B	120	LYS
1	B	144	LEU
1	B	154	SER
1	B	205	MET
1	B	264	ASP
1	D	152	LYS
1	D	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 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	15,15,15	0.29	0	21,21,21	0.80	1 (4%)
2	BMA	E	2	2	11,11,12	1.50	2 (18%)	15,15,17	1.00	1 (6%)
2	NAG	G	1	2	15,15,15	0.24	0	21,21,21	0.52	0
2	BMA	G	2	2	11,11,12	1.54	3 (27%)	15,15,17	1.17	1 (6%)
2	NAG	H	1	2	15,15,15	0.31	0	21,21,21	0.46	0
2	BMA	H	2	2	11,11,12	1.54	3 (27%)	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	2	15,15,15	0.48	0	21,21,21	0.81	0
2	BMA	I	2	2	11,11,12	1.30	2 (18%)	15,15,17	0.95	1 (6%)

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	-	2/6/26/26	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	1/1/1/1
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	BMA	G	2	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2	-	0/6/26/26	0/1/1/1
2	BMA	H	2	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	BMA	I	2	2	-	0/2/19/22	1/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	BMA	C1-C2	3.22	1.59	1.52
2	I	2	BMA	C1-C2	3.11	1.59	1.52
2	G	2	BMA	C2-C3	3.02	1.57	1.52
2	E	2	BMA	C1-C2	2.91	1.58	1.52
2	E	2	BMA	C4-C3	2.61	1.59	1.52
2	G	2	BMA	C1-C2	2.49	1.57	1.52
2	I	2	BMA	C4-C3	2.37	1.58	1.52
2	H	2	BMA	C2-C3	2.23	1.55	1.52
2	H	2	BMA	C4-C3	2.18	1.57	1.52
2	G	2	BMA	C4-C3	2.17	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	BMA	C1-O5-C5	3.53	116.97	112.19
2	H	2	BMA	C1-O5-C5	2.92	116.15	112.19
2	I	2	BMA	C1-O5-C5	2.63	115.76	112.19
2	E	2	BMA	C1-O5-C5	2.50	115.58	112.19
2	H	2	BMA	O2-C2-C1	2.37	114.00	109.15
2	E	1	NAG	O4-C4-C3	-2.07	105.56	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

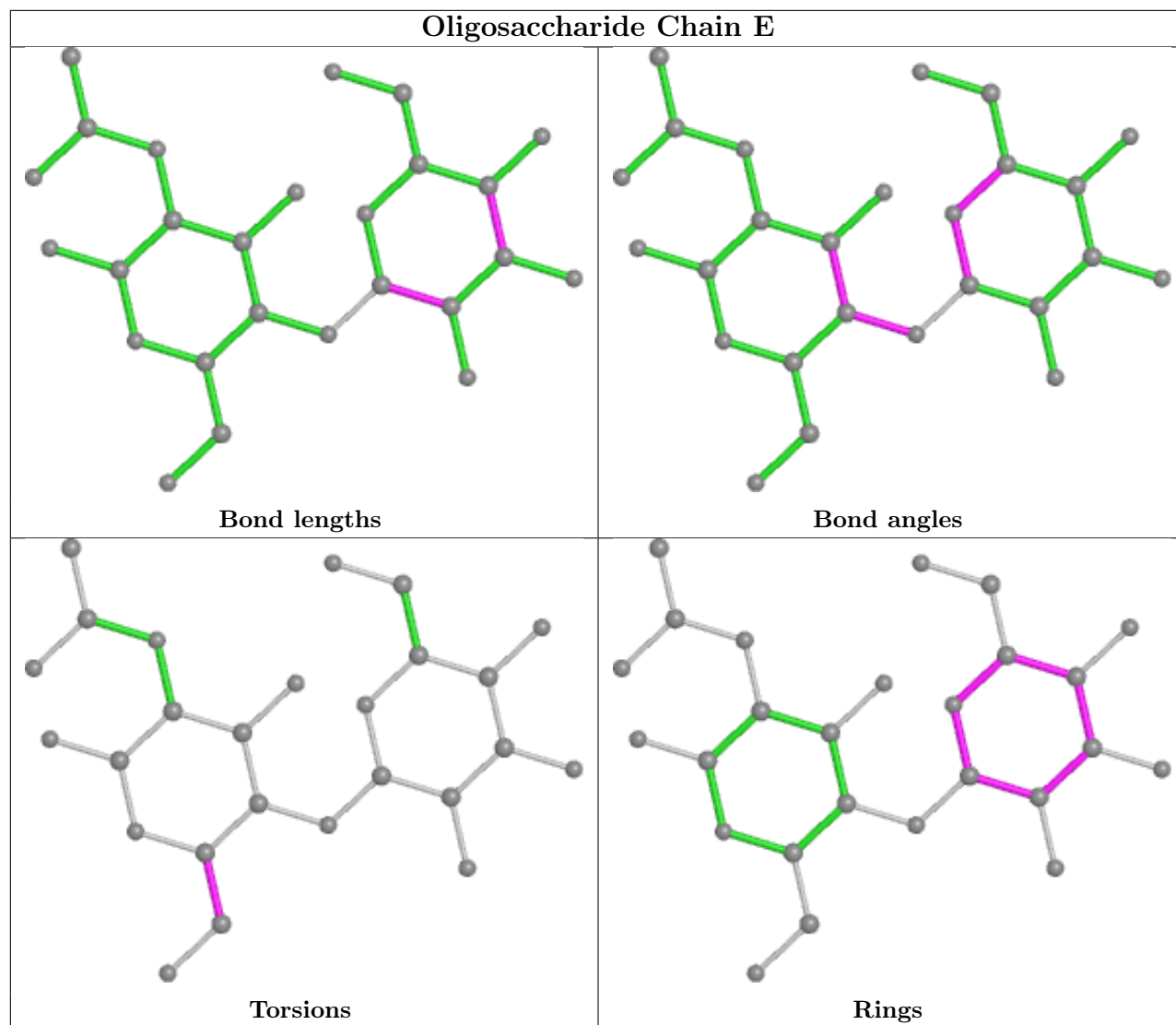
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	BMA	C1-C2-C3-C4-C5-O5
2	I	2	BMA	C1-C2-C3-C4-C5-O5

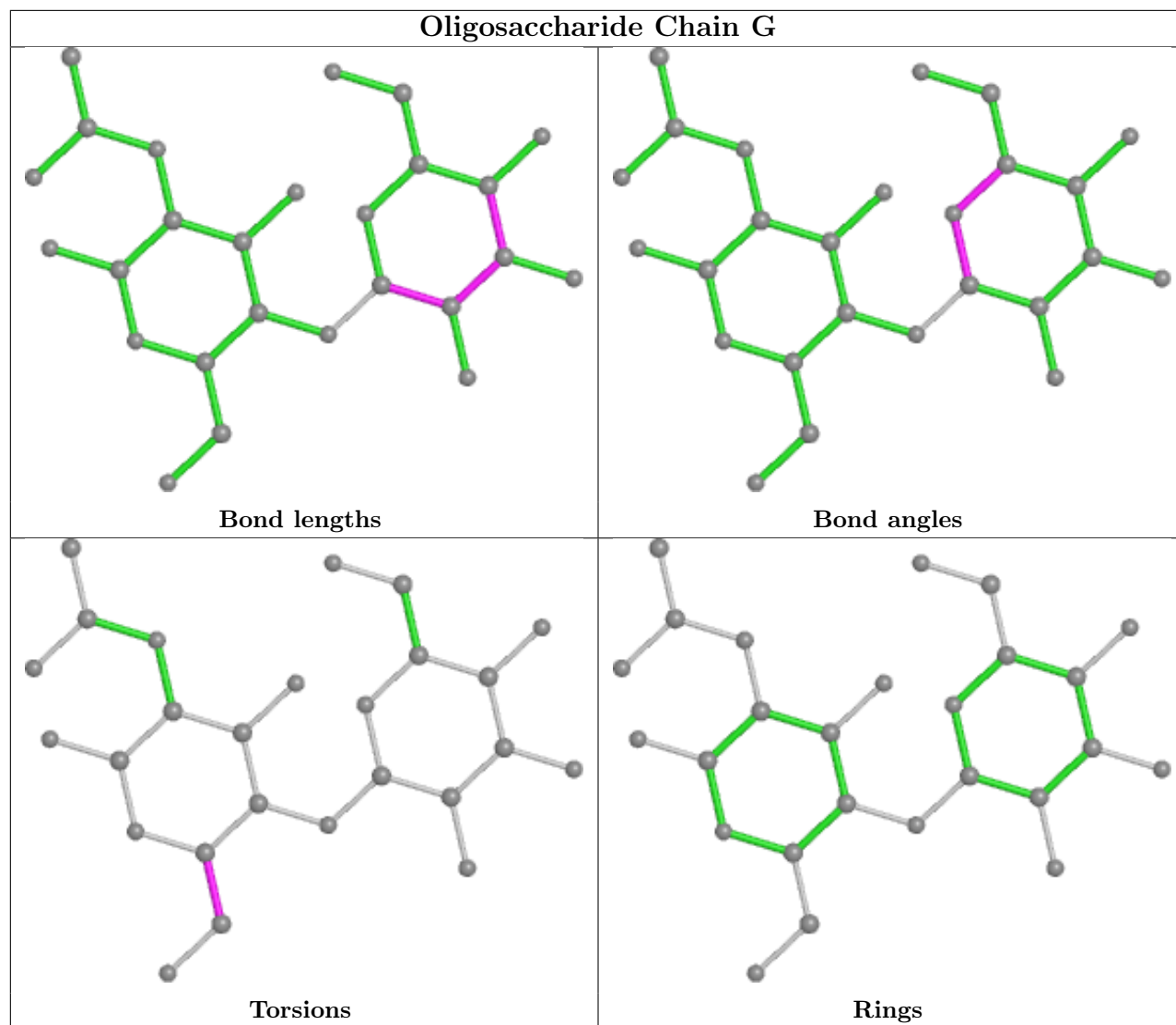
1 monomer is involved in 2 short contacts:

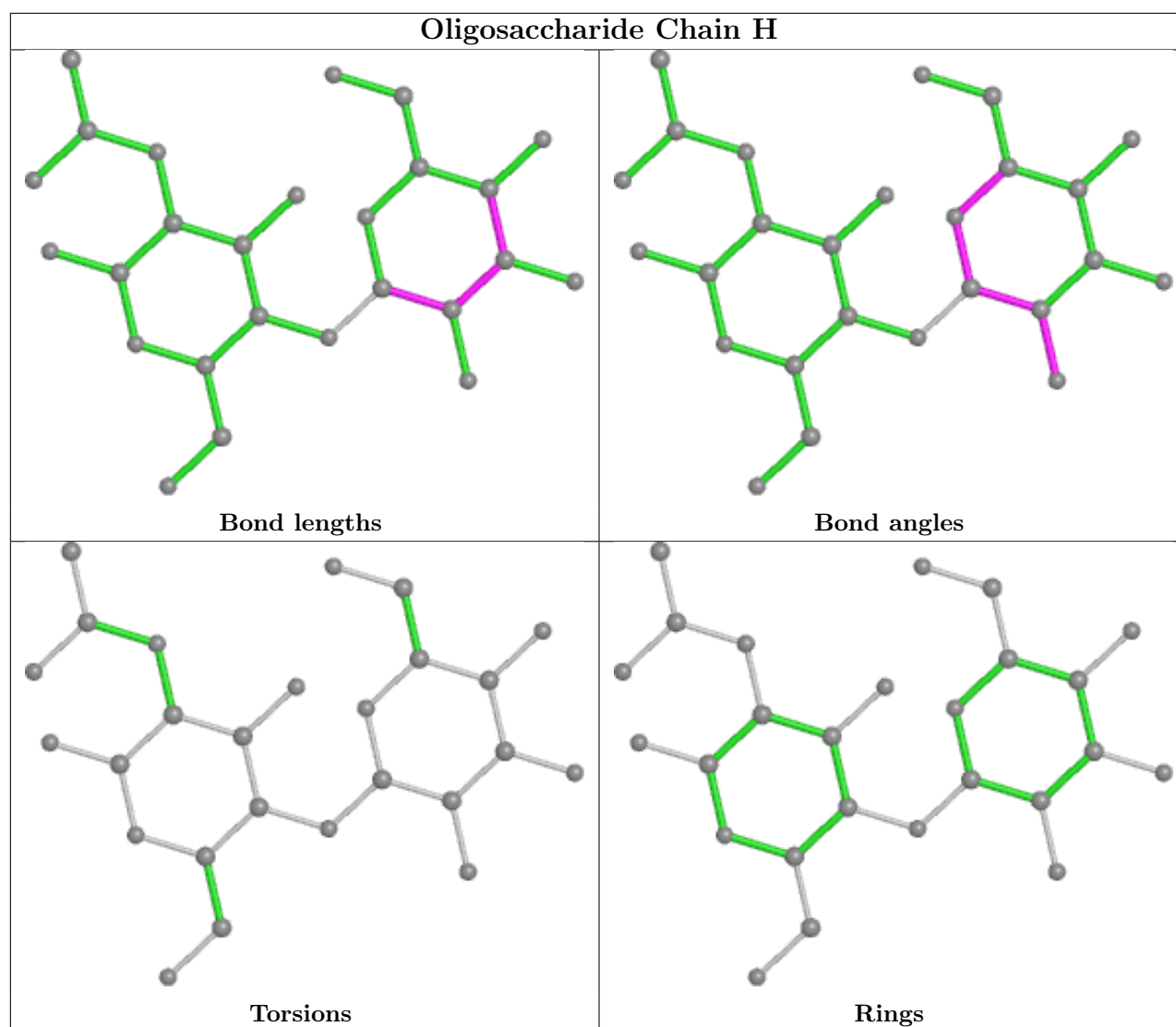
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	2	0

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 G





5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
3	PO4	D	503	-	4,4,4	0.83	0	6,6,6	0.64	0
3	PO4	D	504	-	4,4,4	0.94	0	6,6,6	0.51	0
3	PO4	C	501	-	4,4,4	0.89	0	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	B	501	-	4,4,4	0.84	0	6,6,6	0.52	0
3	PO4	A	504	-	4,4,4	0.85	0	6,6,6	0.42	0
3	PO4	A	503	-	4,4,4	1.00	0	6,6,6	0.41	0
3	PO4	C	502	-	4,4,4	0.75	0	6,6,6	0.61	0
3	PO4	A	502	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	A	501	-	4,4,4	0.81	0	6,6,6	0.59	0
3	PO4	D	501	-	4,4,4	0.84	0	6,6,6	0.65	0
3	PO4	D	502	-	4,4,4	0.86	0	6,6,6	0.59	0
3	PO4	C	503	-	4,4,4	0.83	0	6,6,6	0.46	0
3	PO4	B	502	-	4,4,4	0.86	0	6,6,6	0.59	0
3	PO4	B	503	-	4,4,4	0.85	0	6,6,6	0.41	0
3	PO4	C	504	-	4,4,4	0.88	0	6,6,6	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	424/446 (95%)	0.00	17 (4%)	38 45	33, 45, 66, 105	0
1	B	424/446 (95%)	0.14	27 (6%)	19 25	35, 49, 72, 113	0
1	C	423/446 (94%)	0.01	18 (4%)	35 42	33, 44, 69, 110	0
1	D	423/446 (94%)	0.03	17 (4%)	38 45	32, 47, 72, 108	0
All	All	1694/1784 (94%)	0.05	79 (4%)	31 38	32, 46, 71, 113	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	335	LEU	4.4
1	B	209	HIS	4.3
1	A	87	LEU	4.0
1	C	207	VAL	3.8
1	A	208	ILE	3.7
1	B	208	ILE	3.6
1	B	234	LEU	3.4
1	B	87	LEU	3.4
1	A	254	VAL	3.3
1	C	208	ILE	3.3
1	A	289	TRP	3.2
1	B	210	SER	3.0
1	D	422	PHE	3.0
1	C	234	LEU	2.9
1	B	254	VAL	2.9
1	B	333	SER	2.9
1	A	209	HIS	2.9
1	B	139	ASN	2.8
1	D	334	ALA	2.8
1	B	303	PHE	2.8
1	C	251	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASN	2.8
1	B	207	VAL	2.7
1	B	43	PHE	2.6
1	A	210	SER	2.6
1	D	208	ILE	2.6
1	B	182	VAL	2.6
1	C	249	VAL	2.6
1	D	400	LEU	2.6
1	B	252	GLN	2.6
1	A	140	ALA	2.5
1	B	45	ILE	2.5
1	D	396	GLN	2.5
1	A	251	LEU	2.5
1	C	422	PHE	2.5
1	B	138	GLY	2.5
1	B	140	ALA	2.5
1	C	210	SER	2.4
1	B	407	HIS	2.4
1	D	407	HIS	2.4
1	D	109	ALA	2.4
1	D	110	ASP	2.4
1	C	200	ALA	2.4
1	B	14	PHE	2.4
1	C	182	VAL	2.4
1	B	421	SER	2.4
1	B	86	HIS	2.3
1	C	238	ALA	2.3
1	B	249	VAL	2.3
1	B	251	LEU	2.2
1	B	331	TYR	2.2
1	A	14	PHE	2.2
1	C	209	HIS	2.2
1	D	209	HIS	2.2
1	A	43	PHE	2.2
1	D	395	ALA	2.2
1	A	252	GLN	2.2
1	A	287	THR	2.2
1	D	333	SER	2.2
1	C	335	LEU	2.1
1	C	231	ALA	2.1
1	B	289	TRP	2.1
1	C	73	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	2.1
1	A	253	GLU	2.1
1	A	288	TRP	2.1
1	C	211	TRP	2.1
1	B	181	SER	2.1
1	A	335	LEU	2.1
1	D	251	LEU	2.1
1	B	253	GLU	2.1
1	D	207	VAL	2.1
1	C	407	HIS	2.0
1	C	87	LEU	2.0
1	D	406	GLU	2.0
1	C	138	GLY	2.0
1	D	87	LEU	2.0
1	A	396	GLN	2.0
1	D	376	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

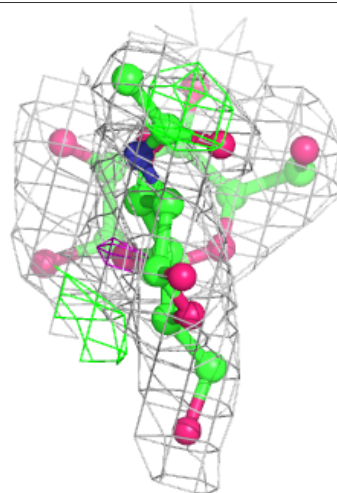
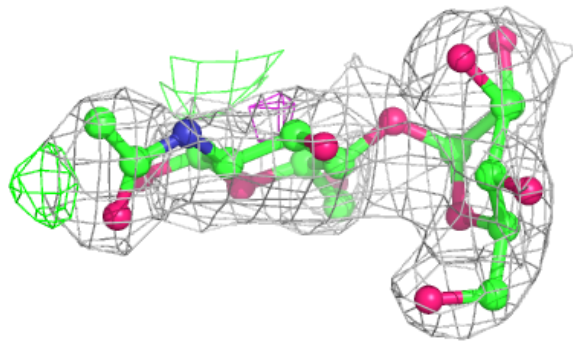
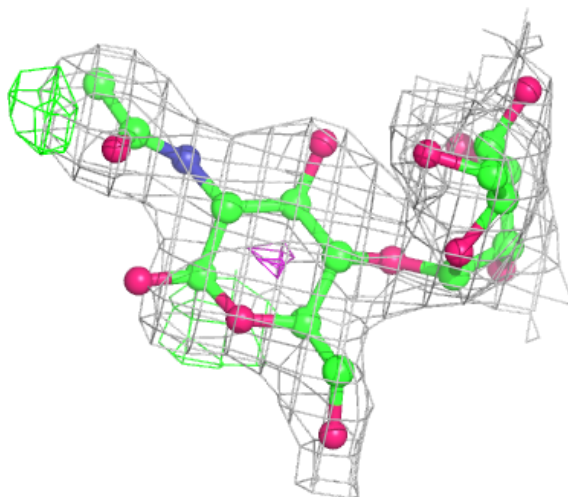
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	1	15/15	0.81	0.28	61,79,98,104	0
2	NAG	H	1	15/15	0.83	0.25	52,80,102,113	0
2	NAG	E	1	15/15	0.84	0.35	57,78,93,100	0
2	NAG	I	1	15/15	0.84	0.24	62,80,91,105	0
2	BMA	G	2	11/12	0.87	0.33	62,70,79,81	0
2	BMA	H	2	11/12	0.88	0.20	51,66,71,74	0
2	BMA	E	2	11/12	0.93	0.28	42,60,67,68	0
2	BMA	I	2	11/12	0.93	0.18	50,57,65,72	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.

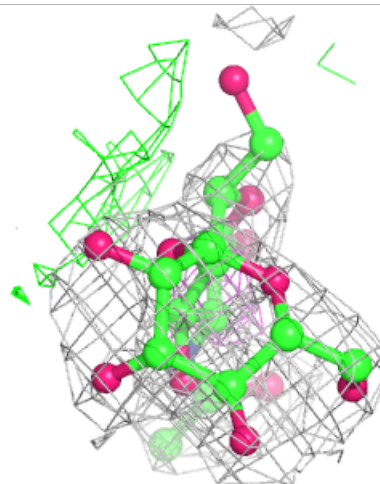
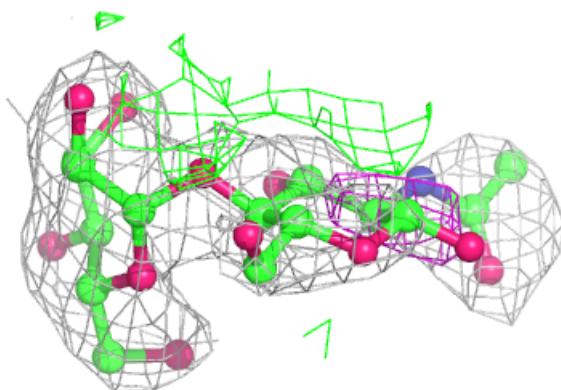
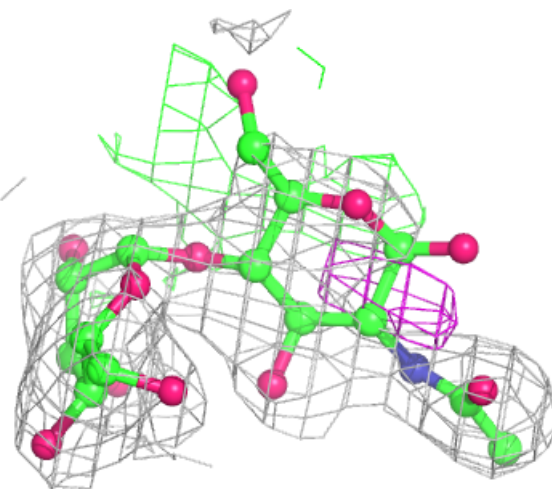
Electron density around Chain E:

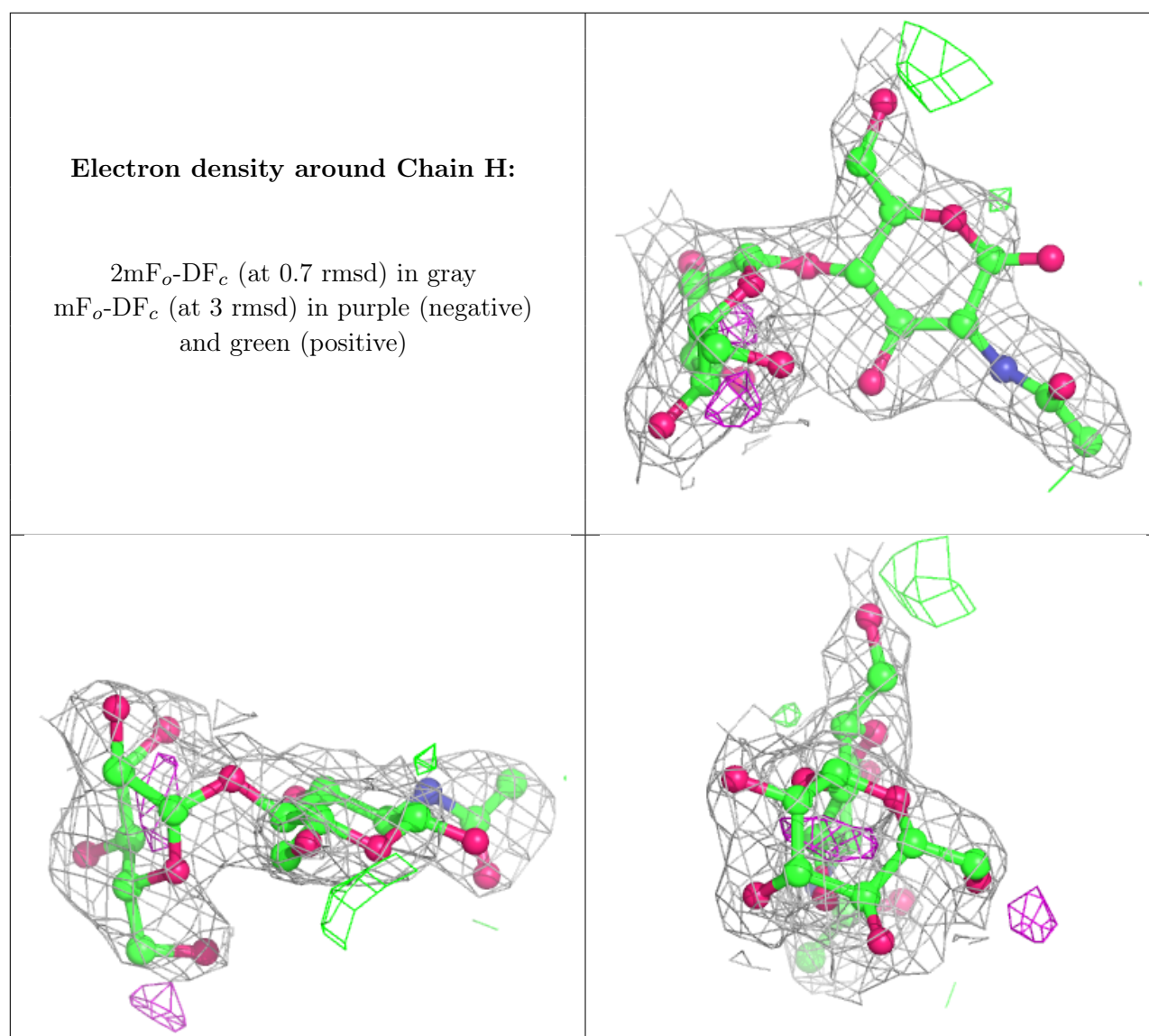
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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
3	PO4	A	502	5/5	0.70	0.51	142,143,145,147	0
3	PO4	A	501	5/5	0.79	0.17	120,122,125,129	0
3	PO4	D	503	5/5	0.82	0.40	123,124,130,131	0
3	PO4	B	503	5/5	0.83	0.48	139,142,146,147	0
3	PO4	B	501	5/5	0.83	0.16	97,97,104,105	0
3	PO4	C	504	5/5	0.84	0.33	122,123,127,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	D	502	5/5	0.85	0.37	113,114,116,119	0
3	PO4	A	504	5/5	0.85	0.32	125,132,134,137	0
3	PO4	C	501	5/5	0.86	0.28	102,104,105,105	0
3	PO4	D	504	5/5	0.88	0.45	138,140,140,143	0
3	PO4	C	503	5/5	0.90	0.33	110,111,114,117	0
3	PO4	C	502	5/5	0.91	0.24	102,103,108,109	0
3	PO4	B	502	5/5	0.92	0.26	110,112,115,118	0
3	PO4	D	501	5/5	0.93	0.23	107,109,112,112	0
3	PO4	A	503	5/5	0.94	0.17	83,86,90,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.