



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 10:10 AM EST

PDB ID : 4LN6
Title : The crystal structure of hemagglutinin from a h7n9 influenza virus (a/shanghai/2/2013)
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2013-07-11
Resolution : 2.12 Å(reported)

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

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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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

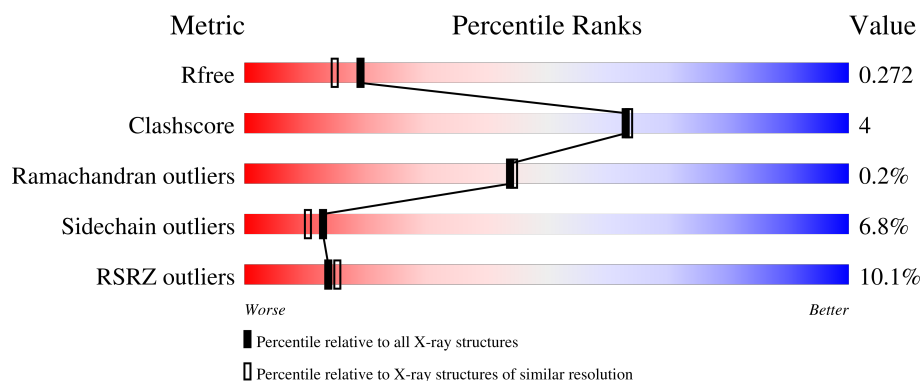
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	325	
1	C	325	
1	E	325	
1	G	325	
1	I	325	

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Mol	Chain	Length	Quality of chain
1	K	325	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
3	M	2	
3	Q	2	
4	N	3	
4	P	3	
4	R	3	
4	S	3	
5	O	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23253 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	C	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	E	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	G	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	I	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	K	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			

- Molecule 2 is a protein called Hemagglutinin.

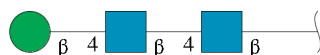
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	D	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	F	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	H	169	Total	C	N	O	S	0	0	0
			1375	849	240	279	7			
2	J	169	Total	C	N	O	S	0	0	0
			1375	849	240	279	7			
2	L	169	Total	C	N	O	S	0	0	0
			1375	849	240	279	7			

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



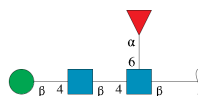
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

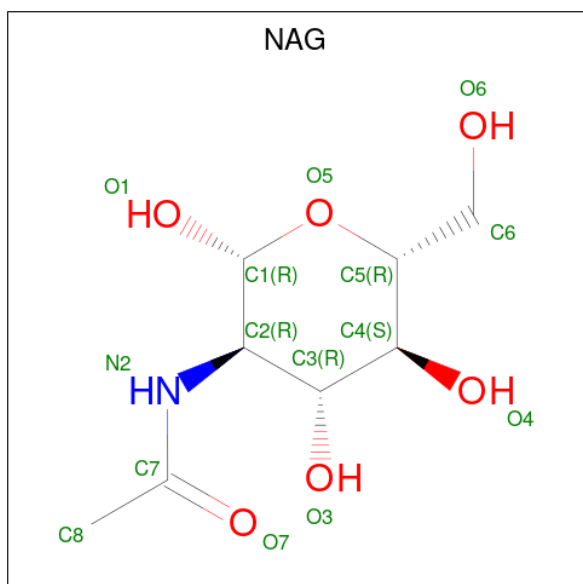


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		
6	G	1	Total	Ca	0	0
			1	1		
6	I	1	Total	Ca	0	0
			1	1		
6	K	1	Total	Ca	0	0
			1	1		

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

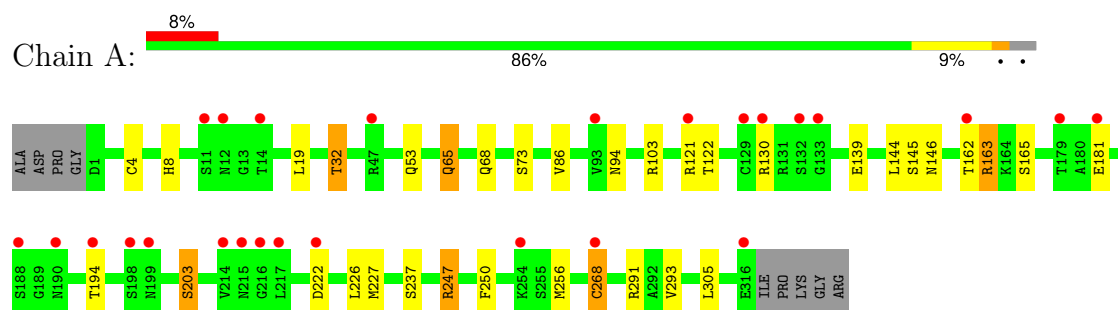
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	12	Total	O	0	0
			12	12		
8	C	32	Total	O	0	0
			32	32		
8	D	12	Total	O	0	0
			12	12		
8	E	24	Total	O	0	0
			24	24		
8	F	15	Total	O	0	0
			15	15		
8	G	24	Total	O	0	0
			24	24		
8	H	15	Total	O	0	0
			15	15		
8	I	16	Total	O	0	0
			16	16		
8	J	14	Total	O	0	0
			14	14		
8	K	18	Total	O	0	0
			18	18		
8	L	11	Total	O	0	0
			11	11		

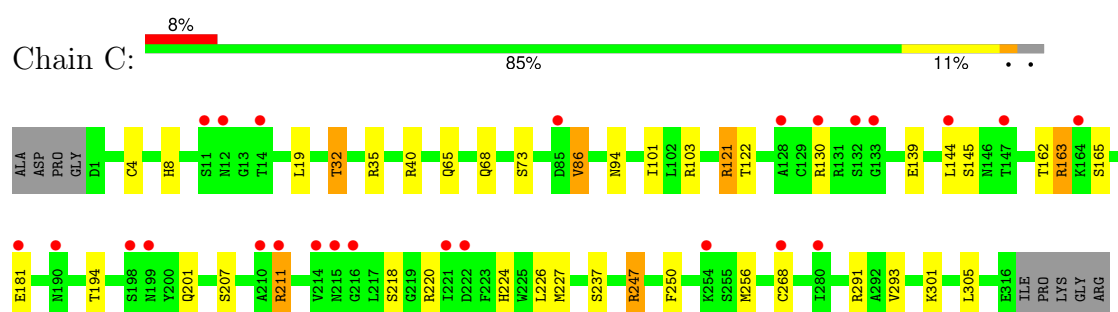
3 Residue-property plots [i](#)

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.

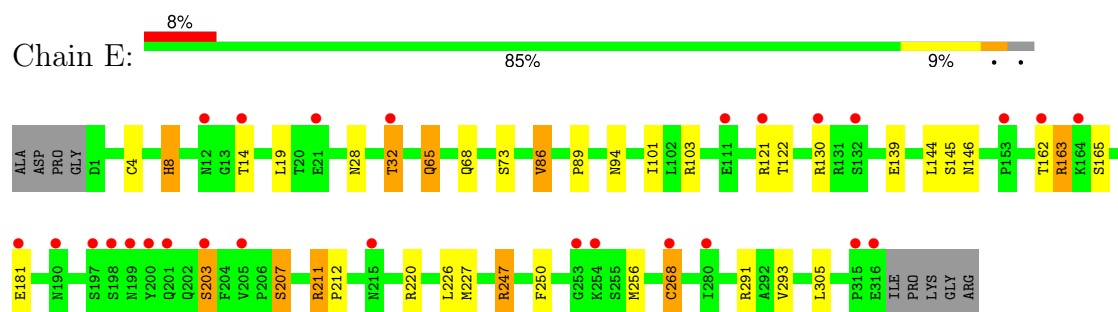
• Molecule 1: Hemagglutinin



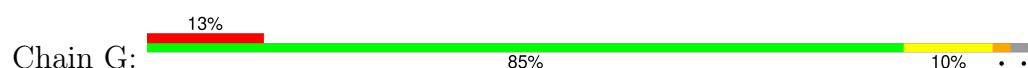
• Molecule 1: Hemagglutinin

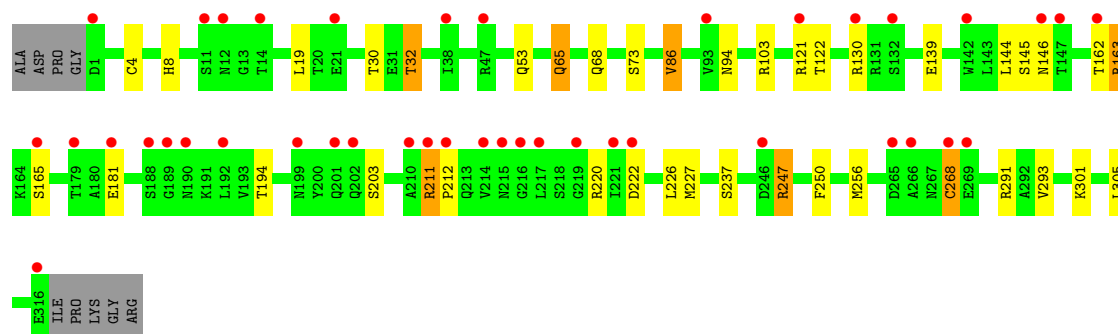


• Molecule 1: Hemagglutinin

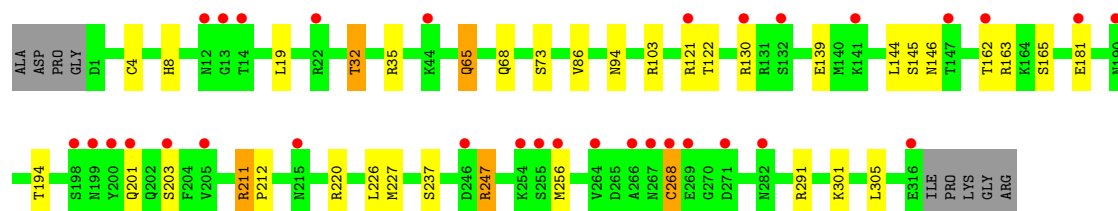
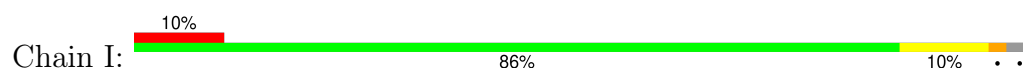


• Molecule 1: Hemagglutinin

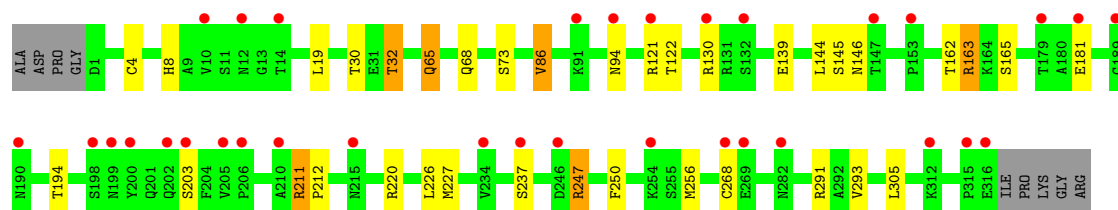
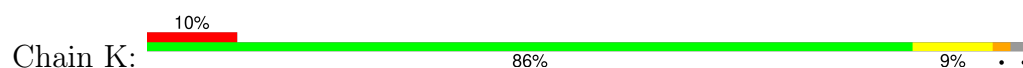




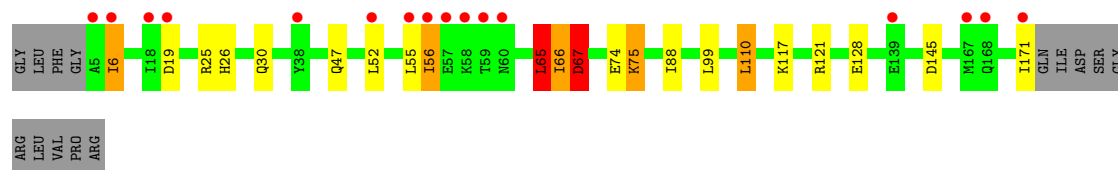
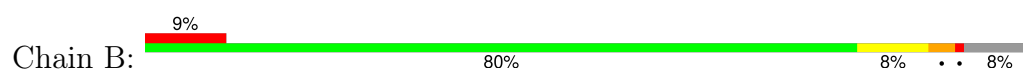
• Molecule 1: Hemagglutinin



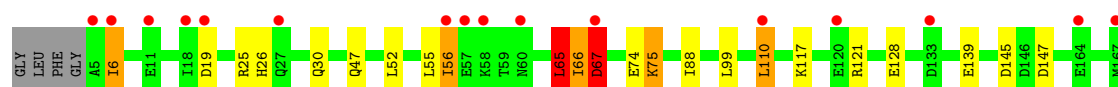
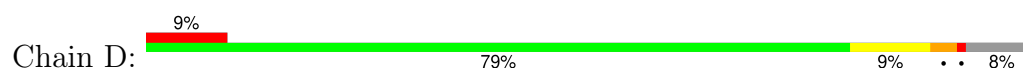
• Molecule 1: Hemagglutinin

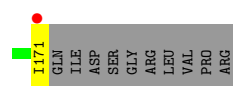


• Molecule 2: Hemagglutinin

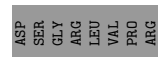
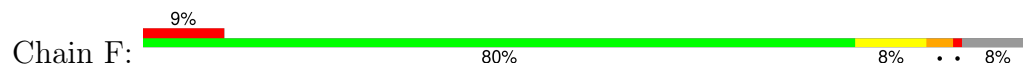


• Molecule 2: Hemagglutinin

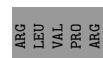
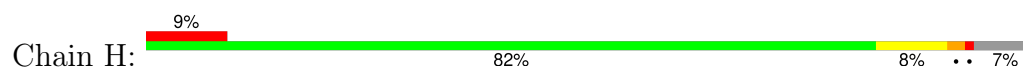




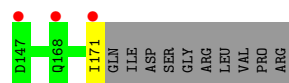
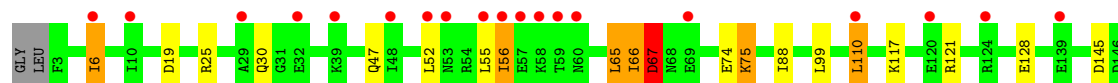
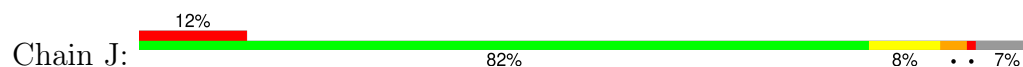
• Molecule 2: Hemagglutinin



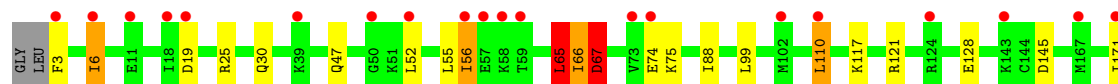
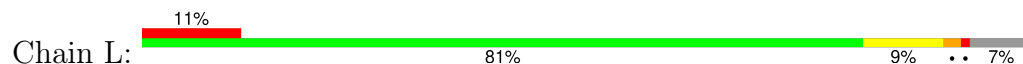
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin




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



MAG1
MAG2

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

Chain Q:  50% 50%

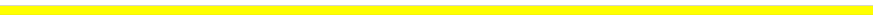
MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain P:  100%


MAG1
MAG2
BMA3

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

Chain R:  33% 67%

MAG1
MAG2
BMA3

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

Chain S:  67% 33%

MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.02Å 152.83Å 155.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 2.12 49.07 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.07-2.12) 96.3 (49.07-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.259 0.249 , 0.272	Depositor DCC
R_{free} test set	16066 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -h,-l,-k 0.000 for k,h,-l 0.096 for l,h,k 0.096 for k,l,h	Xtriage
Reported twinning fraction	0.852 for H, K, L 0.063 for L, H, K 0.085 for -K, -L, H	Depositor
Outliers	0 of 201333 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23253	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: BMA, FUC, NAG, CA

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	1.02	2/2458 (0.1%)	0.98	6/3322 (0.2%)
1	C	1.18	2/2458 (0.1%)	0.99	9/3322 (0.3%)
1	E	1.08	3/2458 (0.1%)	1.00	9/3322 (0.3%)
1	G	0.98	2/2458 (0.1%)	0.98	9/3322 (0.3%)
1	I	1.02	2/2458 (0.1%)	0.96	8/3322 (0.2%)
1	K	0.88	1/2458 (0.0%)	1.00	7/3322 (0.2%)
2	B	0.99	4/1383 (0.3%)	0.99	6/1864 (0.3%)
2	D	0.98	4/1383 (0.3%)	1.02	6/1864 (0.3%)
2	F	0.96	3/1383 (0.2%)	1.00	8/1864 (0.4%)
2	H	0.92	4/1399 (0.3%)	0.99	6/1885 (0.3%)
2	J	0.90	3/1399 (0.2%)	0.99	7/1885 (0.4%)
2	L	0.96	4/1399 (0.3%)	1.01	7/1885 (0.4%)
All	All	1.00	34/23094 (0.1%)	0.99	88/31179 (0.3%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	CYS	CB-SG	-35.85	1.21	1.82
1	I	268	CYS	CB-SG	27.56	2.29	1.82
1	E	268	CYS	CB-SG	23.03	2.21	1.82
1	G	268	CYS	CB-SG	-22.18	1.44	1.82
1	A	268	CYS	CB-SG	-22.00	1.44	1.82

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	268	CYS	CA-CB-SG	16.51	143.71	114.00
2	D	67	ASP	CB-CG-OD1	-14.75	105.03	118.30
2	L	67	ASP	CB-CG-OD1	-14.46	105.28	118.30
2	H	67	ASP	CB-CG-OD1	-14.29	105.44	118.30
1	E	247	ARG	NE-CZ-NH1	13.75	127.17	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2375	19	0
1	C	2412	0	2375	28	0
1	E	2412	0	2374	21	0
1	G	2412	0	2375	18	1
1	I	2412	0	2374	13	1
1	K	2412	0	2375	15	0
2	B	1360	0	1262	15	0
2	D	1360	0	1262	17	0
2	F	1360	0	1262	12	0
2	H	1375	0	1274	11	0
2	J	1375	0	1274	15	0
2	L	1375	0	1274	16	0
3	M	28	0	25	0	0
3	Q	28	0	25	1	0
4	N	39	0	34	0	0
4	P	39	0	34	0	0
4	R	39	0	34	1	0
4	S	39	0	34	1	0
5	O	49	0	43	3	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
7	B	14	0	13	0	0
7	D	14	0	13	0	0
7	F	14	0	13	0	0
7	H	14	0	13	0	0
7	J	14	0	13	1	0
7	L	14	0	13	0	1
8	A	32	0	0	1	0
8	B	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	32	0	0	5	0
8	D	12	0	0	4	0
8	E	24	0	0	1	0
8	F	15	0	0	0	0
8	G	24	0	0	3	1
8	H	15	0	0	0	0
8	I	16	0	0	0	0
8	J	14	0	0	0	0
8	K	18	0	0	0	0
8	L	11	0	0	3	0
All	All	23253	0	22163	175	2

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 4.

The worst 5 of 175 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:121:ARG:NH1	1:C:145:SER:O	1.77	1.18
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.15	1.12
1:A:53:GLN:OE1	8:A:501:HOH:O	1.89	0.89
1:A:222:ASP:OD1	1:C:201:GLN:NE2	2.07	0.87
1:G:53:GLN:OE1	8:G:501:HOH:O	1.96	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:ASP:OD2	1:I:201:GLN:NE2[3_545]	1.66	0.54
7:L:500:NAG:O7	8:G:508:HOH:O[3_555]	2.07	0.13

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	314/325 (97%)	307 (98%)	7 (2%)	0	100	100
1	C	314/325 (97%)	306 (98%)	8 (2%)	0	100	100
1	E	314/325 (97%)	305 (97%)	9 (3%)	0	100	100
1	G	314/325 (97%)	305 (97%)	9 (3%)	0	100	100
1	I	314/325 (97%)	305 (97%)	9 (3%)	0	100	100
1	K	314/325 (97%)	305 (97%)	9 (3%)	0	100	100
2	B	165/181 (91%)	160 (97%)	4 (2%)	1 (1%)	22	18
2	D	165/181 (91%)	161 (98%)	3 (2%)	1 (1%)	22	18
2	F	165/181 (91%)	160 (97%)	4 (2%)	1 (1%)	22	18
2	H	167/181 (92%)	163 (98%)	3 (2%)	1 (1%)	22	18
2	J	167/181 (92%)	163 (98%)	3 (2%)	1 (1%)	22	18
2	L	167/181 (92%)	162 (97%)	4 (2%)	1 (1%)	22	18
All	All	2880/3036 (95%)	2802 (97%)	72 (2%)	6 (0%)	44	44

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	56	ILE
2	J	56	ILE
2	L	56	ILE
2	B	56	ILE
2	D	56	ILE

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	265/271 (98%)	249 (94%)	16 (6%)	16	13
1	C	265/271 (98%)	249 (94%)	16 (6%)	16	13
1	E	265/271 (98%)	247 (93%)	18 (7%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	265/271 (98%)	248 (94%)	17 (6%)	14	12
1	I	265/271 (98%)	248 (94%)	17 (6%)	14	12
1	K	265/271 (98%)	249 (94%)	16 (6%)	16	13
2	B	144/155 (93%)	133 (92%)	11 (8%)	11	8
2	D	144/155 (93%)	132 (92%)	12 (8%)	9	6
2	F	144/155 (93%)	133 (92%)	11 (8%)	11	8
2	H	145/155 (94%)	134 (92%)	11 (8%)	11	8
2	J	145/155 (94%)	134 (92%)	11 (8%)	11	8
2	L	145/155 (94%)	134 (92%)	11 (8%)	11	8
All	All	2457/2556 (96%)	2290 (93%)	167 (7%)	13	10

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	65	GLN
1	K	65	GLN
1	I	94	ASN
2	J	19	ASP
1	K	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	30	GLN
1	K	154	GLN
2	J	30	GLN
1	C	224	HIS
2	F	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
3	NAG	M	1	3,1	14,14,15	0.82	0	17,19,21	1.80	5 (29%)
3	NAG	M	2	3	14,14,15	0.50	0	17,19,21	1.45	2 (11%)
4	NAG	N	1	4,1	14,14,15	0.85	0	17,19,21	2.36	5 (29%)
4	NAG	N	2	4	14,14,15	0.66	0	17,19,21	1.42	4 (23%)
4	BMA	N	3	4	11,11,12	0.83	0	15,15,17	1.67	3 (20%)
5	NAG	O	1	5,1	14,14,15	2.19	5 (35%)	17,19,21	3.70	9 (52%)
5	NAG	O	2	5	14,14,15	1.03	1 (7%)	17,19,21	1.44	4 (23%)
5	BMA	O	3	5	11,11,12	0.75	0	15,15,17	1.81	4 (26%)
5	FUC	O	4	5	10,10,11	0.85	0	14,14,16	1.47	3 (21%)
4	NAG	P	1	4,1	14,14,15	1.20	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	P	2	4	14,14,15	0.68	0	17,19,21	1.32	2 (11%)
4	BMA	P	3	4	11,11,12	0.76	0	15,15,17	2.60	3 (20%)
3	NAG	Q	1	3,1	14,14,15	0.61	0	17,19,21	1.84	4 (23%)
3	NAG	Q	2	3	14,14,15	0.62	0	17,19,21	1.48	2 (11%)
4	NAG	R	1	4,1	14,14,15	0.66	0	17,19,21	1.81	2 (11%)
4	NAG	R	2	4	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
4	BMA	R	3	4	11,11,12	0.67	0	15,15,17	2.32	3 (20%)
4	NAG	S	1	4,1	14,14,15	0.99	0	17,19,21	1.63	5 (29%)
4	NAG	S	2	4	14,14,15	0.71	0	17,19,21	1.29	2 (11%)
4	BMA	S	3	4	11,11,12	0.63	0	15,15,17	0.89	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
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	FUC	O	4	5	-	-	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	1/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1	NAG	C1-C2	6.20	1.60	1.52
4	P	1	NAG	C1-C2	3.01	1.56	1.52
5	O	2	NAG	C1-C2	2.97	1.56	1.52
5	O	1	NAG	C3-C2	2.48	1.57	1.52
5	O	1	NAG	O5-C1	2.30	1.47	1.43

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C1-O5-C5	12.46	128.88	112.19
4	P	3	BMA	C1-O5-C5	8.39	123.43	112.19
4	N	1	NAG	C1-O5-C5	7.38	122.08	112.19
4	R	3	BMA	C1-O5-C5	7.01	121.58	112.19
4	R	1	NAG	C1-C2-N2	-6.08	100.85	110.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

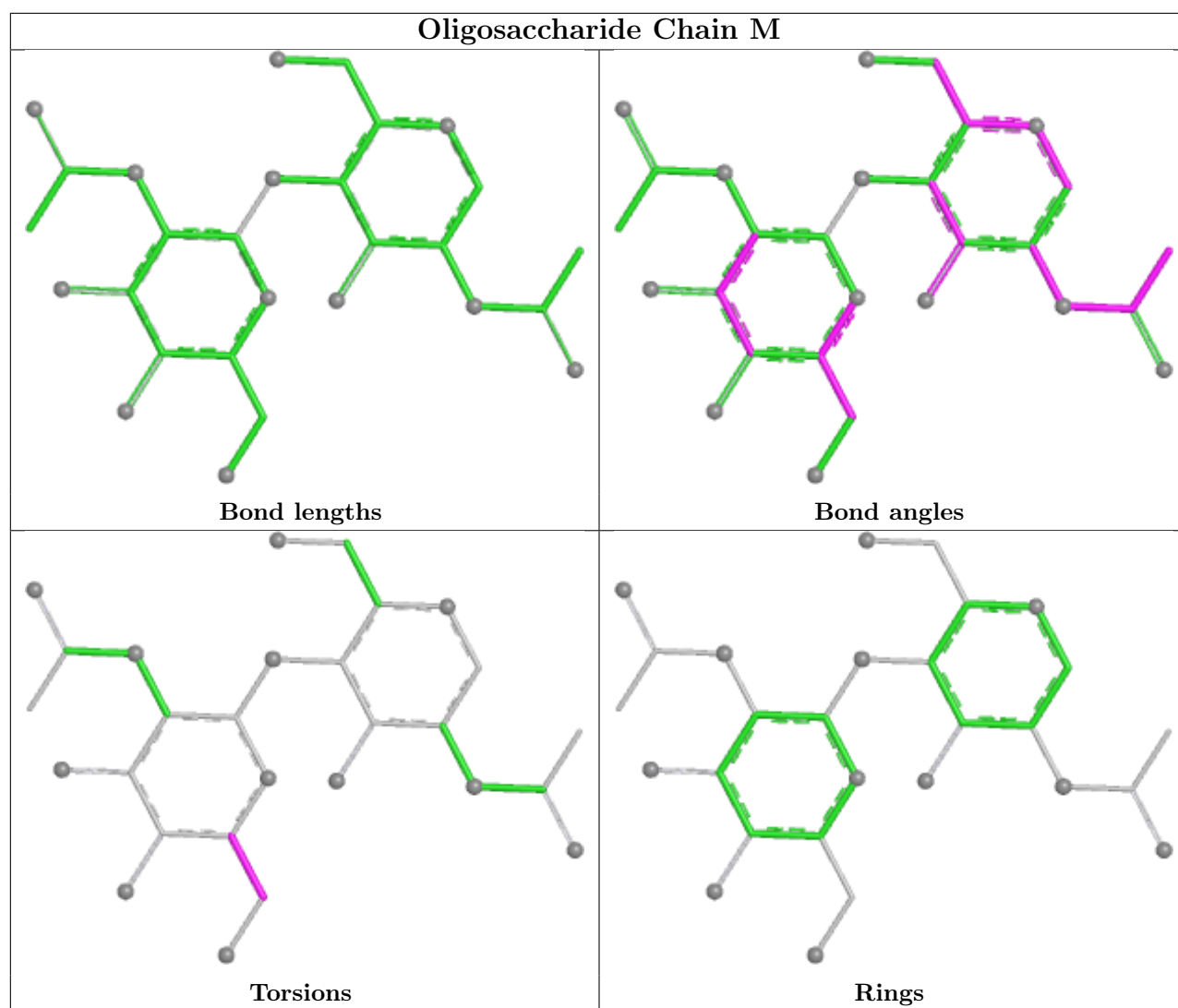
Mol	Chain	Res	Type	Atoms
4	N	2	NAG	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6

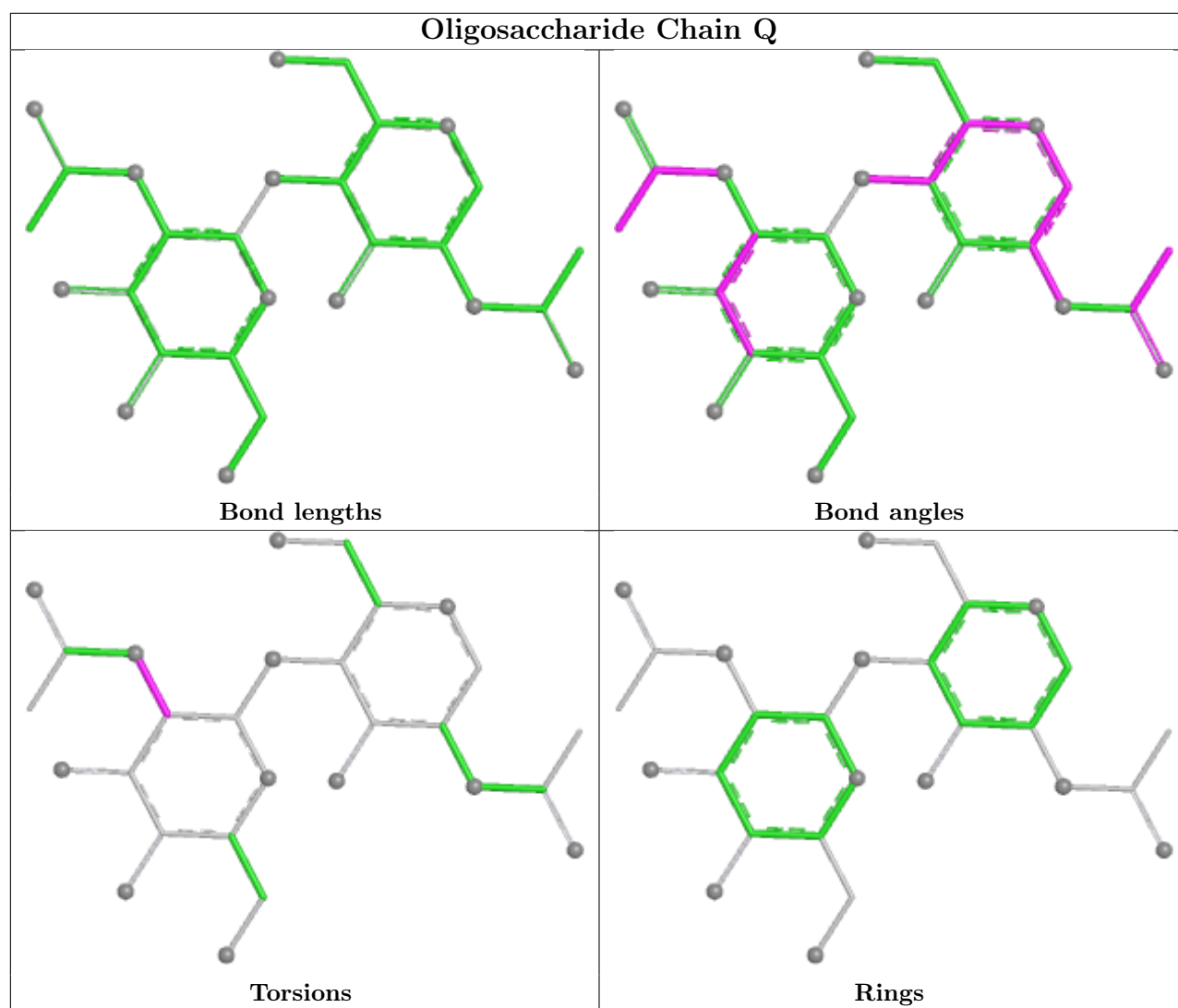
There are no ring outliers.

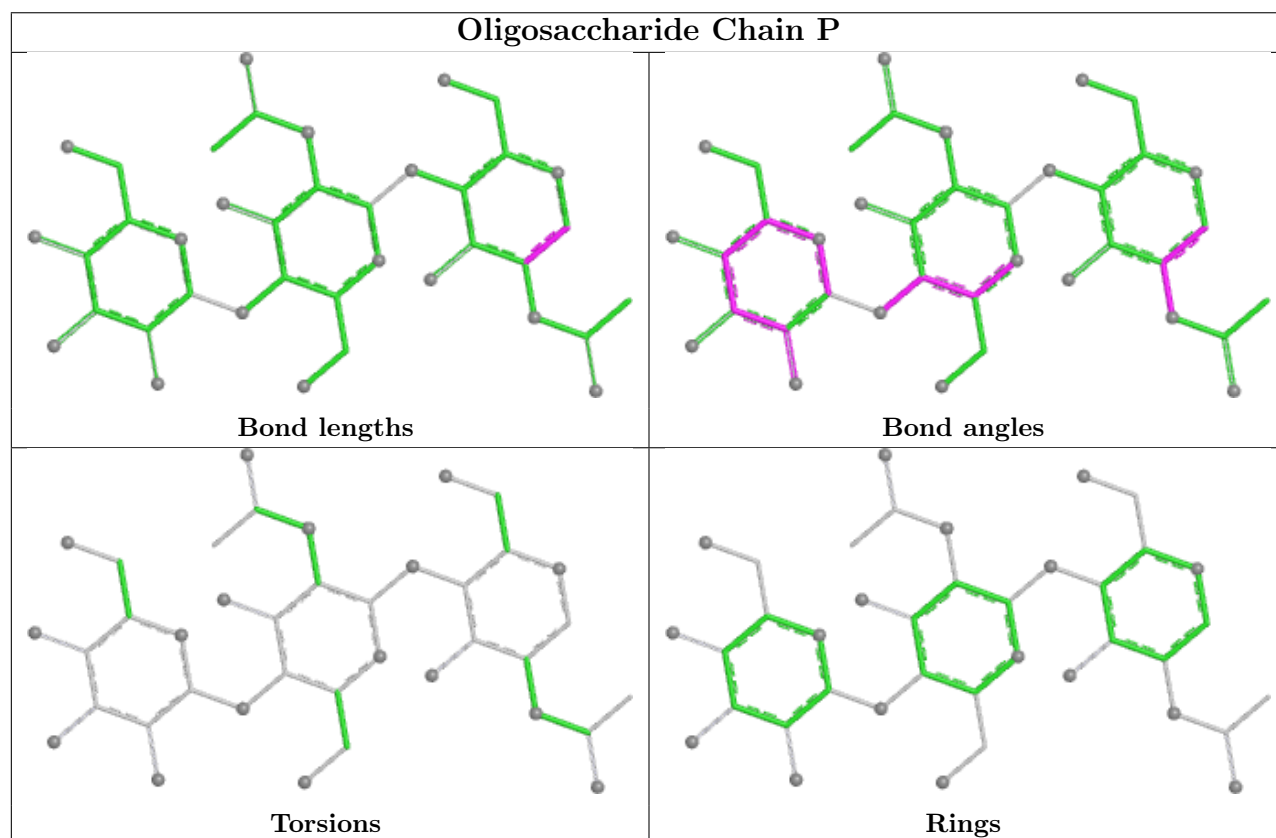
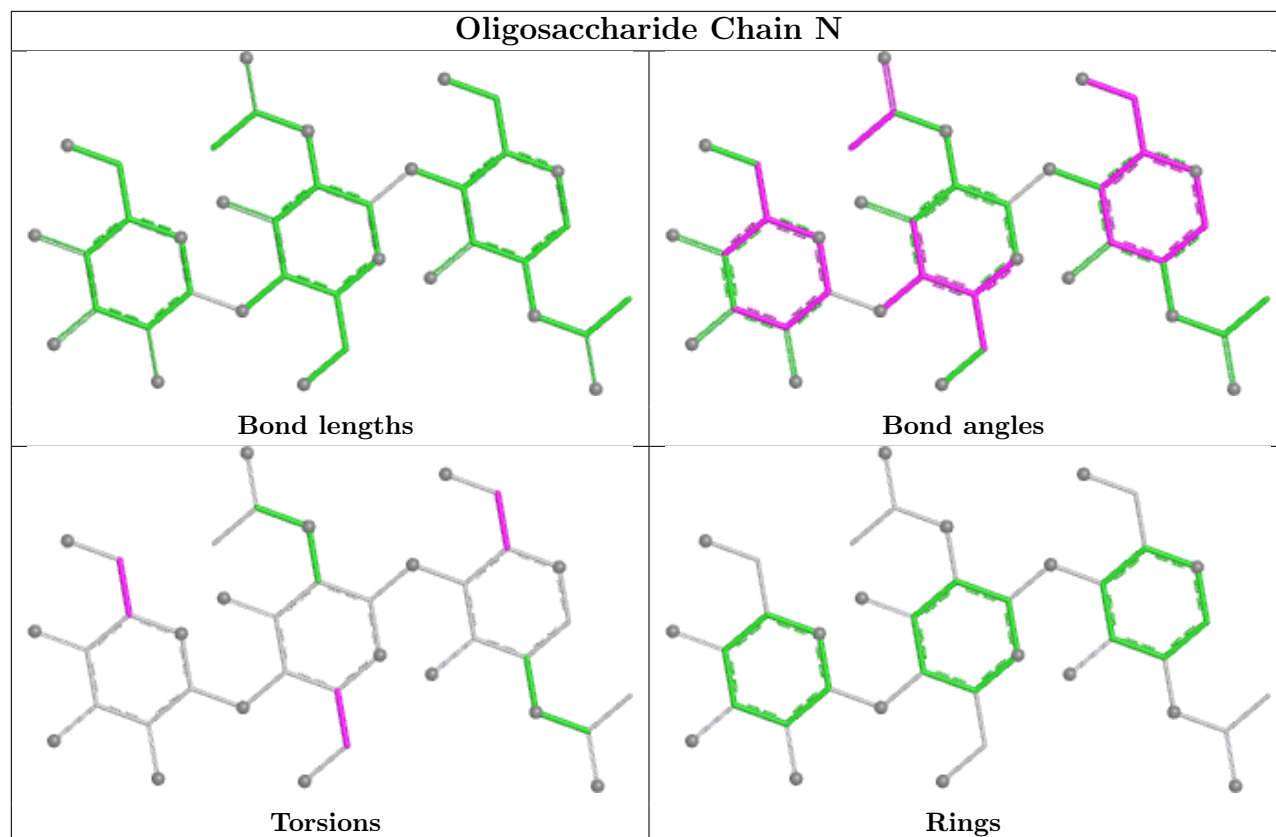
6 monomers are involved in 6 short contacts:

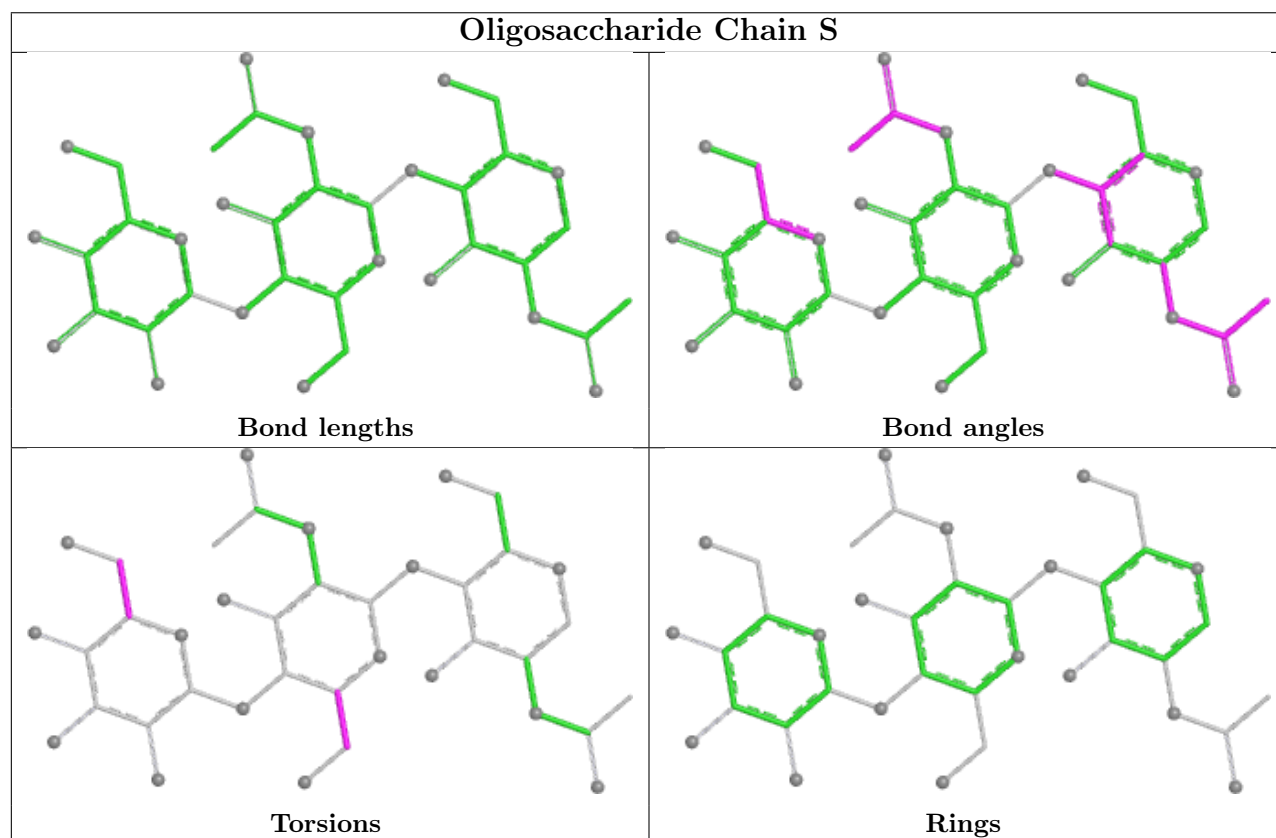
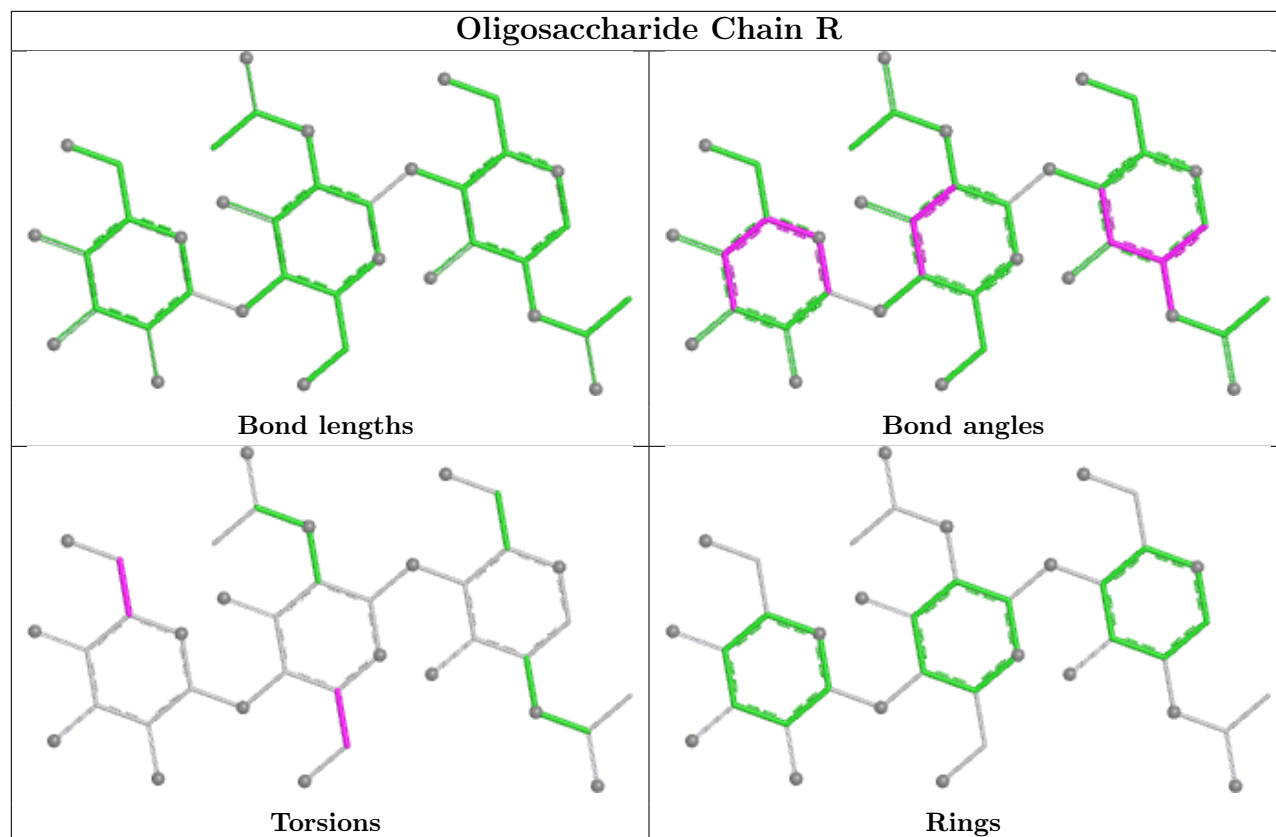
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	2	NAG	1	0
4	S	1	NAG	1	0
5	O	4	FUC	1	0
5	O	1	NAG	2	0
3	Q	1	NAG	1	0
4	R	3	BMA	1	0

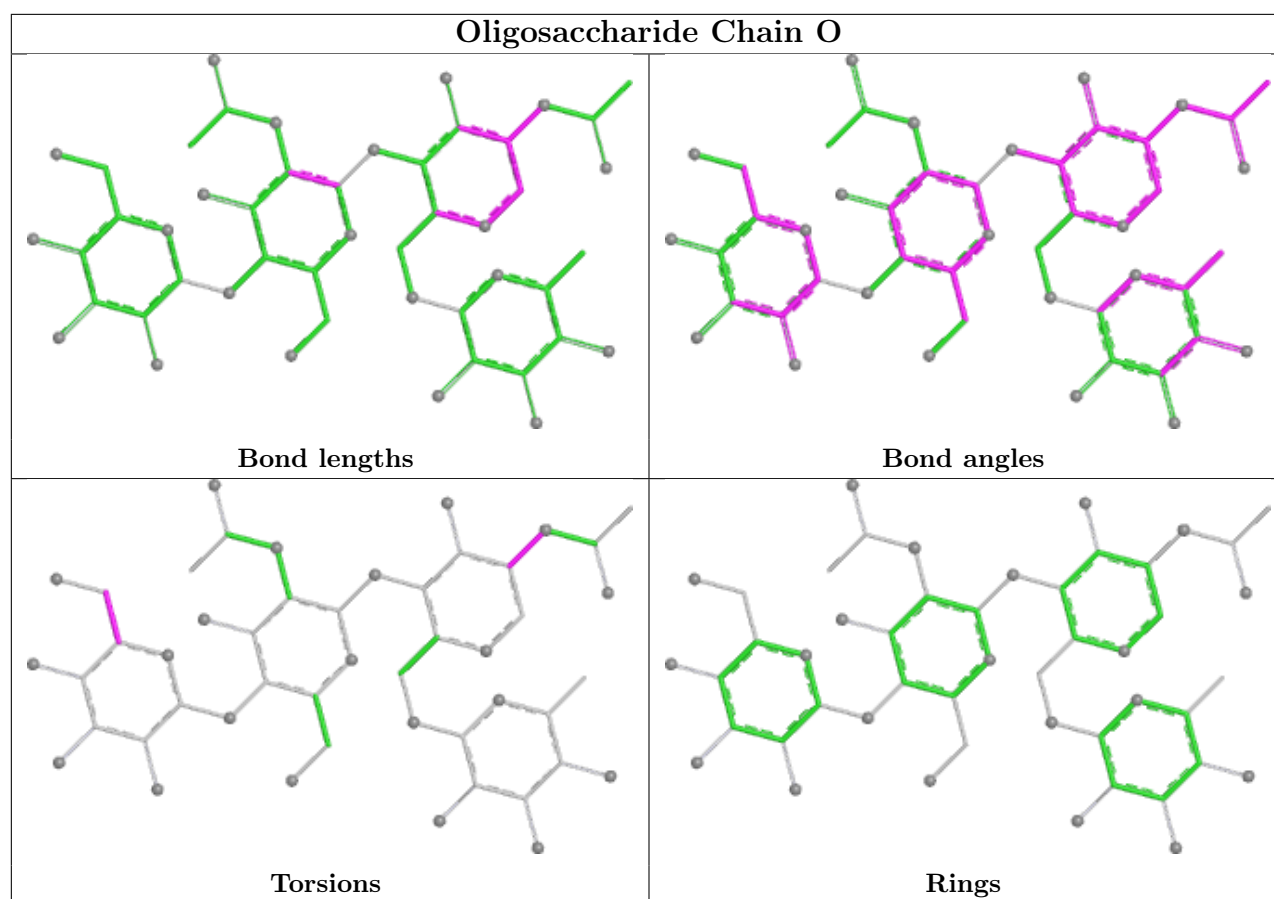
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	F	500	2	14,14,15	0.90	0	17,19,21	2.26	6 (35%)
7	NAG	J	500	2	14,14,15	0.91	1 (7%)	17,19,21	1.99	3 (17%)
7	NAG	D	500	2	14,14,15	0.95	1 (7%)	17,19,21	1.50	2 (11%)
7	NAG	L	500	2	14,14,15	0.79	0	17,19,21	2.66	7 (41%)
7	NAG	B	500	2	14,14,15	0.63	0	17,19,21	2.49	8 (47%)
7	NAG	H	500	2	14,14,15	1.07	1 (7%)	17,19,21	2.45	7 (41%)

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	F	500	2	-	0/6/23/26	0/1/1/1
7	NAG	J	500	2	-	0/6/23/26	0/1/1/1
7	NAG	D	500	2	-	1/6/23/26	0/1/1/1
7	NAG	L	500	2	-	0/6/23/26	0/1/1/1
7	NAG	B	500	2	-	0/6/23/26	0/1/1/1
7	NAG	H	500	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	500	NAG	C1-C2	2.73	1.56	1.52
7	D	500	NAG	O5-C1	2.38	1.47	1.43
7	H	500	NAG	O5-C1	2.15	1.47	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	500	NAG	C1-O5-C5	7.45	122.17	112.19
7	B	500	NAG	C1-O5-C5	6.55	120.97	112.19
7	J	500	NAG	C1-O5-C5	6.47	120.85	112.19
7	H	500	NAG	C1-O5-C5	6.37	120.72	112.19
7	F	500	NAG	C1-O5-C5	4.49	118.20	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	500	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	500	NAG	1	0
7	L	500	NAG	0	1

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	316/325 (97%)	0.65	26 (8%)	19	21	23, 33, 55, 76	1 (0%)
1	C	316/325 (97%)	0.74	25 (7%)	20	22	24, 34, 53, 74	1 (0%)
1	E	316/325 (97%)	0.70	27 (8%)	18	20	24, 33, 52, 81	1 (0%)
1	G	316/325 (97%)	0.90	41 (12%)	9	10	25, 37, 57, 81	1 (0%)
1	I	316/325 (97%)	0.85	32 (10%)	14	15	25, 35, 54, 79	1 (0%)
1	K	316/325 (97%)	0.87	33 (10%)	13	14	26, 36, 55, 81	1 (0%)
2	B	167/181 (92%)	0.82	16 (9%)	15	17	21, 35, 58, 102	0
2	D	167/181 (92%)	0.80	17 (10%)	13	15	22, 36, 54, 103	0
2	F	167/181 (92%)	0.84	16 (9%)	15	17	22, 36, 53, 90	0
2	H	169/181 (93%)	0.94	17 (10%)	14	15	25, 39, 60, 98	0
2	J	169/181 (93%)	0.94	22 (13%)	9	10	23, 38, 57, 100	0
2	L	169/181 (93%)	0.91	20 (11%)	10	11	24, 38, 56, 94	0
All	All	2904/3036 (95%)	0.82	292 (10%)	14	15	21, 36, 56, 103	6 (0%)

The worst 5 of 292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	56	ILE	6.7
1	C	12	ASN	6.5
2	F	171	ILE	6.4
2	D	58	LYS	6.3
2	L	171	ILE	5.9

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

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

6.3 Carbohydrates

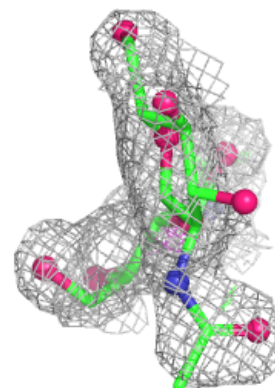
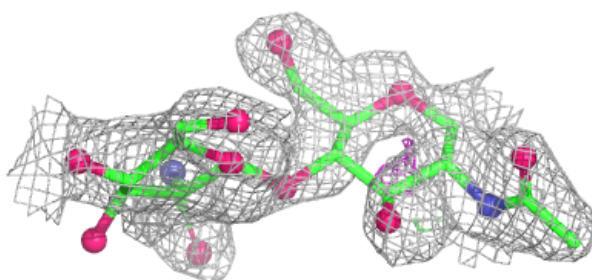
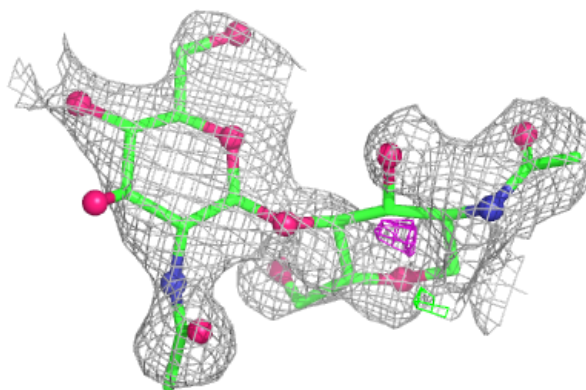
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	O	3	11/12	0.20	0.18	103,109,112,115	0
4	BMA	P	3	11/12	0.34	0.21	76,87,96,99	0
4	BMA	R	3	11/12	0.36	0.16	87,99,102,103	0
4	BMA	N	3	11/12	0.38	0.18	84,95,97,100	0
4	BMA	S	3	11/12	0.40	0.18	92,100,109,112	0
5	NAG	O	2	14/15	0.43	0.19	70,91,94,98	0
5	FUC	O	4	10/11	0.48	0.24	76,86,91,92	0
5	NAG	O	1	14/15	0.56	0.23	69,82,89,90	0
4	NAG	P	2	14/15	0.58	0.17	63,76,85,90	0
3	NAG	Q	2	14/15	0.62	0.15	62,85,91,92	0
3	NAG	M	1	14/15	0.66	0.17	50,67,76,77	0
4	NAG	N	1	14/15	0.68	0.17	41,66,73,73	0
4	NAG	P	1	14/15	0.70	0.17	45,57,62,71	0
4	NAG	S	2	14/15	0.71	0.16	56,70,84,97	0
4	NAG	R	2	14/15	0.72	0.15	58,71,88,96	0
4	NAG	N	2	14/15	0.72	0.16	69,79,84,90	0
3	NAG	Q	1	14/15	0.73	0.15	46,61,68,74	0
3	NAG	M	2	14/15	0.77	0.13	61,76,84,89	0
4	NAG	S	1	14/15	0.78	0.13	44,49,52,58	0
4	NAG	R	1	14/15	0.84	0.12	49,60,64,65	0

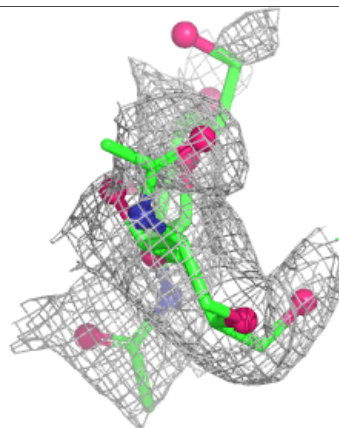
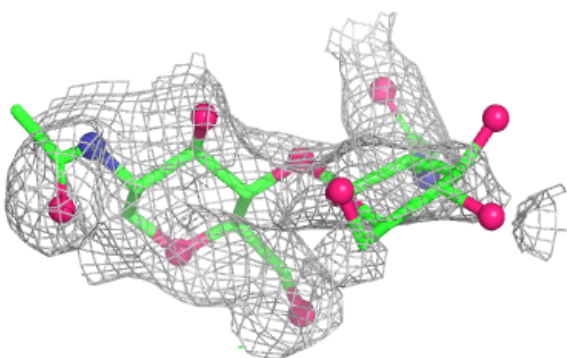
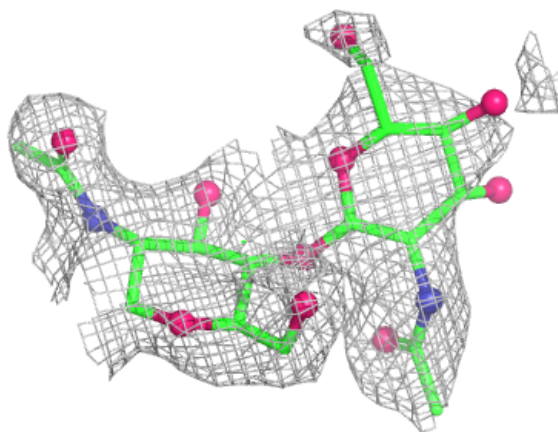
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

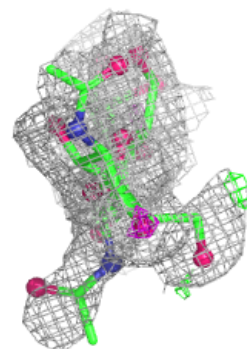
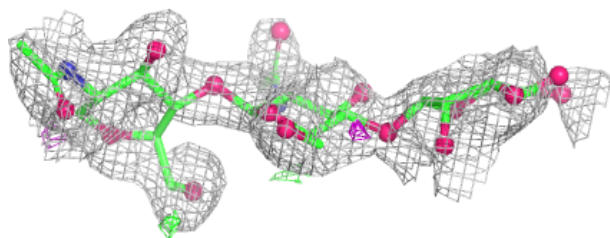
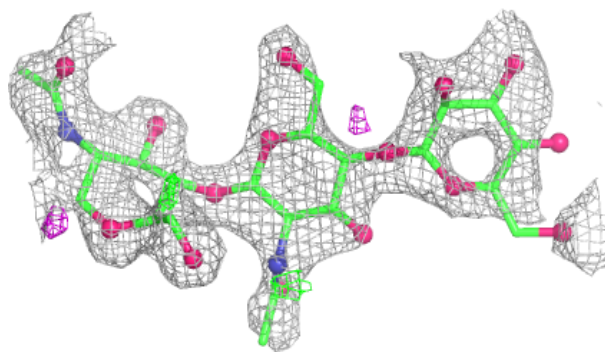
**Electron density around Chain Q:**

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

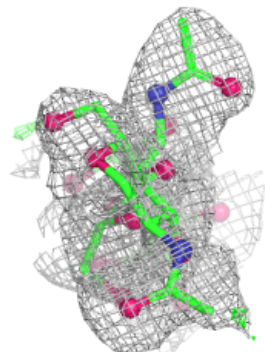
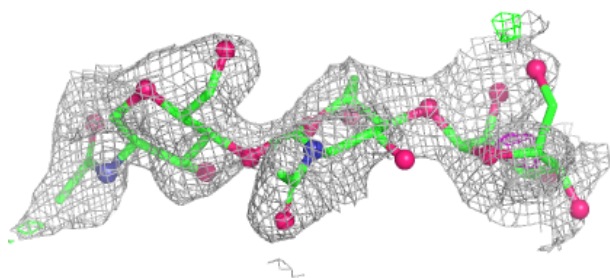
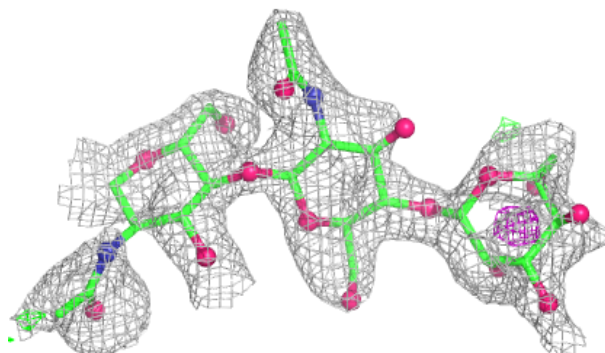


Electron density around Chain N:

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

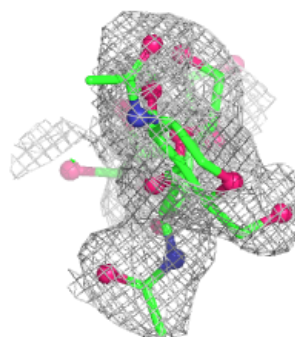
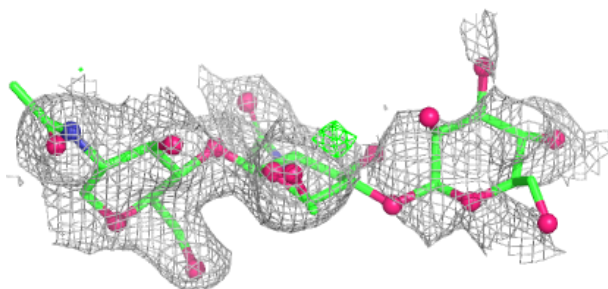
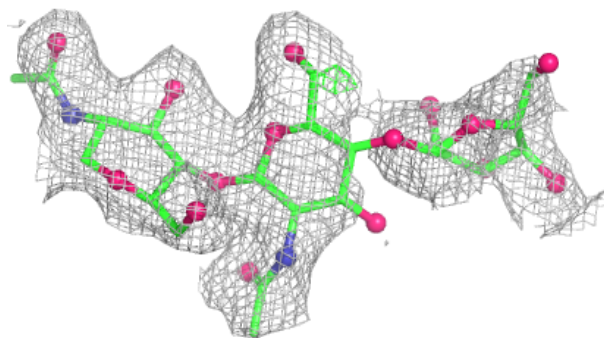
**Electron density around Chain P:**

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

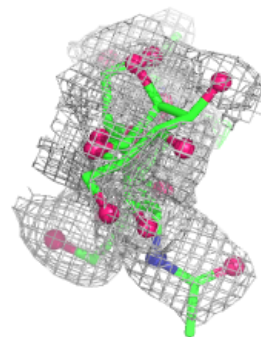
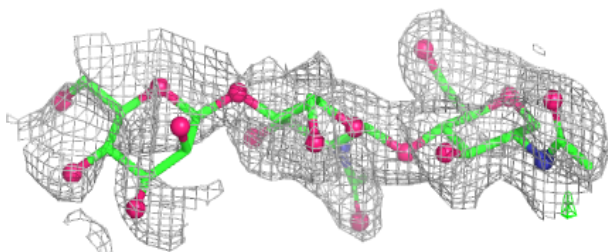
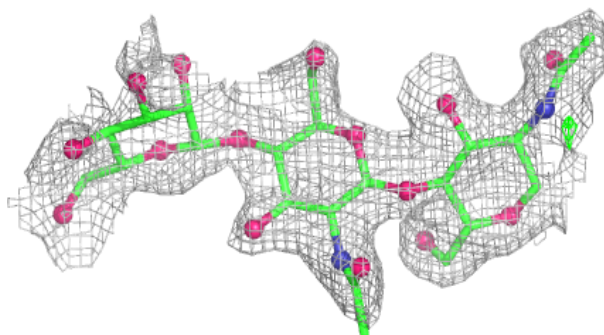


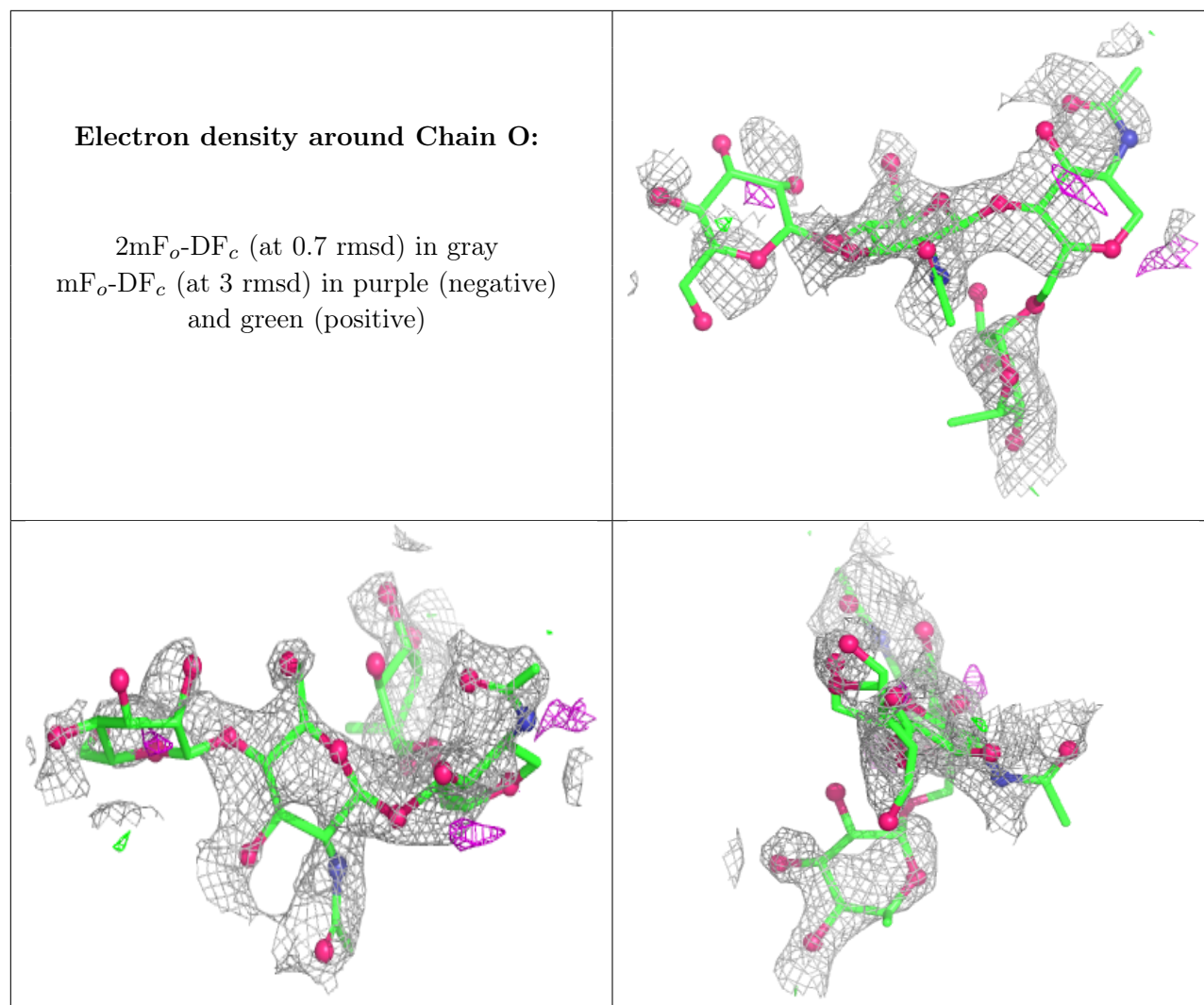
Electron density around Chain R:

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

**Electron density around Chain S:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
7	NAG	J	500	14/15	0.72	0.14	44,54,59,62	0
7	NAG	D	500	14/15	0.77	0.14	44,51,56,59	0
7	NAG	F	500	14/15	0.80	0.13	43,49,54,57	0
7	NAG	B	500	14/15	0.80	0.13	39,46,51,55	0
7	NAG	L	500	14/15	0.82	0.13	45,50,55,55	0
7	NAG	H	500	14/15	0.83	0.12	41,46,53,56	0
6	CA	A	403	1/1	0.88	0.09	42,42,42,42	0
6	CA	C	404	1/1	0.88	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	K	404	1/1	0.88	0.09	44,44,44,44	0
6	CA	G	403	1/1	0.93	0.06	35,35,35,35	0
6	CA	E	408	1/1	0.93	0.08	41,41,41,41	0
6	CA	I	404	1/1	0.95	0.06	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.