



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:04 PM UTC

PDB ID : 5UGY / pdb_00005ugy
Title : Influenza hemagglutinin in complex with a neutralizing antibody
Authors : Whittle, J.R.R.; Jenni, S.; Harrison, S.C.
Deposited on : 2017-01-10
Resolution : 2.80 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

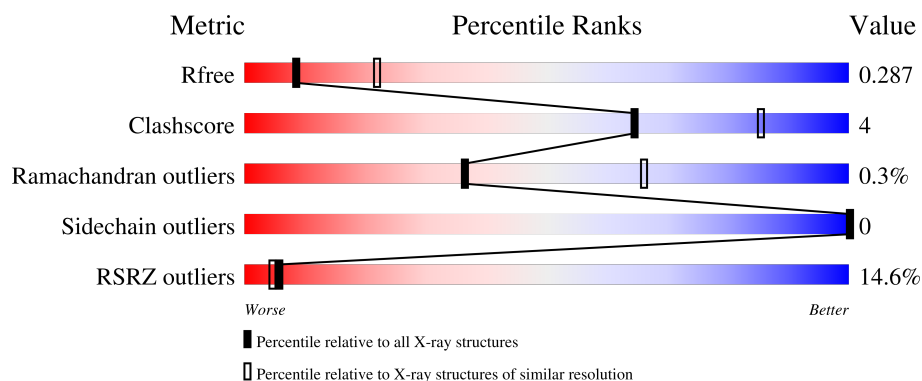
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	323	
1	C	323	
1	E	323	
2	B	173	
2	D	173	

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Mol	Chain	Length	Quality of chain
2	F	173	
3	H	227	
3	I	227	
3	J	227	
4	L	210	
4	M	210	
4	N	210	
5	G	2	
5	O	2	
5	P	2	
5	R	2	
5	S	2	
5	U	2	
6	K	3	
6	Q	3	
6	T	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 42918 atoms, of which 21036 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 HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	H	N	O	S	0	0	0
			4975	1597	2440	441	486	11			
1	C	323	Total	C	H	N	O	S	0	0	0
			4975	1597	2440	441	486	11			
1	E	323	Total	C	H	N	O	S	0	0	0
			4975	1597	2440	441	486	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0
C	4	GLU	-	expression tag	UNP A7UPX0
E	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	173	Total	C	H	N	O	S	0	0	0
			2718	874	1324	238	275	7			
2	D	173	Total	C	H	N	O	S	0	0	0
			2718	874	1324	238	275	7			
2	F	173	Total	C	H	N	O	S	0	0	0
			2718	874	1324	238	275	7			

- Molecule 3 is a protein called CH65 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	221	Total	C	H	N	O	S	0	0	0
			3294	1062	1617	279	328	8			
3	I	221	Total	C	H	N	O	S	0	0	0
			3294	1062	1617	279	328	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	J	221	Total	C	H	N	O	S	0	0	0
			3294	1062	1617	279	328	8			

- Molecule 4 is a protein called CH65 light chain.

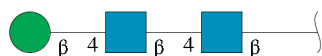
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			
4	M	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			
4	N	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			

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



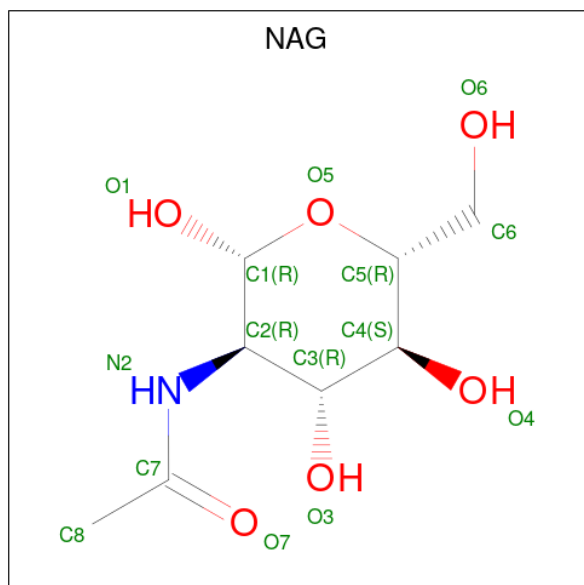
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	O	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	P	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	R	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	S	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	U	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 6 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
6	K	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
6	Q	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
6	T	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

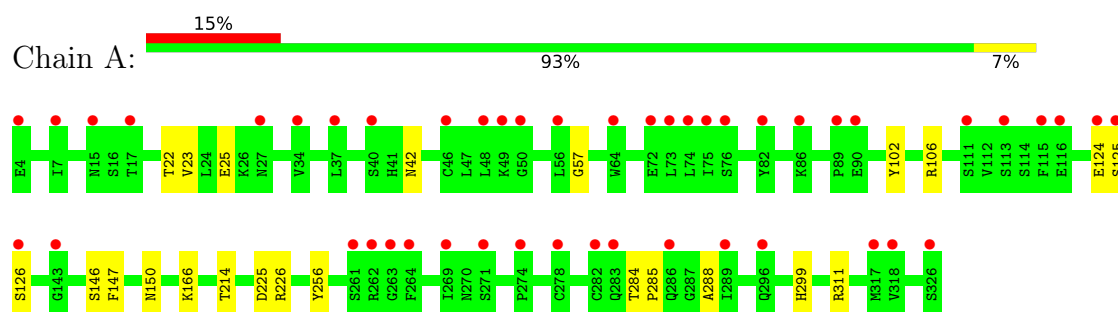


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

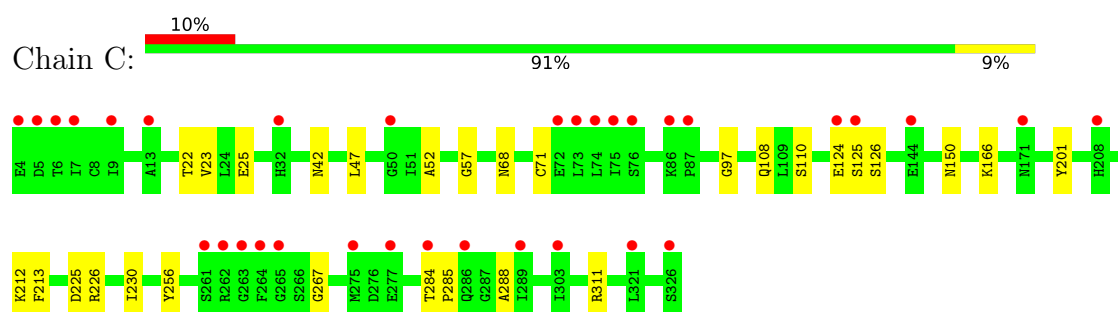
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

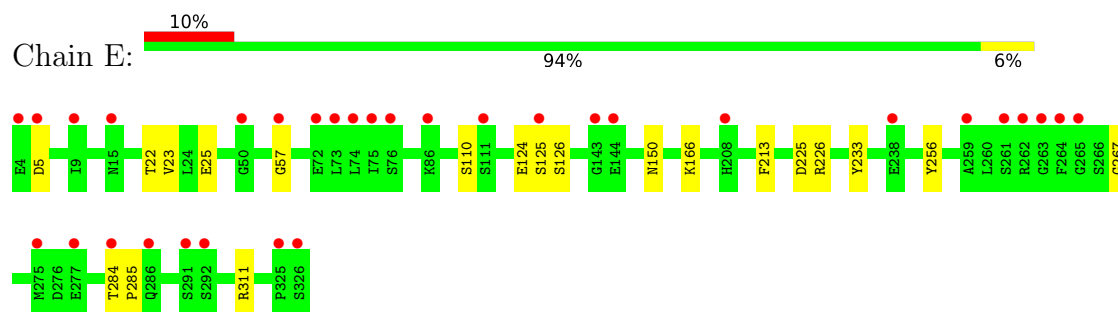
• Molecule 1: Hemagglutinin HA1



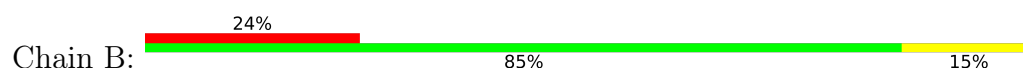
• Molecule 1: Hemagglutinin HA1

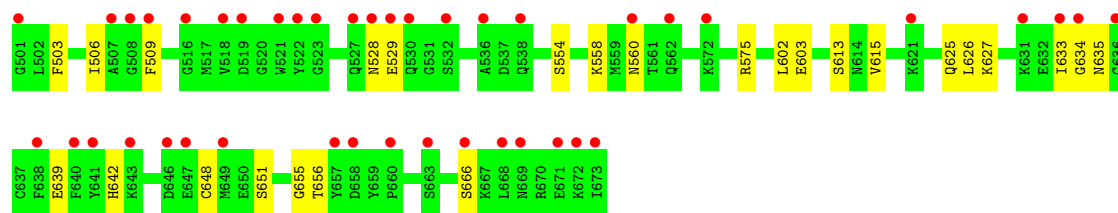


• Molecule 1: Hemagglutinin HA1

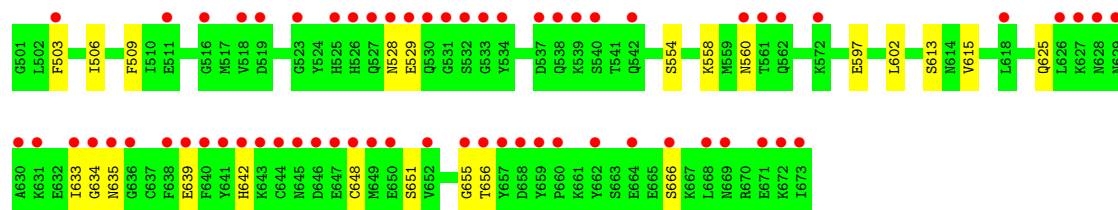
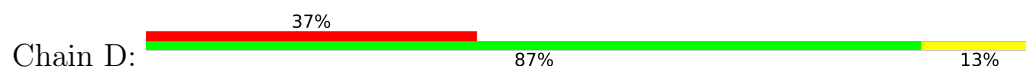


• Molecule 2: Hemagglutinin HA2

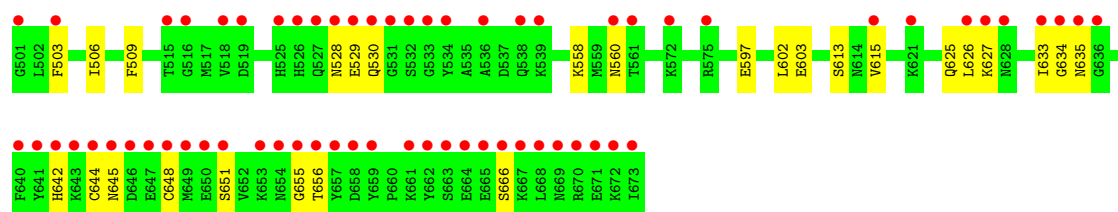
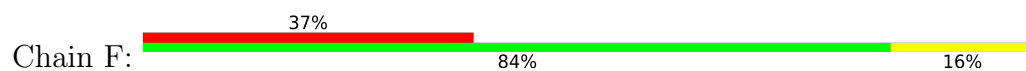




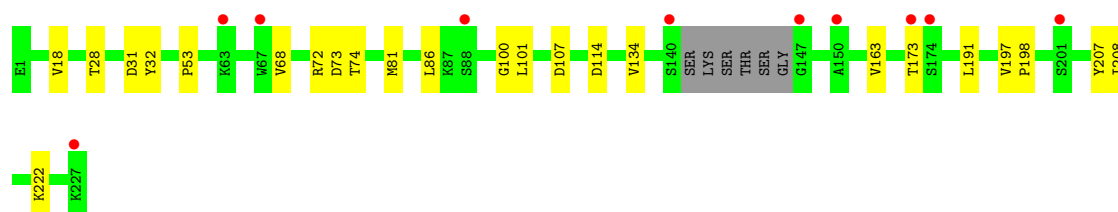
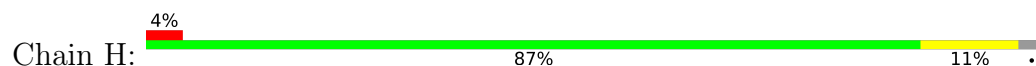
● Molecule 2: Hemagglutinin HA2



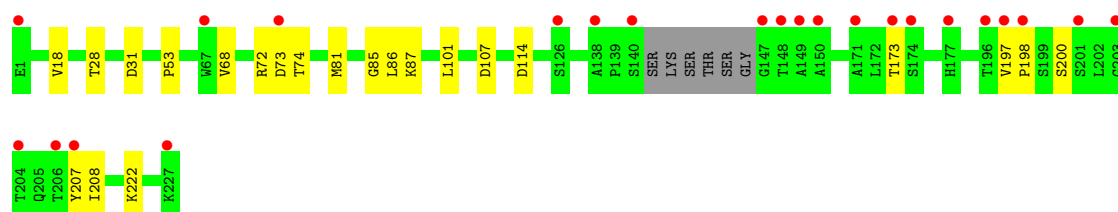
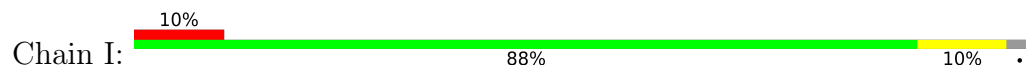
● Molecule 2: Hemagglutinin HA2



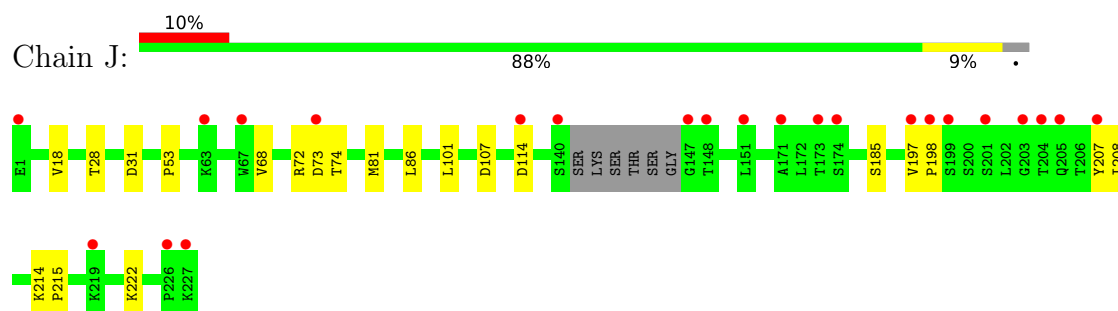
● Molecule 3: CH65 heavy chain



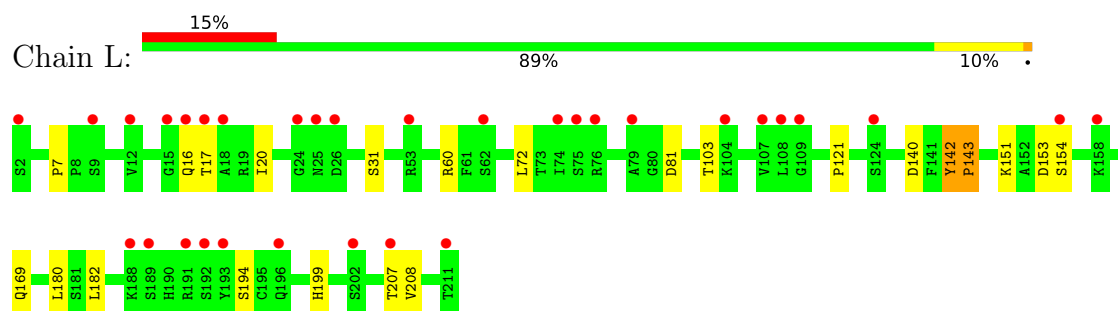
● Molecule 3: CH65 heavy chain



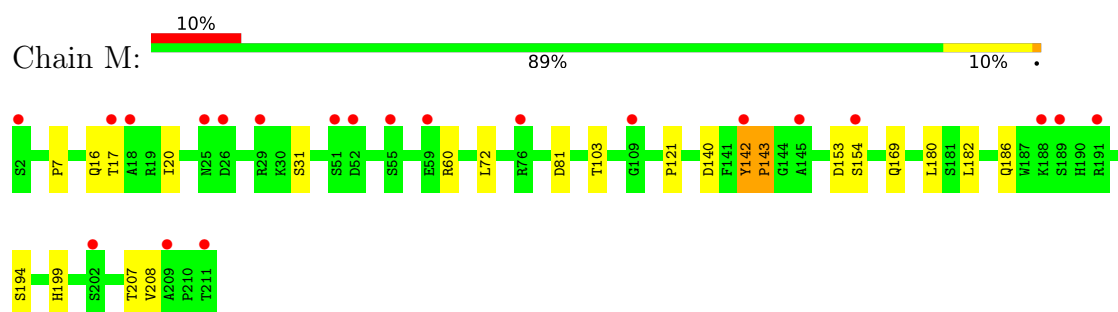
- Molecule 3: CH65 heavy chain



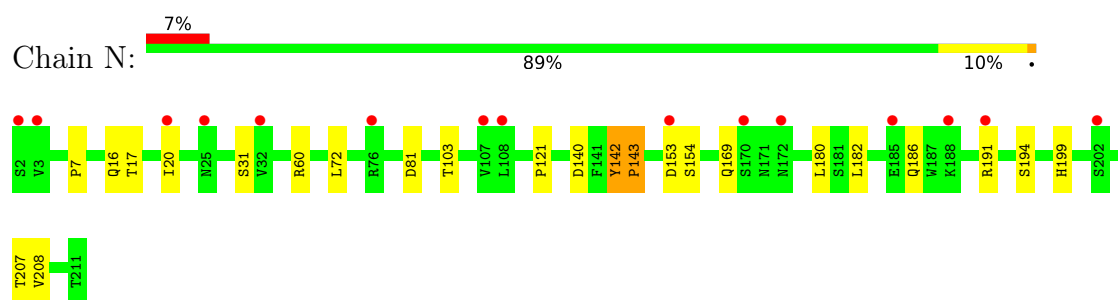
- Molecule 4: CH65 light chain



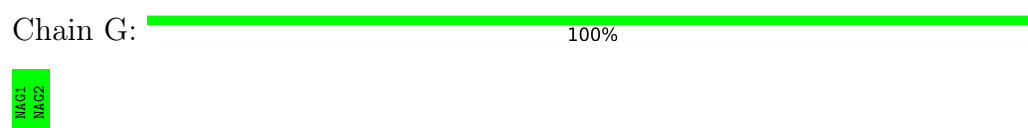
- Molecule 4: CH65 light chain



- Molecule 4: CH65 light chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%



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

Chain K:  100%



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

Chain Q:  100%



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

Chain T:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.82Å 192.19Å 333.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.80 29.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.92-2.80) 91.7 (29.92-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.289 0.260 , 0.287	Depositor DCC
R_{free} test set	2754 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	42918	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 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/2601	0.37	0/3540
1	C	0.14	0/2601	0.37	0/3540
1	E	0.12	0/2601	0.36	0/3540
2	B	0.14	0/1421	0.38	0/1909
2	D	0.14	0/1421	0.37	0/1909
2	F	0.15	0/1421	0.38	0/1909
3	H	0.12	0/1722	0.37	0/2351
3	I	0.13	0/1722	0.38	0/2351
3	J	0.13	0/1722	0.38	0/2351
4	L	0.15	0/1603	0.40	0/2192
4	M	0.16	0/1603	0.42	0/2192
4	N	0.15	0/1603	0.41	0/2192
All	All	0.14	0/22041	0.38	0/29976

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
4	L	0	1
4	M	0	1
4	N	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	142	TYR	Peptide
4	M	142	TYR	Peptide
4	N	142	TYR	Peptide

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	2535	2440	2440	14	0
1	C	2535	2440	2440	17	0
1	E	2535	2440	2440	12	0
2	B	1394	1324	1323	19	0
2	D	1394	1324	1323	16	0
2	F	1394	1324	1323	20	0
3	H	1677	1617	1617	14	1
3	I	1677	1617	1617	13	2
3	J	1677	1617	1617	12	1
4	L	1565	1513	1513	15	0
4	M	1565	1513	1513	15	0
4	N	1565	1513	1513	17	0
5	G	28	27	25	0	0
5	O	28	27	25	0	0
5	P	28	27	25	0	0
5	R	28	27	25	0	0
5	S	28	27	25	0	0
5	U	28	27	25	0	0
6	K	39	36	34	0	0
6	Q	39	36	34	0	0
6	T	39	36	34	0	0
7	A	28	28	26	0	0
7	C	28	28	26	0	0
7	E	28	28	26	0	0
All	All	21882	21036	21009	167	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.

All (167) 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)
2:B:625:GLN:NE2	2:B:655:GLY:O	2.04	0.91
2:D:625:GLN:NE2	2:D:655:GLY:O	2.09	0.86
2:F:625:GLN:NE2	2:F:655:GLY:O	2.11	0.84
1:E:225:ASP:O	1:E:226:ARG:NH1	2.12	0.81
1:C:225:ASP:O	1:C:226:ARG:NH1	2.13	0.79
1:A:225:ASP:O	1:A:226:ARG:NH1	2.17	0.77
4:N:140:ASP:OD1	4:N:169:GLN:NE2	2.20	0.73
1:C:226:ARG:NH2	3:I:107:ASP:OD2	2.23	0.71
4:N:60:ARG:NH1	4:N:81:ASP:OD2	2.24	0.69
4:M:142:TYR:O	4:M:199:HIS:NE2	2.22	0.68
1:A:226:ARG:NH2	3:H:107:ASP:OD2	2.27	0.67
4:L:142:TYR:O	4:L:199:HIS:NE2	2.24	0.67
4:N:142:TYR:O	4:N:199:HIS:NE2	2.25	0.64
1:E:226:ARG:NH2	3:J:107:ASP:OD2	2.32	0.63
4:L:140:ASP:OD1	4:L:169:GLN:NE2	2.32	0.63
4:L:20:ILE:CG2	4:L:72:LEU:HB3	2.30	0.62
1:C:23:VAL:HG21	2:D:602:LEU:HD23	1.84	0.59
4:M:20:ILE:CG2	4:M:72:LEU:HB3	2.32	0.59
4:N:20:ILE:CG2	4:N:72:LEU:HB3	2.32	0.59
4:M:140:ASP:OD1	4:M:169:GLN:NE2	2.36	0.58
1:E:23:VAL:HG21	2:F:602:LEU:HD23	1.85	0.57
1:A:23:VAL:HG21	2:B:602:LEU:HD23	1.87	0.56
3:J:197:VAL:HG21	3:J:207:TYR:CZ	2.43	0.53
3:H:197:VAL:HG21	3:H:207:TYR:CZ	2.43	0.53
4:L:142:TYR:CD2	4:L:143:PRO:HD3	2.45	0.52
3:I:28:THR:OG1	3:I:31:ASP:OD2	2.28	0.51
4:M:142:TYR:CD2	4:M:143:PRO:HD3	2.46	0.50
4:N:142:TYR:CD2	4:N:143:PRO:HD3	2.46	0.50
2:B:506:ILE:HG13	2:B:615:VAL:HG21	1.94	0.50
1:C:311:ARG:HD2	2:F:560:ASN:HD22	1.76	0.50
4:M:20:ILE:HD13	4:M:103:THR:HG21	1.93	0.50
4:L:20:ILE:HG23	4:L:72:LEU:HB3	1.94	0.49
3:I:85:GLY:O	3:I:87:LYS:NZ	2.44	0.49
1:C:124:GLU:O	1:C:125:SER:HB3	2.12	0.49
4:N:20:ILE:HD13	4:N:103:THR:HG21	1.94	0.49
3:I:197:VAL:HG21	3:I:207:TYR:CZ	2.48	0.49
2:F:503:PHE:HE2	2:F:613:SER:HB2	1.77	0.49
3:I:53:PRO:HA	3:I:72:ARG:HD3	1.95	0.49
1:A:214:THR:O	1:C:212:LYS:NZ	2.46	0.49
3:H:53:PRO:HA	3:H:72:ARG:HD3	1.95	0.49
3:J:28:THR:OG1	3:J:31:ASP:OD2	2.31	0.48
2:F:651:SER:HB3	2:F:656:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ASP:OD2	2:F:644:CYS:N	2.38	0.48
1:E:124:GLU:O	1:E:125:SER:HB3	2.13	0.48
4:M:182:LEU:HB2	4:M:186:GLN:OE1	2.13	0.48
4:L:20:ILE:HD13	4:L:103:THR:HG21	1.94	0.47
1:A:124:GLU:O	1:A:125:SER:HB3	2.14	0.47
1:A:311:ARG:HD2	2:D:560:ASN:HD22	1.80	0.47
2:B:558:LYS:HD2	2:F:597:GLU:OE1	2.14	0.47
2:B:560:ASN:HD22	1:E:311:ARG:HD2	1.78	0.47
4:L:60:ARG:NH1	4:L:81:ASP:OD2	2.35	0.47
2:B:651:SER:HB3	2:B:656:THR:O	2.15	0.47
3:J:208:ILE:HA	3:J:222:LYS:O	2.15	0.47
4:N:194:SER:HB3	4:N:207:THR:HG22	1.95	0.47
4:N:142:TYR:CD2	4:N:143:PRO:CD	2.98	0.47
4:L:194:SER:HB3	4:L:207:THR:HG22	1.97	0.47
2:D:506:ILE:HG13	2:D:615:VAL:HG21	1.97	0.47
4:L:121:PRO:HB3	4:L:208:VAL:HG11	1.97	0.47
4:M:20:ILE:HG23	4:M:72:LEU:HB3	1.97	0.46
1:C:110:SER:OG	1:C:267:GLY:N	2.49	0.46
3:J:53:PRO:HA	3:J:72:ARG:HD3	1.96	0.46
2:F:506:ILE:HG13	2:F:615:VAL:HG21	1.98	0.46
3:I:197:VAL:HG22	3:I:198:PRO:HD2	1.98	0.46
4:M:153:ASP:O	4:M:154:SER:OG	2.23	0.46
4:L:142:TYR:CD2	4:L:143:PRO:CD	2.99	0.46
2:B:648:CYS:O	2:B:651:SER:HB2	2.15	0.46
4:M:142:TYR:CD2	4:M:143:PRO:CD	2.98	0.46
4:N:121:PRO:HB3	4:N:208:VAL:HG11	1.98	0.46
2:D:651:SER:HB3	2:D:656:THR:O	2.16	0.46
3:I:197:VAL:HG21	3:I:207:TYR:CE1	2.51	0.46
4:L:153:ASP:O	4:L:154:SER:OG	2.25	0.45
4:M:60:ARG:NH1	4:M:81:ASP:OD2	2.33	0.45
4:N:20:ILE:HG23	4:N:72:LEU:HB3	1.97	0.45
3:H:197:VAL:CG2	3:H:198:PRO:HD2	2.47	0.45
4:N:180:LEU:HD21	4:N:182:LEU:HD23	1.98	0.45
2:B:503:PHE:HE2	2:B:613:SER:HB2	1.81	0.44
2:F:530:GLN:HE22	2:F:645:ASN:HB2	1.81	0.44
3:J:18:VAL:HG13	3:J:86:LEU:HD11	2.00	0.44
4:L:16:GLN:HG2	4:L:17:THR:H	1.81	0.44
4:N:153:ASP:O	4:N:154:SER:OG	2.22	0.44
4:M:16:GLN:HG2	4:M:17:THR:H	1.82	0.44
1:C:126:SER:O	1:C:166:LYS:HE2	2.17	0.44
3:I:18:VAL:HG13	3:I:86:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:VAL:HG13	3:J:81:MET:SD	2.58	0.44
2:D:528:ASN:O	2:D:529:GLU:C	2.61	0.44
4:L:180:LEU:HD21	4:L:182:LEU:HD23	1.99	0.44
4:M:194:SER:HB3	4:M:207:THR:HG22	1.98	0.44
2:B:528:ASN:O	2:B:529:GLU:C	2.60	0.44
2:D:509:PHE:O	2:D:635:ASN:HB3	2.18	0.44
2:F:528:ASN:O	2:F:529:GLU:C	2.60	0.44
4:M:180:LEU:HD21	4:M:182:LEU:HD23	1.99	0.44
2:B:603:GLU:OE2	2:F:602:LEU:HD22	2.18	0.43
2:D:642:HIS:HD2	2:D:666:SER:OG	2.00	0.43
2:D:648:CYS:O	2:D:651:SER:HB2	2.18	0.43
2:F:642:HIS:HD2	2:F:666:SER:OG	2.01	0.43
2:F:509:PHE:O	2:F:635:ASN:HB3	2.18	0.43
1:A:284:THR:OG1	1:A:285:PRO:HD2	2.19	0.43
2:D:633:ILE:HD13	2:D:639:GLU:HB2	2.00	0.43
1:E:126:SER:O	1:E:166:LYS:HE2	2.18	0.43
4:N:182:LEU:HB2	4:N:186:GLN:OE1	2.19	0.43
3:H:208:ILE:HA	3:H:222:LYS:O	2.18	0.43
2:D:554:SER:O	2:D:558:LYS:CG	2.66	0.43
4:L:7:PRO:HG2	4:L:20:ILE:CD1	2.48	0.43
1:A:126:SER:O	1:A:166:LYS:HE2	2.19	0.43
3:H:73:ASP:O	3:H:74:THR:HB	2.19	0.43
2:D:597:GLU:OE1	2:F:558:LYS:HD2	2.19	0.43
3:H:32:TYR:CD1	3:H:100:GLY:HA2	2.54	0.43
1:A:150:ASN:OD1	1:A:256:TYR:HB2	2.19	0.42
3:H:134:VAL:HG12	3:H:222:LYS:HG3	2.00	0.42
1:A:284:THR:OG1	1:A:299:HIS:HB3	2.19	0.42
2:D:503:PHE:HE2	2:D:613:SER:HB2	1.84	0.42
2:F:626:LEU:O	2:F:627:LYS:C	2.62	0.42
4:M:121:PRO:HB3	4:M:208:VAL:HG11	2.00	0.42
1:E:150:ASN:OD1	1:E:256:TYR:HB2	2.19	0.42
2:D:602:LEU:HD22	2:F:603:GLU:OE2	2.19	0.42
1:E:213:PHE:CE1	1:E:233:TYR:CE2	3.08	0.42
3:I:73:ASP:O	3:I:74:THR:HB	2.19	0.42
3:I:208:ILE:HA	3:I:222:LYS:O	2.20	0.42
2:B:575:ARG:HG3	1:C:108:GLN:HG2	2.02	0.42
3:J:101:LEU:HG	3:J:114:ASP:OD1	2.19	0.42
3:J:214:LYS:N	3:J:215:PRO:CD	2.82	0.42
2:B:642:HIS:HD2	2:B:666:SER:OG	2.02	0.42
2:D:633:ILE:HG21	2:D:639:GLU:HB2	2.02	0.42
4:M:7:PRO:HG2	4:M:20:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:ILE:HD13	2:B:639:GLU:HB2	2.02	0.42
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.60	0.42
3:J:197:VAL:CG2	3:J:198:PRO:HD2	2.50	0.42
4:N:7:PRO:HG2	4:N:20:ILE:CD1	2.50	0.42
1:A:42:ASN:OD1	1:A:288:ALA:N	2.52	0.42
2:B:503:PHE:CZ	2:F:503:PHE:HE1	2.38	0.42
3:H:68:VAL:HG13	3:H:81:MET:SD	2.59	0.42
3:J:197:VAL:HG22	3:J:198:PRO:HD2	2.02	0.42
1:C:22:THR:HB	1:C:25:GLU:O	2.19	0.42
2:F:633:ILE:O	2:F:634:GLY:C	2.63	0.42
3:H:197:VAL:HG22	3:H:198:PRO:HD2	2.00	0.42
1:C:42:ASN:OD1	1:C:288:ALA:N	2.53	0.41
3:I:68:VAL:HG13	3:I:81:MET:SD	2.60	0.41
3:J:73:ASP:O	3:J:74:THR:HB	2.19	0.41
4:N:7:PRO:HG2	4:N:20:ILE:HD11	2.02	0.41
2:B:509:PHE:O	2:B:635:ASN:HB3	2.20	0.41
3:I:101:LEU:HG	3:I:114:ASP:OD1	2.20	0.41
1:E:22:THR:HB	1:E:25:GLU:O	2.20	0.41
3:I:197:VAL:CG2	3:I:198:PRO:HD2	2.51	0.41
2:D:633:ILE:O	2:D:634:GLY:C	2.63	0.41
2:B:626:LEU:O	2:B:627:LYS:C	2.63	0.41
2:B:651:SER:O	2:B:656:THR:O	2.39	0.41
1:C:97:GLY:HA3	1:C:230:ILE:O	2.21	0.41
3:H:101:LEU:HG	3:H:114:ASP:OD1	2.21	0.41
1:C:150:ASN:OD1	1:C:256:TYR:HB2	2.21	0.41
3:H:18:VAL:HG13	3:H:86:LEU:HD11	2.02	0.41
1:C:47:LEU:HB2	1:C:52:ALA:HA	2.03	0.40
1:E:110:SER:OG	1:E:267:GLY:N	2.54	0.40
1:A:102:TYR:CE2	1:A:106:ARG:HD2	2.56	0.40
2:F:648:CYS:O	2:F:651:SER:HB2	2.20	0.40
3:H:163:VAL:HG13	3:H:191:LEU:HD21	2.03	0.40
1:A:22:THR:HB	1:A:25:GLU:O	2.22	0.40
2:B:554:SER:O	2:B:558:LYS:CG	2.69	0.40
1:C:284:THR:O	1:C:285:PRO:C	2.65	0.40
4:L:151:LYS:HB2	4:L:194:SER:OG	2.22	0.40
4:N:16:GLN:HG2	4:N:17:THR:H	1.86	0.40
2:B:633:ILE:O	2:B:634:GLY:C	2.65	0.40
1:E:284:THR:O	1:E:285:PRO:C	2.63	0.40
2:F:651:SER:O	2:F:656:THR:O	2.40	0.40
3:H:28:THR:OG1	3:H:31:ASP:OD2	2.39	0.40
4:N:191:ARG:O	4:N:191:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.40
1:C:201:TYR:HA	1:C:213:PHE:O	2.21	0.40

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)
3:H:173:THR:OG1	3:I:173:THR:OG1[8_555]	2.11	0.09
3:I:200:SER:OG	3:J:185:SER:OG[3_545]	2.13	0.07

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	321/323 (99%)	304 (95%)	16 (5%)	1 (0%)	36	66
1	C	321/323 (99%)	305 (95%)	15 (5%)	1 (0%)	36	66
1	E	321/323 (99%)	305 (95%)	15 (5%)	1 (0%)	36	66
2	B	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	D	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	F	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
3	H	217/227 (96%)	205 (94%)	12 (6%)	0	100	100
3	I	217/227 (96%)	207 (95%)	10 (5%)	0	100	100
3	J	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
4	L	208/210 (99%)	196 (94%)	10 (5%)	2 (1%)	12	38
4	M	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	12	38
4	N	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	12	38
All	All	2751/2799 (98%)	2593 (94%)	149 (5%)	9 (0%)	36	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	143	PRO
4	M	143	PRO
4	N	143	PRO
4	L	31	SER
4	M	31	SER
4	N	31	SER
1	C	57	GLY
1	E	57	GLY
1	A	57	GLY

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	283/283 (100%)	283 (100%)	0	100	100
1	C	283/283 (100%)	283 (100%)	0	100	100
1	E	283/283 (100%)	283 (100%)	0	100	100
2	B	149/149 (100%)	149 (100%)	0	100	100
2	D	149/149 (100%)	149 (100%)	0	100	100
2	F	149/149 (100%)	149 (100%)	0	100	100
3	H	185/190 (97%)	185 (100%)	0	100	100
3	I	185/190 (97%)	185 (100%)	0	100	100
3	J	185/190 (97%)	185 (100%)	0	100	100
4	L	177/177 (100%)	177 (100%)	0	100	100
4	M	177/177 (100%)	177 (100%)	0	100	100
4	N	177/177 (100%)	177 (100%)	0	100	100
All	All	2382/2397 (99%)	2382 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	270	ASN
1	C	183	HIS
1	C	184	HIS
1	C	270	ASN
1	C	296	GLN
1	E	183	HIS
3	H	33	HIS
3	I	33	HIS
4	M	35	ASN
4	N	35	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 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	$\# Z > 2$
5	NAG	G	1	5,1	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	K	1	1,6	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.20	0	17,19,21	0.40	0
6	BMA	K	3	6	11,11,12	0.55	0	15,15,17	0.95	0
5	NAG	O	1	5,1	14,14,15	0.33	0	17,19,21	0.62	0
5	NAG	O	2	5	14,14,15	0.18	0	17,19,21	0.50	0
5	NAG	P	1	5,1	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	P	2	5	14,14,15	0.25	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	Q	1	1,6	14,14,15	0.18	0	17,19,21	0.43	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.42	0
6	BMA	Q	3	6	11,11,12	0.55	0	15,15,17	0.94	0
5	NAG	R	1	5,1	14,14,15	0.30	0	17,19,21	0.66	0
5	NAG	R	2	5	14,14,15	0.17	0	17,19,21	0.49	0
5	NAG	S	1	5,1	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	S	2	5	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	T	1	1,6	14,14,15	0.17	0	17,19,21	0.43	0
6	NAG	T	2	6	14,14,15	0.20	0	17,19,21	0.42	0
6	BMA	T	3	6	11,11,12	0.57	0	15,15,17	0.94	0
5	NAG	U	1	5,1	14,14,15	0.33	0	17,19,21	0.64	1 (5%)
5	NAG	U	2	5	14,14,15	0.19	0	17,19,21	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	BMA	T	3	6	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

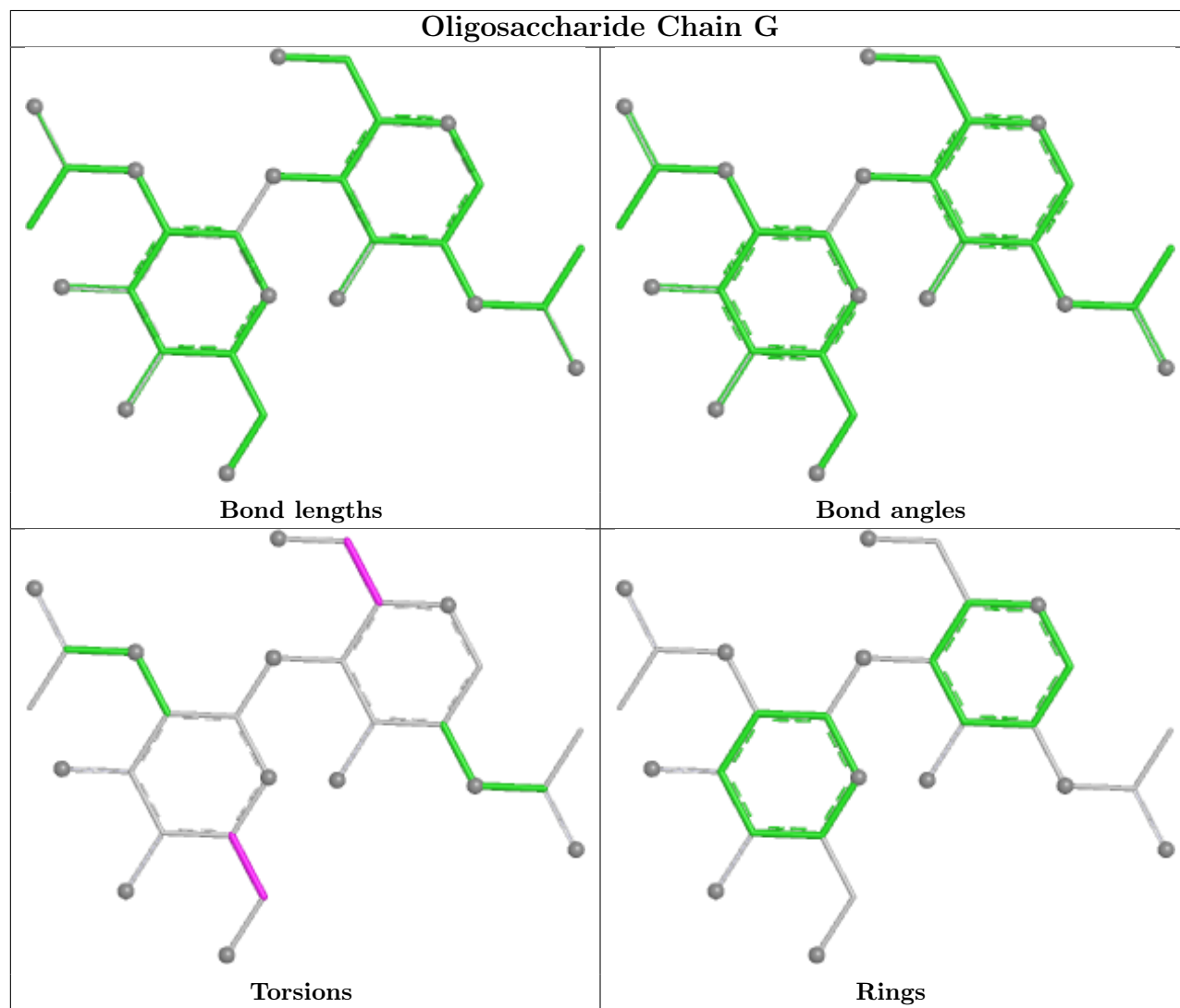
All (28) torsion outliers are listed below:

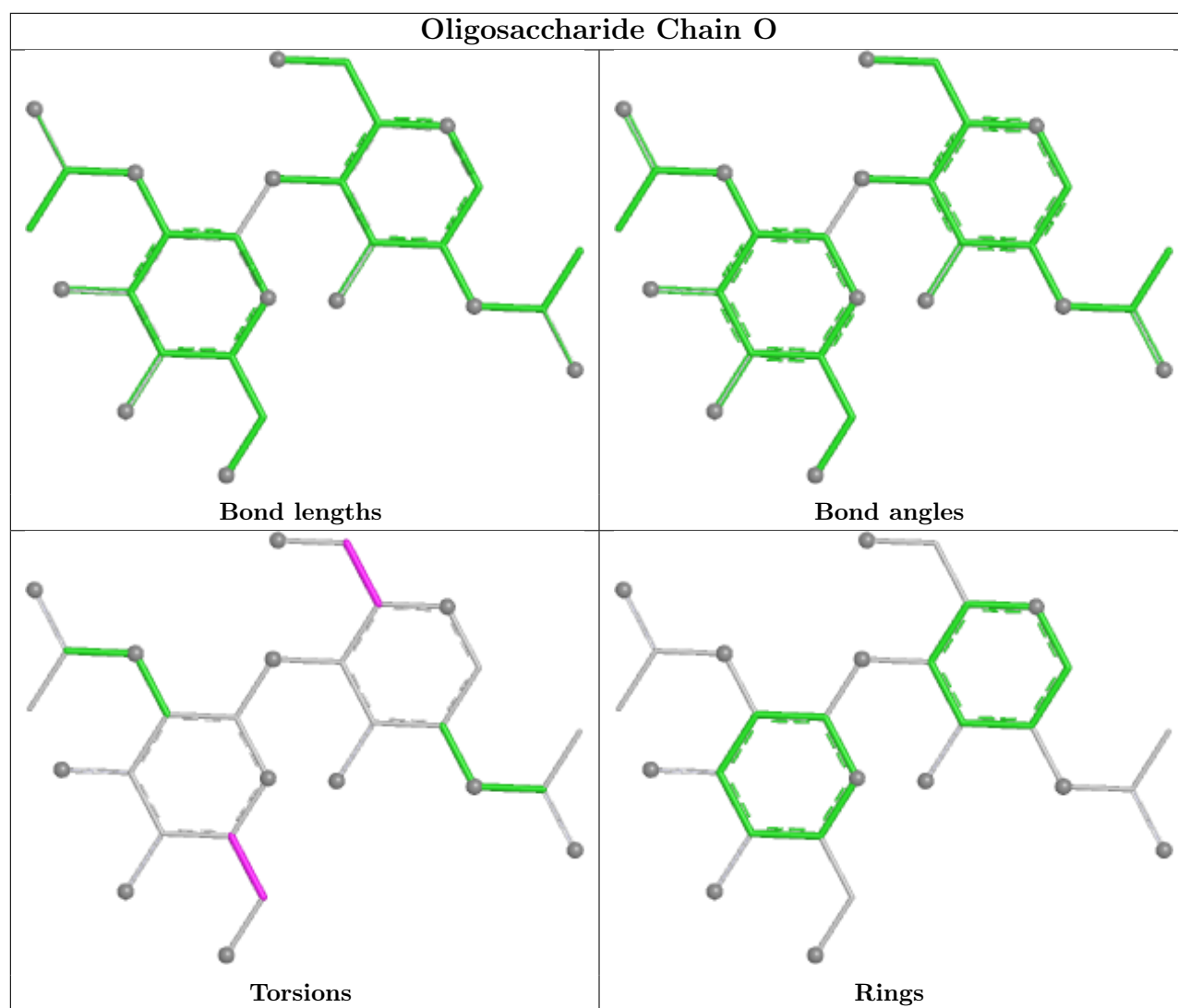
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6

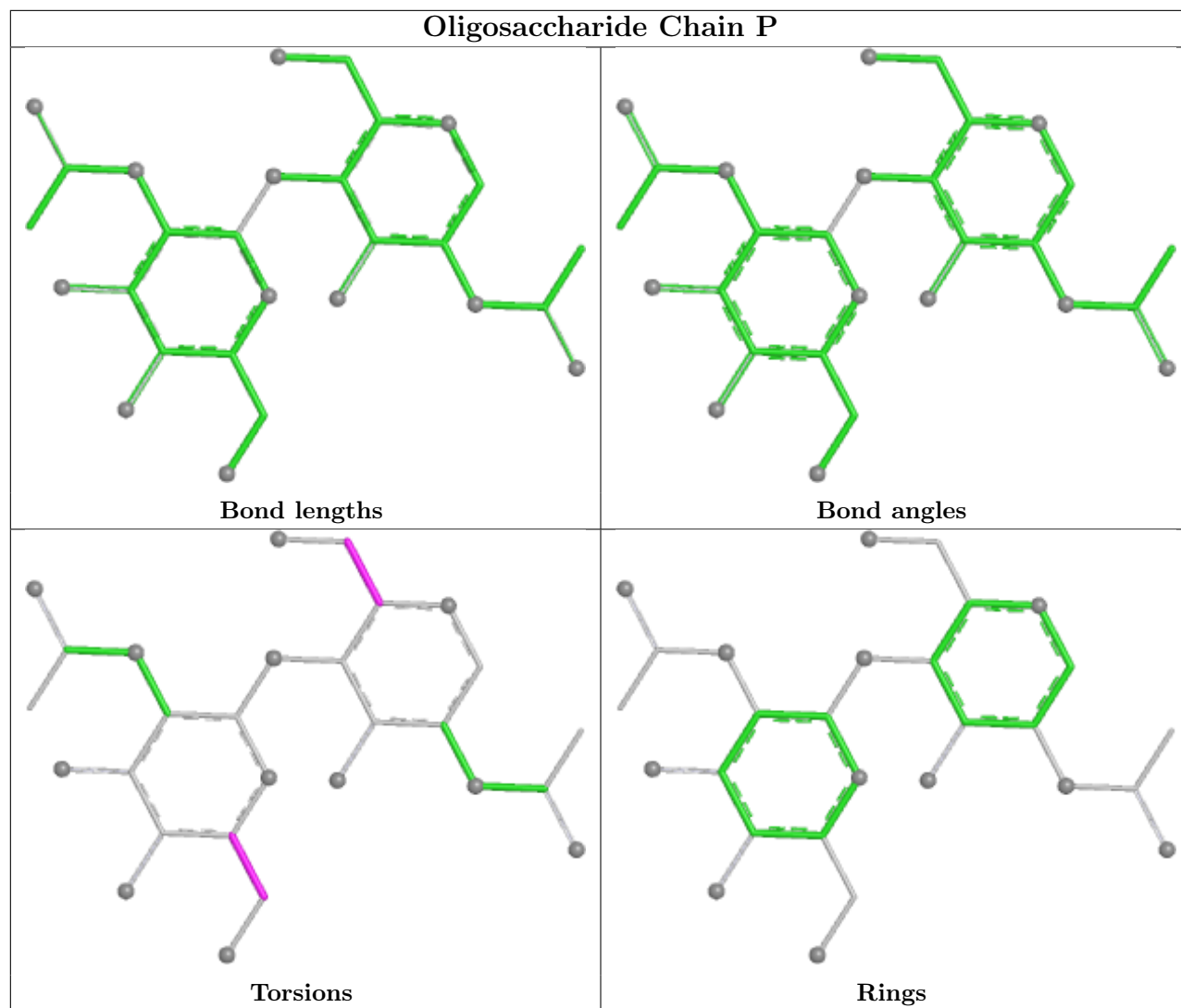
There are no ring outliers.

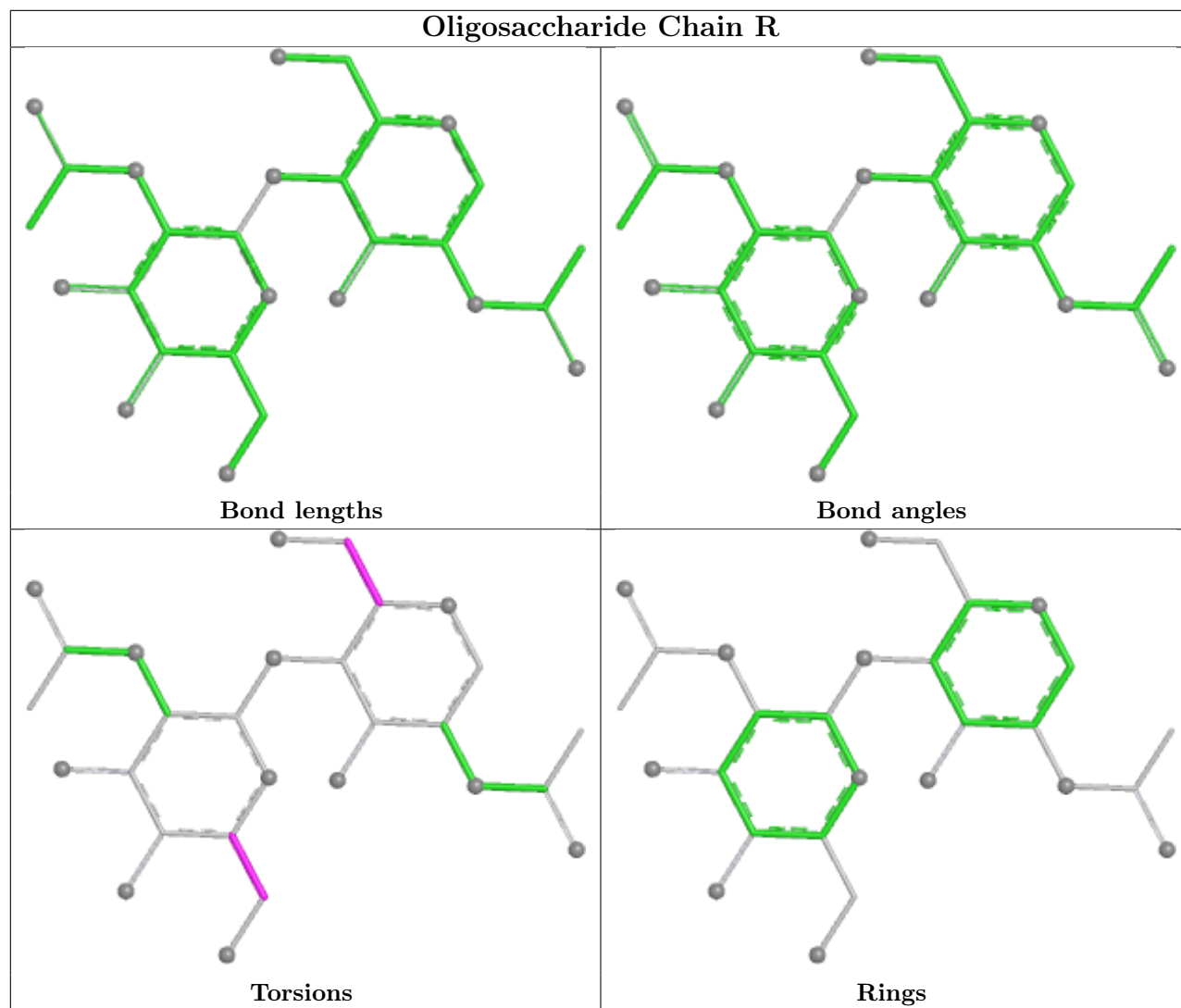
No monomer is involved in short contacts.

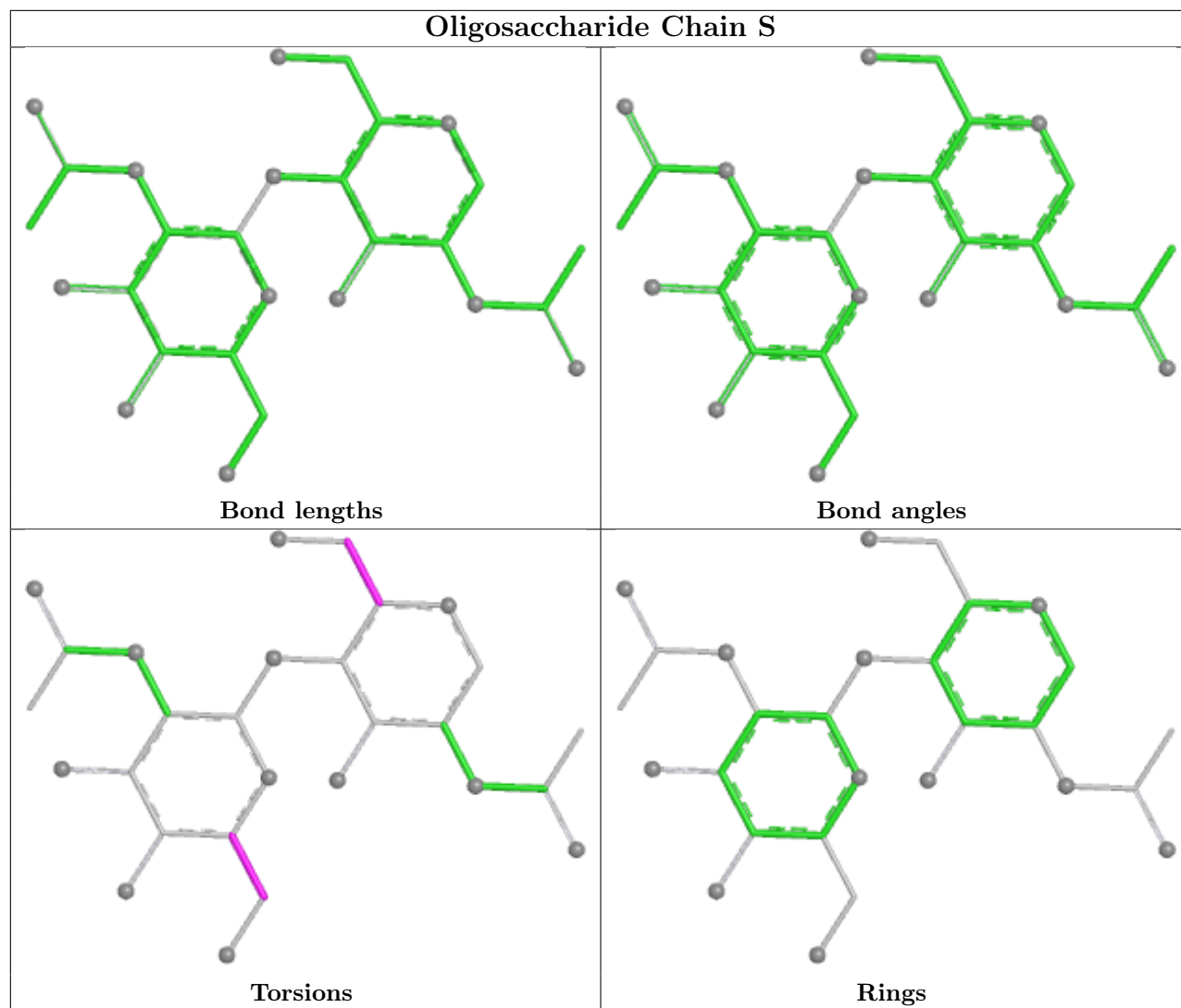
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

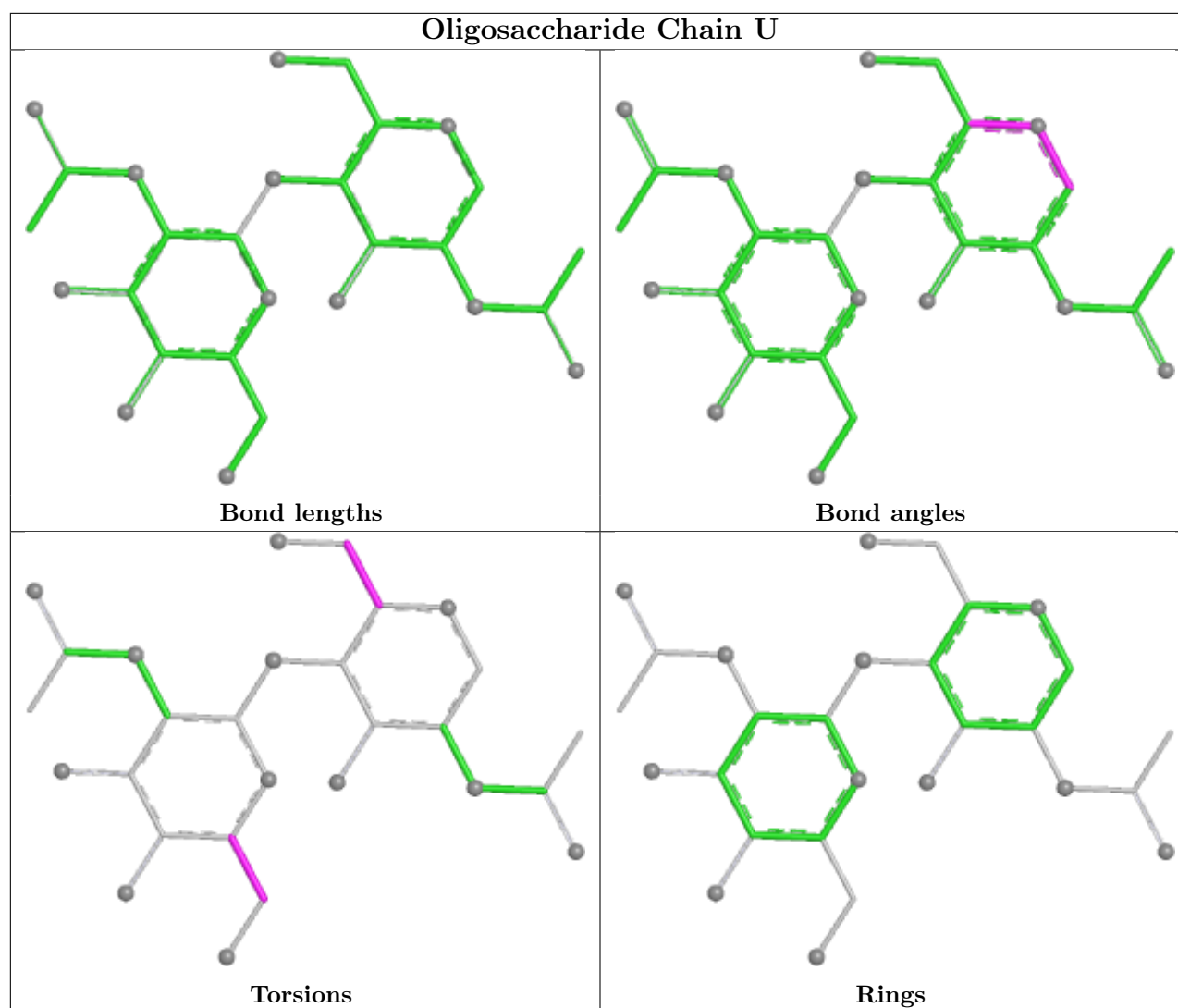


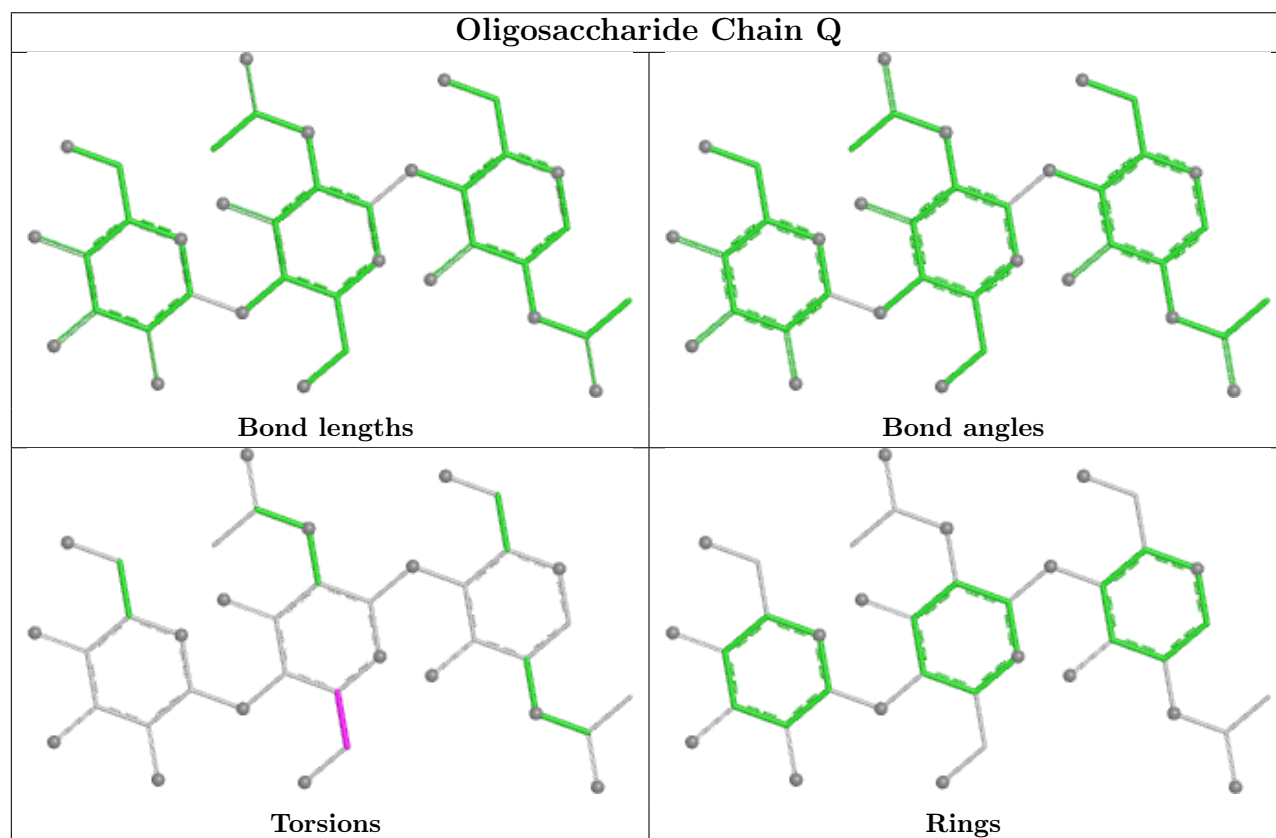
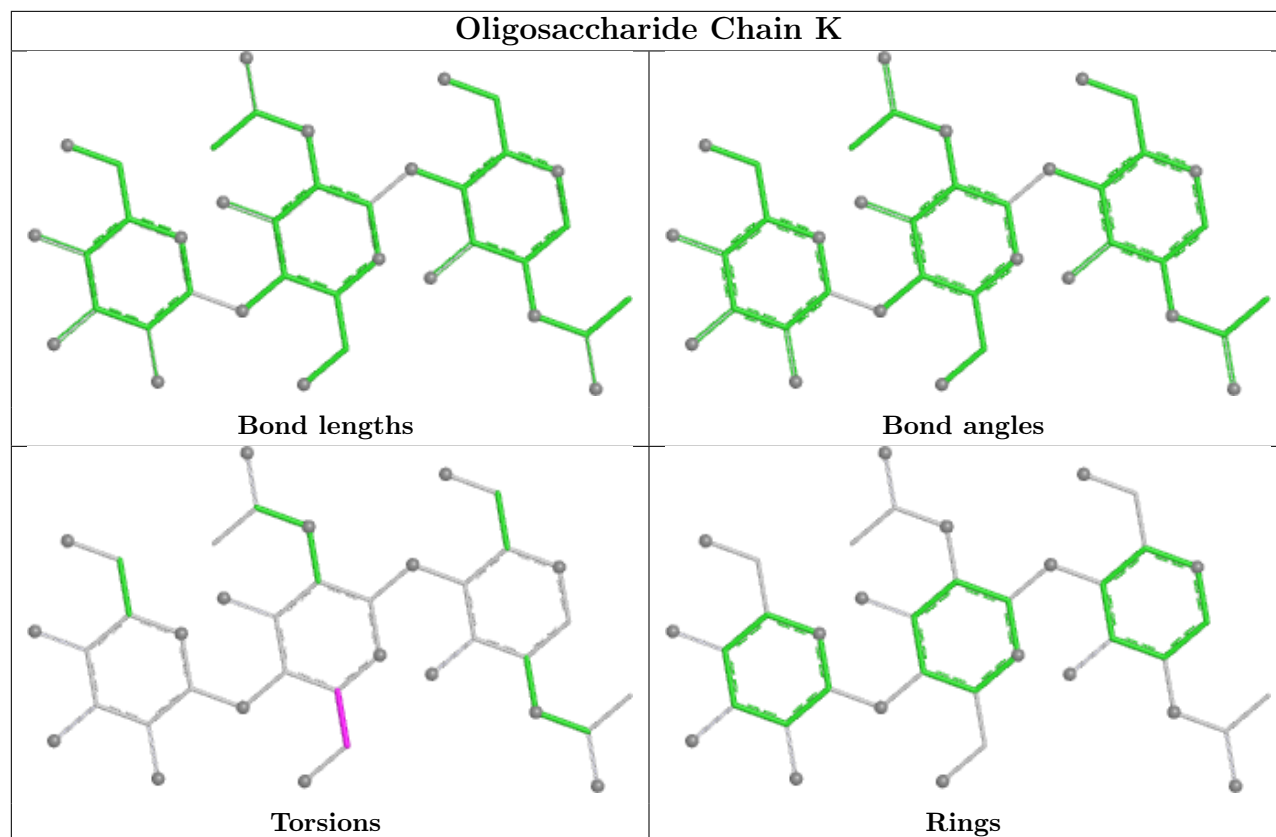


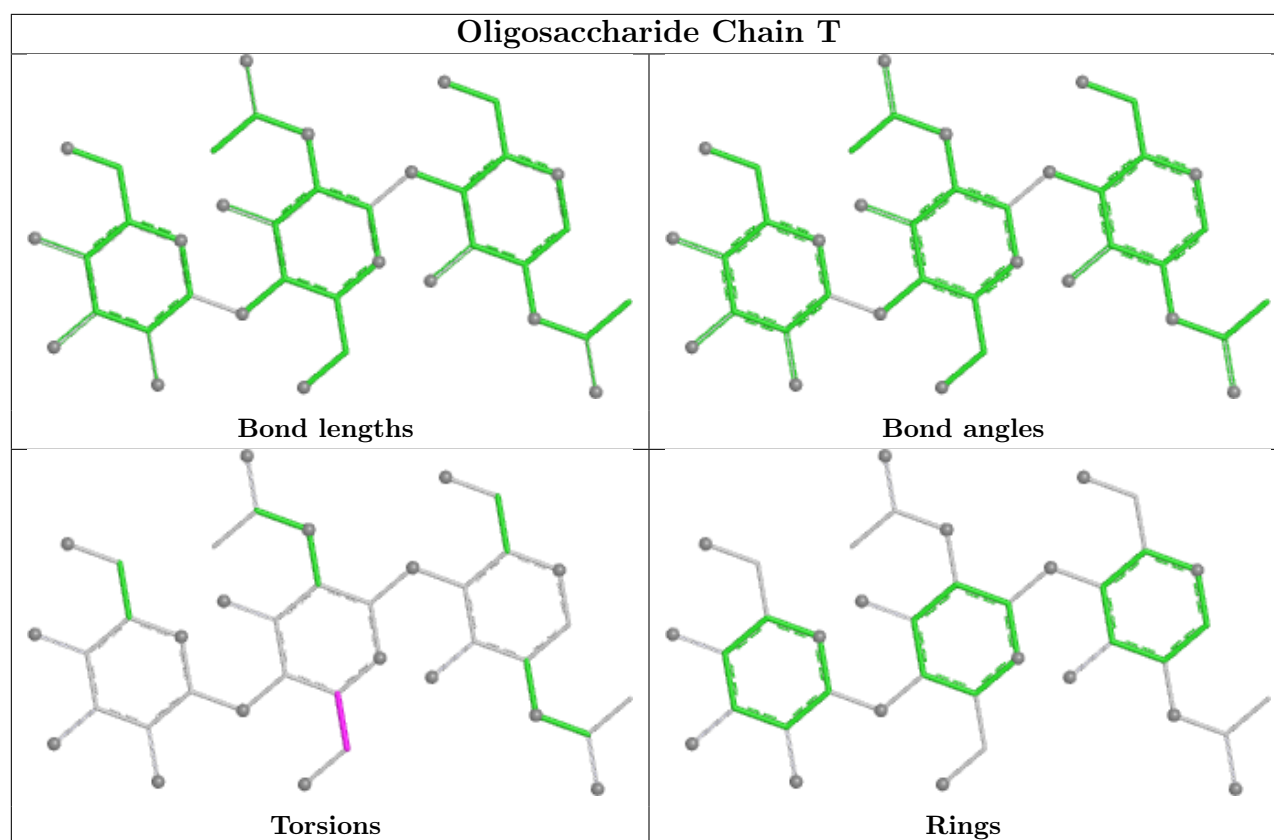












5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
7	NAG	A	406	1	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	E	406	1	14,14,15	0.25	0	17,19,21	0.52	0
7	NAG	C	406	1	14,14,15	0.27	0	17,19,21	0.50	0
7	NAG	A	407	1	14,14,15	0.15	0	17,19,21	0.47	0
7	NAG	E	407	1	14,14,15	0.16	0	17,19,21	0.46	0
7	NAG	C	407	1	14,14,15	0.17	0	17,19,21	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	406	1	-	2/6/23/26	0/1/1/1
7	NAG	E	406	1	-	2/6/23/26	0/1/1/1
7	NAG	C	406	1	-	1/6/23/26	0/1/1/1
7	NAG	A	407	1	-	0/6/23/26	0/1/1/1
7	NAG	E	407	1	-	0/6/23/26	0/1/1/1
7	NAG	C	407	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	NAG	O5-C5-C6-O6
7	E	406	NAG	O5-C5-C6-O6
7	C	406	NAG	O5-C5-C6-O6
7	A	406	NAG	C4-C5-C6-O6
7	E	406	NAG	C4-C5-C6-O6

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	323/323 (100%)	1.07	47 (14%) 6 4	32, 56, 86, 118	0
1	C	323/323 (100%)	0.77	33 (10%) 12 9	18, 41, 77, 110	0
1	E	323/323 (100%)	0.76	32 (9%) 13 9	19, 39, 74, 115	0
2	B	173/173 (100%)	1.40	42 (24%) 2 1	18, 59, 100, 118	0
2	D	173/173 (100%)	1.70	64 (36%) 1 0	12, 59, 112, 133	0
2	F	173/173 (100%)	1.59	64 (36%) 1 0	17, 50, 117, 126	0
3	H	221/227 (97%)	0.31	10 (4%) 38 30	16, 37, 61, 92	0
3	I	221/227 (97%)	0.48	23 (10%) 11 8	14, 31, 80, 117	0
3	J	221/227 (97%)	0.49	23 (10%) 11 8	13, 31, 73, 104	0
4	L	210/210 (100%)	1.04	32 (15%) 5 4	28, 56, 84, 115	0
4	M	210/210 (100%)	0.69	21 (10%) 12 9	22, 46, 77, 109	0
4	N	210/210 (100%)	0.67	15 (7%) 22 16	16, 39, 64, 91	0
All	All	2781/2799 (99%)	0.88	406 (14%) 6 4	12, 44, 90, 133	0

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	673	ILE	9.0
2	B	673	ILE	8.2
2	F	673	ILE	7.5
1	A	326	SER	7.3
1	A	73	LEU	7.0
2	B	643	LYS	6.7
1	E	75	ILE	6.7
2	D	527	GLN	6.4
1	E	326	SER	6.4
3	I	227	LYS	6.4
1	E	74	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
2	F	533	GLY	5.9
2	D	640	PHE	5.9
3	J	227	LYS	5.8
1	E	73	LEU	5.6
1	E	264	PHE	5.6
1	C	264	PHE	5.5
2	F	530	GLN	5.5
1	A	75	ILE	5.5
1	A	264	PHE	5.5
2	F	658	ASP	5.3
3	I	174	SER	5.3
2	F	644	CYS	5.2
4	N	191	ARG	5.1
2	B	672	LYS	5.1
2	D	641	TYR	5.1
3	I	140	SER	5.1
2	F	531	GLY	5.0
1	C	72	GLU	5.0
3	I	147	GLY	5.0
2	D	643	LYS	5.0
2	D	627	LYS	4.9
4	N	2	SER	4.8
2	F	526	HIS	4.8
1	A	74	LEU	4.8
1	E	72	GLU	4.7
2	B	668	LEU	4.7
2	F	529	GLU	4.7
2	D	528	ASN	4.7
2	D	533	GLY	4.7
3	H	140	SER	4.6
2	D	560	ASN	4.6
1	E	4	GLU	4.5
3	J	204	THR	4.5
4	L	108	LEU	4.5
1	C	76	SER	4.5
2	B	647	GLU	4.4
2	F	538	GLN	4.4
2	D	538	GLN	4.4
2	F	527	GLN	4.4
2	D	526	HIS	4.4
1	C	73	LEU	4.3
1	C	326	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	76	SER	4.3
2	F	532	SER	4.3
2	D	642	HIS	4.3
1	C	125	SER	4.2
2	F	633	ILE	4.2
1	C	74	LEU	4.1
3	J	147	GLY	4.1
2	F	643	LYS	4.1
4	M	211	THR	4.1
2	D	662	TYR	4.1
2	F	627	LYS	4.1
3	H	227	LYS	4.1
1	A	115	PHE	4.1
3	J	207	TYR	4.1
1	E	144	GLU	4.1
2	F	650	GLU	4.1
4	L	202	SER	4.1
2	D	638	PHE	4.1
4	N	202	SER	4.0
1	C	75	ILE	4.0
2	D	669	ASN	4.0
2	F	668	LEU	4.0
2	D	658	ASP	4.0
2	D	652	VAL	4.0
2	F	663	SER	3.9
3	I	173	THR	3.9
2	F	647	GLU	3.9
2	F	656	THR	3.9
3	I	203	GLY	3.9
2	D	672	LYS	3.8
2	F	672	LYS	3.8
2	B	538	GLN	3.8
2	F	628	ASN	3.8
3	J	140	SER	3.8
2	F	519	ASP	3.8
2	F	626	LEU	3.8
2	D	531	GLY	3.8
2	F	664	GLU	3.7
2	F	651	SER	3.7
4	L	76	ARG	3.7
2	F	560	ASN	3.7
2	F	669	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
4	L	17	THR	3.7
1	E	15	ASN	3.7
2	D	660	PRO	3.7
2	B	560	ASN	3.7
2	D	655	GLY	3.7
3	I	148	THR	3.7
2	F	646	ASP	3.6
3	H	67	TRP	3.6
3	J	203	GLY	3.6
1	C	286	GLN	3.6
1	A	40	SER	3.6
4	L	191	ARG	3.6
2	B	634	GLY	3.6
2	B	658	ASP	3.6
2	D	628	ASN	3.6
1	A	49	LYS	3.6
2	D	561	THR	3.6
3	I	149	ALA	3.5
1	C	261	SER	3.5
2	D	636	GLY	3.5
4	N	20	ILE	3.5
2	F	662	TYR	3.5
3	I	204	THR	3.5
2	D	656	THR	3.5
2	B	646	ASP	3.5
2	B	530	GLN	3.5
2	D	530	GLN	3.5
1	C	303	ILE	3.5
1	A	262	ARG	3.4
1	A	125	SER	3.4
2	F	634	GLY	3.4
4	M	2	SER	3.4
1	C	124	GLU	3.4
2	B	519	ASP	3.4
4	L	109	GLY	3.3
2	D	529	GLU	3.3
2	B	621	LYS	3.3
1	A	286	GLN	3.3
2	F	561	THR	3.3
3	H	88	SER	3.3
3	I	207	TYR	3.3
3	J	197	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	635	ASN	3.3
4	M	191	ARG	3.3
2	D	516	GLY	3.3
2	F	501	GLY	3.3
2	F	528	ASN	3.3
2	D	542	GLN	3.3
2	D	646	ASP	3.2
2	D	629	ASN	3.2
3	H	63	LYS	3.2
2	F	635	ASN	3.2
1	C	7	ILE	3.2
1	E	86	LYS	3.2
4	L	2	SER	3.2
4	L	189	SER	3.2
1	E	262	ARG	3.2
2	B	528	ASN	3.2
2	D	626	LEU	3.2
2	B	562	GLN	3.2
4	L	16	GLN	3.2
1	C	275	MET	3.2
2	D	633	ILE	3.2
2	B	527	GLN	3.1
2	F	516	GLY	3.1
2	F	645	ASN	3.1
1	A	4	GLU	3.1
1	A	90	GLU	3.1
1	E	5	ASP	3.1
2	D	519	ASP	3.1
2	B	523	GLY	3.1
4	L	211	THR	3.1
2	B	649	MET	3.0
4	M	154	SER	3.0
2	F	653	LYS	3.0
4	N	185	GLU	3.0
1	C	9	ILE	3.0
2	D	634	GLY	3.0
1	E	57	GLY	3.0
1	E	263	GLY	3.0
4	N	76	ARG	3.0
4	M	51	SER	3.0
2	D	523	GLY	3.0
3	J	205	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	666	SER	3.0
1	A	317	MET	3.0
2	F	536	ALA	3.0
2	F	621	LYS	2.9
2	F	654	ASN	2.9
1	E	125	SER	2.9
2	F	671	GLU	2.9
4	M	202	SER	2.9
3	J	171	ALA	2.9
2	B	636	GLY	2.9
2	F	659	TYR	2.9
3	I	150	ALA	2.9
4	N	3	VAL	2.9
2	B	501	GLY	2.9
2	B	508	GLY	2.9
3	J	198	PRO	2.9
1	C	277	GLU	2.9
4	L	75	SER	2.9
1	E	208	HIS	2.9
2	D	644	CYS	2.9
2	F	572	LYS	2.9
3	I	198	PRO	2.8
2	D	650	GLU	2.8
2	D	659	TYR	2.8
4	L	188	LYS	2.8
1	C	13	ALA	2.8
4	M	29	ARG	2.8
1	A	271	SER	2.8
1	C	32	HIS	2.8
2	D	618	LEU	2.8
2	B	641	TYR	2.8
2	D	668	LEU	2.8
1	E	325	PRO	2.8
4	L	26	ASP	2.8
3	J	148	THR	2.8
2	D	562	GLN	2.8
4	M	76	ARG	2.8
3	I	177	HIS	2.8
2	B	631	LYS	2.8
2	D	657	TYR	2.7
2	B	572	LYS	2.7
3	H	201	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	201	SER	2.7
4	L	24	GLY	2.7
3	J	226	PRO	2.7
2	B	663	SER	2.7
1	A	278	CYS	2.7
1	C	265	GLY	2.7
1	C	4	GLU	2.7
2	B	529	GLU	2.7
1	C	289	ILE	2.7
2	F	640	PHE	2.7
1	C	86	LYS	2.7
1	E	286	GLN	2.7
4	L	12	VAL	2.7
3	J	174	SER	2.7
1	C	208	HIS	2.6
3	J	67	TRP	2.6
3	I	197	VAL	2.6
3	J	63	LYS	2.6
1	E	291	SER	2.6
2	D	532	SER	2.6
3	I	126	SER	2.6
4	L	154	SER	2.6
1	C	6	THR	2.6
4	L	207	THR	2.6
1	E	259	ALA	2.6
3	I	171	ALA	2.6
4	L	192	SER	2.6
2	F	661	LYS	2.6
1	A	72	GLU	2.6
2	B	671	GLU	2.6
2	D	645	ASN	2.6
2	D	647	GLU	2.6
2	B	509	PHE	2.6
1	A	111	SER	2.6
1	A	86	LYS	2.6
2	F	615	VAL	2.6
3	I	206	THR	2.6
4	N	107	VAL	2.6
1	A	283	GLN	2.6
3	I	138	ALA	2.6
4	M	25	ASN	2.6
1	C	87	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	263	GLY	2.5
4	L	74	ILE	2.5
4	L	18	ALA	2.5
2	F	525	HIS	2.5
2	D	631	LYS	2.5
2	F	636	GLY	2.5
1	A	17	THR	2.5
1	A	116	GLU	2.5
3	J	73	ASP	2.5
4	N	153	ASP	2.5
1	A	143	GLY	2.5
3	I	67	TRP	2.5
2	D	671	GLU	2.5
2	D	648	CYS	2.5
4	L	25	ASN	2.5
4	N	25	ASN	2.5
4	M	52	ASP	2.5
2	D	525	HIS	2.5
2	B	536	ALA	2.4
2	D	572	LYS	2.4
2	F	642	HIS	2.4
1	E	9	ILE	2.4
3	J	199	SER	2.4
4	L	9	SER	2.4
4	M	55	SER	2.4
1	A	124	GLU	2.4
2	F	539	LYS	2.4
4	L	196	GLN	2.4
2	B	660	PRO	2.4
2	F	648	CYS	2.4
2	D	518	VAL	2.4
4	L	15	GLY	2.4
1	C	144	GLU	2.4
2	F	503	PHE	2.4
2	B	669	ASN	2.4
2	B	640	PHE	2.4
2	D	503	PHE	2.4
1	E	292	SER	2.4
2	F	666	SER	2.4
3	J	201	SER	2.4
4	L	124	SER	2.4
4	M	189	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	657	TYR	2.4
3	H	173	THR	2.4
3	I	196	THR	2.4
1	A	289	ILE	2.4
2	F	670	ARG	2.3
3	J	1	GLU	2.3
4	M	209	ALA	2.3
4	M	188	LYS	2.3
2	D	511	GLU	2.3
2	F	665	GLU	2.3
4	M	59	GLU	2.3
1	A	261	SER	2.3
2	F	641	TYR	2.3
1	A	27	ASN	2.3
1	A	296	GLN	2.3
1	A	64	TRP	2.3
1	A	76	SER	2.3
3	H	174	SER	2.3
1	E	284	THR	2.3
1	C	262	ARG	2.3
2	F	657	TYR	2.3
1	E	50	GLY	2.3
2	F	655	GLY	2.3
2	D	649	MET	2.3
2	D	664	GLU	2.3
1	C	5	ASP	2.3
2	B	532	SER	2.3
4	N	32	VAL	2.3
1	A	274	PRO	2.2
1	E	111	SER	2.2
1	E	261	SER	2.2
2	B	522	TYR	2.2
2	D	534	TYR	2.2
2	D	540	SER	2.2
4	L	62	SER	2.2
2	B	507	ALA	2.2
3	H	150	ALA	2.2
3	I	1	GLU	2.2
4	L	104	LYS	2.2
4	L	158	LYS	2.2
3	J	114	ASP	2.2
4	M	26	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	518	VAL	2.2
4	L	107	VAL	2.2
1	A	263	GLY	2.2
1	C	50	GLY	2.2
2	F	649	MET	2.2
1	A	37	LEU	2.2
1	A	56	LEU	2.2
4	M	145	ALA	2.2
1	A	34	VAL	2.2
1	A	50	GLY	2.2
2	F	534	TYR	2.2
3	J	151	LEU	2.2
2	D	639	GLU	2.2
2	F	575	ARG	2.2
2	D	537	ASP	2.2
2	F	515	THR	2.2
1	E	143	GLY	2.2
1	A	46	CYS	2.2
2	D	539	LYS	2.2
2	F	667	LYS	2.2
2	B	638	PHE	2.2
2	D	666	SER	2.2
4	N	170	SER	2.2
4	L	53	ARG	2.1
4	N	172	ASN	2.1
1	A	89	PRO	2.1
3	I	73	ASP	2.1
1	C	284	THR	2.1
3	J	173	THR	2.1
4	M	17	THR	2.1
1	C	321	LEU	2.1
4	N	108	LEU	2.1
4	L	193	TYR	2.1
1	A	7	ILE	2.1
1	E	275	MET	2.1
1	A	48	LEU	2.1
4	M	18	ALA	2.1
4	M	142	TYR	2.1
1	A	113	SER	2.1
1	A	269	ILE	2.1
4	M	109	GLY	2.1
2	B	633	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	282	CYS	2.1
2	F	518	VAL	2.1
1	E	265	GLY	2.1
2	B	516	GLY	2.1
4	L	79	ALA	2.1
1	A	82	TYR	2.1
2	D	630	ALA	2.0
3	J	219	LYS	2.0
4	N	188	LYS	2.0
1	A	126	SER	2.0
1	A	15	ASN	2.0
1	C	171	ASN	2.0
3	H	147	GLY	2.0
1	E	238	GLU	2.0
1	E	277	GLU	2.0
2	B	521	TRP	2.0
1	A	318	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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

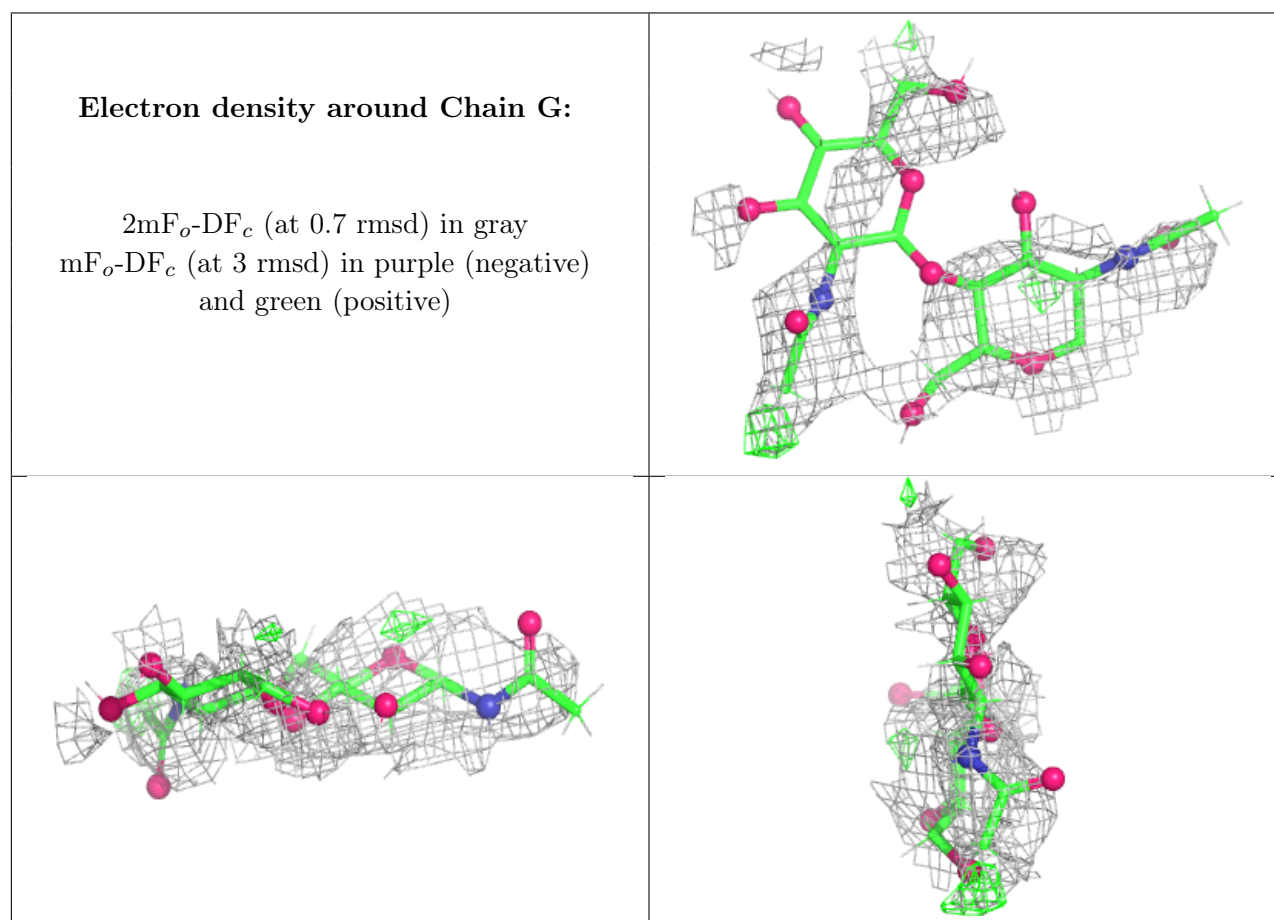
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	76,116,140,147	0
5	NAG	G	2	14/15	-	-	67,127,159,164	0
5	NAG	P	2	14/15	0.22	0.29	85,134,170,175	0
6	BMA	Q	3	11/12	0.24	0.27	85,106,127,130	0
6	BMA	T	3	11/12	0.34	0.24	64,98,117,123	0
5	NAG	R	2	14/15	0.36	0.28	82,115,142,153	0
5	NAG	S	2	14/15	0.42	0.24	81,127,159,167	0
5	NAG	U	2	14/15	0.43	0.25	61,123,160,162	0
5	NAG	P	1	14/15	0.48	0.25	91,111,135,155	0
5	NAG	O	2	14/15	0.54	0.21	55,110,137,139	0
5	NAG	R	1	14/15	0.63	0.20	61,87,116,133	0

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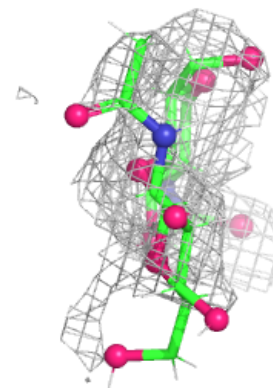
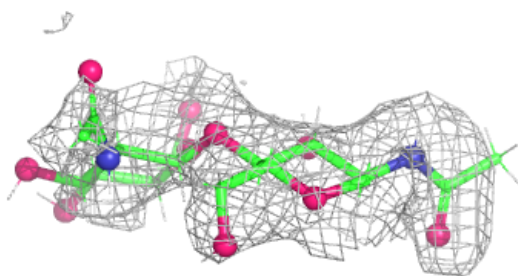
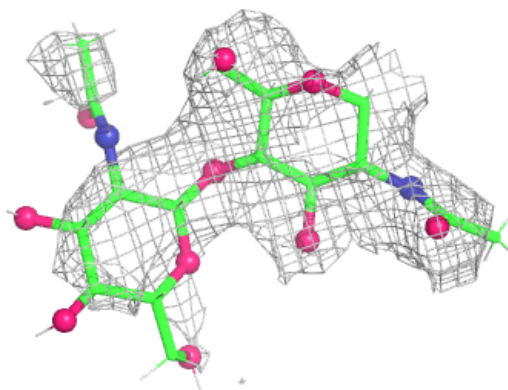
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	S	1	14/15	0.64	0.21	73,97,122,140	0
6	NAG	K	1	14/15	-	-	40,73,120,125	0
6	NAG	K	2	14/15	-	-	55,92,118,125	0
6	BMA	K	3	11/12	-	-	74,97,115,138	0
6	NAG	Q	2	14/15	0.70	0.22	50,97,117,124	0
6	NAG	T	2	14/15	0.76	0.20	51,82,101,117	0
5	NAG	U	1	14/15	0.77	0.17	50,81,120,127	0
5	NAG	O	1	14/15	0.77	0.14	56,87,110,121	0
6	NAG	T	1	14/15	0.82	0.17	36,56,93,103	0
6	NAG	Q	1	14/15	0.85	0.14	33,60,97,103	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.

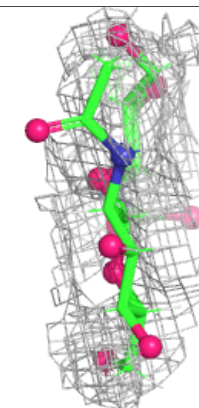
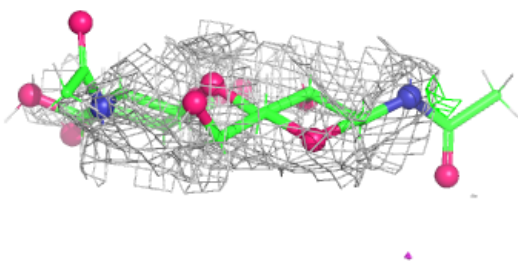
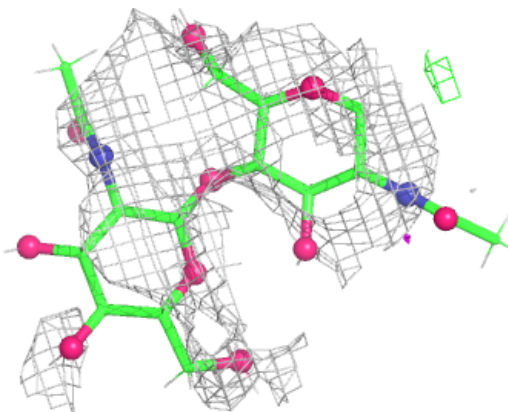


Electron density around Chain O:

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

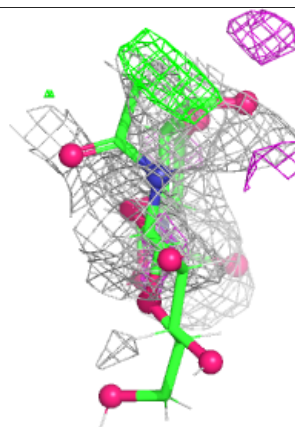
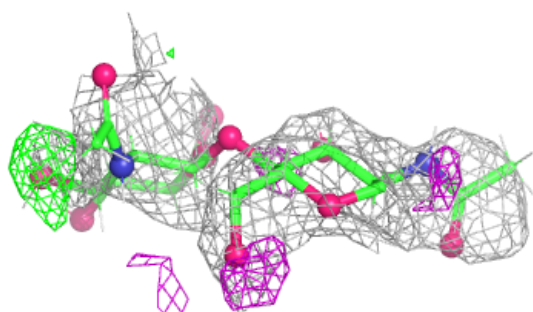
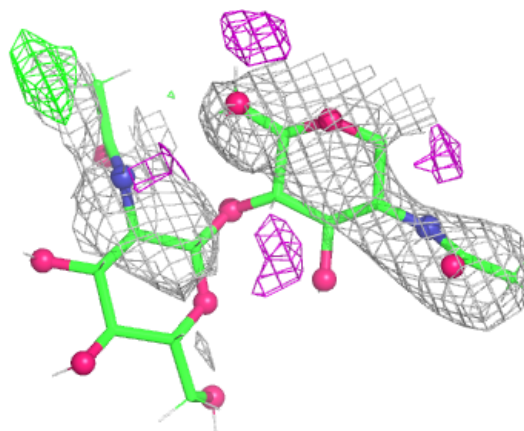
**Electron density around Chain P:**

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

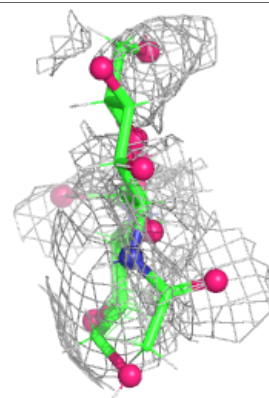
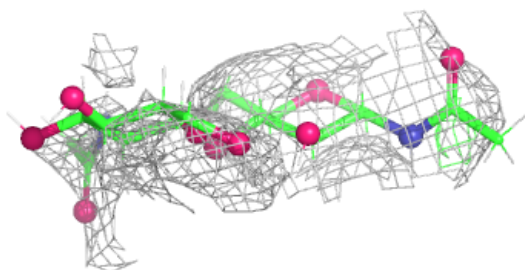
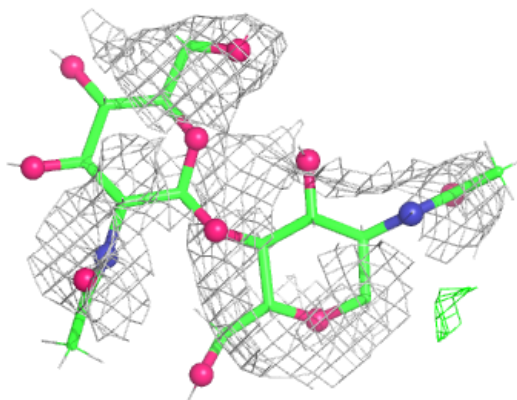


Electron density around Chain R:

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

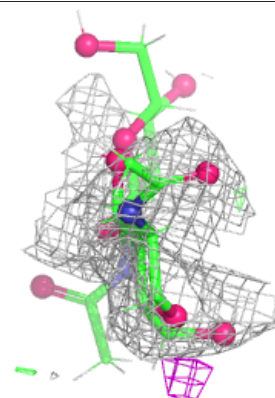
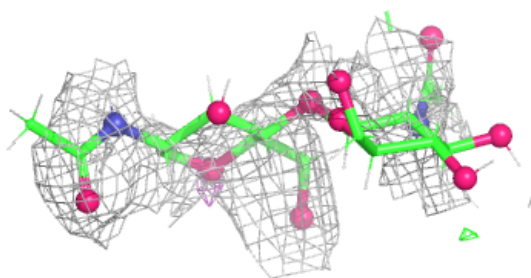
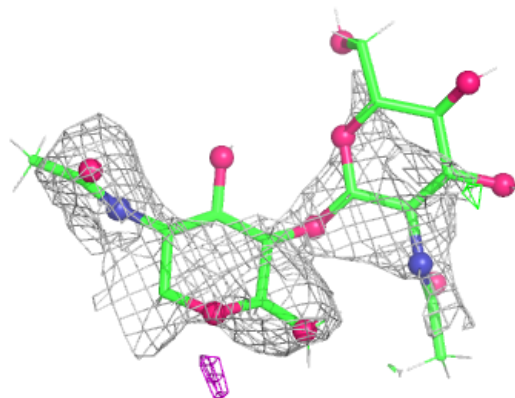
**Electron density around Chain S:**

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

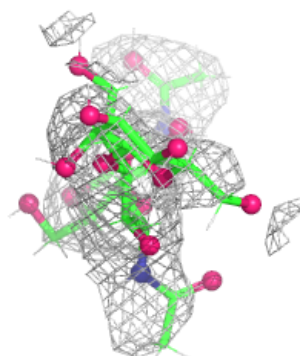
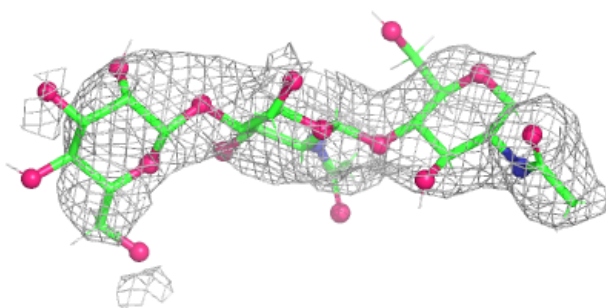
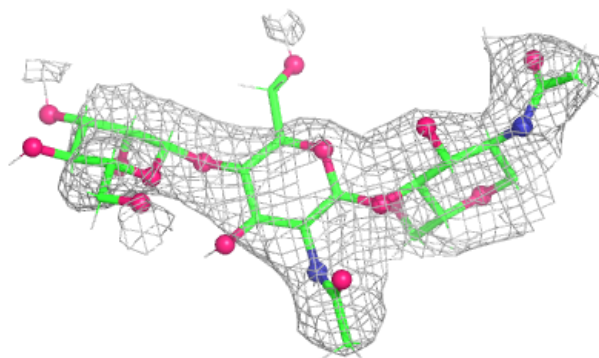


Electron density around Chain U:

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

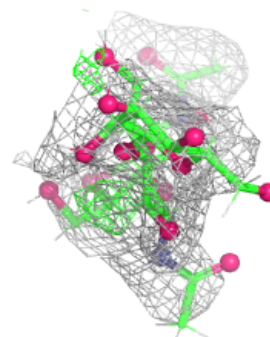
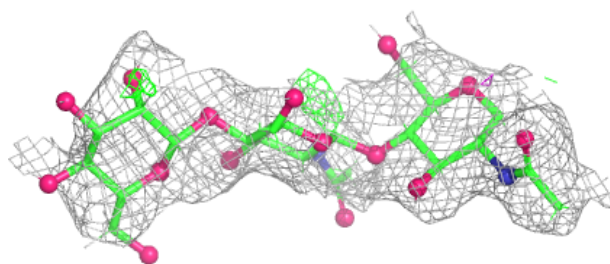
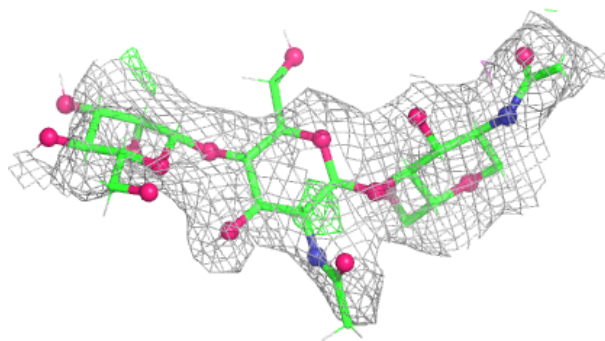
**Electron density around Chain K:**

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

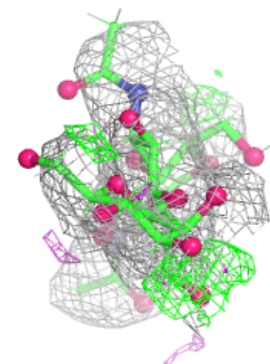
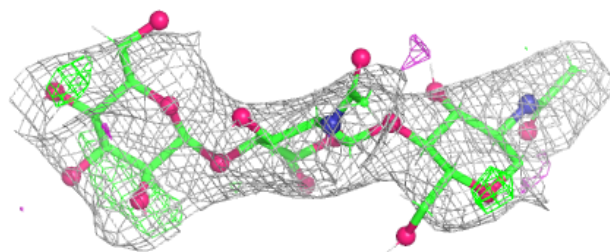
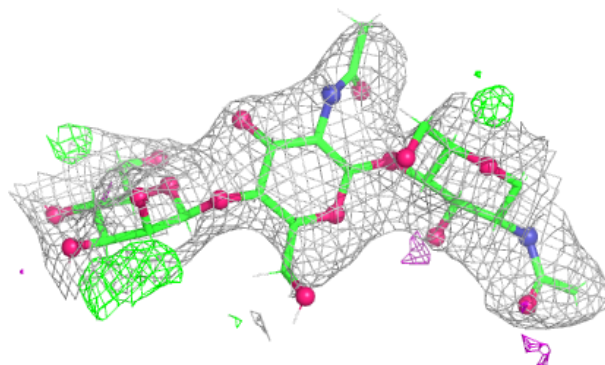


Electron density around Chain Q:

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

**Electron density around Chain T:**

$2mF_o-DF_c$ (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
7	NAG	E	407	14/15	0.34	0.27	58,104,151,154	0
7	NAG	A	407	14/15	0.47	0.22	53,97,139,154	0
7	NAG	C	406	14/15	0.51	0.21	83,108,138,146	0
7	NAG	C	407	14/15	0.52	0.25	51,107,132,155	0
7	NAG	A	406	14/15	0.55	0.21	75,111,140,149	0
7	NAG	E	406	14/15	0.56	0.23	78,110,139,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.