



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 08:01 pm BST

PDB ID : 3ZTJ
Title : Structure of influenza A neutralizing antibody selected from cultures of single human plasma cells in complex with human H3 Influenza haemagglutinin.
Authors : Voss, J.E.; Vachieri, S.G.; Gamblin, S.J.; Collins, P.J.; Haire, L.F.; Skehel, J.J.
Deposited on : 2011-07-08
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

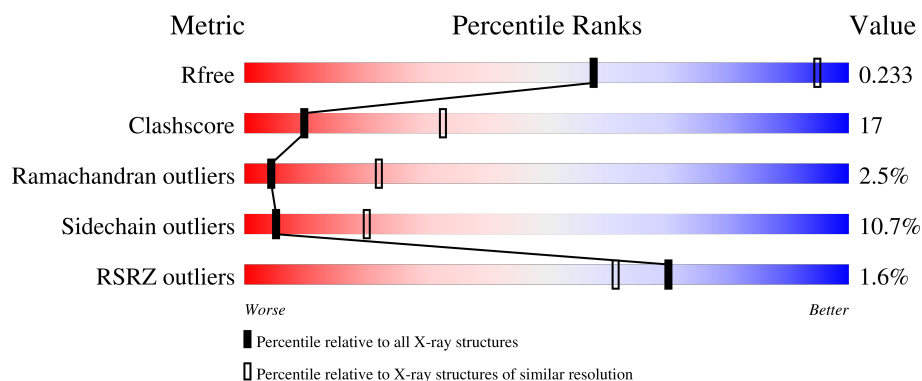
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1112 (3.48-3.36)
Clashscore	180529	1144 (3.48-3.36)
Ramachandran outliers	177936	1146 (3.48-3.36)
Sidechain outliers	177891	1146 (3.48-3.36)
RSRZ outliers	164620	1112 (3.48-3.36)

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	329	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>34%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	329	<div> <div></div> <div> <div>53%</div> <div>37%</div> <div>5%</div> <div>.</div> </div> </div>
1	E	329	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>.</div> <div>.</div> </div> </div>
2	B	175	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>
2	D	175	<div> <div></div> <div> <div>59%</div> <div>33%</div> <div>6%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	175	
3	G	226	
3	I	226	
3	K	226	
4	H	218	
4	J	218	
4	L	218	
5	M	3	
5	O	3	
5	T	3	
5	X	3	
6	N	2	
6	P	2	
6	Q	2	
6	R	2	
6	S	2	
6	U	2	
6	V	2	
6	W	2	
6	Y	2	
6	Z	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	M	1	X	-	-	-
6	NAG	R	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Z	1	X	-	-	-
7	NAG	D	410	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20384 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 HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			
1	C	316	Total	C	N	O	S	0	0	0
			2425	1521	422	469	13			
1	E	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	863	244	279	6			
2	D	172	Total	C	N	O	S	0	0	0
			1382	856	243	277	6			
2	F	172	Total	C	N	O	S	0	0	0
			1379	854	244	275	6			

- Molecule 3 is a protein called FI6V3 ANTIBODY HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	S	0	0	0
			1004	642	167	191	4			
3	I	226	Total	C	N	O	S	0	0	0
			1712	1089	285	332	6			
3	K	224	Total	C	N	O	S	0	0	0
			1697	1082	281	328	6			

- Molecule 4 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

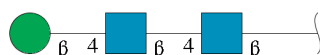
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	107	Total	C	N	O	S	0	0	0
			771	485	129	154	3			

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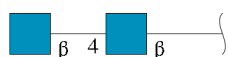
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	216	Total	C	N	O	S	0	0	0
			1647	1035	278	329	5			
4	L	216	Total	C	N	O	S	0	0	0
			1623	1018	273	327	5			

- Molecule 5 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
5	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



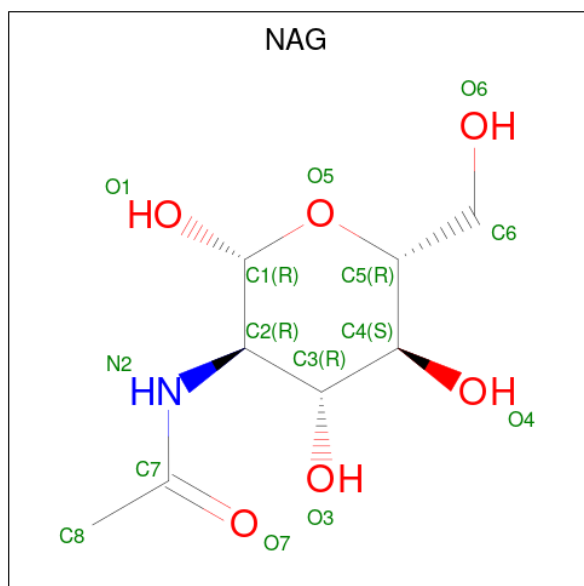
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

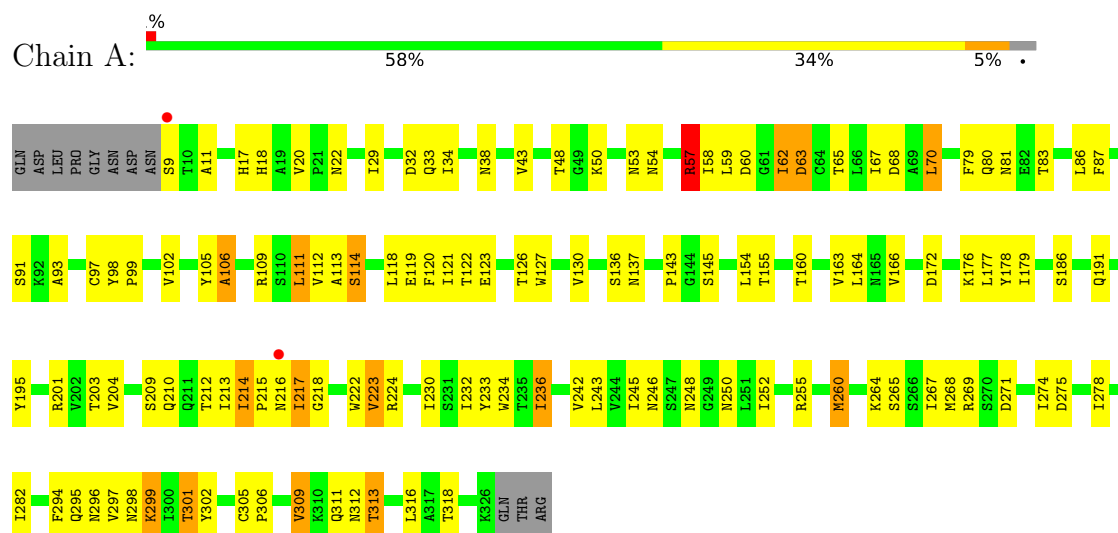


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

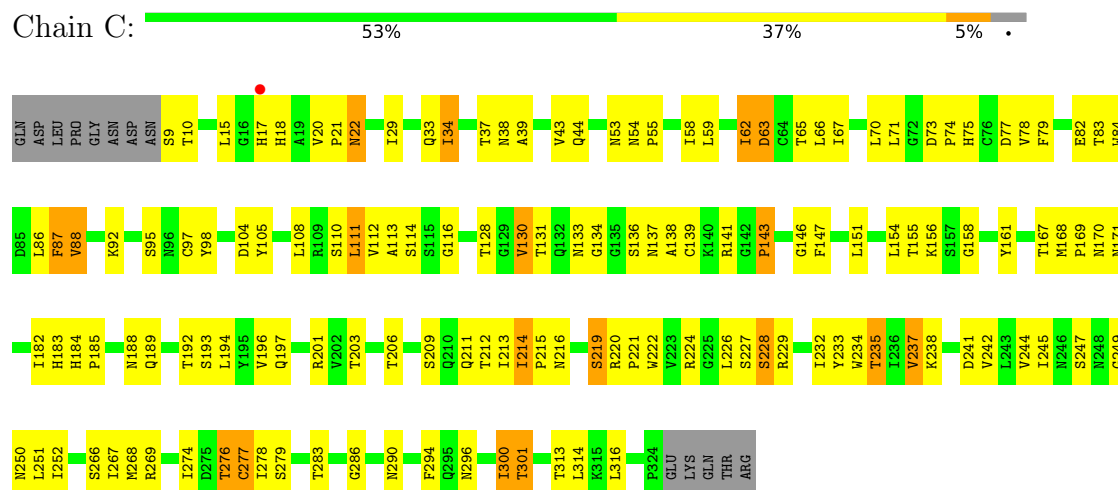
3 Residue-property plots

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 CHAIN

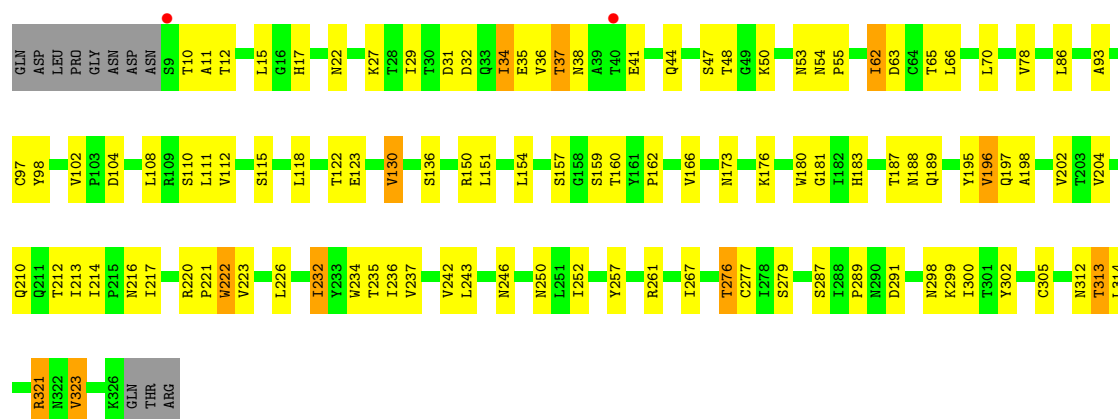


• Molecule 1: HEMAGGLUTININ HA1 CHAIN

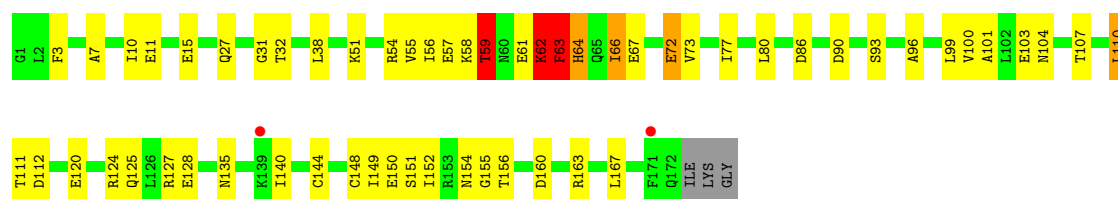


• Molecule 1: HEMAGGLUTININ HA1 CHAIN

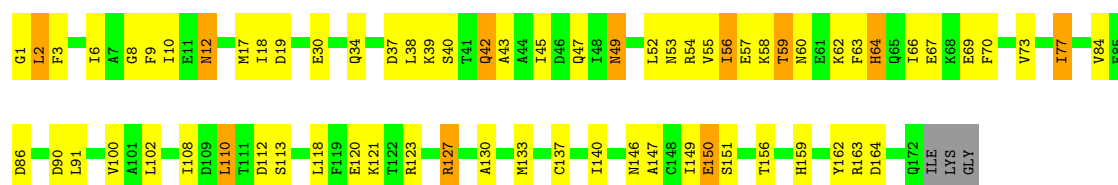




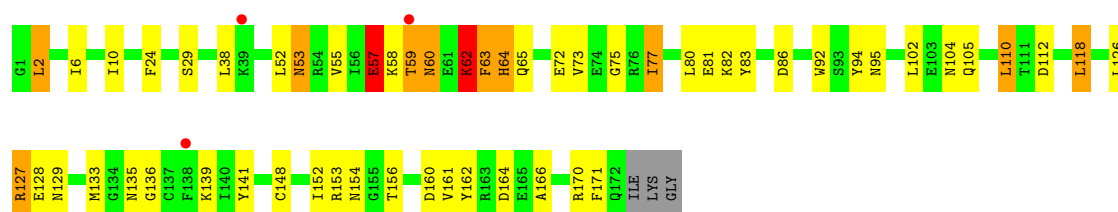
• Molecule 2: HEMAGGLUTININ HA2 CHAIN



• Molecule 2: HEMAGGLUTININ HA2 CHAIN

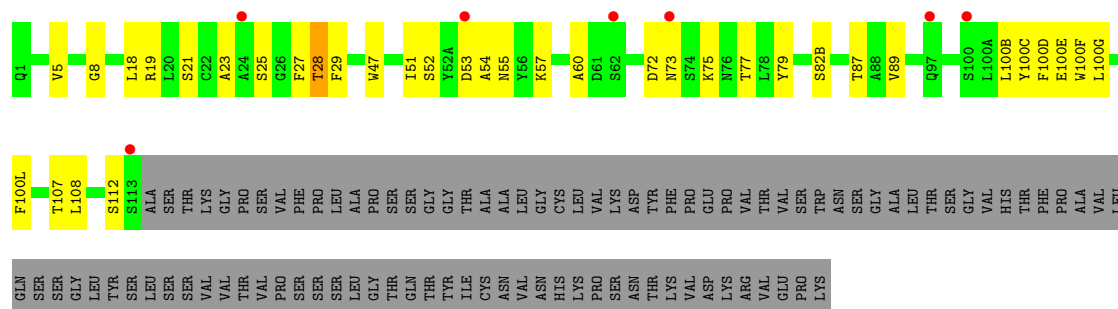


• Molecule 2: HEMAGGLUTININ HA2 CHAIN

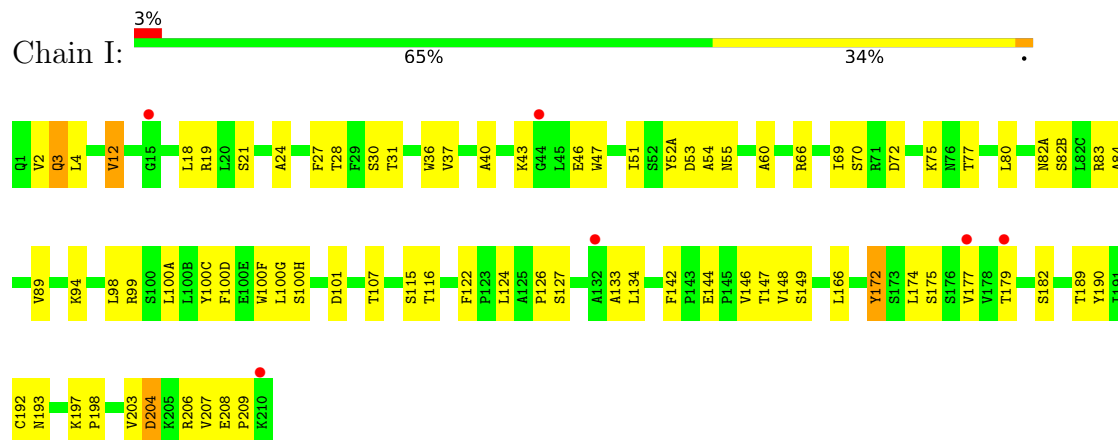


• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

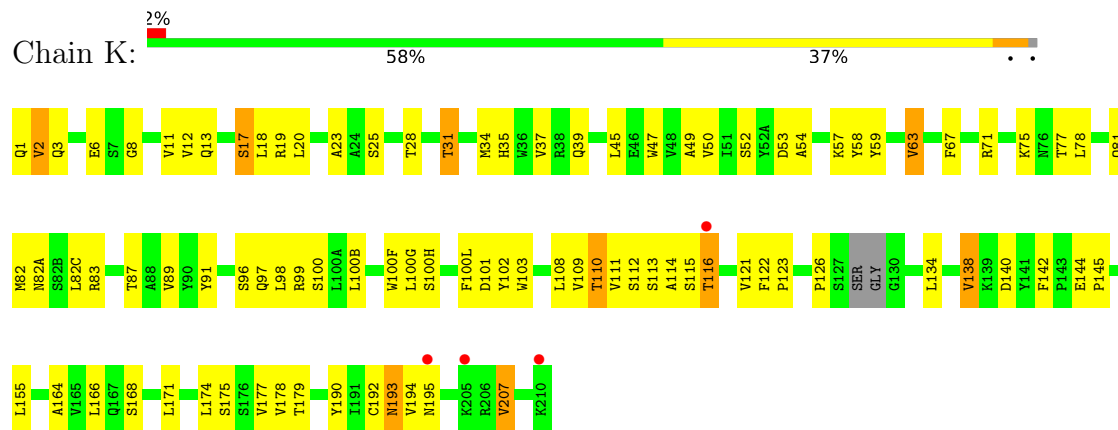




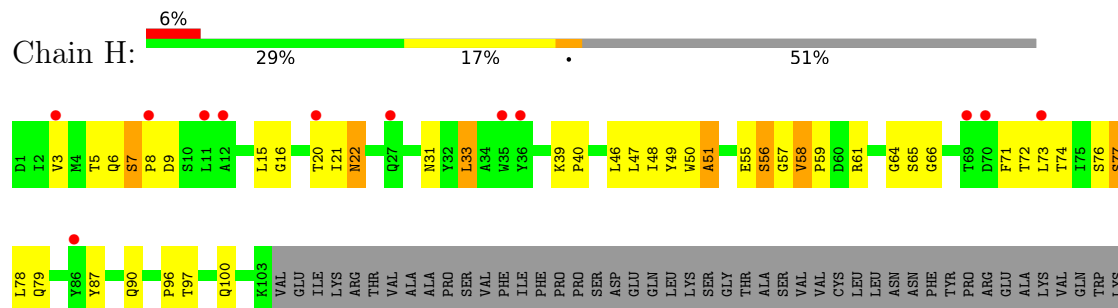
• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

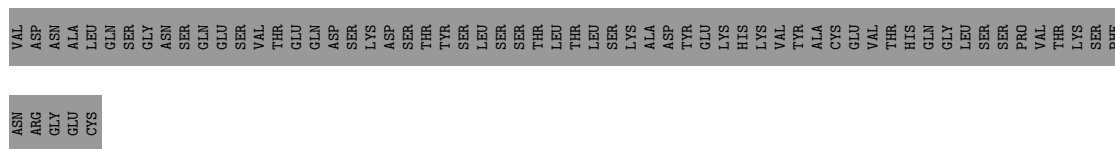


• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

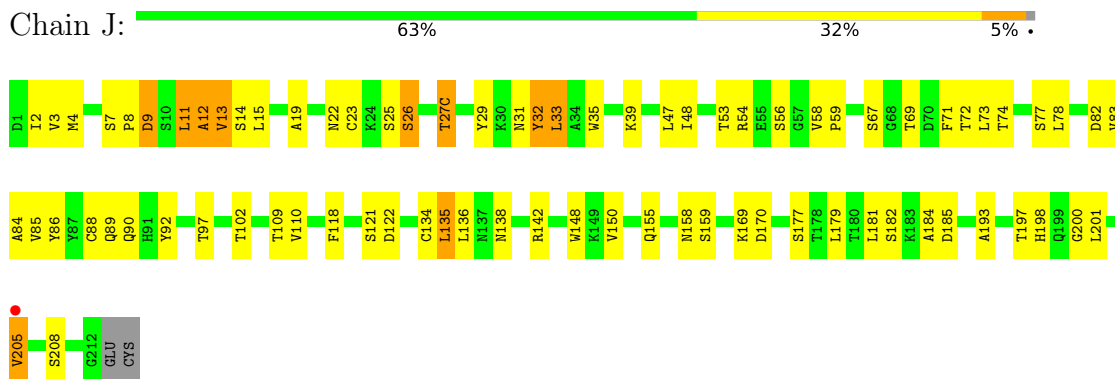


• Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN

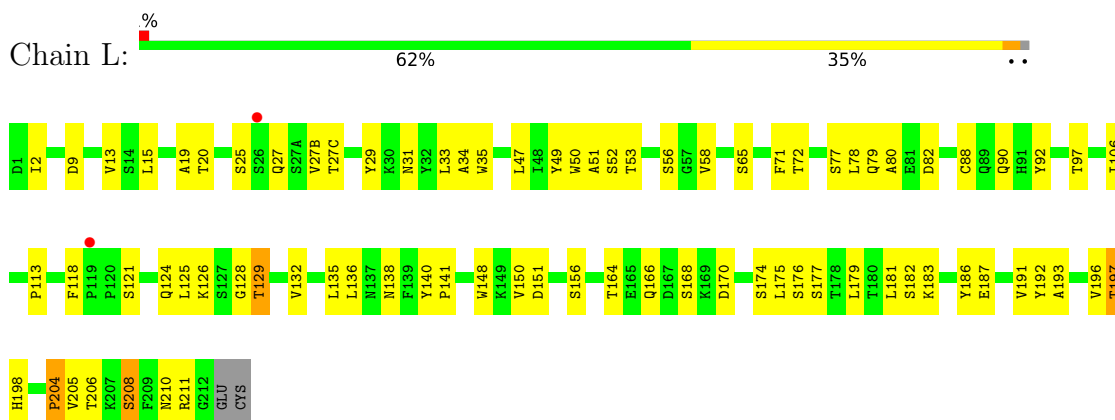




• Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN



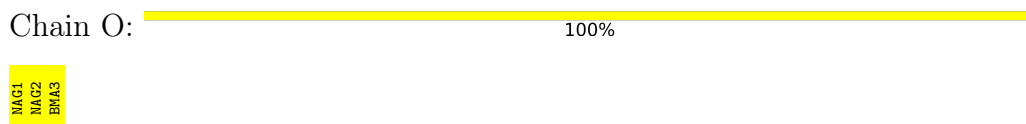
● Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN



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



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




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

Chain T:  100%

NAG1
NAG2
BMA3

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

Chain X:  100%

NAG1
NAG2
BMA3

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

Chain N:  100%



NAG1
NAG2

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

Chain P:  100%

NAG1
NAG2

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

Chain Q:  50%  50%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain S:  100%


NAG1
NAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.49Å 193.43Å 213.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.42 – 3.41 143.42 – 3.41	Depositor EDS
% Data completeness (in resolution range)	95.6 (143.42-3.41) 95.3 (143.42-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.284 0.236 , 0.233	Depositor DCC
R_{free} test set	4644 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	116.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20384	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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	0.73	0/2507	0.82	1/3417 (0.0%)
1	C	0.78	1/2481 (0.0%)	0.83	0/3384
1	E	0.78	1/2507 (0.0%)	0.86	1/3417 (0.0%)
2	B	0.87	4/1416 (0.3%)	0.82	1/1905 (0.1%)
2	D	0.92	3/1406 (0.2%)	0.87	2/1893 (0.1%)
2	F	0.86	2/1402 (0.1%)	0.85	1/1887 (0.1%)
3	G	0.52	0/1030	0.63	0/1401
3	I	0.67	0/1757	0.73	0/2399
3	K	0.73	0/1741	0.77	0/2376
4	H	0.54	0/792	0.63	0/1088
4	J	0.70	0/1686	0.77	0/2299
4	L	0.61	0/1662	0.71	0/2272
All	All	0.75	11/20387 (0.1%)	0.79	6/27738 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	3
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	GLU	CB-CG	7.17	1.65	1.52
2	F	59	THR	CA-CB	7.02	1.71	1.53
2	D	150	GLU	CG-CD	6.83	1.62	1.51
1	C	277	CYS	CB-SG	6.16	1.92	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	GLU	CG-CD	5.71	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	63	PHE	N-CA-C	-9.09	86.45	111.00
1	A	57	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	D	54	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	D	54	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	B	63	PHE	N-CA-CB	5.36	120.25	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	62	LYS	Peptide
2	F	57	GLU	Peptide
2	F	62	LYS	Peptide
2	F	75	GLY	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	2451	0	2395	90	0
1	C	2425	0	2364	99	0
1	E	2451	0	2395	68	0
2	B	1392	0	1298	60	0
2	D	1382	0	1276	77	0
2	F	1379	0	1285	46	0
3	G	1004	0	937	17	0
3	I	1712	0	1638	68	0
3	K	1697	0	1628	75	0
4	H	771	0	666	30	0
4	J	1647	0	1562	55	0
4	L	1623	0	1497	57	0
5	M	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	39	0	34	0	0
5	T	39	0	34	0	0
5	X	39	0	34	0	0
6	N	28	0	25	2	0
6	P	28	0	25	0	0
6	Q	28	0	25	1	0
6	R	28	0	25	2	0
6	S	28	0	25	1	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	1	0
6	Y	28	0	25	0	0
6	Z	28	0	25	2	0
7	D	14	0	13	7	0
All	All	20384	0	19340	682	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 682 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:D:52:LEU:O	2:D:56:ILE:HD11	1.43	1.17
2:D:56:ILE:HD12	2:D:56:ILE:N	1.68	1.08
2:D:56:ILE:HD12	2:D:56:ILE:H	1.15	1.00
4:L:13:VAL:HG11	4:L:19:ALA:HB2	1.45	0.98
1:C:53:ASN:HD21	1:C:276:THR:HG23	1.25	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/329 (96%)	276 (87%)	32 (10%)	8 (2%)	4	22
1	C	314/329 (95%)	269 (86%)	36 (12%)	9 (3%)	3	20
1	E	316/329 (96%)	278 (88%)	33 (10%)	5 (2%)	8	29
2	B	170/175 (97%)	143 (84%)	23 (14%)	4 (2%)	5	23
2	D	170/175 (97%)	140 (82%)	23 (14%)	7 (4%)	2	15
2	F	170/175 (97%)	146 (86%)	20 (12%)	4 (2%)	5	23
3	G	127/226 (56%)	109 (86%)	14 (11%)	4 (3%)	3	19
3	I	224/226 (99%)	189 (84%)	33 (15%)	2 (1%)	14	43
3	K	220/226 (97%)	195 (89%)	22 (10%)	3 (1%)	9	32
4	H	105/218 (48%)	81 (77%)	21 (20%)	3 (3%)	3	20
4	J	214/218 (98%)	189 (88%)	19 (9%)	6 (3%)	4	20
4	L	214/218 (98%)	177 (83%)	28 (13%)	9 (4%)	2	14
All	All	2560/2844 (90%)	2192 (86%)	304 (12%)	64 (2%)	4	22

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA
2	D	64	HIS
2	D	127	ARG
2	D	163	ARG
2	F	58	LYS

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	279/290 (96%)	249 (89%)	30 (11%)	5	20
1	C	276/290 (95%)	238 (86%)	38 (14%)	3	11
1	E	279/290 (96%)	249 (89%)	30 (11%)	5	20
2	B	145/149 (97%)	134 (92%)	11 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	142/149 (95%)	125 (88%)	17 (12%)	4	16
2	F	142/149 (95%)	127 (89%)	15 (11%)	5	20
3	G	102/191 (53%)	95 (93%)	7 (7%)	13	38
3	I	185/191 (97%)	170 (92%)	15 (8%)	9	31
3	K	184/191 (96%)	164 (89%)	20 (11%)	5	19
4	H	74/193 (38%)	65 (88%)	9 (12%)	4	15
4	J	181/193 (94%)	158 (87%)	23 (13%)	3	14
4	L	173/193 (90%)	157 (91%)	16 (9%)	7	26
All	All	2162/2469 (88%)	1931 (89%)	231 (11%)	5	20

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	222	TRP
4	L	129	THR
3	G	28	THR
4	L	77	SER
3	K	31	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	296	ASN
4	H	31	ASN
4	L	124	GLN
2	F	49	ASN
3	G	1	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 ⓘ

32 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	M	1	1,5	14,14,15	0.79	0	17,19,21	1.80	7 (41%)
5	NAG	M	2	5	14,14,15	1.06	1 (7%)	17,19,21	2.06	4 (23%)
5	BMA	M	3	5	11,11,12	1.32	2 (18%)	15,15,17	1.70	4 (26%)
6	NAG	N	1	1,6	14,14,15	1.05	1 (7%)	17,19,21	2.16	6 (35%)
6	NAG	N	2	6	14,14,15	1.28	3 (21%)	17,19,21	2.05	4 (23%)
5	NAG	O	1	1,5	14,14,15	0.73	1 (7%)	17,19,21	1.09	1 (5%)
5	NAG	O	2	5	14,14,15	0.81	0	17,19,21	1.16	3 (17%)
5	BMA	O	3	5	11,11,12	0.94	0	15,15,17	1.84	4 (26%)
6	NAG	P	1	1,6	14,14,15	0.62	0	17,19,21	1.42	5 (29%)
6	NAG	P	2	6	14,14,15	1.30	3 (21%)	17,19,21	1.88	7 (41%)
6	NAG	Q	1	2,6	14,14,15	1.25	1 (7%)	17,19,21	1.36	4 (23%)
6	NAG	Q	2	6	14,14,15	1.34	2 (14%)	17,19,21	1.76	7 (41%)
6	NAG	R	1	1,6	14,14,15	1.47	2 (14%)	17,19,21	2.63	5 (29%)
6	NAG	R	2	6	14,14,15	1.33	2 (14%)	17,19,21	3.19	7 (41%)
6	NAG	S	1	1,6	14,14,15	1.04	1 (7%)	17,19,21	3.22	10 (58%)
6	NAG	S	2	6	14,14,15	1.34	1 (7%)	17,19,21	1.97	4 (23%)
5	NAG	T	1	1,5	14,14,15	0.62	0	17,19,21	1.69	4 (23%)
5	NAG	T	2	5	14,14,15	0.65	0	17,19,21	1.81	4 (23%)
5	BMA	T	3	5	11,11,12	0.75	0	15,15,17	1.27	2 (13%)
6	NAG	U	1	1,6	14,14,15	0.81	0	17,19,21	1.78	4 (23%)
6	NAG	U	2	6	14,14,15	1.20	1 (7%)	17,19,21	2.26	5 (29%)
6	NAG	V	1	1,6	14,14,15	1.18	2 (14%)	17,19,21	2.41	4 (23%)
6	NAG	V	2	6	14,14,15	1.30	2 (14%)	17,19,21	2.07	4 (23%)
6	NAG	W	1	1,6	14,14,15	0.91	1 (7%)	17,19,21	1.87	7 (41%)
6	NAG	W	2	6	14,14,15	1.15	3 (21%)	17,19,21	1.79	4 (23%)
5	NAG	X	1	1,5	14,14,15	0.70	0	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	X	2	5	14,14,15	0.98	1 (7%)	17,19,21	1.05	2 (11%)
5	BMA	X	3	5	11,11,12	1.04	1 (9%)	15,15,17	2.20	8 (53%)
6	NAG	Y	1	1,6	14,14,15	1.03	0	17,19,21	2.30	5 (29%)
6	NAG	Y	2	6	14,14,15	1.21	1 (7%)	17,19,21	1.92	3 (17%)
6	NAG	Z	1	2,6	14,14,15	1.30	1 (7%)	17,19,21	1.89	3 (17%)
6	NAG	Z	2	6	14,14,15	0.96	0	17,19,21	2.15	4 (23%)

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	M	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	3/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
6	NAG	P	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Q	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	1,6	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	2,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	1	NAG	C1-C2	4.17	1.58	1.52
6	S	2	NAG	C1-C2	3.62	1.57	1.52
6	Z	1	NAG	C1-C2	3.28	1.57	1.52
6	R	2	NAG	C1-C2	3.00	1.56	1.52
6	Q	2	NAG	C1-C2	2.91	1.56	1.52

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	2	NAG	C1-O5-C5	8.60	123.84	112.19
6	S	1	NAG	O3-C3-C2	-7.20	94.58	109.47
6	R	1	NAG	O5-C1-C2	-6.96	100.30	111.29
6	S	2	NAG	C1-C2-N2	5.80	120.39	110.49
6	Y	1	NAG	C2-N2-C7	5.62	130.91	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1	NAG	C1
6	R	1	NAG	C1
6	Z	1	NAG	C1

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
6	Y	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6

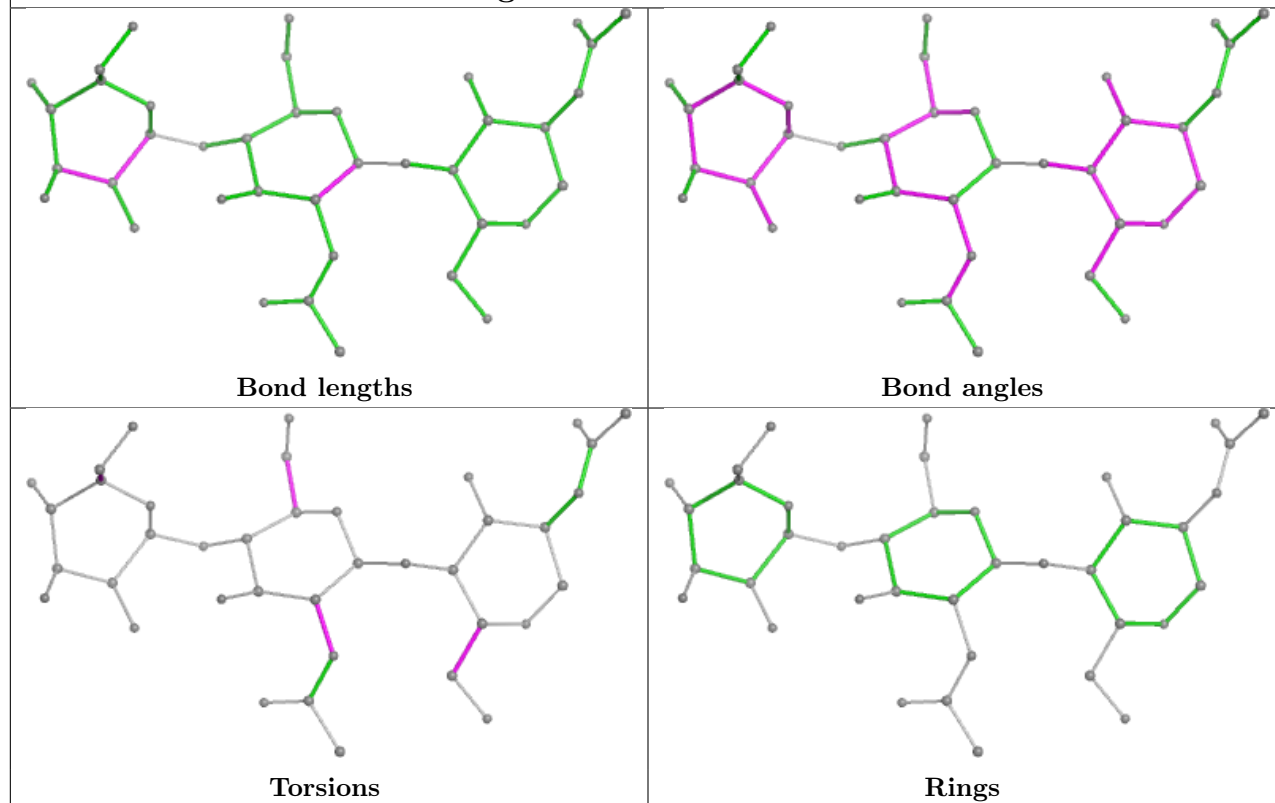
There are no ring outliers.

12 monomers are involved in 11 short contacts:

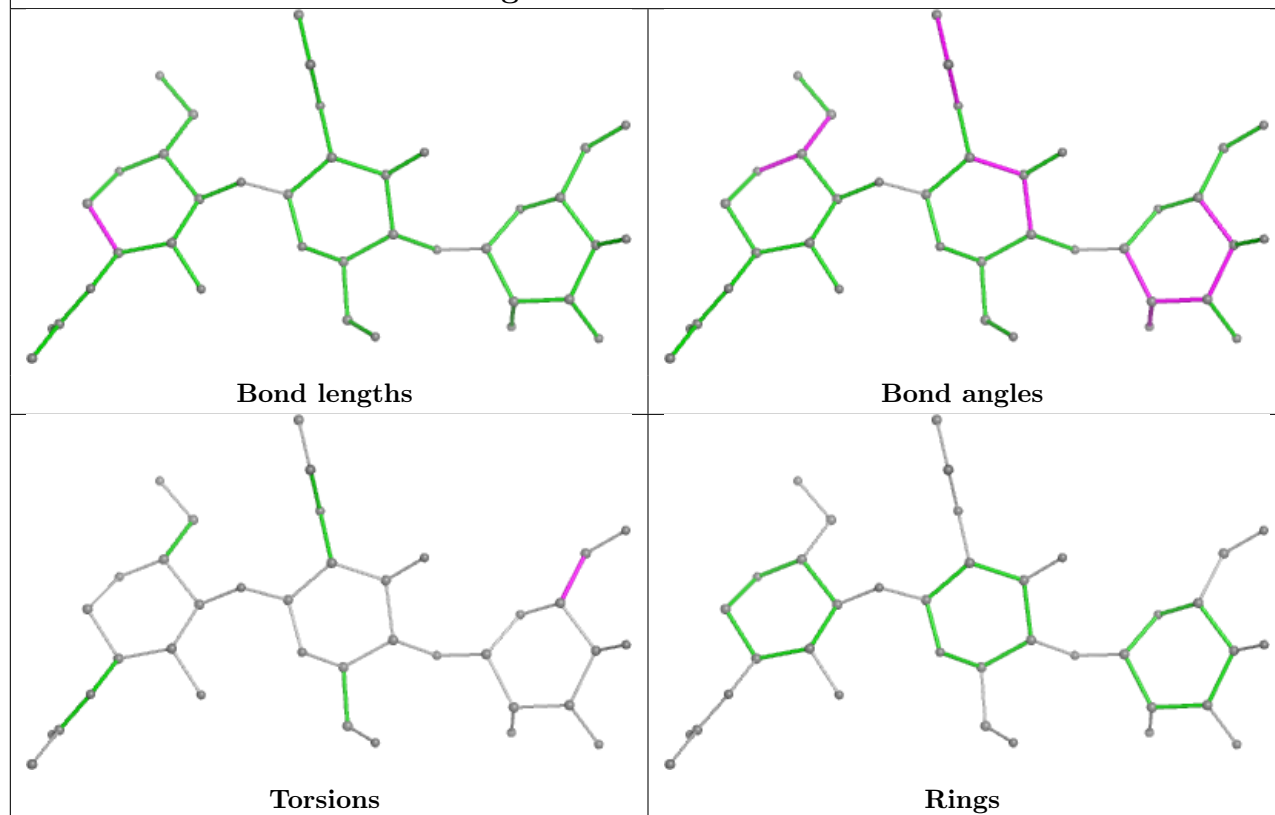
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	2	NAG	2	0
6	S	2	NAG	1	0
6	N	1	NAG	2	0
6	R	2	NAG	2	0
5	M	2	NAG	2	0
6	Z	1	NAG	2	0
6	W	1	NAG	1	0
5	M	1	NAG	1	0
6	W	2	NAG	1	0
6	R	1	NAG	2	0
6	S	1	NAG	1	0
6	Q	1	NAG	1	0

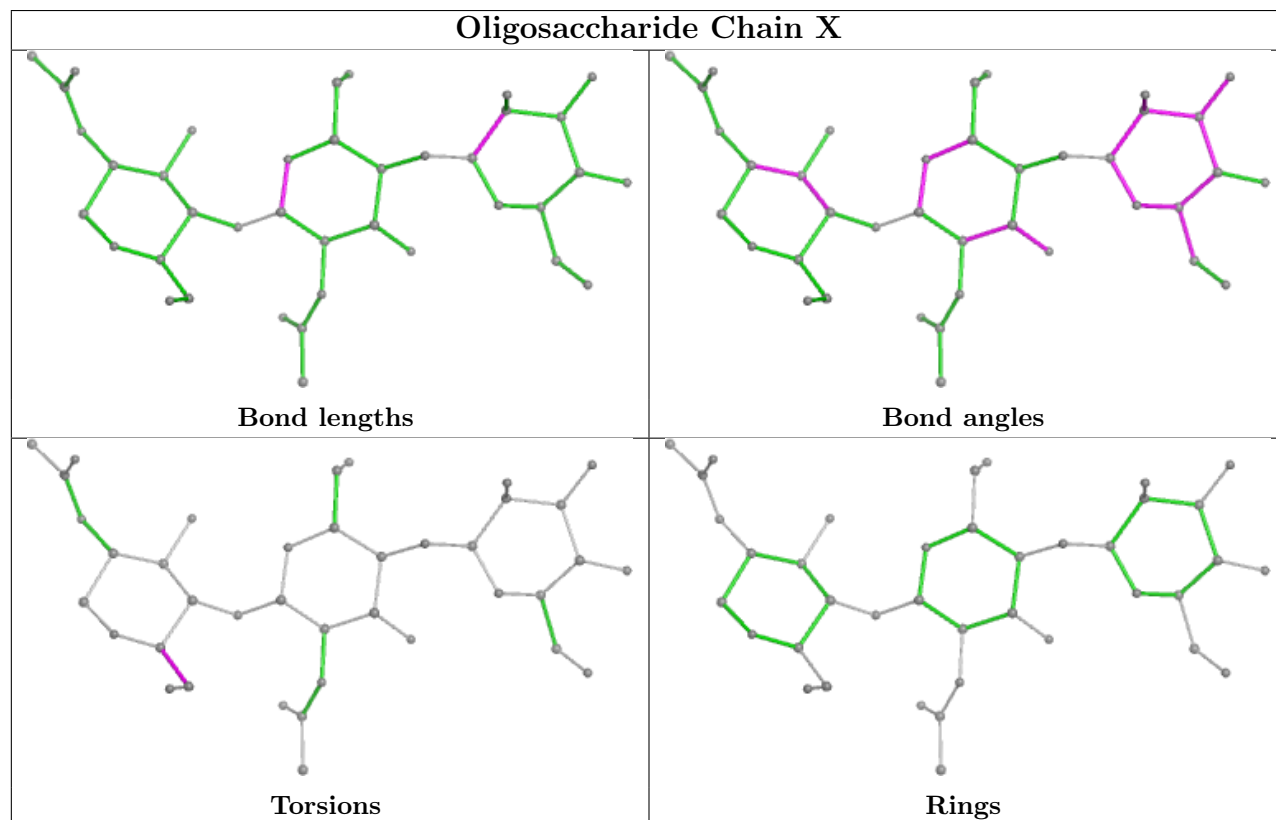
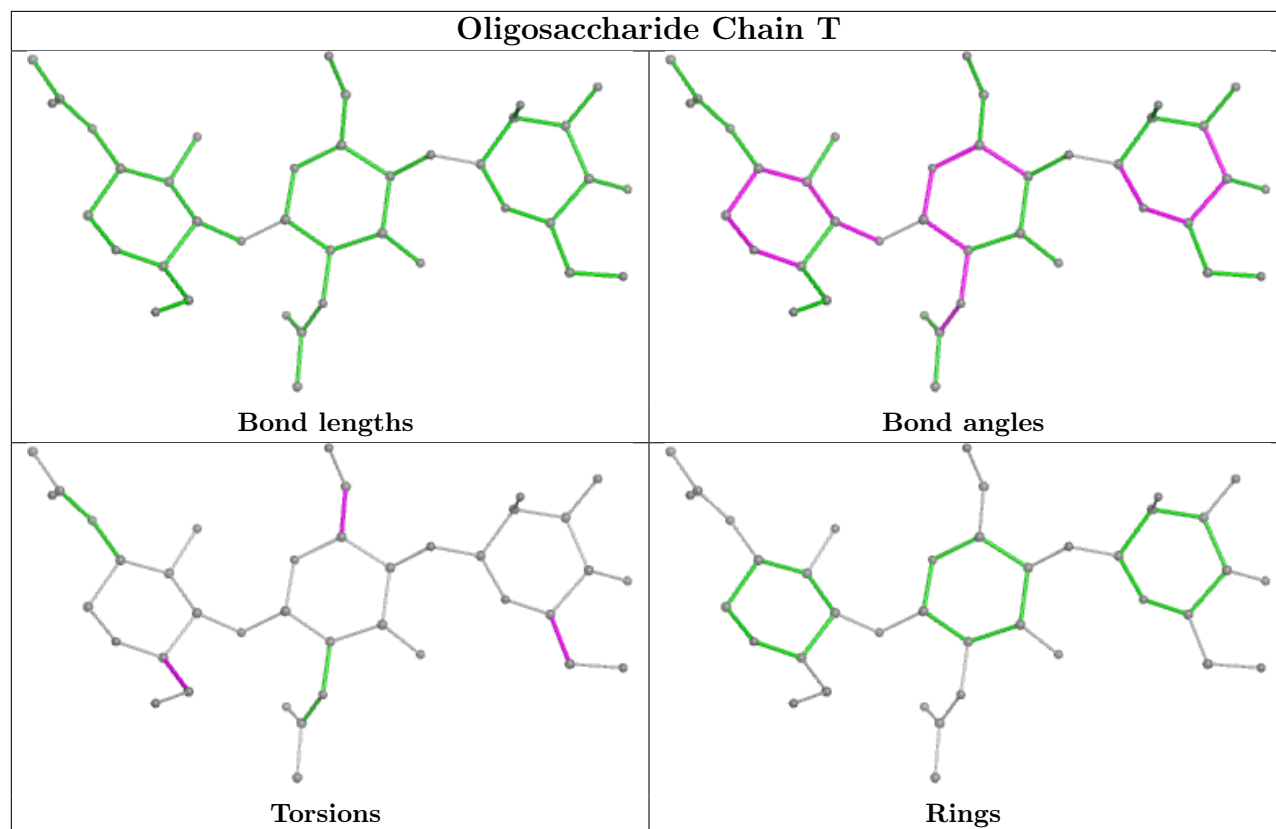
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

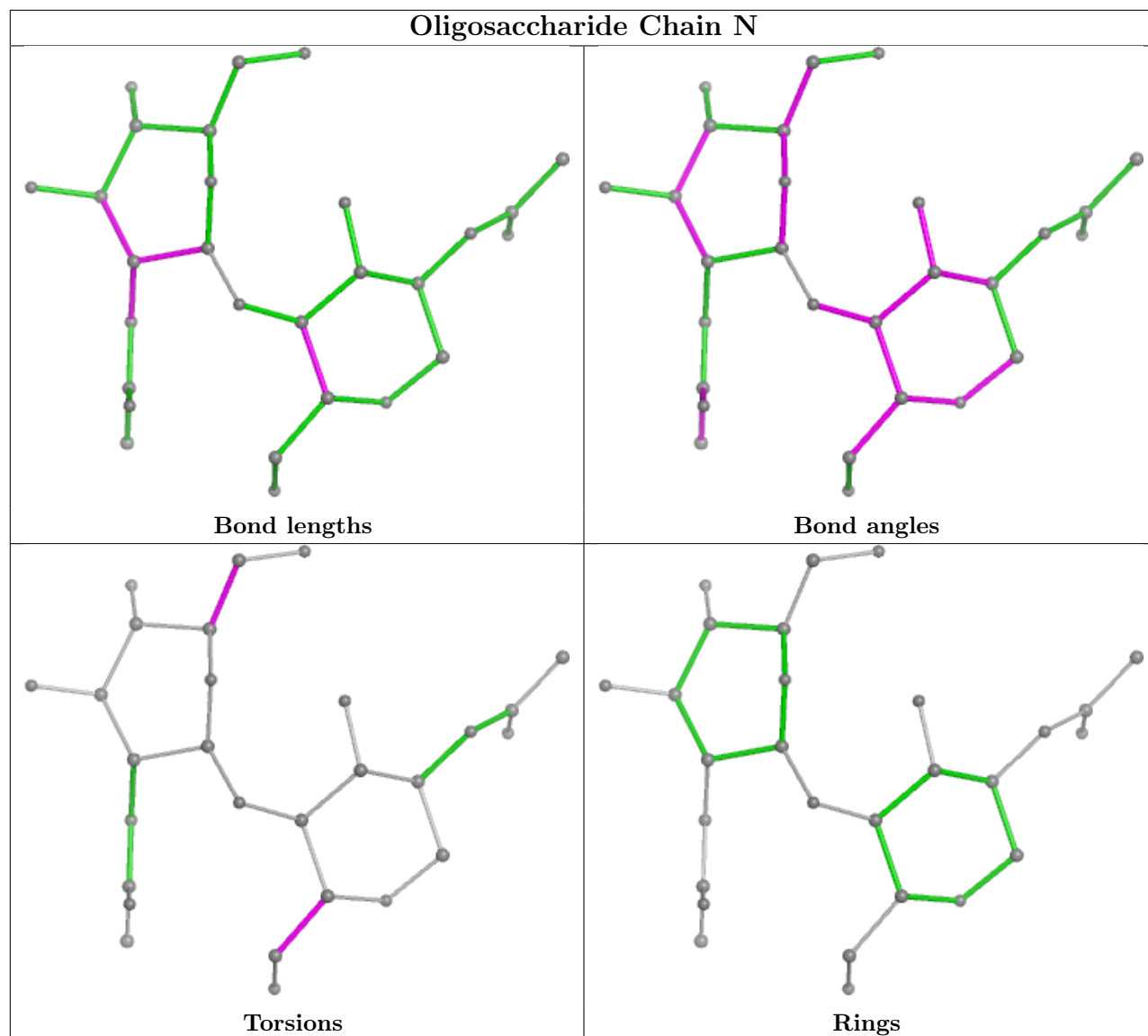
Oligosaccharide Chain M



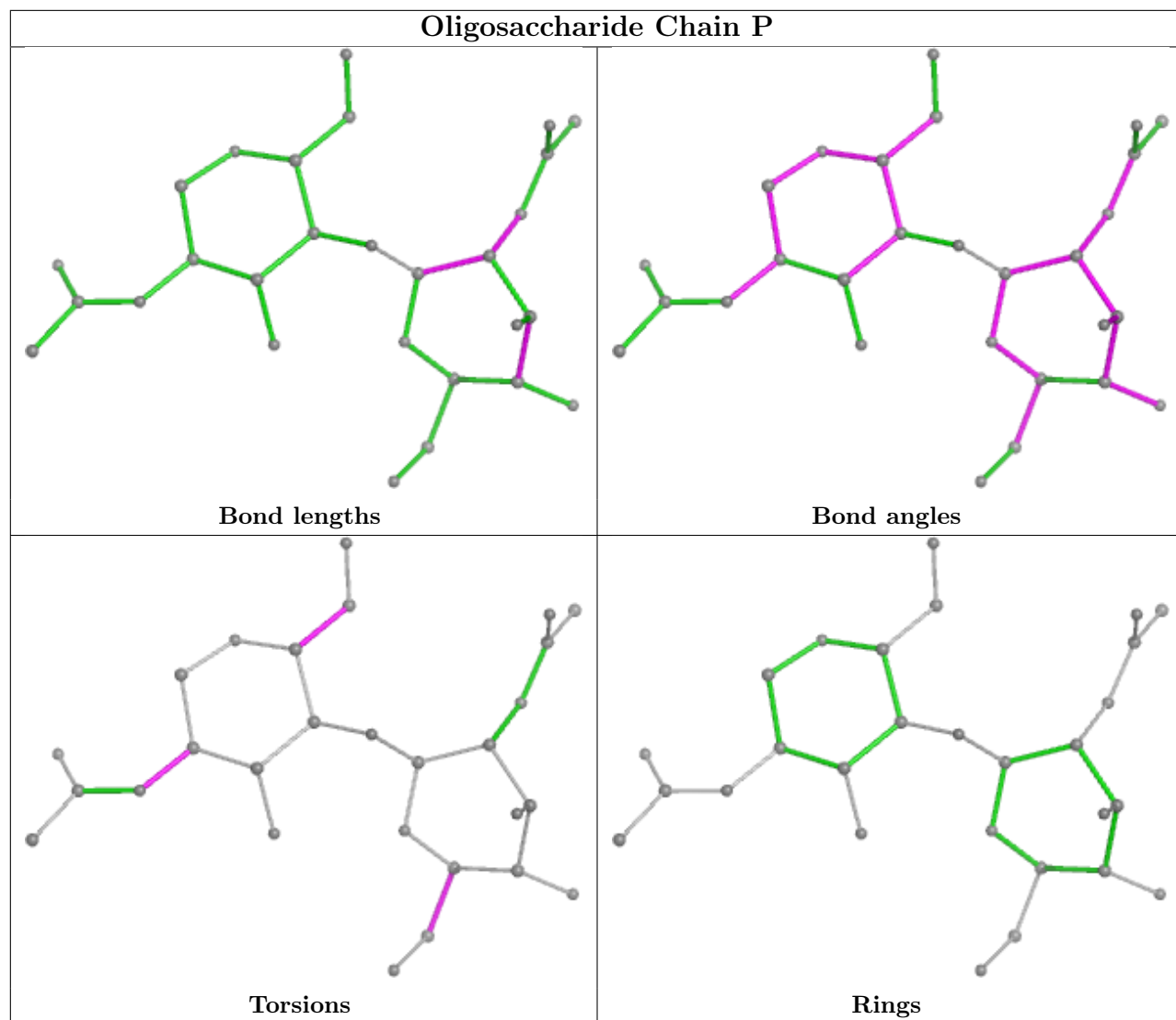
Oligosaccharide Chain O

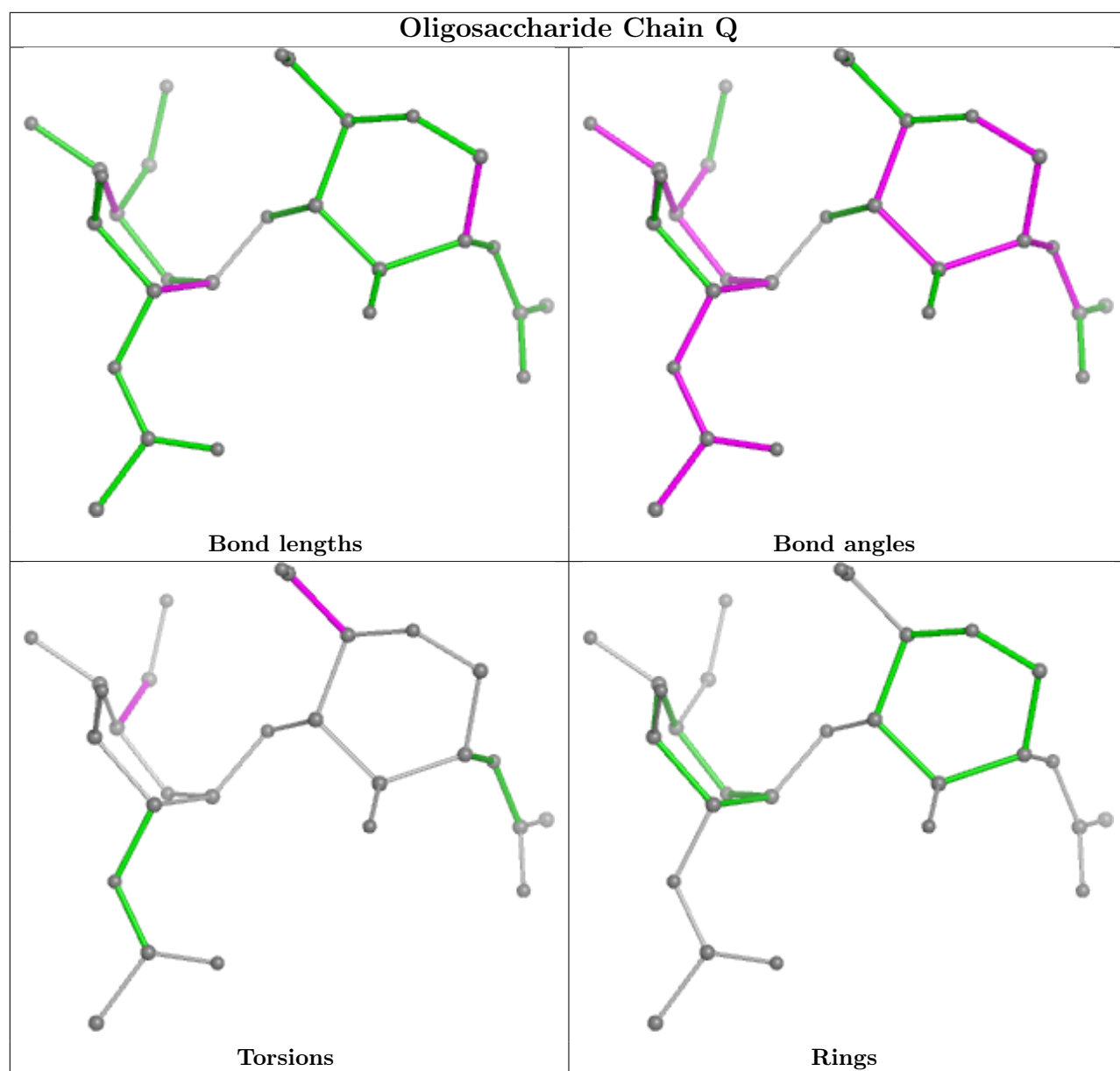


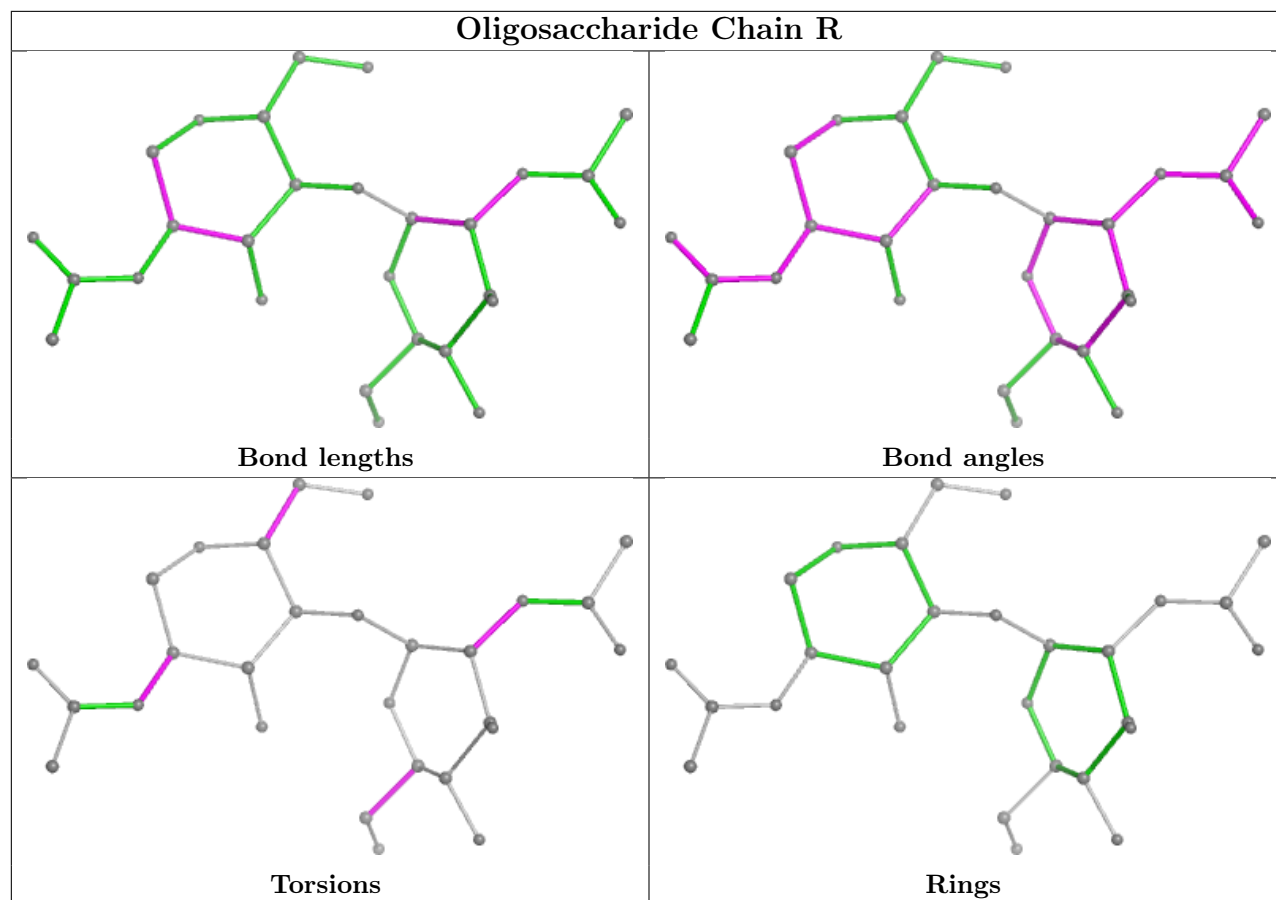


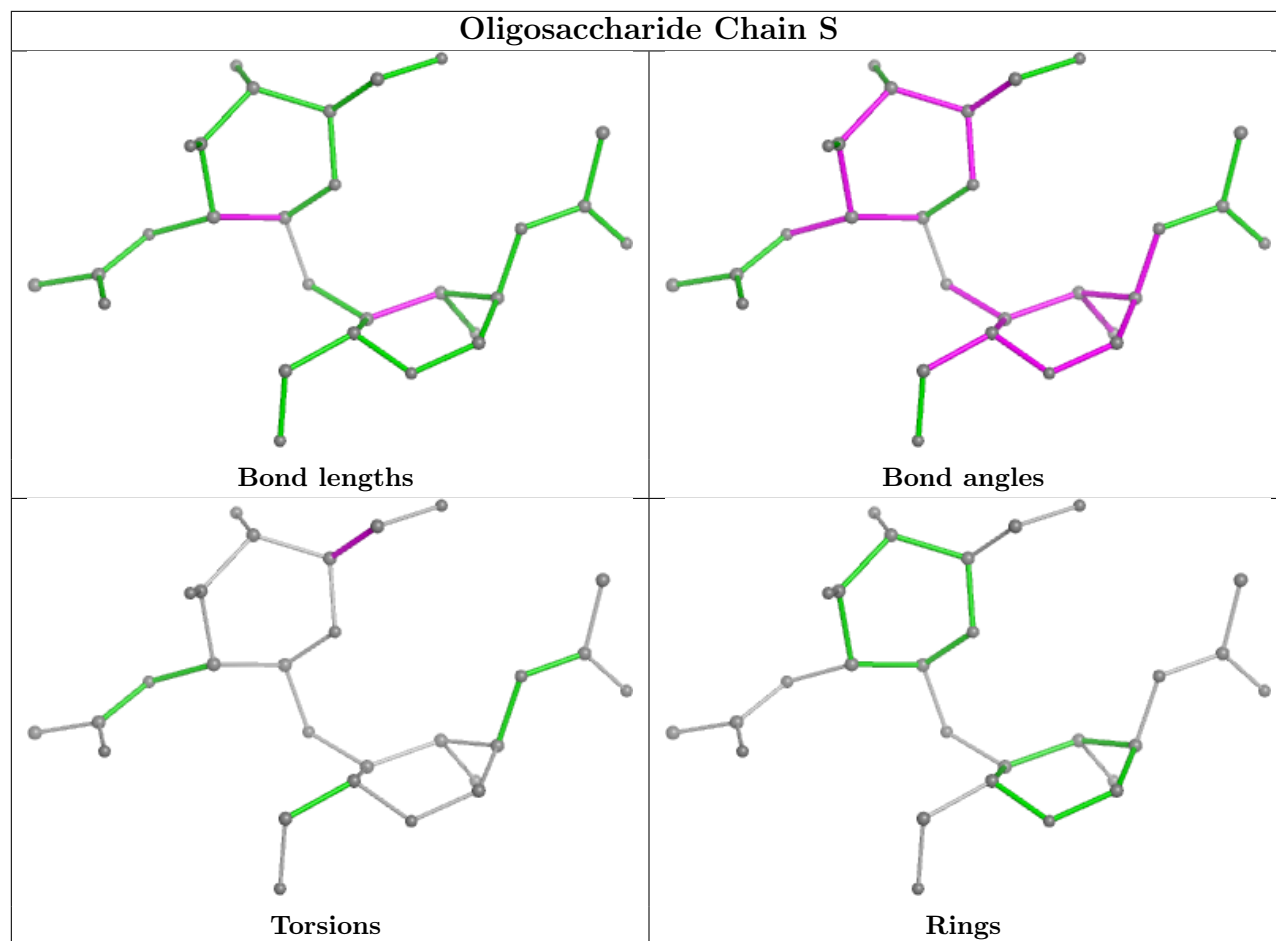


Oligosaccharide Chain P

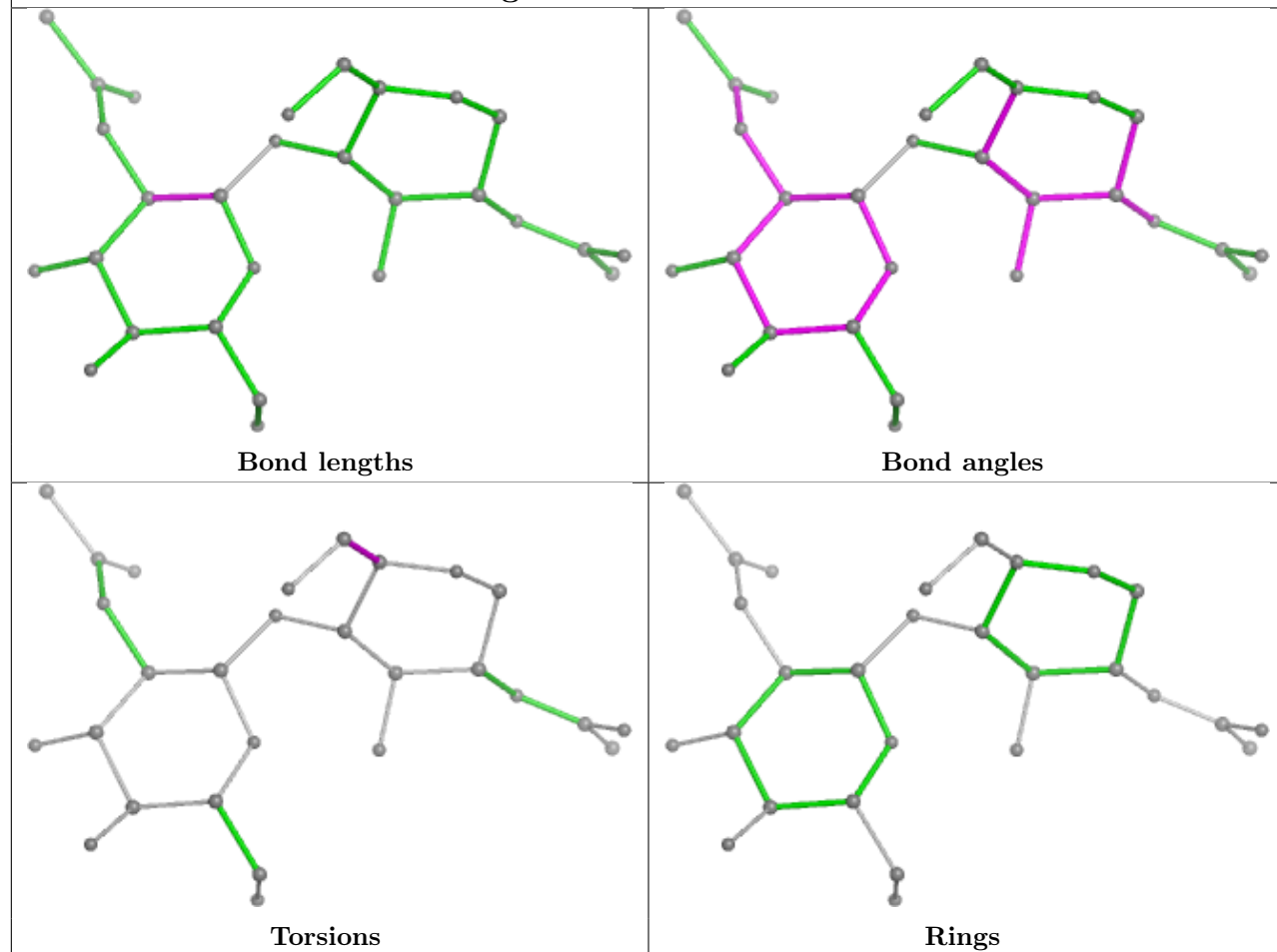


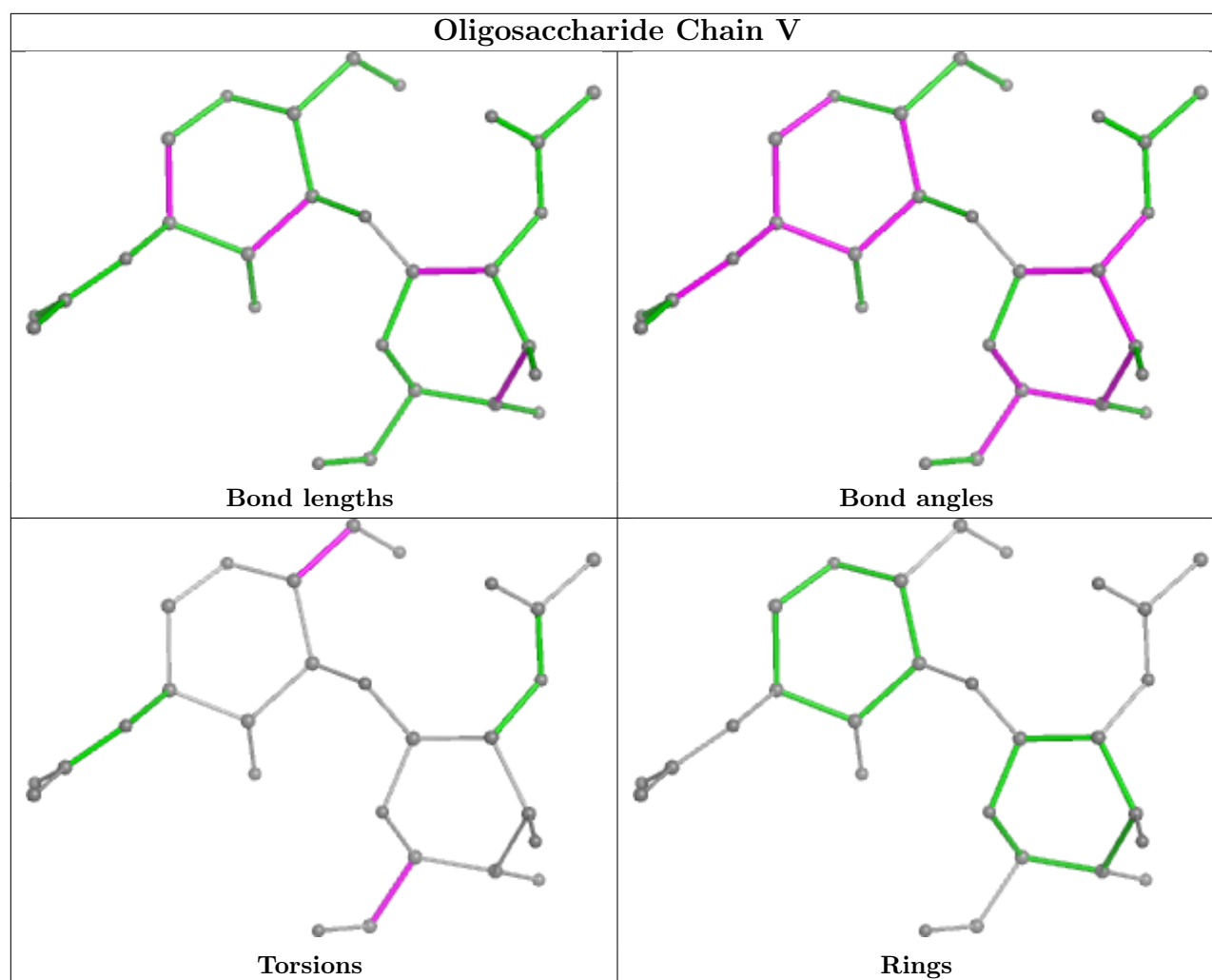


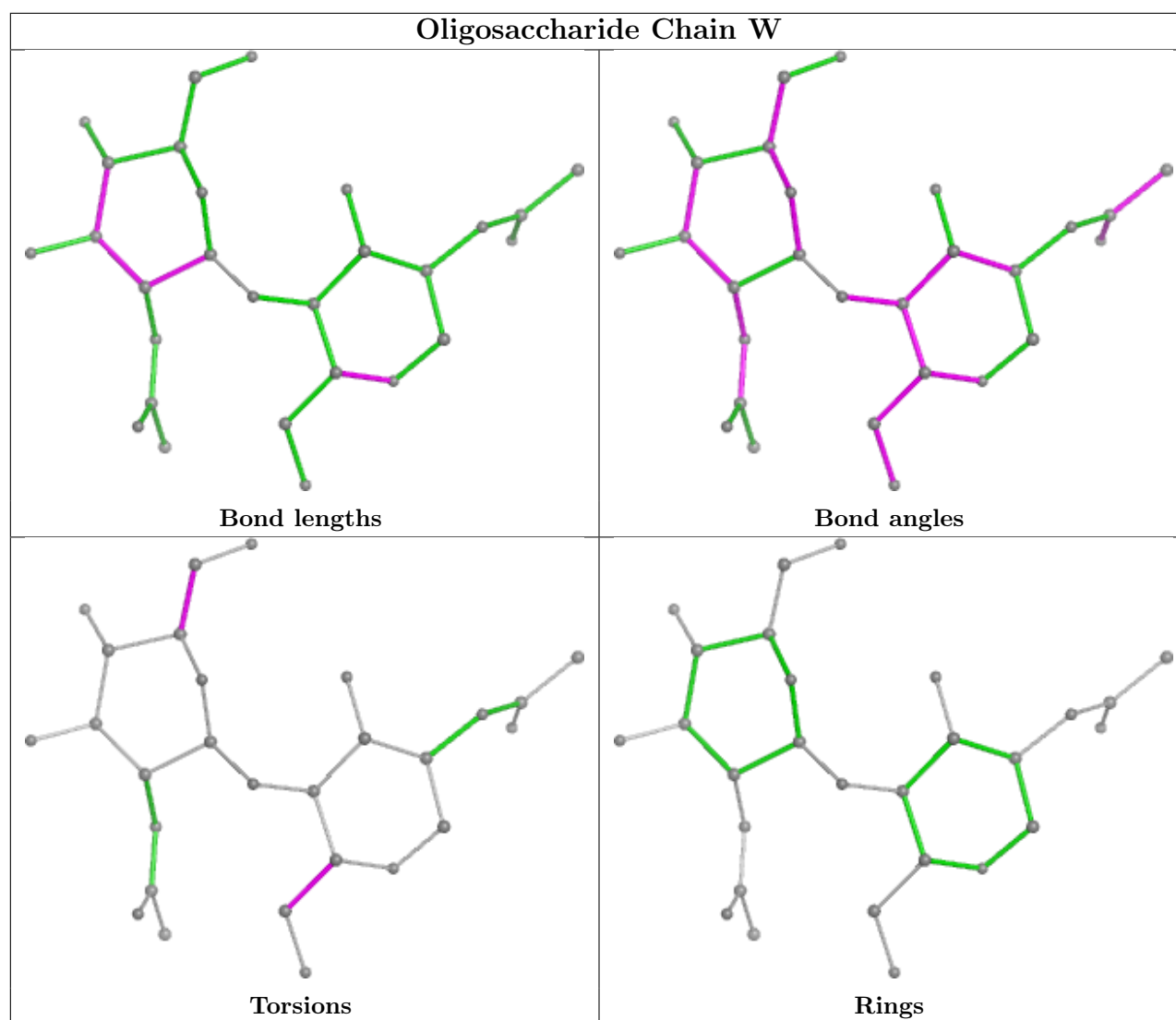


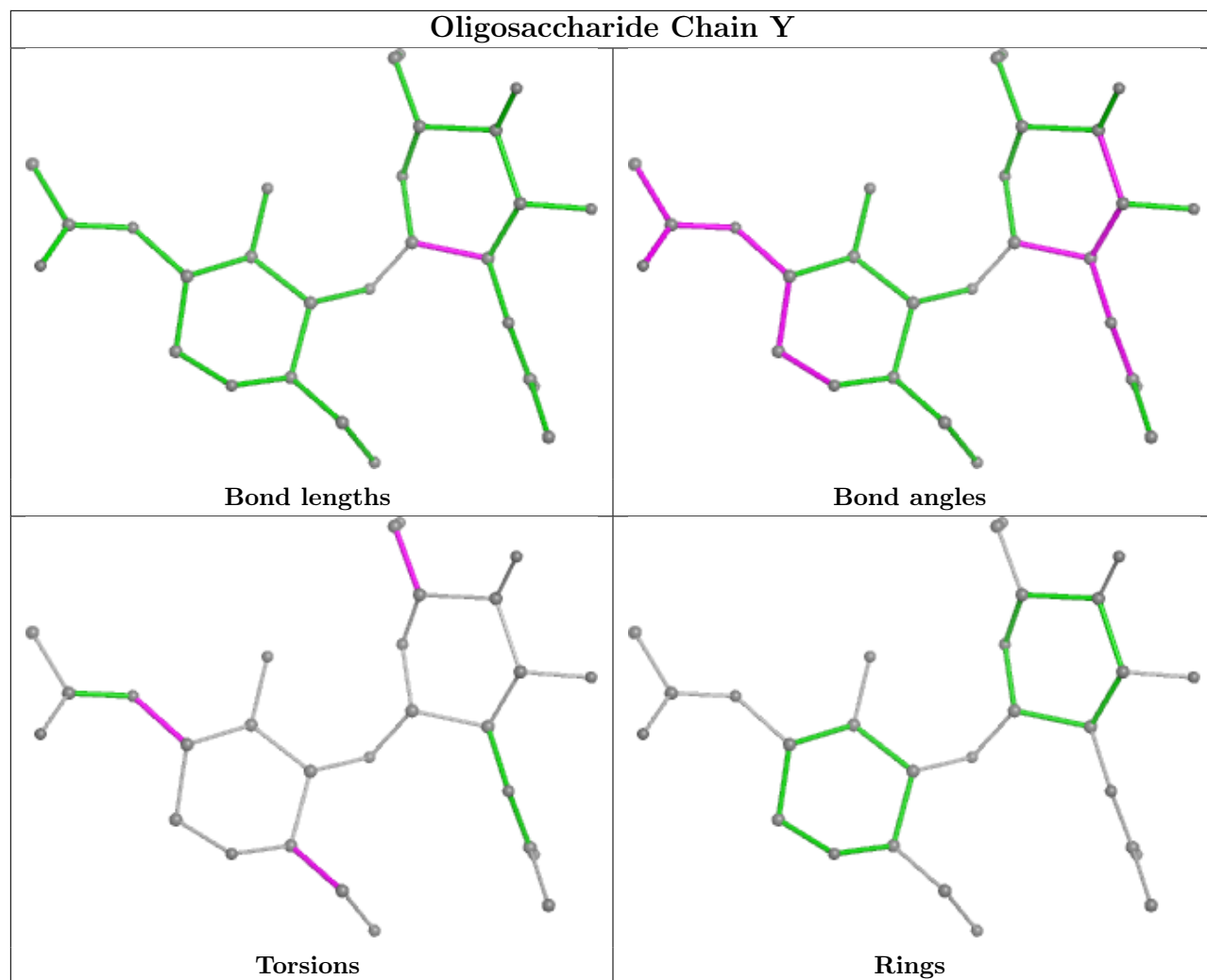


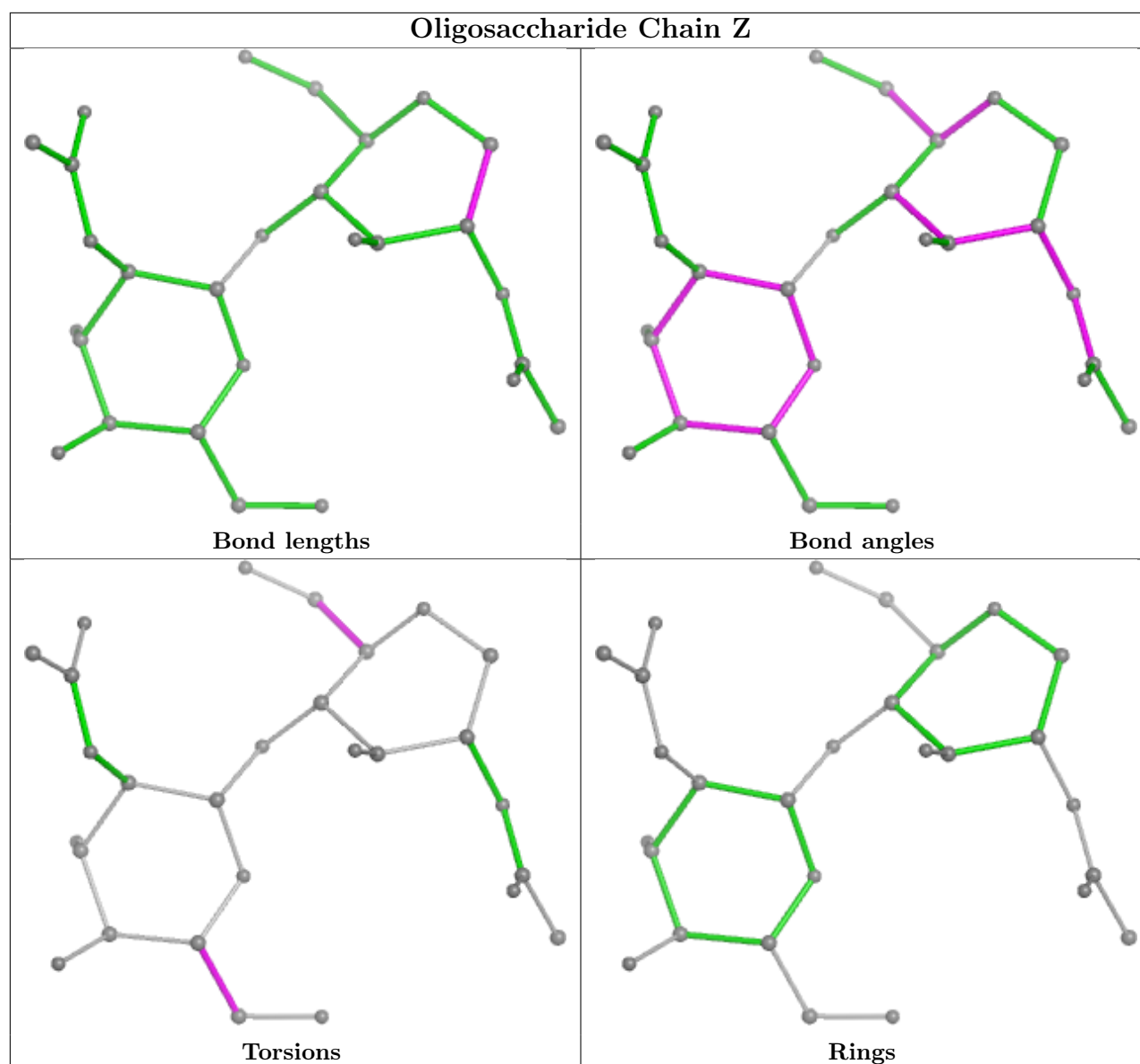
Oligosaccharide Chain U











5.6 Ligand geometry [i](#)

1 ligand is 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	D	410	2	14,14,15	1.33	1 (7%)	17,19,21	1.65	4 (23%)

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	D	410	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	410	NAG	C4-C5	2.81	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	410	NAG	C3-C4-C5	3.57	116.60	110.24
7	D	410	NAG	O5-C1-C2	-3.15	106.32	111.29
7	D	410	NAG	O5-C5-C6	2.55	111.19	107.20
7	D	410	NAG	O7-C7-C8	-2.26	117.86	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	410	NAG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	318/329 (96%)	-0.29	2 (0%) 85 80	110, 138, 165, 184	0
1	C	316/329 (96%)	-0.32	1 (0%) 90 89	104, 126, 153, 180	0
1	E	318/329 (96%)	-0.35	2 (0%) 85 80	106, 125, 149, 185	0
2	B	172/175 (98%)	-0.26	2 (1%) 76 68	98, 143, 196, 219	0
2	D	172/175 (98%)	-0.30	0 100 100	97, 135, 196, 233	0
2	F	172/175 (98%)	-0.21	3 (1%) 69 60	102, 138, 195, 226	0
3	G	129/226 (57%)	0.21	7 (5%) 32 29	163, 221, 268, 289	0
3	I	226/226 (100%)	-0.19	6 (2%) 56 49	114, 150, 223, 253	0
3	K	224/226 (99%)	-0.23	4 (1%) 67 59	109, 141, 229, 251	0
4	H	107/218 (49%)	0.61	12 (11%) 11 14	189, 240, 266, 273	0
4	J	216/218 (99%)	-0.28	1 (0%) 87 83	113, 142, 196, 223	0
4	L	216/218 (99%)	0.03	2 (0%) 81 73	121, 183, 215, 234	0
All	All	2586/2844 (90%)	-0.19	42 (1%) 70 61	97, 140, 233, 289	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	62	SER	5.0
3	K	205	LYS	4.2
4	H	36	TYR	4.0
2	B	171	PHE	3.8
3	K	116	THR	3.5

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

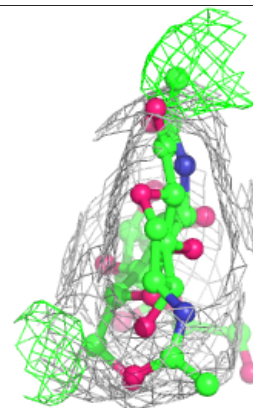
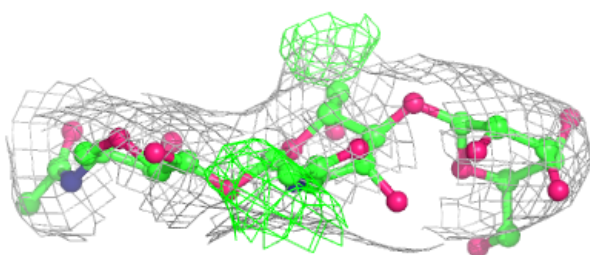
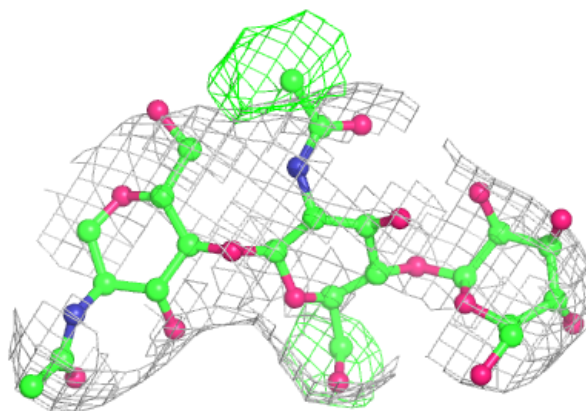
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	R	2	14/15	0.13	0.23	200,206,210,215	0
6	NAG	P	2	14/15	0.33	0.14	181,188,190,191	0
5	BMA	T	3	11/12	0.36	0.19	243,248,254,258	0
6	NAG	U	2	14/15	0.45	0.14	167,171,175,178	0
6	NAG	S	2	14/15	0.46	0.18	207,214,219,222	0
5	BMA	O	3	11/12	0.52	0.24	230,232,237,240	0
5	BMA	X	3	11/12	0.53	0.18	201,205,212,213	0
6	NAG	Q	2	14/15	0.55	0.16	267,273,284,291	0
6	NAG	Q	1	14/15	0.55	0.18	232,248,258,261	0
6	NAG	Z	2	14/15	0.55	0.16	258,264,271,277	0
6	NAG	Y	2	14/15	0.59	0.14	190,196,203,203	0
6	NAG	N	2	14/15	0.65	0.12	212,217,225,226	0
5	NAG	M	2	14/15	0.68	0.15	197,203,217,217	0
6	NAG	Z	1	14/15	0.72	0.12	223,239,248,250	0
6	NAG	W	2	14/15	0.72	0.12	191,197,204,209	0
6	NAG	V	2	14/15	0.76	0.13	190,200,204,205	0
6	NAG	S	1	14/15	0.80	0.15	172,183,192,204	0
5	BMA	M	3	11/12	0.81	0.10	214,220,223,226	0
6	NAG	V	1	14/15	0.84	0.14	175,187,190,191	0
5	NAG	O	2	14/15	0.85	0.31	209,217,228,228	0
5	NAG	T	1	14/15	0.86	0.14	183,195,200,203	0
6	NAG	W	1	14/15	0.86	0.15	162,171,175,184	0
5	NAG	M	1	14/15	0.86	0.12	178,188,193,196	0
5	NAG	T	2	14/15	0.87	0.25	210,221,233,237	0
6	NAG	R	1	14/15	0.88	0.15	170,180,186,193	0
6	NAG	Y	1	14/15	0.89	0.11	156,164,172,180	0
6	NAG	U	1	14/15	0.89	0.08	143,149,159,160	0
6	NAG	N	1	14/15	0.90	0.15	180,186,194,202	0
6	NAG	P	1	14/15	0.92	0.09	152,160,164,170	0
5	NAG	X	2	14/15	0.92	0.17	177,183,195,196	0
5	NAG	O	1	14/15	0.92	0.21	192,203,213,213	0
5	NAG	X	1	14/15	0.94	0.18	155,164,168,171	0

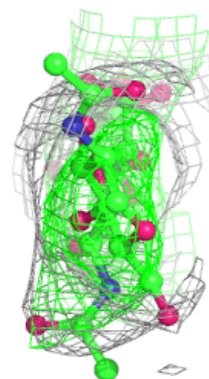
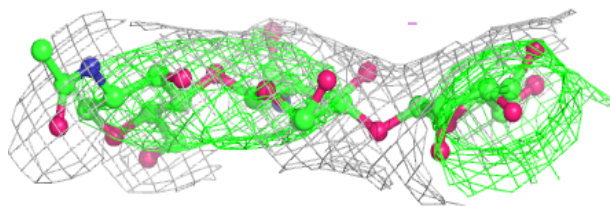
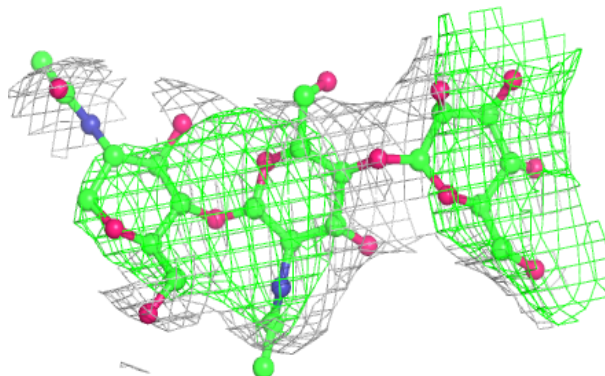
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

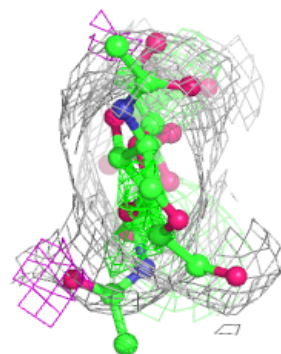
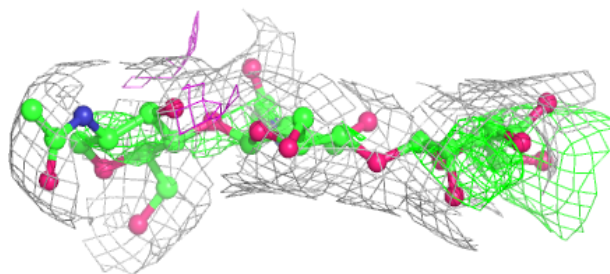
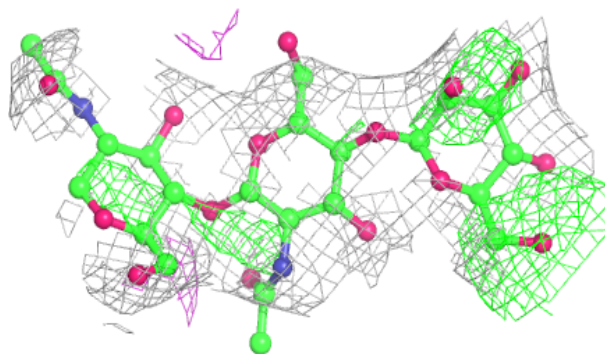
**Electron density around Chain O:**

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

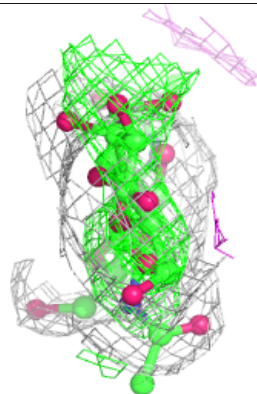
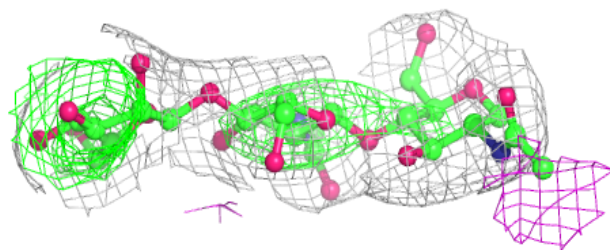
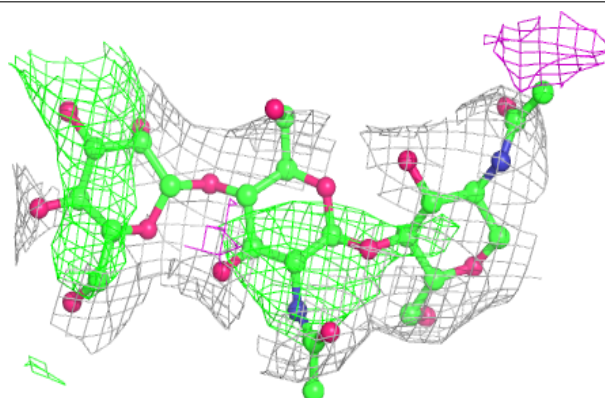


Electron density around Chain T:

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

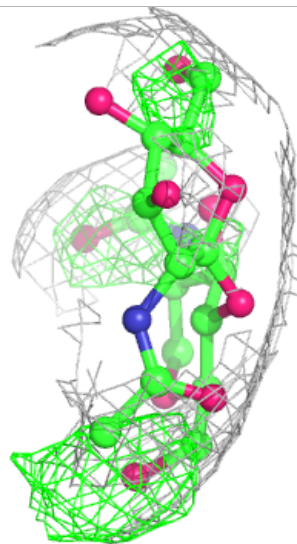
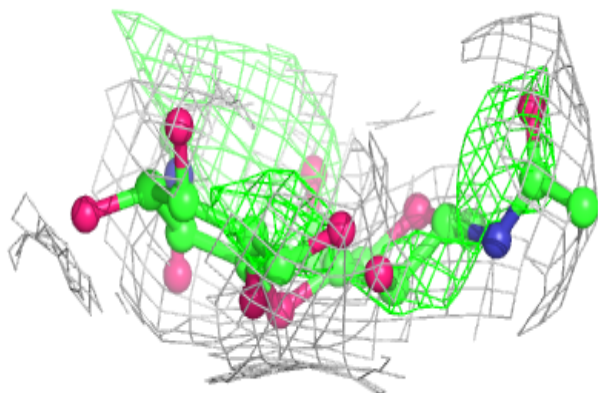
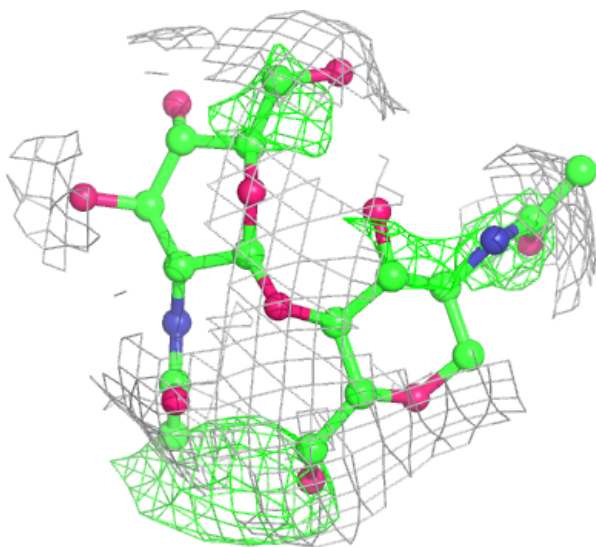
**Electron density around Chain X:**

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



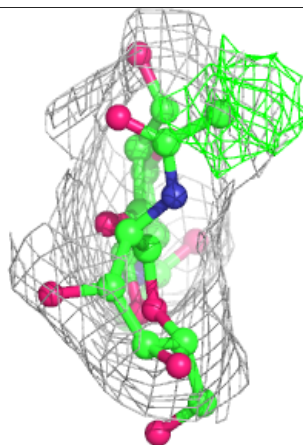
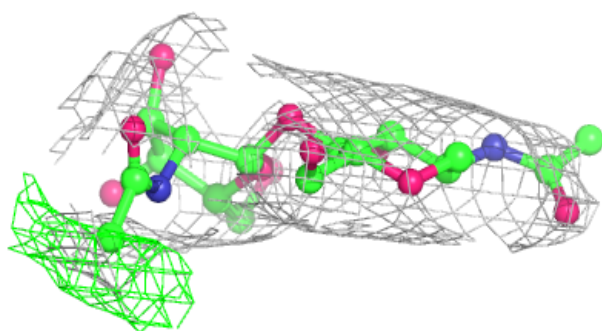
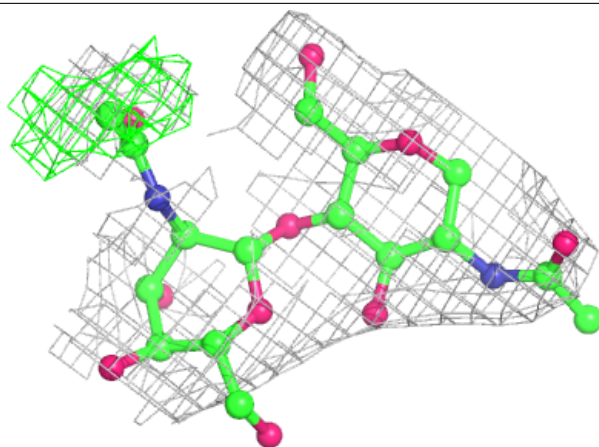
Electron density around Chain N:

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



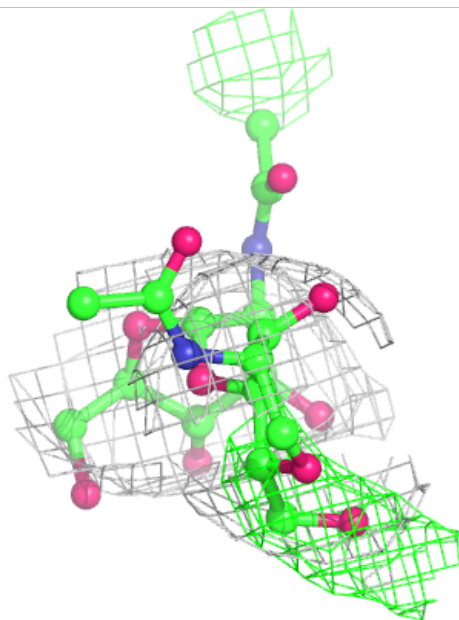
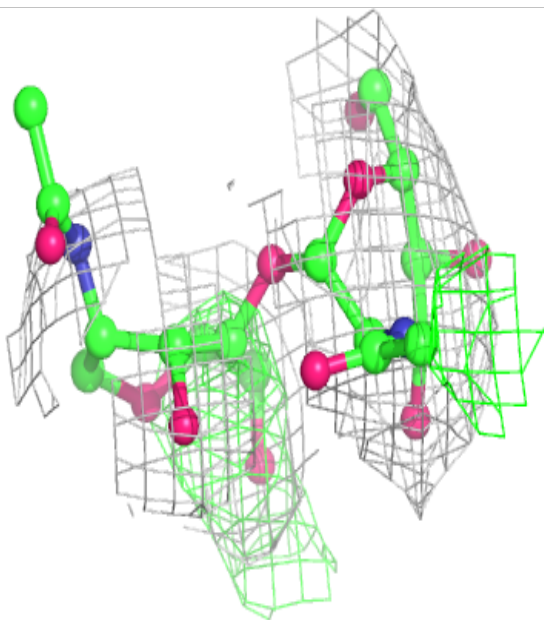
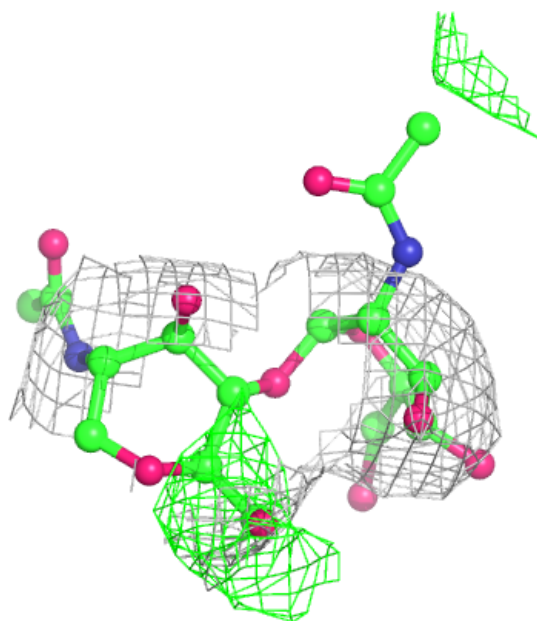
Electron density around Chain P:

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



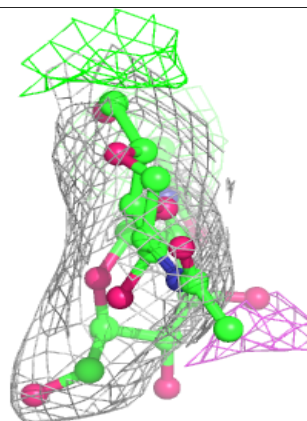
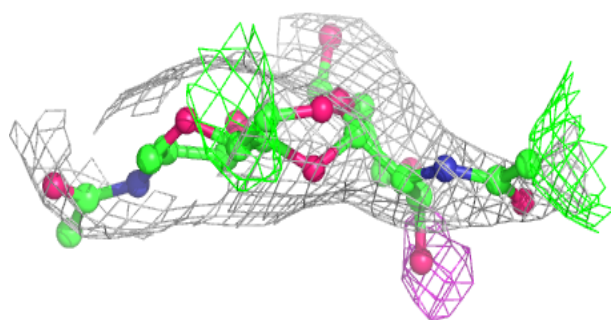
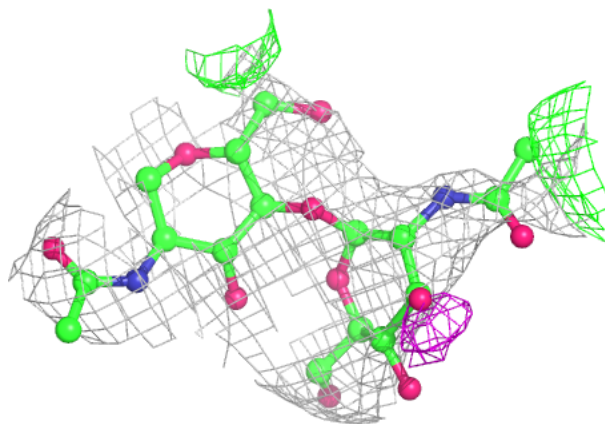
Electron density around Chain Q:

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



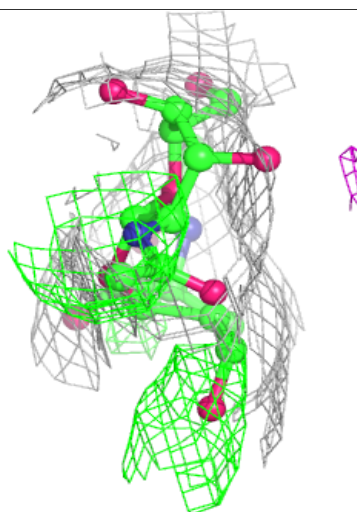
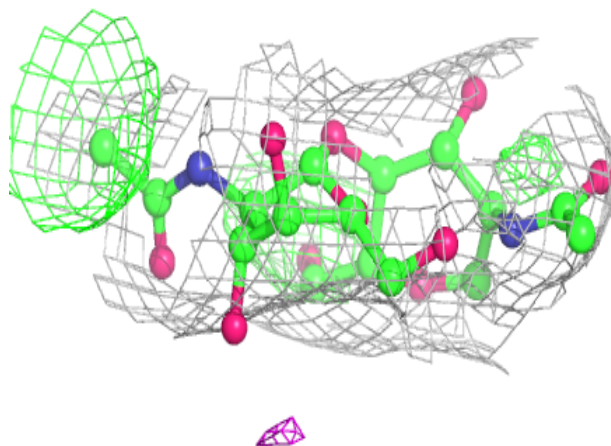
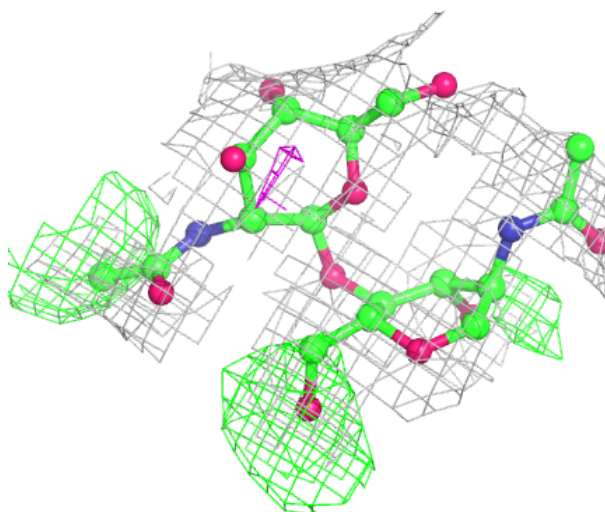
Electron density around Chain R:

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



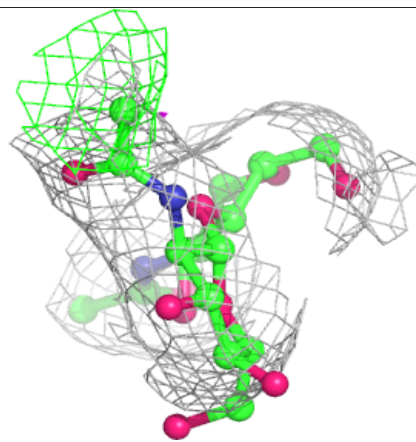
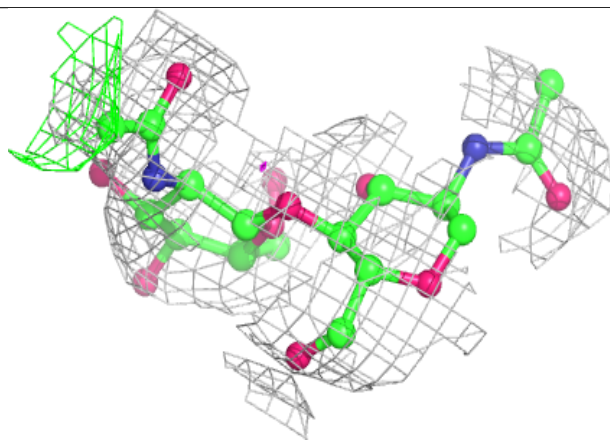
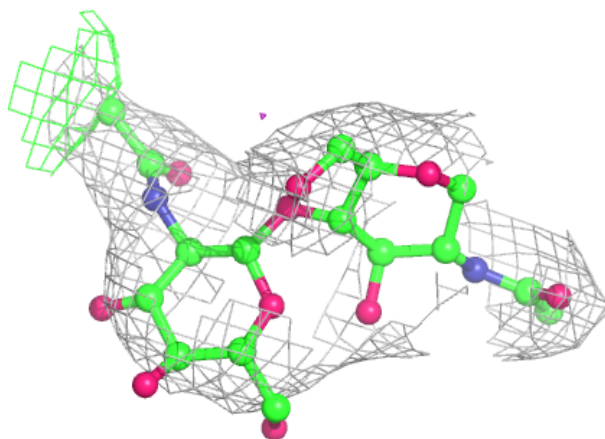
Electron density around Chain S:

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



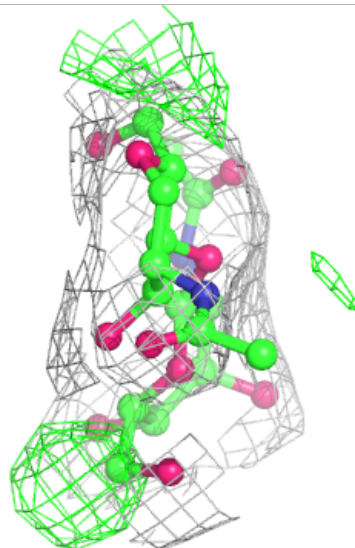
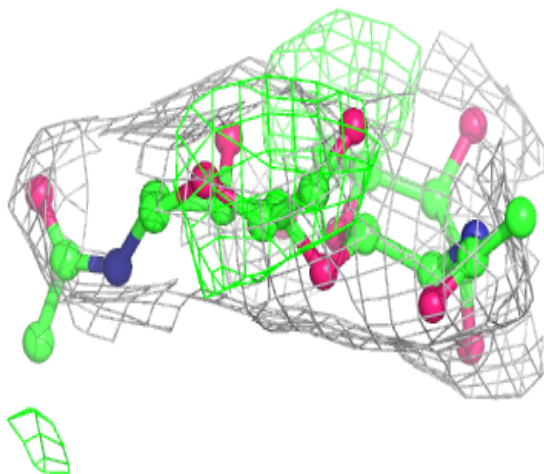
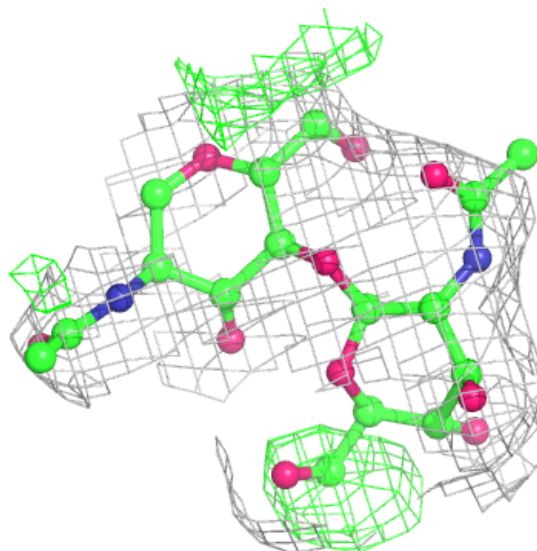
Electron density around Chain U:

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



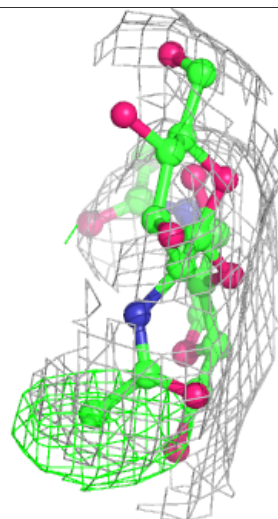
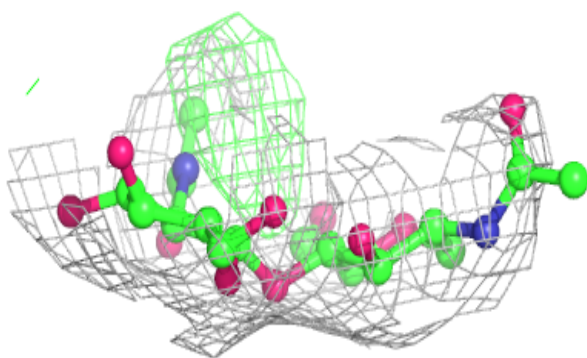
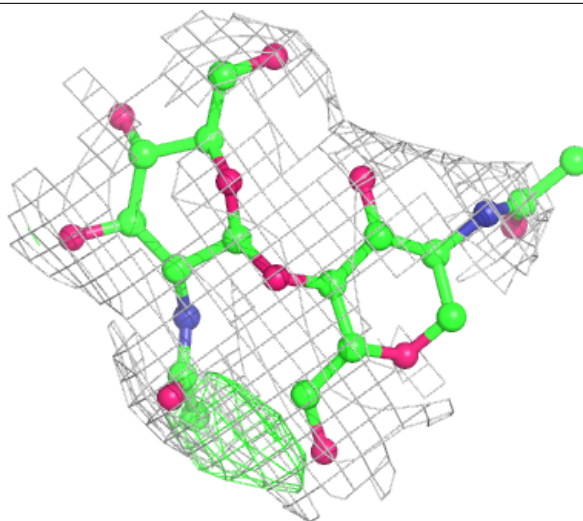
Electron density around Chain V:

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



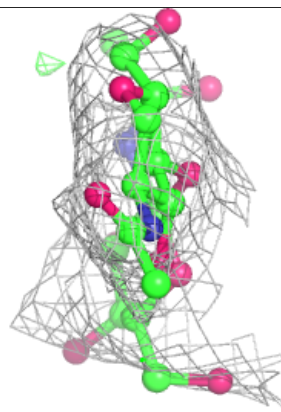
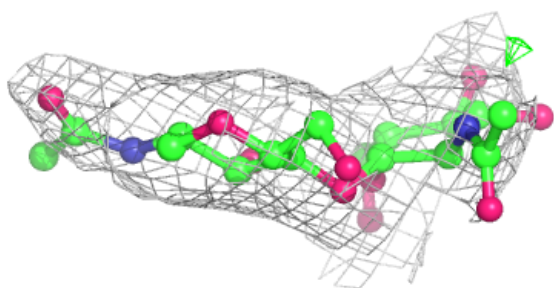
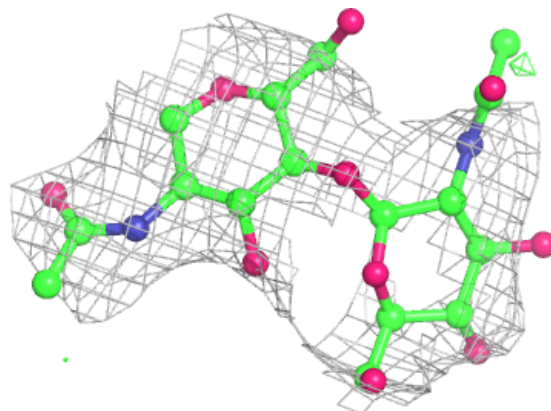
Electron density around Chain W:

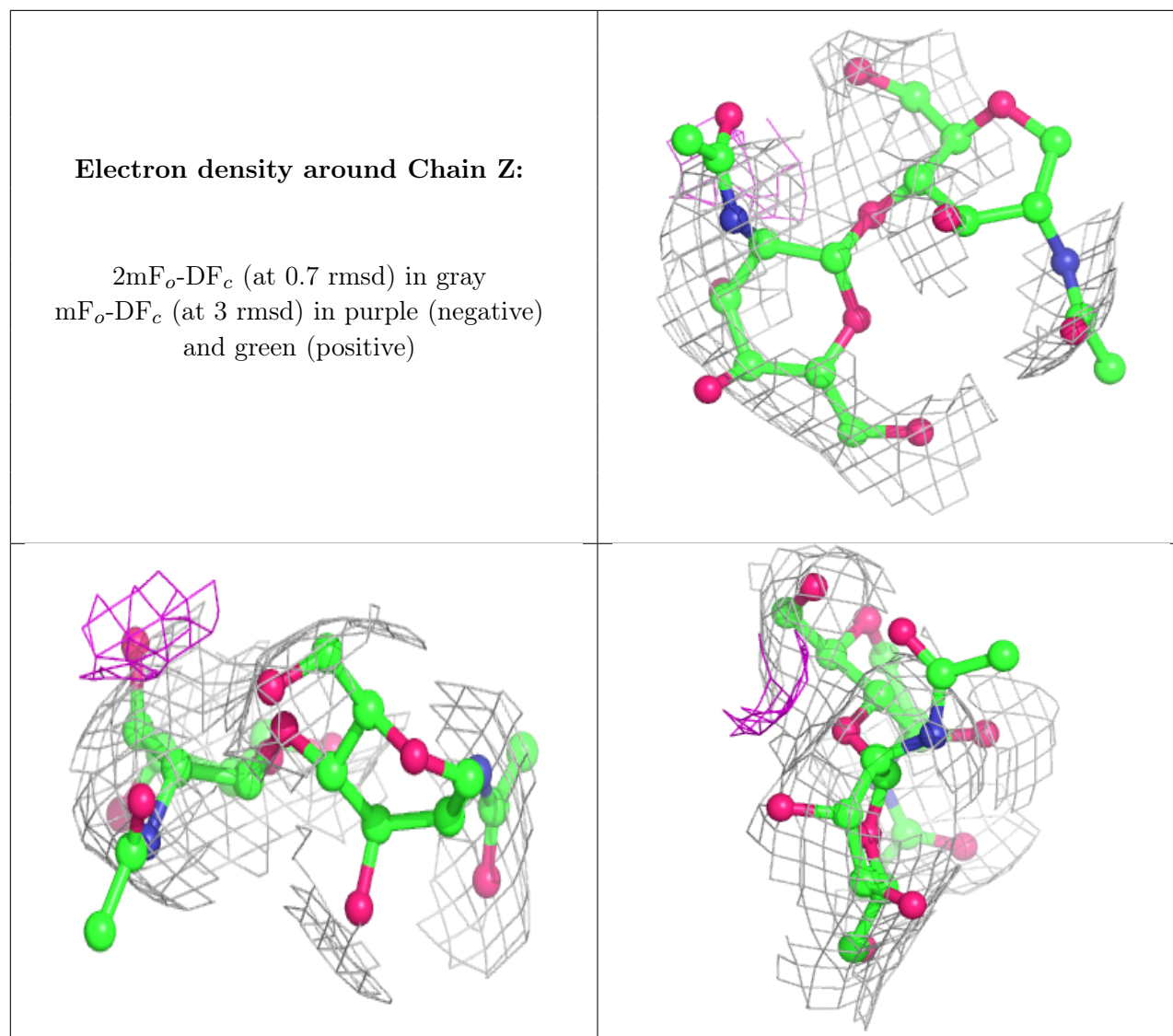
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Y:

$2mF_o-DF_c$ (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	D	410	14/15	0.57	0.26	201,215,222,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.