



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 01:44 am BST

PDB ID : 4AY1
Title : Human YKL-39 is a pseudo-chitinase with retained chitooligosaccharide binding properties
Authors : Schimpl, M.; Rush, C.L.; Betou, M.; Eggleston, I.M.; Penman, G.A.; Recklies, A.D.; van Aalten, D.M.F.
Deposited on : 2012-06-17
Resolution : 1.95 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

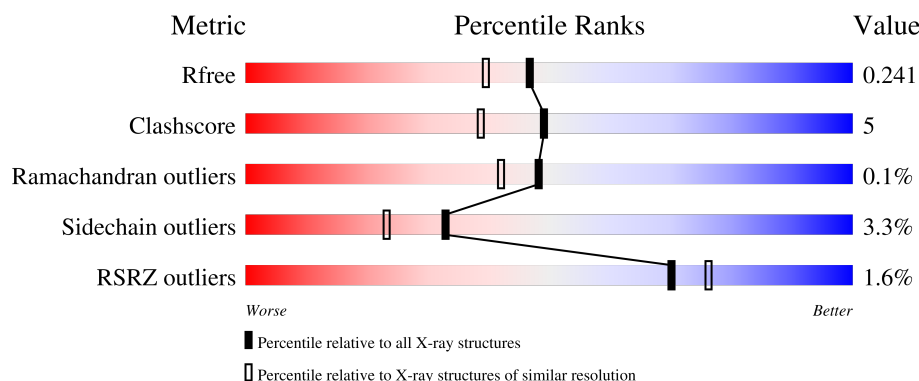
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



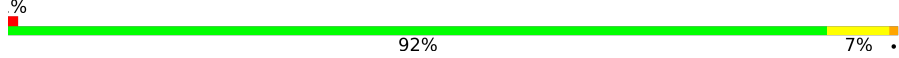

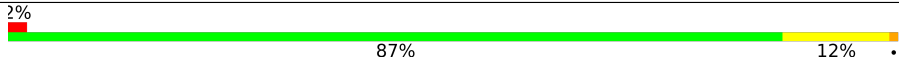
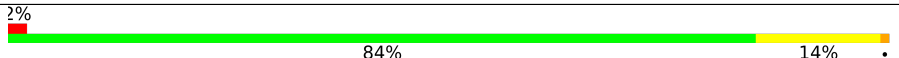
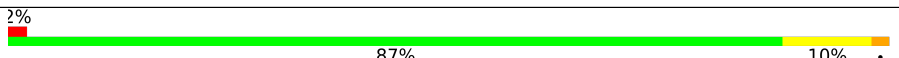
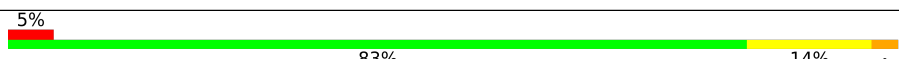
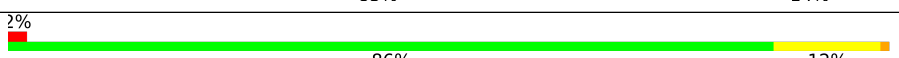
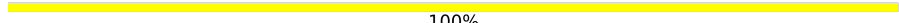
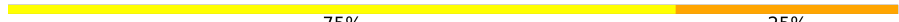
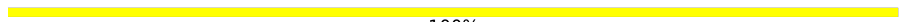









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	365	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	365	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	365	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	365	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	E	365	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	365	
1	G	365	
1	H	365	
1	I	365	
1	J	365	
1	K	365	
1	L	365	
2	M	4	
2	N	4	
2	O	4	
2	P	4	
2	Q	4	
2	R	4	
2	S	4	
2	T	4	
2	U	4	
2	V	4	
2	W	4	
2	X	4	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37104 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 CHITINASE-3-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	B	364	Total	C	N	O	S	0	0	0
			2869	1847	474	536	12			
1	C	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	D	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	E	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	F	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	G	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	H	364	Total	C	N	O	S	0	0	0
			2874	1852	474	536	12			
1	I	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	J	364	Total	C	N	O	S	0	0	0
			2866	1846	472	536	12			
1	K	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	L	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	N	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	O	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	P	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	Q	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	R	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	S	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	T	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	U	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	V	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	W	4	Total	C	N	O	0	0	0
			57	32	4	21			
2	X	4	Total	C	N	O	0	0	0
			57	32	4	21			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		
3	B	137	Total	O	0	0
			137	137		
3	C	181	Total	O	0	0
			181	181		
3	D	165	Total	O	0	0
			165	165		
3	E	190	Total	O	0	0
			190	190		
3	F	180	Total	O	0	0
			180	180		
3	G	174	Total	O	0	0
			174	174		
3	H	167	Total	O	0	0
			167	167		

Continued on next page...

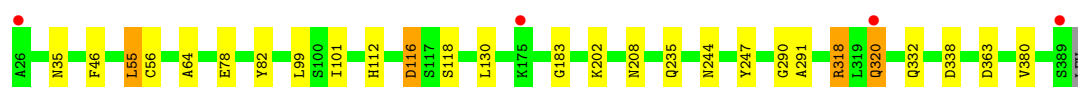
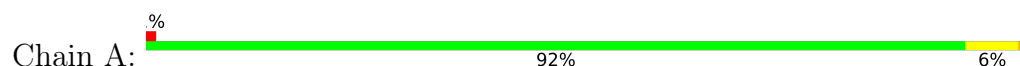
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	125	Total 125	O 125	0	0
3	J	162	Total 162	O 162	0	0
3	K	83	Total 83	O 83	0	0
3	L	127	Total 127	O 127	0	0

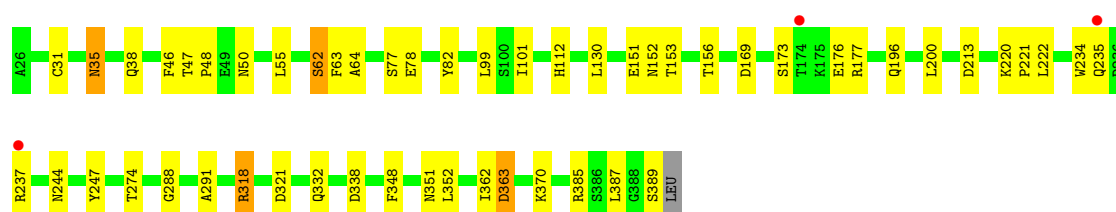
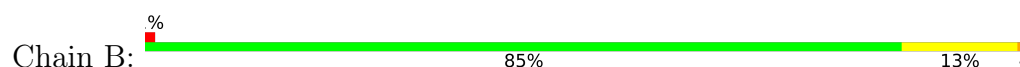
3 Residue-property plots [i](#)

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

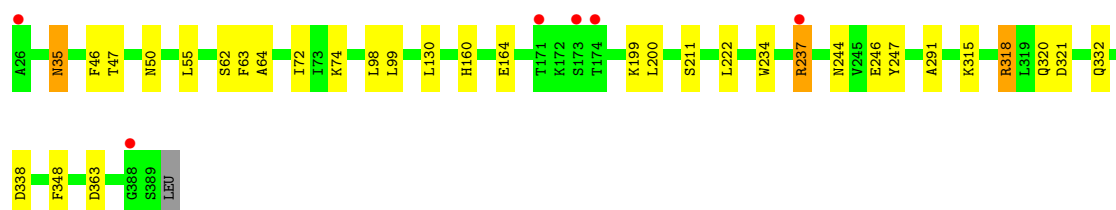
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



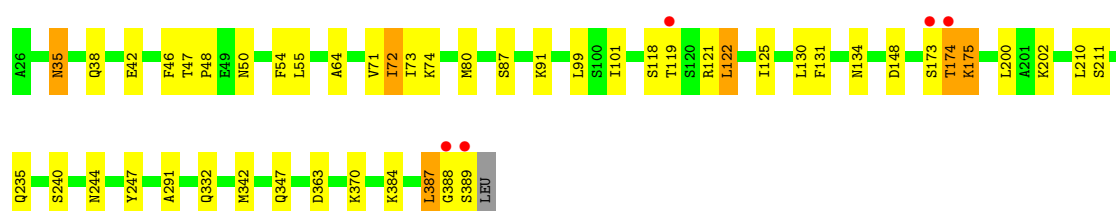
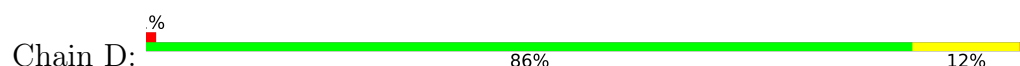
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



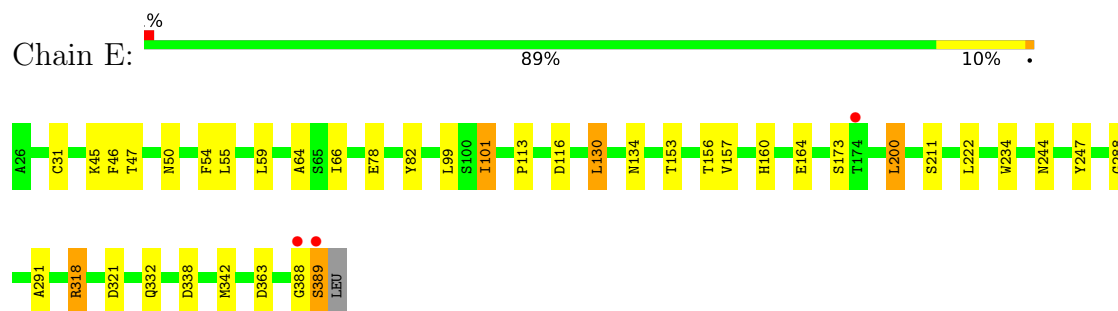
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



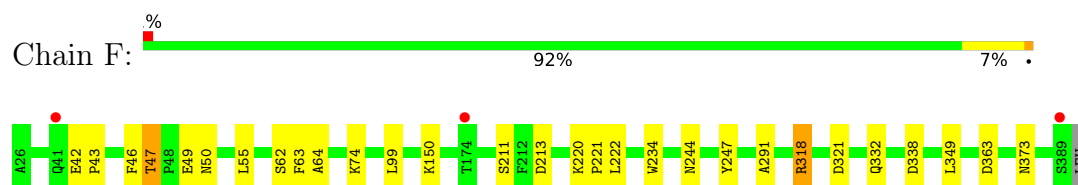
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



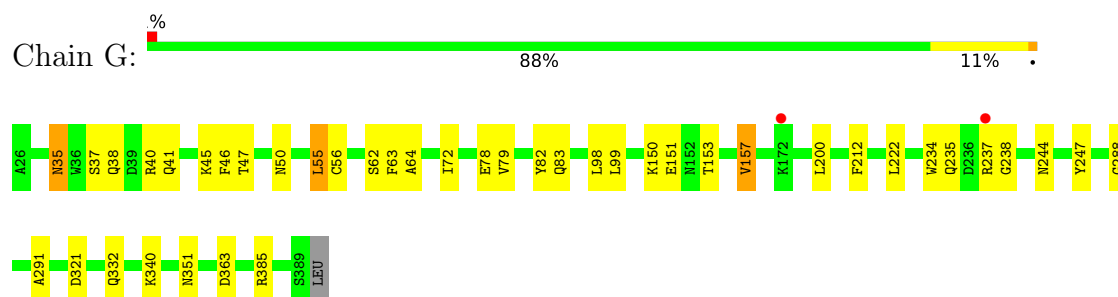
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



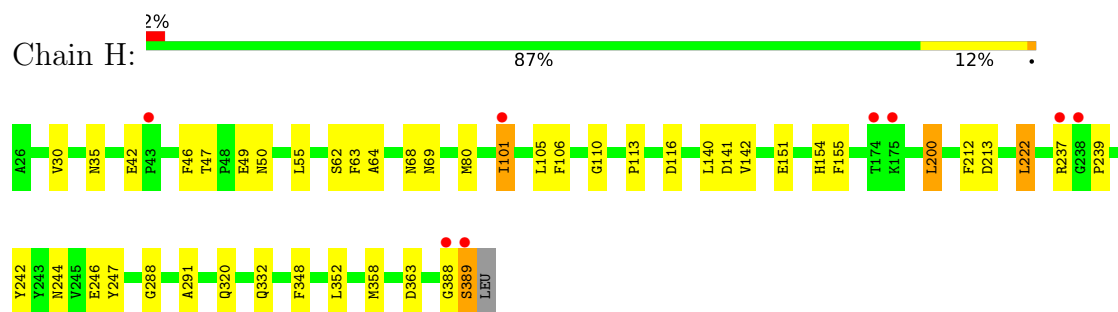
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



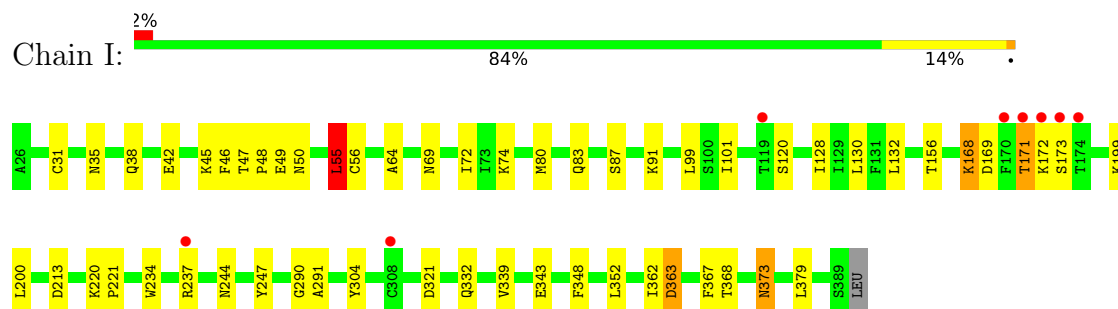
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



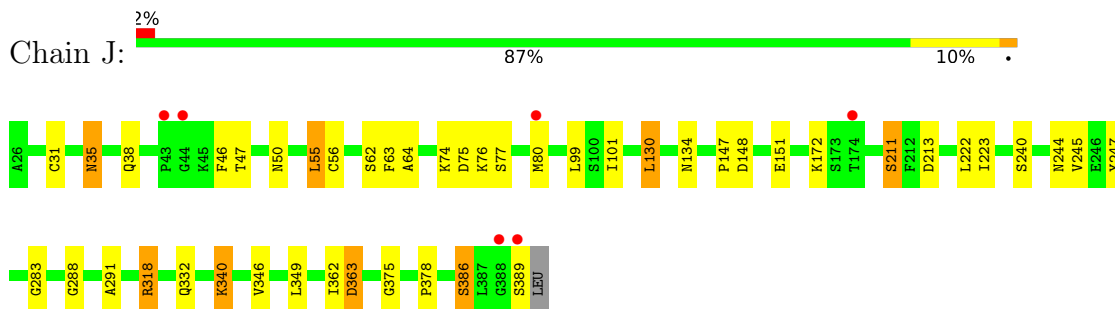
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



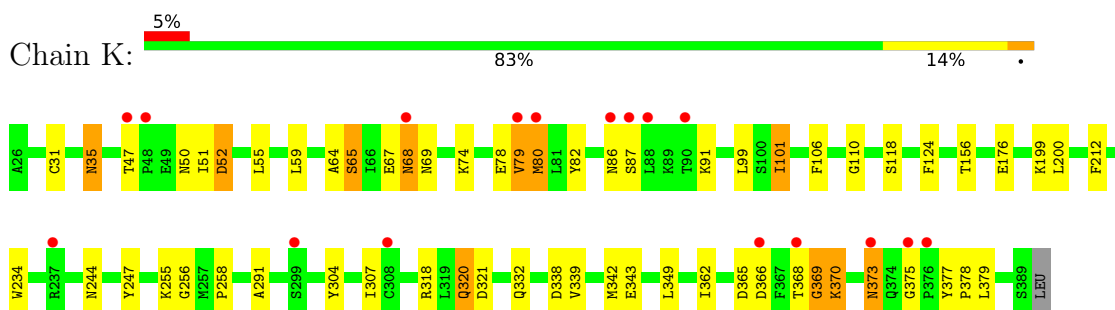
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



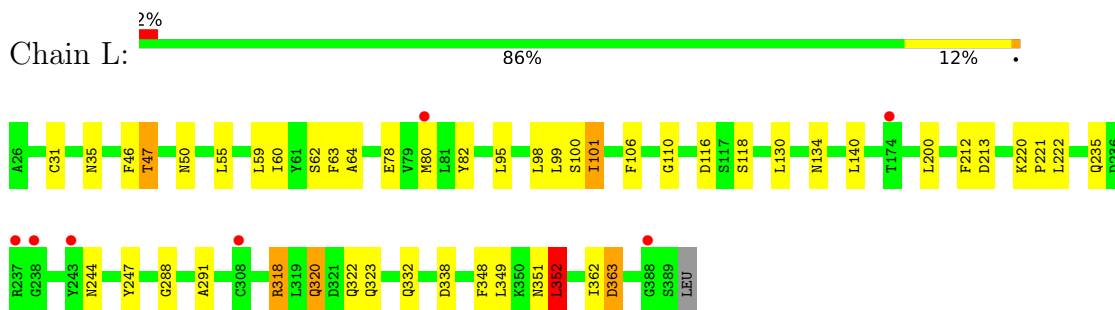
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



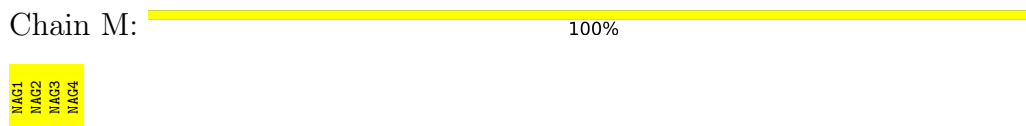
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



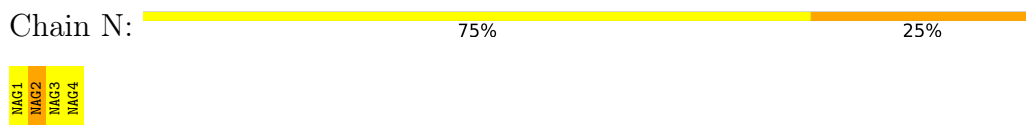
- Molecule 1: CHITINASE-3-LIKE PROTEIN 2



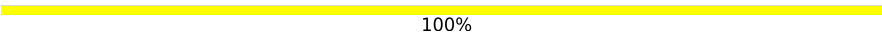
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain O:  100%

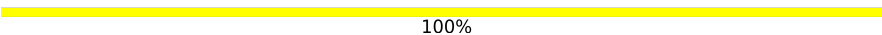
NAG1
NAG2
NAG3
NAG4

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

Chain P:  25% 25% 50%

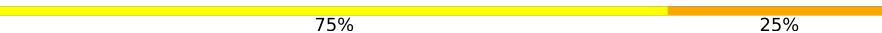
NAG1
NAG2
NAG3
NAG4

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

Chain Q:  100%

NAG1
NAG2
NAG3
NAG4

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

Chain R:  75% 25%

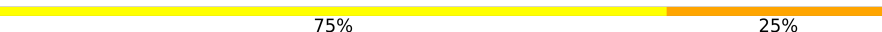
NAG1
NAG2
NAG3
NAG4

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

Chain S:  25% 75%

NAG1
NAG2
NAG3
NAG4

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

Chain T:  75% 25%



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

Chain U: 25% 50% 25%



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

Chain V: 100%



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

Chain W: 50% 50%



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

Chain X: 25% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	255.69Å 152.54Å 138.19Å 90.00° 94.62° 90.00°	Depositor
Resolution (Å)	137.36 – 1.95 137.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (137.36-1.95) 99.4 (137.36-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.191 , 0.239 0.191 , 0.241	Depositor DCC
R_{free} test set	1911 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37104	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	0/2954	0.67	2/4002 (0.0%)
1	B	0.50	0/2944	0.64	1/3985 (0.0%)
1	C	0.53	0/2958	0.65	2/4006 (0.0%)
1	D	0.55	0/2958	0.64	1/4006 (0.0%)
1	E	0.57	0/2958	0.67	4/4006 (0.1%)
1	F	0.57	0/2954	0.67	2/4002 (0.0%)
1	G	0.55	0/2958	0.63	0/4006
1	H	0.54	0/2950	0.64	1/3996 (0.0%)
1	I	0.49	0/2954	0.60	1/4002 (0.0%)
1	J	0.54	0/2942	0.64	0/3988
1	K	0.60	2/2954 (0.1%)	0.64	0/4002
1	L	0.50	0/2954	0.65	2/4002 (0.0%)
All	All	0.55	2/35438 (0.0%)	0.65	16/48003 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	52	ASP	CG-OD2	12.61	1.54	1.25
1	K	86	ASN	C-O	7.66	1.37	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	318	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	318	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	318	ARG	CG-CD-NE	-7.20	96.68	111.80
1	D	342	MET	CA-CB-CG	-6.93	101.52	113.30
1	B	318	ARG	NE-CZ-NH2	-6.28	117.16	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	387	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2878	0	2819	19	0
1	B	2869	0	2811	34	0
1	C	2882	0	2830	18	1
1	D	2882	0	2830	43	1
1	E	2882	0	2830	26	0
1	F	2878	0	2819	19	0
1	G	2882	0	2830	31	0
1	H	2874	0	2820	33	0
1	I	2878	0	2819	48	0
1	J	2866	0	2798	29	0
1	K	2878	0	2819	49	0
1	L	2878	0	2819	28	0
2	M	57	0	51	0	0
2	N	57	0	51	1	0
2	O	57	0	51	0	0
2	P	57	0	51	2	0
2	Q	57	0	51	0	0
2	R	57	0	51	1	0
2	S	57	0	51	0	0
2	T	57	0	51	1	0
2	U	57	0	51	1	0
2	V	57	0	51	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	57	0	51	1	0
2	X	57	0	51	1	0
3	A	202	0	0	0	0
3	B	137	0	0	3	0
3	C	181	0	0	0	0
3	D	165	0	0	1	0
3	E	190	0	0	1	0
3	F	180	0	0	2	0
3	G	174	0	0	2	0
3	H	167	0	0	1	0
3	I	125	0	0	1	0
3	J	162	0	0	2	0
3	K	83	0	0	2	0
3	L	127	0	0	2	0
All	All	37104	0	34456	370	1

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 5.

The worst 5 of 370 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:ASN:HB3	3:K:575:HOH:O	1.47	1.14
1:I:168:LYS:O	1:I:171:THR:HG22	1.47	1.14
1:I:47:THR:HG21	1:I:80:MET:CE	1.81	1.09
1:I:47:THR:CG2	1:I:80:MET:CE	2.37	1.02
1:L:351:ASN:HB2	3:L:550:HOH:O	1.60	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLN:NE2	1:D:347:GLN:OE1[4_546]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	B	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
1	C	362/365 (99%)	360 (99%)	2 (1%)	0	100	100
1	D	362/365 (99%)	357 (99%)	3 (1%)	2 (1%)	22	13
1	E	362/365 (99%)	356 (98%)	6 (2%)	0	100	100
1	F	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	G	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
1	H	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	I	362/365 (99%)	356 (98%)	6 (2%)	0	100	100
1	J	362/365 (99%)	359 (99%)	2 (1%)	1 (0%)	37	29
1	K	362/365 (99%)	351 (97%)	10 (3%)	1 (0%)	37	29
1	L	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
All	All	4344/4380 (99%)	4284 (99%)	56 (1%)	4 (0%)	48	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	LYS
1	K	369	GLY
1	D	148	ASP
1	J	148	ASP

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	315/317 (99%)	308 (98%)	7 (2%)	47	41
1	B	313/317 (99%)	301 (96%)	12 (4%)	28	18
1	C	316/317 (100%)	307 (97%)	9 (3%)	38	29
1	D	316/317 (100%)	303 (96%)	13 (4%)	26	15
1	E	316/317 (100%)	309 (98%)	7 (2%)	47	41
1	F	315/317 (99%)	307 (98%)	8 (2%)	42	34
1	G	316/317 (100%)	306 (97%)	10 (3%)	34	24
1	H	314/317 (99%)	305 (97%)	9 (3%)	37	28
1	I	315/317 (99%)	306 (97%)	9 (3%)	37	28
1	J	312/317 (98%)	299 (96%)	13 (4%)	25	15
1	K	315/317 (99%)	301 (96%)	14 (4%)	24	13
1	L	315/317 (99%)	302 (96%)	13 (4%)	26	15
All	All	3778/3804 (99%)	3654 (97%)	124 (3%)	33	23

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	55	LEU
1	K	373	ASN
1	H	222	LEU
1	K	370	LYS
1	L	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	373	ASN
1	K	320	GLN
1	J	149	GLN
1	J	373	ASN
1	L	235	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 ⓘ

48 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	M	1	2	15,15,15	1.16	1 (6%)	21,21,21	1.35	3 (14%)
2	NAG	M	2	2	14,14,15	1.22	2 (14%)	17,19,21	0.99	0
2	NAG	M	3	2	14,14,15	0.95	0	17,19,21	1.66	3 (17%)
2	NAG	M	4	2	14,14,15	1.07	1 (7%)	17,19,21	0.97	0
2	NAG	N	1	2	15,15,15	0.69	0	21,21,21	1.43	4 (19%)
2	NAG	N	2	2	14,14,15	0.99	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	N	3	2	14,14,15	1.21	1 (7%)	17,19,21	1.46	2 (11%)
2	NAG	N	4	2	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	O	1	2	15,15,15	0.76	0	21,21,21	1.40	3 (14%)
2	NAG	O	2	2	14,14,15	0.95	0	17,19,21	1.02	1 (5%)
2	NAG	O	3	2	14,14,15	1.21	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	O	4	2	14,14,15	0.83	1 (7%)	17,19,21	0.96	0
2	NAG	P	1	2	15,15,15	0.73	0	21,21,21	1.46	4 (19%)
2	NAG	P	2	2	14,14,15	1.03	1 (7%)	17,19,21	1.31	2 (11%)
2	NAG	P	3	2	14,14,15	0.98	1 (7%)	17,19,21	1.15	2 (11%)
2	NAG	P	4	2	14,14,15	0.87	0	17,19,21	0.93	0
2	NAG	Q	1	2	15,15,15	1.06	2 (13%)	21,21,21	1.66	4 (19%)
2	NAG	Q	2	2	14,14,15	0.83	0	17,19,21	1.32	2 (11%)
2	NAG	Q	3	2	14,14,15	0.91	0	17,19,21	1.10	2 (11%)
2	NAG	Q	4	2	14,14,15	0.92	0	17,19,21	0.98	2 (11%)
2	NAG	R	1	2	15,15,15	0.88	1 (6%)	21,21,21	1.50	4 (19%)
2	NAG	R	2	2	14,14,15	1.02	2 (14%)	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	R	3	2	14,14,15	1.32	2 (14%)	17,19,21	1.32	3 (17%)
2	NAG	R	4	2	14,14,15	0.80	1 (7%)	17,19,21	1.13	1 (5%)
2	NAG	S	1	2	15,15,15	0.87	0	21,21,21	1.29	2 (9%)
2	NAG	S	2	2	14,14,15	0.91	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	S	3	2	14,14,15	1.41	3 (21%)	17,19,21	1.37	2 (11%)
2	NAG	S	4	2	14,14,15	0.97	0	17,19,21	0.92	0
2	NAG	T	1	2	15,15,15	0.78	0	21,21,21	1.17	2 (9%)
2	NAG	T	2	2	14,14,15	0.94	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	T	3	2	14,14,15	0.89	0	17,19,21	1.33	2 (11%)
2	NAG	T	4	2	14,14,15	0.83	0	17,19,21	0.91	1 (5%)
2	NAG	U	1	2	15,15,15	0.90	0	21,21,21	1.10	2 (9%)
2	NAG	U	2	2	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
2	NAG	U	3	2	14,14,15	0.90	0	17,19,21	1.29	3 (17%)
2	NAG	U	4	2	14,14,15	0.40	0	17,19,21	1.02	0
2	NAG	V	1	2	15,15,15	0.86	0	21,21,21	1.50	3 (14%)
2	NAG	V	2	2	14,14,15	0.86	0	17,19,21	0.86	0
2	NAG	V	3	2	14,14,15	1.08	1 (7%)	17,19,21	1.40	3 (17%)
2	NAG	V	4	2	14,14,15	0.95	0	17,19,21	1.00	1 (5%)
2	NAG	W	1	2	15,15,15	0.98	0	21,21,21	1.39	4 (19%)
2	NAG	W	2	2	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
2	NAG	W	3	2	14,14,15	1.03	1 (7%)	17,19,21	1.73	6 (35%)
2	NAG	W	4	2	14,14,15	0.98	1 (7%)	17,19,21	0.70	0
2	NAG	X	1	2	15,15,15	0.98	1 (6%)	21,21,21	1.17	2 (9%)
2	NAG	X	2	2	14,14,15	0.90	0	17,19,21	1.19	2 (11%)
2	NAG	X	3	2	14,14,15	0.99	1 (7%)	17,19,21	1.25	3 (17%)
2	NAG	X	4	2	14,14,15	0.73	0	17,19,21	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1	2	-	0/6/26/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	3	2	-	0/6/23/26	0/1/1/1
2	NAG	M	4	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	1	2	-	0/6/26/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1
2	NAG	N	4	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2	-	0/6/26/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	3	2	-	0/6/23/26	0/1/1/1
2	NAG	O	4	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2	-	0/6/26/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	3	2	-	0/6/23/26	0/1/1/1
2	NAG	P	4	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2	-	0/6/26/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	3	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	4	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	2	-	0/6/26/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	3	2	-	0/6/23/26	0/1/1/1
2	NAG	R	4	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2	-	0/6/26/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	3	2	-	0/6/23/26	0/1/1/1
2	NAG	S	4	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2	-	0/6/26/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	3	2	-	0/6/23/26	0/1/1/1
2	NAG	T	4	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	2	-	0/6/26/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	3	2	-	0/6/23/26	0/1/1/1
2	NAG	U	4	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	2	-	2/6/26/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	3	2	-	0/6/23/26	0/1/1/1
2	NAG	V	4	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	2	-	0/6/26/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	3	2	-	0/6/23/26	0/1/1/1
2	NAG	W	4	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	2	-	0/6/26/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	X	3	2	-	0/6/23/26	0/1/1/1
2	NAG	X	4	2	-	0/6/23/26	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	4	NAG	C8-C7	3.03	1.56	1.50
2	N	3	NAG	C8-C7	2.78	1.56	1.50
2	T	2	NAG	O5-C1	-2.65	1.39	1.43
2	Q	1	NAG	C1-C2	2.62	1.56	1.52
2	O	3	NAG	C1-C2	2.60	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	NAG	C1-O5-C5	5.15	119.17	112.19
2	V	3	NAG	C1-O5-C5	4.05	117.68	112.19
2	N	3	NAG	C1-O5-C5	3.95	117.54	112.19
2	Q	1	NAG	O1-C1-C2	3.65	116.80	109.22
2	P	1	NAG	O1-C1-O5	-3.64	99.45	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	1	NAG	O5-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 9 short contacts:

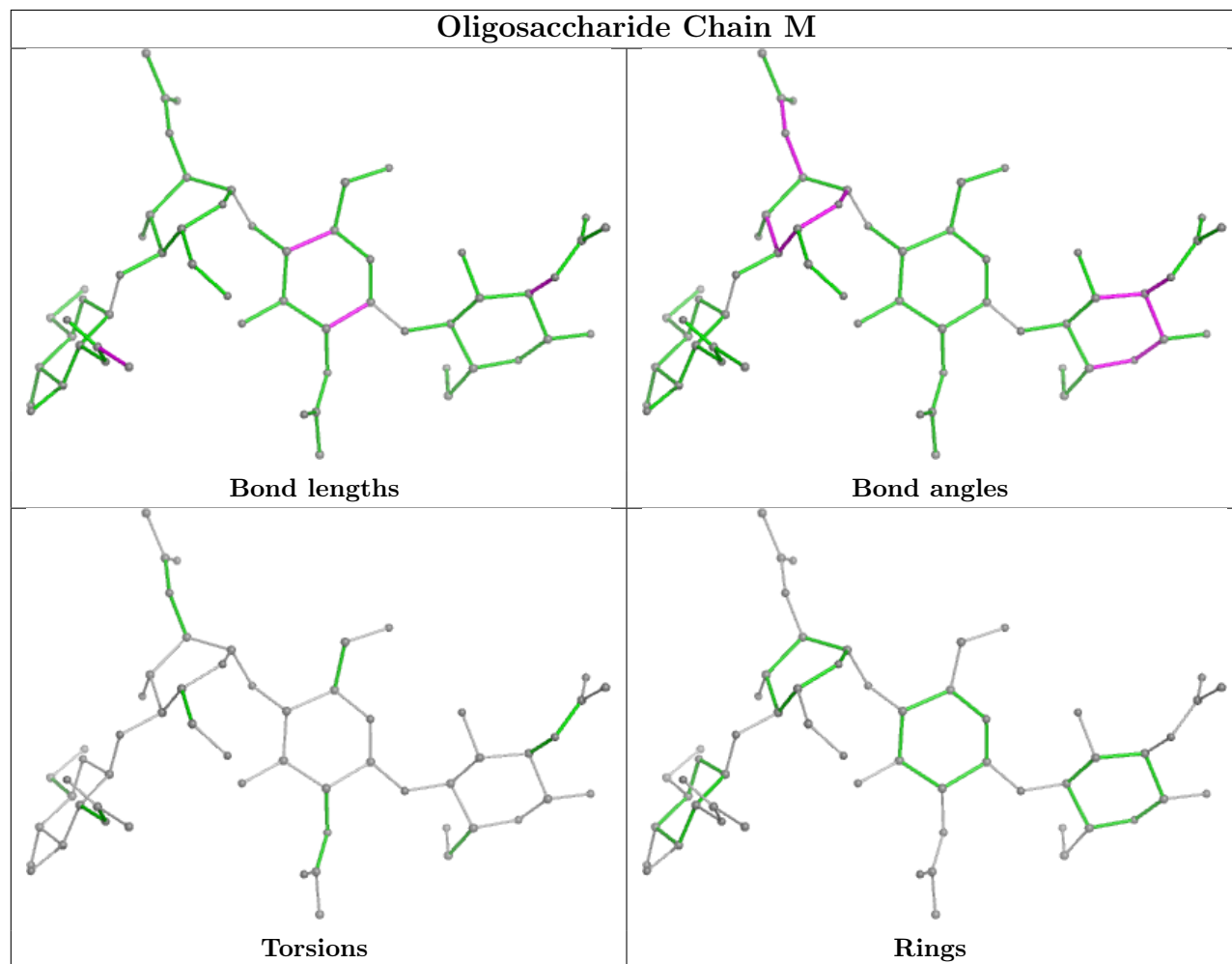
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	2	NAG	1	0
2	U	2	NAG	1	0
2	N	2	NAG	1	0
2	P	2	NAG	1	0
2	T	2	NAG	1	0
2	R	2	NAG	1	0
2	X	2	NAG	1	0
2	W	3	NAG	1	0
2	P	3	NAG	2	0

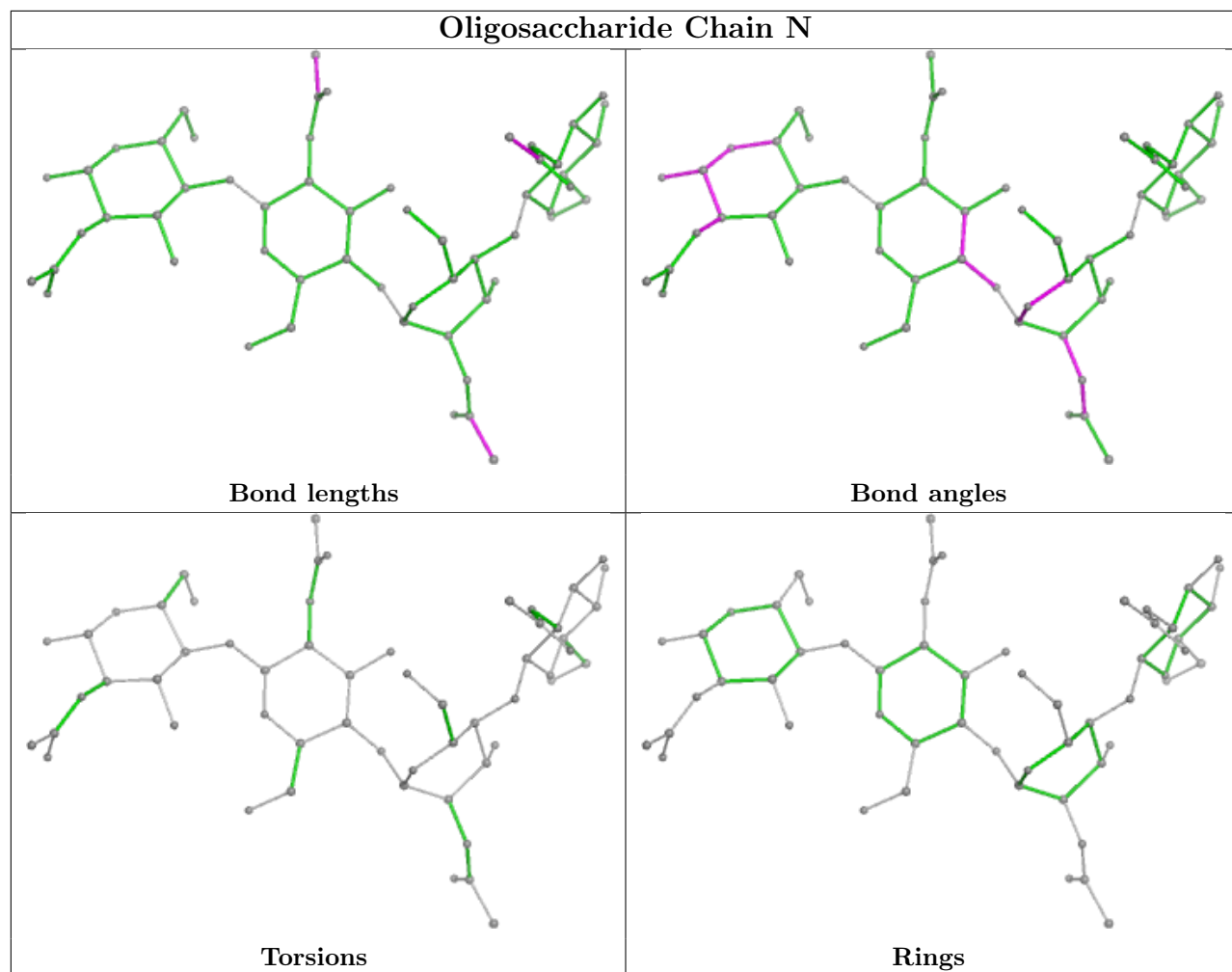
Continued on next page...

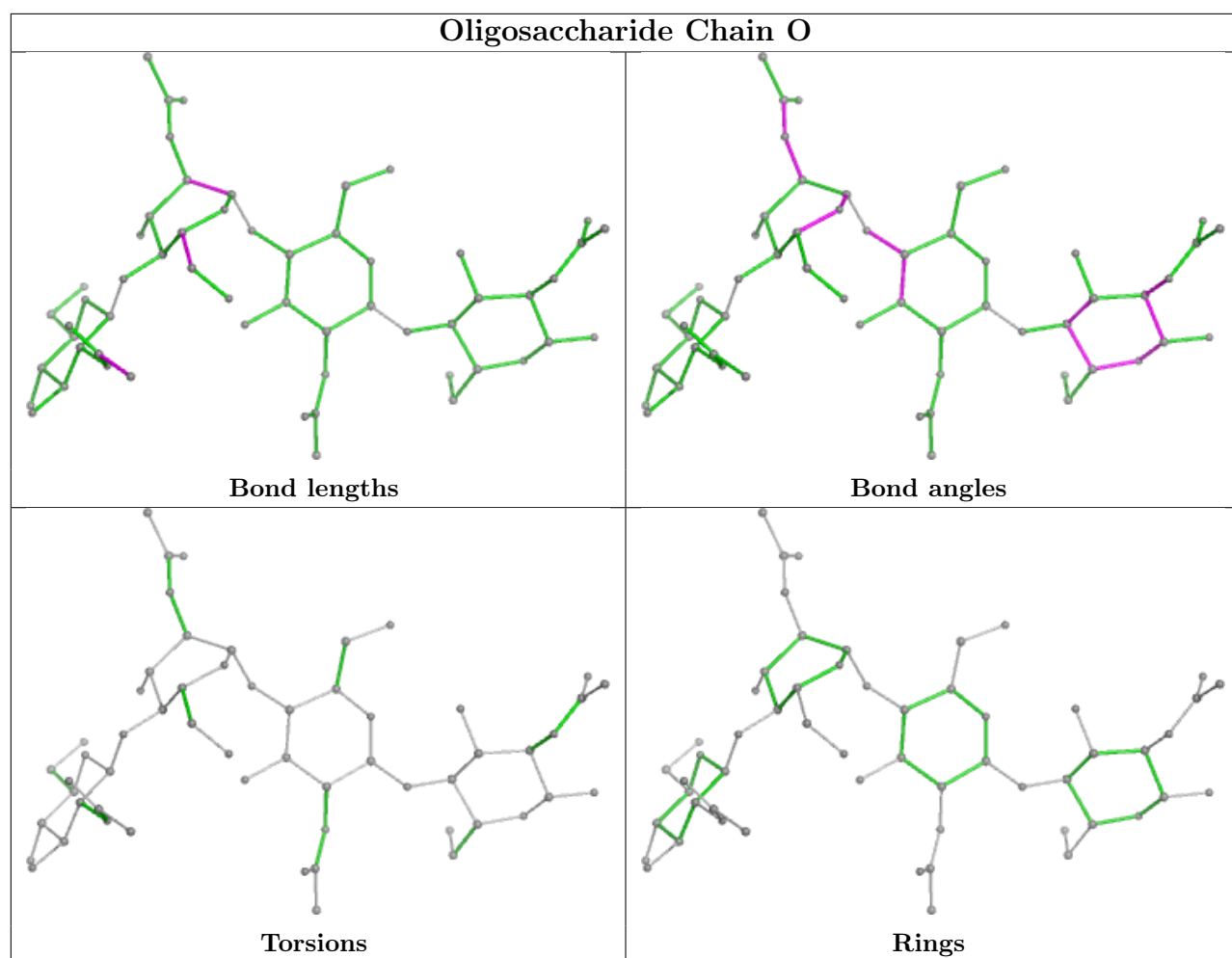
Continued from previous page...

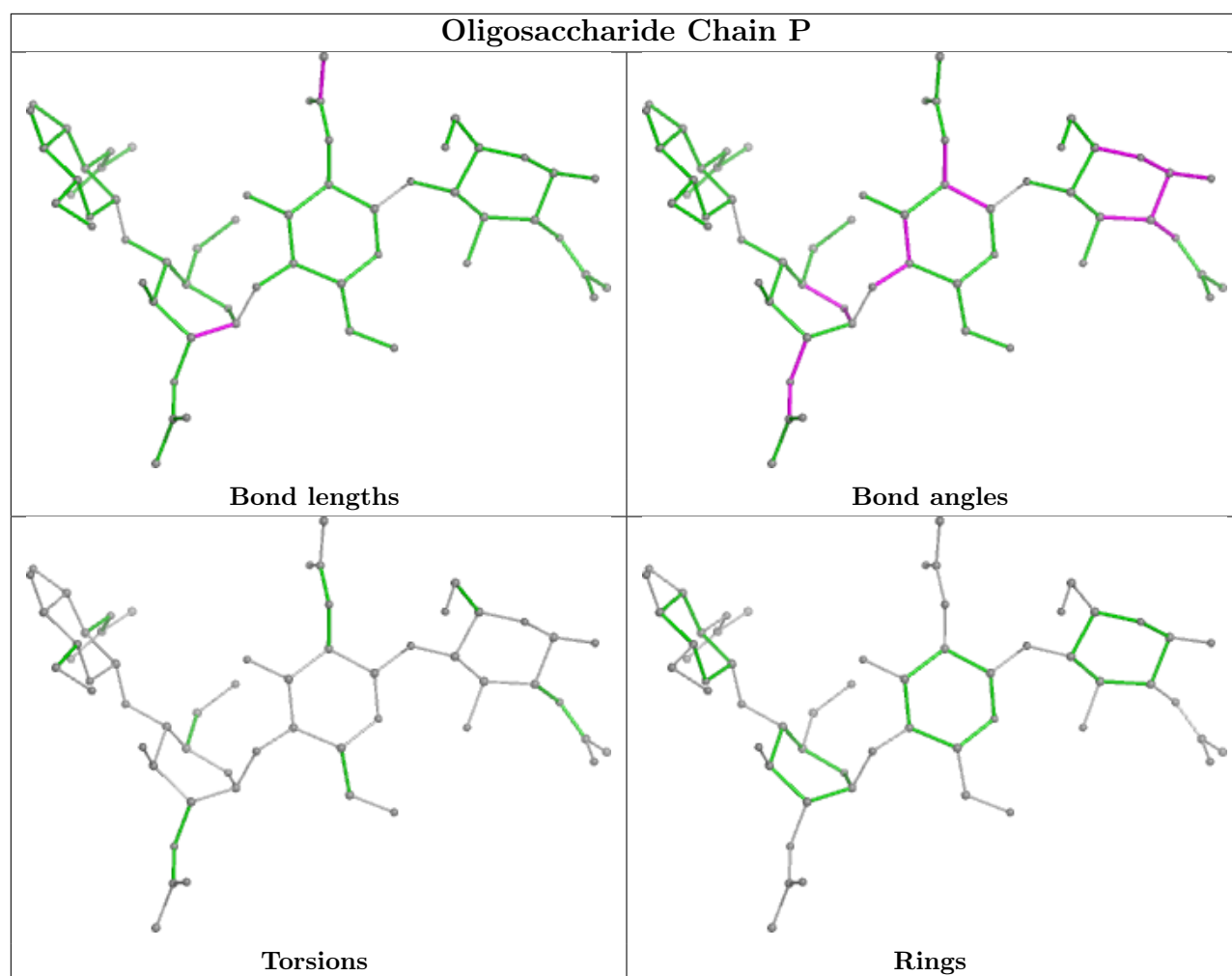
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	2	NAG	1	0

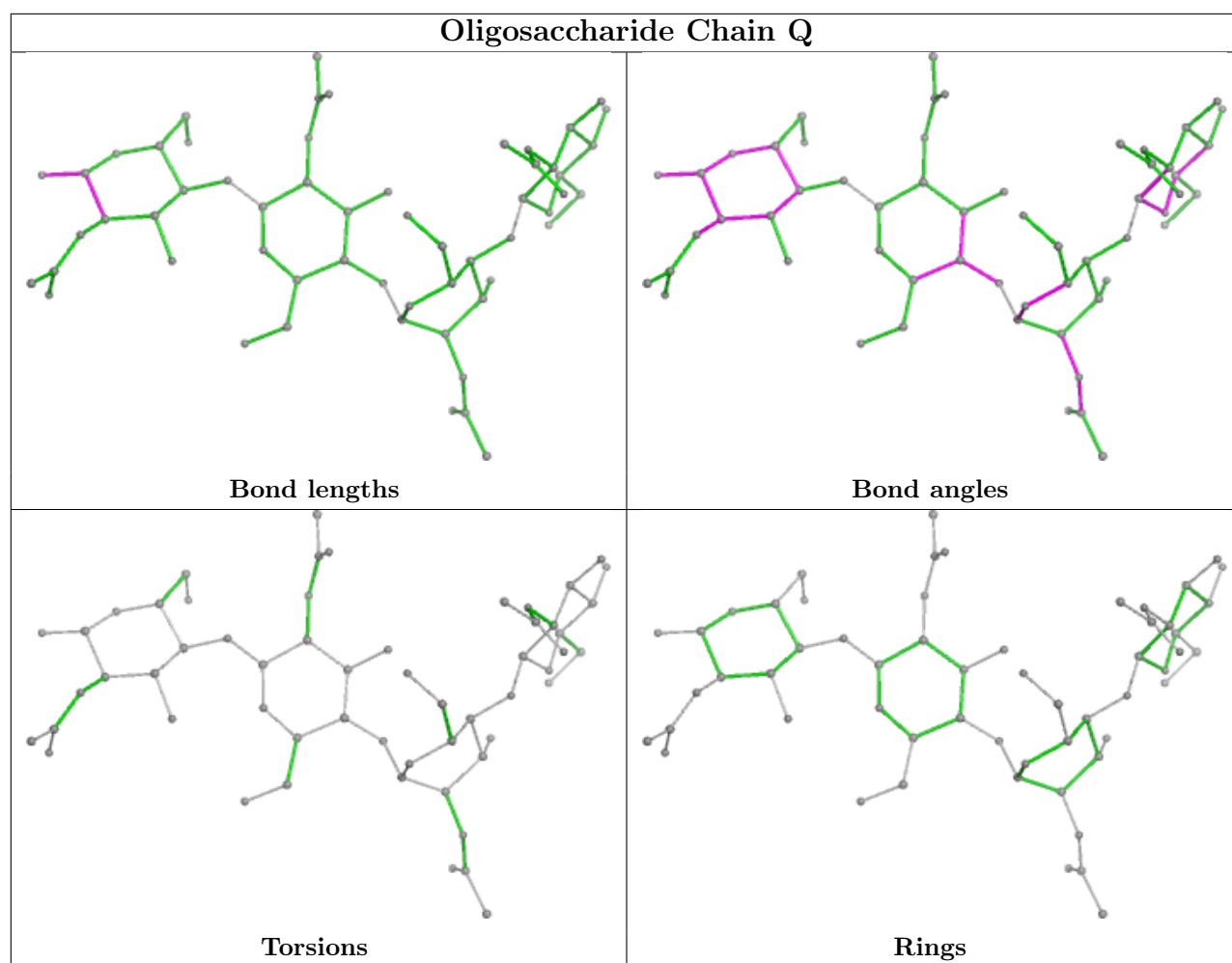
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

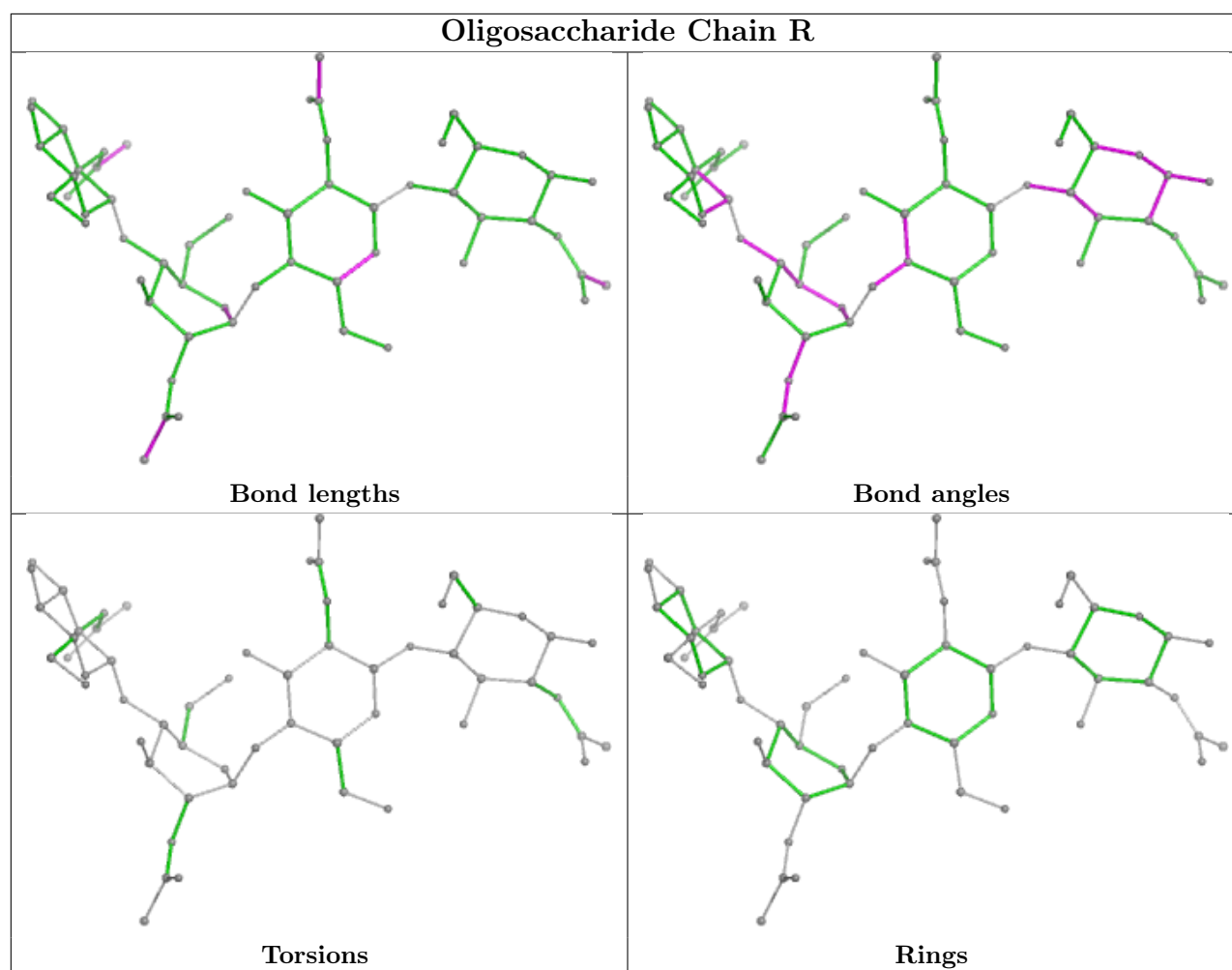


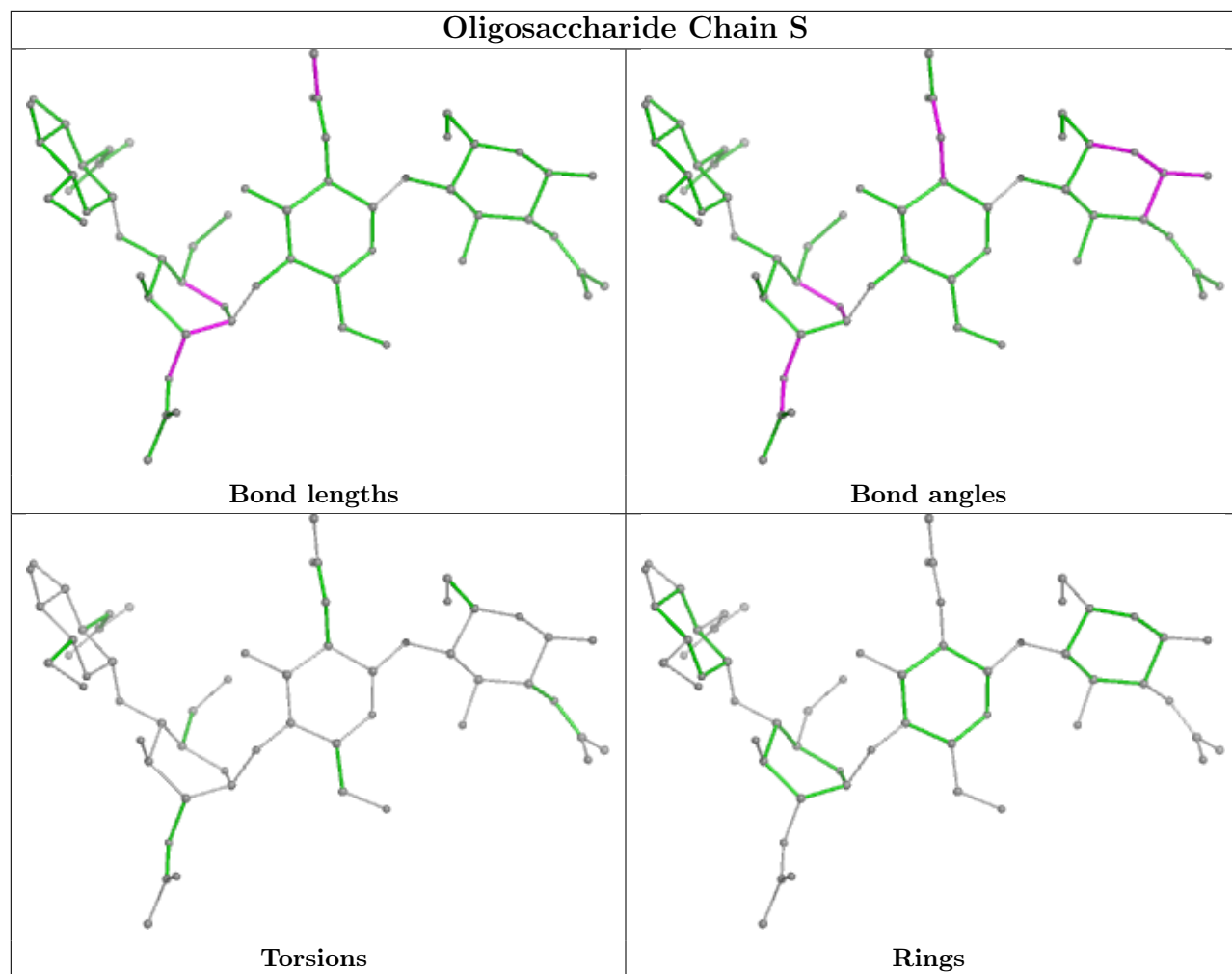


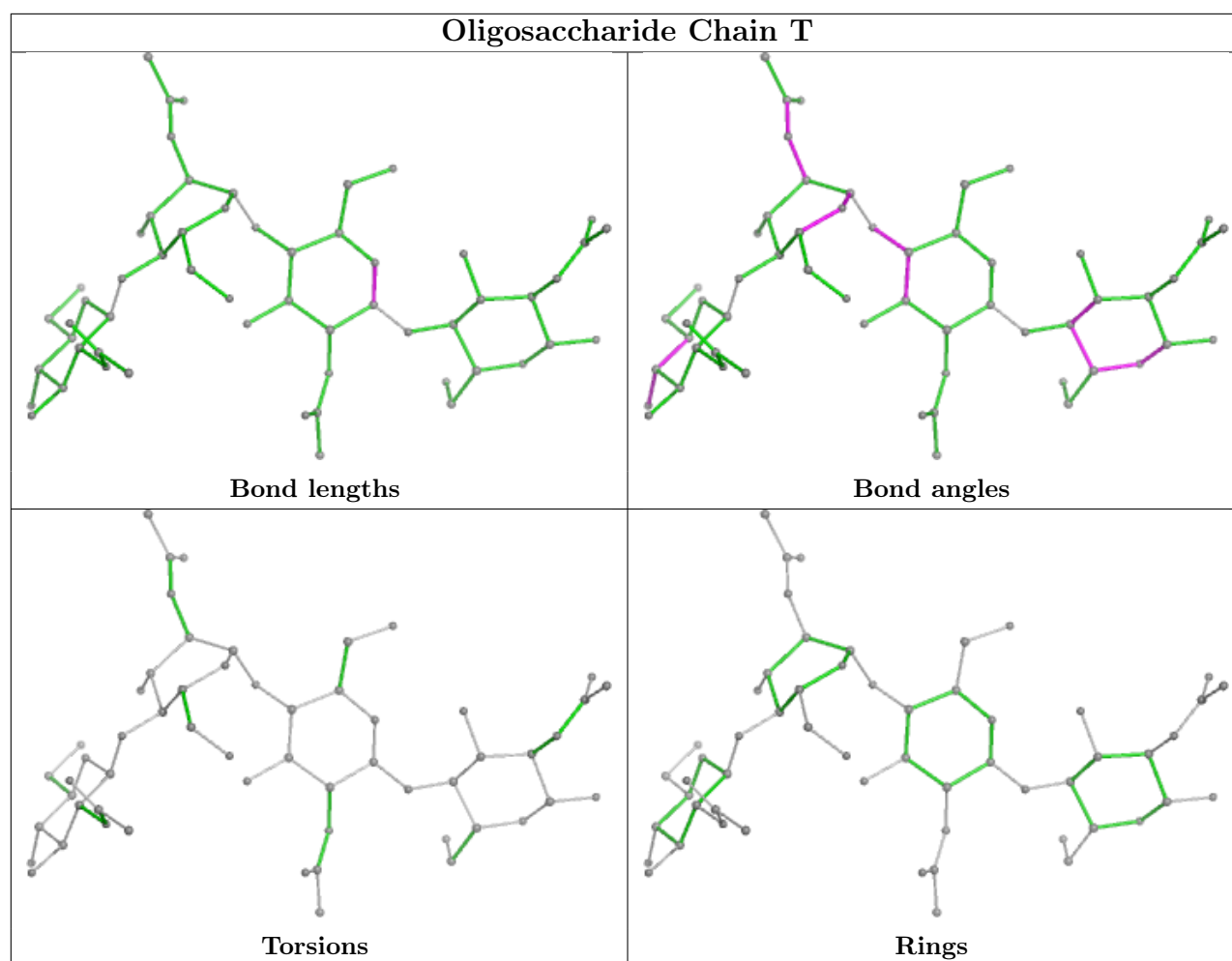


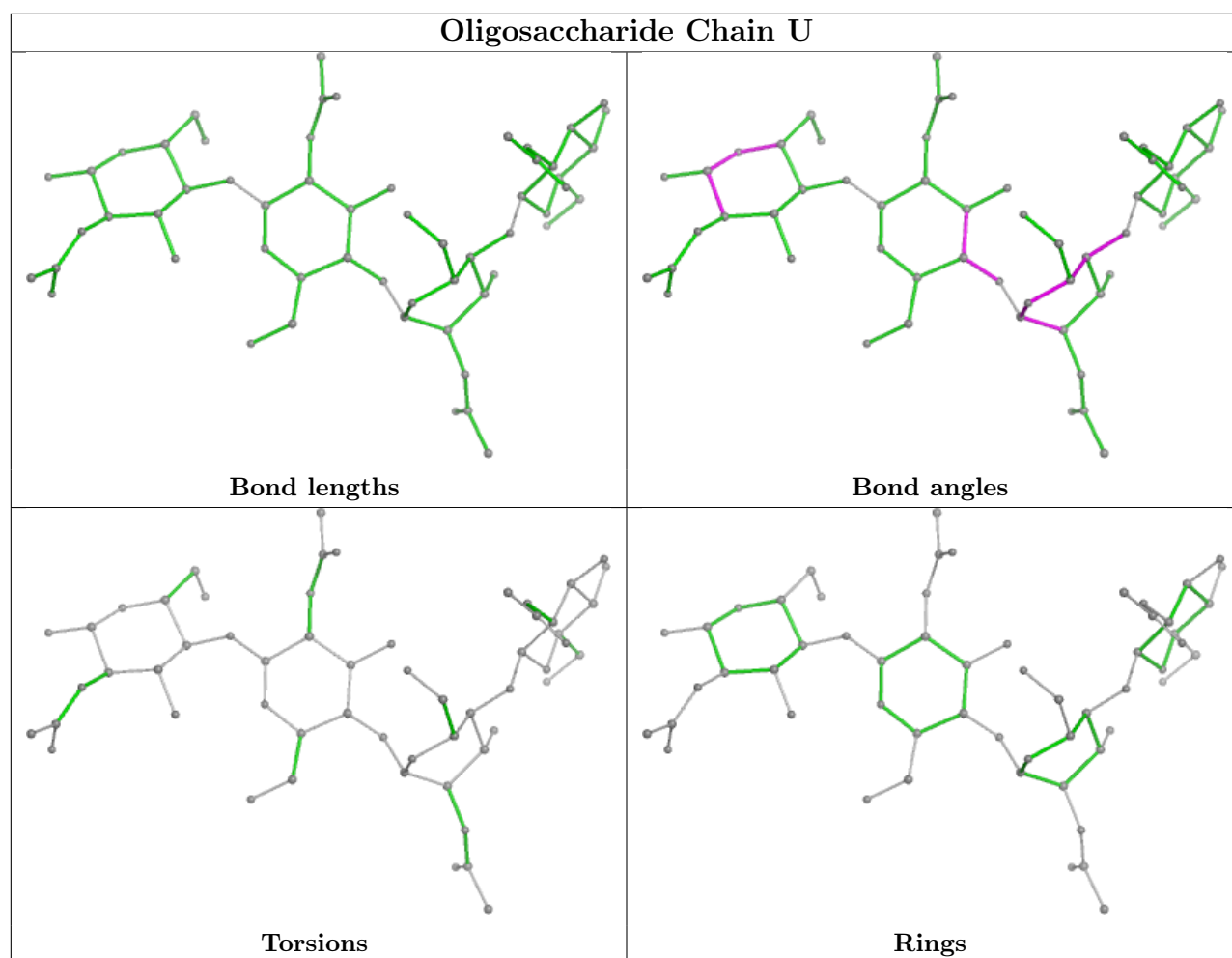


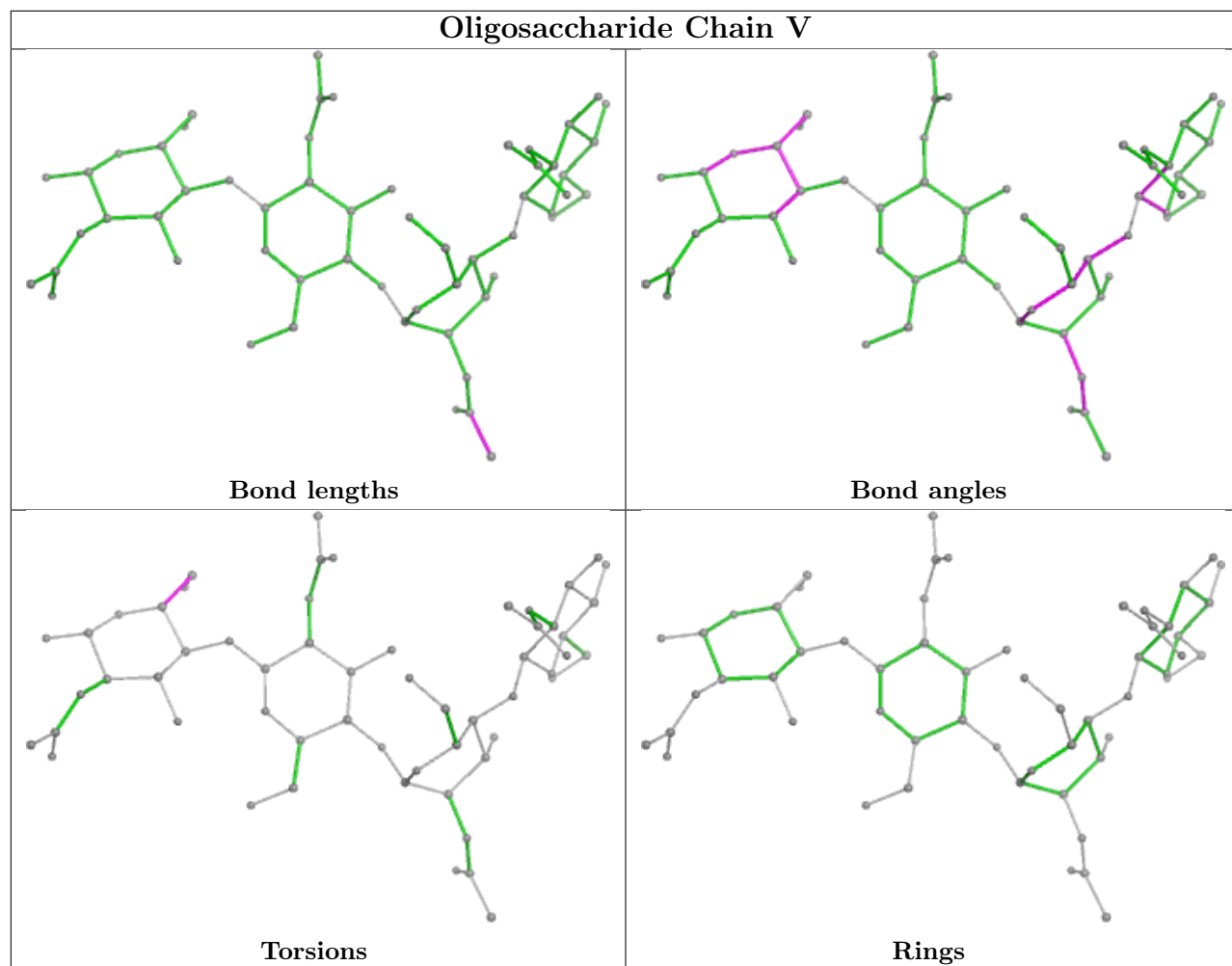




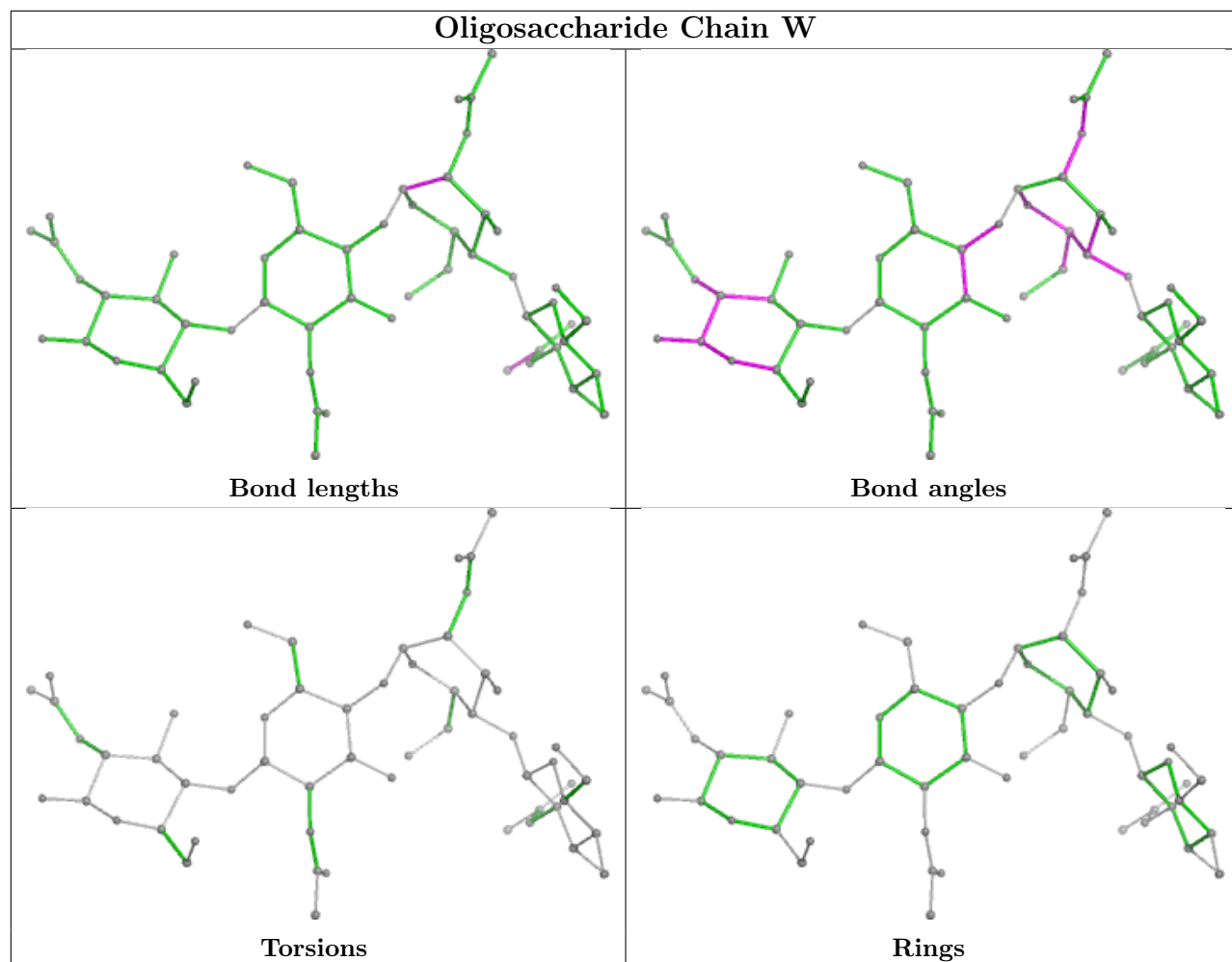


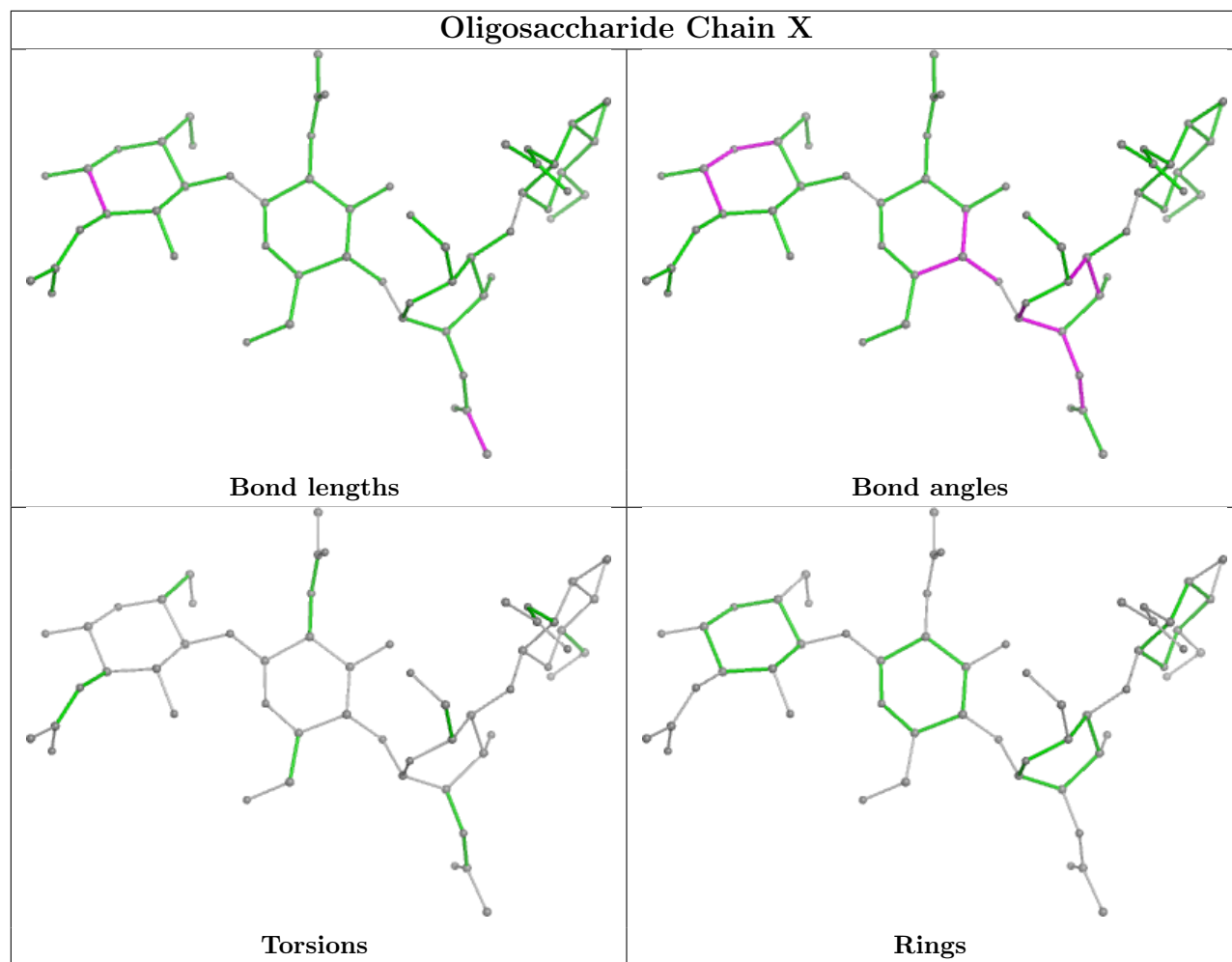






Oligosaccharide Chain W





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/365 (99%)	-0.47	4 (1%) 77 82	12, 22, 33, 50	0
1	B	364/365 (99%)	-0.23	3 (0%) 82 85	17, 27, 43, 57	0
1	C	364/365 (99%)	-0.33	6 (1%) 70 76	15, 24, 38, 57	0
1	D	364/365 (99%)	-0.26	5 (1%) 73 78	14, 25, 42, 59	0
1	E	364/365 (99%)	-0.42	3 (0%) 82 85	13, 23, 36, 50	0
1	F	364/365 (99%)	-0.39	3 (0%) 82 85	14, 23, 38, 52	0
1	G	364/365 (99%)	-0.36	2 (0%) 87 89	15, 24, 37, 53	0
1	H	364/365 (99%)	-0.32	8 (2%) 62 68	15, 24, 37, 51	0
1	I	364/365 (99%)	-0.08	8 (2%) 62 68	17, 30, 48, 58	0
1	J	364/365 (99%)	-0.22	6 (1%) 70 76	16, 27, 40, 50	0
1	K	364/365 (99%)	0.18	17 (4%) 37 44	21, 33, 56, 65	0
1	L	364/365 (99%)	-0.12	7 (1%) 66 72	15, 29, 45, 57	0
All	All	4368/4380 (99%)	-0.25	72 (1%) 70 76	12, 26, 43, 65	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	388	GLY	6.5
1	D	174	THR	5.8
1	I	171	THR	4.8
1	D	388	GLY	4.8
1	I	172	LYS	4.6

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

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

6.3 Carbohydrates

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

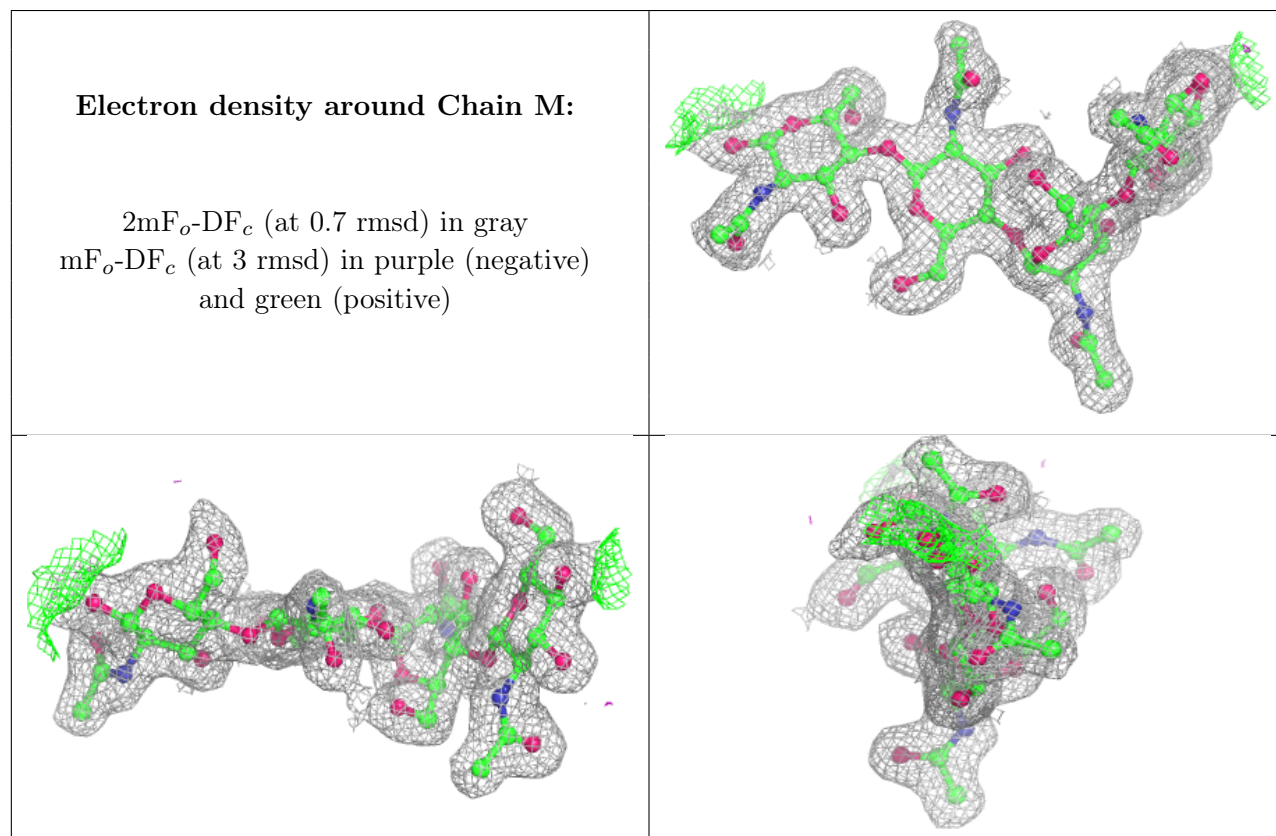
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	W	1	15/15	0.93	0.07	20,23,30,33	0
2	NAG	X	1	15/15	0.94	0.07	21,24,29,33	0
2	NAG	P	1	15/15	0.95	0.06	17,22,26,29	0
2	NAG	S	1	15/15	0.95	0.06	15,18,23,23	0
2	NAG	U	1	15/15	0.95	0.06	24,26,35,39	0
2	NAG	U	4	14/15	0.95	0.06	25,30,33,35	0
2	NAG	N	1	15/15	0.95	0.07	20,23,28,30	0
2	NAG	W	4	14/15	0.95	0.07	27,31,34,35	0
2	NAG	O	1	15/15	0.95	0.06	16,21,28,29	0
2	NAG	R	1	15/15	0.96	0.05	13,17,23,24	0
2	NAG	N	4	14/15	0.96	0.06	21,23,26,27	0
2	NAG	T	1	15/15	0.96	0.06	18,21,28,28	0
2	NAG	M	1	15/15	0.96	0.06	12,19,23,26	0
2	NAG	U	3	14/15	0.96	0.06	23,24,26,26	0
2	NAG	N	2	14/15	0.96	0.06	19,20,23,24	0
2	NAG	V	1	15/15	0.96	0.05	19,22,29,31	0
2	NAG	V	2	14/15	0.96	0.06	19,21,23,23	0
2	NAG	V	4	14/15	0.96	0.05	19,22,25,25	0
2	NAG	P	4	14/15	0.96	0.06	18,19,21,22	0
2	NAG	Q	1	15/15	0.96	0.05	17,22,28,30	0
2	NAG	Q	2	14/15	0.96	0.06	15,17,21,21	0
2	NAG	X	4	14/15	0.96	0.06	20,22,24,25	0
2	NAG	U	2	14/15	0.97	0.05	22,24,32,33	0
2	NAG	Q	3	14/15	0.97	0.04	13,15,17,18	0
2	NAG	P	3	14/15	0.97	0.05	16,17,19,21	0
2	NAG	R	3	14/15	0.97	0.05	13,16,18,19	0
2	NAG	O	4	14/15	0.97	0.05	14,17,19,20	0
2	NAG	V	3	14/15	0.97	0.05	18,20,21,21	0
2	NAG	S	2	14/15	0.97	0.06	15,17,19,20	0
2	NAG	S	3	14/15	0.97	0.05	13,15,18,21	0
2	NAG	W	2	14/15	0.97	0.05	21,22,27,28	0
2	NAG	W	3	14/15	0.97	0.05	22,24,26,27	0
2	NAG	O	3	14/15	0.97	0.05	13,15,17,19	0
2	NAG	T	4	14/15	0.97	0.04	15,17,18,18	0
2	NAG	X	2	14/15	0.97	0.05	19,20,24,28	0
2	NAG	P	2	14/15	0.97	0.05	17,18,21,23	0
2	NAG	S	4	14/15	0.98	0.03	15,17,18,18	0

Continued on next page...

Continued from previous page...

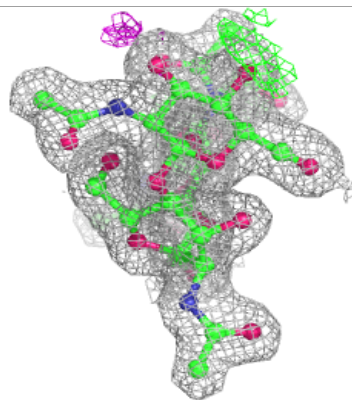
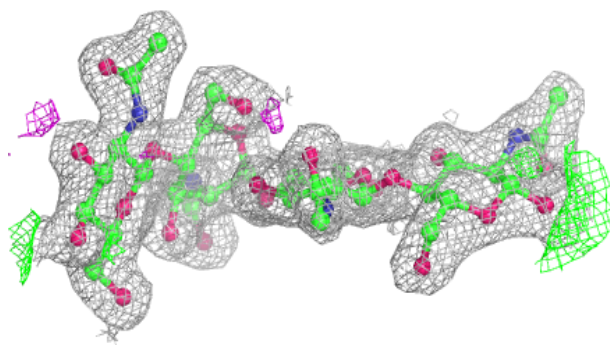
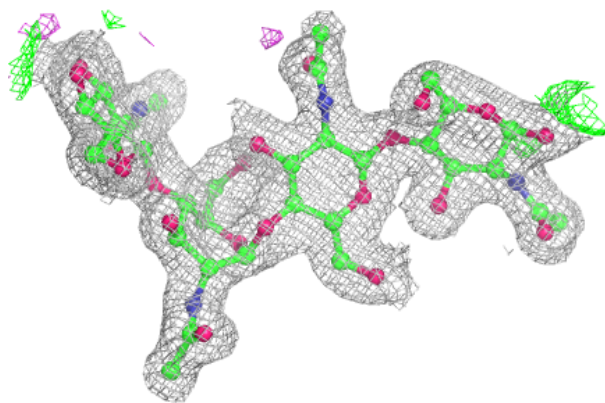
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	O	2	14/15	0.98	0.04	15,17,21,24	0
2	NAG	T	2	14/15	0.98	0.04	14,16,20,21	0
2	NAG	T	3	14/15	0.98	0.04	13,15,17,17	0
2	NAG	R	2	14/15	0.98	0.04	13,15,19,21	0
2	NAG	M	3	14/15	0.98	0.05	11,13,15,18	0
2	NAG	R	4	14/15	0.98	0.04	15,17,18,20	0
2	NAG	N	3	14/15	0.98	0.04	16,19,21,21	0
2	NAG	M	4	14/15	0.98	0.04	14,16,19,19	0
2	NAG	X	3	14/15	0.98	0.04	18,19,22,23	0
2	NAG	M	2	14/15	0.98	0.04	12,15,20,23	0
2	NAG	Q	4	14/15	0.99	0.04	14,17,22,22	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.

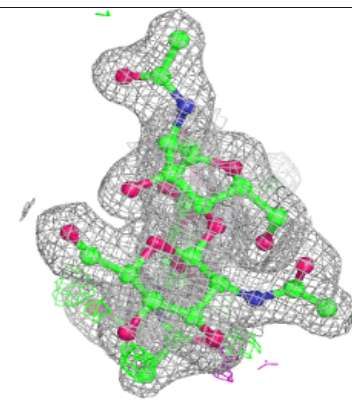
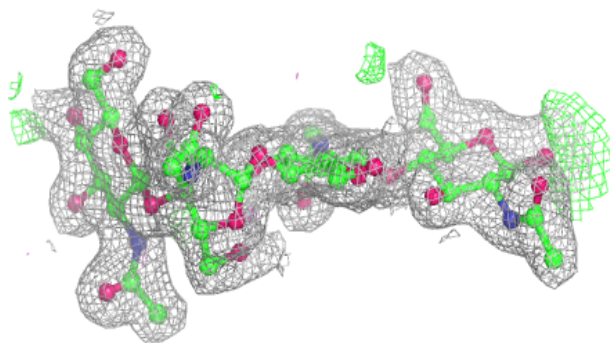
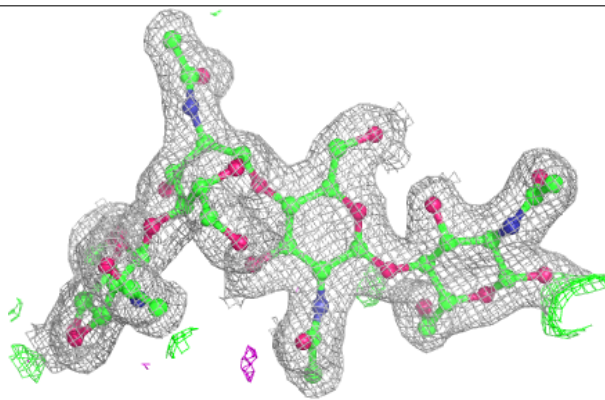


Electron density around Chain N:

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

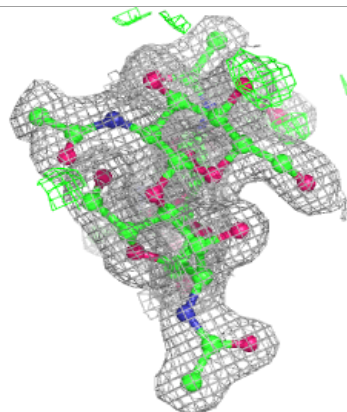
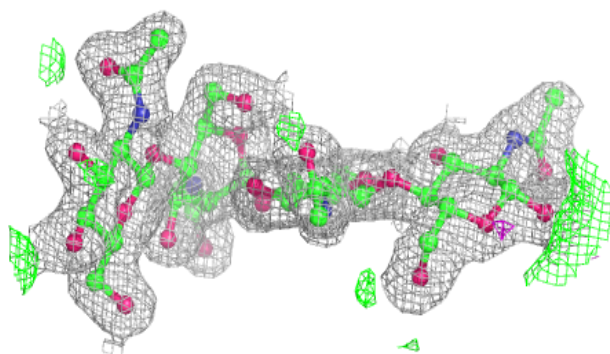
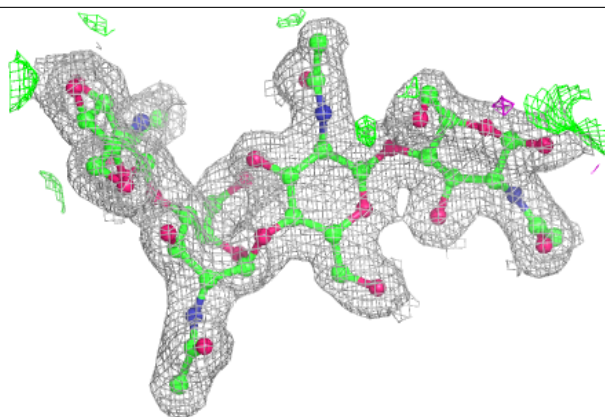
**Electron density around Chain O:**

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

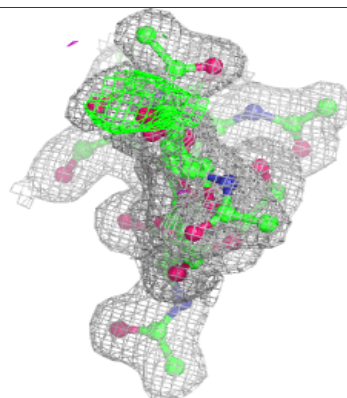
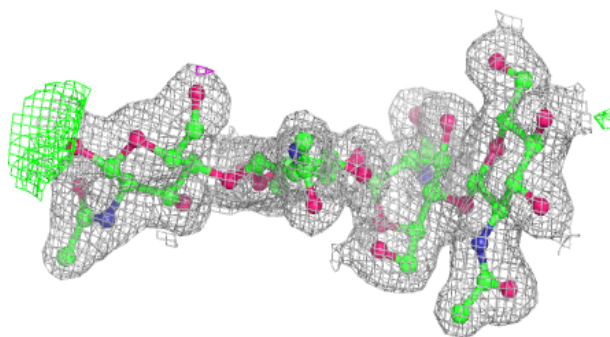
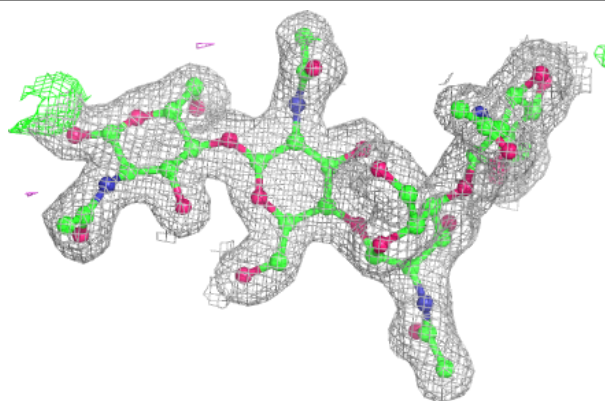


Electron density around Chain P:

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

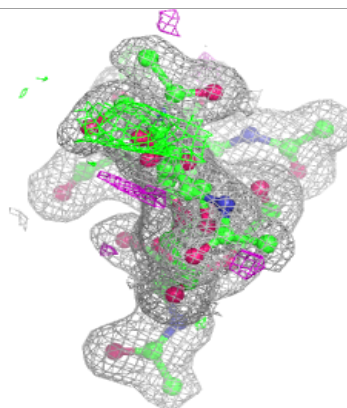
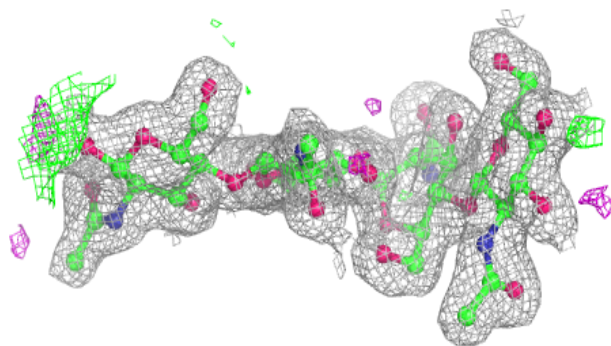
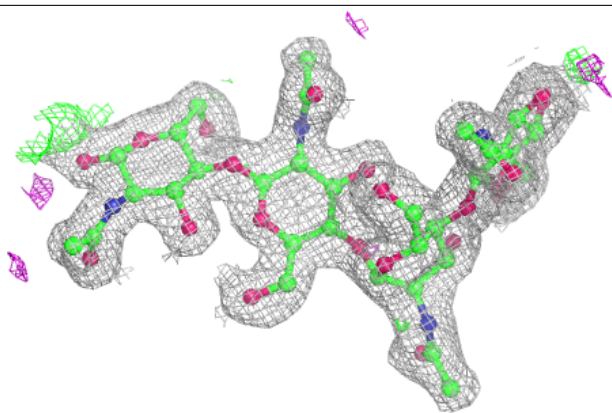
**Electron density around Chain Q:**

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

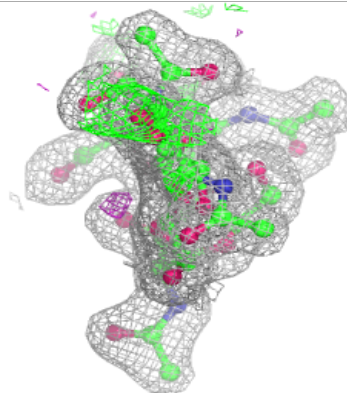
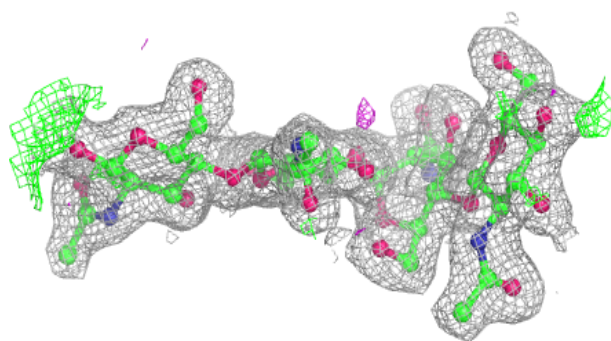
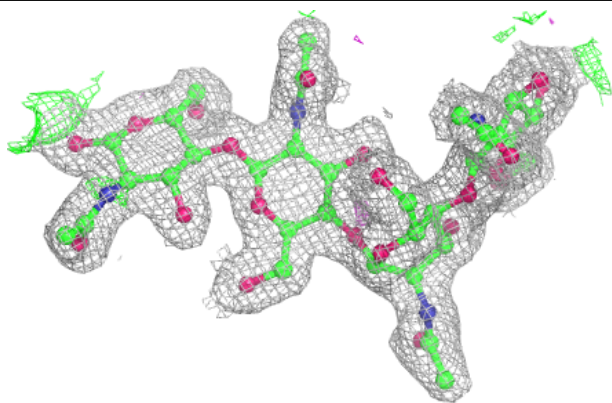


Electron density around Chain R:

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

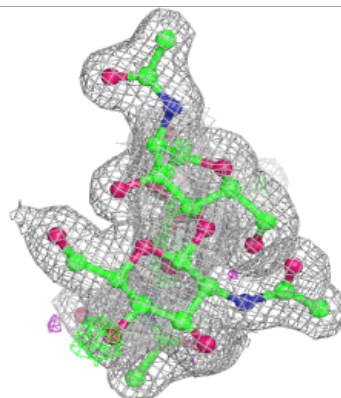
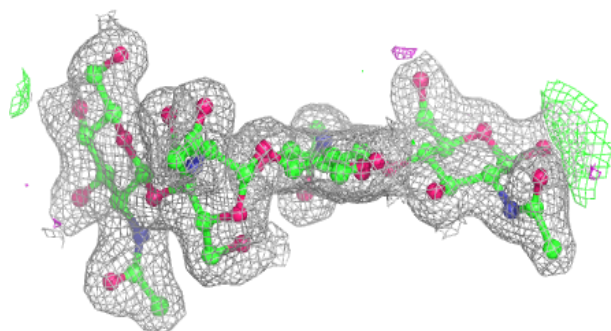
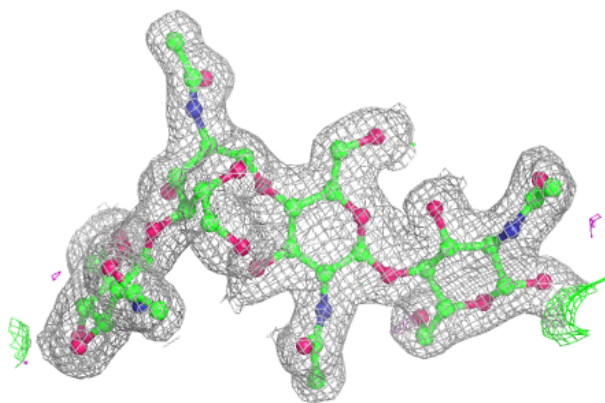
**Electron density around Chain S:**

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

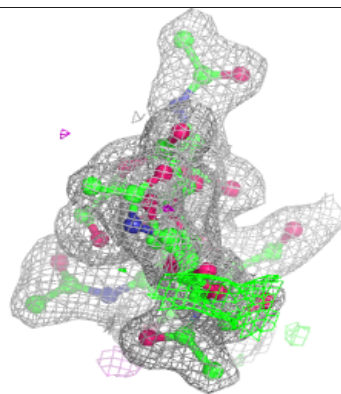
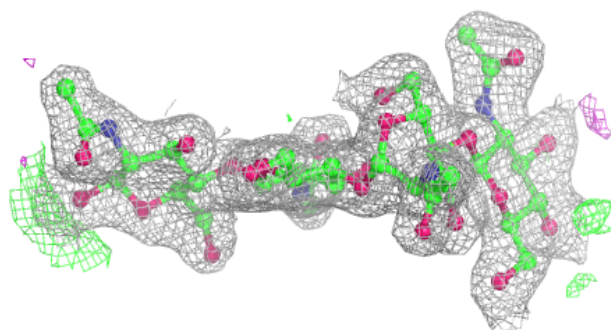
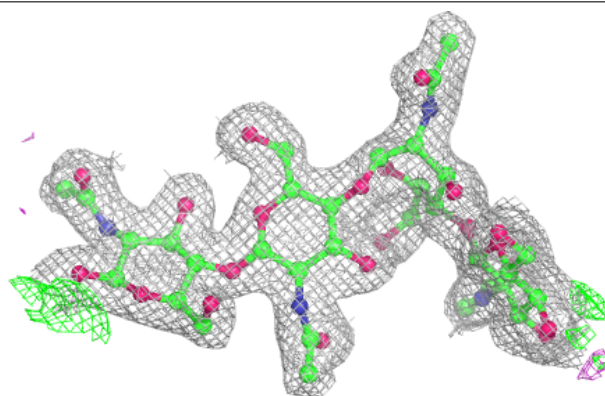


Electron density around Chain T:

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

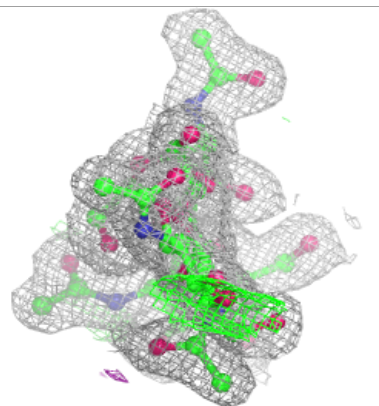
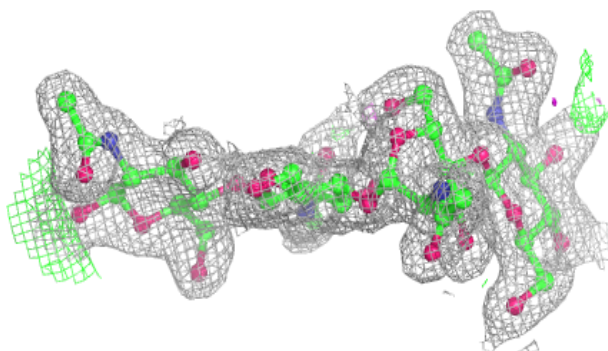
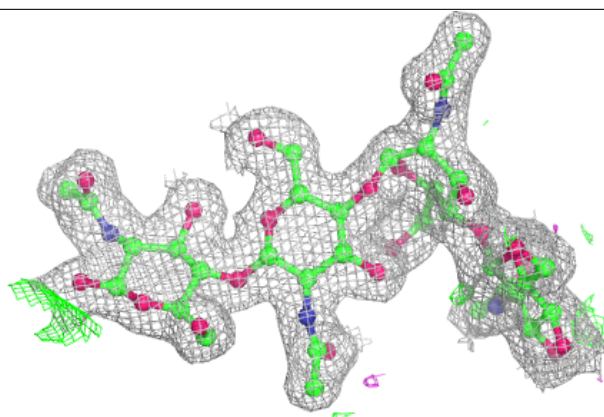
**Electron density around Chain U:**

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

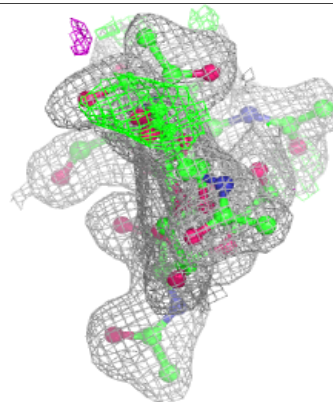
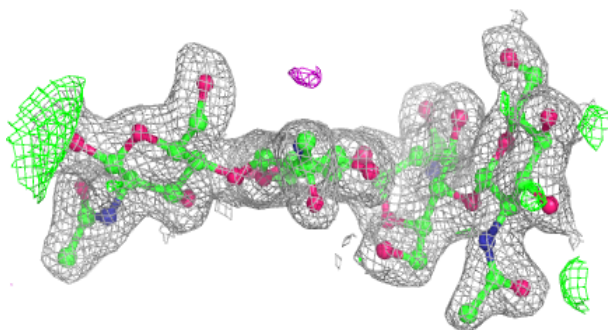
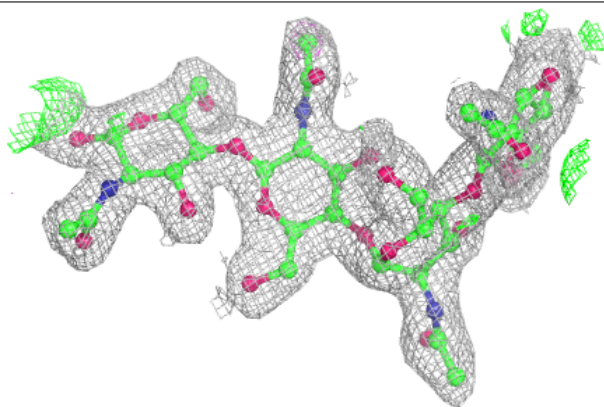


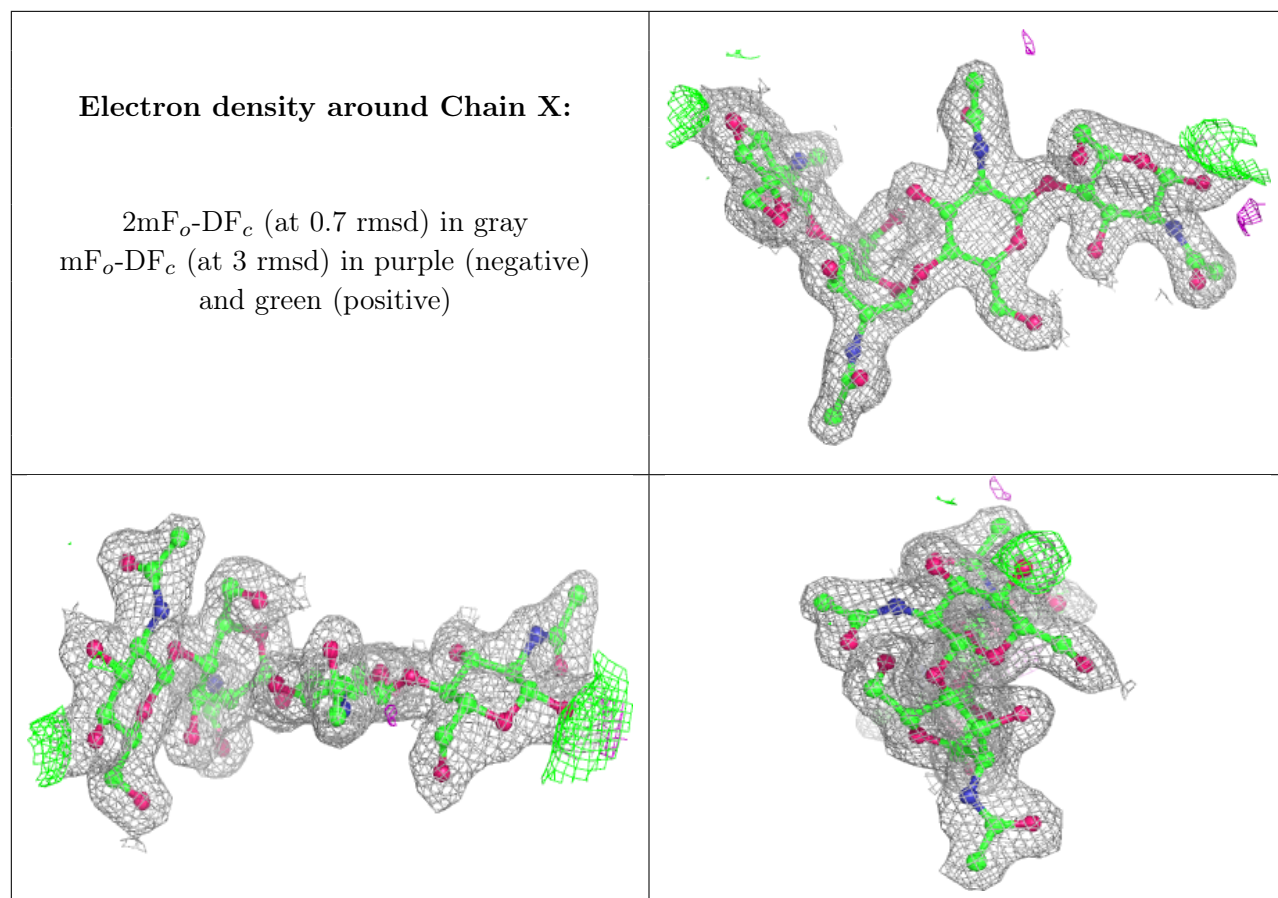
Electron density around Chain V:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.