



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:41 PM UTC

PDB ID : 2XQR / pdb_00002xqr
Title : Crystal structure of plant cell wall invertase in complex with a specific protein inhibitor
Authors : Hothorn, M.; Van den Ende, W.; Lammens, W.; Rybin, V.; Scheffzek, K.
Deposited on : 2010-09-07
Resolution : 2.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

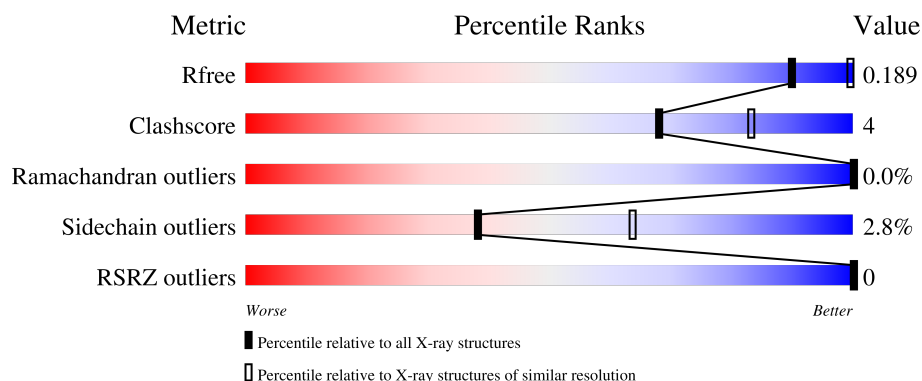
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



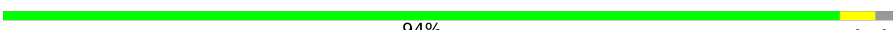
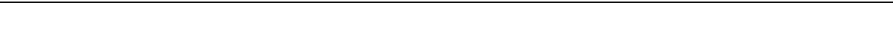
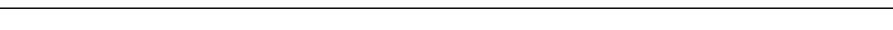
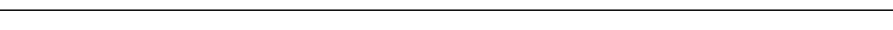
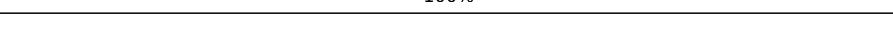
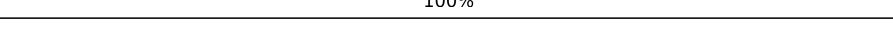
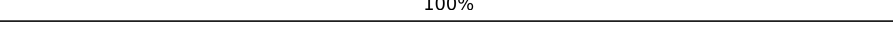
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	537	
1	C	537	
1	E	537	
1	G	537	
1	I	537	

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Mol	Chain	Length	Quality of chain
1	K	537	 88% 12%
2	B	149	 85% 13% .
2	D	149	 94% . .
2	F	149	 87% 11% . .
2	H	149	 92% 6% .
2	J	149	 90% 8% .
2	L	149	 92% 6% .
3	M	6	 33% 50% 17%
3	O	6	 17% 67% 17%
3	Q	6	 17% 33% 50%
3	S	6	 33% 67%
3	U	6	 83% 17%
3	W	6	 33% 67%
4	N	2	 100%
4	P	2	 50% 50%
4	R	2	 100%
4	T	2	 100%
4	V	2	 50% 50%
4	X	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	1	X	-	-	-
3	NAG	M	2	X	-	-	-
3	NAG	O	1	X	-	-	-
3	NAG	O	2	X	-	-	-
3	NAG	Q	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	Q	2	X	-	-	-
3	NAG	S	1	X	-	-	-
3	NAG	S	2	X	-	-	-
3	NAG	U	1	X	-	-	-
3	NAG	U	2	X	-	-	-
3	NAG	W	1	X	-	-	-
3	NAG	W	2	X	-	-	-
4	NAG	N	1	X	-	-	-
4	NAG	P	1	X	-	-	-
4	NAG	R	1	X	-	-	-
4	NAG	T	1	X	-	-	-
4	NAG	V	1	X	-	-	-
4	NAG	X	1	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 34132 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 BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	C	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	E	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	G	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	I	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	K	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			

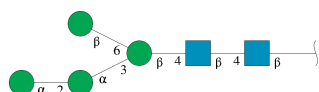
- Molecule 2 is a protein called INVERTASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	D	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	F	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	H	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	J	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	L	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O49908
D	-1	GLY	-	expression tag	UNP O49908
F	-1	GLY	-	expression tag	UNP O49908
H	-1	GLY	-	expression tag	UNP O49908
J	-1	GLY	-	expression tag	UNP O49908
L	-1	GLY	-	expression tag	UNP O49908

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]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
3	M	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	O	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	S	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	U	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



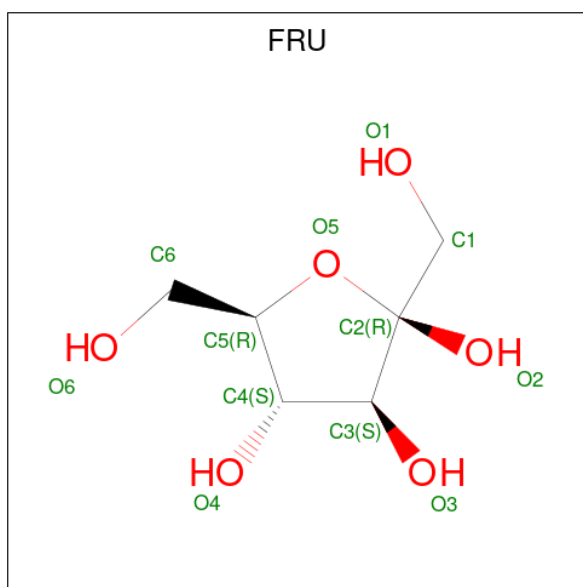
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

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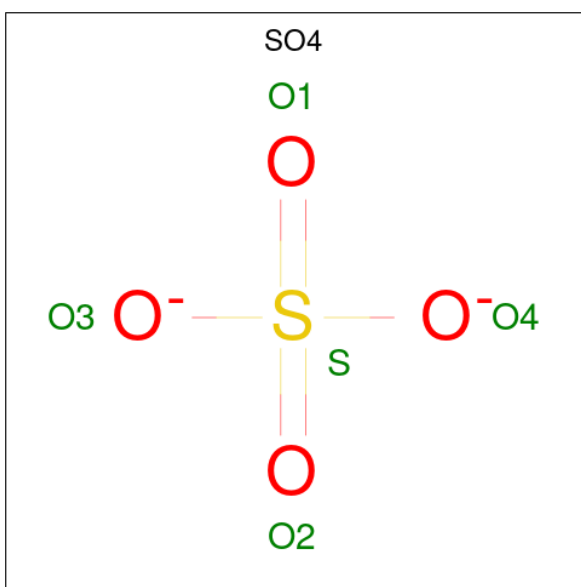
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is beta-D-fructofuranose (CCD ID: FRU) (formula: $C_6H_{12}O_6$).



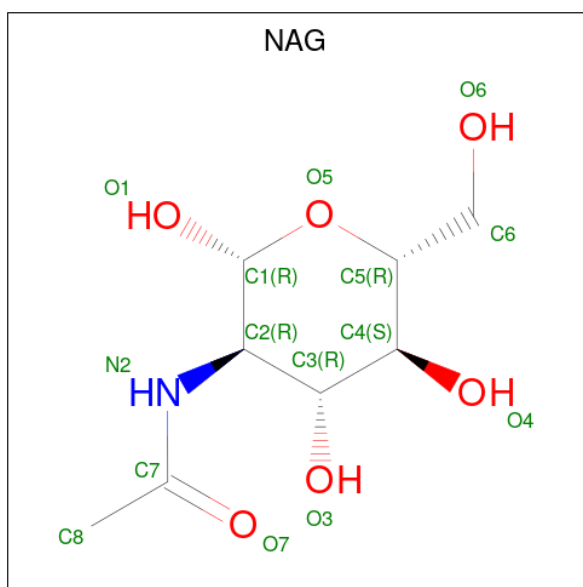
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		
5	G	1	Total	C	O	0	0
			12	6	6		
5	I	1	Total	C	O	0	0
			12	6	6		
5	K	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



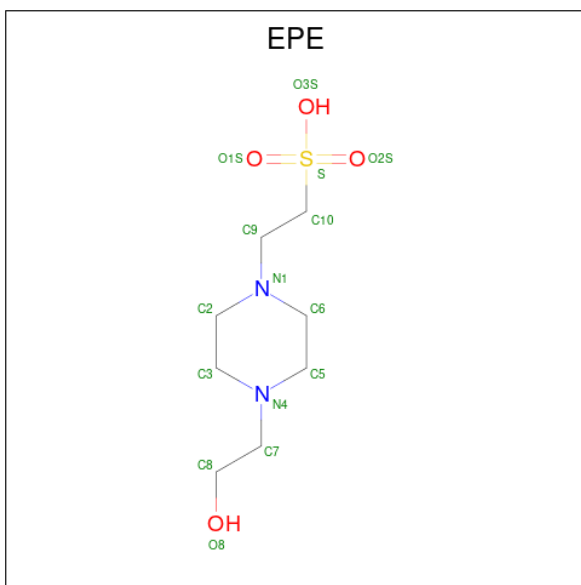
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	121	Total	O	0	0
			121	121		
9	B	27	Total	O	0	0
			27	27		
9	C	117	Total	O	0	0
			117	117		
9	D	26	Total	O	0	0
			26	26		
9	E	109	Total	O	0	0
			109	109		
9	F	17	Total	O	0	0
			17	17		

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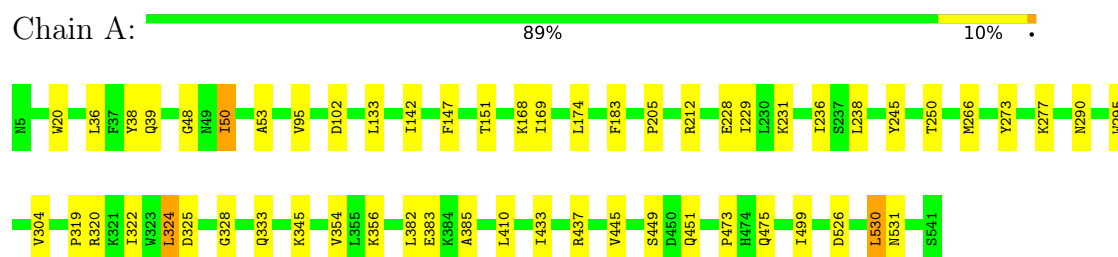
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	99	Total 99	O 99	0	0
9	H	20	Total 20	O 20	0	0
9	I	106	Total 106	O 106	0	0
9	J	29	Total 29	O 29	0	0
9	K	98	Total 98	O 98	0	0
9	L	22	Total 22	O 22	0	0

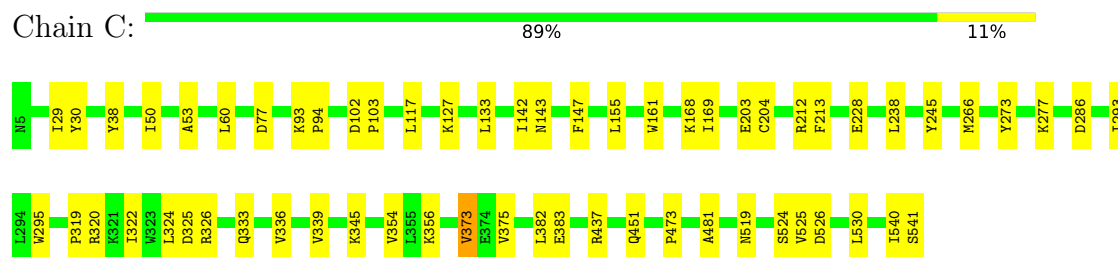
3 Residue-property plots

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.

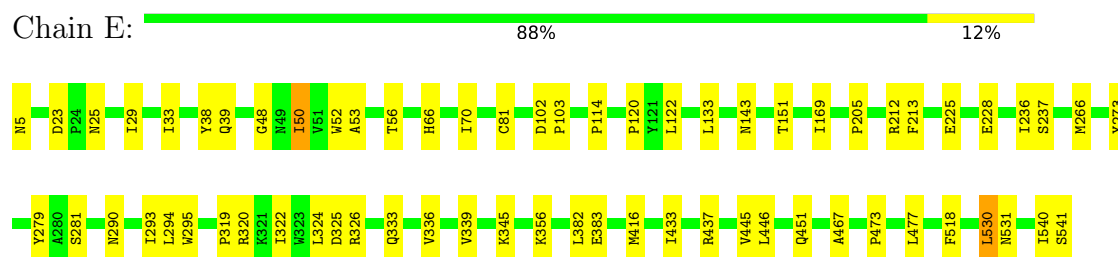
• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1



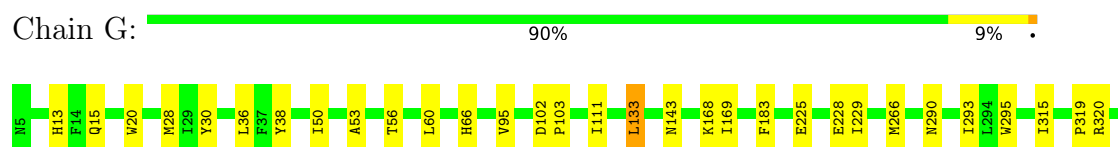
• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

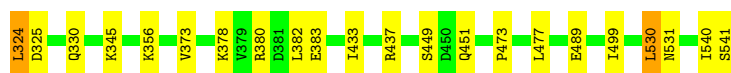


• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1



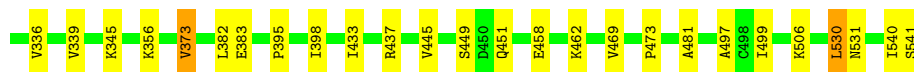
• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1





- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

Chain I: 89% 11%



- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

Chain K: 88% 12%



- Molecule 2: INVERTASE INHIBITOR

Chain B: 85% 13%



- Molecule 2: INVERTASE INHIBITOR

Chain D: 94%



- Molecule 2: INVERTASE INHIBITOR

Chain F: 87% 11%



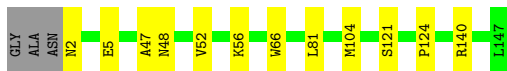
- Molecule 2: INVERTASE INHIBITOR

Chain H: 92% 6%



- Molecule 2: INVERTASE INHIBITOR

Chain J:  90% 8%

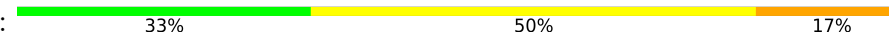


- Molecule 2: INVERTASE INHIBITOR

Chain L:  92% 6%

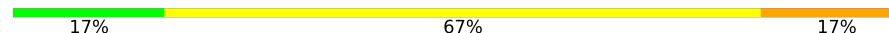


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 50% 17%



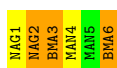
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  17% 67% 17%



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  17% 33% 50%

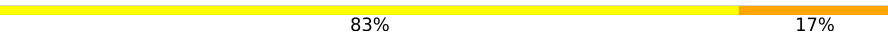


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67%

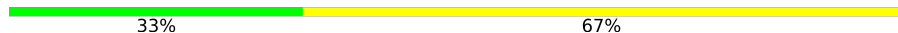


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  83% 17%

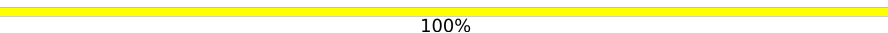
 NAG1
NAG2
BMA3
MAN4
MAN5
BMA6

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  33% 67%

 NAG1
NAG2
BMA3
MAN4
MAN5
BMA6

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

Chain N:  100%

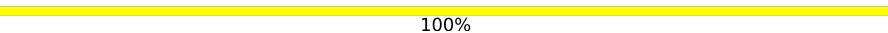
 NAG1
NAG2

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

Chain P:  50% 50%

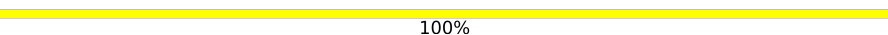
 NAG1
NAG2

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

Chain R:  100%

 NAG1
NAG2

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

Chain T:  100%

 NAG1
NAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain X:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	199.98Å 199.98Å 111.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.57 – 2.58 48.57 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.57-2.58) 99.4 (48.57-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0043	Depositor
R, R_{free}	0.183 , 0.210 0.188 , 0.189	Depositor DCC
R_{free} test set	7782 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 5.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l 0.058 for h,-h-k,-l 0.145 for -k,-h,-l	Xtriage
Reported twinning fraction	0.818 for H, K, L 0.182 for -H, H+K, -L	Depositor
Outliers	0 of 155624 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34132	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NAG, MAN, FRU, SO4, BMA

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	0.42	0/4442	0.65	0/6034
1	C	0.42	0/4442	0.64	0/6034
1	E	0.42	0/4442	0.64	1/6034 (0.0%)
1	G	0.42	0/4442	0.63	0/6034
1	I	0.42	0/4442	0.65	0/6034
1	K	0.42	0/4442	0.64	0/6034
2	B	0.46	0/1112	0.82	1/1506 (0.1%)
2	D	0.44	0/1112	0.80	0/1506
2	F	0.45	0/1112	0.80	2/1506 (0.1%)
2	H	0.46	0/1112	0.84	0/1506
2	J	0.48	0/1112	0.79	0/1506
2	L	0.45	0/1112	0.77	0/1506
All	All	0.43	0/33324	0.68	4/45240 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	GLY	N-CA-C	-6.26	105.85	114.67
1	E	23	ASP	N-CA-C	5.08	115.44	109.60
2	F	96	ASP	CA-C-N	5.07	125.35	119.47
2	F	96	ASP	C-N-CA	5.07	125.35	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4315	0	4219	32	0
1	C	4315	0	4219	34	0
1	E	4315	0	4219	38	0
1	G	4315	0	4219	26	0
1	I	4315	0	4219	33	0
1	K	4315	0	4219	36	0
2	B	1095	0	1118	14	0
2	D	1095	0	1118	4	0
2	F	1095	0	1118	9	0
2	H	1095	0	1118	6	0
2	J	1095	0	1118	8	0
2	L	1095	0	1118	7	0
3	M	72	0	61	2	0
3	O	72	0	61	1	0
3	Q	72	0	61	2	0
3	S	72	0	61	0	0
3	U	72	0	61	2	0
3	W	72	0	61	0	0
4	N	28	0	25	0	0
4	P	28	0	25	1	0
4	R	28	0	25	0	0
4	T	28	0	25	0	0
4	V	28	0	25	0	0
4	X	28	0	25	1	0
5	A	12	0	12	1	0
5	C	12	0	12	0	0
5	E	12	0	12	0	0
5	G	12	0	12	0	0
5	I	12	0	12	0	0
5	K	12	0	12	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
6	I	5	0	0	1	0
6	K	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	14	0	13	0	0
7	K	14	0	13	0	0
8	B	15	0	17	3	0
8	D	15	0	17	2	0
8	F	15	0	17	3	0
8	H	15	0	17	2	0
8	J	15	0	17	2	0
8	L	15	0	17	2	0
9	A	121	0	0	0	0
9	B	27	0	0	1	0
9	C	117	0	0	1	0
9	D	26	0	0	1	0
9	E	109	0	0	1	0
9	F	17	0	0	0	0
9	G	99	0	0	1	0
9	H	20	0	0	0	0
9	I	106	0	0	0	0
9	J	29	0	0	0	0
9	K	98	0	0	4	0
9	L	22	0	0	0	0
All	All	34132	0	32790	241	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 4.

All (241) 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:G:530:LEU:HD12	1:G:530:LEU:C	2.14	0.73
1:G:382:LEU:HD21	1:G:473:PRO:HB2	1.72	0.71
1:A:433:ILE:HD12	1:A:445:VAL:HG22	1.72	0.71
2:F:51:ALA:HB1	8:F:1000:EPE:H82	1.74	0.69
1:K:382:LEU:HD21	1:K:473:PRO:HB2	1.75	0.69
1:K:433:ILE:HD12	1:K:445:VAL:HG22	1.76	0.68
1:C:354:VAL:HG22	1:C:526:ASP:OD1	1.94	0.67
1:E:382:LEU:HD21	1:E:473:PRO:HB2	1.76	0.67
1:A:530:LEU:C	1:A:530:LEU:HD12	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD11	1:C:293:ILE:HD13	1.78	0.66
2:B:81:LEU:HD12	8:B:1000:EPE:H32	1.78	0.65
2:B:11:THR:HG22	2:B:141:ALA:HB3	1.79	0.65
1:C:77:ASP:OD2	1:C:127:LYS:NZ	2.29	0.64
1:C:286:ASP:HB2	1:C:293:ILE:HD12	1.81	0.63
1:G:433:ILE:HD11	1:G:477:LEU:HD21	1.79	0.62
1:E:433:ILE:HD11	1:E:477:LEU:HD21	1.80	0.62
1:K:530:LEU:C	1:K:530:LEU:HD12	2.25	0.61
1:I:530:LEU:HD12	1:I:531:ASN:N	2.14	0.61
1:I:213:PHE:CZ	1:I:326:ARG:HG2	2.36	0.60
1:C:266:MET:HA	1:C:266:MET:HE3	1.83	0.60
1:C:373:VAL:HG13	1:C:481:ALA:HB3	1.82	0.60
1:C:382:LEU:HD21	1:C:473:PRO:HB2	1.85	0.59
1:E:48:GLY:O	1:E:50:ILE:HD12	2.04	0.58
9:C:4040:HOH:O	4:P:1:NAG:H83	2.04	0.58
1:C:213:PHE:CZ	1:C:326:ARG:HG2	2.39	0.57
1:I:382:LEU:HD21	1:I:473:PRO:HB2	1.87	0.57
1:A:385:ALA:HB2	1:A:410:LEU:HD23	1.86	0.57
2:J:81:LEU:HD12	8:J:1000:EPE:H32	1.87	0.57
1:G:143:ASN:OD1	1:G:169:ILE:HD13	2.05	0.56
1:I:71:PHE:CE2	2:L:52:VAL:HG21	2.41	0.56
1:I:322:ILE:HG22	1:I:333:GLN:HG2	1.89	0.55
1:K:322:ILE:HG22	1:K:333:GLN:HG2	1.89	0.55
1:G:530:LEU:C	1:G:530:LEU:CD1	2.80	0.55
1:K:155:LEU:HD13	1:K:161:TRP:CE2	2.42	0.54
1:E:322:ILE:HG22	1:E:333:GLN:HG2	1.90	0.54
1:E:530:LEU:HD12	1:E:531:ASN:N	2.22	0.54
2:J:47:ALA:HB3	2:J:81:LEU:HD21	1.89	0.54
1:C:213:PHE:CD1	1:E:213:PHE:CE1	2.96	0.53
1:E:433:ILE:HD12	1:E:445:VAL:HG22	1.91	0.53
1:I:238:LEU:HD12	1:I:245:TYR:CE1	2.44	0.53
1:K:417:VAL:HG12	1:K:515:LEU:CD1	2.39	0.53
2:B:81:LEU:HD12	8:B:1000:EPE:C3	2.39	0.53
2:F:81:LEU:HD12	8:F:1000:EPE:H32	1.90	0.53
1:I:530:LEU:HD12	1:I:530:LEU:C	2.34	0.53
2:J:81:LEU:HD12	8:J:1000:EPE:C3	2.39	0.53
2:D:81:LEU:HD12	8:D:1000:EPE:H32	1.91	0.52
2:D:119:LYS:NZ	9:D:4023:HOH:O	2.41	0.52
1:A:38:TYR:CZ	1:A:53:ALA:HB3	2.45	0.52
1:C:238:LEU:HD12	1:C:245:TYR:CE1	2.44	0.52
1:I:155:LEU:HD13	1:I:161:TRP:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:ARG:NH1	9:K:4042:HOH:O	2.43	0.51
1:E:281:SER:HB2	1:E:294:LEU:HD11	1.93	0.51
2:B:51:ALA:HB1	8:B:1000:EPE:H82	1.93	0.51
1:C:322:ILE:HG22	1:C:333:GLN:HG2	1.93	0.51
1:C:375:VAL:HB	1:C:530:LEU:HD13	1.92	0.51
1:I:71:PHE:CZ	2:L:52:VAL:HG21	2.45	0.51
1:C:213:PHE:HB3	1:E:213:PHE:CD2	2.46	0.51
1:A:36:LEU:HD22	1:A:295:TRP:CH2	2.45	0.51
1:I:277:LYS:NZ	3:U:1:NAG:H61	2.26	0.50
1:K:28:MET:HE1	1:K:94:PRO:CB	2.41	0.50
1:E:530:LEU:HD12	1:E:530:LEU:C	2.36	0.50
2:F:66:TRP:CH2	2:F:124:PRO:HG3	2.47	0.50
1:E:273:TYR:CA	1:E:333:GLN:HE22	2.24	0.50
2:F:139:GLY:O	2:F:143:VAL:HG23	2.11	0.50
1:C:38:TYR:CE2	1:C:53:ALA:HB3	2.46	0.50
1:A:295:TRP:CH2	1:A:319:PRO:HG3	2.47	0.49
1:C:93:LYS:HG3	1:C:117:LEU:HD21	1.93	0.49
1:C:213:PHE:CE1	1:E:213:PHE:CE1	3.00	0.49
1:K:143:ASN:OD1	1:K:169:ILE:HD13	2.12	0.49
1:A:277:LYS:NZ	3:M:1:NAG:H61	2.27	0.49
1:C:295:TRP:CH2	1:C:319:PRO:HG3	2.47	0.49
1:K:530:LEU:HD12	1:K:531:ASN:N	2.26	0.49
1:A:433:ILE:CD1	1:A:445:VAL:HG22	2.42	0.49
1:E:236:ILE:HG12	1:E:266:MET:HE2	1.93	0.49
2:B:66:TRP:CH2	2:B:124:PRO:HG3	2.48	0.49
1:E:295:TRP:CH2	1:E:319:PRO:HG3	2.48	0.49
1:A:151:THR:HG22	1:A:205:PRO:O	2.12	0.49
1:A:229:ILE:HD13	1:G:229:ILE:HD12	1.94	0.49
2:L:81:LEU:HD12	8:L:1000:EPE:H32	1.93	0.49
2:H:81:LEU:HD12	8:H:1000:EPE:H32	1.95	0.48
1:A:324:LEU:HD22	1:A:328:GLY:HA2	1.94	0.48
1:K:295:TRP:CH2	1:K:319:PRO:HG3	2.48	0.48
1:G:95:VAL:HG21	1:G:183:PHE:CE2	2.48	0.48
1:K:61:ILE:CG2	1:K:342:LEU:HD11	2.44	0.48
1:E:336:VAL:O	1:E:339:VAL:HG12	2.13	0.48
1:G:530:LEU:HD12	1:G:531:ASN:N	2.27	0.48
1:G:324:LEU:HD23	1:G:330:GLN:O	2.14	0.48
1:G:449:SER:HB3	1:G:499:ILE:HG21	1.95	0.48
1:A:382:LEU:HD21	1:A:473:PRO:HB2	1.95	0.48
1:G:266:MET:HE3	1:G:266:MET:HA	1.96	0.48
1:I:295:TRP:CH2	1:I:319:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:66:TRP:CH2	2:J:124:PRO:HG3	2.49	0.48
1:K:213:PHE:CZ	1:K:326:ARG:HG2	2.49	0.48
2:H:20:THR:HG21	2:H:39:MET:SD	2.54	0.47
1:I:277:LYS:HZ1	3:U:1:NAG:H61	1.79	0.47
1:I:469:VAL:HG22	1:I:497:ALA:CB	2.44	0.47
2:B:5:GLU:OE1	2:B:14:TYR:OH	2.25	0.47
1:E:114:PRO:HB3	1:E:122:LEU:HD22	1.97	0.47
1:G:378:LYS:NZ	9:G:4081:HOH:O	2.41	0.47
1:G:540:ILE:O	1:G:541:SER:C	2.57	0.47
2:D:51:ALA:HB1	8:D:1000:EPE:H82	1.96	0.47
1:I:469:VAL:HG22	1:I:497:ALA:HB2	1.96	0.47
1:E:25:ASN:HB3	1:E:52:TRP:CH2	2.50	0.47
1:E:433:ILE:CD1	1:E:445:VAL:HG22	2.45	0.47
1:I:449:SER:HB3	1:I:499:ILE:HG21	1.96	0.47
1:E:416:MET:HE3	1:E:518:PHE:CG	2.50	0.46
1:K:235:LYS:NZ	1:K:281:SER:O	2.36	0.46
1:G:28:MET:HE2	1:G:30:TYR:HB2	1.96	0.46
1:G:36:LEU:HD22	1:G:295:TRP:CH2	2.50	0.46
1:I:143:ASN:OD1	1:I:169:ILE:HD13	2.15	0.46
1:A:48:GLY:H	1:A:50:ILE:HD13	1.80	0.46
1:A:277:LYS:HZ3	3:M:1:NAG:H61	1.80	0.46
1:I:336:VAL:O	1:I:339:VAL:HG12	2.16	0.46
1:E:213:PHE:CZ	1:E:326:ARG:HG2	2.51	0.46
1:I:28:MET:CE	1:I:30:TYR:HB2	2.45	0.46
1:K:25:ASN:HB3	1:K:52:TRP:CH2	2.51	0.46
1:K:102:ASP:HB2	1:K:103:PRO:CD	2.46	0.46
1:E:273:TYR:C	1:E:333:GLN:HE22	2.24	0.46
1:I:433:ILE:HD12	1:I:445:VAL:HG22	1.98	0.46
1:I:540:ILE:O	1:I:541:SER:C	2.57	0.46
1:K:111:ILE:HB	1:K:133:LEU:HD22	1.98	0.45
1:E:237:SER:HB3	1:E:279:TYR:CZ	2.51	0.45
1:A:266:MET:HE3	1:A:266:MET:HA	1.97	0.45
1:I:151:THR:HG22	1:I:205:PRO:O	2.16	0.45
1:E:540:ILE:O	1:E:541:SER:C	2.58	0.45
2:F:51:ALA:CB	8:F:1000:EPE:H82	2.46	0.45
2:F:105:VAL:HG11	3:Q:2:NAG:C7	2.47	0.45
1:G:38:TYR:CZ	1:G:53:ALA:HB3	2.52	0.45
1:K:13:HIS:NE2	1:K:489:GLU:OE2	2.47	0.45
1:E:33:ILE:HD12	1:E:120:PRO:HB2	1.99	0.45
1:G:295:TRP:CH2	1:G:319:PRO:HG3	2.51	0.45
1:C:373:VAL:CG1	1:C:481:ALA:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:VAL:HG13	2:F:85:LEU:HD22	1.99	0.45
2:B:11:THR:HG22	2:B:141:ALA:CB	2.46	0.45
1:C:213:PHE:HB3	1:E:213:PHE:CE2	2.51	0.45
1:K:266:MET:HE3	1:K:266:MET:HA	1.99	0.44
1:A:449:SER:HB3	1:A:499:ILE:HG21	1.99	0.44
1:E:102:ASP:HB2	1:E:103:PRO:CD	2.48	0.44
1:C:155:LEU:HD13	1:C:161:TRP:CE2	2.52	0.44
1:G:15:GLN:HB3	1:G:315:ILE:HG22	2.00	0.44
1:G:102:ASP:HB2	1:G:103:PRO:CD	2.48	0.44
2:B:2:ASN:HB2	2:B:5:GLU:HB2	1.99	0.44
2:F:119:LYS:C	2:F:121:SER:H	2.26	0.44
2:J:2:ASN:HB2	2:J:5:GLU:HB3	2.00	0.44
1:A:238:LEU:HD12	1:A:245:TYR:CE1	2.53	0.43
2:H:2:ASN:HB2	2:H:5:GLU:HB2	2.00	0.43
1:I:395:PRO:HA	1:I:398:ILE:HD12	2.01	0.43
1:K:344:THR:HG21	9:K:4065:HOH:O	2.18	0.43
1:E:70:ILE:HG22	1:E:81:CYS:SG	2.58	0.43
2:J:48:ASN:O	2:J:52:VAL:HG23	2.18	0.43
1:C:143:ASN:OD1	1:C:169:ILE:HD13	2.18	0.43
1:E:446:LEU:HD12	1:E:467:ALA:O	2.17	0.43
1:I:143:ASN:ND2	6:I:2002:SO4:O1	2.50	0.43
1:K:151:THR:HG22	1:K:205:PRO:O	2.18	0.43
1:K:231:LYS:HZ1	1:K:250:THR:HG23	1.83	0.43
5:A:1000:FRU:O2	2:B:98:LYS:NZ	2.52	0.43
2:L:51:ALA:HB1	8:L:1000:EPE:H82	2.01	0.43
1:C:273:TYR:C	1:C:333:GLN:HE22	2.27	0.43
2:J:47:ALA:CB	2:J:81:LEU:HD21	2.48	0.43
2:B:24:ASP:HB3	2:B:38:ILE:HD13	2.00	0.43
1:C:38:TYR:CZ	1:C:53:ALA:HB3	2.54	0.43
1:C:60:LEU:CD1	1:C:293:ILE:HD13	2.46	0.43
1:A:236:ILE:HD12	1:A:238:LEU:HD21	2.01	0.43
1:A:322:ILE:HG22	1:A:333:GLN:HG2	2.00	0.43
1:I:373:VAL:HG23	1:I:530:LEU:CD1	2.48	0.43
1:K:237:SER:HB3	1:K:279:TYR:CZ	2.54	0.43
1:K:325:ASP:CB	1:K:332:ILE:HD11	2.48	0.43
1:A:530:LEU:HD12	1:A:531:ASN:N	2.32	0.43
1:K:38:TYR:CZ	1:K:53:ALA:HB3	2.53	0.43
1:E:143:ASN:OD1	1:E:169:ILE:HD13	2.19	0.42
2:H:66:TRP:CH2	2:H:124:PRO:HG3	2.54	0.42
1:K:169:ILE:HG12	1:K:174:LEU:HD11	2.00	0.42
1:E:151:THR:HG22	1:E:205:PRO:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:OE1	1:A:50:ILE:HG21	2.19	0.42
1:A:385:ALA:CB	1:A:410:LEU:HD23	2.48	0.42
2:H:47:ALA:HB3	2:H:81:LEU:HD21	2.01	0.42
1:K:231:LYS:NZ	1:K:250:THR:HG23	2.34	0.42
2:B:28:ALA:HB3	9:B:4008:HOH:O	2.18	0.42
1:I:131:ASN:OD1	1:I:133:LEU:HD13	2.19	0.42
2:D:66:TRP:CH2	2:D:124:PRO:HG3	2.54	0.42
1:G:60:LEU:CD1	1:G:293:ILE:HD13	2.50	0.42
1:K:131:ASN:OD1	1:K:133:LEU:HD13	2.19	0.42
1:G:13:HIS:NE2	1:G:489:GLU:OE2	2.48	0.42
1:K:114:PRO:HB2	1:K:117:LEU:HD23	2.01	0.42
1:C:373:VAL:HG23	1:C:530:LEU:HD11	2.02	0.42
1:K:29:ILE:HG23	9:K:4055:HOH:O	2.20	0.42
1:K:540:ILE:O	1:K:541:SER:C	2.63	0.42
1:C:356:LYS:HA	1:C:524:SER:HB3	2.00	0.42
1:E:5:ASN:N	9:E:4002:HOH:O	2.52	0.42
1:A:236:ILE:HG12	1:A:266:MET:HE2	2.01	0.42
1:C:540:ILE:O	1:C:541:SER:C	2.63	0.42
1:C:277:LYS:NZ	3:O:1:NAG:H61	2.35	0.42
1:E:29:ILE:HD12	1:E:33:ILE:O	2.20	0.42
1:I:169:ILE:HG22	1:I:170:HIS:CD2	2.55	0.42
1:K:170:HIS:H	4:X:1:NAG:H83	1.84	0.42
1:A:273:TYR:C	1:A:333:GLN:HE22	2.27	0.41
1:C:142:ILE:HG21	1:C:147:PHE:CD1	2.55	0.41
1:C:203:GLU:O	1:C:204:CYS:C	2.63	0.41
1:E:273:TYR:O	1:E:333:GLN:NE2	2.51	0.41
1:E:293:ILE:HD13	1:E:336:VAL:HG11	2.02	0.41
2:F:104:MET:HB3	2:F:140:ARG:HG3	2.02	0.41
1:I:30:TYR:CD2	1:I:122:LEU:HD11	2.54	0.41
1:I:121:TYR:O	1:I:122:LEU:C	2.63	0.41
1:C:102:ASP:HB2	1:C:103:PRO:CD	2.50	0.41
1:G:111:ILE:HB	1:G:133:LEU:CD2	2.50	0.41
1:K:169:ILE:HG22	1:K:170:HIS:CD2	2.55	0.41
1:A:142:ILE:HG21	1:A:147:PHE:CD1	2.56	0.41
2:H:81:LEU:HD12	8:H:1000:EPE:C3	2.50	0.41
2:B:111:ALA:HB2	2:B:132:VAL:HG12	2.01	0.41
1:G:449:SER:CB	1:G:499:ILE:HG21	2.50	0.41
2:J:104:MET:HB3	2:J:140:ARG:HG3	2.02	0.41
1:A:304:VAL:HG13	2:B:79:VAL:HG11	2.02	0.41
1:A:354:VAL:HG22	1:A:526:ASP:OD1	2.20	0.41
1:K:61:ILE:HG21	1:K:342:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG21	1:A:183:PHE:CE2	2.55	0.41
1:E:56:THR:HG23	1:E:66:HIS:CD2	2.56	0.41
1:I:458:GLU:HA	1:I:462:LYS:HZ1	1.85	0.41
1:A:38:TYR:CE2	1:A:53:ALA:HB3	2.56	0.41
1:E:102:ASP:OD1	1:E:102:ASP:C	2.63	0.41
1:G:373:VAL:HG23	1:G:530:LEU:CD1	2.51	0.41
2:B:57:LEU:HB2	2:B:70:LEU:HD21	2.03	0.41
1:K:326:ARG:NH2	9:K:4060:HOH:O	2.53	0.41
1:A:20:TRP:CD1	1:A:20:TRP:C	2.99	0.41
1:A:231:LYS:HZ1	1:A:250:THR:HG23	1.86	0.41
1:E:39:GLN:OE1	1:E:50:ILE:HG21	2.20	0.41
1:G:20:TRP:CD1	1:G:20:TRP:C	2.98	0.41
5:K:1000:FRU:O2	2:L:98:LYS:NZ	2.53	0.41
1:C:519:ASN:ND2	1:C:525:VAL:HG22	2.36	0.40
1:A:169:ILE:HG12	1:A:174:LEU:HD11	2.03	0.40
1:C:30:TYR:CE1	1:C:94:PRO:HD3	2.57	0.40
1:C:336:VAL:O	1:C:339:VAL:HG12	2.20	0.40
1:E:38:TYR:CZ	1:E:53:ALA:HB3	2.56	0.40
1:G:56:THR:HG23	1:G:66:HIS:CD2	2.57	0.40
2:L:104:MET:HB3	2:L:140:ARG:HG3	2.02	0.40
3:Q:3:BMA:H62	3:Q:6:BMA:C6	2.51	0.40
1:I:102:ASP:HB2	1:I:103:PRO:HD3	2.03	0.40
1:I:373:VAL:HG23	1:I:530:LEU:HD11	2.03	0.40
1:I:373:VAL:HG13	1:I:481:ALA:HB3	2.04	0.40
1:I:458:GLU:HA	1:I:462:LYS:NZ	2.36	0.40
2:L:66:TRP:CH2	2:L:124:PRO:HG3	2.57	0.40
1:K:109:GLN:HB2	1:K:134:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/537 (100%)	508 (95%)	27 (5%)	0	100	100
1	C	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
1	E	535/537 (100%)	509 (95%)	26 (5%)	0	100	100
1	G	535/537 (100%)	513 (96%)	22 (4%)	0	100	100
1	I	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
1	K	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
2	B	144/149 (97%)	136 (94%)	8 (6%)	0	100	100
2	D	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
2	F	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
2	H	144/149 (97%)	137 (95%)	6 (4%)	1 (1%)	18	36
2	J	144/149 (97%)	137 (95%)	6 (4%)	1 (1%)	18	36
2	L	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
All	All	4074/4116 (99%)	3887 (95%)	185 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	121	SER
2	J	121	SER

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	473/473 (100%)	456 (96%)	17 (4%)	31	56
1	C	473/473 (100%)	459 (97%)	14 (3%)	36	62
1	E	473/473 (100%)	458 (97%)	15 (3%)	34	59
1	G	473/473 (100%)	457 (97%)	16 (3%)	32	58
1	I	473/473 (100%)	456 (96%)	17 (4%)	31	56
1	K	473/473 (100%)	460 (97%)	13 (3%)	39	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	120/121 (99%)	120 (100%)	0	100	100
2	D	120/121 (99%)	119 (99%)	1 (1%)	73	87
2	F	120/121 (99%)	116 (97%)	4 (3%)	33	59
2	H	120/121 (99%)	120 (100%)	0	100	100
2	J	120/121 (99%)	119 (99%)	1 (1%)	73	87
2	L	120/121 (99%)	119 (99%)	1 (1%)	73	87
All	All	3558/3564 (100%)	3459 (97%)	99 (3%)	38	64

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	102	ASP
1	A	133	LEU
1	A	168	LYS
1	A	212	ARG
1	A	228	GLU
1	A	290	ASN
1	A	320	ARG
1	A	324	LEU
1	A	325	ASP
1	A	345	LYS
1	A	356	LYS
1	A	383	GLU
1	A	437	ARG
1	A	451	GLN
1	A	475	GLN
1	A	530	LEU
1	C	29	ILE
1	C	50	ILE
1	C	133	LEU
1	C	168	LYS
1	C	212	ARG
1	C	228	GLU
1	C	320	ARG
1	C	324	LEU
1	C	325	ASP
1	C	345	LYS
1	C	373	VAL
1	C	383	GLU

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Mol	Chain	Res	Type
1	C	437	ARG
1	C	451	GLN
2	D	70	LEU
1	E	50	ILE
1	E	133	LEU
1	E	212	ARG
1	E	225	GLU
1	E	228	GLU
1	E	290	ASN
1	E	320	ARG
1	E	324	LEU
1	E	325	ASP
1	E	345	LYS
1	E	356	LYS
1	E	383	GLU
1	E	437	ARG
1	E	451	GLN
1	E	530	LEU
2	F	56	LYS
2	F	70	LEU
2	F	112	GLN
2	F	119	LYS
1	G	50	ILE
1	G	133	LEU
1	G	168	LYS
1	G	225	GLU
1	G	228	GLU
1	G	290	ASN
1	G	320	ARG
1	G	324	LEU
1	G	325	ASP
1	G	345	LYS
1	G	356	LYS
1	G	380	ARG
1	G	383	GLU
1	G	437	ARG
1	G	451	GLN
1	G	530	LEU
1	I	50	ILE
1	I	168	LYS
1	I	212	ARG
1	I	228	GLU

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Mol	Chain	Res	Type
1	I	239	ASP
1	I	290	ASN
1	I	320	ARG
1	I	324	LEU
1	I	325	ASP
1	I	345	LYS
1	I	356	LYS
1	I	373	VAL
1	I	383	GLU
1	I	437	ARG
1	I	451	GLN
1	I	506	LYS
1	I	530	LEU
2	J	56	LYS
1	K	49	ASN
1	K	50	ILE
1	K	228	GLU
1	K	320	ARG
1	K	324	LEU
1	K	325	ASP
1	K	345	LYS
1	K	356	LYS
1	K	373	VAL
1	K	383	GLU
1	K	437	ARG
1	K	451	GLN
1	K	530	LEU
2	L	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	441	ASN
2	B	61	ASN
1	C	106	GLN
1	C	333	GLN
1	C	349	ASN
1	C	422	ASN
1	C	439	ASN
1	C	441	ASN
1	C	451	GLN

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Mol	Chain	Res	Type
1	C	475	GLN
1	C	529	ASN
2	D	10	ASN
2	D	61	ASN
1	E	105	ASN
1	E	262	ASN
1	E	333	GLN
1	E	475	GLN
2	F	10	ASN
1	G	170	HIS
1	G	262	ASN
1	G	316	GLN
1	G	333	GLN
1	G	349	ASN
1	G	441	ASN
1	G	529	ASN
2	H	2	ASN
2	H	10	ASN
2	H	49	GLN
2	J	2	ASN
2	J	59	HIS
1	K	170	HIS
1	K	333	GLN
1	K	349	ASN
1	K	422	ASN
1	K	529	ASN
2	L	61	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
3	NAG	M	1	1,3	14,14,15	0.55	0	17,19,21	1.23	1 (5%)
3	NAG	M	2	3	14,14,15	0.59	0	17,19,21	1.29	2 (11%)
3	BMA	M	3	3	11,11,12	0.58	0	15,15,17	2.06	4 (26%)
3	MAN	M	4	3	11,11,12	0.64	0	15,15,17	0.61	0
3	MAN	M	5	3	11,11,12	0.47	0	15,15,17	0.73	0
3	BMA	M	6	3	11,11,12	0.51	0	15,15,17	2.50	3 (20%)
4	NAG	N	1	1,4	14,14,15	0.48	0	17,19,21	1.44	3 (17%)
4	NAG	N	2	4	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.50	0	17,19,21	1.15	1 (5%)
3	NAG	O	2	3	14,14,15	0.59	0	17,19,21	1.36	1 (5%)
3	BMA	O	3	3	11,11,12	0.43	0	15,15,17	2.11	4 (26%)
3	MAN	O	4	3	11,11,12	0.61	0	15,15,17	0.75	1 (6%)
3	MAN	O	5	3	11,11,12	0.57	0	15,15,17	0.66	0
3	BMA	O	6	3	11,11,12	0.48	0	15,15,17	2.57	3 (20%)
4	NAG	P	1	1,4	14,14,15	0.61	0	17,19,21	1.55	4 (23%)
4	NAG	P	2	4	14,14,15	0.53	0	17,19,21	0.87	0
3	NAG	Q	1	1,3	14,14,15	0.48	0	17,19,21	1.23	1 (5%)
3	NAG	Q	2	3	14,14,15	0.58	0	17,19,21	1.43	1 (5%)
3	BMA	Q	3	3	11,11,12	0.56	0	15,15,17	1.90	3 (20%)
3	MAN	Q	4	3	11,11,12	0.57	0	15,15,17	0.69	1 (6%)
3	MAN	Q	5	3	11,11,12	0.51	0	15,15,17	0.63	0
3	BMA	Q	6	3	11,11,12	0.47	0	15,15,17	2.45	3 (20%)
4	NAG	R	1	1,4	14,14,15	0.55	0	17,19,21	1.38	2 (11%)
4	NAG	R	2	4	14,14,15	0.50	0	17,19,21	1.12	2 (11%)
3	NAG	S	1	1,3	14,14,15	0.58	0	17,19,21	1.33	2 (11%)
3	NAG	S	2	3	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
3	BMA	S	3	3	11,11,12	0.59	0	15,15,17	2.19	4 (26%)
3	MAN	S	4	3	11,11,12	0.64	0	15,15,17	0.59	0
3	MAN	S	5	3	11,11,12	0.59	0	15,15,17	0.76	0
3	BMA	S	6	3	11,11,12	0.53	0	15,15,17	2.39	3 (20%)
4	NAG	T	1	1,4	14,14,15	0.58	0	17,19,21	1.19	2 (11%)
4	NAG	T	2	4	14,14,15	0.52	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	U	1	1,3	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
3	NAG	U	2	3	14,14,15	0.64	0	17,19,21	1.02	1 (5%)
3	BMA	U	3	3	11,11,12	0.61	0	15,15,17	2.23	3 (20%)
3	MAN	U	4	3	11,11,12	0.55	0	15,15,17	1.01	1 (6%)
3	MAN	U	5	3	11,11,12	0.66	0	15,15,17	1.11	2 (13%)
3	BMA	U	6	3	11,11,12	0.48	0	15,15,17	2.42	3 (20%)
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	1.45	3 (17%)
4	NAG	V	2	4	14,14,15	0.53	0	17,19,21	0.76	0
3	NAG	W	1	1,3	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
3	NAG	W	2	3	14,14,15	0.61	0	17,19,21	1.44	2 (11%)
3	BMA	W	3	3	11,11,12	0.52	0	15,15,17	2.43	3 (20%)
3	MAN	W	4	3	11,11,12	0.62	0	15,15,17	0.66	0
3	MAN	W	5	3	11,11,12	0.56	0	15,15,17	0.67	0
3	BMA	W	6	3	11,11,12	0.47	0	15,15,17	2.55	3 (20%)
4	NAG	X	1	1,4	14,14,15	0.57	0	17,19,21	1.21	2 (11%)
4	NAG	X	2	4	14,14,15	0.52	0	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	M	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	MAN	M	4	3	-	0/2/19/22	0/1/1/1
3	MAN	M	5	3	-	1/2/19/22	0/1/1/1
3	BMA	M	6	3	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	O	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
3	MAN	O	5	3	-	2/2/19/22	0/1/1/1
3	BMA	O	6	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	2/2/19/22	0/1/1/1
3	BMA	Q	6	3	-	2/2/19/22	0/1/1/1
4	NAG	R	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
3	NAG	S	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	S	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
3	MAN	S	4	3	-	0/2/19/22	0/1/1/1
3	MAN	S	5	3	-	1/2/19/22	0/1/1/1
3	BMA	S	6	3	-	2/2/19/22	0/1/1/1
4	NAG	T	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	U	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	MAN	U	4	3	-	1/2/19/22	0/1/1/1
3	MAN	U	5	3	-	2/2/19/22	0/1/1/1
3	BMA	U	6	3	-	2/2/19/22	0/1/1/1
4	NAG	V	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	3/6/23/26	0/1/1/1
3	NAG	W	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	W	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	BMA	W	3	3	-	2/2/19/22	0/1/1/1
3	MAN	W	4	3	-	0/2/19/22	0/1/1/1
3	MAN	W	5	3	-	2/2/19/22	0/1/1/1
3	BMA	W	6	3	-	2/2/19/22	0/1/1/1
4	NAG	X	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	6	BMA	C1-O5-C5	8.79	123.97	112.19
3	O	6	BMA	C1-O5-C5	8.67	123.80	112.19
3	Q	6	BMA	C1-O5-C5	8.40	123.44	112.19
3	M	6	BMA	C1-O5-C5	8.32	123.34	112.19
3	U	6	BMA	C1-O5-C5	8.30	123.31	112.19
3	W	3	BMA	C1-O5-C5	8.04	122.96	112.19
3	S	6	BMA	C1-O5-C5	7.88	122.75	112.19
3	S	3	BMA	C1-O5-C5	6.85	121.37	112.19
3	U	3	BMA	C1-O5-C5	6.68	121.14	112.19
3	O	3	BMA	C1-O5-C5	5.88	120.06	112.19
3	M	3	BMA	C1-O5-C5	5.60	119.69	112.19
3	Q	3	BMA	C1-O5-C5	5.03	118.93	112.19
3	Q	2	NAG	C1-O5-C5	4.58	118.33	112.19
3	O	2	NAG	C1-O5-C5	4.39	118.07	112.19
3	W	2	NAG	C1-O5-C5	4.37	118.05	112.19
4	V	1	NAG	C2-N2-C7	4.15	128.46	122.90
4	N	1	NAG	C2-N2-C7	4.01	128.28	122.90
3	M	2	NAG	C1-O5-C5	3.74	117.19	112.19
4	P	1	NAG	C2-N2-C7	3.69	127.84	122.90
3	M	3	BMA	C3-C4-C5	3.63	116.81	110.23
3	W	1	NAG	C1-O5-C5	3.61	117.02	112.19
3	O	3	BMA	C3-C4-C5	3.54	116.65	110.23
3	U	3	BMA	C3-C4-C5	3.50	116.58	110.23
3	Q	3	BMA	C3-C4-C5	3.46	116.51	110.23
3	M	1	NAG	C1-O5-C5	3.43	116.78	112.19
3	Q	1	NAG	C1-O5-C5	3.26	116.55	112.19
3	S	1	NAG	C1-O5-C5	3.12	116.37	112.19
3	O	6	BMA	O5-C5-C4	3.11	118.38	110.83
3	O	1	NAG	C1-O5-C5	3.07	116.30	112.19
3	S	6	BMA	C3-C4-C5	3.03	115.73	110.23
3	W	6	BMA	O5-C5-C4	3.02	118.17	110.83
4	X	2	NAG	O5-C1-C2	-3.02	106.62	111.29
3	Q	6	BMA	C3-C4-C5	3.01	115.69	110.23
3	M	6	BMA	O5-C5-C4	3.00	118.13	110.83
3	U	4	MAN	C1-O5-C5	2.98	116.18	112.19
3	M	6	BMA	C3-C4-C5	2.96	115.59	110.23
3	O	6	BMA	C3-C4-C5	2.87	115.43	110.23
3	U	3	BMA	O5-C5-C4	2.82	117.69	110.83
3	U	1	NAG	C1-O5-C5	2.81	115.95	112.19
3	S	3	BMA	C3-C4-C5	2.80	115.31	110.23
4	R	1	NAG	C2-N2-C7	2.73	126.56	122.90
3	S	6	BMA	O5-C5-C4	2.71	117.43	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	6	BMA	O5-C5-C4	2.70	117.41	110.83
3	Q	6	BMA	O5-C5-C4	2.67	117.32	110.83
3	W	6	BMA	C3-C4-C5	2.64	115.02	110.23
3	W	3	BMA	O5-C5-C4	2.62	117.19	110.83
3	O	3	BMA	O3-C3-C4	-2.59	104.27	110.38
4	R	2	NAG	O5-C1-C2	-2.56	107.34	111.29
3	W	3	BMA	C3-C4-C5	2.55	114.86	110.23
4	R	1	NAG	C1-O5-C5	2.54	115.59	112.19
4	P	1	NAG	C1-O5-C5	2.53	115.58	112.19
3	U	6	BMA	C3-C4-C5	2.52	114.79	110.23
4	N	2	NAG	O5-C1-C2	-2.51	107.40	111.29
4	X	1	NAG	C2-N2-C7	2.51	126.26	122.90
4	N	1	NAG	O7-C7-N2	2.44	126.30	121.98
3	S	1	NAG	O5-C5-C6	2.43	112.39	107.66
4	T	1	NAG	C1-O5-C5	2.40	115.40	112.19
4	P	1	NAG	O7-C7-N2	2.39	126.20	121.98
3	S	2	NAG	C1-O5-C5	2.36	115.34	112.19
3	O	3	BMA	C6-C5-C4	-2.35	107.26	113.02
3	U	5	MAN	C1-C2-C3	2.29	112.98	109.64
3	Q	3	BMA	O5-C5-C4	2.27	116.34	110.83
4	T	1	NAG	C2-N2-C7	2.25	125.92	122.90
4	N	1	NAG	C1-O5-C5	2.23	115.18	112.19
4	P	1	NAG	O7-C7-C8	-2.23	118.08	122.05
3	M	3	BMA	O5-C5-C4	2.22	116.23	110.83
4	V	1	NAG	O7-C7-N2	2.15	125.78	121.98
3	W	2	NAG	C1-C2-N2	2.14	113.81	110.43
3	Q	4	MAN	C1-O5-C5	2.12	115.03	112.19
3	U	5	MAN	C3-C4-C5	2.10	114.05	110.23
3	M	3	BMA	O3-C3-C4	-2.10	105.43	110.38
4	V	1	NAG	O7-C7-C8	-2.08	118.36	122.05
3	M	2	NAG	C1-C2-N2	2.07	113.70	110.43
3	S	3	BMA	O3-C3-C4	-2.07	105.50	110.38
4	T	2	NAG	O5-C1-C2	-2.05	108.11	111.29
4	X	1	NAG	O7-C7-N2	2.05	125.60	121.98
3	U	2	NAG	C1-O5-C5	2.05	114.93	112.19
3	S	3	BMA	C6-C5-C4	-2.03	108.05	113.02
4	R	2	NAG	C1-C2-N2	2.02	113.62	110.43
3	O	4	MAN	C1-O5-C5	2.01	114.88	112.19

All (18) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	M	1	NAG	C1
3	M	2	NAG	C1
3	O	1	NAG	C1
3	O	2	NAG	C1
3	Q	1	NAG	C1
3	Q	2	NAG	C1
3	S	1	NAG	C1
3	S	2	NAG	C1
3	U	1	NAG	C1
3	U	2	NAG	C1
3	W	1	NAG	C1
3	W	2	NAG	C1
4	N	1	NAG	C1
4	P	1	NAG	C1
4	R	1	NAG	C1
4	T	1	NAG	C1
4	V	1	NAG	C1
4	X	1	NAG	C1

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C3-C2-N2-C7
4	P	1	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
3	U	1	NAG	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	M	6	BMA	O5-C5-C6-O6
3	U	6	BMA	O5-C5-C6-O6
3	W	6	BMA	O5-C5-C6-O6
3	W	3	BMA	C4-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	O	3	BMA	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
3	Q	6	BMA	O5-C5-C6-O6
3	S	6	BMA	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
3	O	6	BMA	O5-C5-C6-O6
3	W	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	W	5	MAN	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	S	6	BMA	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
3	Q	6	BMA	C4-C5-C6-O6
3	Q	5	MAN	C4-C5-C6-O6
3	W	5	MAN	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	U	5	MAN	C4-C5-C6-O6
3	W	6	BMA	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6

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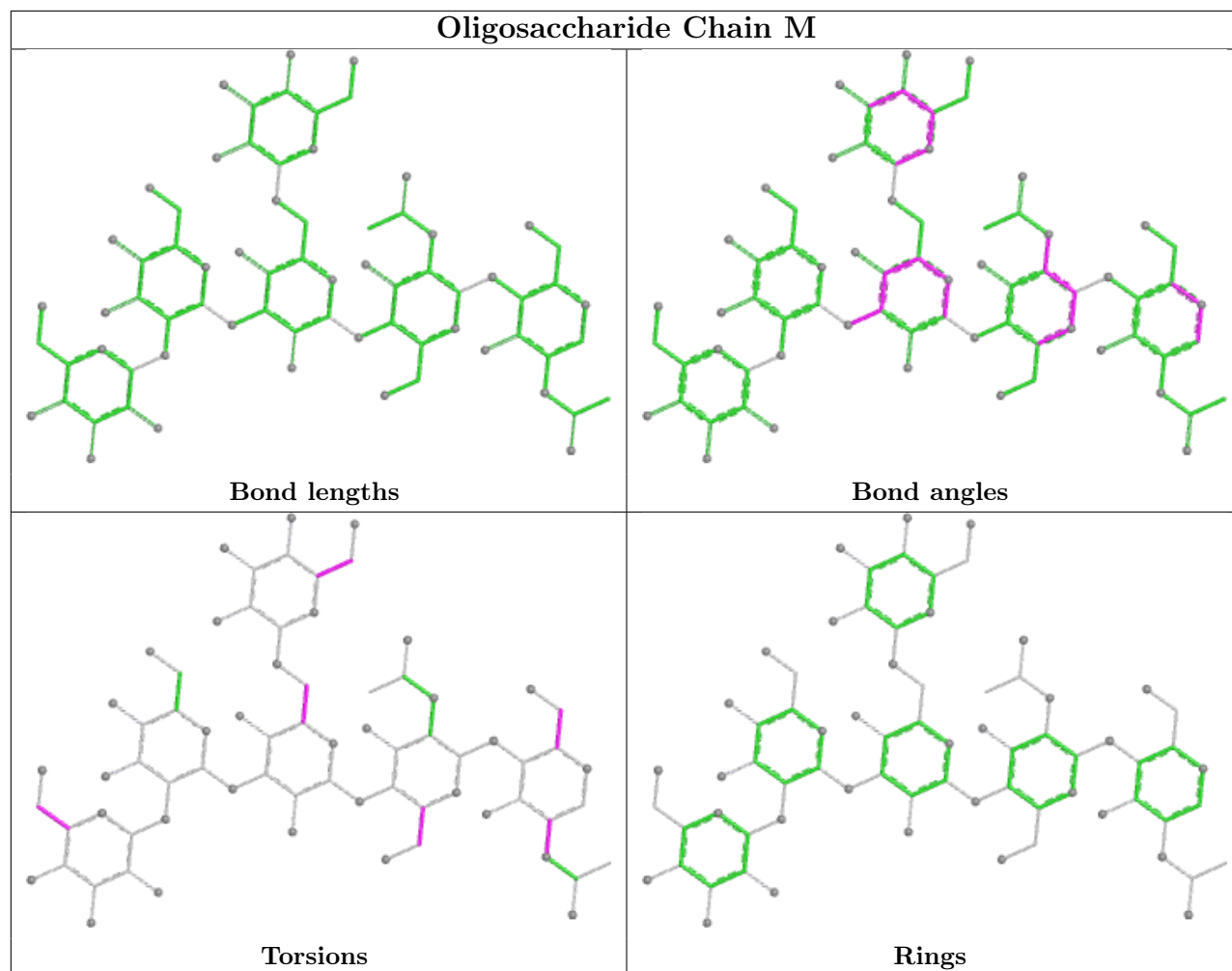
Mol	Chain	Res	Type	Atoms
4	R	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
3	O	5	MAN	C4-C5-C6-O6
3	Q	5	MAN	O5-C5-C6-O6
4	T	1	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	N	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
3	U	6	BMA	C4-C5-C6-O6
3	S	5	MAN	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	U	5	MAN	O5-C5-C6-O6
3	O	5	MAN	O5-C5-C6-O6
3	M	6	BMA	C4-C5-C6-O6
3	M	1	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	V	2	NAG	C1-C2-N2-C7
4	X	2	NAG	C1-C2-N2-C7
3	U	4	MAN	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	5	MAN	C4-C5-C6-O6

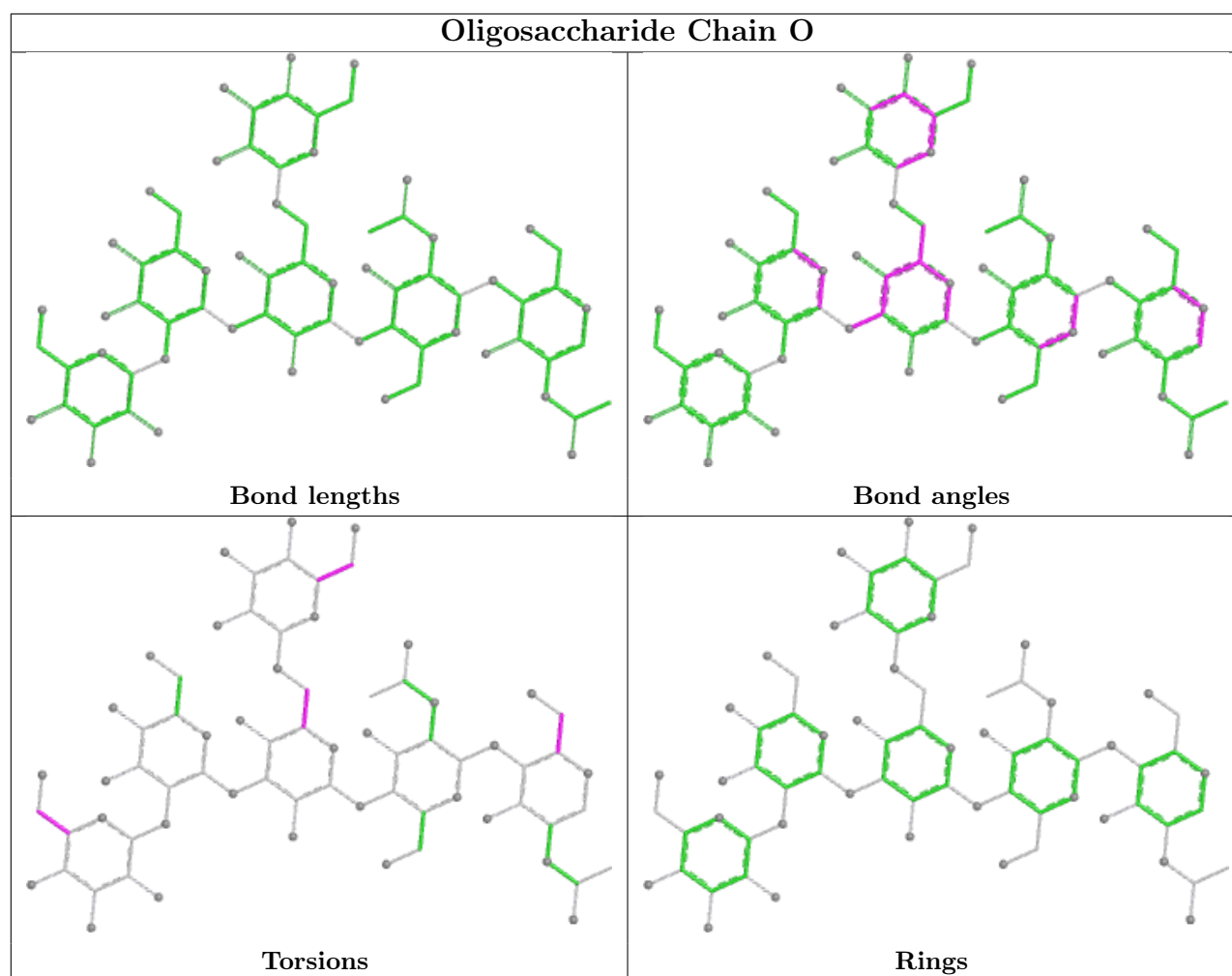
There are no ring outliers.

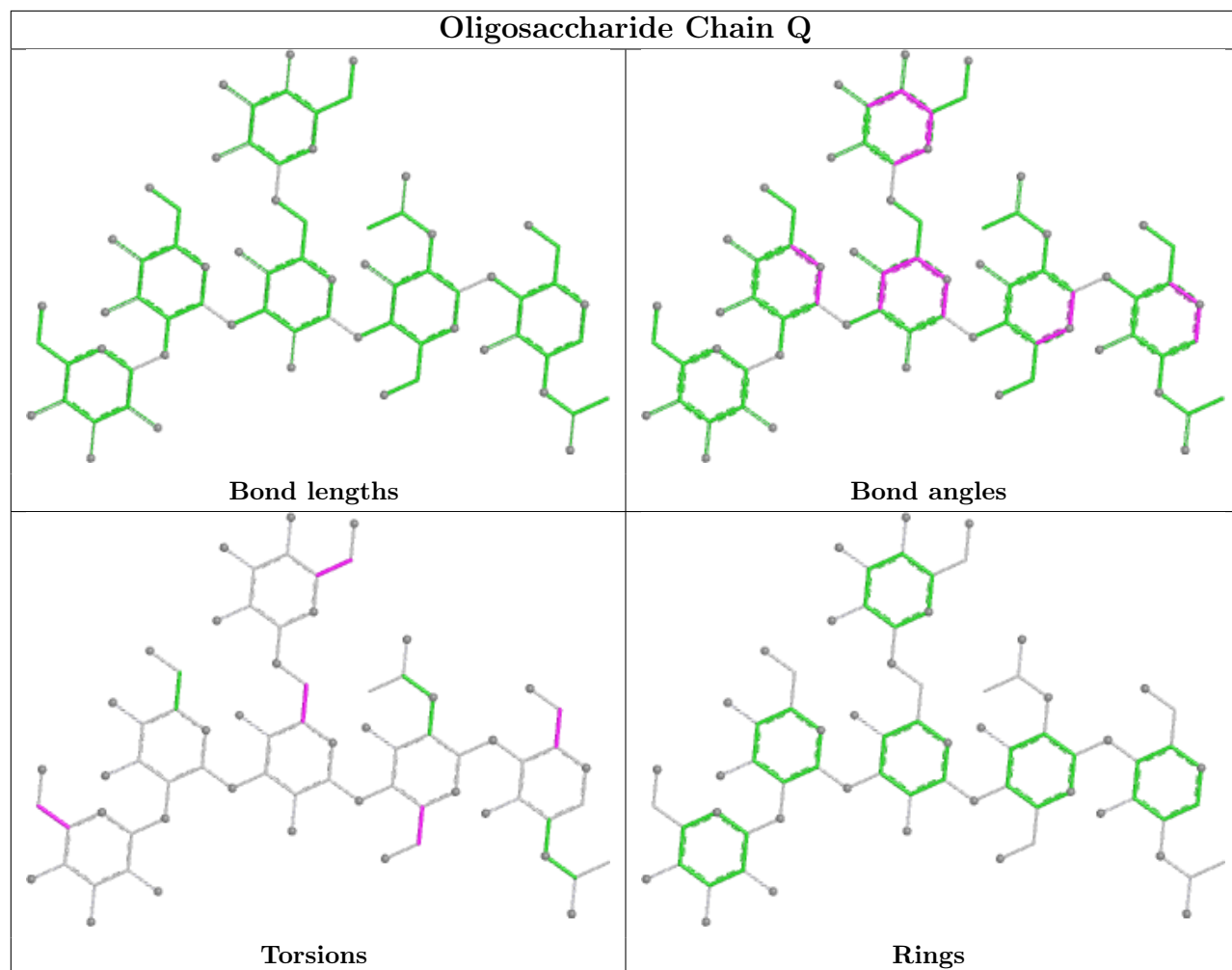
8 monomers are involved in 9 short contacts:

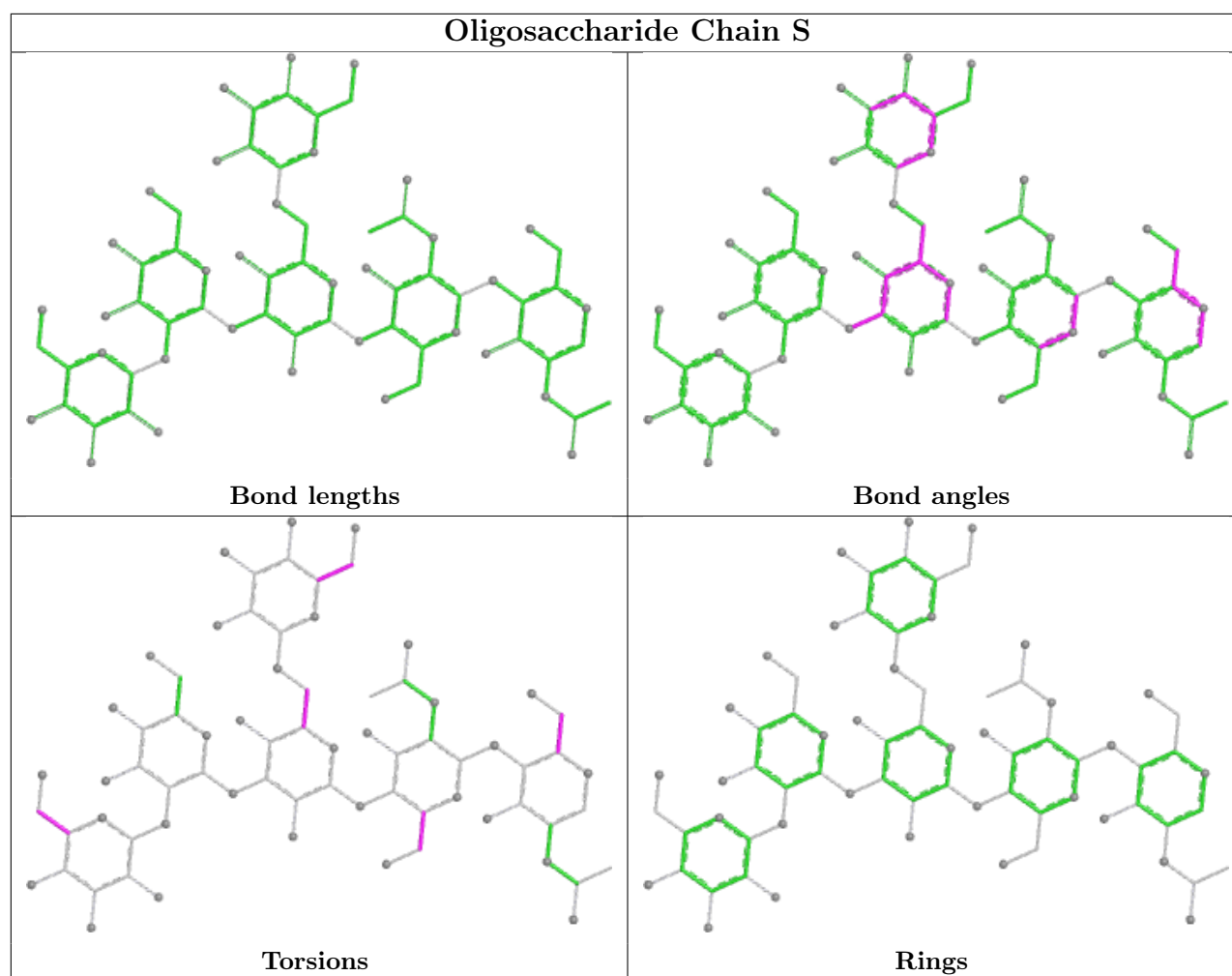
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1	NAG	1	0
3	M	1	NAG	2	0
4	X	1	NAG	1	0
3	Q	6	BMA	1	0
3	Q	3	BMA	1	0
3	Q	2	NAG	1	0
3	U	1	NAG	2	0
3	O	1	NAG	1	0

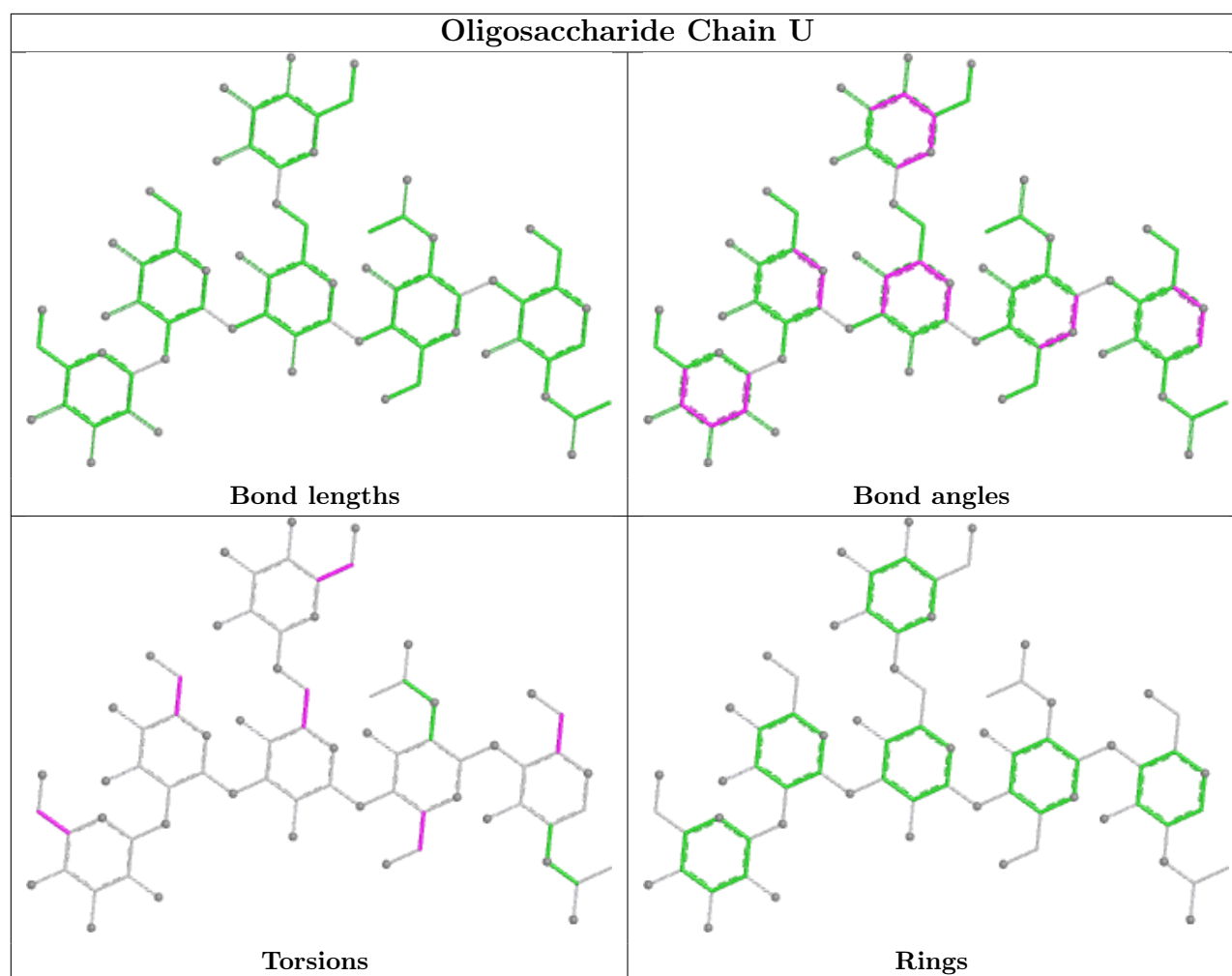
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

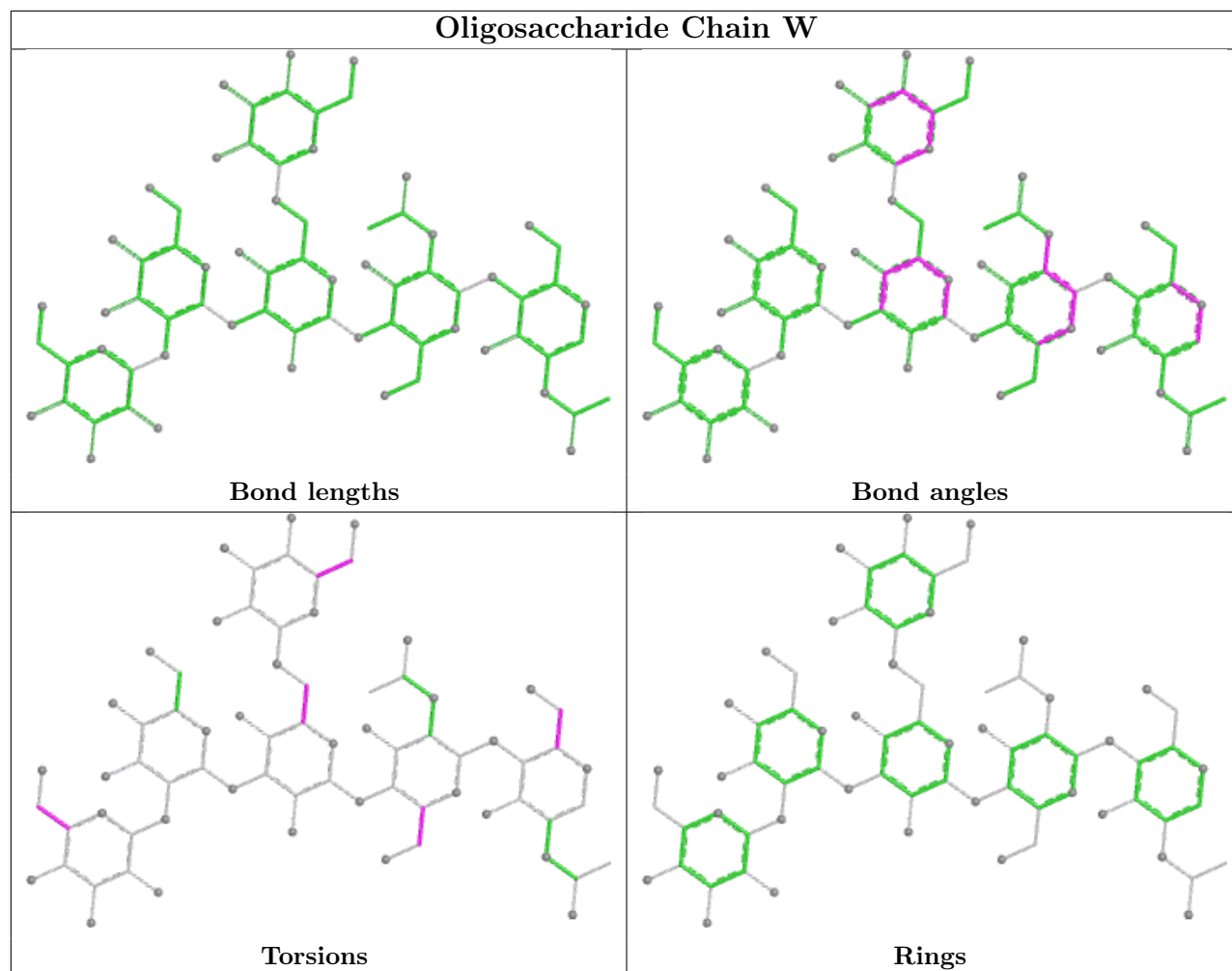


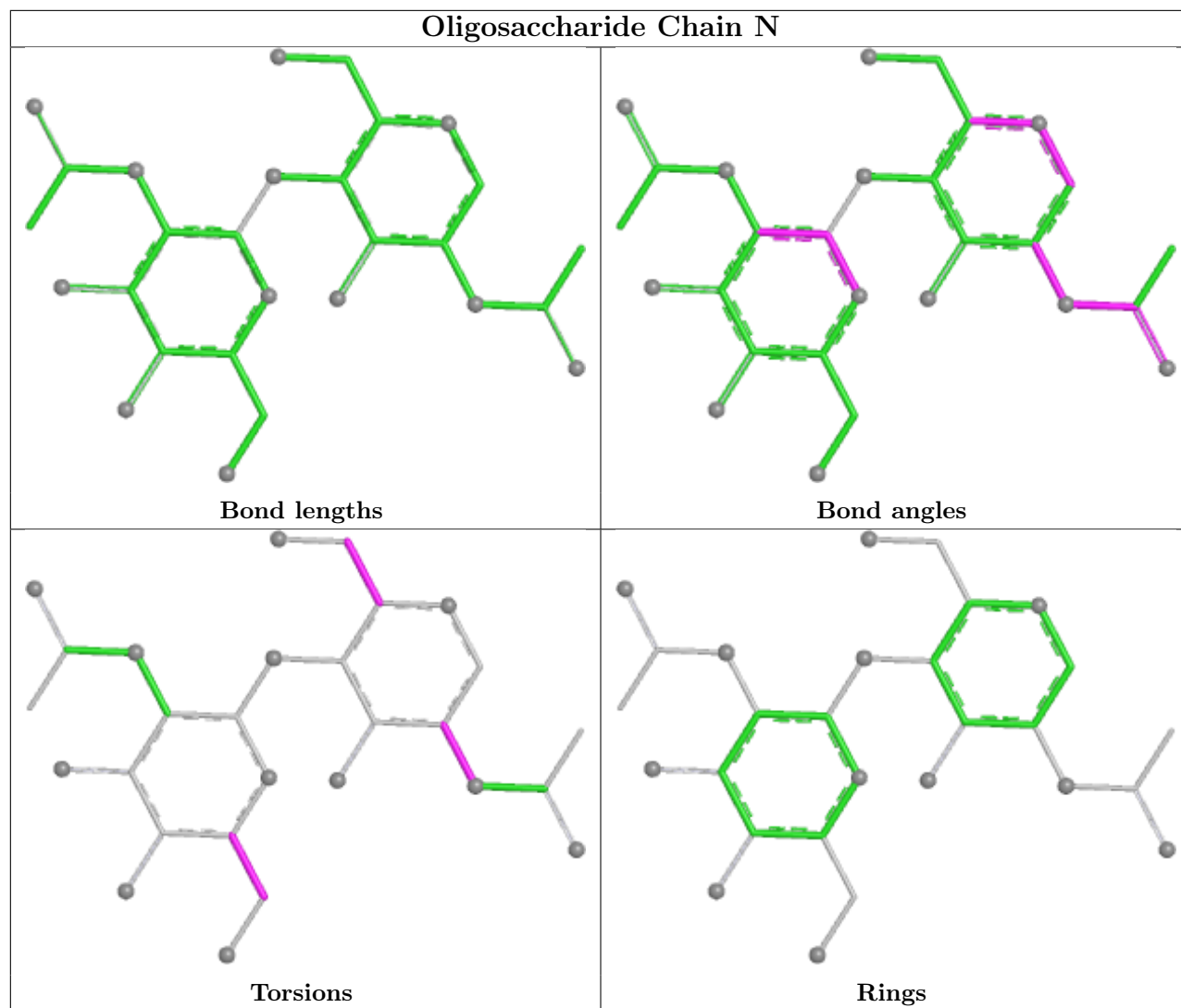


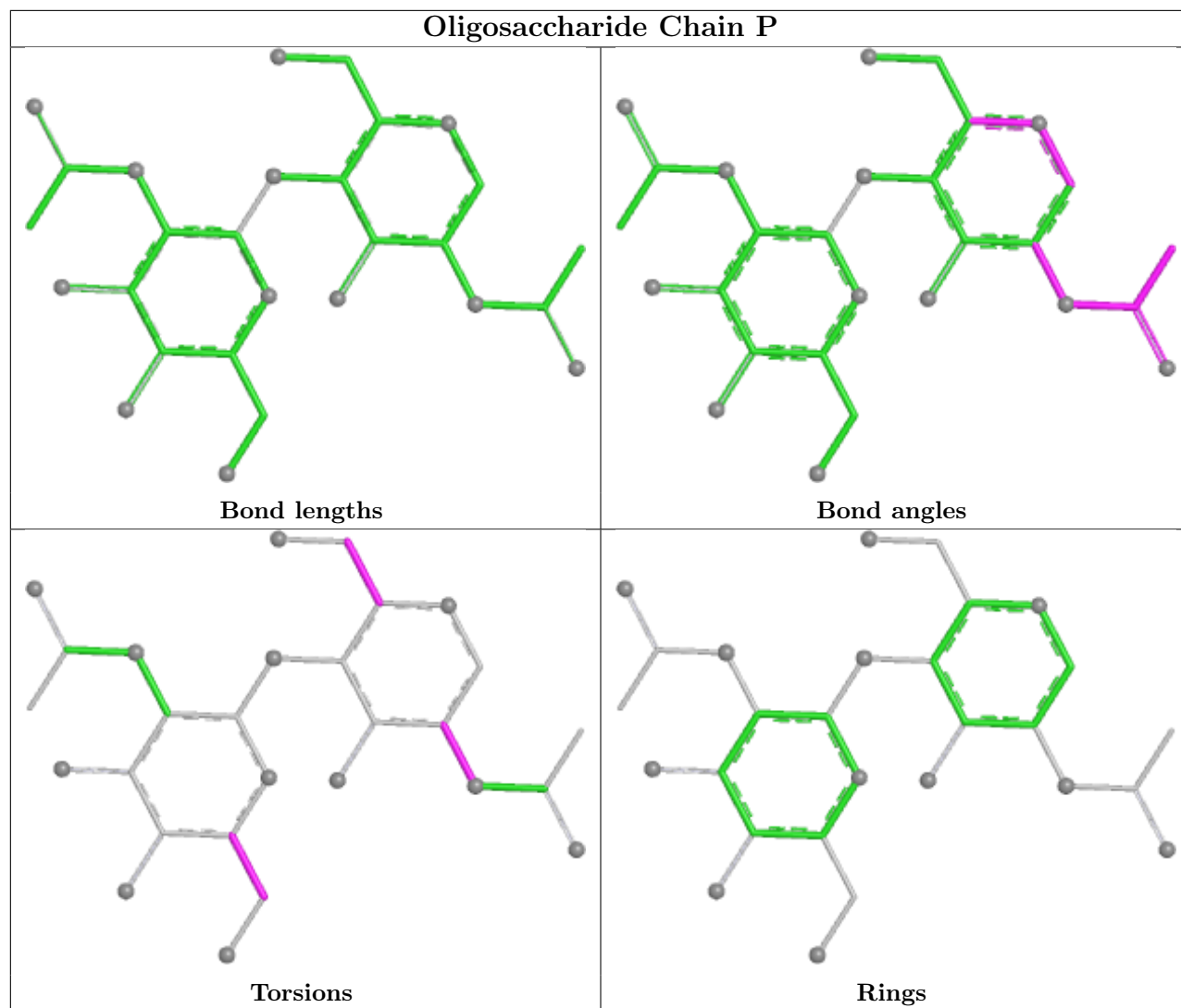


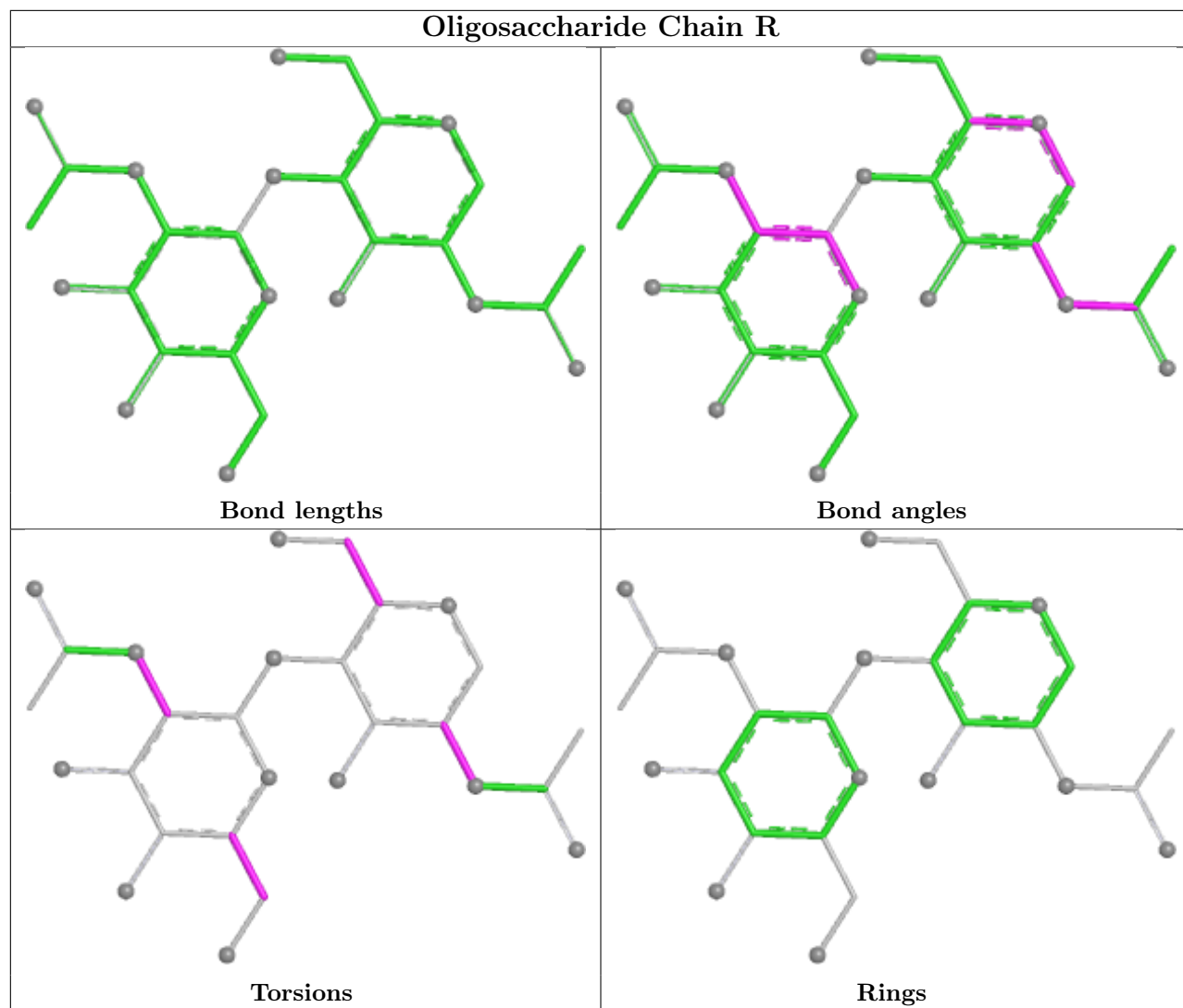


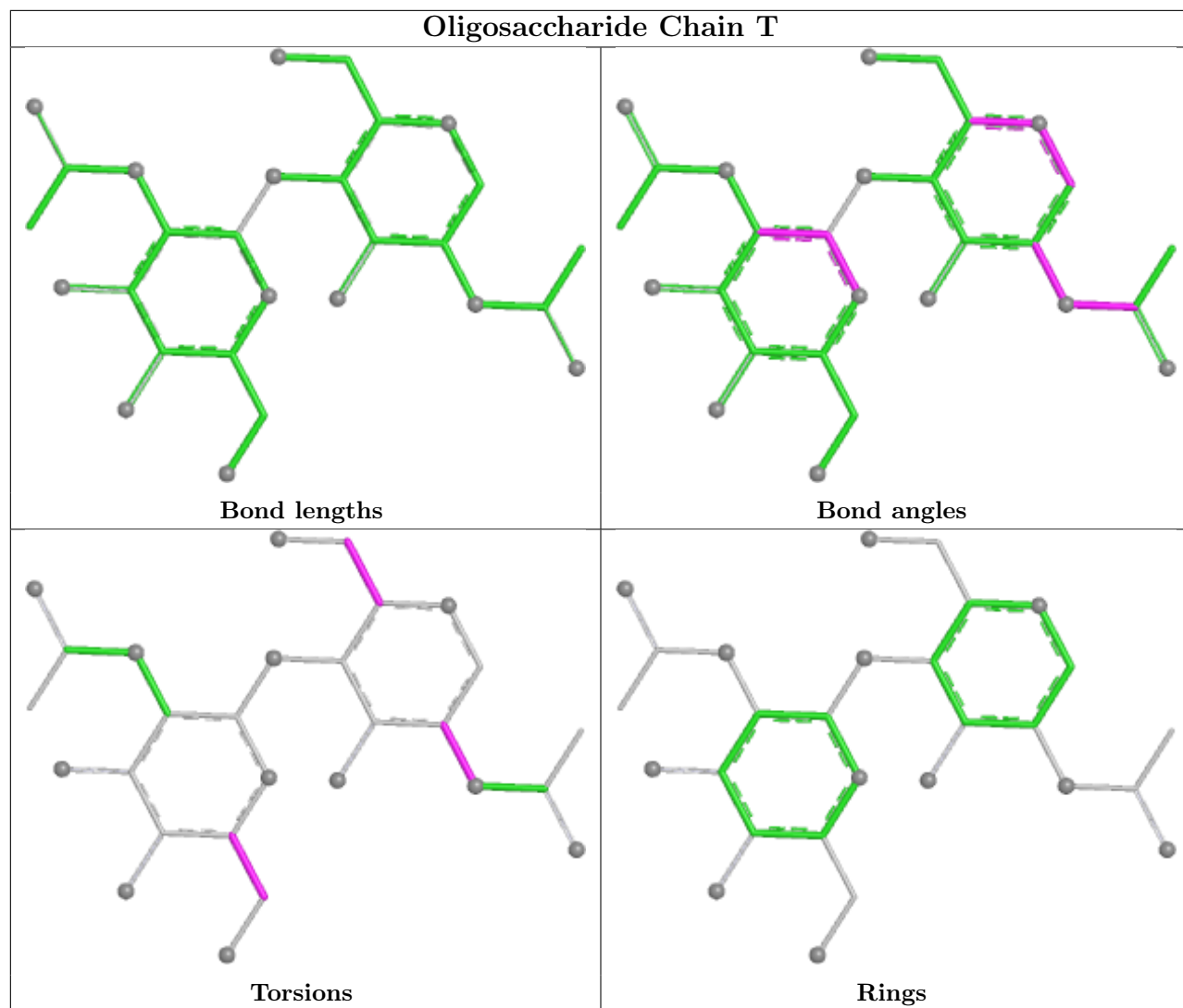


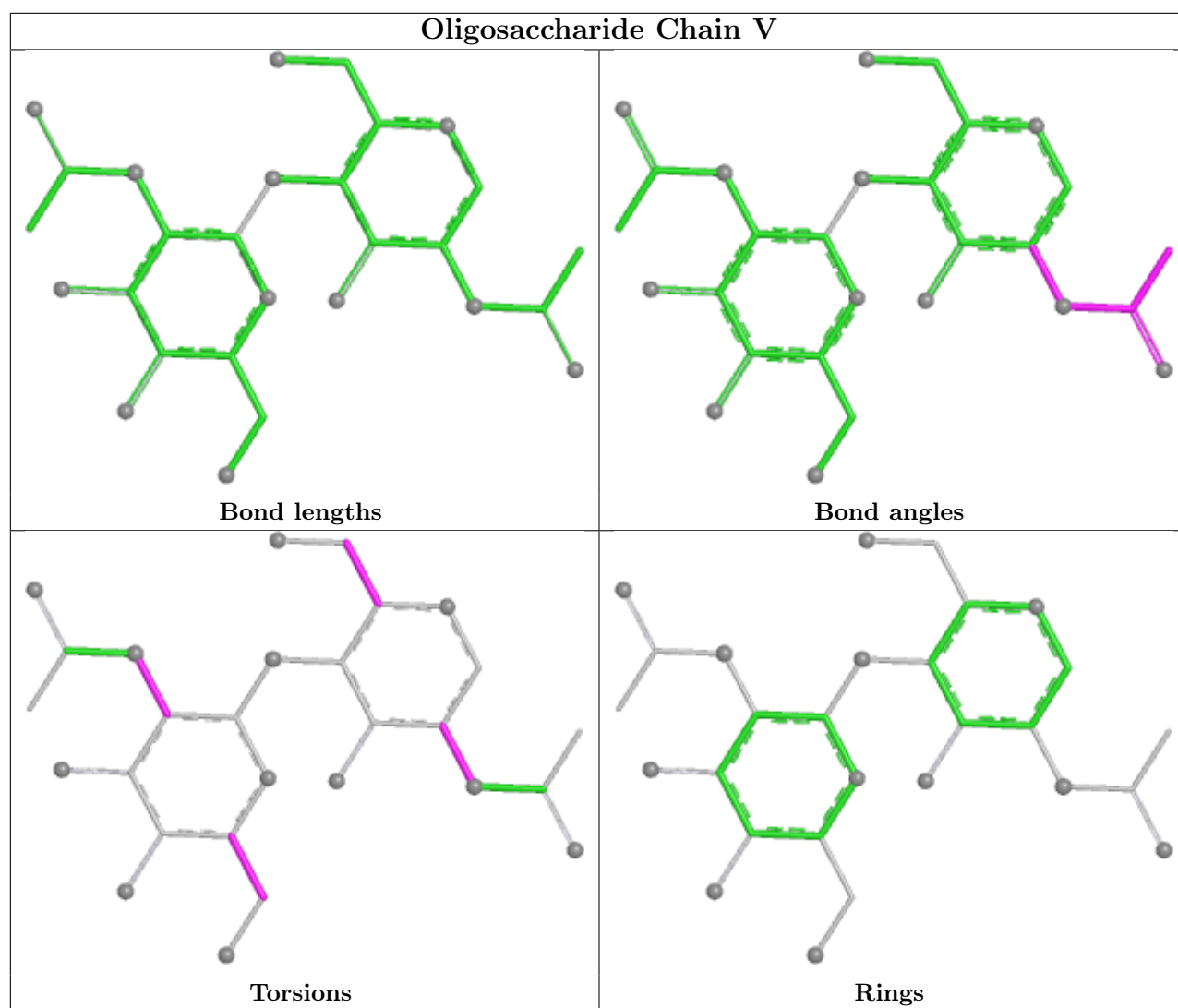


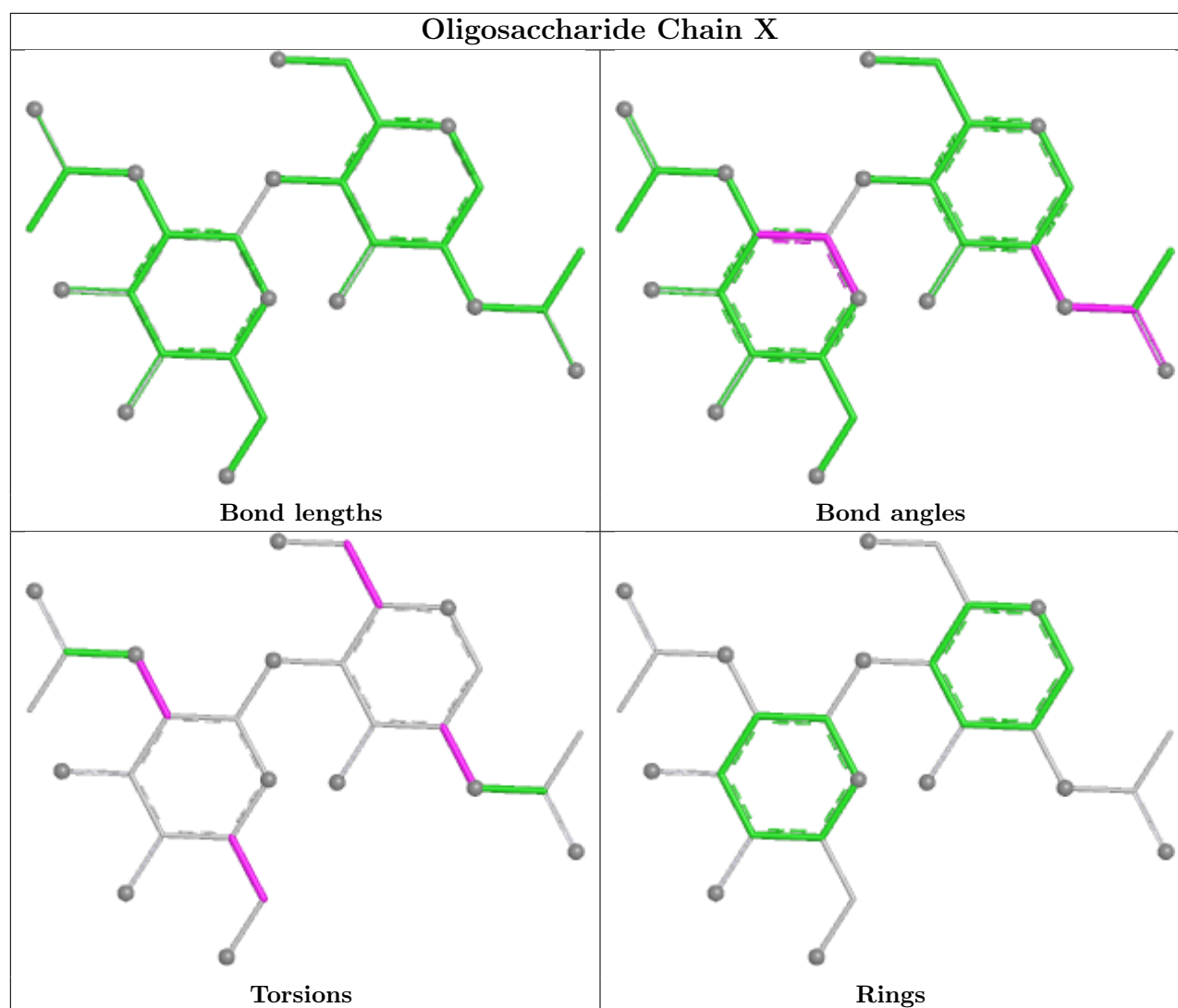












5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FRU	K	1000	-	11,12,12	0.64	0	10,18,18	0.53	0
8	EPE	J	1000	-	15,15,15	0.94	1 (6%)	19,20,20	1.07	1 (5%)
5	FRU	E	1000	-	11,12,12	0.57	0	10,18,18	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	I	2002	-	4,4,4	0.24	0	6,6,6	0.20	0
5	FRU	A	1000	-	11,12,12	0.67	0	10,18,18	0.45	0
6	SO4	E	2002	-	4,4,4	0.26	0	6,6,6	0.13	0
5	FRU	C	1000	-	11,12,12	0.54	0	10,18,18	0.52	0
6	SO4	A	2002	-	4,4,4	0.26	0	6,6,6	0.17	0
8	EPE	F	1000	-	15,15,15	0.90	1 (6%)	19,20,20	1.00	0
6	SO4	C	2002	-	4,4,4	0.25	0	6,6,6	0.16	0
8	EPE	H	1000	-	15,15,15	1.02	1 (6%)	19,20,20	1.07	1 (5%)
8	EPE	B	1000	-	15,15,15	0.91	1 (6%)	19,20,20	1.05	0
7	NAG	G	3000	1	14,14,15	0.44	0	17,19,21	1.04	1 (5%)
7	NAG	E	3000	1	14,14,15	0.44	0	17,19,21	0.86	0
8	EPE	D	1000	-	15,15,15	0.89	1 (6%)	19,20,20	1.06	1 (5%)
7	NAG	A	3000	1	14,14,15	0.50	0	17,19,21	1.09	2 (11%)
7	NAG	K	3000	1	14,14,15	0.44	0	17,19,21	1.03	1 (5%)
6	SO4	K	2002	-	4,4,4	0.25	0	6,6,6	0.10	0
7	NAG	C	3000	1	14,14,15	0.45	0	17,19,21	0.83	0
7	NAG	I	3000	1	14,14,15	0.41	0	17,19,21	0.92	0
5	FRU	G	1000	-	11,12,12	0.61	0	10,18,18	0.33	0
6	SO4	B	1001	-	4,4,4	0.25	0	6,6,6	0.11	0
8	EPE	L	1000	-	15,15,15	0.90	1 (6%)	19,20,20	1.07	2 (10%)
5	FRU	I	1000	-	11,12,12	0.56	0	10,18,18	0.53	0
6	SO4	G	2002	-	4,4,4	0.24	0	6,6,6	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FRU	C	1000	-	-	5/5/24/24	0/1/1/1
5	FRU	K	1000	-	-	5/5/24/24	0/1/1/1
7	NAG	C	3000	1	-	0/6/23/26	0/1/1/1
7	NAG	I	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	J	1000	-	-	2/9/19/19	0/1/1/1
5	FRU	G	1000	-	-	4/5/24/24	0/1/1/1
8	EPE	L	1000	-	-	2/9/19/19	0/1/1/1
8	EPE	B	1000	-	-	5/9/19/19	0/1/1/1
7	NAG	G	3000	1	-	0/6/23/26	0/1/1/1
5	FRU	E	1000	-	-	5/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FRU	I	1000	-	-	3/5/24/24	0/1/1/1
7	NAG	E	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	F	1000	-	-	2/9/19/19	0/1/1/1
8	EPE	D	1000	-	-	4/9/19/19	0/1/1/1
7	NAG	A	3000	1	-	2/6/23/26	0/1/1/1
7	NAG	K	3000	1	-	1/6/23/26	0/1/1/1
5	FRU	A	1000	-	-	5/5/24/24	0/1/1/1
8	EPE	H	1000	-	-	5/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1000	EPE	C10-S	3.54	1.82	1.77
8	J	1000	EPE	C10-S	3.14	1.82	1.77
8	L	1000	EPE	C10-S	3.06	1.81	1.77
8	B	1000	EPE	C10-S	3.02	1.81	1.77
8	F	1000	EPE	C10-S	2.96	1.81	1.77
8	D	1000	EPE	C10-S	2.93	1.81	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	3000	NAG	C1-O5-C5	3.03	116.24	112.19
7	A	3000	NAG	O5-C1-C2	-2.89	106.81	111.29
8	D	1000	EPE	O1S-S-C10	2.43	110.41	106.73
7	A	3000	NAG	C1-O5-C5	2.41	115.41	112.19
8	J	1000	EPE	O3S-S-C10	2.37	110.64	106.00
8	L	1000	EPE	O2S-S-C10	2.18	110.03	106.73
8	L	1000	EPE	O3S-S-C10	2.18	110.27	106.00
8	H	1000	EPE	O3S-S-C10	2.08	110.07	106.00
7	K	3000	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1000	FRU	O1-C1-C2-O2
5	C	1000	FRU	O1-C1-C2-O2
5	G	1000	FRU	O1-C1-C2-O2
5	I	1000	FRU	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	I	1000	FRU	O1-C1-C2-O2
5	K	1000	FRU	O1-C1-C2-O2
8	D	1000	EPE	S-C10-C9-N1
8	D	1000	EPE	C9-C10-S-O1S
5	K	1000	FRU	C4-C5-C6-O6
7	A	3000	NAG	O5-C5-C6-O6
7	A	3000	NAG	C4-C5-C6-O6
5	I	1000	FRU	O1-C1-C2-O5
8	B	1000	EPE	C9-C10-S-O3S
8	D	1000	EPE	C9-C10-S-O3S
8	J	1000	EPE	N4-C7-C8-O8
5	A	1000	FRU	C4-C5-C6-O6
5	K	1000	FRU	O5-C5-C6-O6
8	L	1000	EPE	N4-C7-C8-O8
5	C	1000	FRU	O1-C1-C2-C3
5	A	1000	FRU	O5-C5-C6-O6
8	B	1000	EPE	N4-C7-C8-O8
5	E	1000	FRU	C4-C5-C6-O6
8	H	1000	EPE	N4-C7-C8-O8
5	C	1000	FRU	C4-C5-C6-O6
5	A	1000	FRU	O1-C1-C2-C3
5	E	1000	FRU	O1-C1-C2-C3
5	G	1000	FRU	O1-C1-C2-C3
5	K	1000	FRU	O1-C1-C2-C3
8	H	1000	EPE	C9-C10-S-O3S
8	B	1000	EPE	C9-C10-S-O1S
8	B	1000	EPE	C9-C10-S-O2S
8	D	1000	EPE	C9-C10-S-O2S
8	H	1000	EPE	C9-C10-S-O1S
8	H	1000	EPE	C9-C10-S-O2S
8	B	1000	EPE	S-C10-C9-N1
8	F	1000	EPE	S-C10-C9-N1
8	H	1000	EPE	S-C10-C9-N1
8	J	1000	EPE	S-C10-C9-N1
8	L	1000	EPE	S-C10-C9-N1
5	C	1000	FRU	O1-C1-C2-O5
5	E	1000	FRU	O1-C1-C2-O2
5	G	1000	FRU	C4-C5-C6-O6
5	A	1000	FRU	O1-C1-C2-O5
5	E	1000	FRU	O5-C5-C6-O6
5	G	1000	FRU	O1-C1-C2-O5
8	F	1000	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
5	E	1000	FRU	O1-C1-C2-O5
5	K	1000	FRU	O1-C1-C2-O5
5	C	1000	FRU	O5-C5-C6-O6
7	K	3000	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1000	FRU	1	0
8	J	1000	EPE	2	0
6	I	2002	SO4	1	0
5	A	1000	FRU	1	0
8	F	1000	EPE	3	0
8	H	1000	EPE	2	0
8	B	1000	EPE	3	0
8	D	1000	EPE	2	0
8	L	1000	EPE	2	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 [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	537/537 (100%)	-1.67	0 100 100	14, 27, 43, 56	0
1	C	537/537 (100%)	-1.66	0 100 100	17, 31, 45, 60	0
1	E	537/537 (100%)	-1.64	0 100 100	16, 30, 45, 61	0
1	G	537/537 (100%)	-1.65	0 100 100	17, 31, 46, 59	0
1	I	537/537 (100%)	-1.66	0 100 100	15, 29, 46, 59	0
1	K	537/537 (100%)	-1.63	0 100 100	19, 33, 51, 64	0
2	B	146/149 (97%)	-1.59	0 100 100	19, 32, 55, 62	0
2	D	146/149 (97%)	-1.58	0 100 100	20, 33, 50, 55	0
2	F	146/149 (97%)	-1.60	0 100 100	20, 33, 48, 57	0
2	H	146/149 (97%)	-1.56	0 100 100	22, 31, 51, 56	0
2	J	146/149 (97%)	-1.60	0 100 100	18, 27, 48, 55	0
2	L	146/149 (97%)	-1.60	0 100 100	18, 31, 48, 53	0
All	All	4098/4116 (99%)	-1.64	0 100 100	14, 30, 47, 64	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

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

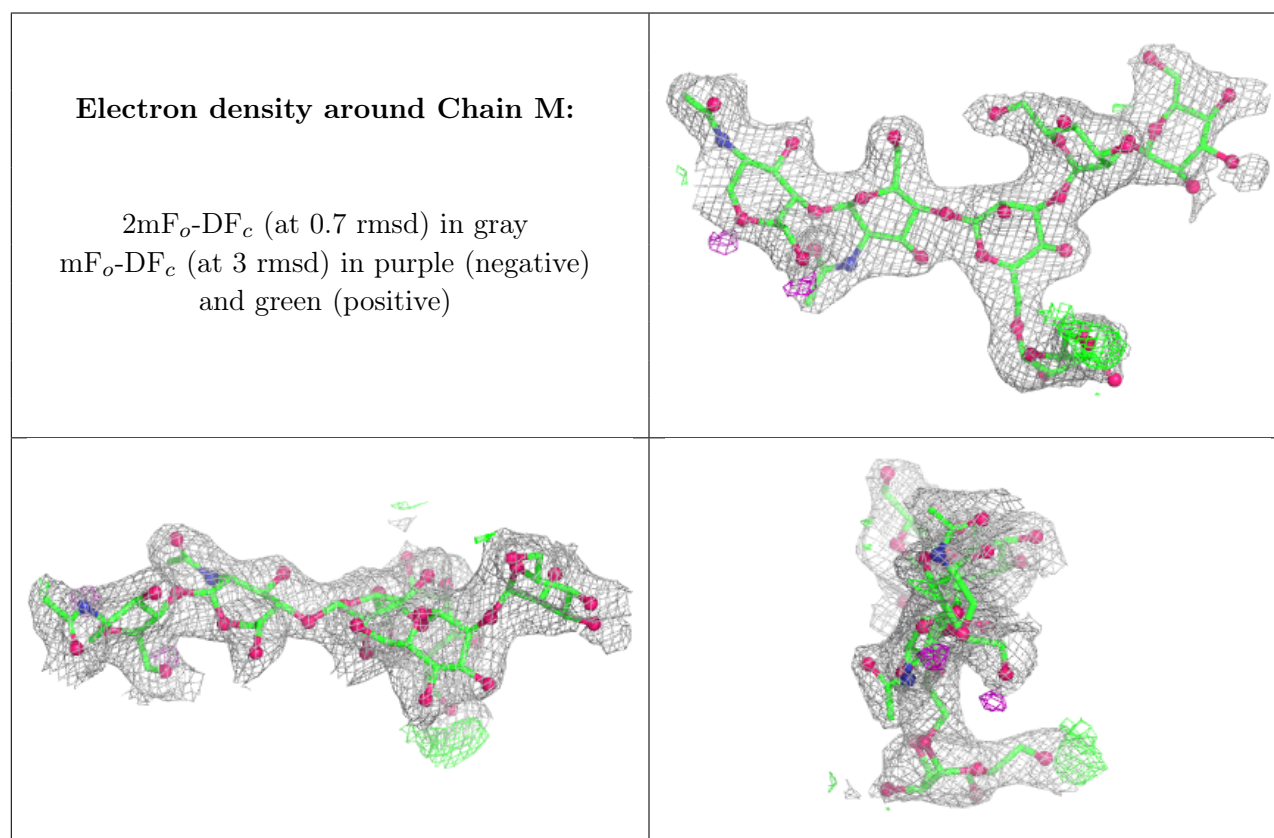
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	Q	5	11/12	0.95	0.06	51,52,52,53	0
4	NAG	V	2	14/15	0.96	0.05	41,42,45,45	0
3	BMA	S	6	11/12	0.97	0.05	40,41,42,43	0
3	BMA	W	6	11/12	0.97	0.05	42,43,44,45	0
4	NAG	P	2	14/15	0.97	0.04	42,44,45,46	0
4	NAG	R	2	14/15	0.97	0.06	44,45,46,46	0
4	NAG	T	2	14/15	0.97	0.04	39,41,43,43	0
3	BMA	Q	6	11/12	0.97	0.05	47,48,49,49	0
4	NAG	X	2	14/15	0.97	0.05	43,44,46,46	0
3	BMA	O	6	11/12	0.98	0.04	43,45,45,46	0
4	NAG	N	2	14/15	0.98	0.04	40,42,43,43	0
3	MAN	S	5	11/12	0.98	0.04	41,42,43,43	0
3	BMA	M	6	11/12	0.98	0.04	37,39,40,40	0
3	MAN	U	5	11/12	0.98	0.04	40,42,43,43	0
3	BMA	U	6	11/12	0.98	0.04	37,38,39,40	0
3	MAN	W	5	11/12	0.98	0.05	44,46,47,47	0
3	NAG	S	2	14/15	0.99	0.02	25,26,28,30	0
3	BMA	S	3	11/12	0.99	0.02	33,35,37,38	0
3	MAN	S	4	11/12	0.99	0.02	38,38,39,40	0
3	NAG	M	1	14/15	0.99	0.02	15,18,21,21	0
3	NAG	O	1	14/15	0.99	0.03	21,22,25,26	0
3	BMA	U	3	11/12	0.99	0.02	30,32,34,36	0
3	MAN	U	4	11/12	0.99	0.03	34,35,36,38	0
3	BMA	O	3	11/12	0.99	0.02	35,37,39,41	0
3	MAN	O	4	11/12	0.99	0.02	38,39,39,42	0
3	NAG	W	1	14/15	0.99	0.03	20,22,24,24	0
3	NAG	W	2	14/15	0.99	0.03	24,26,28,31	0
3	BMA	W	3	11/12	0.99	0.03	33,35,37,39	0
3	MAN	W	4	11/12	0.99	0.03	39,40,41,42	0
3	MAN	O	5	11/12	0.99	0.03	44,45,45,46	0
3	NAG	M	2	14/15	0.99	0.03	22,23,25,28	0
4	NAG	N	1	14/15	0.99	0.03	32,36,37,38	0
3	NAG	Q	1	14/15	0.99	0.03	23,25,27,31	0
4	NAG	P	1	14/15	0.99	0.03	33,36,38,40	0
3	NAG	Q	2	14/15	0.99	0.04	33,35,37,39	0
4	NAG	R	1	14/15	0.99	0.03	34,37,40,41	0
3	BMA	Q	3	11/12	0.99	0.03	41,43,45,45	0
3	MAN	Q	4	11/12	0.99	0.04	46,47,48,49	0
4	NAG	V	1	14/15	0.99	0.04	33,36,38,39	0
3	MAN	M	4	11/12	0.99	0.03	35,36,36,39	0
4	NAG	X	1	14/15	0.99	0.03	32,35,38,39	0
3	MAN	M	5	11/12	0.99	0.03	41,42,43,43	0
4	NAG	T	1	14/15	1.00	0.02	31,34,37,37	0

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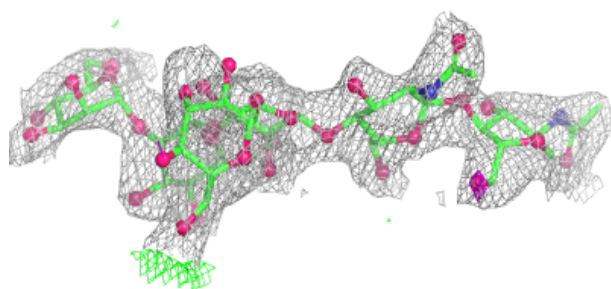
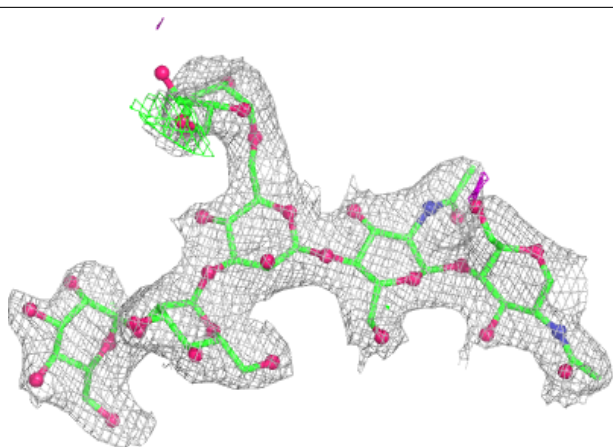
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	M	3	11/12	1.00	0.01	30,32,34,35	0
3	NAG	O	2	14/15	1.00	0.02	27,28,30,33	0
3	NAG	U	1	14/15	1.00	0.03	21,22,23,24	0
3	NAG	U	2	14/15	1.00	0.04	24,26,27,28	0
3	NAG	S	1	14/15	1.00	0.02	21,22,24,24	0

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

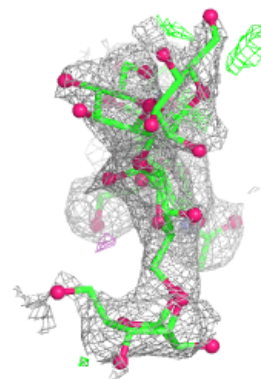
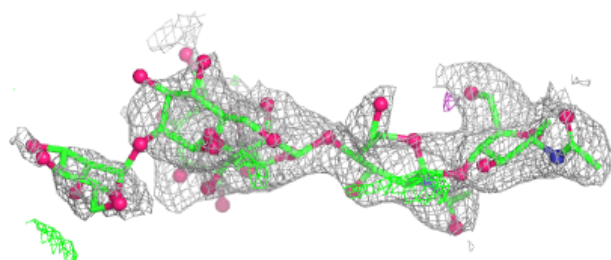
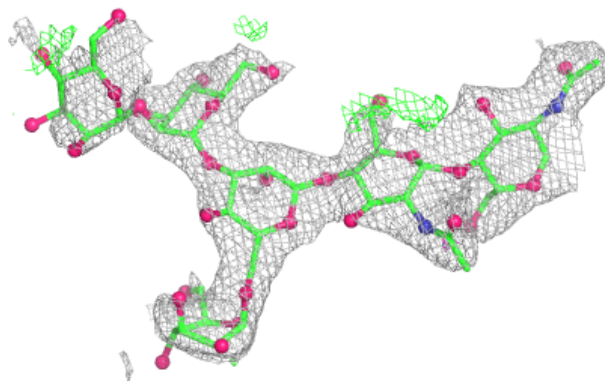


Electron density around Chain O:

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

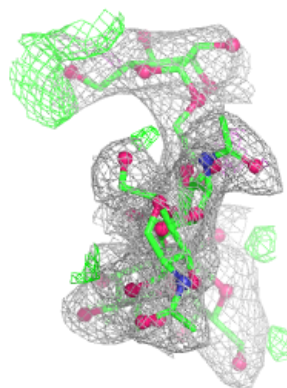
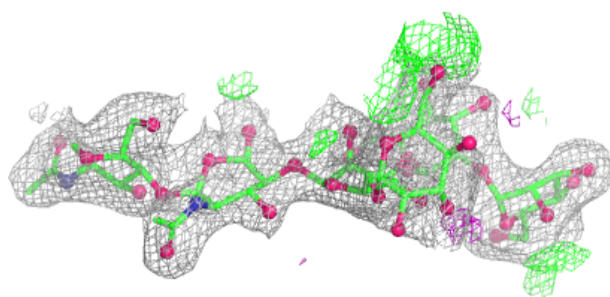
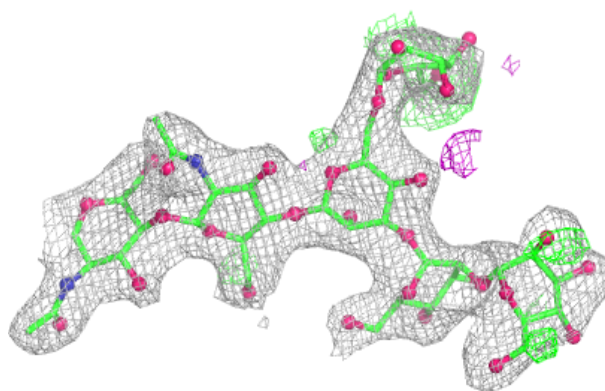
**Electron density around Chain Q:**

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

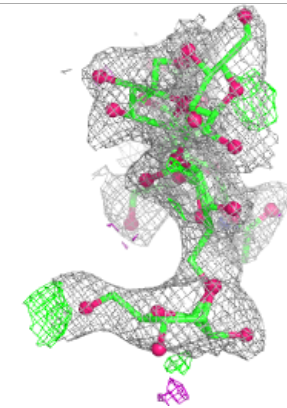
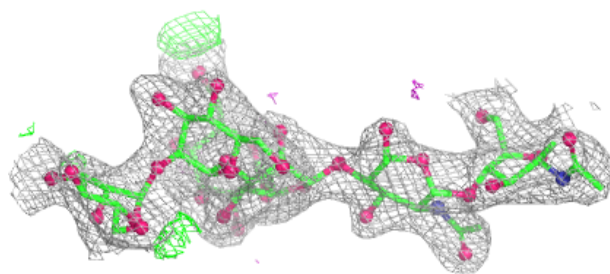
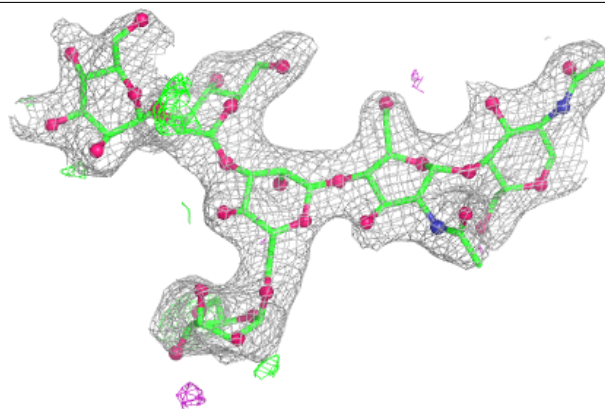


Electron density around Chain S:

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

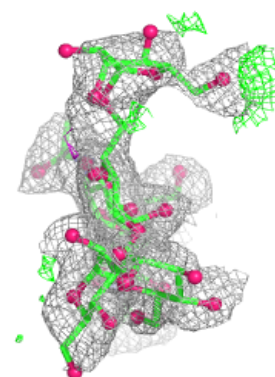
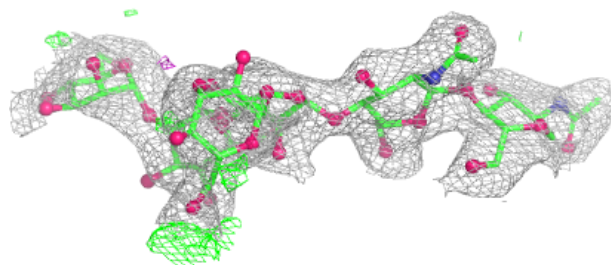
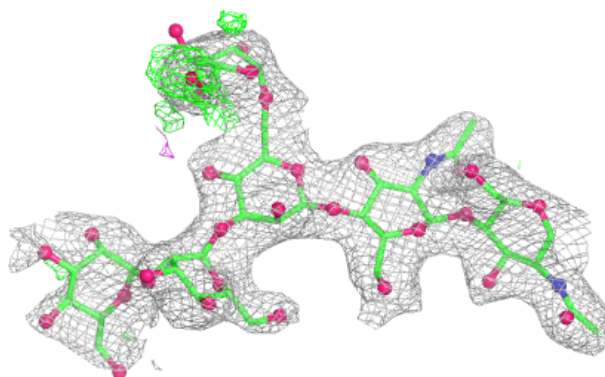
**Electron density around Chain U:**

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

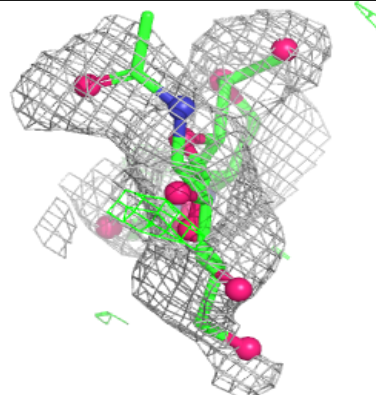
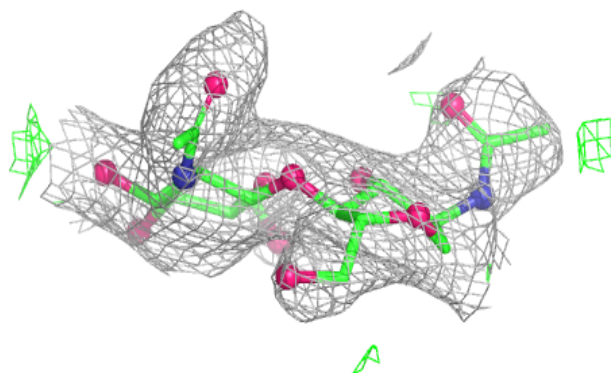
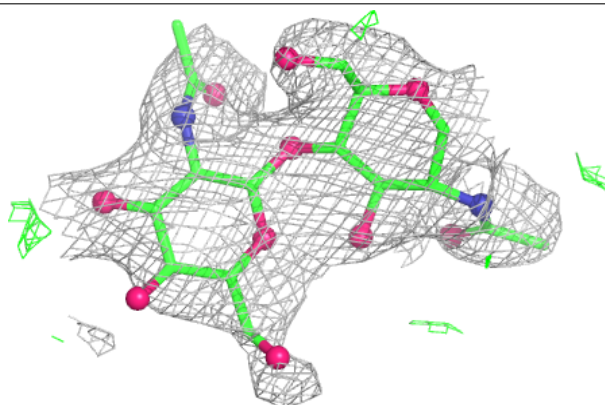


Electron density around Chain W:

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

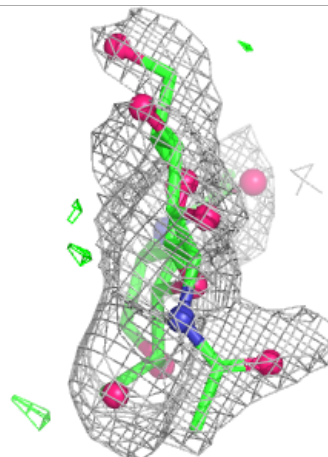
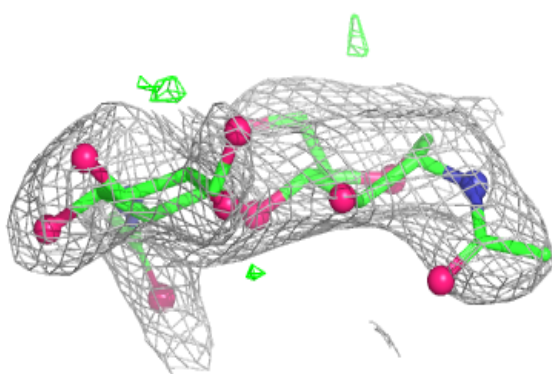
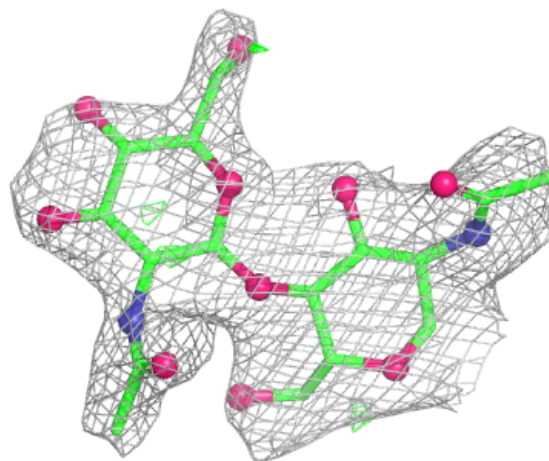
**Electron density around Chain N:**

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



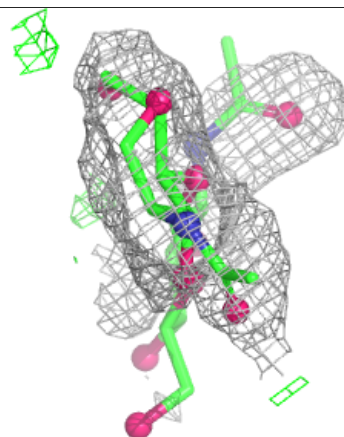
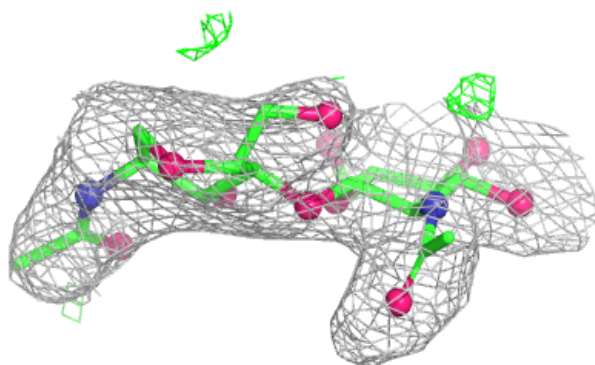
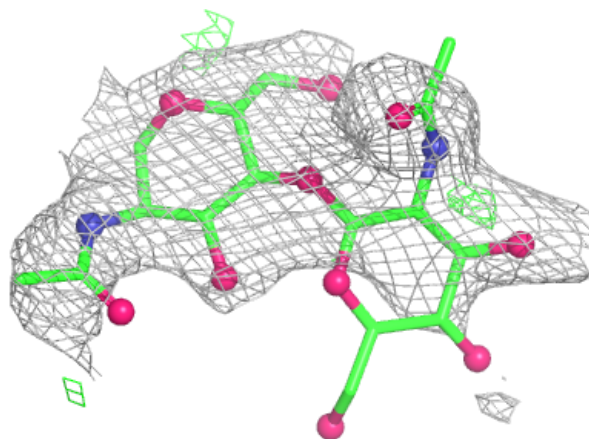
Electron density around Chain P:

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



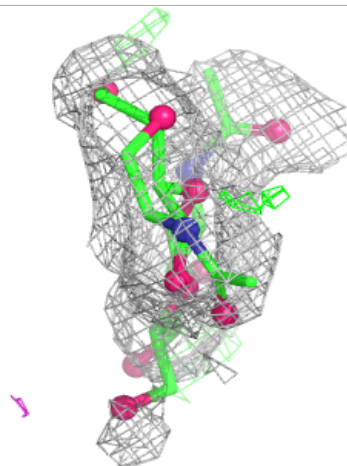
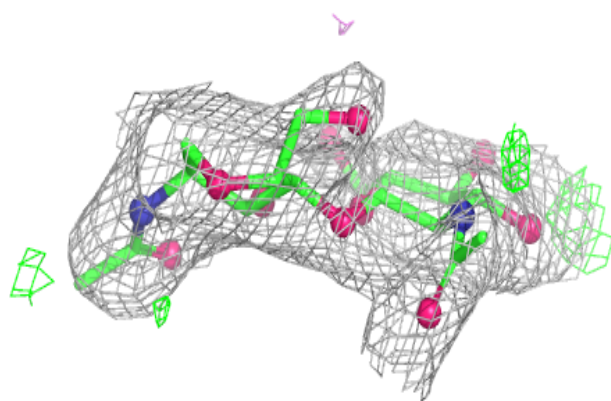
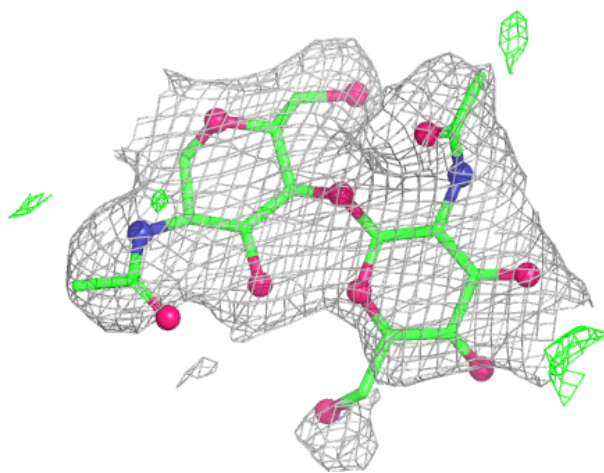
Electron density around Chain R:

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



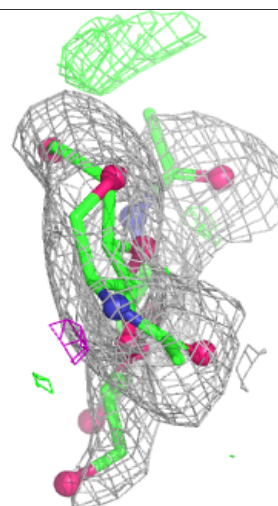
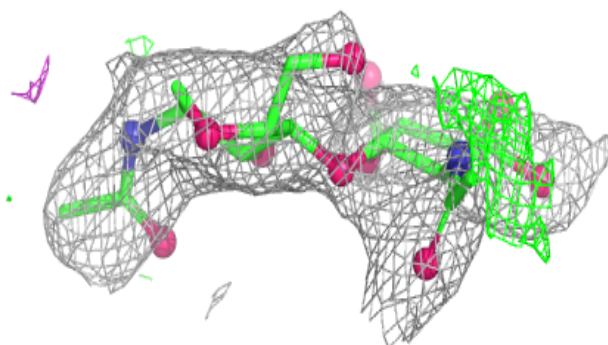
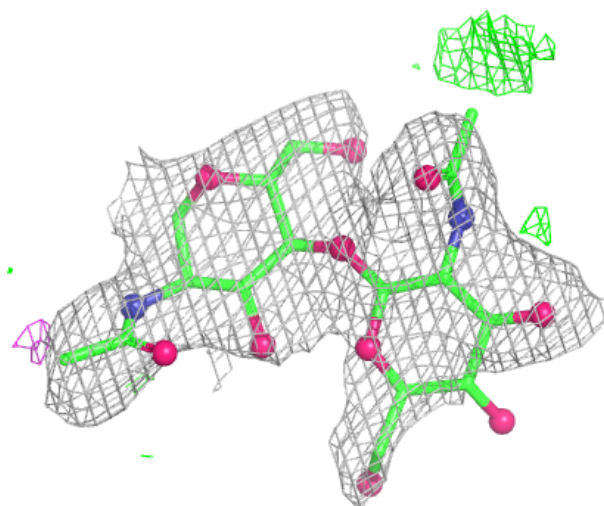
Electron density around Chain T:

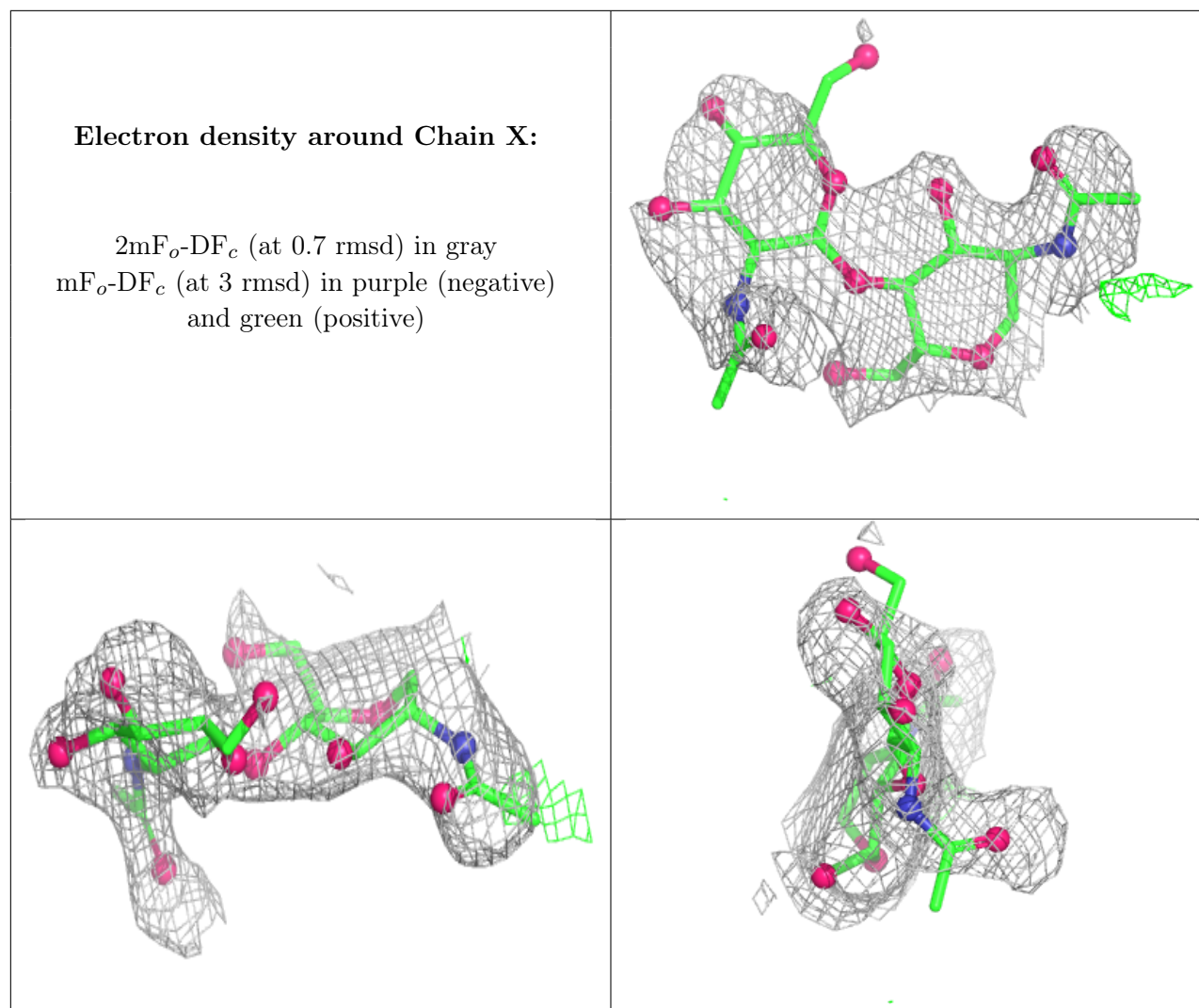
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain V:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	NAG	C	3000	14/15	0.98	0.04	33,35,38,39	0
7	NAG	E	3000	14/15	0.98	0.04	33,36,37,37	0
8	EPE	D	1000	15/15	0.98	0.06	43,45,51,52	0
6	SO4	E	2002	5/5	0.99	0.07	56,57,57,57	0
6	SO4	G	2002	5/5	0.99	0.04	63,64,64,64	0
6	SO4	I	2002	5/5	0.99	0.05	49,49,50,50	0
6	SO4	K	2002	5/5	0.99	0.05	51,51,52,52	0
7	NAG	A	3000	14/15	0.99	0.03	34,37,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FRU	K	1000	12/12	0.99	0.03	22,23,23,23	0
6	SO4	A	2002	5/5	0.99	0.06	43,43,44,44	0
7	NAG	G	3000	14/15	0.99	0.03	32,35,37,37	0
7	NAG	I	3000	14/15	0.99	0.03	30,33,34,34	0
7	NAG	K	3000	14/15	0.99	0.03	33,35,36,36	0
8	EPE	B	1000	15/15	0.99	0.04	34,37,44,44	0
6	SO4	B	1001	5/5	0.99	0.04	45,45,45,45	0
8	EPE	F	1000	15/15	0.99	0.05	43,46,51,52	0
8	EPE	H	1000	15/15	0.99	0.04	46,47,52,52	0
8	EPE	J	1000	15/15	0.99	0.05	40,42,48,48	0
8	EPE	L	1000	15/15	0.99	0.05	45,46,50,50	0
5	FRU	E	1000	12/12	1.00	0.02	21,22,22,23	0
6	SO4	C	2002	5/5	1.00	0.04	54,54,55,55	0
5	FRU	G	1000	12/12	1.00	0.03	18,21,22,22	0
5	FRU	I	1000	12/12	1.00	0.03	22,23,24,24	0
5	FRU	A	1000	12/12	1.00	0.02	18,19,19,20	0
5	FRU	C	1000	12/12	1.00	0.03	20,20,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.