



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:27 AM UTC

PDB ID : 4MIV / pdb_00004miv
Title : Crystal Structure of Sulfamidase, Crystal Form L
Authors : Sidhu, N.S.; Uson, I.; Schreiber, K.; Proepper, K.; Becker, S.; Sheldrick, G.M.;
Gaertner, J.; Kraetzner, R.; Steinfeld, R.
Deposited on : 2013-09-02
Resolution : 2.40 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

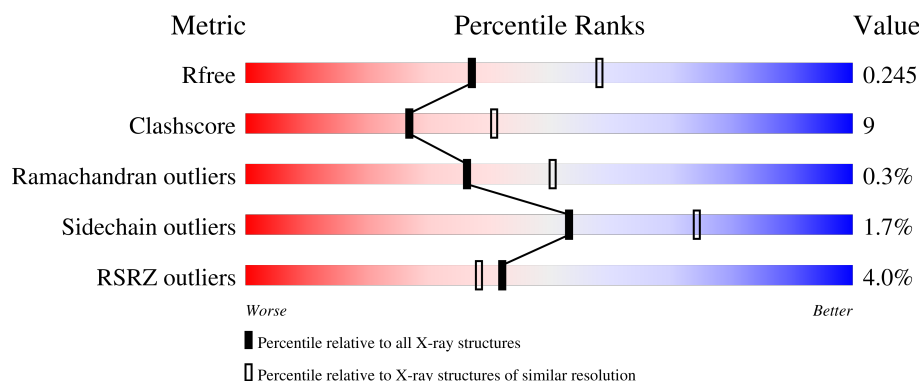
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	510	80% 14% • 5%
1	B	510	78% 15% • 6%
1	C	510	80% 14% • 5%
1	D	510	80% 13% • 6%
1	E	510	6% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	F	510	 4% 79% 14% • 6%
1	G	510	 5% 80% 13% • 6%
1	H	510	 12% 79% 14% • 5%
2	I	2	 100%
2	J	2	 100%
2	K	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 100%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 50% 50%
2	R	2	 50% 50%
2	S	2	 100%
2	T	2	 100%
2	U	2	 50% 50%
2	V	2	 50% 50%
2	W	2	 100%
2	X	2	 50% 50%
2	Y	2	 100%
2	Z	2	 50% 50%
2	a	2	 50% 50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31167 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 N-sulphoglucosamine sulphonydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	P	S	0	2	0
			3869	2478	670	708	1	12			
1	B	481	Total	C	N	O	P	S	0	2	0
			3860	2467	676	705	1	11			
1	C	484	Total	C	N	O	P	S	0	0	0
			3854	2467	670	705	1	11			
1	D	480	Total	C	N	O	P	S	0	1	0
			3835	2454	671	698	1	11			
1	E	483	Total	C	N	O	P	S	0	1	0
			3607	2308	617	670	1	11			
1	F	478	Total	C	N	O	P	S	0	0	0
			3703	2373	636	682	1	11			
1	G	479	Total	C	N	O	S		0	1	0
			3685	2362	641	671	11				
1	H	482	Total	C	N	O	S		0	0	0
			3617	2317	627	663	10				

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	FGP	CYS	modified residue	UNP P51688
A	503	ARG	-	expression tag	UNP P51688
A	504	SER	-	expression tag	UNP P51688
A	505	HIS	-	expression tag	UNP P51688
A	506	HIS	-	expression tag	UNP P51688
A	507	HIS	-	expression tag	UNP P51688
A	508	HIS	-	expression tag	UNP P51688
A	509	HIS	-	expression tag	UNP P51688
A	510	HIS	-	expression tag	UNP P51688
B	70	FGP	CYS	modified residue	UNP P51688
B	503	ARG	-	expression tag	UNP P51688
B	504	SER	-	expression tag	UNP P51688
B	505	HIS	-	expression tag	UNP P51688

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Chain	Residue	Modelled	Actual	Comment	Reference
B	506	HIS	-	expression tag	UNP P51688
B	507	HIS	-	expression tag	UNP P51688
B	508	HIS	-	expression tag	UNP P51688
B	509	HIS	-	expression tag	UNP P51688
B	510	HIS	-	expression tag	UNP P51688
C	70	FGP	CYS	modified residue	UNP P51688
C	503	ARG	-	expression tag	UNP P51688
C	504	SER	-	expression tag	UNP P51688
C	505	HIS	-	expression tag	UNP P51688
C	506	HIS	-	expression tag	UNP P51688
C	507	HIS	-	expression tag	UNP P51688
C	508	HIS	-	expression tag	UNP P51688
C	509	HIS	-	expression tag	UNP P51688
C	510	HIS	-	expression tag	UNP P51688
D	70	FGP	CYS	modified residue	UNP P51688
D	503	ARG	-	expression tag	UNP P51688
D	504	SER	-	expression tag	UNP P51688
D	505	HIS	-	expression tag	UNP P51688
D	506	HIS	-	expression tag	UNP P51688
D	507	HIS	-	expression tag	UNP P51688
D	508	HIS	-	expression tag	UNP P51688
D	509	HIS	-	expression tag	UNP P51688
D	510	HIS	-	expression tag	UNP P51688
E	70	FGP	CYS	modified residue	UNP P51688
E	503	ARG	-	expression tag	UNP P51688
E	504	SER	-	expression tag	UNP P51688
E	505	HIS	-	expression tag	UNP P51688
E	506	HIS	-	expression tag	UNP P51688
E	507	HIS	-	expression tag	UNP P51688
E	508	HIS	-	expression tag	UNP P51688
E	509	HIS	-	expression tag	UNP P51688
E	510	HIS	-	expression tag	UNP P51688
F	70	FGP	CYS	modified residue	UNP P51688
F	503	ARG	-	expression tag	UNP P51688
F	504	SER	-	expression tag	UNP P51688
F	505	HIS	-	expression tag	UNP P51688
F	506	HIS	-	expression tag	UNP P51688
F	507	HIS	-	expression tag	UNP P51688
F	508	HIS	-	expression tag	UNP P51688
F	509	HIS	-	expression tag	UNP P51688
F	510	HIS	-	expression tag	UNP P51688
G	70	FGP	CYS	modified residue	UNP P51688

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Chain	Residue	Modelled	Actual	Comment	Reference
G	503	ARG	-	expression tag	UNP P51688
G	504	SER	-	expression tag	UNP P51688
G	505	HIS	-	expression tag	UNP P51688
G	506	HIS	-	expression tag	UNP P51688
G	507	HIS	-	expression tag	UNP P51688
G	508	HIS	-	expression tag	UNP P51688
G	509	HIS	-	expression tag	UNP P51688
G	510	HIS	-	expression tag	UNP P51688
H	70	FGP	CYS	modified residue	UNP P51688
H	503	ARG	-	expression tag	UNP P51688
H	504	SER	-	expression tag	UNP P51688
H	505	HIS	-	expression tag	UNP P51688
H	506	HIS	-	expression tag	UNP P51688
H	507	HIS	-	expression tag	UNP P51688
H	508	HIS	-	expression tag	UNP P51688
H	509	HIS	-	expression tag	UNP P51688
H	510	HIS	-	expression tag	UNP P51688

- Molecule 2 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
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			27	16	2	9			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			27	16	2	9			
2	P	2	Total	C	N	O	0	0	0
			27	16	2	9			

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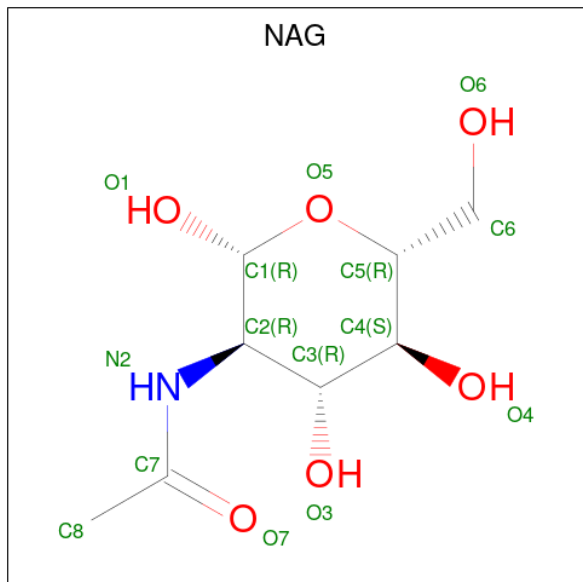
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Y	2	Total	C	N	O	0	0	0
			25	14	2	9			
2	Z	2	Total	C	N	O	0	0	0
			27	16	2	9			
2	a	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			10	6	1	3		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

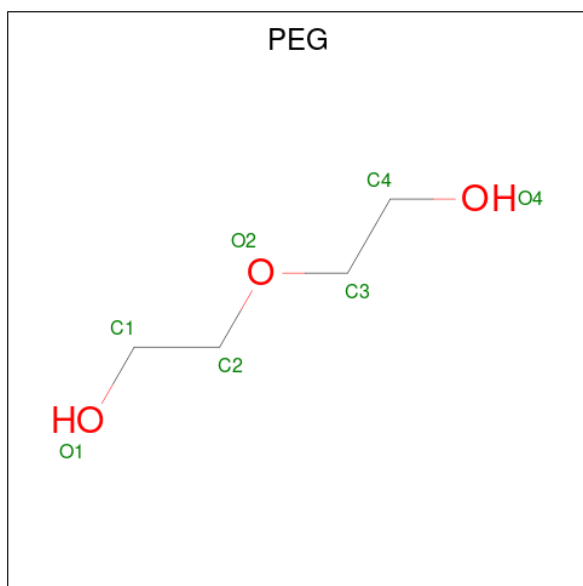
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	97	Total	O	0	0
			97	97		
7	B	112	Total	O	0	0
			112	112		
7	C	87	Total	O	0	0
			87	87		
7	D	107	Total	O	0	0
			107	107		
7	E	8	Total	O	0	0
			8	8		
7	F	26	Total	O	0	0
			26	26		
7	G	29	Total	O	0	0
			29	29		

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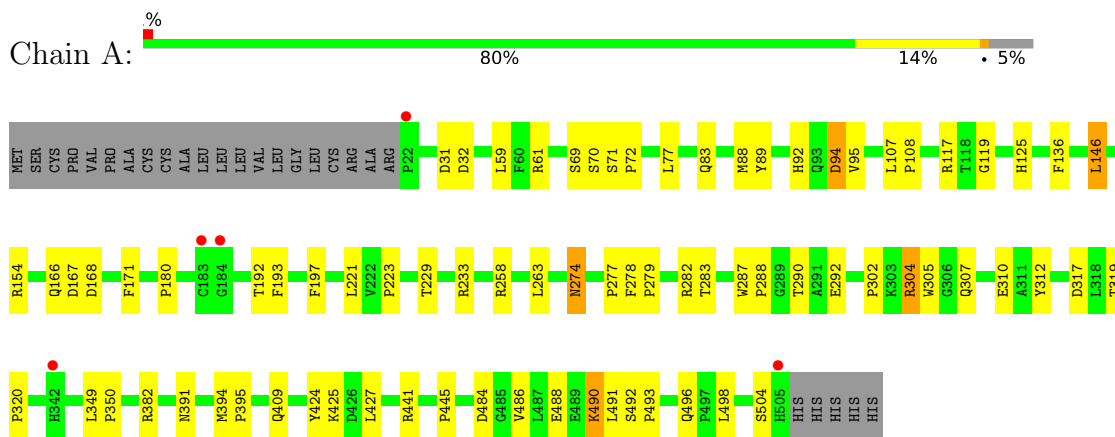
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	9	Total	O	0	0
			9	9		

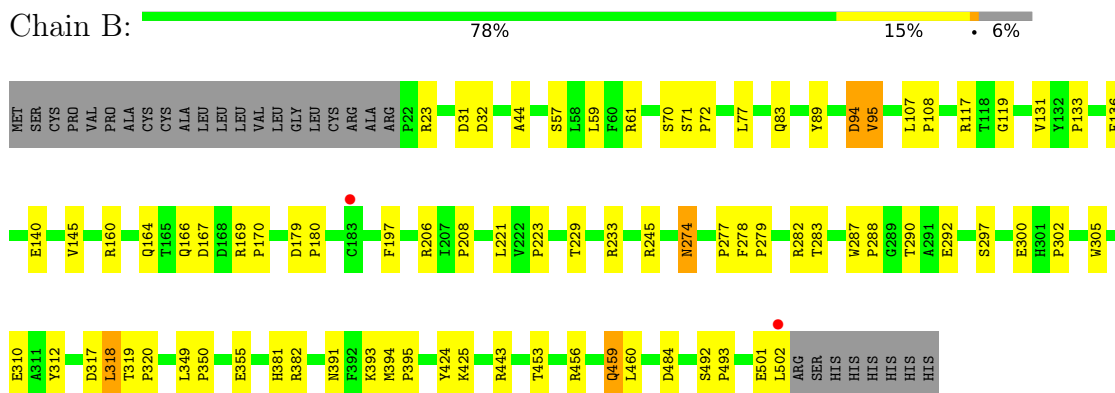
3 Residue-property plots [i](#)

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.

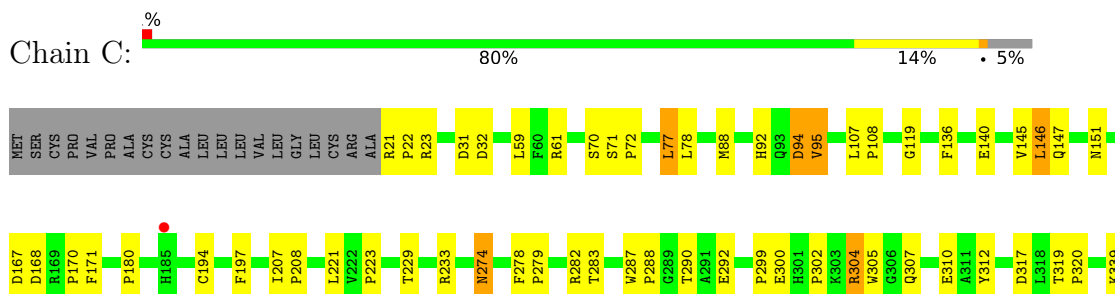
- Molecule 1: N-sulphoglucosamine sulphohydrolase



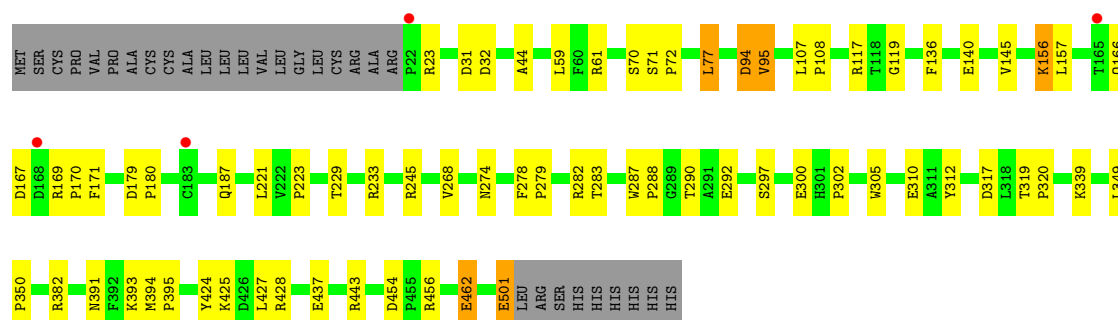
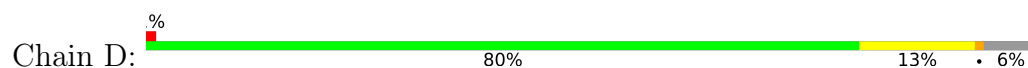
- Molecule 1: N-sulphoglucosamine sulphohydrolase



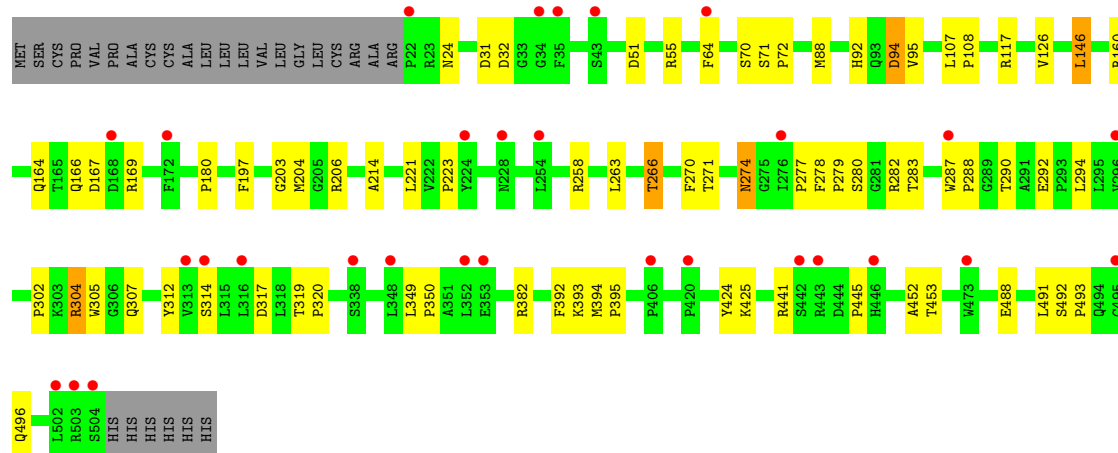
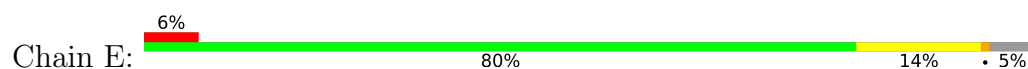
- Molecule 1: N-sulphoglucosamine sulphohydrolase



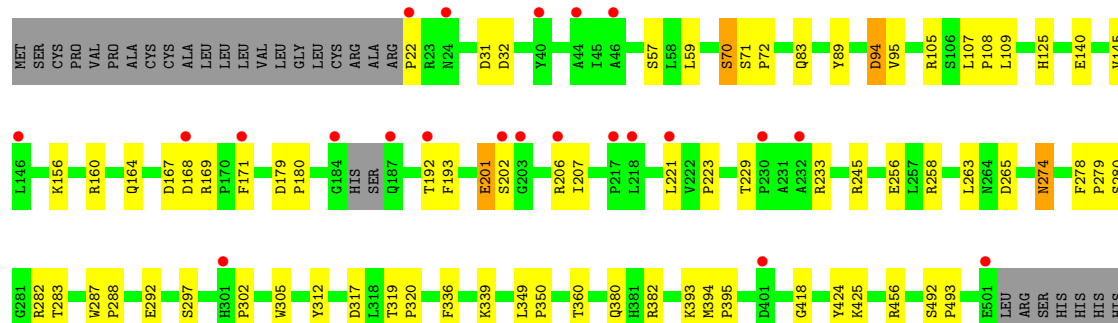
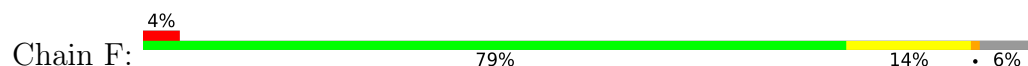
- Molecule 1: N-sulphoglucosamine sulphonydrolase



- Molecule 1: N-sulphoglucosamine sulphonydrolase



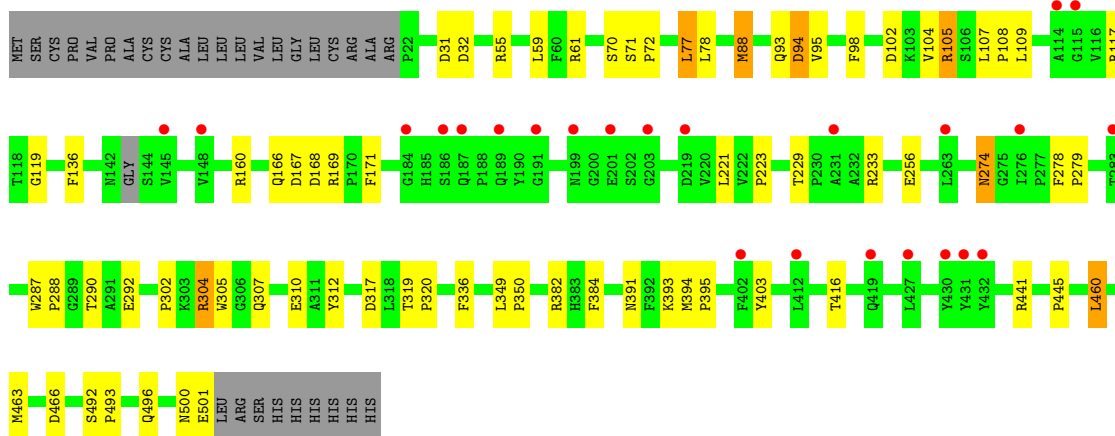
- Molecule 1: N-sulphoglucosamine sulphonydrolase



HIS
HIS

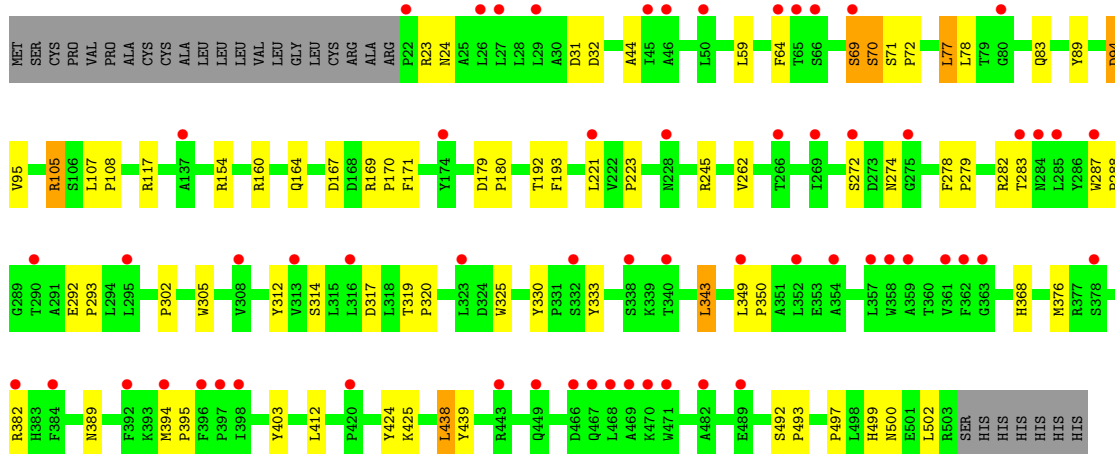
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain G: 5% 80% 13% 6%



- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain H: 12% 79% 14% 5%



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

Chain I: 100%

WAG1
WAG2

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

Chain J: 100%



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

Chain K:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  100%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 50%

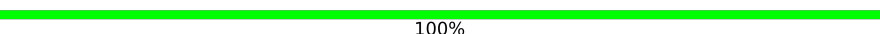


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

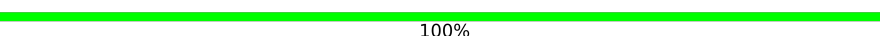


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



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

Chain T:  100%



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

Chain U:  50% 50%

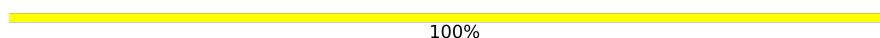


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%



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

Chain W:  100%

MAG1
MAG2

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

Chain X:  50% 50%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain a:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.93Å 211.45Å 108.35Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	48.85 – 2.40 48.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.85-2.40) 99.4 (48.85-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.245 0.217 , 0.245	Depositor DCC
R_{free} test set	8462 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31167	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6261e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, FGP, PEG, CA, CL

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	0.32	0/3986	0.68	0/5443
1	B	0.33	0/3977	0.68	0/5429
1	C	0.33	0/3964	0.70	0/5415
1	D	0.33	0/3946	0.68	0/5387
1	E	0.31	0/3710	0.69	0/5081
1	F	0.30	0/3809	0.68	0/5202
1	G	0.31	0/3794	0.68	0/5187
1	H	0.30	0/3725	0.69	0/5100
All	All	0.32	0/30911	0.68	0/42244

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	A	0	1
1	H	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	SER	Mainchain
1	H	69	SER	Mainchain
1	H	70	FGP	Mainchain

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	3869	0	3671	63	0
1	B	3860	0	3696	75	0
1	C	3854	0	3664	66	0
1	D	3835	0	3648	58	0
1	E	3607	0	3130	70	0
1	F	3703	0	3368	61	0
1	G	3685	0	3350	85	0
1	H	3617	0	3180	80	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	1	0
2	M	27	0	22	4	0
2	N	28	0	25	1	0
2	O	27	0	22	0	0
2	P	27	0	22	0	0
2	Q	28	0	25	2	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	3	0
2	X	28	0	25	0	0
2	Y	25	0	21	1	0
2	Z	27	0	22	2	0
2	a	28	0	25	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	14	0	13	2	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	2	0
4	D	14	0	13	0	0
4	F	28	0	26	0	0
4	G	24	0	19	0	0
4	H	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	D	5	0	4	1	0
7	A	97	0	0	5	0
7	B	112	0	0	1	0
7	C	87	0	0	0	0
7	D	107	0	0	2	0
7	E	8	0	0	2	0
7	F	26	0	0	2	0
7	G	29	0	0	2	0
7	H	9	0	0	0	0
All	All	31167	0	28280	541	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 9.

All (541) 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:88:MET:HE1	1:G:98:PHE:C	1.66	1.19
1:G:88:MET:CE	1:G:98:PHE:HB3	1.79	1.11
1:E:24:ASN:HB2	1:E:266:THR:HG22	1.30	1.08
1:A:394[A]:MET:HG3	1:B:391[A]:ASN:OD1	1.53	1.06
1:G:88:MET:HE3	1:G:88:MET:HA	1.33	1.06
1:E:24:ASN:HB2	1:E:266:THR:CG2	1.88	1.04
1:B:453:THR:HG22	7:B:800:HOH:O	1.59	1.03
1:B:460:LEU:HD11	1:G:463:MET:HE1	1.42	1.02
1:E:271:THR:CG2	1:E:294:LEU:HD13	1.89	1.02
1:G:88:MET:CE	1:G:98:PHE:CB	2.41	0.99
1:B:61:ARG:HD2	1:B:310:GLU:OE2	1.63	0.97
1:E:271:THR:HG21	1:E:294:LEU:HD13	1.48	0.95
1:D:268:VAL:HG13	1:D:297:SER:HB3	1.47	0.94
1:G:391:ASN:OD1	1:H:394:MET:HG3	1.67	0.94
1:C:140:GLU:HB3	1:C:145:VAL:HG22	1.51	0.92
1:B:140:GLU:HB3	1:B:145:VAL:HG22	1.52	0.91
1:D:140:GLU:HB3	1:D:145:VAL:HG22	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ARG:HG3	1:F:256:GLU:OE1	1.70	0.91
1:C:140:GLU:CB	1:C:145:VAL:HG22	2.00	0.91
1:D:140:GLU:CB	1:D:145:VAL:HG22	2.00	0.91
1:B:140:GLU:CB	1:B:145:VAL:HG22	2.01	0.90
1:A:484:ASP:OD2	1:A:504:SER:HA	1.73	0.89
1:C:394:MET:HG3	1:D:391:ASN:OD1	1.71	0.88
1:E:271:THR:CG2	1:E:294:LEU:CD1	2.52	0.88
1:F:140:GLU:CB	1:F:145:VAL:HG22	2.03	0.88
1:C:77:LEU:C	1:C:77:LEU:HD23	2.00	0.87
1:F:202:SER:HA	7:F:720:HOH:O	1.75	0.87
1:G:88:MET:HE2	1:G:98:PHE:HB3	1.57	0.86
1:G:77:LEU:HD23	1:G:77:LEU:C	2.01	0.86
1:D:501:GLU:OE1	1:D:501:GLU:C	2.18	0.86
1:D:268:VAL:CG1	1:D:297:SER:HB3	2.05	0.85
1:D:462:GLU:HG2	7:D:796:HOH:O	1.76	0.85
1:F:140:GLU:HB3	1:F:145:VAL:HG22	1.55	0.85
1:G:88:MET:HE2	1:G:98:PHE:CB	2.06	0.85
1:H:77:LEU:C	1:H:77:LEU:HD23	2.01	0.84
1:E:453:THR:HG22	1:G:167:ASP:HA	1.59	0.84
1:D:145:VAL:HG23	7:D:723:HOH:O	1.78	0.84
1:B:460:LEU:CD1	1:G:463:MET:HE1	2.07	0.83
1:B:208:PRO:HG3	2:M:2:NAG:C6	2.08	0.83
1:G:88:MET:HE1	1:G:98:PHE:CB	2.07	0.83
1:G:88:MET:HE1	1:G:98:PHE:O	1.80	0.82
1:H:23:ARG:HD2	1:H:325:TRP:CZ2	2.15	0.82
1:H:330:TYR:CG	1:H:343:LEU:HD21	2.15	0.82
1:H:330:TYR:CD2	1:H:343:LEU:HD21	2.15	0.82
1:E:88:MET:HE1	1:E:92:HIS:HB2	1.64	0.80
1:C:88:MET:HE1	1:C:92:HIS:HB2	1.64	0.79
1:E:24:ASN:CB	1:E:266:THR:HG22	2.10	0.79
1:A:61:ARG:HD2	1:A:310:GLU:OE2	1.83	0.78
1:B:459:GLN:HG2	1:G:384:PHE:CZ	2.20	0.77
1:C:304:ARG:HG3	1:C:307:GLN:CD	2.10	0.77
1:A:88:MET:HE1	1:A:92:HIS:HB2	1.65	0.76
1:A:304:ARG:HG3	1:A:307:GLN:CD	2.10	0.76
2:a:1:NAG:H61	2:a:2:NAG:O5	1.85	0.76
1:E:304:ARG:HG3	1:E:307:GLN:CD	2.11	0.75
1:A:394[B]:MET:HE1	7:A:779:HOH:O	1.85	0.75
1:G:304:ARG:HG3	1:G:307:GLN:CD	2.11	0.74
1:H:272:SER:O	1:H:292:GLU:HG2	1.88	0.74
1:F:160:ARG:O	1:F:164:GLN:HG2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:MET:CE	1:G:88:MET:HA	2.15	0.74
1:C:299:PRO:O	2:Q:1:NAG:H62	1.88	0.73
1:E:203:GLY:C	1:E:204:MET:HE2	2.15	0.72
1:G:160:ARG:HB2	1:G:256:GLU:OE1	1.89	0.72
1:G:77:LEU:HD22	1:G:78:LEU:HG	1.72	0.71
1:H:77:LEU:HD22	1:H:78:LEU:HG	1.72	0.71
2:a:1:NAG:O3	2:a:2:NAG:C7	2.38	0.71
1:C:23:ARG:NH2	1:C:300:GLU:OE1	2.24	0.70
1:D:117:ARG:HD3	1:D:166:GLN:OE1	1.92	0.70
1:H:69:SER:HB2	1:H:368:HIS:ND1	2.07	0.70
1:B:77:LEU:CD1	1:B:318:LEU:HD23	2.21	0.69
1:C:77:LEU:HD22	1:C:78:LEU:HG	1.73	0.69
1:G:61:ARG:HD2	1:G:310:GLU:OE2	1.92	0.69
1:H:438:LEU:HD23	1:H:439:TYR:N	2.07	0.69
1:B:117:ARG:HD3	1:B:166:GLN:OE1	1.92	0.69
1:G:105:ARG:NH1	1:G:109:LEU:HD21	2.07	0.69
1:A:391:ASN:O	1:A:394[B]:MET:HG2	1.93	0.69
1:A:117:ARG:HD3	1:A:166:GLN:OE1	1.93	0.68
1:H:343:LEU:N	1:H:343:LEU:HD22	2.08	0.68
1:B:61:ARG:NH2	2:L:1:NAG:O3	2.27	0.68
1:E:117:ARG:HD3	1:E:166:GLN:OE1	1.94	0.68
1:E:203:GLY:O	1:E:204:MET:HE2	1.93	0.68
1:B:460:LEU:CD1	1:G:463:MET:CE	2.72	0.68
1:F:160:ARG:CG	1:F:256:GLU:OE1	2.41	0.68
1:E:51:ASP:O	1:E:55:ARG:CD	2.43	0.67
1:A:304:ARG:HG3	1:A:307:GLN:OE1	1.95	0.67
1:E:214:ALA:HA	7:E:704:HOH:O	1.95	0.66
1:C:77:LEU:HD23	1:C:78:LEU:N	2.11	0.66
1:C:167:ASP:O	1:C:168:ASP:HB2	1.95	0.66
1:G:117:ARG:HD3	1:G:166:GLN:OE1	1.94	0.66
1:B:71:SER:HB2	1:B:72:PRO:HD3	1.78	0.66
1:D:71:SER:HB2	1:D:72:PRO:HD3	1.77	0.66
1:E:452:ALA:O	1:G:168:ASP:CB	2.43	0.66
1:C:304:ARG:HG3	1:C:307:GLN:OE1	1.95	0.66
1:H:438:LEU:HD23	1:H:438:LEU:C	2.21	0.66
1:C:71:SER:HB2	1:C:72:PRO:HD3	1.78	0.66
1:H:71:SER:HB2	1:H:72:PRO:HD3	1.78	0.66
1:G:71:SER:HB2	1:G:72:PRO:HD3	1.78	0.65
1:E:71:SER:HB2	1:E:72:PRO:HD3	1.78	0.65
1:G:88:MET:HE1	1:G:98:PHE:CA	2.26	0.65
1:E:304:ARG:HG3	1:E:307:GLN:OE1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2:NAG:H2	2:Z:2:NAG:C6	2.26	0.65
1:D:61:ARG:NE	1:D:310:GLU:OE2	2.30	0.65
1:F:71:SER:HB2	1:F:72:PRO:HD3	1.78	0.65
1:D:140:GLU:CB	1:D:145:VAL:CG2	2.74	0.65
1:G:88:MET:HE2	1:G:98:PHE:HB2	1.78	0.65
1:A:71:SER:HB2	1:A:72:PRO:HD3	1.78	0.64
1:F:287:TRP:HB3	1:F:288:PRO:HD3	1.79	0.64
1:F:418:GLY:O	1:G:102:ASP:HB3	1.97	0.64
1:A:287:TRP:HB3	1:A:288:PRO:HD3	1.80	0.64
1:F:418:GLY:HA3	7:G:712:HOH:O	1.97	0.63
1:G:287:TRP:HB3	1:G:288:PRO:HD3	1.80	0.63
1:H:77:LEU:HD23	1:H:78:LEU:N	2.13	0.63
1:A:167:ASP:O	1:A:168:ASP:HB2	1.97	0.63
1:G:77:LEU:HD23	1:G:78:LEU:N	2.12	0.63
1:G:109:LEU:HD22	7:G:705:HOH:O	1.96	0.63
1:G:304:ARG:HG3	1:G:307:GLN:OE1	1.98	0.63
1:E:287:TRP:HB3	1:E:288:PRO:HD3	1.80	0.63
1:F:70:FGP:OG1	1:F:125:HIS:ND1	2.30	0.63
1:F:201:GLU:N	1:F:201:GLU:OE1	2.32	0.63
1:H:287:TRP:HB3	1:H:288:PRO:HD3	1.81	0.63
1:B:140:GLU:CB	1:B:145:VAL:CG2	2.75	0.62
1:F:160:ARG:HG3	1:F:256:GLU:CD	2.22	0.62
1:C:140:GLU:CB	1:C:145:VAL:CG2	2.75	0.62
1:D:287:TRP:HB3	1:D:288:PRO:HD3	1.82	0.62
1:H:330:TYR:CD2	1:H:343:LEU:CD2	2.82	0.62
1:G:416:THR:HG21	1:H:499:HIS:CE1	2.34	0.62
1:H:376:MET:HE3	1:H:389:ASN:OD1	2.00	0.61
1:C:287:TRP:HB3	1:C:288:PRO:HD3	1.81	0.61
1:B:287:TRP:HB3	1:B:288:PRO:HD3	1.81	0.61
1:B:57:SER:HB3	1:B:297:SER:HB2	1.82	0.61
1:F:140:GLU:CB	1:F:145:VAL:CG2	2.77	0.61
1:B:501:GLU:O	1:B:502:LEU:HD23	2.01	0.61
1:G:319:THR:HB	1:G:320:PRO:HD3	1.83	0.60
1:H:31:ASP:O	1:H:180:PRO:HD2	2.01	0.60
1:H:23:ARG:HG3	1:H:325:TRP:NE1	2.16	0.60
1:H:319:THR:HB	1:H:320:PRO:HD3	1.82	0.60
1:B:460:LEU:HD11	1:G:463:MET:CE	2.25	0.60
1:H:438:LEU:C	1:H:438:LEU:CD2	2.74	0.60
1:A:441:ARG:NH1	1:A:445:PRO:O	2.35	0.60
1:B:459:GLN:HB3	1:G:460:LEU:HD11	1.82	0.60
1:H:272:SER:HB3	1:H:292:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:THR:HB	1:F:320:PRO:HD3	1.83	0.59
1:B:44:ALA:HB2	1:B:221:LEU:HD13	1.85	0.59
1:C:77:LEU:CD2	1:C:78:LEU:HG	2.33	0.59
1:D:319:THR:HB	1:D:320:PRO:HD3	1.84	0.59
1:B:424:TYR:CZ	1:B:425:LYS:HD2	2.38	0.59
1:C:319:THR:HB	1:C:320:PRO:HD3	1.84	0.59
1:A:319:THR:HB	1:A:320:PRO:HD3	1.84	0.59
1:H:44:ALA:HB2	1:H:221:LEU:HD13	1.83	0.59
1:B:44:ALA:CB	1:B:221:LEU:HD13	2.32	0.59
1:B:23:ARG:O	1:B:170:PRO:HB3	2.02	0.59
1:D:23:ARG:O	1:D:170:PRO:HB3	2.03	0.59
1:D:424:TYR:CZ	1:D:425:LYS:HD2	2.38	0.59
1:A:424:TYR:CZ	1:A:425:LYS:HD2	2.38	0.59
1:G:77:LEU:CD2	1:G:78:LEU:HG	2.32	0.59
1:E:424:TYR:CZ	1:E:425:LYS:HD2	2.38	0.59
1:H:77:LEU:CD2	1:H:78:LEU:HG	2.31	0.59
1:E:319:THR:HB	1:E:320:PRO:HD3	1.84	0.59
1:F:424:TYR:CZ	1:F:425:LYS:HD2	2.38	0.59
1:B:319:THR:HB	1:B:320:PRO:HD3	1.85	0.58
1:G:441:ARG:NH1	1:G:445:PRO:O	2.36	0.58
1:F:201:GLU:OE1	1:F:201:GLU:CA	2.51	0.58
1:H:424:TYR:CZ	1:H:425:LYS:HD2	2.38	0.58
1:E:24:ASN:HB2	1:E:266:THR:HG23	1.80	0.58
2:Z:2:NAG:C6	2:Z:2:NAG:C2	2.82	0.58
1:C:140:GLU:HB3	1:C:145:VAL:CG2	2.31	0.58
1:C:424:TYR:CZ	1:C:425:LYS:HD2	2.39	0.58
1:D:77:LEU:HD12	1:D:77:LEU:C	2.28	0.58
1:H:105:ARG:NH2	1:H:333:TYR:HB3	2.19	0.58
1:B:140:GLU:HB3	1:B:145:VAL:CG2	2.31	0.57
1:G:88:MET:CE	1:G:98:PHE:C	2.60	0.57
1:B:501:GLU:O	1:B:501:GLU:HG2	2.04	0.57
1:D:44:ALA:CB	1:D:221:LEU:HD13	2.34	0.57
1:B:77:LEU:HD13	1:B:318:LEU:HD23	1.85	0.57
1:E:441:ARG:NH1	1:E:445:PRO:O	2.37	0.57
1:H:23:ARG:O	1:H:170:PRO:HB3	2.05	0.57
1:C:492:SER:HA	1:C:493:PRO:C	2.29	0.57
1:C:441:ARG:NH1	1:C:445:PRO:O	2.37	0.57
1:D:140:GLU:HB2	1:D:145:VAL:CG2	2.34	0.57
1:F:125:HIS:HA	7:F:726:HOH:O	2.05	0.57
1:F:140:GLU:HB2	1:F:145:VAL:CG2	2.35	0.57
1:D:140:GLU:HB3	1:D:145:VAL:CG2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ALA:HB2	1:D:221:LEU:HD13	1.87	0.56
1:E:271:THR:CG2	1:E:294:LEU:HD12	2.35	0.56
1:H:262:VAL:O	1:H:262:VAL:HG12	2.05	0.56
1:A:278:PHE:HB3	1:A:279:PRO:HD2	1.88	0.56
1:C:140:GLU:HB2	1:C:145:VAL:CG2	2.35	0.56
1:D:437:GLU:HG2	6:D:609:PEG:H22	1.88	0.56
1:F:278:PHE:HB3	1:F:279:PRO:HD2	1.88	0.56
1:G:278:PHE:HB3	1:G:279:PRO:HD2	1.88	0.56
1:D:278:PHE:HB3	1:D:279:PRO:HD2	1.88	0.56
1:E:278:PHE:HB3	1:E:279:PRO:HD2	1.88	0.56
1:H:44:ALA:CB	1:H:221:LEU:HD13	2.36	0.55
1:H:171:PHE:HE2	1:H:262:VAL:HG11	1.71	0.55
1:G:274:ASN:HA	1:G:292:GLU:OE2	2.06	0.55
1:B:140:GLU:HB2	1:B:145:VAL:CG2	2.35	0.55
1:A:274:ASN:HA	1:A:292:GLU:OE2	2.07	0.55
1:G:107:LEU:N	1:G:108:PRO:HD2	2.21	0.55
1:B:355:GLU:H	1:G:492:SER:CB	2.20	0.55
1:C:278:PHE:HB3	1:C:279:PRO:HD2	1.88	0.55
1:H:171:PHE:CE2	1:H:262:VAL:HG11	2.42	0.55
1:H:412:LEU:O	1:H:412:LEU:HD23	2.06	0.55
2:a:2:NAG:O3	2:a:2:NAG:H82	2.07	0.55
1:G:88:MET:CE	1:G:98:PHE:HB2	2.32	0.55
1:F:274:ASN:HA	1:F:292:GLU:OE2	2.07	0.54
2:M:1:NAG:O4	2:M:2:NAG:H4	2.07	0.54
1:B:59:LEU:C	1:B:59:LEU:HD23	2.33	0.54
1:F:59:LEU:HD23	1:F:59:LEU:C	2.32	0.54
1:B:274:ASN:HA	1:B:292:GLU:OE2	2.08	0.54
1:E:274:ASN:HA	1:E:292:GLU:OE2	2.07	0.54
1:C:274:ASN:HA	1:C:292:GLU:OE2	2.08	0.54
1:D:274:ASN:HA	1:D:292:GLU:OE2	2.08	0.54
1:G:77:LEU:C	1:G:77:LEU:CD2	2.75	0.54
1:H:278:PHE:HB3	1:H:279:PRO:HD2	1.88	0.54
1:A:59:LEU:HD23	1:A:59:LEU:C	2.33	0.54
1:B:278:PHE:HB3	1:B:279:PRO:HD2	1.89	0.54
1:C:394:MET:HE3	1:C:395:PRO:HD2	1.89	0.53
1:D:107:LEU:N	1:D:108:PRO:HD2	2.23	0.53
1:E:270:PHE:O	1:E:271:THR:HG23	2.08	0.53
1:A:409:GLN:HB3	4:A:608:NAG:H82	1.90	0.53
1:H:59:LEU:C	1:H:59:LEU:HD23	2.33	0.53
1:C:59:LEU:C	1:C:59:LEU:HD23	2.34	0.53
1:A:107:LEU:N	1:A:108:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:LEU:HB3	1:H:108:PRO:CD	2.39	0.53
1:H:107:LEU:N	1:H:108:PRO:HD2	2.24	0.53
1:H:343:LEU:HD22	1:H:343:LEU:H	1.72	0.53
2:N:1:NAG:H61	2:N:2:NAG:C1	2.39	0.53
1:F:394:MET:HE3	1:F:395:PRO:HD2	1.91	0.53
1:C:77:LEU:C	1:C:77:LEU:CD2	2.74	0.53
1:A:492:SER:HA	1:A:493:PRO:C	2.33	0.53
1:E:492:SER:HA	1:E:493:PRO:C	2.34	0.52
1:A:107:LEU:HB3	1:A:108:PRO:CD	2.40	0.52
1:B:394:MET:HE3	1:B:395:PRO:HD2	1.92	0.52
1:F:94:ASP:OD1	1:F:95:VAL:N	2.39	0.52
1:F:107:LEU:N	1:F:108:PRO:HD2	2.24	0.52
1:G:94:ASP:OD1	1:G:95:VAL:N	2.38	0.52
1:A:192:THR:HG23	1:A:193:PHE:HD1	1.75	0.52
1:B:107:LEU:N	1:B:108:PRO:HD2	2.24	0.52
1:C:23:ARG:O	1:C:170:PRO:HB3	2.10	0.52
1:E:394:MET:HE3	1:E:395:PRO:HD2	1.90	0.52
1:D:394:MET:HE3	1:D:395:PRO:HD2	1.91	0.52
1:H:394:MET:HE3	1:H:395:PRO:HD2	1.90	0.52
1:G:59:LEU:C	1:G:59:LEU:HD23	2.34	0.52
1:B:459:GLN:CB	1:G:460:LEU:HD11	2.40	0.52
1:B:107:LEU:HB3	1:B:108:PRO:CD	2.39	0.52
1:D:107:LEU:HB3	1:D:108:PRO:CD	2.40	0.52
1:E:271:THR:HG22	1:E:294:LEU:HD13	1.87	0.52
1:F:107:LEU:HB3	1:F:108:PRO:CD	2.40	0.52
1:C:94:ASP:OD1	1:C:95:VAL:N	2.37	0.52
1:G:55:ARG:HA	1:G:55:ARG:NE	2.25	0.52
1:D:274:ASN:C	1:D:292:GLU:OE2	2.53	0.51
1:F:274:ASN:C	1:F:292:GLU:OE2	2.54	0.51
1:H:77:LEU:C	1:H:77:LEU:CD2	2.75	0.51
1:B:459:GLN:HG2	1:G:384:PHE:CE2	2.45	0.51
1:D:59:LEU:C	1:D:59:LEU:HD23	2.35	0.51
1:B:179:ASP:OD2	1:B:245:ARG:HD2	2.11	0.51
1:G:394:MET:HE3	1:G:395:PRO:HD2	1.91	0.51
1:G:107:LEU:HB3	1:G:108:PRO:CD	2.40	0.51
1:A:394[A]:MET:HE3	1:A:395:PRO:HD2	1.92	0.51
1:G:395:PRO:HG3	1:H:502:LEU:HD11	1.92	0.51
1:H:23:ARG:O	1:H:24:ASN:ND2	2.44	0.51
1:H:282:ARG:O	1:H:283:THR:CB	2.58	0.51
1:B:287:TRP:N	1:B:288:PRO:CD	2.73	0.51
1:C:107:LEU:N	1:C:108:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:N	1:E:108:PRO:HD2	2.25	0.51
1:C:107:LEU:HB3	1:C:108:PRO:CD	2.40	0.50
1:C:287:TRP:N	1:C:288:PRO:CD	2.73	0.50
1:F:140:GLU:HB3	1:F:145:VAL:CG2	2.34	0.50
1:G:393:LYS:HB2	1:H:394:MET:SD	2.50	0.50
1:H:192:THR:HG23	1:H:193:PHE:HD1	1.76	0.50
1:H:262:VAL:O	1:H:262:VAL:CG1	2.58	0.50
1:E:107:LEU:HB3	1:E:108:PRO:CD	2.40	0.50
1:A:31:ASP:O	1:A:180:PRO:HD2	2.11	0.50
1:C:221:LEU:O	1:C:223:PRO:HD3	2.11	0.50
1:D:31:ASP:O	1:D:180:PRO:HD2	2.11	0.50
1:D:179:ASP:OD2	1:D:245:ARG:HD2	2.12	0.50
1:F:31:ASP:O	1:F:180:PRO:HD2	2.12	0.50
1:H:500:ASN:OD1	1:H:502:LEU:HB2	2.12	0.50
1:A:274:ASN:C	1:A:292:GLU:OE2	2.55	0.50
1:E:31:ASP:O	1:E:180:PRO:HD2	2.11	0.50
1:A:94:ASP:OD1	1:A:95:VAL:N	2.43	0.50
1:E:287:TRP:N	1:E:288:PRO:CD	2.74	0.50
1:F:282:ARG:O	1:F:283:THR:OG1	2.22	0.50
1:E:274:ASN:C	1:E:292:GLU:OE2	2.55	0.50
1:F:179:ASP:OD2	1:F:245:ARG:HD2	2.12	0.50
1:C:274:ASN:C	1:C:292:GLU:OE2	2.55	0.49
1:E:282:ARG:O	1:E:283:THR:OG1	2.22	0.49
2:a:1:NAG:C6	2:a:2:NAG:O5	2.58	0.49
1:A:488:GLU:OE1	1:A:490:LYS:NZ	2.46	0.49
1:B:274:ASN:C	1:B:292:GLU:OE2	2.55	0.49
1:A:221:LEU:O	1:A:223:PRO:HD3	2.12	0.49
1:A:287:TRP:N	1:A:288:PRO:CD	2.74	0.49
1:A:229:THR:O	1:A:233:ARG:HG3	2.13	0.49
1:G:287:TRP:N	1:G:288:PRO:CD	2.75	0.49
1:H:343:LEU:CD2	1:H:343:LEU:H	2.26	0.49
1:D:349:LEU:N	1:D:350:PRO:CD	2.75	0.49
1:E:394:MET:SD	1:F:393:LYS:HB2	2.52	0.49
1:G:492:SER:HA	1:G:493:PRO:C	2.37	0.49
1:F:192:THR:HG23	1:F:193:PHE:HD1	1.77	0.49
1:G:274:ASN:C	1:G:292:GLU:OE2	2.56	0.49
1:H:221:LEU:O	1:H:223:PRO:HD3	2.12	0.49
1:H:343:LEU:N	1:H:343:LEU:CD2	2.74	0.49
1:D:94:ASP:OD1	1:D:95:VAL:N	2.38	0.49
1:F:167:ASP:C	1:F:169:ARG:H	2.21	0.49
1:H:179:ASP:OD2	1:H:245:ARG:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:O	1:C:233:ARG:HG3	2.13	0.49
1:E:31:ASP:O	1:E:32:ASP:HB2	2.13	0.49
1:E:258:ARG:HG3	1:E:263:LEU:HD22	1.95	0.49
1:B:349:LEU:HB2	1:B:350:PRO:HD3	1.95	0.49
1:D:287:TRP:N	1:D:288:PRO:CD	2.75	0.49
1:F:258:ARG:HG3	1:F:263:LEU:HD22	1.95	0.49
1:G:416:THR:HG21	1:H:499:HIS:ND1	2.27	0.49
1:H:330:TYR:CD1	1:H:343:LEU:HD21	2.48	0.49
1:H:412:LEU:HD23	1:H:412:LEU:C	2.38	0.49
1:A:504:SER:CB	7:A:746:HOH:O	2.61	0.48
1:A:282:ARG:O	1:A:283:THR:OG1	2.23	0.48
1:B:349:LEU:N	1:B:350:PRO:CD	2.76	0.48
1:E:271:THR:HG22	1:E:294:LEU:CD1	2.39	0.48
1:D:282:ARG:O	1:D:283:THR:OG1	2.25	0.48
1:G:312:TYR:CZ	1:G:382:ARG:HA	2.48	0.48
1:E:349:LEU:HB2	1:E:350:PRO:HD3	1.95	0.48
1:B:94:ASP:OD1	1:B:95:VAL:N	2.40	0.48
1:E:271:THR:HG23	1:E:294:LEU:CD1	2.41	0.48
1:G:278:PHE:HB3	1:G:279:PRO:CD	2.44	0.48
1:B:31:ASP:O	1:B:180:PRO:HD2	2.14	0.48
1:C:380:GLN:OE1	1:C:385:ARG:HD2	2.14	0.48
1:F:278:PHE:HB3	1:F:279:PRO:CD	2.44	0.47
1:H:107:LEU:HB3	1:H:108:PRO:HD3	1.96	0.47
1:G:349:LEU:N	1:G:350:PRO:CD	2.77	0.47
1:H:287:TRP:N	1:H:288:PRO:CD	2.77	0.47
1:H:349:LEU:HB2	1:H:350:PRO:HD3	1.95	0.47
1:H:69:SER:OG	1:H:72:PRO:HG2	2.13	0.47
1:A:349:LEU:HB2	1:A:350:PRO:HD3	1.96	0.47
1:C:349:LEU:N	1:C:350:PRO:CD	2.77	0.47
1:D:221:LEU:O	1:D:223:PRO:HD3	2.15	0.47
1:E:160:ARG:O	1:E:164:GLN:HG3	2.14	0.47
1:E:392:PHE:O	7:E:702:HOH:O	2.20	0.47
1:A:258:ARG:HG3	1:A:263:LEU:HD22	1.96	0.47
1:G:229:THR:O	1:G:233:ARG:HG3	2.14	0.47
1:G:349:LEU:HB2	1:G:350:PRO:HD3	1.96	0.47
1:C:278:PHE:HB3	1:C:279:PRO:CD	2.45	0.47
1:C:349:LEU:HB2	1:C:350:PRO:HD3	1.97	0.47
1:F:287:TRP:N	1:F:288:PRO:CD	2.77	0.47
1:F:349:LEU:N	1:F:350:PRO:CD	2.78	0.47
1:B:221:LEU:O	1:B:223:PRO:HD3	2.14	0.47
1:E:271:THR:HG23	1:E:294:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HB3	1:B:108:PRO:HD3	1.97	0.47
1:E:278:PHE:HB3	1:E:279:PRO:CD	2.45	0.47
1:E:302:PRO:HA	1:E:305:TRP:CD1	2.50	0.47
1:A:302:PRO:HA	1:A:305:TRP:CD1	2.50	0.47
1:H:492:SER:HA	1:H:493:PRO:C	2.39	0.47
1:D:349:LEU:HB2	1:D:350:PRO:HD3	1.97	0.46
1:G:31:ASP:O	1:G:32:ASP:HB2	2.15	0.46
1:G:221:LEU:O	1:G:223:PRO:HD3	2.15	0.46
1:C:31:ASP:O	1:C:32:ASP:HB2	2.15	0.46
1:C:302:PRO:HA	1:C:305:TRP:CD1	2.50	0.46
1:H:278:PHE:HB3	1:H:279:PRO:CD	2.44	0.46
1:B:31:ASP:O	1:B:32:ASP:HB2	2.14	0.46
1:E:146:LEU:HD22	1:E:197:PHE:CZ	2.50	0.46
1:E:221:LEU:O	1:E:223:PRO:HD3	2.14	0.46
1:H:94:ASP:OD1	1:H:95:VAL:N	2.40	0.46
1:C:31:ASP:O	1:C:180:PRO:HD2	2.16	0.46
1:F:221:LEU:O	1:F:223:PRO:HD3	2.16	0.46
1:F:302:PRO:HA	1:F:305:TRP:CD1	2.50	0.46
1:B:278:PHE:HB3	1:B:279:PRO:CD	2.46	0.46
1:C:88:MET:HE1	1:C:92:HIS:CB	2.41	0.46
1:F:31:ASP:O	1:F:32:ASP:HB2	2.14	0.46
1:D:278:PHE:HB3	1:D:279:PRO:CD	2.45	0.46
1:H:302:PRO:HA	1:H:305:TRP:CD1	2.50	0.46
1:A:409:GLN:CB	4:A:608:NAG:H82	2.46	0.46
1:C:107:LEU:HB3	1:C:108:PRO:HD3	1.98	0.46
1:C:409:GLN:CB	4:C:608:NAG:H82	2.46	0.46
1:E:94:ASP:OD1	1:E:95:VAL:N	2.44	0.46
1:E:167:ASP:C	1:E:169:ARG:H	2.24	0.46
1:F:492:SER:HA	1:F:493:PRO:C	2.40	0.46
1:A:125:HIS:HA	7:A:794:HOH:O	2.16	0.45
1:A:146:LEU:HD22	1:A:197:PHE:CZ	2.50	0.45
1:A:394[A]:MET:SD	1:B:393:LYS:HB2	2.56	0.45
1:C:61:ARG:NE	1:C:310:GLU:OE2	2.48	0.45
1:C:146:LEU:HD22	1:C:197:PHE:CZ	2.51	0.45
1:F:107:LEU:HB3	1:F:108:PRO:HD3	1.97	0.45
1:F:349:LEU:HB2	1:F:350:PRO:HD3	1.97	0.45
1:A:278:PHE:HB3	1:A:279:PRO:CD	2.45	0.45
1:A:312:TYR:CZ	1:A:382:ARG:HA	2.51	0.45
1:A:107:LEU:HB3	1:A:108:PRO:HD3	1.97	0.45
1:D:23:ARG:NH2	1:D:300:GLU:OE2	2.45	0.45
1:D:302:PRO:HA	1:D:305:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:PHE:O	1:E:314:SER:HA	2.15	0.45
1:B:381:HIS:NE2	1:G:466:ASP:OD2	2.49	0.45
1:D:31:ASP:O	1:D:32:ASP:HB2	2.15	0.45
1:E:107:LEU:HB3	1:E:108:PRO:HD3	1.98	0.45
2:M:2:NAG:O5	2:M:2:NAG:O7	2.34	0.45
2:a:1:NAG:H4	2:a:2:NAG:H2	1.52	0.45
1:D:229:THR:O	1:D:233:ARG:HG3	2.17	0.45
1:F:312:TYR:CZ	1:F:382:ARG:HA	2.52	0.45
1:D:290:THR:O	1:D:292:GLU:HG2	2.16	0.45
1:E:32:ASP:HB3	1:E:277:PRO:HD3	1.98	0.45
1:A:31:ASP:O	1:A:32:ASP:HB2	2.16	0.45
1:A:317:ASP:C	1:A:320:PRO:HD2	2.41	0.45
1:B:355:GLU:H	1:G:492:SER:HB2	1.80	0.45
1:C:304:ARG:CG	1:C:307:GLN:OE1	2.65	0.45
1:E:349:LEU:N	1:E:350:PRO:CD	2.78	0.45
1:H:349:LEU:N	1:H:350:PRO:CD	2.79	0.45
2:Y:1:NAG:H61	2:Y:2:NAG:C1	2.46	0.45
1:B:23:ARG:NH2	1:B:300:GLU:OE2	2.39	0.45
1:B:167:ASP:OD1	1:B:167:ASP:N	2.50	0.45
1:G:336:PHE:CE1	1:H:94:ASP:HA	2.51	0.45
1:G:463:MET:HE3	1:G:463:MET:HB2	1.89	0.45
1:B:282:ARG:O	1:B:283:THR:OG1	2.24	0.45
1:B:355:GLU:H	1:G:492:SER:HB3	1.79	0.45
1:F:57:SER:OG	1:F:297:SER:HB2	2.16	0.45
1:H:292:GLU:HG3	1:H:293:PRO:HD2	1.99	0.45
1:A:304:ARG:CG	1:A:307:GLN:OE1	2.64	0.45
1:A:349:LEU:N	1:A:350:PRO:CD	2.79	0.45
1:H:23:ARG:C	1:H:24:ASN:ND2	2.75	0.45
1:B:160:ARG:O	1:B:164:GLN:HG3	2.17	0.44
1:E:88:MET:HE1	1:E:92:HIS:CB	2.42	0.44
1:E:317:ASP:C	1:E:320:PRO:HD2	2.42	0.44
1:C:282:ARG:O	1:C:283:THR:OG1	2.24	0.44
1:H:330:TYR:CE2	1:H:343:LEU:HD21	2.51	0.44
1:G:107:LEU:HB3	1:G:108:PRO:HD3	1.98	0.44
1:D:107:LEU:HB3	1:D:108:PRO:HD3	1.98	0.44
1:G:302:PRO:HA	1:G:305:TRP:CD1	2.53	0.44
1:H:160:ARG:O	1:H:164:GLN:HG3	2.17	0.44
1:A:319:THR:N	1:A:320:PRO:CD	2.80	0.44
1:A:484:ASP:OD1	1:A:484:ASP:N	2.48	0.44
1:B:229:THR:O	1:B:233:ARG:HG3	2.18	0.44
1:H:167:ASP:C	1:H:169:ARG:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:ASP:C	1:H:320:PRO:HD2	2.43	0.44
1:B:312:TYR:CZ	1:B:382:ARG:HA	2.52	0.44
1:D:319:THR:N	1:D:320:PRO:CD	2.81	0.44
1:E:117:ARG:CD	1:E:166:GLN:OE1	2.65	0.44
1:E:312:TYR:CZ	1:E:382:ARG:HA	2.52	0.44
1:F:319:THR:N	1:F:320:PRO:CD	2.81	0.44
1:E:271:THR:HG22	1:E:294:LEU:HA	2.00	0.44
1:G:319:THR:N	1:G:320:PRO:CD	2.81	0.43
1:D:117:ARG:CD	1:D:166:GLN:OE1	2.64	0.43
1:E:94:ASP:HA	1:F:336:PHE:CE1	2.53	0.43
1:A:504:SER:HB3	7:A:746:HOH:O	2.19	0.43
1:D:274:ASN:CA	1:D:292:GLU:OE2	2.67	0.43
1:H:312:TYR:CZ	1:H:382:ARG:HA	2.54	0.43
1:B:117:ARG:CD	1:B:166:GLN:OE1	2.63	0.43
1:D:317:ASP:C	1:D:320:PRO:HD2	2.43	0.43
1:A:117:ARG:CD	1:A:166:GLN:OE1	2.65	0.43
1:B:319:THR:N	1:B:320:PRO:CD	2.82	0.43
1:B:484:ASP:OD1	1:B:484:ASP:N	2.48	0.43
1:C:484:ASP:OD1	1:C:484:ASP:N	2.47	0.43
1:H:31:ASP:O	1:H:32:ASP:HB2	2.19	0.43
1:A:274:ASN:CA	1:A:292:GLU:OE2	2.67	0.43
1:C:317:ASP:C	1:C:320:PRO:HD2	2.43	0.43
1:D:119:GLY:HA2	1:D:136:PHE:O	2.19	0.43
1:F:317:ASP:C	1:F:320:PRO:HD2	2.43	0.43
1:G:496:GLN:HB3	1:H:403:TYR:OH	2.19	0.43
1:B:302:PRO:HA	1:B:305:TRP:CD1	2.53	0.43
1:B:317:ASP:C	1:B:320:PRO:HD2	2.44	0.43
1:C:491:LEU:HD13	1:C:496:GLN:NE2	2.34	0.43
1:F:279:PRO:O	1:F:280:SER:HB2	2.19	0.43
1:G:105:ARG:NH1	1:G:109:LEU:CD2	2.81	0.43
1:A:491:LEU:HD13	1:A:496:GLN:NE2	2.34	0.43
1:B:197:PHE:O	1:B:245:ARG:NH2	2.52	0.43
1:E:491:LEU:HD13	1:E:496:GLN:NE2	2.34	0.43
1:G:317:ASP:C	1:G:320:PRO:HD2	2.43	0.43
1:B:501:GLU:O	1:B:501:GLU:CG	2.66	0.42
1:C:319:THR:N	1:C:320:PRO:CD	2.82	0.42
1:G:304:ARG:CG	1:G:307:GLN:OE1	2.67	0.42
1:H:64:PHE:O	1:H:314:SER:HA	2.18	0.42
1:E:393:LYS:HB2	1:F:394:MET:SD	2.59	0.42
1:G:500:ASN:O	1:G:501:GLU:C	2.62	0.42
2:Q:1:NAG:H61	2:Q:2:NAG:C7	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:THR:N	1:E:320:PRO:CD	2.83	0.42
1:G:274:ASN:CA	1:G:292:GLU:OE2	2.67	0.42
1:H:105:ARG:HH21	1:H:333:TYR:HB3	1.83	0.42
1:A:88:MET:HE1	1:A:92:HIS:CB	2.42	0.42
1:C:312:TYR:CZ	1:C:382:ARG:HA	2.54	0.42
1:E:279:PRO:O	1:E:280:SER:HB2	2.19	0.42
1:E:304:ARG:CG	1:E:307:GLN:OE1	2.65	0.42
1:G:119:GLY:HA2	1:G:136:PHE:O	2.20	0.42
1:A:290:THR:O	1:A:292:GLU:HG2	2.19	0.42
1:B:167:ASP:C	1:B:169:ARG:H	2.28	0.42
1:F:274:ASN:CA	1:F:292:GLU:OE2	2.67	0.42
1:D:167:ASP:OD1	1:D:167:ASP:N	2.53	0.42
1:D:454:ASP:OD1	1:D:456:ARG:HD3	2.18	0.42
1:B:119:GLY:HA2	1:B:136:PHE:O	2.19	0.42
1:D:156:LYS:HG3	1:D:157:LEU:N	2.34	0.42
1:E:270:PHE:C	1:E:271:THR:HG23	2.45	0.42
1:A:488:GLU:HB2	1:A:491:LEU:HD11	2.02	0.42
1:C:207:ILE:HA	1:C:208:PRO:HD2	1.92	0.42
1:E:274:ASN:CA	1:E:292:GLU:OE2	2.67	0.42
1:H:105:ARG:NE	1:H:333:TYR:CG	2.88	0.42
1:A:425:LYS:CE	7:A:752:HOH:O	2.67	0.41
1:D:167:ASP:C	1:D:169:ARG:H	2.28	0.41
1:E:290:THR:O	1:E:292:GLU:HG2	2.19	0.41
1:H:105:ARG:HD3	1:H:333:TYR:CE2	2.55	0.41
1:E:88:MET:HE3	1:E:126:VAL:HA	2.01	0.41
1:G:167:ASP:C	1:G:169:ARG:H	2.28	0.41
1:G:171:PHE:CD1	1:G:171:PHE:C	2.98	0.41
1:A:32:ASP:HB3	1:A:277:PRO:HD3	2.02	0.41
1:B:32:ASP:HB3	1:B:277:PRO:HD3	2.02	0.41
1:C:21:ARG:HA	1:C:22:PRO:HD2	1.89	0.41
1:C:146:LEU:HD22	1:C:197:PHE:CE2	2.55	0.41
1:F:167:ASP:N	1:F:167:ASP:OD1	2.53	0.41
1:G:290:THR:O	1:G:292:GLU:HG2	2.20	0.41
2:W:1:NAG:H61	2:W:2:NAG:C1	2.51	0.41
1:B:290:THR:O	1:B:292:GLU:HG2	2.21	0.41
1:D:171:PHE:CD1	1:D:171:PHE:C	2.98	0.41
1:A:119:GLY:HA2	1:A:136:PHE:O	2.21	0.41
1:B:274:ASN:CA	1:B:292:GLU:OE2	2.67	0.41
1:C:147:GLN:O	1:C:151:ASN:HB3	2.21	0.41
1:C:171:PHE:CD1	1:C:171:PHE:C	2.99	0.41
1:C:290:THR:O	1:C:292:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:PHE:CD1	1:F:171:PHE:C	2.98	0.41
1:H:171:PHE:CD1	1:H:171:PHE:C	2.99	0.41
1:F:83:GLN:OE1	1:F:89:TYR:HA	2.21	0.41
1:F:207:ILE:HG13	2:W:1:NAG:H82	2.03	0.41
1:E:488:GLU:HB2	1:E:491:LEU:HD11	2.03	0.41
1:F:22:PRO:O	1:F:265:ASP:HB3	2.21	0.41
1:F:206:ARG:N	2:W:1:NAG:H83	2.35	0.41
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.87	0.41
1:B:83:GLN:OE1	1:B:89:TYR:HA	2.21	0.41
1:C:140:GLU:HB2	1:C:145:VAL:HG22	1.89	0.41
1:C:274:ASN:CA	1:C:292:GLU:OE2	2.68	0.41
1:C:409:GLN:HB2	4:C:608:NAG:H82	2.03	0.41
1:G:104:VAL:C	1:G:105:ARG:HE	2.28	0.41
1:H:83:GLN:OE1	1:H:89:TYR:HA	2.21	0.41
2:M:1:NAG:H61	2:M:2:NAG:H2	2.02	0.41
1:A:486:VAL:CG2	1:A:498:LEU:HD21	2.51	0.41
1:D:312:TYR:CZ	1:D:382:ARG:HA	2.55	0.41
1:F:360:THR:HA	1:F:380:GLN:O	2.21	0.41
1:B:131:VAL:C	1:B:133:PRO:HD3	2.46	0.40
1:B:492:SER:HA	1:B:493:PRO:C	2.45	0.40
1:C:394:MET:SD	1:D:393:LYS:HB2	2.61	0.40
1:G:403:TYR:OH	1:H:497:PRO:O	2.38	0.40
1:A:171:PHE:CD1	1:A:171:PHE:C	2.99	0.40
1:C:119:GLY:HA2	1:C:136:PHE:O	2.21	0.40
1:C:394:MET:HE2	1:D:391:ASN:HA	2.04	0.40
1:G:117:ARG:CD	1:G:166:GLN:OE1	2.66	0.40
1:B:77:LEU:HD13	1:B:318:LEU:CD2	2.52	0.40
1:D:427:LEU:HD23	1:D:427:LEU:HA	1.88	0.40
1:H:154:ARG:HA	1:H:154:ARG:NE	2.36	0.40
1:A:83:GLN:OE1	1:A:89:TYR:HA	2.22	0.40
1:F:105:ARG:HG3	1:F:109:LEU:HD23	2.04	0.40
1:F:229:THR:O	1:F:233:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/510 (95%)	472 (98%)	11 (2%)	1 (0%)	43	58
1	B	480/510 (94%)	464 (97%)	15 (3%)	1 (0%)	43	58
1	C	481/510 (94%)	469 (98%)	10 (2%)	2 (0%)	30	43
1	D	478/510 (94%)	463 (97%)	13 (3%)	2 (0%)	30	43
1	E	480/510 (94%)	468 (98%)	11 (2%)	1 (0%)	43	58
1	F	473/510 (93%)	459 (97%)	11 (2%)	3 (1%)	21	32
1	G	474/510 (93%)	460 (97%)	13 (3%)	1 (0%)	43	58
1	H	479/510 (94%)	466 (97%)	12 (2%)	1 (0%)	43	58
All	All	3829/4080 (94%)	3721 (97%)	96 (2%)	12 (0%)	36	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	B	94	ASP
1	C	94	ASP
1	D	94	ASP
1	E	94	ASP
1	F	94	ASP
1	G	94	ASP
1	H	94	ASP
1	F	168	ASP
1	F	339	LYS
1	D	339	LYS
1	C	339	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/442 (93%)	404 (98%)	6 (2%)	57	77
1	B	414/442 (94%)	407 (98%)	7 (2%)	53	74
1	C	408/442 (92%)	401 (98%)	7 (2%)	53	74
1	D	404/442 (91%)	396 (98%)	8 (2%)	48	70
1	E	325/442 (74%)	320 (98%)	5 (2%)	57	77
1	F	361/442 (82%)	357 (99%)	4 (1%)	65	82
1	G	358/442 (81%)	351 (98%)	7 (2%)	48	70
1	H	331/442 (75%)	325 (98%)	6 (2%)	51	73
All	All	3011/3536 (85%)	2961 (98%)	50 (2%)	53	74

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	146	LEU
1	A	154	ARG
1	A	274	ASN
1	A	304	ARG
1	A	490	LYS
1	B	95	VAL
1	B	206	ARG
1	B	274	ASN
1	B	318	LEU
1	B	443	ARG
1	B	456	ARG
1	B	459	GLN
1	C	77	LEU
1	C	95	VAL
1	C	146	LEU
1	C	194	CYS
1	C	274	ASN
1	C	304	ARG
1	C	385	ARG
1	D	77	LEU
1	D	95	VAL
1	D	156	LYS
1	D	187	GLN
1	D	428	ARG
1	D	443	ARG
1	D	462	GLU

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Mol	Chain	Res	Type
1	D	501	GLU
1	E	146	LEU
1	E	206	ARG
1	E	266	THR
1	E	274	ASN
1	E	304	ARG
1	F	156	LYS
1	F	201	GLU
1	F	274	ASN
1	F	456	ARG
1	G	77	LEU
1	G	88	MET
1	G	93	GLN
1	G	105	ARG
1	G	274	ASN
1	G	304	ARG
1	G	460	LEU
1	H	77	LEU
1	H	105	ARG
1	H	117	ARG
1	H	274	ASN
1	H	343	LEU
1	H	438	LEU

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

Mol	Chain	Res	Type
1	A	274	ASN
1	A	472	GLN
1	A	496	GLN
1	C	496	GLN
1	D	381	HIS
1	D	383	HIS
1	D	472	GLN
1	E	496	GLN
1	F	274	ASN
1	G	274	ASN
1	H	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	FGP	F	70	1,3	7,10,11	1.03	0	9,14,16	1.31	1 (11%)
1	FGP	A	70	1,3	7,10,11	1.06	0	9,14,16	1.35	1 (11%)
1	FGP	C	70	1,3	7,10,11	1.08	0	9,14,16	1.24	1 (11%)
1	FGP	B	70	1,3	7,10,11	1.05	0	9,14,16	1.33	1 (11%)
1	FGP	H	70	1,3	4,6,11	1.25	0	3,7,16	1.46	1 (33%)
1	FGP	G	70	1,3	4,6,11	1.37	0	3,7,16	1.57	1 (33%)
1	FGP	D	70	1,3	7,10,11	1.08	0	9,14,16	1.27	1 (11%)
1	FGP	E	70	1,3	7,10,11	1.06	0	9,14,16	1.15	1 (11%)

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
1	FGP	F	70	1,3	-	0/5/11/13	-
1	FGP	A	70	1,3	-	0/5/11/13	-
1	FGP	C	70	1,3	-	2/5/11/13	-
1	FGP	B	70	1,3	-	1/5/11/13	-
1	FGP	H	70	1,3	-	0/2/6/13	-
1	FGP	G	70	1,3	-	0/2/6/13	-
1	FGP	D	70	1,3	-	0/5/11/13	-
1	FGP	E	70	1,3	-	0/5/11/13	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	FGP	O-C-CA	-2.88	117.36	124.77
1	B	70	FGP	O-C-CA	-2.84	117.46	124.77
1	D	70	FGP	O-C-CA	-2.81	117.54	124.77
1	F	70	FGP	O-C-CA	-2.76	117.67	124.77
1	G	70	FGP	O-C-CA	-2.63	118.01	124.77
1	C	70	FGP	O-C-CA	-2.47	118.41	124.77
1	H	70	FGP	O-C-CA	-2.29	118.87	124.77
1	E	70	FGP	O-C-CA	-2.26	118.96	124.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	70	FGP	CA-CB-OG2-P
1	C	70	FGP	CA-CB-OG2-P
1	C	70	FGP	CB-OG2-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	70	FGP	1	0

5.5 Carbohydrates [i](#)

38 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	I	1	2,1	14,14,15	0.56	0	17,19,21	0.75	0
2	NAG	I	2	2	14,14,15	0.54	0	17,19,21	0.80	0
2	NAG	J	1	2,1	14,14,15	0.60	0	17,19,21	0.75	0
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	1	2,1	14,14,15	0.42	0	17,19,21	0.87	1 (5%)
2	NAG	K	2	2	14,14,15	0.53	0	17,19,21	0.67	0
2	NAG	L	1	2,1	14,14,15	0.51	0	17,19,21	0.87	0
2	NAG	L	2	2	14,14,15	0.54	0	17,19,21	0.65	0
2	NAG	M	1	2,1	14,14,15	0.61	0	17,19,21	1.08	2 (11%)
2	NAG	M	2	2	13,13,15	0.48	0	16,18,21	1.09	1 (6%)
2	NAG	N	1	2,1	14,14,15	0.55	0	17,19,21	0.79	1 (5%)
2	NAG	N	2	2	14,14,15	0.53	0	17,19,21	0.63	0
2	NAG	O	1	2,1	14,14,15	0.48	0	17,19,21	0.55	0
2	NAG	O	2	2	13,13,15	0.65	0	16,18,21	1.78	3 (18%)
2	NAG	P	1	2,1	14,14,15	0.58	0	17,19,21	0.74	0
2	NAG	P	2	2	13,13,15	0.58	0	16,18,21	0.62	0
2	NAG	Q	1	2,1	14,14,15	0.52	0	17,19,21	0.87	1 (5%)
2	NAG	Q	2	2	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	R	1	2,1	14,14,15	0.55	0	17,19,21	0.74	0
2	NAG	R	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	S	1	2,1	14,14,15	0.58	0	17,19,21	0.83	0
2	NAG	S	2	2	14,14,15	0.57	0	17,19,21	0.67	0
2	NAG	T	1	2,1	14,14,15	0.56	0	17,19,21	0.70	0
2	NAG	T	2	2	14,14,15	0.58	0	17,19,21	0.54	0
2	NAG	U	1	2,1	14,14,15	0.47	0	17,19,21	0.59	0
2	NAG	U	2	2	14,14,15	0.46	0	17,19,21	1.05	2 (11%)
2	NAG	V	1	2,1	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
2	NAG	V	2	2	14,14,15	0.59	0	17,19,21	0.79	0
2	NAG	W	1	2,1	14,14,15	0.57	0	17,19,21	0.72	0
2	NAG	W	2	2	14,14,15	0.55	0	17,19,21	0.70	0
2	NAG	X	1	2,1	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
2	NAG	X	2	2	14,14,15	0.49	0	17,19,21	0.80	0
2	NAG	Y	1	2,1	14,14,15	0.52	0	17,19,21	0.70	0
2	NAG	Y	2	2	11,11,15	0.59	0	13,15,21	0.63	0
2	NAG	Z	1	2,1	14,14,15	0.60	0	17,19,21	0.65	0
2	NAG	Z	2	2	13,13,15	0.52	0	16,18,21	0.77	0
2	NAG	a	1	2,1	14,14,15	0.49	0	17,19,21	0.79	1 (5%)
2	NAG	a	2	2	14,14,15	0.56	0	17,19,21	0.60	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	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/4/21/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/4/21/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/4/21/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/2/19/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/4/21/26	0/1/1/1
2	NAG	a	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	NAG	C3-C4-C5	4.82	117.14	109.81
2	O	2	NAG	O5-C1-C2	-3.18	106.38	111.29
2	O	2	NAG	O5-C5-C4	3.08	115.10	109.55
2	M	2	NAG	C4-C3-C2	-3.00	106.62	111.02
2	M	1	NAG	C4-C3-C2	2.92	115.29	111.02
2	X	1	NAG	C1-O5-C5	2.70	115.81	112.19
2	Q	1	NAG	O5-C1-C2	-2.60	107.27	111.29
2	U	2	NAG	O5-C1-C2	-2.43	107.53	111.29
2	M	1	NAG	O5-C1-C2	-2.42	107.55	111.29
2	U	2	NAG	C4-C3-C2	-2.31	107.63	111.02
2	K	1	NAG	O5-C1-C2	-2.17	107.94	111.29
2	V	1	NAG	O5-C1-C2	-2.11	108.02	111.29
2	a	1	NAG	C4-C3-C2	-2.11	107.93	111.02
2	N	1	NAG	C2-N2-C7	-2.09	120.10	122.90
2	R	2	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C1-C2-N2-C7
2	M	2	NAG	C1-C2-N2-C7
2	T	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	S	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	a	2	NAG	C8-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	N	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C1-C2-N2-C7
2	M	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 19 short contacts:

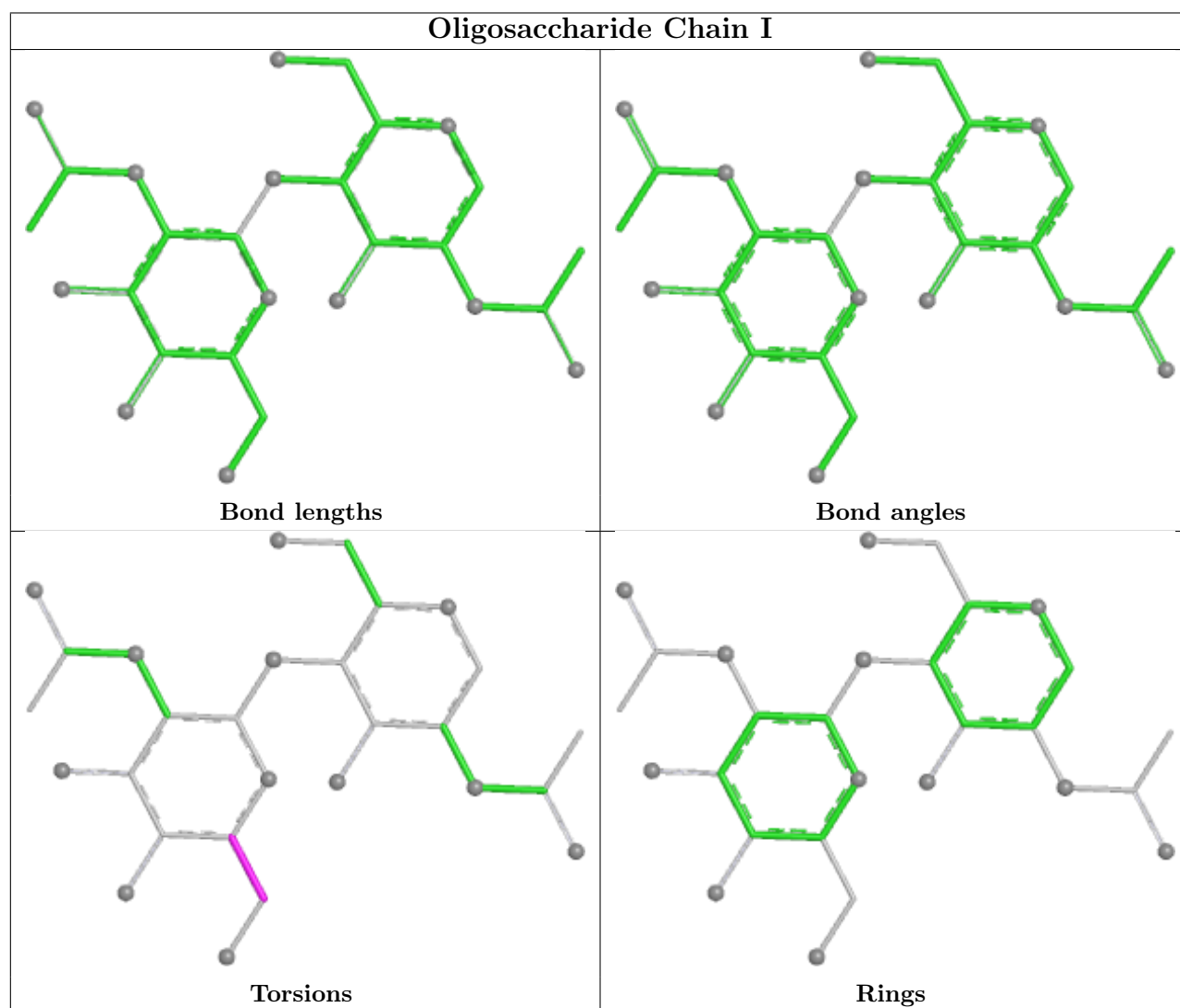
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	1	NAG	1	0
2	Q	1	NAG	2	0
2	N	1	NAG	1	0
2	M	1	NAG	2	0
2	W	1	NAG	3	0
2	W	2	NAG	1	0
2	M	2	NAG	4	0

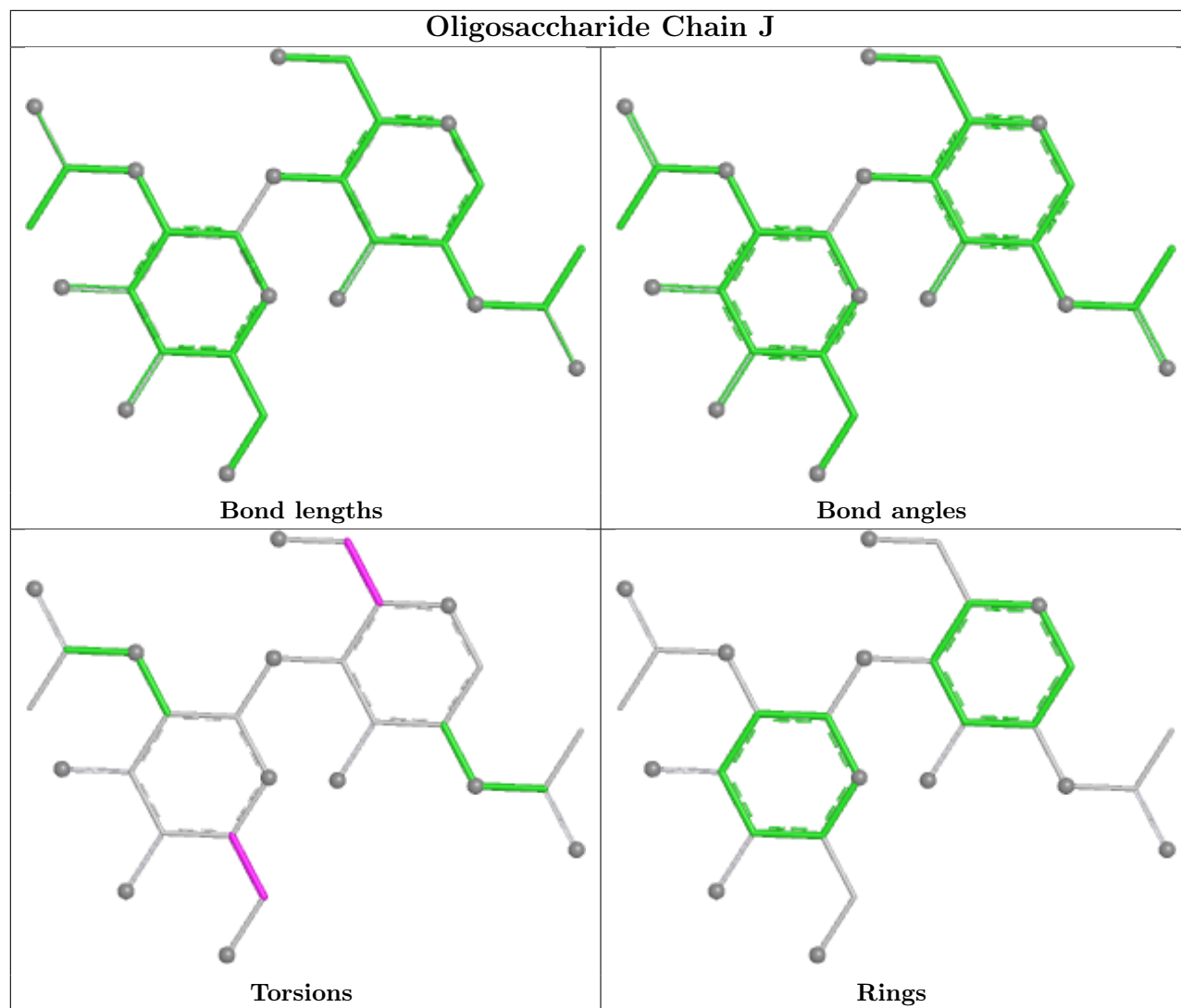
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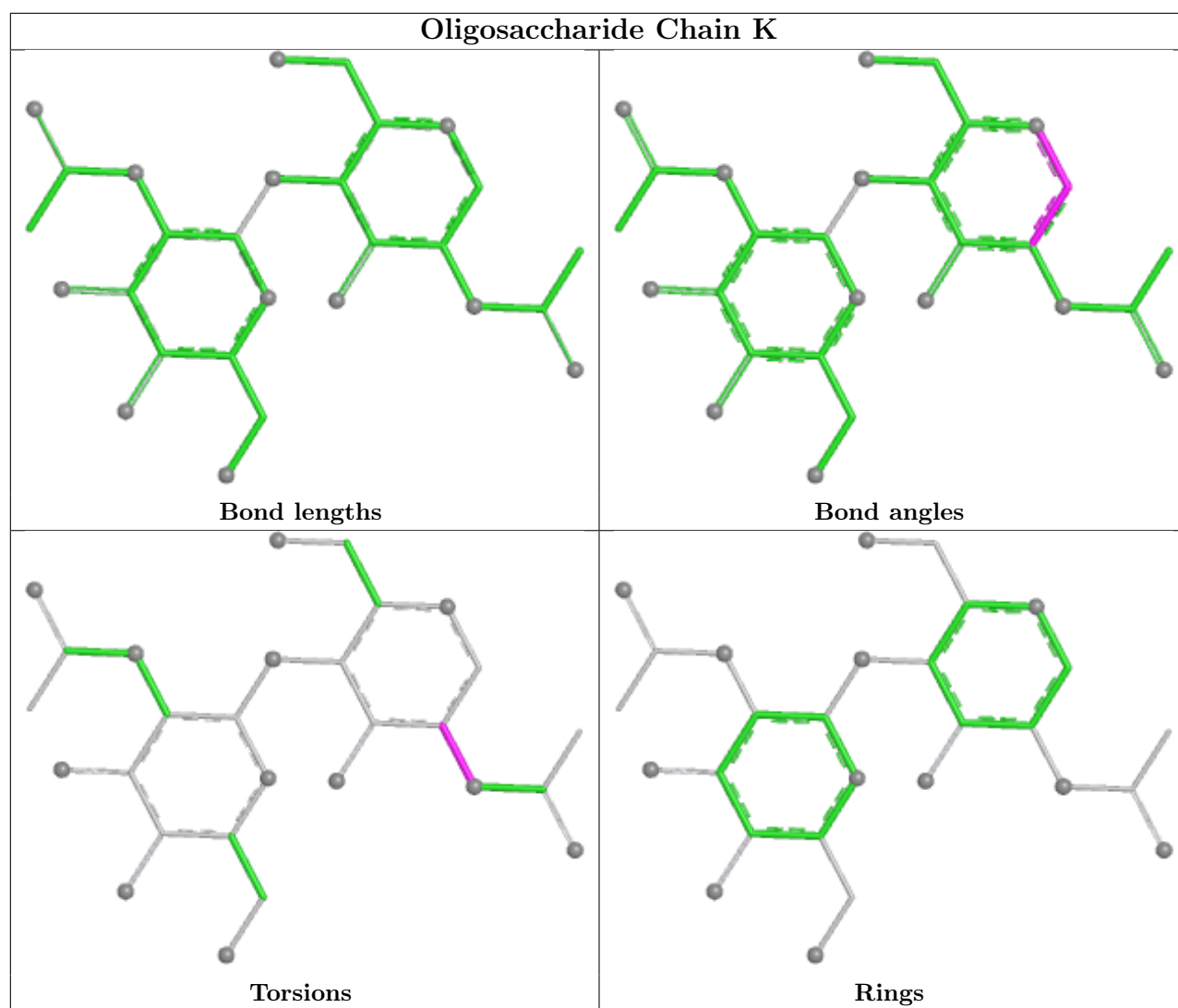
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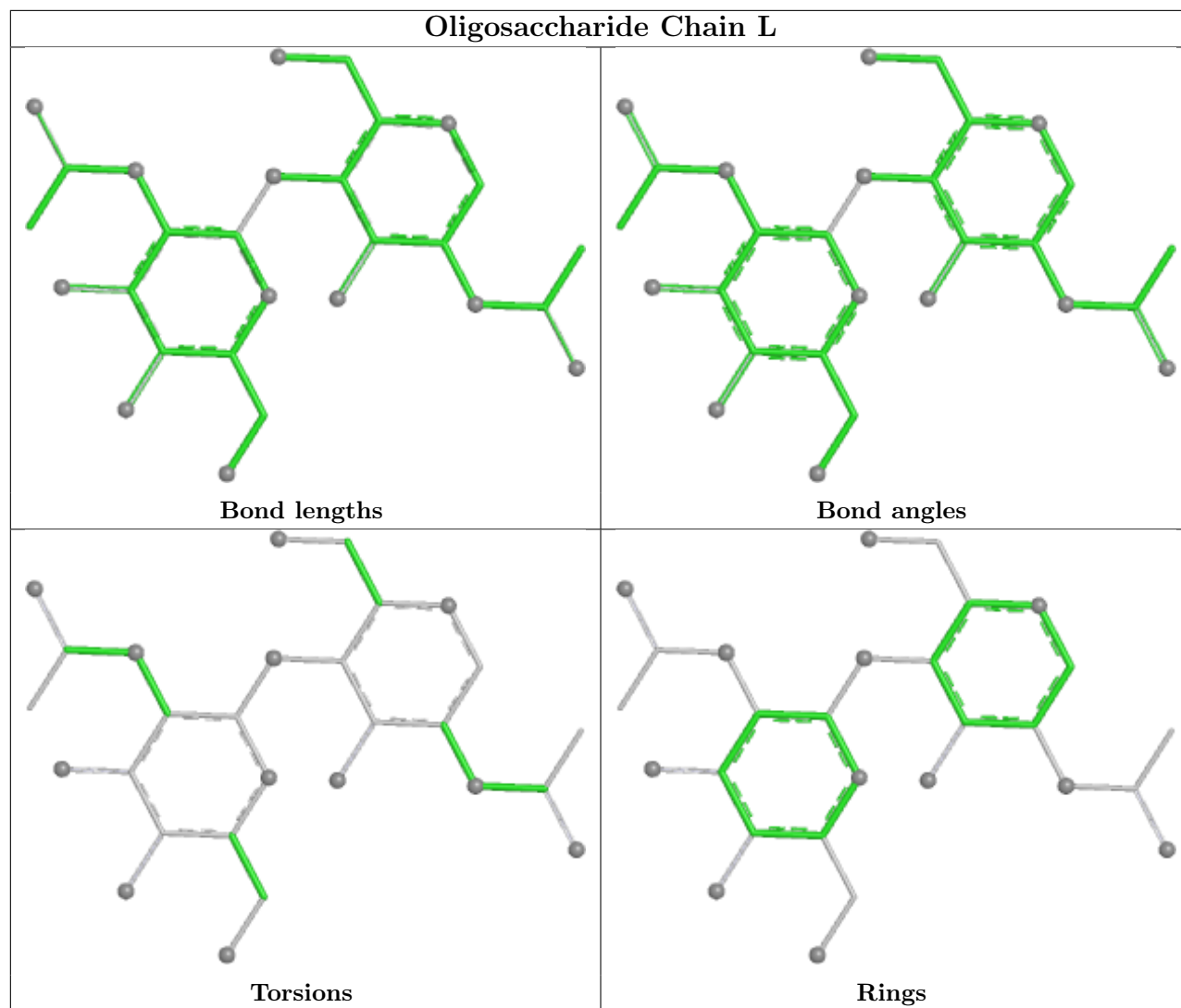
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	1	NAG	4	0
2	Q	2	NAG	1	0
2	N	2	NAG	1	0
2	a	2	NAG	5	0
2	Y	2	NAG	1	0
2	L	1	NAG	1	0
2	Z	2	NAG	2	0

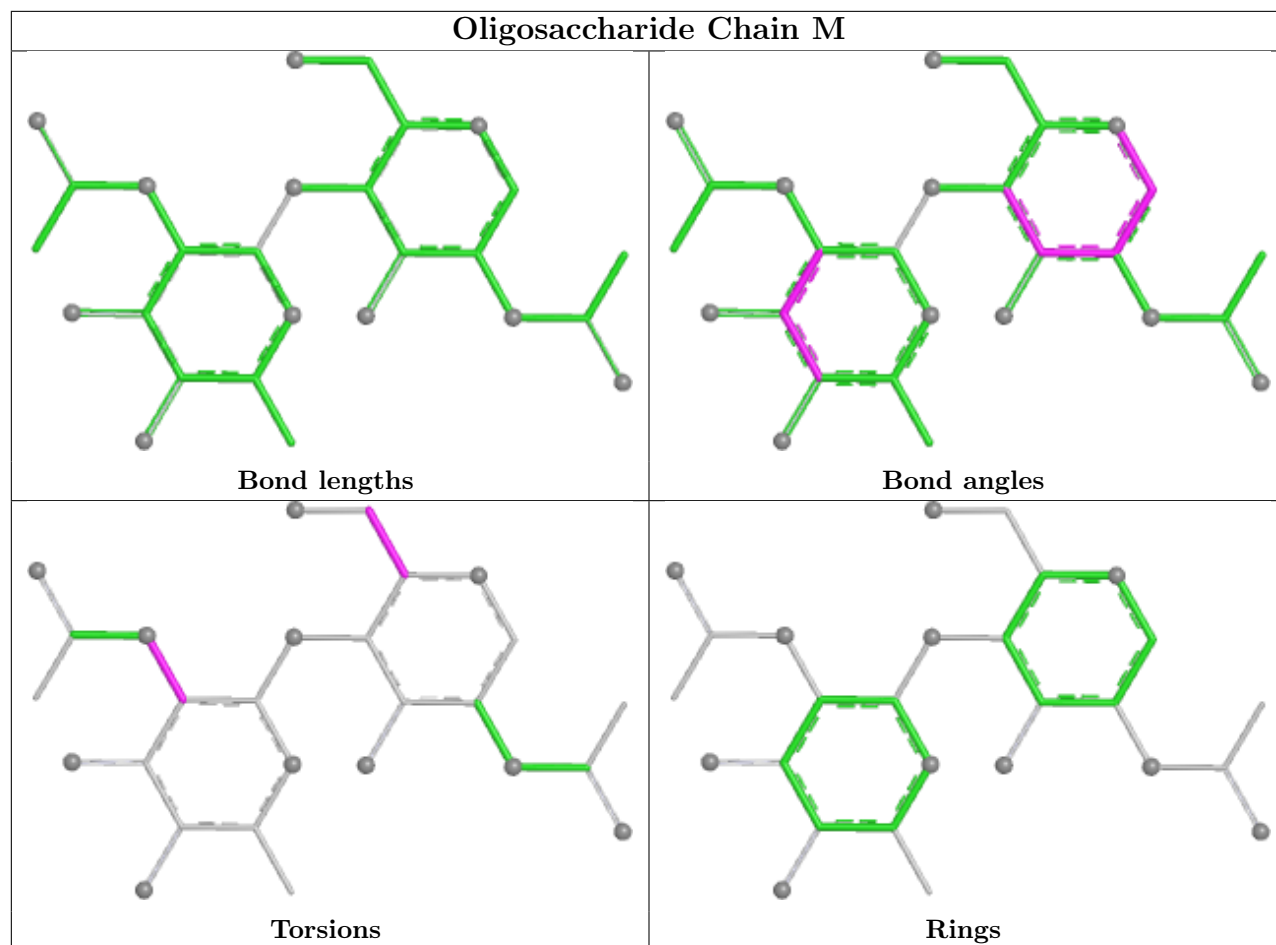
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

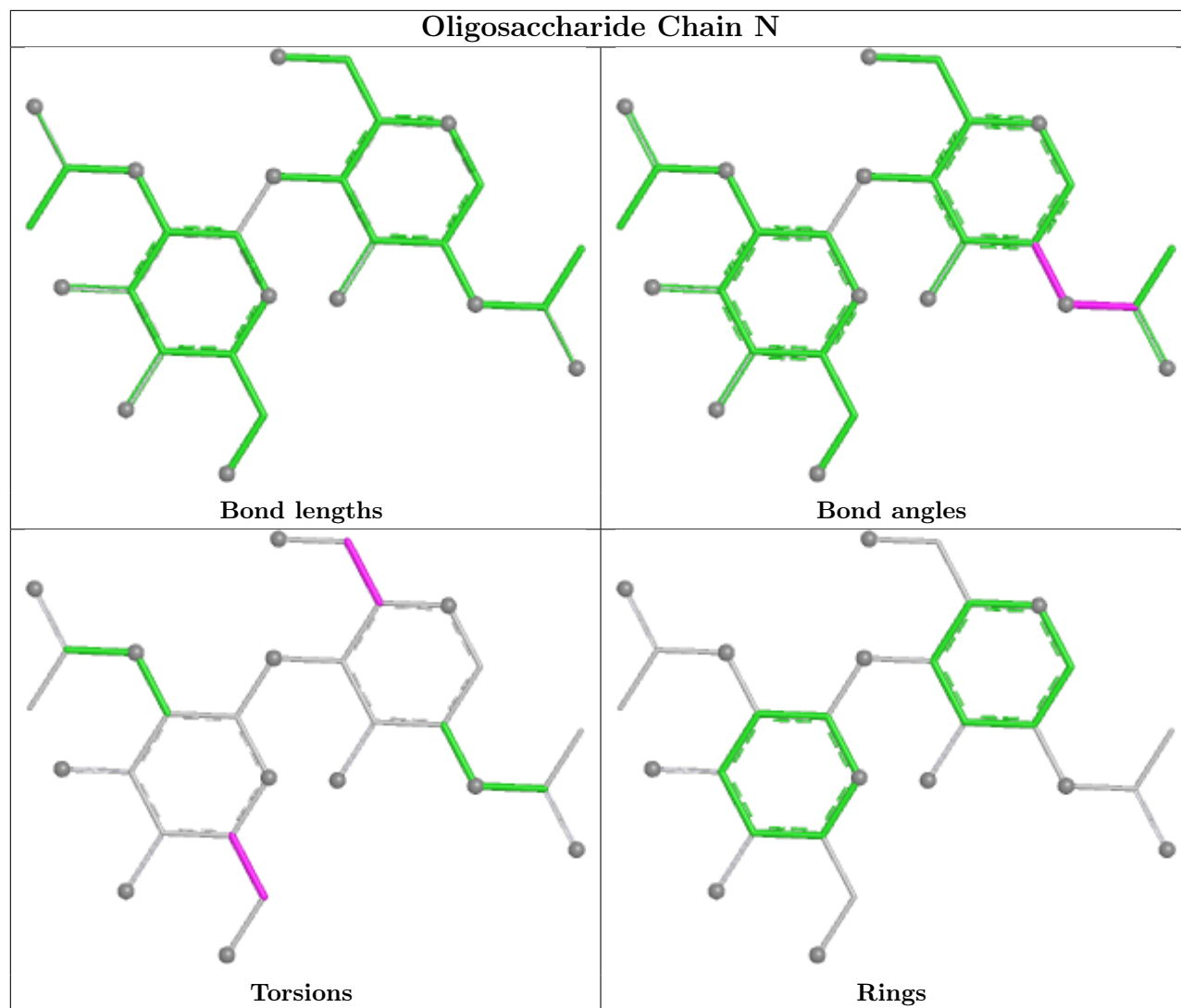


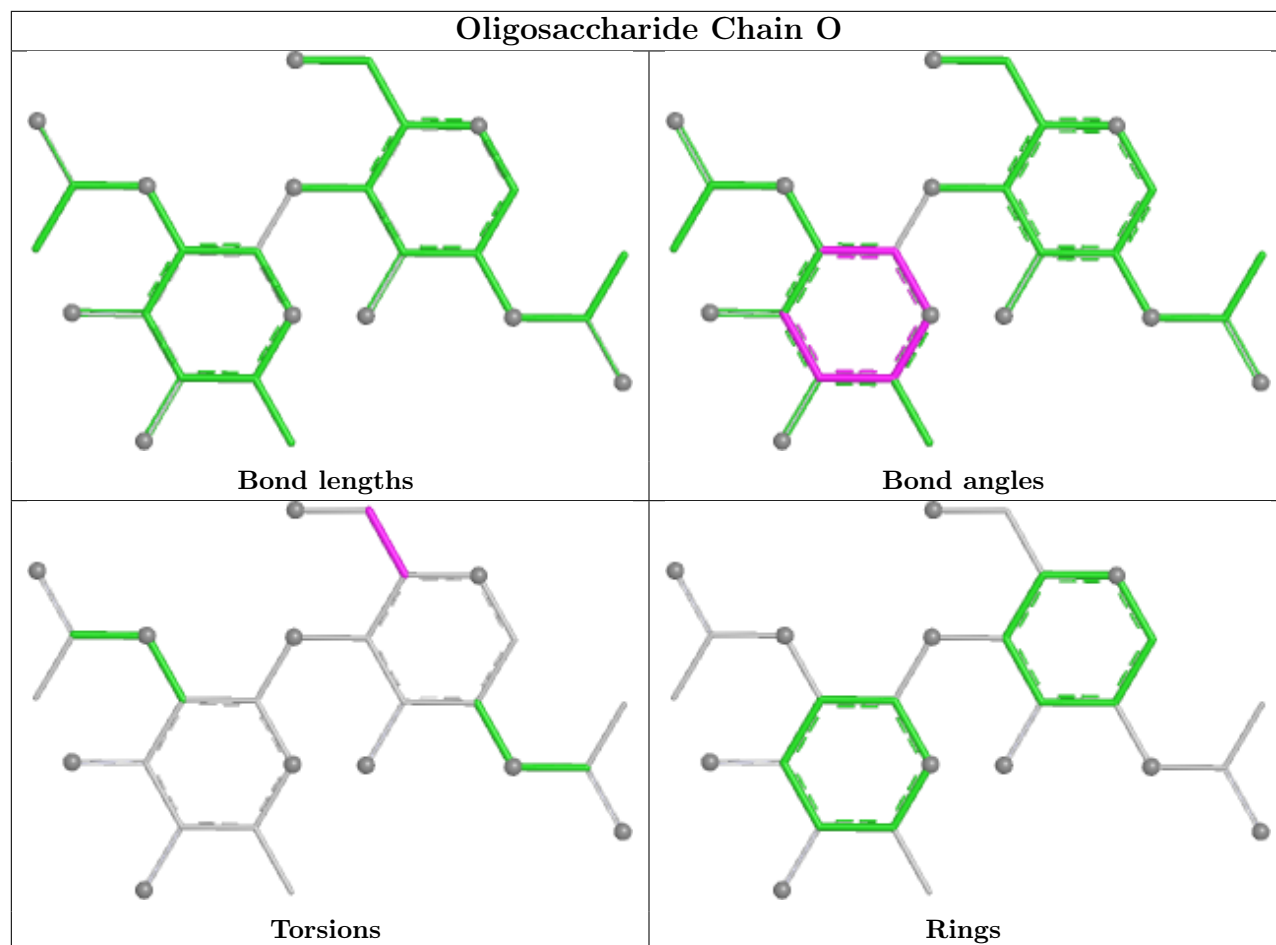


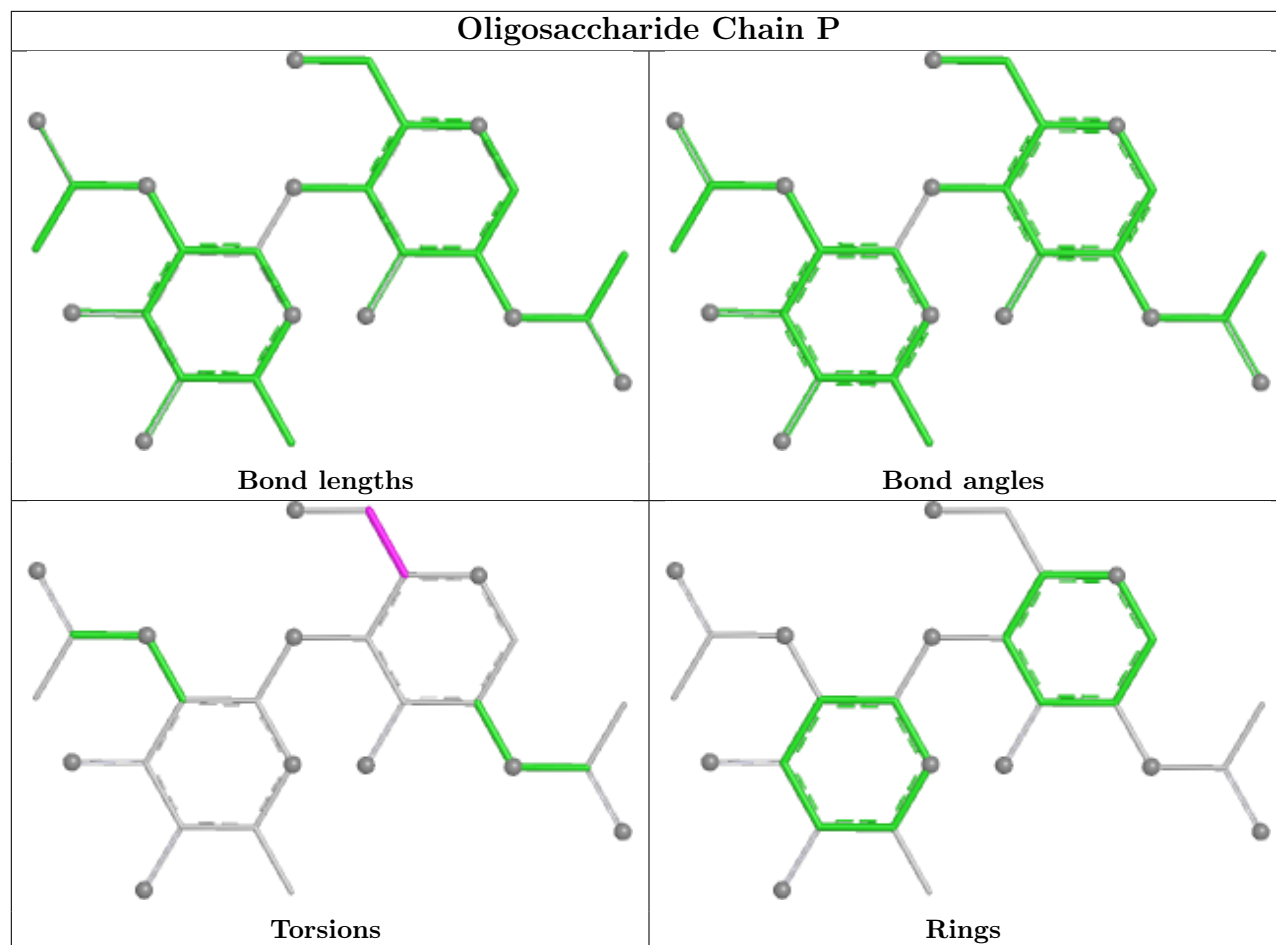


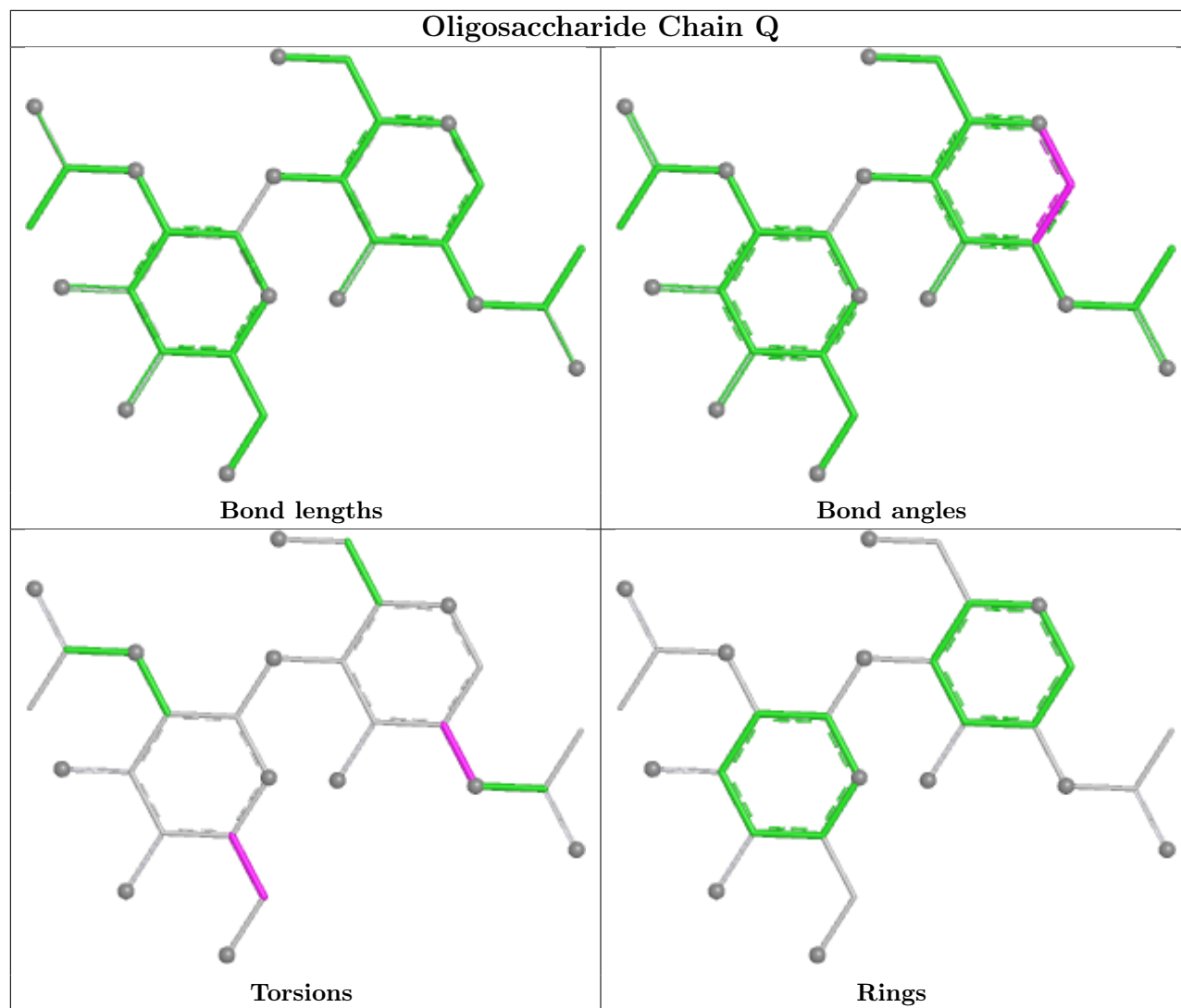


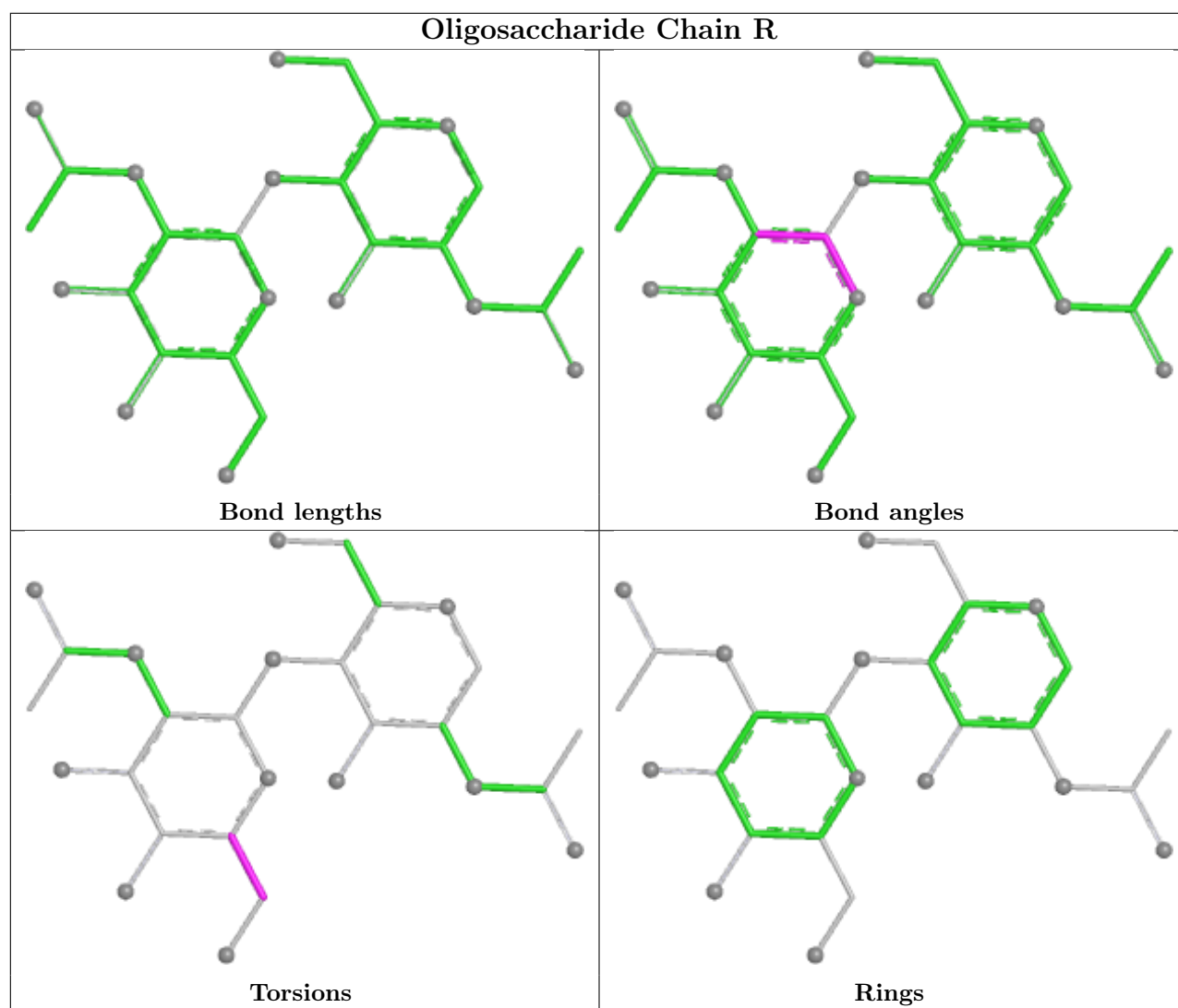


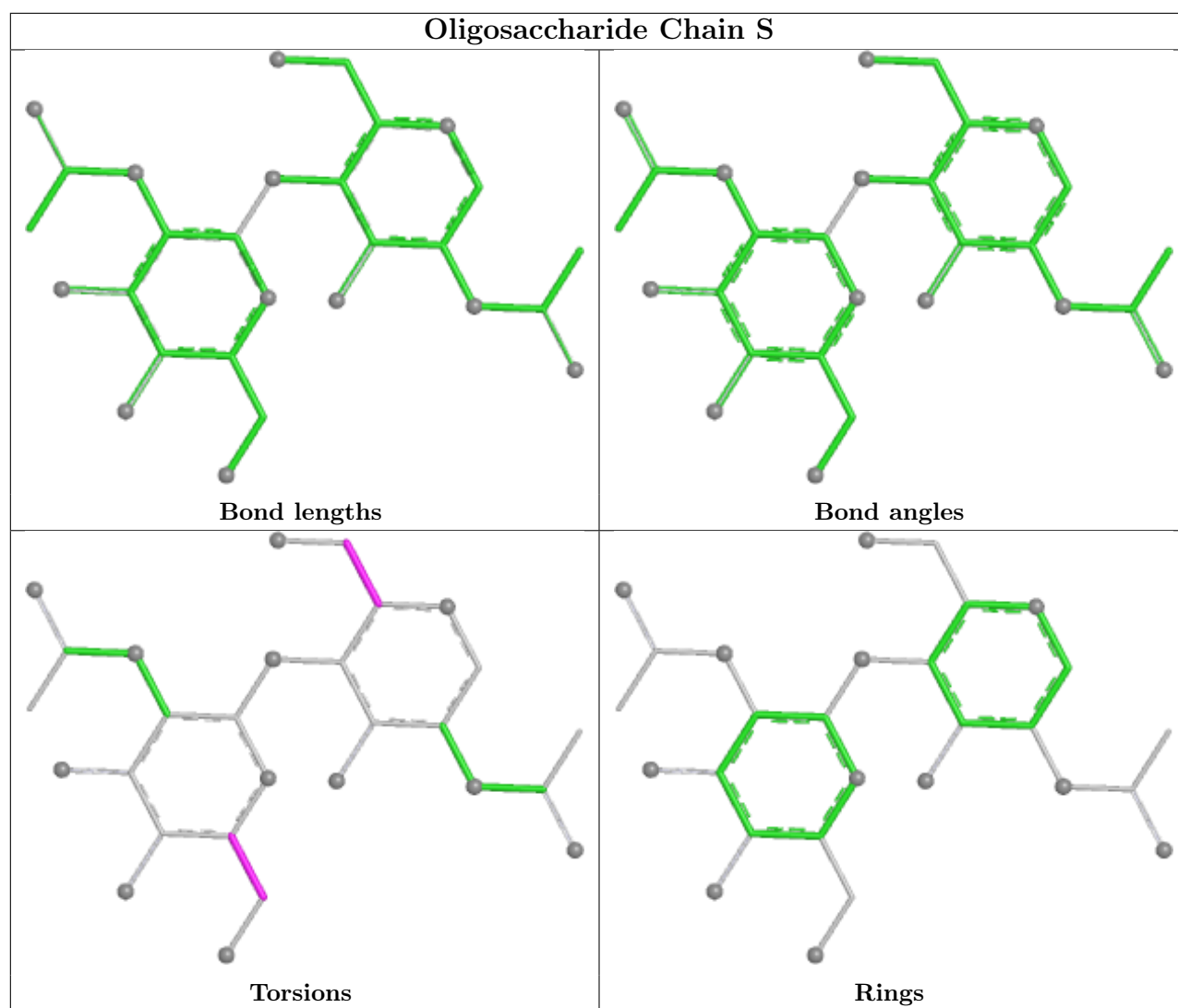


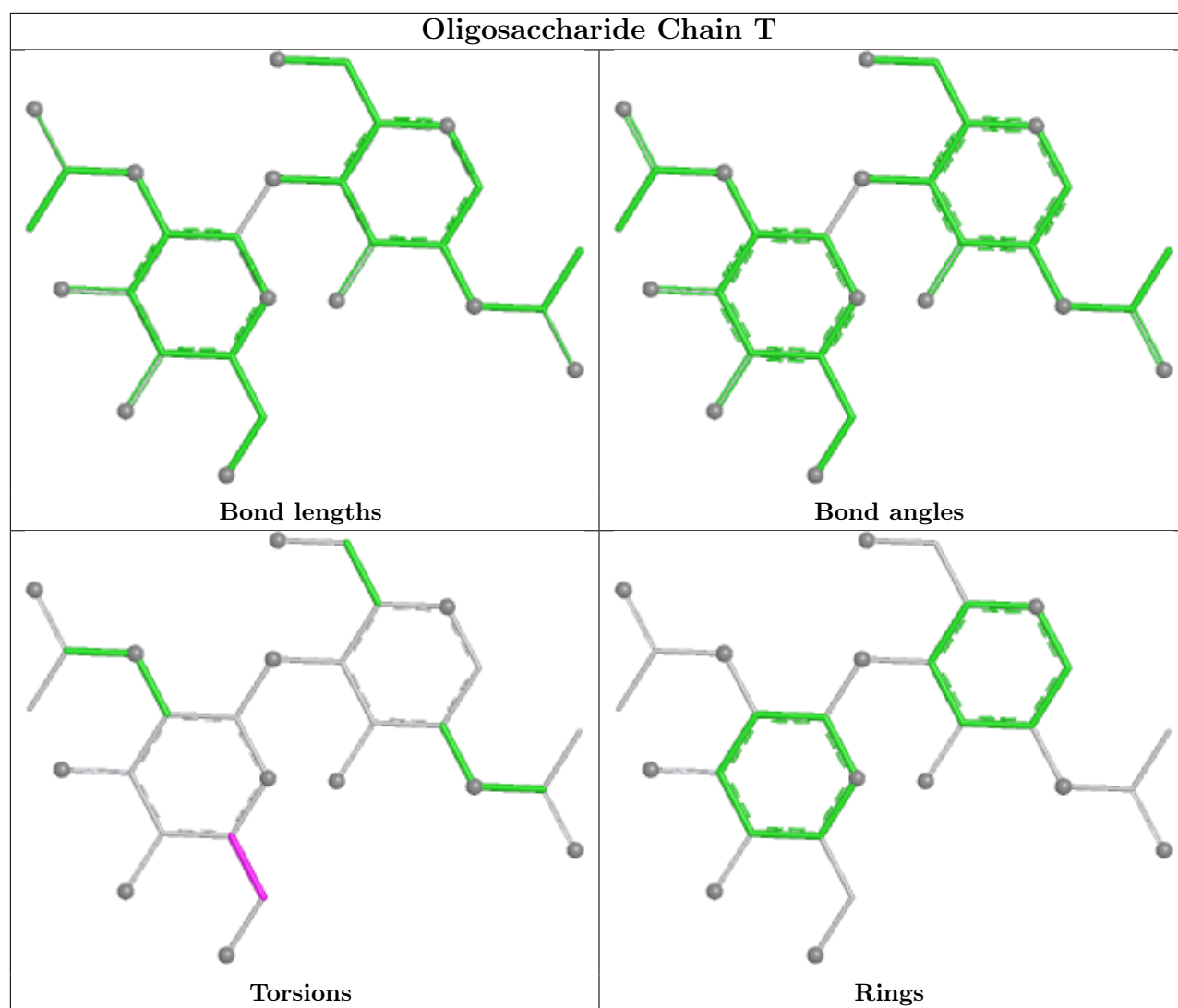


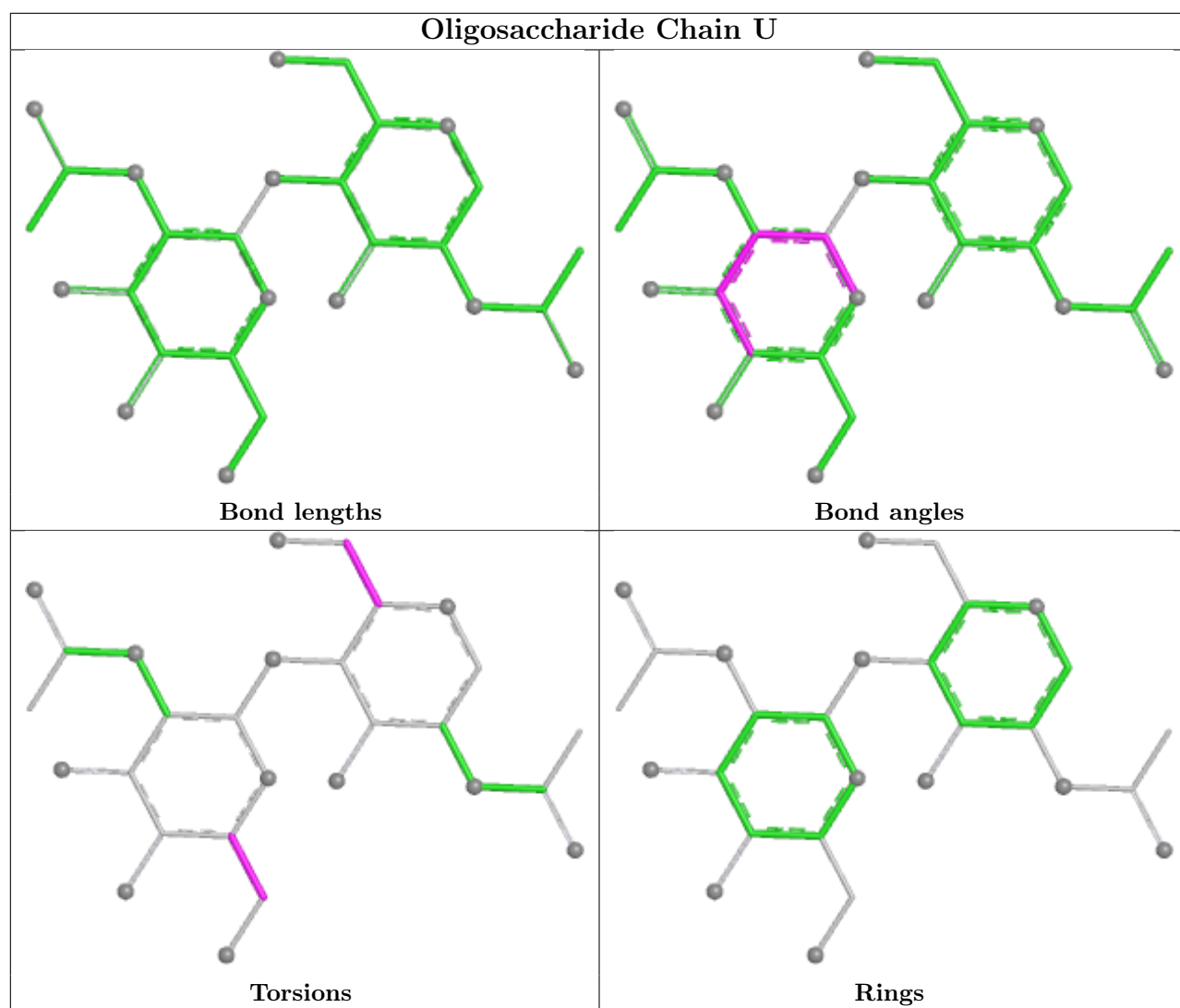


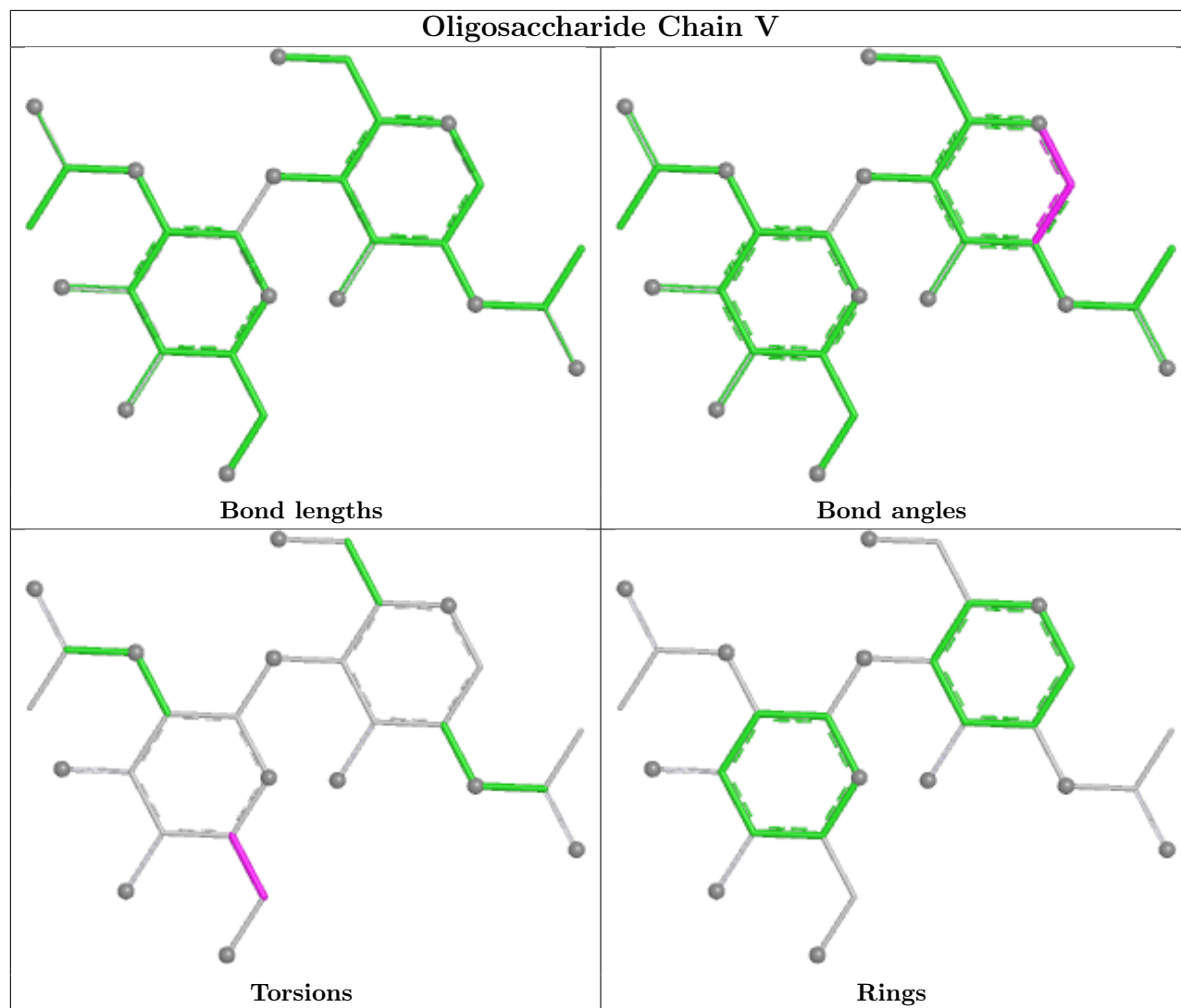


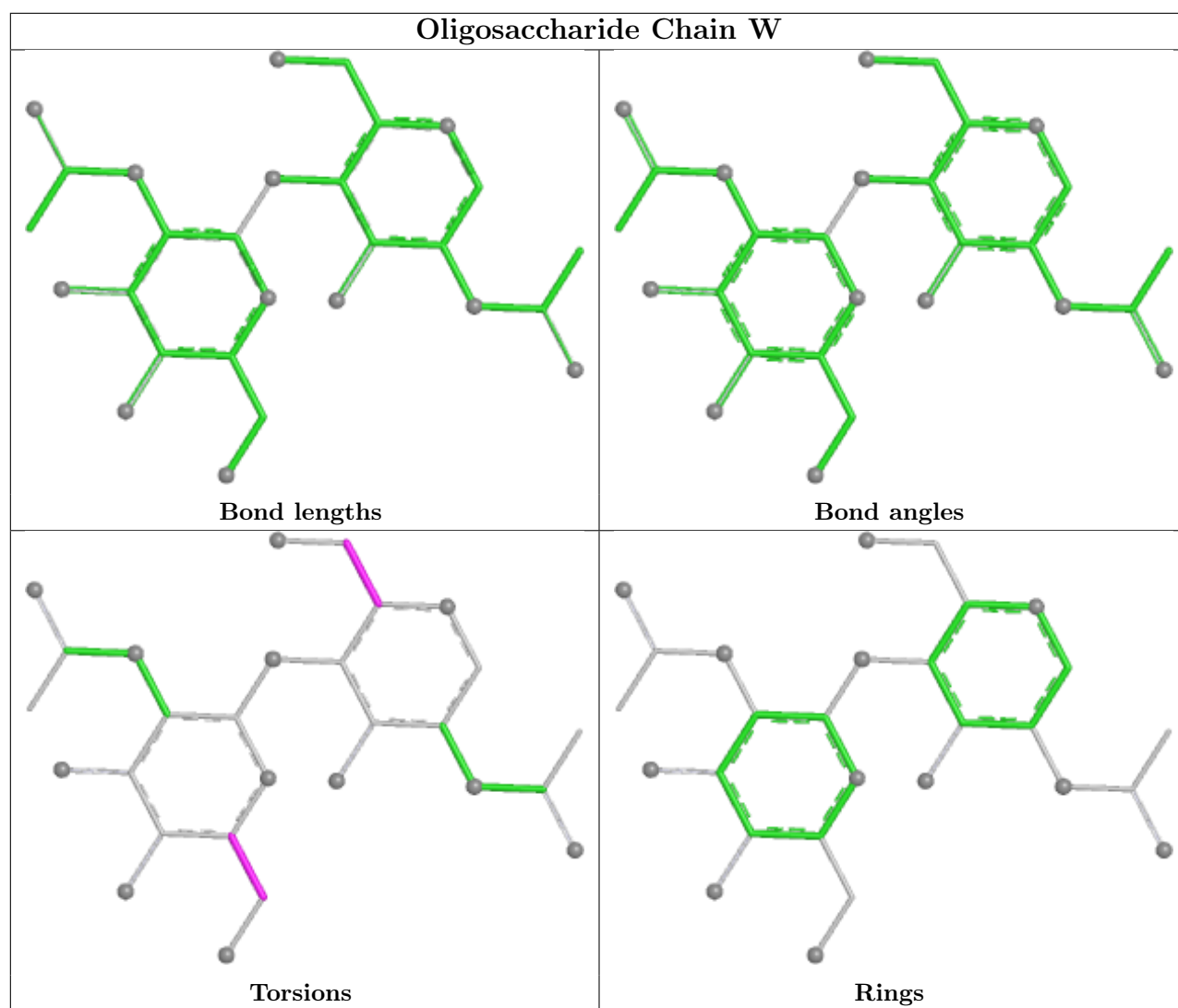


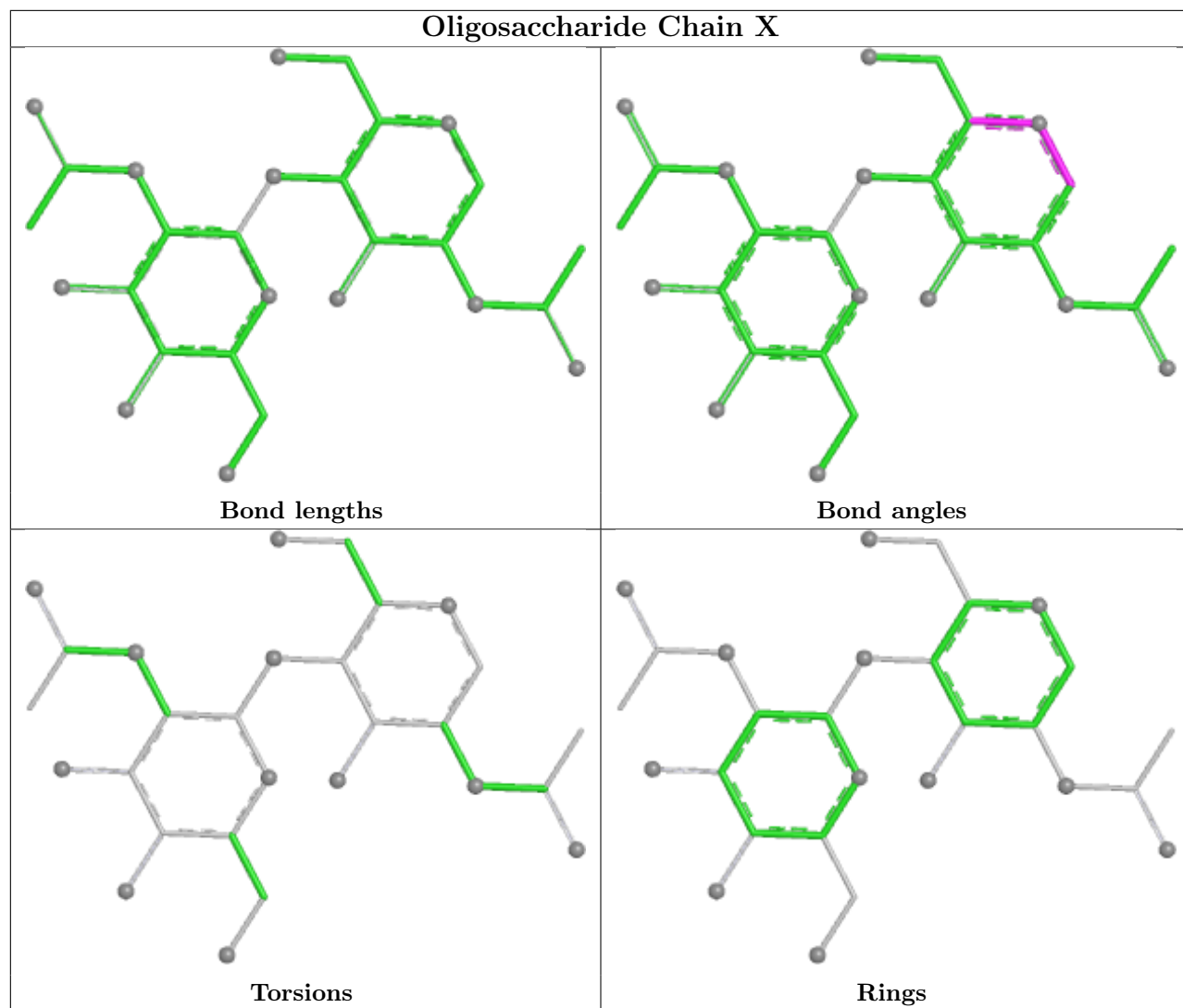


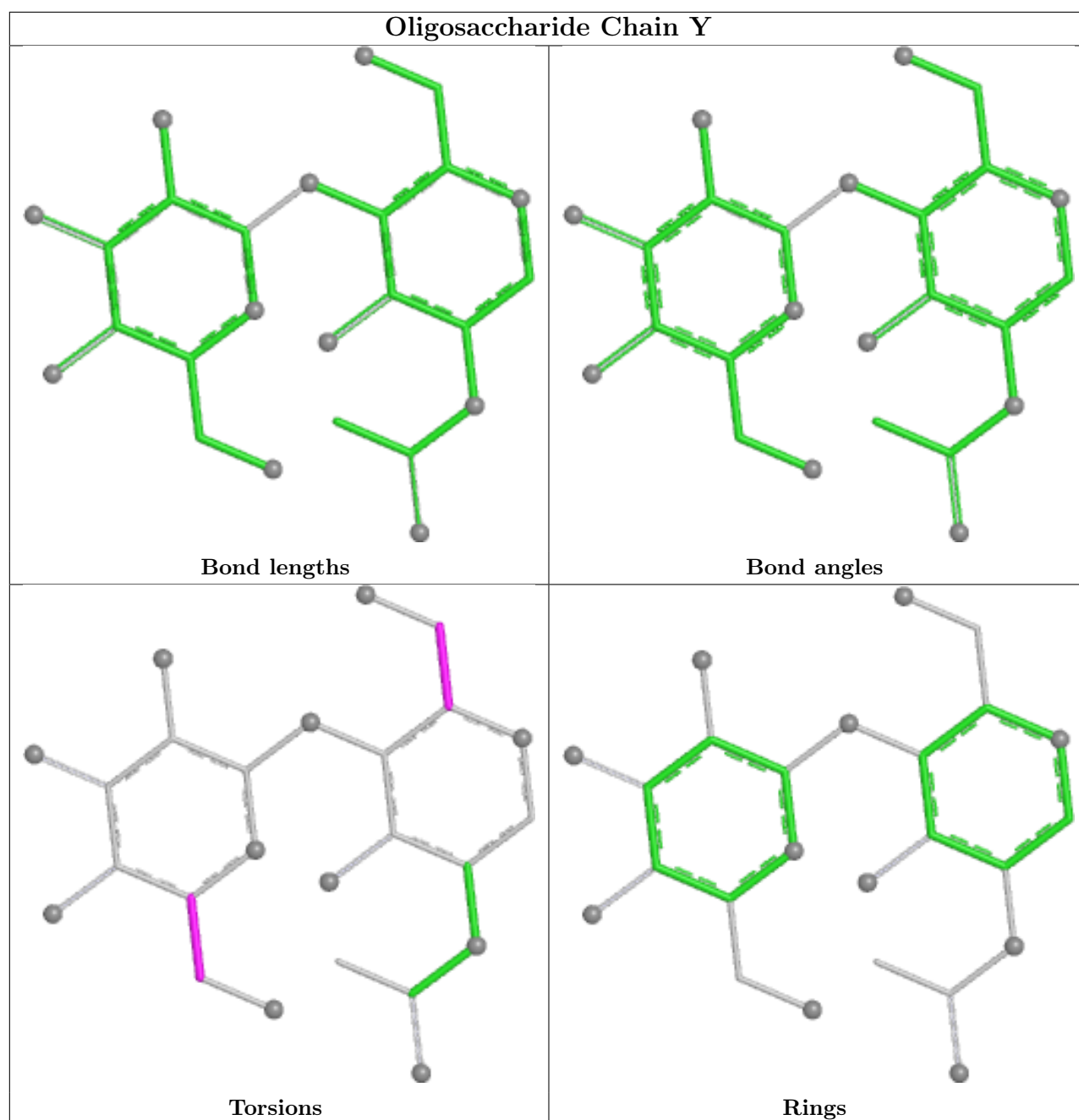


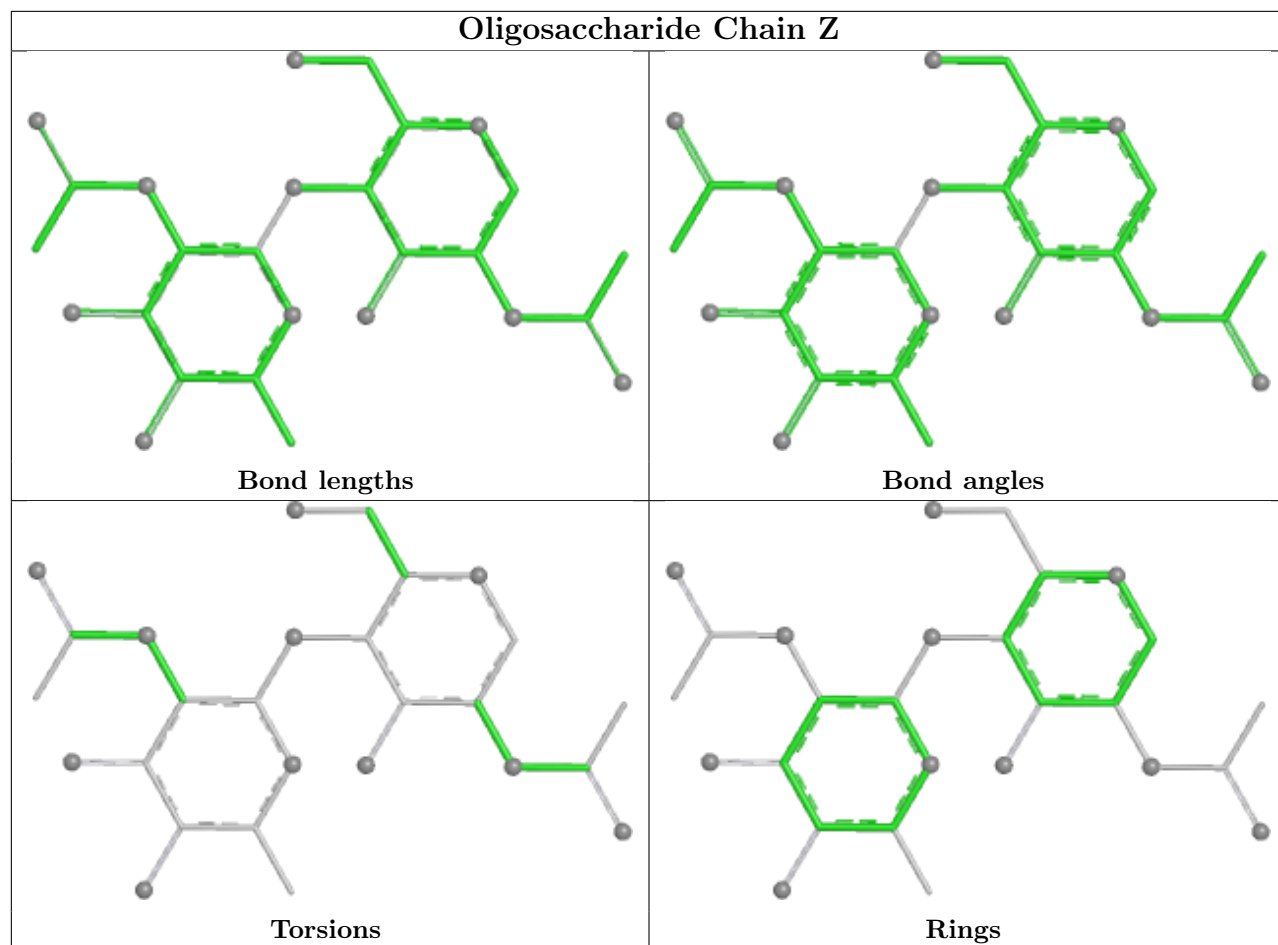


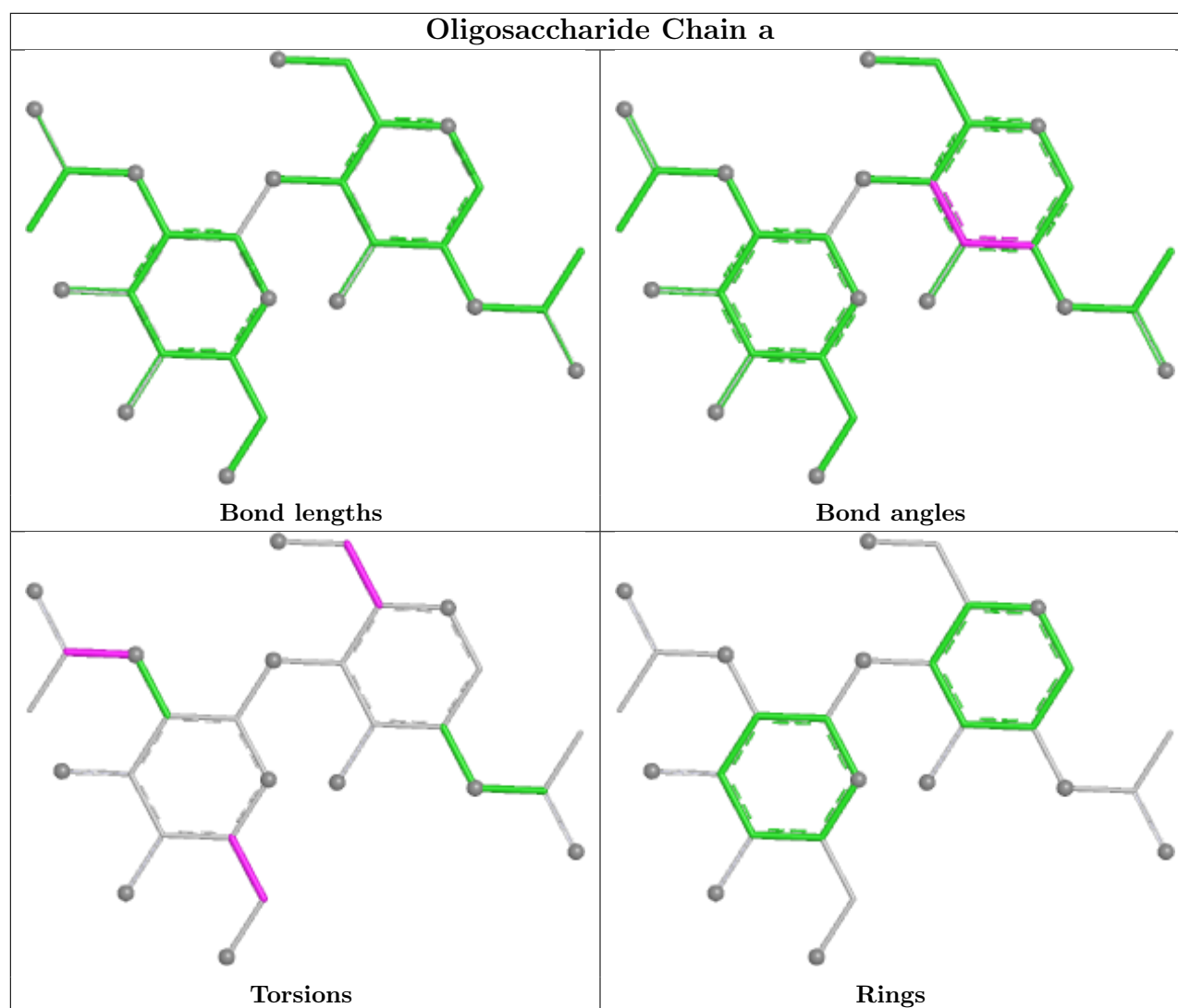












5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	605	1	10,10,15	0.61	0	12,14,21	0.62	0
4	NAG	A	608	1	14,14,15	0.55	0	17,19,21	0.79	0
4	NAG	H	606	1	14,14,15	0.47	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	605	1	14,14,15	0.50	0	17,19,21	0.64	0
4	NAG	B	607	1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
4	NAG	C	608	1	14,14,15	0.56	0	17,19,21	0.83	0
4	NAG	F	602	1	14,14,15	0.48	0	17,19,21	0.82	0
4	NAG	D	608	1	14,14,15	0.52	0	17,19,21	1.37	1 (5%)
6	PEG	D	609	-	4,4,6	0.59	0	3,3,5	0.20	0
4	NAG	G	604	1	14,14,15	0.54	0	17,19,21	0.92	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
4	NAG	G	605	1	-	-	0/1/1/1
4	NAG	A	608	1	-	2/6/23/26	0/1/1/1
4	NAG	H	606	1	-	4/6/23/26	0/1/1/1
4	NAG	F	605	1	-	2/6/23/26	0/1/1/1
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1
4	NAG	C	608	1	-	0/6/23/26	0/1/1/1
4	NAG	F	602	1	-	0/6/23/26	0/1/1/1
4	NAG	D	608	1	-	0/6/23/26	0/1/1/1
6	PEG	D	609	-	-	2/2/2/4	-
4	NAG	G	604	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	608	NAG	C1-O5-C5	4.41	118.10	112.19
4	G	604	NAG	C1-O5-C5	2.33	115.31	112.19
4	B	607	NAG	C1-O5-C5	2.23	115.17	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	604	NAG	O5-C5-C6-O6
4	G	604	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	605	NAG	O5-C5-C6-O6
4	F	605	NAG	C4-C5-C6-O6
4	H	606	NAG	O5-C5-C6-O6
4	H	606	NAG	C8-C7-N2-C2
4	H	606	NAG	O7-C7-N2-C2
4	H	606	NAG	C4-C5-C6-O6
4	A	608	NAG	O5-C5-C6-O6
4	A	608	NAG	C4-C5-C6-O6
6	D	609	PEG	C1-C2-O2-C3
6	D	609	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	NAG	2	0
4	C	608	NAG	2	0
6	D	609	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/510 (94%)	-0.14	5 (1%) 79 76	19, 47, 70, 100	2 (0%)
1	B	480/510 (94%)	-0.22	2 (0%) 88 86	18, 41, 71, 101	2 (0%)
1	C	483/510 (94%)	-0.14	5 (1%) 79 76	28, 46, 75, 105	0
1	D	479/510 (93%)	-0.25	4 (0%) 82 80	26, 42, 67, 114	1 (0%)
1	E	482/510 (94%)	0.76	30 (6%) 26 23	54, 83, 119, 135	0
1	F	477/510 (93%)	0.57	22 (4%) 37 33	53, 75, 99, 126	0
1	G	478/510 (93%)	0.63	24 (5%) 34 30	44, 77, 122, 160	0
1	H	481/510 (94%)	1.07	61 (12%) 8 6	62, 91, 128, 142	0
All	All	3843/4080 (94%)	0.29	153 (3%) 42 38	18, 63, 111, 160	5 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	357	LEU	4.6
1	H	396	PHE	4.4
1	E	168	ASP	4.3
1	F	501	GLU	4.0
1	E	473	TRP	3.9
1	F	168	ASP	3.9
1	H	283	THR	3.9
1	H	362	PHE	3.8
1	C	504	SER	3.8
1	E	504	SER	3.7
1	H	174	TYR	3.7
1	H	471	TRP	3.6
1	G	430	TYR	3.6
1	H	361	VAL	3.6
1	B	502	LEU	3.6
1	F	217	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	187	GLN	3.5
1	G	184	GLY	3.5
1	E	224	TYR	3.5
1	E	442	SER	3.5
1	F	202	SER	3.5
1	H	397	PRO	3.5
1	H	384	PHE	3.5
1	G	191	GLY	3.4
1	H	46	ALA	3.4
1	H	27	LEU	3.3
1	H	22	PRO	3.3
1	G	115	GLY	3.2
1	G	114	ALA	3.2
1	A	22	PRO	3.2
1	D	22	PRO	3.2
1	E	22	PRO	3.1
1	F	203	GLY	3.1
1	E	503	ARG	3.1
1	H	65	THR	3.1
1	H	466	ASP	3.1
1	G	231	ALA	3.0
1	H	272	SER	3.0
1	E	254	LEU	3.0
1	H	363	GLY	3.0
1	H	354	ALA	2.9
1	F	401	ASP	2.9
1	H	29	LEU	2.9
1	F	44	ALA	2.9
1	E	314	SER	2.8
1	F	24	ASN	2.8
1	H	378	SER	2.8
1	E	348	LEU	2.8
1	H	66	SER	2.8
1	D	168	ASP	2.8
1	H	64	PHE	2.7
1	E	443	ARG	2.7
1	H	275	GLY	2.7
1	F	221	LEU	2.6
1	H	469	ALA	2.6
1	G	186	SER	2.6
1	G	419	GLN	2.6
1	E	502	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	495	CYS	2.5
1	H	332	SER	2.5
1	H	359	ALA	2.5
1	F	184	GLY	2.5
1	E	172	PHE	2.5
1	G	427	LEU	2.5
1	H	352	LEU	2.5
1	H	137	ALA	2.5
1	H	221	LEU	2.5
1	H	338	SER	2.5
1	H	398	ILE	2.4
1	G	189	GLN	2.4
1	E	287	TRP	2.4
1	H	290	THR	2.4
1	H	26	LEU	2.4
1	A	342[A]	HIS	2.4
1	E	64	PHE	2.4
1	G	145	VAL	2.4
1	C	492	SER	2.4
1	H	449	GLN	2.4
1	H	382	ARG	2.4
1	H	313	VAL	2.4
1	F	22	PRO	2.3
1	G	283	THR	2.3
1	H	287	TRP	2.4
1	H	340	THR	2.3
1	G	412	LEU	2.3
1	H	349	LEU	2.3
1	G	199	ASN	2.3
1	E	316	LEU	2.3
1	H	468	LEU	2.3
1	H	394	MET	2.3
1	H	358	TRP	2.3
1	C	185	HIS	2.3
1	E	228	ASN	2.3
1	F	218	LEU	2.3
1	G	148	VAL	2.3
1	E	420	PRO	2.3
1	F	232	ALA	2.2
1	H	266	THR	2.2
1	E	276	ILE	2.2
1	F	146	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	201	GLU	2.2
1	E	35	PHE	2.2
1	C	383	HIS	2.2
1	G	263	LEU	2.2
1	E	353	GLU	2.2
1	H	443	ARG	2.2
1	E	313	VAL	2.2
1	E	406	PRO	2.2
1	A	183	CYS	2.2
1	H	284	ASN	2.2
1	G	187	GLN	2.2
1	H	467	GLN	2.2
1	A	184	GLY	2.2
1	G	276	ILE	2.2
1	E	296	VAL	2.1
1	F	46	ALA	2.1
1	B	183	CYS	2.1
1	G	219	ASP	2.1
1	G	402	PHE	2.1
1	H	228	ASN	2.1
1	D	165	THR	2.1
1	E	352	LEU	2.1
1	G	203	GLY	2.1
1	H	50	LEU	2.1
1	H	80	GLY	2.1
1	F	40	TYR	2.1
1	H	470	LYS	2.1
1	F	301	HIS	2.1
1	F	206	ARG	2.1
1	H	45	ILE	2.1
1	H	269	ILE	2.1
1	G	432	TYR	2.1
1	F	171	PHE	2.1
1	H	308	VAL	2.1
1	H	482	ALA	2.1
1	H	323	LEU	2.1
1	E	34	GLY	2.1
1	H	489	GLU	2.1
1	G	431	TYR	2.1
1	E	338	SER	2.1
1	D	183	CYS	2.1
1	F	230	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	420	PRO	2.1
1	H	285	LEU	2.0
1	H	295	LEU	2.0
1	H	316	LEU	2.0
1	E	43	SER	2.0
1	H	392	PHE	2.0
1	C	491	LEU	2.0
1	F	192	THR	2.0
1	A	505	HIS	2.0
1	E	446	HIS	2.0
1	H	69	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FGP	G	70	7/12	0.84	0.11	72,75,80,83	0
1	FGP	F	70	11/12	0.91	0.11	61,72,131,141	0
1	FGP	E	70	11/12	0.91	0.19	68,80,139,144	0
1	FGP	D	70	11/12	0.92	0.12	29,40,93,95	0
1	FGP	H	70	7/12	0.92	0.10	66,68,70,75	0
1	FGP	C	70	11/12	0.94	0.11	32,40,91,115	0
1	FGP	A	70	11/12	0.95	0.12	33,50,105,123	0
1	FGP	B	70	11/12	0.96	0.12	26,34,85,101	0

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(Å ²)	Q<0.9
2	NAG	Y	2	11/15	0.56	0.13	80,116,138,142	0
2	NAG	Q	2	14/15	0.64	0.11	80,116,146,150	0
2	NAG	U	2	14/15	0.65	0.14	71,119,139,145	0
2	NAG	Z	2	13/15	0.65	0.15	69,98,115,115	0

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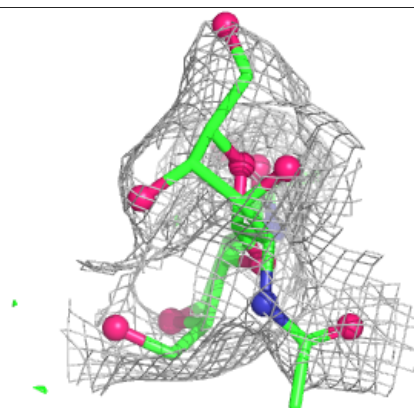
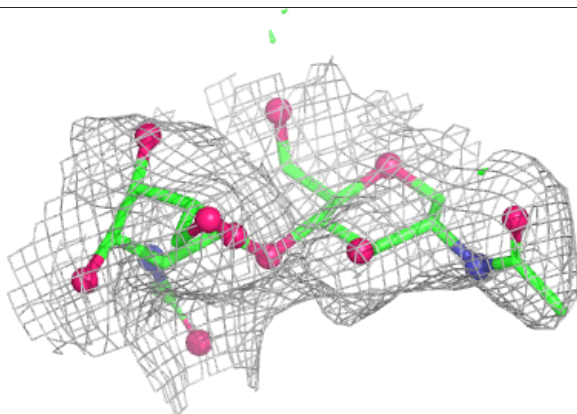
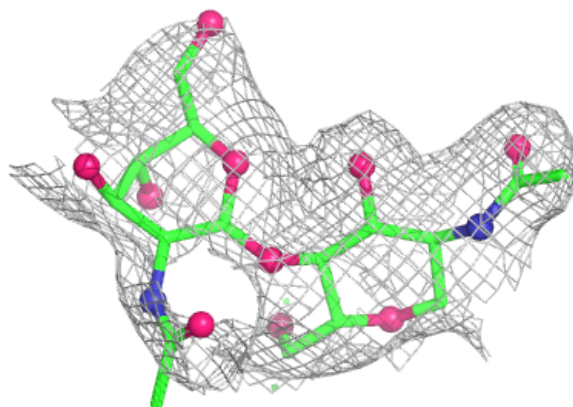
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	M	2	13/15	0.67	0.14	55,103,128,139	0
2	NAG	I	2	14/15	0.68	0.13	78,106,134,140	0
2	NAG	T	2	14/15	0.70	0.11	72,101,118,120	0
2	NAG	K	2	14/15	0.70	0.12	74,102,124,126	0
2	NAG	U	1	14/15	0.71	0.14	80,128,152,152	0
2	NAG	O	2	13/15	0.71	0.14	84,105,126,132	0
2	NAG	R	2	14/15	0.72	0.10	71,104,136,136	0
2	NAG	Q	1	14/15	0.72	0.12	71,112,124,129	0
2	NAG	L	2	14/15	0.73	0.13	73,97,111,114	0
2	NAG	P	2	13/15	0.74	0.12	60,92,106,120	0
2	NAG	W	2	14/15	0.74	0.12	58,74,92,96	0
2	NAG	O	1	14/15	0.75	0.12	55,78,105,130	0
2	NAG	R	1	14/15	0.76	0.11	48,80,128,145	0
2	NAG	S	2	14/15	0.78	0.10	53,76,115,118	0
2	NAG	X	1	14/15	0.81	0.10	58,73,85,86	0
2	NAG	V	2	14/15	0.81	0.12	56,77,85,90	0
2	NAG	N	2	14/15	0.81	0.10	70,87,99,104	0
2	NAG	J	2	14/15	0.83	0.10	47,83,104,116	0
2	NAG	K	1	14/15	0.84	0.09	54,72,94,97	0
2	NAG	L	1	14/15	0.85	0.09	49,64,88,90	0
2	NAG	I	1	14/15	0.85	0.10	60,98,132,137	0
2	NAG	W	1	14/15	0.86	0.11	44,78,94,95	0
2	NAG	Y	1	14/15	0.86	0.11	52,80,105,114	0
2	NAG	Z	1	14/15	0.87	0.09	47,64,74,77	0
2	NAG	X	2	14/15	0.87	0.09	60,75,94,100	0
2	NAG	T	1	14/15	0.89	0.09	56,65,92,100	0
2	NAG	N	1	14/15	0.90	0.07	48,63,78,81	0
2	NAG	V	1	14/15	0.91	0.09	49,63,77,79	0
2	NAG	M	1	14/15	0.91	0.09	44,65,85,107	0
2	NAG	J	1	14/15	0.93	0.07	36,48,61,70	0
2	NAG	S	1	14/15	0.94	0.06	36,43,61,69	0
2	NAG	P	1	14/15	0.94	0.06	39,49,67,68	0
2	NAG	a	1	14/15	-	-	76,127,145,153	0
2	NAG	a	2	14/15	-	-	86,132,149,150	0

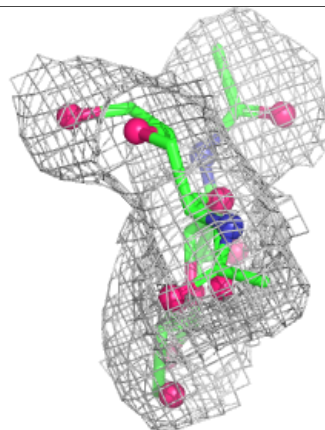
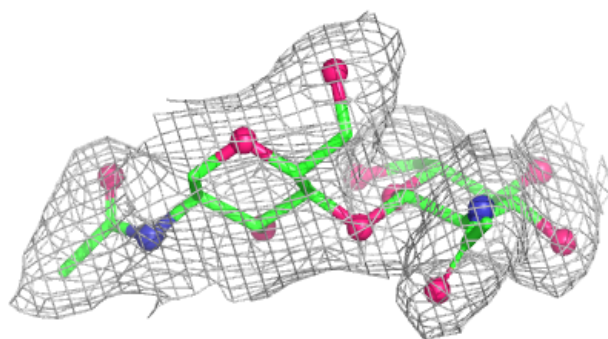
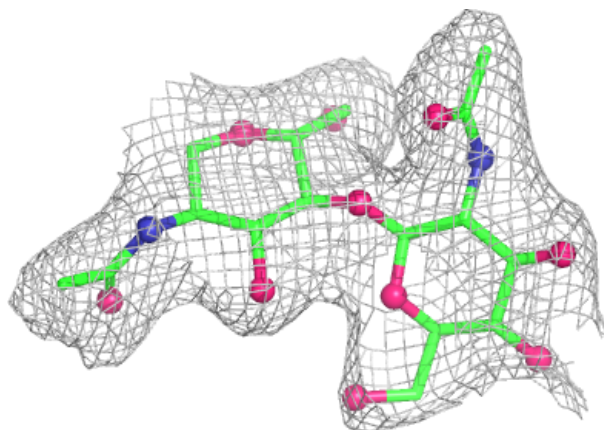
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

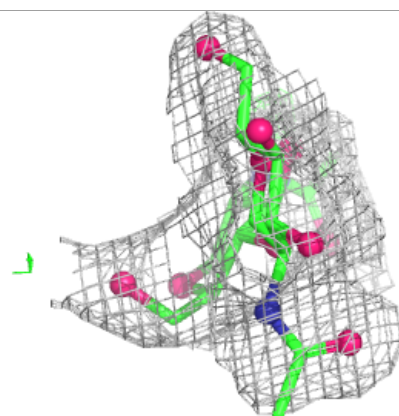
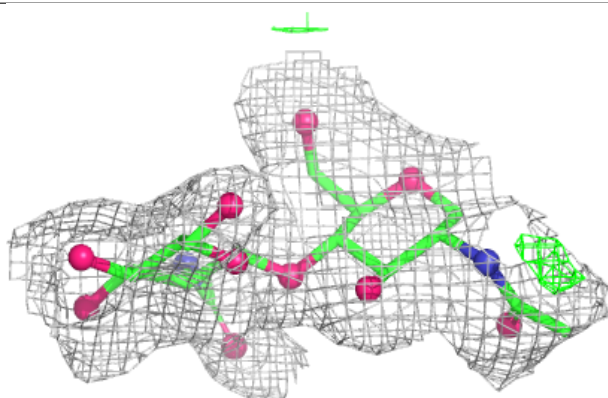
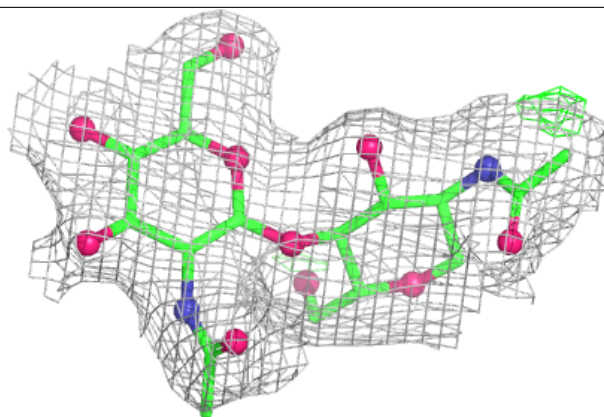
**Electron density around Chain J:**

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

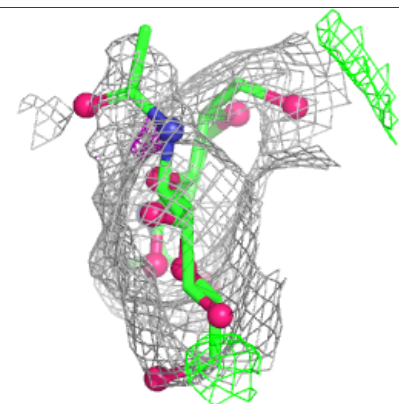
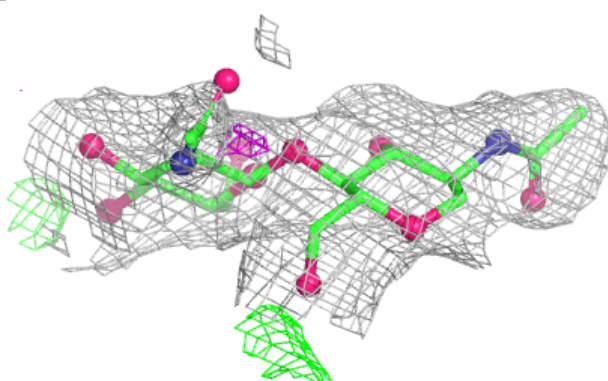
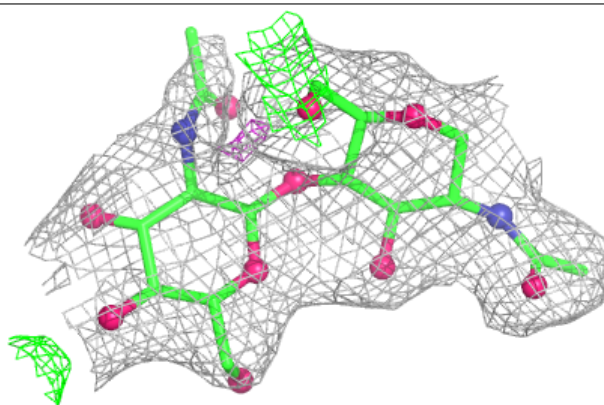


Electron density around Chain K:

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

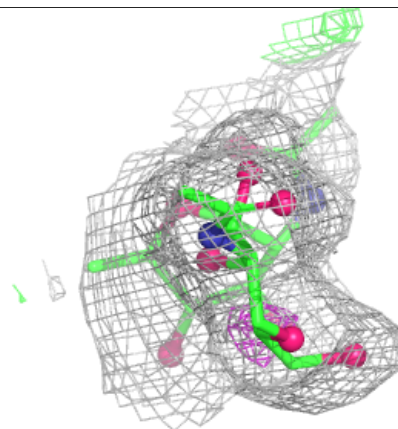
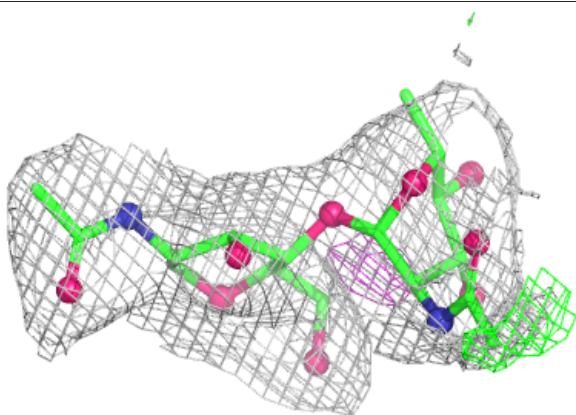
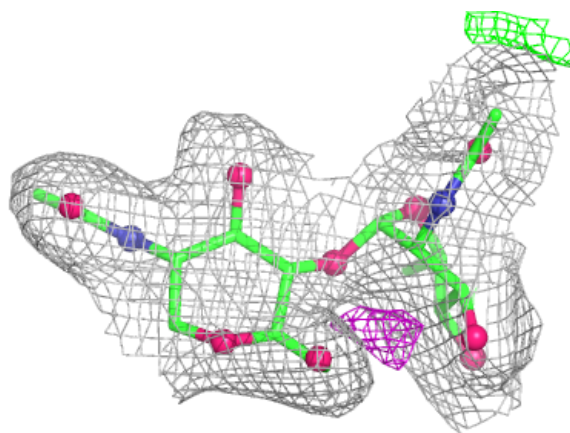
**Electron density around Chain L:**

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



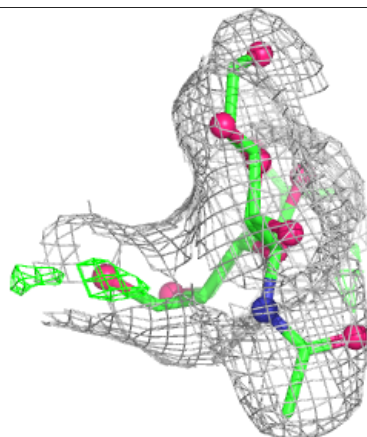
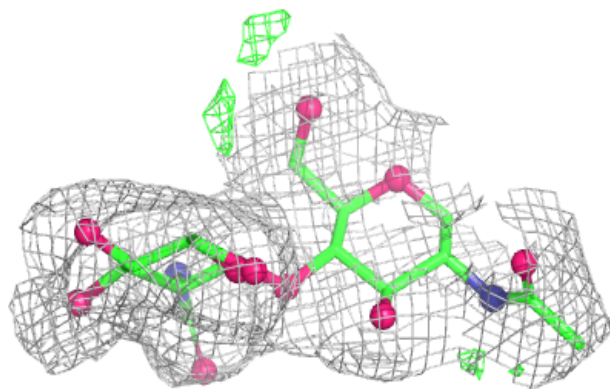
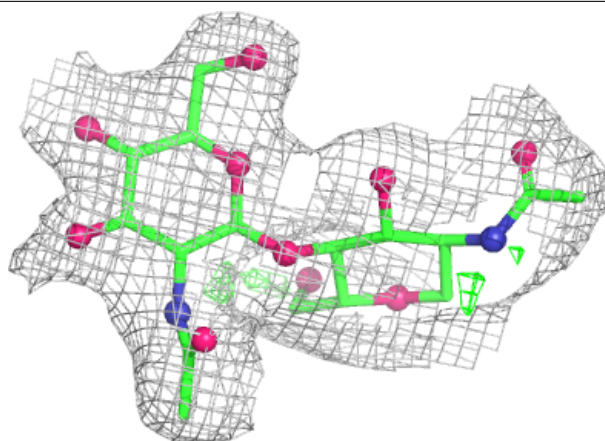
Electron density around Chain M:

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



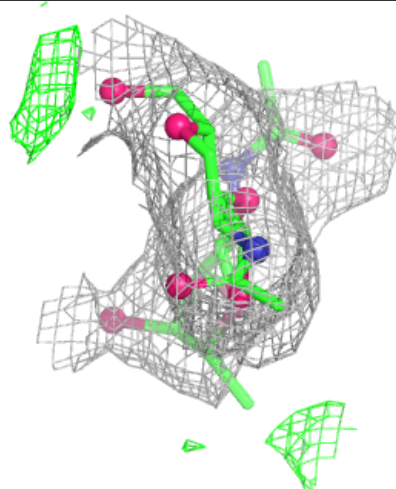
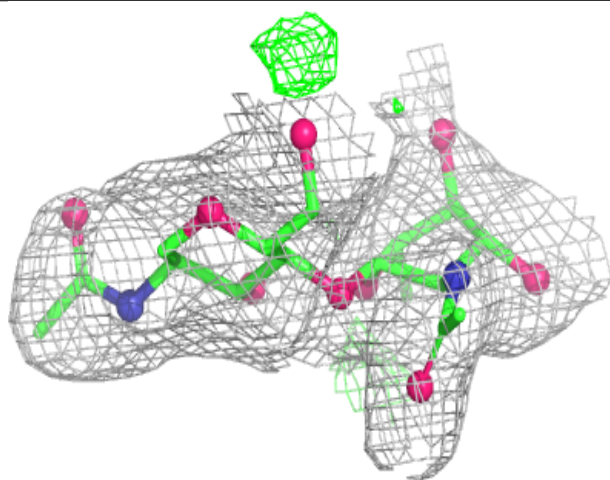
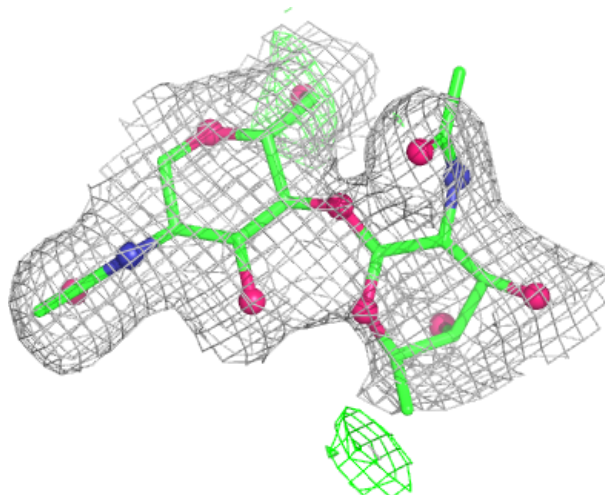
Electron density around Chain N:

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



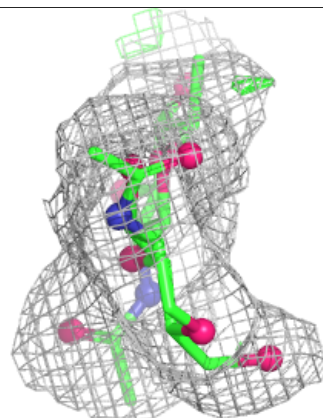
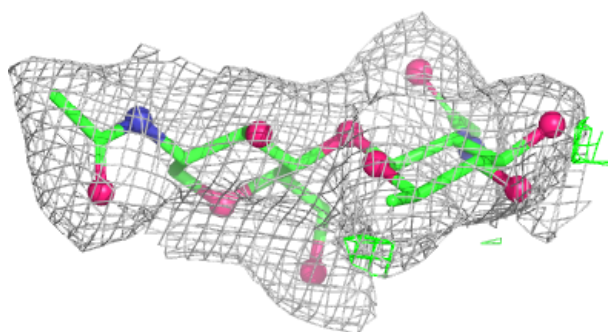
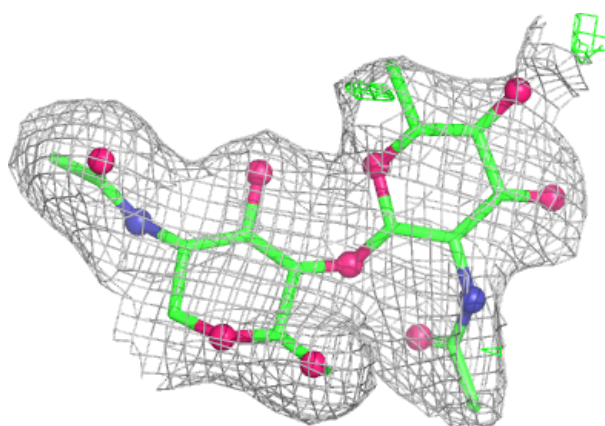
Electron density around Chain O:

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

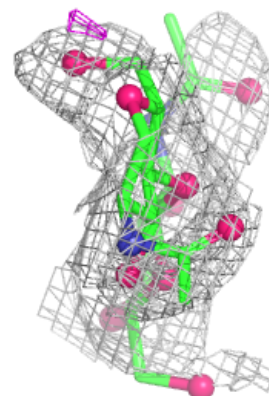
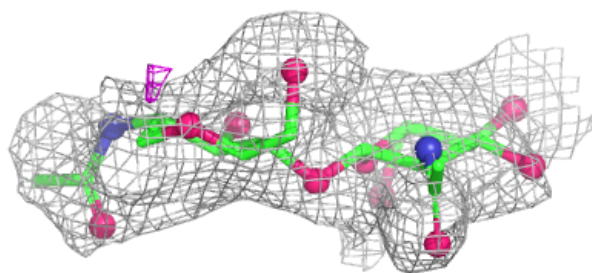
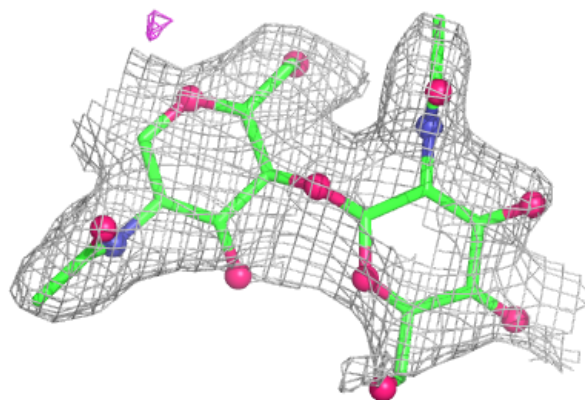


Electron density around Chain P:

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

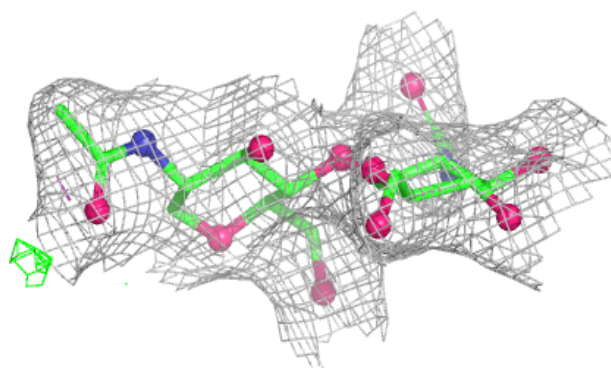
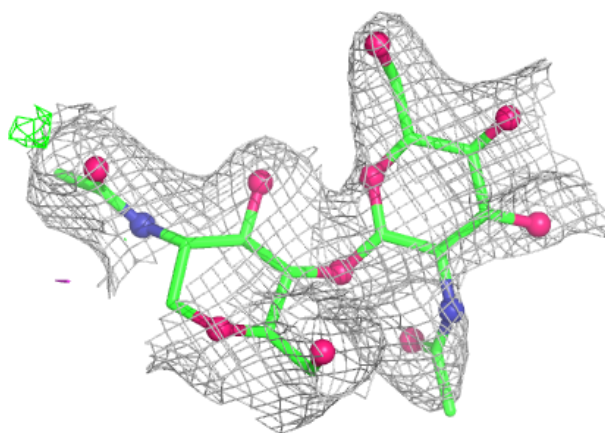
**Electron density around Chain Q:**

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



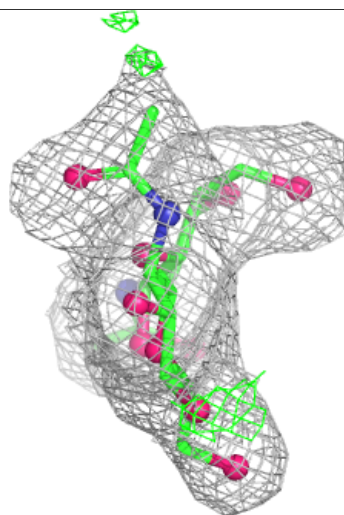
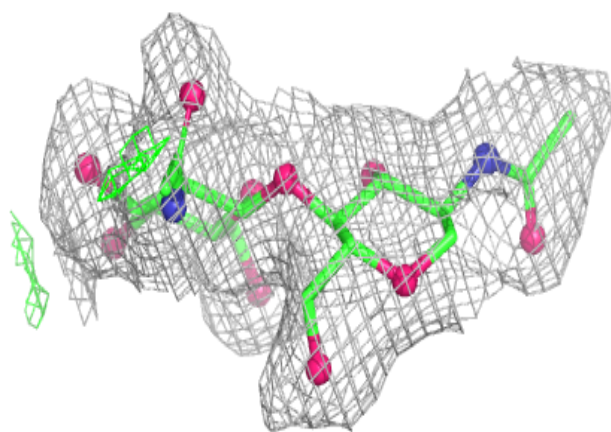
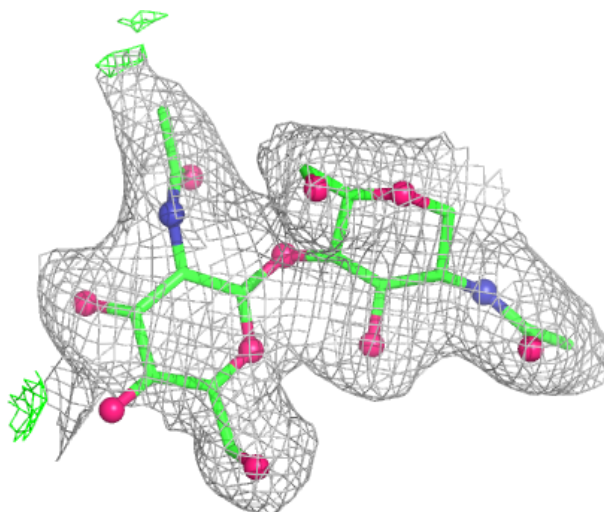
Electron density around Chain R:

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



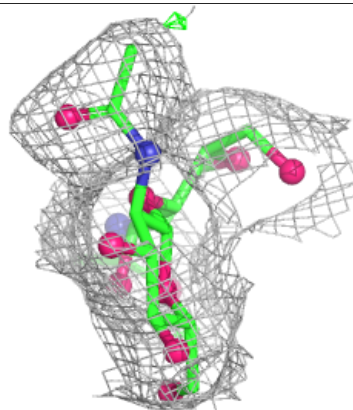
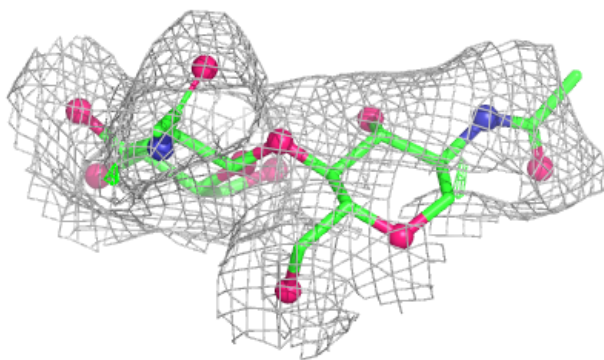
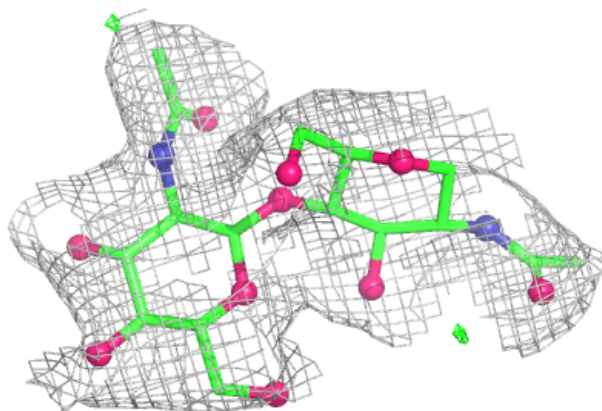
Electron density around Chain S:

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



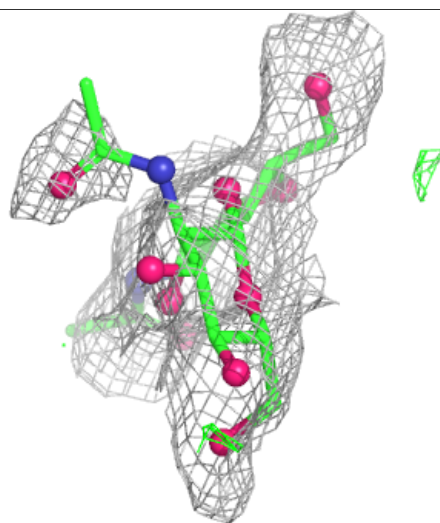
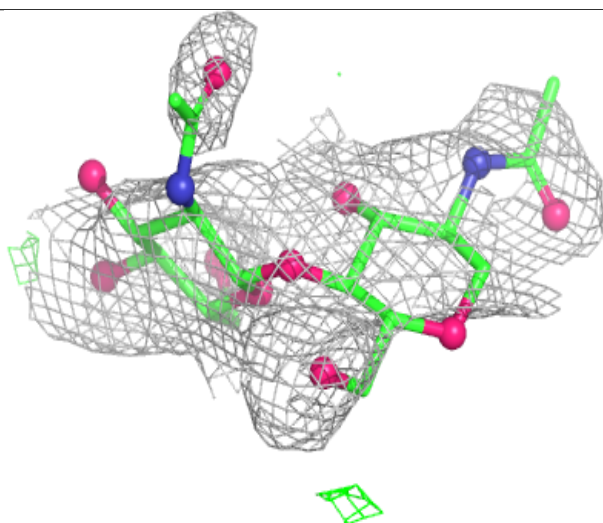
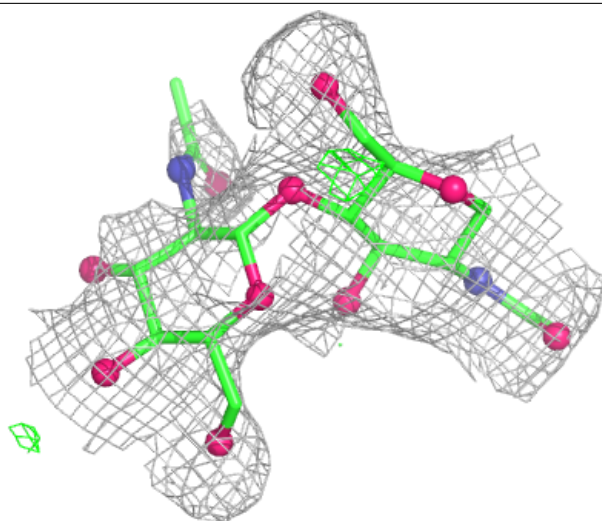
Electron density around Chain T:

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



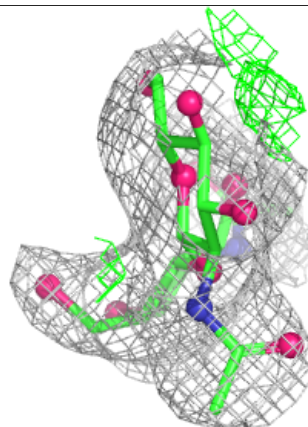
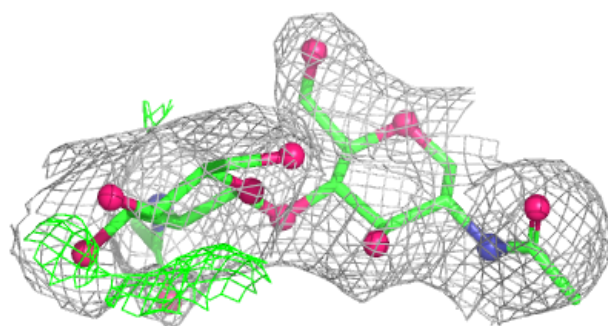
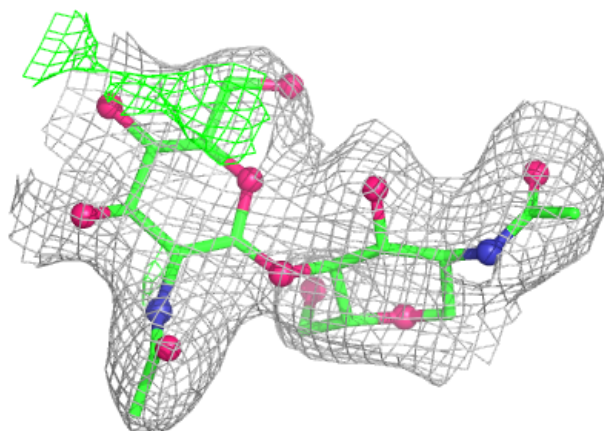
Electron density around Chain U:

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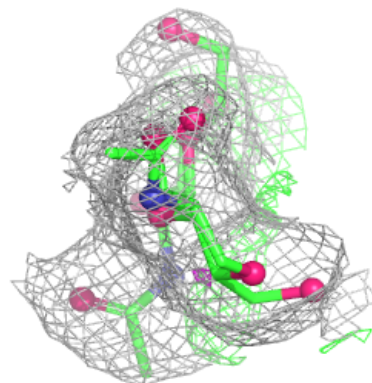
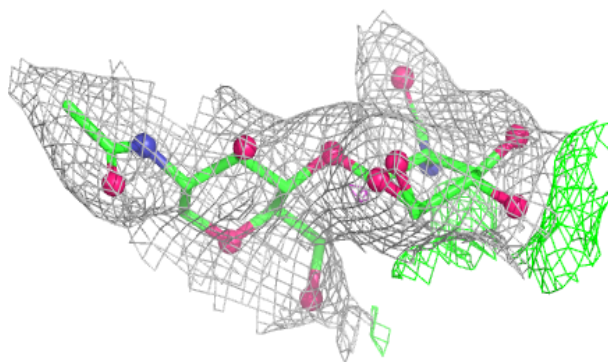
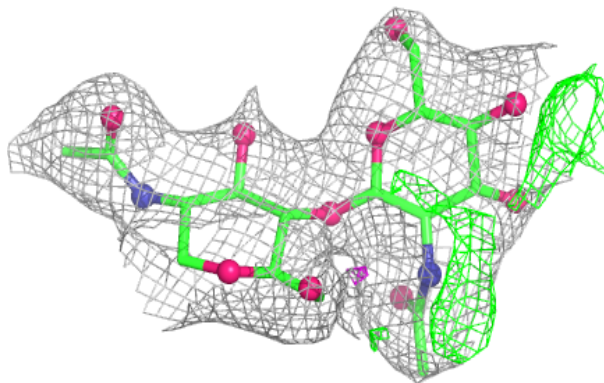


Electron density around Chain V:

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

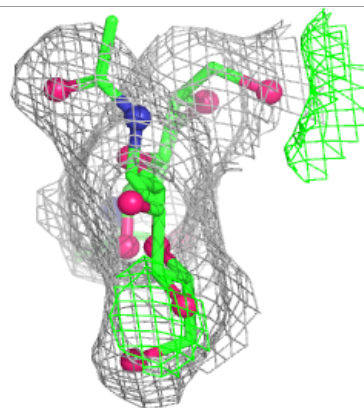
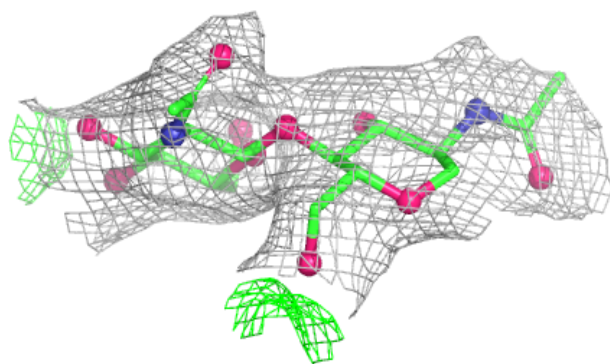
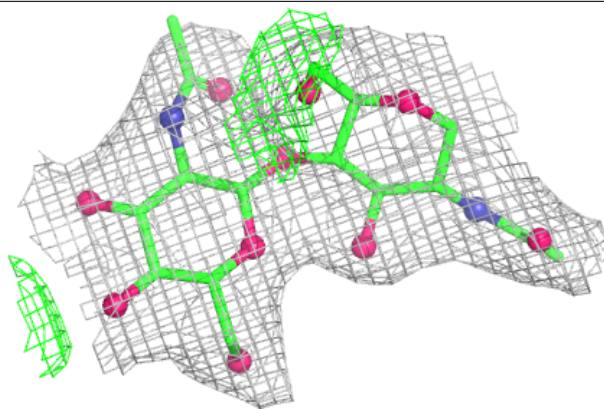
**Electron density around Chain W:**

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

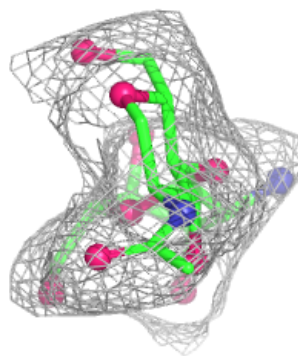
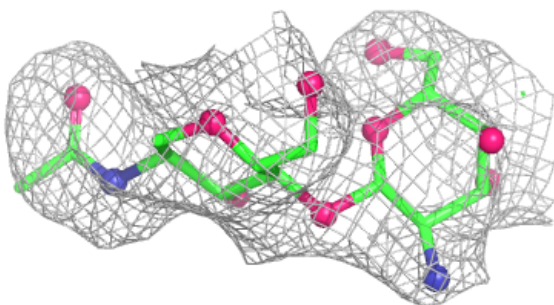
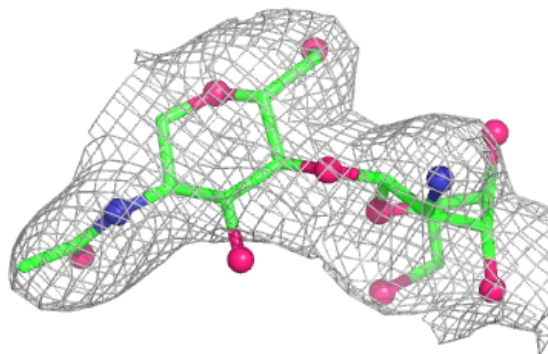


Electron density around Chain X:

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

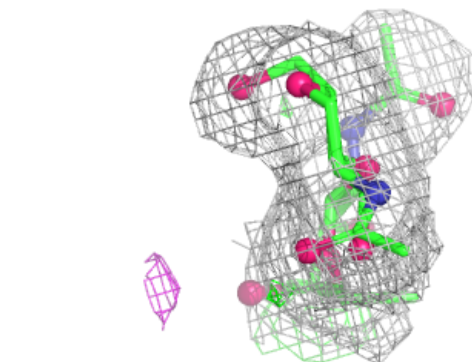
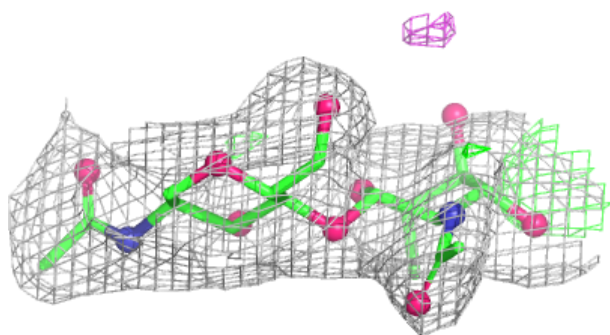
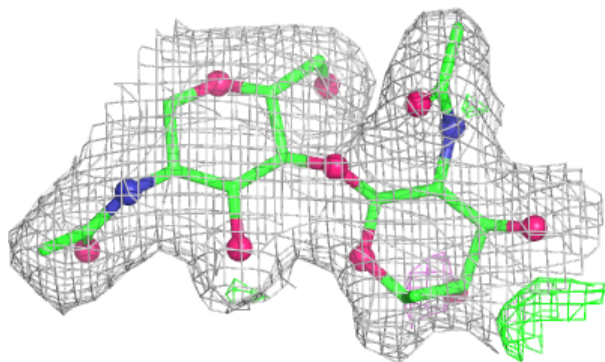
**Electron density around Chain Y:**

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

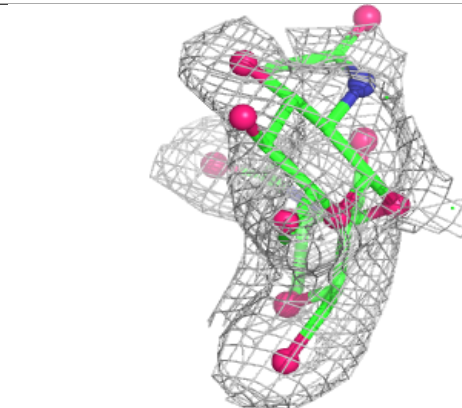
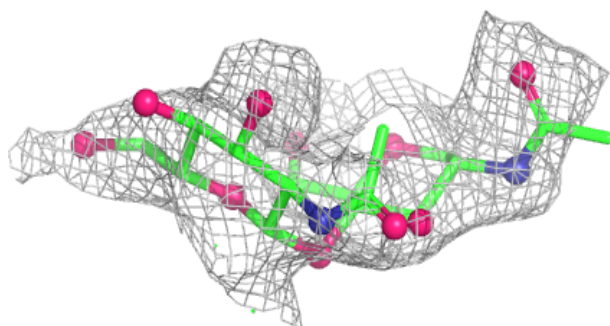
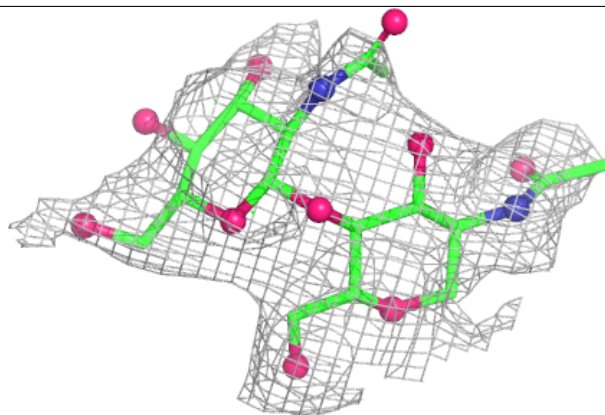


Electron density around Chain Z:

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

**Electron density around Chain a:**

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



6.4 Ligands

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
4	NAG	A	608	14/15	0.60	0.15	73,114,126,128	0
4	NAG	F	605	14/15	0.71	0.09	77,105,120,129	0
4	NAG	G	605	10/15	0.75	0.11	72,88,104,107	0
4	NAG	G	604	14/15	0.76	0.12	61,83,117,120	0
4	NAG	H	606	14/15	0.79	0.10	81,99,115,117	0
4	NAG	F	602	14/15	0.80	0.12	63,87,110,118	0
4	NAG	D	608	14/15	0.81	0.11	37,62,87,91	0
4	NAG	C	608	14/15	0.84	0.09	56,79,108,112	0
4	NAG	B	607	14/15	0.86	0.10	50,71,89,101	0
6	PEG	D	609	5/7	0.87	0.20	27,33,49,54	0
5	CL	C	609	1/1	0.92	0.19	64,64,64,64	0
3	CA	G	601	1/1	0.93	0.07	107,107,107,107	0
3	CA	H	601	1/1	0.96	0.08	75,75,75,75	0
3	CA	F	601	1/1	0.97	0.07	73,73,73,73	0
3	CA	C	601	1/1	0.98	0.10	50,50,50,50	0
3	CA	D	601	1/1	0.98	0.08	43,43,43,43	0
5	CL	A	609	1/1	0.98	0.05	43,43,43,43	0
3	CA	A	601	1/1	0.98	0.10	57,57,57,57	0
3	CA	B	600	1/1	0.98	0.09	52,52,52,52	0
3	CA	E	600	1/1	0.99	0.09	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.