



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2021 – 12:21 PM EDT

PDB ID : 4MIV
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

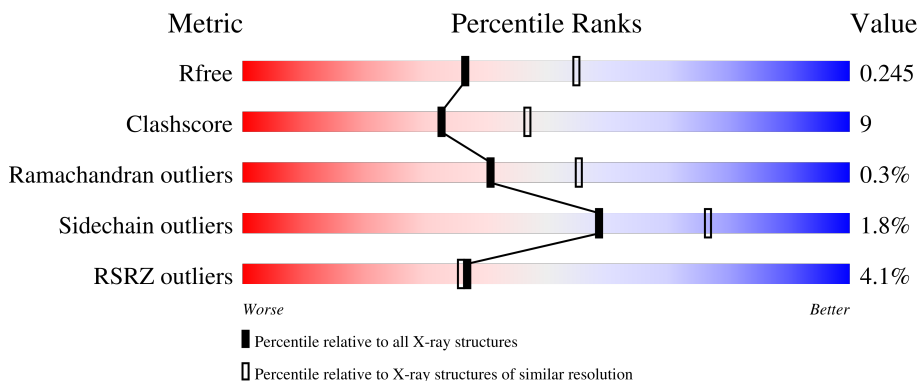
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	80% 13% • 6%
1	C	510	80% 13% • 5%
1	D	510	81% 12% • 6%
1	E	510	7% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
1	F	510	 4% 80% 13% • 6%
1	G	510	 7% 81% 12% • 6%
1	H	510	 10% 80% 13% • 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	 100%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 50% 50%
2	R	2	 100%
2	S	2	 100%
2	T	2	 50% 50%
2	U	2	 50% 50%
2	V	2	 50% 50%
2	W	2	 100%
2	X	2	 100%
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
			Total	C	N	O	P	S			
1	A	484	Total 3869	C 2478	N 670	O 708	P 1	S 12	0	2	0
1	B	481	Total 3860	C 2467	N 676	O 705	P 1	S 11	0	2	0
1	C	484	Total 3854	C 2467	N 670	O 705	P 1	S 11	0	0	0
1	D	480	Total 3835	C 2454	N 671	O 698	P 1	S 11	0	1	0
1	E	483	Total 3607	C 2308	N 617	O 670	P 1	S 11	0	1	0
1	F	478	Total 3703	C 2373	N 636	O 682	P 1	S 11	0	0	0
1	G	479	Total 3685	C 2362	N 641	O 671		S 11	0	1	0
1	H	482	Total 3617	C 2317	N 627	O 663		S 10	0	0	0

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

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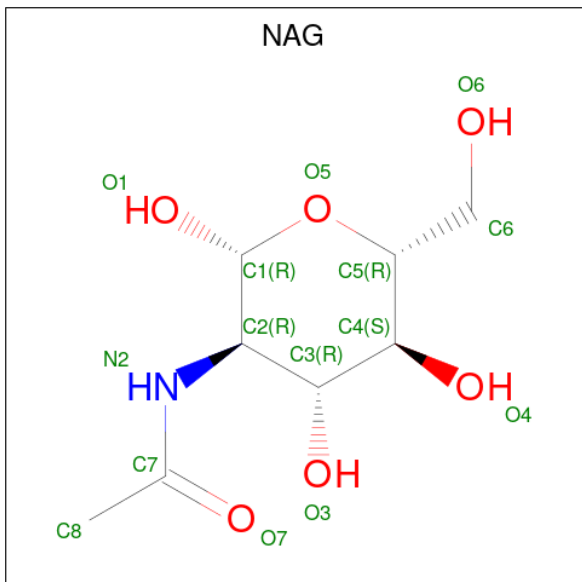
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	Q	2	28	16	2	10	0	0	0
2	R	2	28	16	2	10	0	0	0
2	S	2	28	16	2	10	0	0	0
2	T	2	28	16	2	10	0	0	0
2	U	2	28	16	2	10	0	0	0
2	V	2	28	16	2	10	0	0	0
2	W	2	28	16	2	10	0	0	0
2	X	2	28	16	2	10	0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

- Molecule 3 is CALCIUM ION (three-letter code: 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

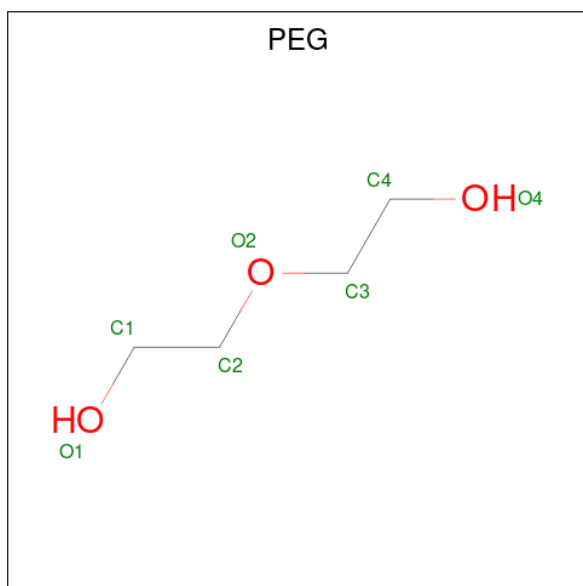
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is water.

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

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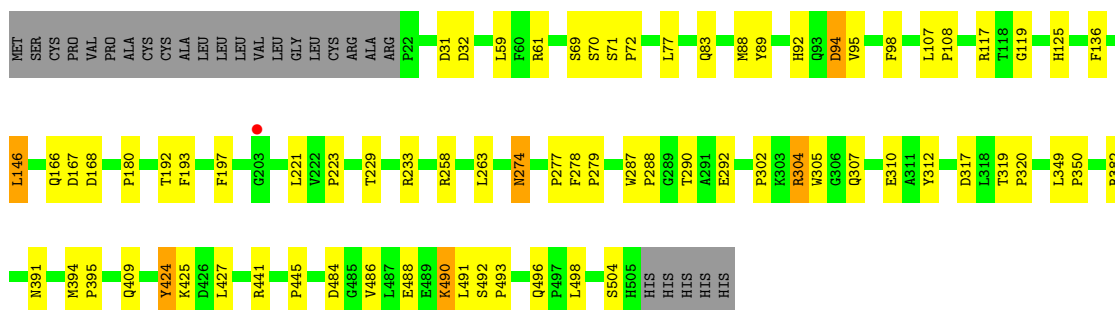
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	9	Total	O	0	0
			9	9		

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.

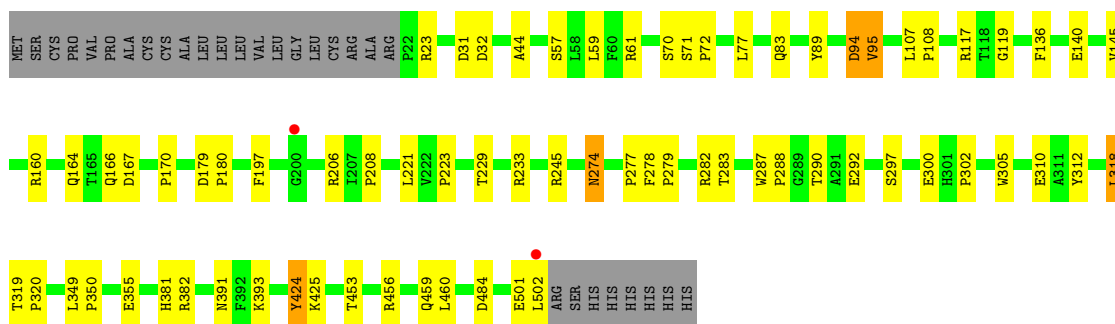
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain A: 




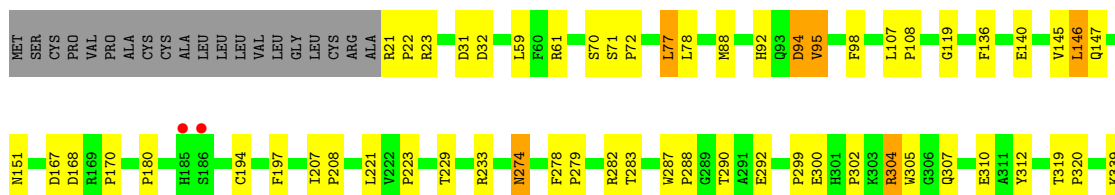
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain B: 



- Molecule 1: N-sulphoglucosamine sulphohydrolase

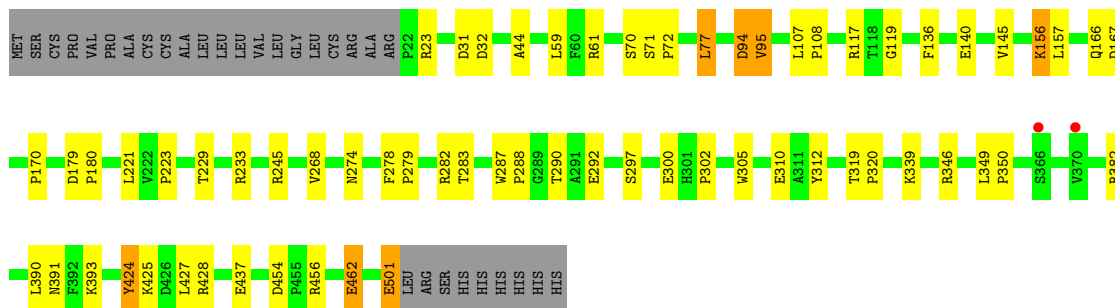
Chain C: 





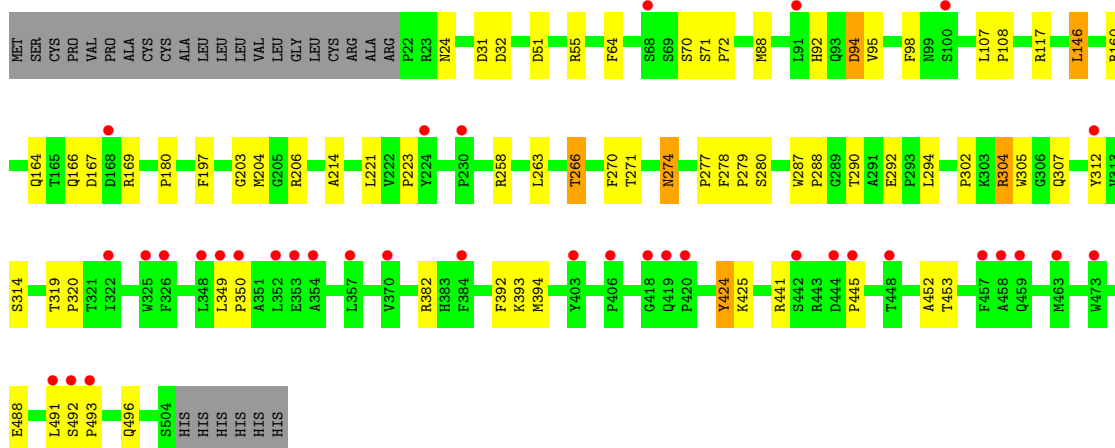
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain D: 81% 12% 6%



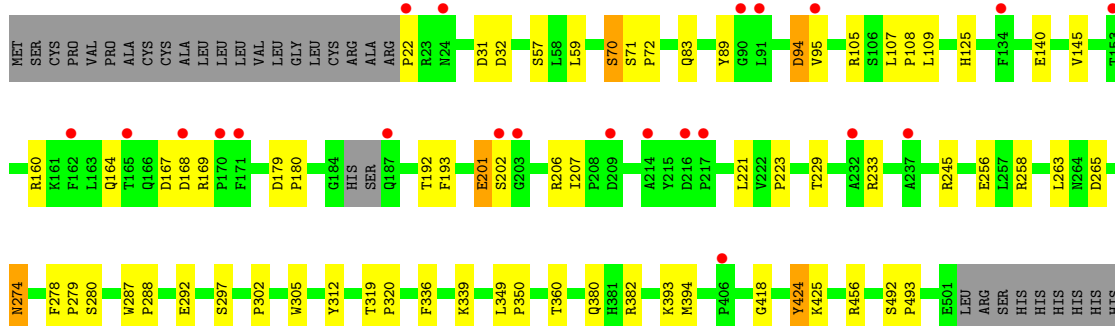
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain E: 7% 81% 13% 5%




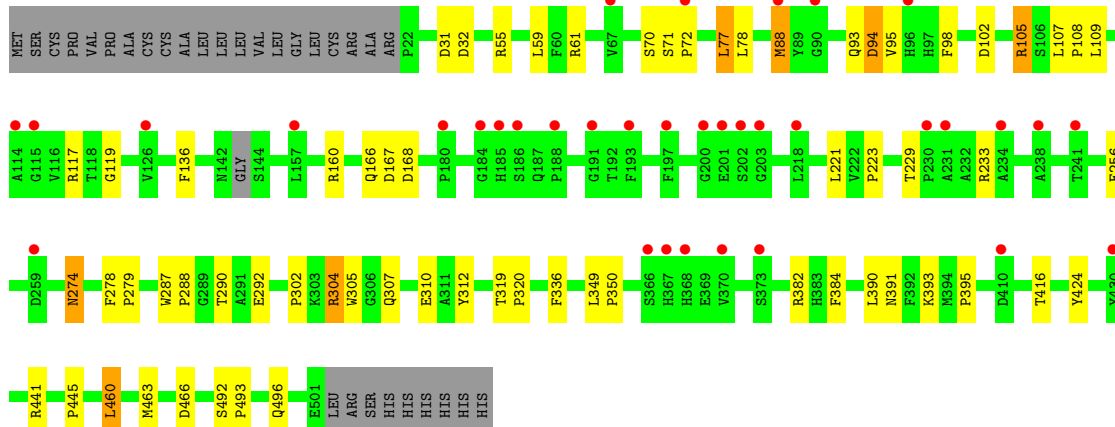
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain F: 4% 80% 13% 6%




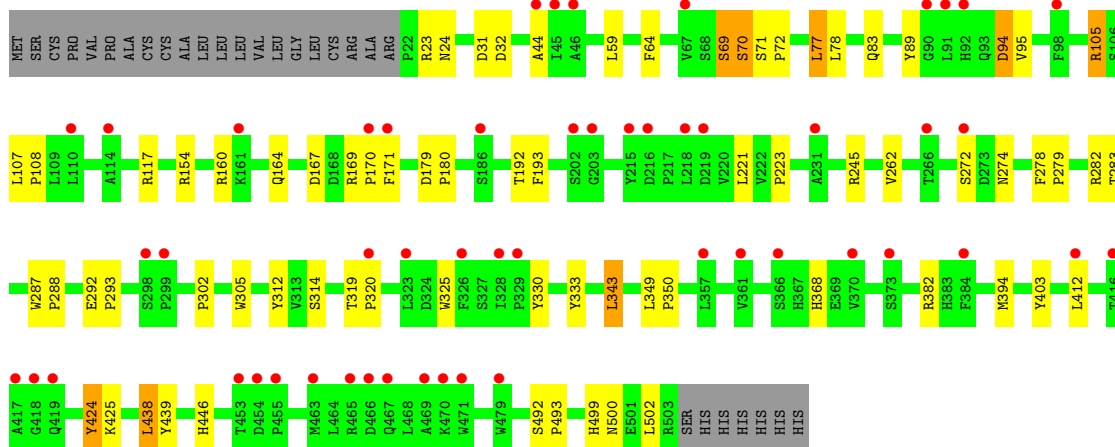
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain G:  7% 81% 12% 6%



- Molecule 1: N-sulphoglucosamine sulphonydrolase

Chain H:  10% 80% 13% 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%

WAG1
WAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

- 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:  100%

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) 99.3 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.275	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: CL, FGP, NAG, PEG, CA

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	0.24	0/3986	0.41	0/5443
1	B	0.25	0/3977	0.41	0/5429
1	C	0.25	0/3964	0.42	0/5415
1	D	0.25	0/3946	0.41	0/5387
1	E	0.23	0/3710	0.39	0/5081
1	F	0.23	0/3809	0.39	0/5202
1	G	0.23	0/3794	0.39	0/5187
1	H	0.22	0/3725	0.39	0/5100
All	All	0.24	0/30911	0.40	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3869	0	3671	61	0
1	B	3860	0	3696	70	0
1	C	3854	0	3663	64	0
1	D	3835	0	3648	55	0
1	E	3607	0	3129	65	0
1	F	3703	0	3368	58	0
1	G	3685	0	3350	80	0
1	H	3617	0	3180	76	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	0	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	4	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	28278	507	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 (507) 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:CE	1:G:98:PHE:HB3	1.79	1.11
1:G:88:MET:HE1	1:G:98:PHE:CB	1.80	1.09
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: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:E:271:THR:CG2	1:E:294:LEU:HD13	1.89	1.02
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:G:88:MET:CE	1:G:98:PHE:CB	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:88:MET:HE1	1:G:98:PHE:HB2	1.56	0.87
1:F:202:SER:HA	7:F:720:HOH:O	1.75	0.87
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: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:208:PRO:HG3	2:M:2:NAG:C6	2.08	0.83
1:C:77:LEU:C	1:C:77:LEU:HD23	2.00	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:D:501:GLU:OE1	1:D:501:GLU:C	2.18	0.81
1:G:77:LEU:HD23	1:G:77:LEU:C	2.01	0.81
1:H:77:LEU:C	1:H:77:LEU:HD23	2.01	0.80
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:G:88:MET:CE	1:G:88:MET:HA	2.15	0.76
1:G:88:MET:HE2	1:G:98:PHE:HB3	1.69	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
1:C:299:PRO:O	2:Q:1:NAG:H62	1.88	0.73
1:C:304:ARG:HG3	1:C:307:GLN:CD	2.10	0.72
1:G:160:ARG:HB2	1:G:256:GLU:OE1	1.89	0.72
1:B:460:LEU:HD11	1:G:463:MET:HE1	1.72	0.71
1:G:77:LEU:HD22	1:G:78:LEU:HG	1.72	0.71
1:A:304:ARG:HG3	1:A:307:GLN:CD	2.10	0.71
1:E:88:MET:HE3	1:E:92:HIS:HB2	1.71	0.71
1:H:77:LEU:HD22	1:H:78:LEU:HG	1.72	0.71
1:E:304:ARG:HG3	1:E:307:GLN:CD	2.11	0.71
1:G:88:MET:HE1	1:G:98:PHE:C	2.11	0.70
1:G:88:MET:CE	1:G:98:PHE:C	2.60	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ARG:HG3	1:G:307:GLN:CD	2.11	0.70
1:H:69:SER:HB2	1:H:368:HIS:ND1	2.07	0.70
1:A:88:MET:HE3	1:A:92:HIS:HB2	1.73	0.69
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:B:460:LEU:CD1	1:G:463:MET:CE	2.72	0.68
1:C:88:MET:HE3	1:C:92:HIS:HB2	1.75	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:B:460:LEU:HD11	1:G:463:MET:CE	2.25	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: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:88:MET:HA	1:G:88:MET:HE2	1.77	0.65
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:E:304:ARG:HG3	1:E:307:GLN:OE1	1.95	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TRP:HB3	1:A:288:PRO:HD3	1.80	0.64
1:B:460:LEU:CD1	1:G:463:MET:HE3	2.28	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: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: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: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:H:438:LEU:HD23	1:H:438:LEU:C	2.21	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: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
1:F:70:FGP:HOG	1:F:125:HIS:CE1	2.18	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:MET:HE1	1:G:98:PHE:CA	2.33	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:F:160:ARG:HG3	1:F:256:GLU:CD	2.22	0.58
1:C:424:TYR:CZ	1:C:425:LYS:HD2	2.39	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:F:70:FGP:OG1	1:F:125:HIS:ND1	2.30	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: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
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:H:438:LEU:C	1:H:438:LEU:CD2	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:H:278:PHE:HB3	1:H:279:PRO:HD2	1.88	0.54
1:B:278:PHE:HB3	1:B:279:PRO:HD2	1.89	0.54
1:C:492:SER:HA	1:C:493:PRO:C	2.29	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:A:107:LEU:N	1:A:108:PRO:HD2	2.23	0.53
1:D:77:LEU:HD12	1:D:77:LEU:C	2.28	0.53
1:G:88:MET:HE3	1:G:98:PHE:C	2.29	0.53
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:G:77:LEU:C	1:G:77:LEU:CD2	2.75	0.52
1:A:107:LEU:HB3	1:A:108:PRO:CD	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:459:GLN:HG2	1:G:384:PHE:CE2	2.45	0.51
1:B:179:ASP:OD2	1:B:245:ARG:HD2	2.11	0.51
1:G:107:LEU:HB3	1:G:108:PRO:CD	2.40	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
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: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:179:ASP:OD2	1:F:245:ARG:HD2	2.12	0.50
1:G:88:MET:HA	1:G:88:MET:HE3	1.94	0.50
1:B:59:LEU:C	1:B:59:LEU:HD23	2.33	0.49
1:A:488:GLU:OE1	1:A:490:LYS:NZ	2.46	0.49
1:F:59:LEU:HD23	1:F:59:LEU:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD23	1:A:59:LEU:C	2.33	0.49
1:F:192:THR:HG23	1:F:193:PHE:HD1	1.77	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:H:179:ASP:OD2	1:H:245:ARG:HD2	2.13	0.49
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:A:504:SER:CB	7:A:746:HOH:O	2.61	0.48
1:C:59:LEU:C	1:C:59:LEU:HD23	2.34	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:H:59:LEU:C	1:H:59:LEU:HD23	2.33	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:A:492:SER:HA	1:A:493:PRO:C	2.33	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:E:492:SER:HA	1:E:493:PRO:C	2.34	0.47
1:G:59:LEU:C	1:G:59:LEU:HD23	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:MET:HE1	1:G:98:PHE:O	2.14	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
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:F:274:ASN:C	1:F:292:GLU:OE2	2.54	0.47
1:D:274:ASN:C	1:D:292:GLU:OE2	2.53	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:C:77:LEU:C	1:C:77:LEU:CD2	2.74	0.47
1:D:59:LEU:C	1:D:59:LEU:HD23	2.35	0.47
1:C:394:MET:HE1	1:D:390:LEU:O	2.14	0.46
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:D:31:ASP:O	1:D:32:ASP:HB2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:LEU:C	1:H:77:LEU:CD2	2.75	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:274:ASN:C	1:A:292:GLU:OE2	2.55	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:G:492:SER:HA	1:G:493:PRO:C	2.37	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
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: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
1:D:229:THR:O	1:D:233:ARG:HG3	2.17	0.45
1:E:274:ASN:C	1:E:292:GLU:OE2	2.55	0.45
1:F:312:TYR:CZ	1:F:382:ARG:HA	2.52	0.45
1:C:274:ASN:C	1:C:292:GLU:OE2	2.55	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:B:274:ASN:C	1:B:292:GLU:OE2	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:O	1:B:164:GLN:HG3	2.17	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:A:88:MET:CE	1:A:92:HIS:HB2	2.45	0.44
1:D:107:LEU:HB3	1:D:108:PRO:HD3	1.98	0.44
1:F:167:ASP:C	1:F:169:ARG:H	2.21	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:H:412:LEU:HD23	1:H:412:LEU:C	2.38	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: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:G:274:ASN:C	1:G:292:GLU:OE2	2.56	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:88:MET:CE	1:E:92:HIS:HB2	2.45	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:C:88:MET:CE	1:C:92:HIS:HB2	2.45	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:A:88:MET:HE1	1:A:98:PHE:O	2.18	0.43
1:B:117:ARG:CD	1:B:166:GLN:OE1	2.63	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:D:119:GLY:HA2	1:D:136:PHE:O	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:390:LEU:O	1:H:394:MET:HE1	2.19	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
2:Q:1:NAG:H61	2:Q:2:NAG:C7	2.49	0.42
1:C:88:MET:HE1	1:C:98:PHE:O	2.19	0.42
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: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:E:203:GLY:O	1:E:204:MET:HE2	2.20	0.42
1:A:290:THR:O	1:A:292:GLU:HG2	2.19	0.42
1:F:274:ASN:CA	1:F:292:GLU:OE2	2.67	0.42
1:G:88:MET:HE2	1:G:88:MET:CA	2.46	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: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:G:88:MET:CE	1:G:98:PHE:O	2.68	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: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:H:492:SER:HA	1:H:493:PRO:C	2.39	0.41
1:E:88:MET:HE1	1:E:98:PHE:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:ARG:O	1:D:346:ARG:HG2	2.19	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:290:THR:O	1:C:292:GLU:HG2	2.20	0.41
1:E:167:ASP:C	1:E:169:ARG:H	2.24	0.41
1:F:492:SER:HA	1:F:493:PRO:C	2.40	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: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:C:394:MET:SD	1:D:393:LYS:HB2	2.61	0.40
1:C:119:GLY:HA2	1:C:136:PHE:O	2.21	0.40
1:G:117:ARG:CD	1:G:166:GLN:OE1	2.66	0.40
1:H:23:ARG:C	1:H:24:ASN:ND2	2.75	0.40
1:A:317:ASP:C	1:A:320:PRO:HD2	2.41	0.40
1:B:77:LEU:HD13	1:B:318:LEU:CD2	2.52	0.40
1:A:394[A]:MET:HE3	1:A:395:PRO:HD2	2.04	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:H:167:ASP:C	1:H:169:ARG:H	2.25	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%)	47	62
1	B	480/510 (94%)	464 (97%)	15 (3%)	1 (0%)	47	62
1	C	481/510 (94%)	469 (98%)	10 (2%)	2 (0%)	34	48
1	D	478/510 (94%)	463 (97%)	13 (3%)	2 (0%)	34	48
1	E	480/510 (94%)	468 (98%)	11 (2%)	1 (0%)	47	62
1	F	473/510 (93%)	459 (97%)	11 (2%)	3 (1%)	25	36
1	G	474/510 (93%)	460 (97%)	13 (3%)	1 (0%)	47	62
1	H	479/510 (94%)	466 (97%)	12 (2%)	1 (0%)	47	62
All	All	3829/4080 (94%)	3721 (97%)	96 (2%)	12 (0%)	41	55

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 [i](#)

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%)	65	80
1	B	414/442 (94%)	408 (99%)	6 (1%)	67	82
1	C	408/442 (92%)	400 (98%)	8 (2%)	55	74
1	D	404/442 (91%)	397 (98%)	7 (2%)	60	78
1	E	325/442 (74%)	319 (98%)	6 (2%)	59	76
1	F	361/442 (82%)	357 (99%)	4 (1%)	73	87
1	G	358/442 (81%)	350 (98%)	8 (2%)	52	71
1	H	331/442 (75%)	323 (98%)	8 (2%)	49	68
All	All	3011/3536 (85%)	2958 (98%)	53 (2%)	59	76

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	146	LEU
1	A	274	ASN
1	A	304	ARG
1	A	424	TYR
1	A	490	LYS
1	B	95	VAL
1	B	206	ARG
1	B	274	ASN
1	B	318	LEU
1	B	424	TYR
1	B	456	ARG
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	C	424	TYR
1	D	77	LEU
1	D	95	VAL
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	424	TYR
1	D	428	ARG
1	D	462	GLU
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	E	424	TYR
1	F	201	GLU
1	F	274	ASN
1	F	424	TYR
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	424	TYR
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	424	TYR
1	H	438	LEU
1	H	446	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	C	70	3,1	7,10,11	1.06	0	8,14,16	1.25	1 (12%)
1	FGP	H	70	3,1	4,6,11	1.23	0	3,7,16	1.44	1 (33%)
1	FGP	G	70	3,1	4,6,11	1.34	0	3,7,16	1.55	1 (33%)
1	FGP	E	70	3,1	7,10,11	1.04	0	8,14,16	1.19	1 (12%)
1	FGP	B	70	3,1	7,10,11	1.03	0	8,14,16	1.37	1 (12%)
1	FGP	A	70	3,1	7,10,11	1.04	0	8,14,16	1.37	1 (12%)
1	FGP	F	70	3,1	7,10,11	1.01	0	8,14,16	1.33	1 (12%)
1	FGP	D	70	3,1	7,10,11	1.06	0	8,14,16	1.32	1 (12%)

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	C	70	3,1	-	2/5/11/13	-
1	FGP	H	70	3,1	-	0/2/6/13	-
1	FGP	G	70	3,1	-	0/2/6/13	-
1	FGP	E	70	3,1	-	1/5/11/13	-
1	FGP	B	70	3,1	-	1/5/11/13	-
1	FGP	A	70	3,1	-	0/5/11/13	-
1	FGP	F	70	3,1	-	0/5/11/13	-
1	FGP	D	70	3,1	-	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	-2.83	117.36	124.78
1	B	70	FGP	O-C-CA	-2.79	117.46	124.78
1	D	70	FGP	O-C-CA	-2.76	117.54	124.78
1	F	70	FGP	O-C-CA	-2.71	117.67	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	70	FGP	O-C-CA	-2.58	118.01	124.78
1	C	70	FGP	O-C-CA	-2.43	118.41	124.78
1	H	70	FGP	O-C-CA	-2.25	118.87	124.78
1	E	70	FGP	O-C-CA	-2.22	118.96	124.78

There are no chirality outliers.

All (4) 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
1	E	70	FGP	CB-OG2-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	70	FGP	2	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	1,2	14,14,15	0.57	0	17,19,21	0.82	0
2	NAG	I	2	2	14,14,15	0.55	0	17,19,21	0.82	0
2	NAG	J	1	1,2	14,14,15	0.61	0	17,19,21	0.78	0
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	0.68	0
2	NAG	K	1	1,2	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
2	NAG	K	2	2	14,14,15	0.54	0	17,19,21	0.74	0
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	2	2	14,14,15	0.55	0	17,19,21	0.68	0
2	NAG	M	1	1,2	14,14,15	0.62	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	1,2	14,14,15	0.56	0	17,19,21	0.79	0
2	NAG	N	2	2	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	O	1	1,2	14,14,15	0.49	0	17,19,21	0.64	0
2	NAG	O	2	2	13,13,15	0.67	0	16,18,21	1.75	3 (18%)
2	NAG	P	1	1,2	14,14,15	0.59	0	17,19,21	0.75	0
2	NAG	P	2	2	13,13,15	0.58	0	16,18,21	0.60	0
2	NAG	Q	1	1,2	14,14,15	0.53	0	17,19,21	0.87	1 (5%)
2	NAG	Q	2	2	14,14,15	0.57	0	17,19,21	0.66	0
2	NAG	R	1	1,2	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	R	2	2	14,14,15	0.50	0	17,19,21	0.97	0
2	NAG	S	1	1,2	14,14,15	0.59	0	17,19,21	0.82	0
2	NAG	S	2	2	14,14,15	0.58	0	17,19,21	0.70	0
2	NAG	T	1	1,2	14,14,15	0.57	0	17,19,21	0.77	1 (5%)
2	NAG	T	2	2	14,14,15	0.59	0	17,19,21	0.60	0
2	NAG	U	1	1,2	14,14,15	0.48	0	17,19,21	0.64	0
2	NAG	U	2	2	14,14,15	0.48	0	17,19,21	1.06	2 (11%)
2	NAG	V	1	1,2	14,14,15	0.61	0	17,19,21	0.89	1 (5%)
2	NAG	V	2	2	14,14,15	0.60	0	17,19,21	0.79	0
2	NAG	W	1	1,2	14,14,15	0.58	0	17,19,21	0.74	0
2	NAG	W	2	2	14,14,15	0.56	0	17,19,21	0.73	0
2	NAG	X	1	1,2	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
2	NAG	X	2	2	14,14,15	0.50	0	17,19,21	0.87	1 (5%)
2	NAG	Y	1	1,2	14,14,15	0.52	0	17,19,21	0.73	0
2	NAG	Y	2	2	11,11,15	0.62	0	12,15,21	0.71	0
2	NAG	Z	1	1,2	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	0.78	0
2	NAG	a	1	1,2	14,14,15	0.50	0	17,19,21	0.81	1 (5%)
2	NAG	a	2	2	14,14,15	0.58	0	17,19,21	0.63	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	4.73	117.14	109.77
2	O	2	NAG	O5-C1-C2	-3.11	106.38	111.29
2	O	2	NAG	O5-C5-C4	3.11	115.10	109.52
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	2.67	115.81	112.19
2	Q	1	NAG	O5-C1-C2	-2.54	107.27	111.29
2	U	2	NAG	O5-C1-C2	-2.38	107.53	111.29
2	M	1	NAG	O5-C1-C2	-2.37	107.55	111.29
2	U	2	NAG	C4-C3-C2	-2.31	107.63	111.02
2	K	1	NAG	O5-C1-C2	-2.12	107.94	111.29
2	X	2	NAG	O5-C5-C6	2.12	110.52	107.20
2	a	1	NAG	C4-C3-C2	-2.11	107.93	111.02
2	V	1	NAG	O5-C1-C2	-2.07	108.02	111.29
2	T	1	NAG	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	U	2	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	I	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	Y	1	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	a	2	NAG	C8-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	I	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6

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

There are no ring outliers.

12 monomers are involved in 14 short contacts:

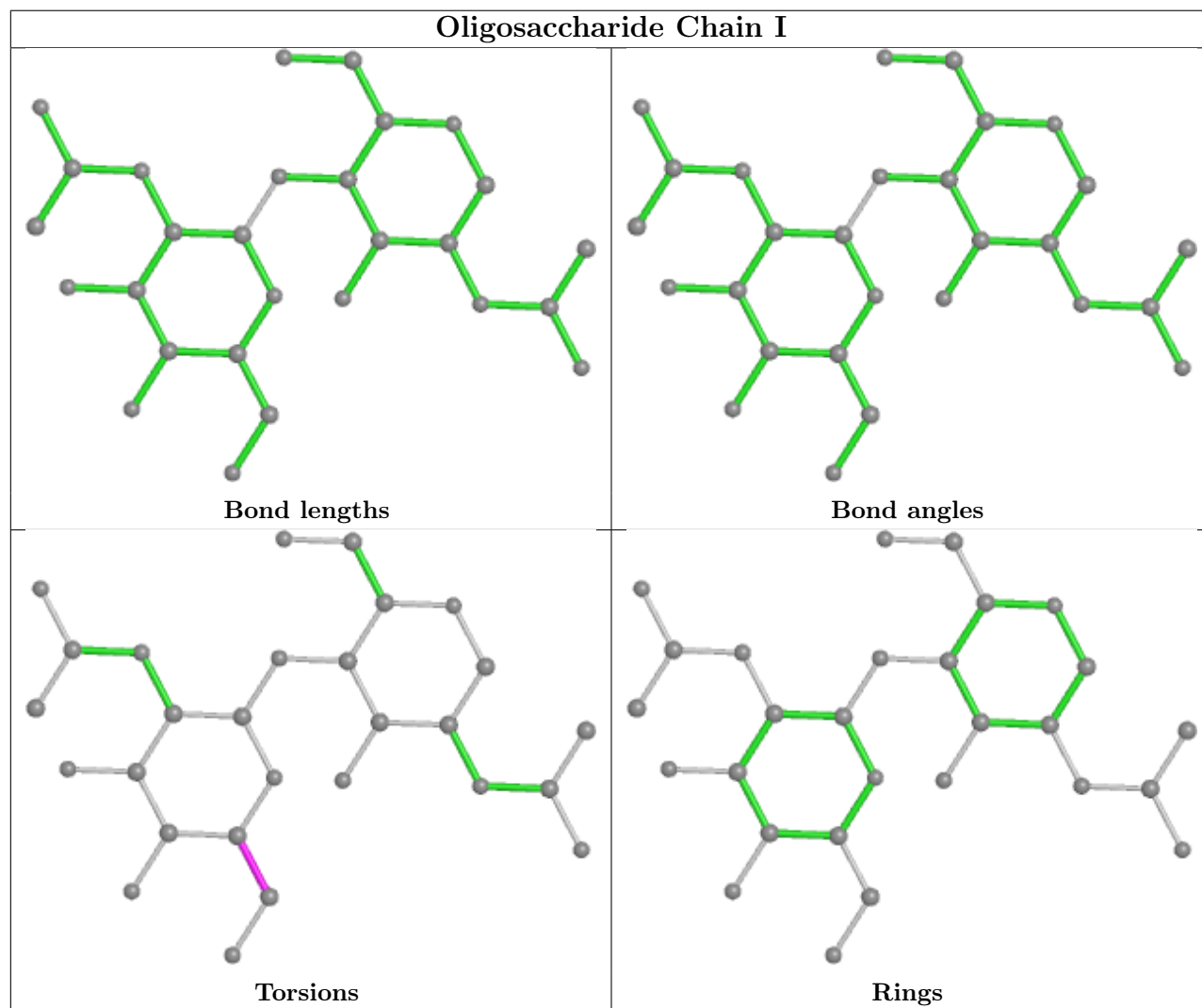
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	1	0
2	W	2	NAG	1	0
2	Y	2	NAG	1	0
2	N	1	NAG	1	0
2	M	1	NAG	2	0
2	W	1	NAG	3	0
2	N	2	NAG	1	0
2	Q	2	NAG	1	0

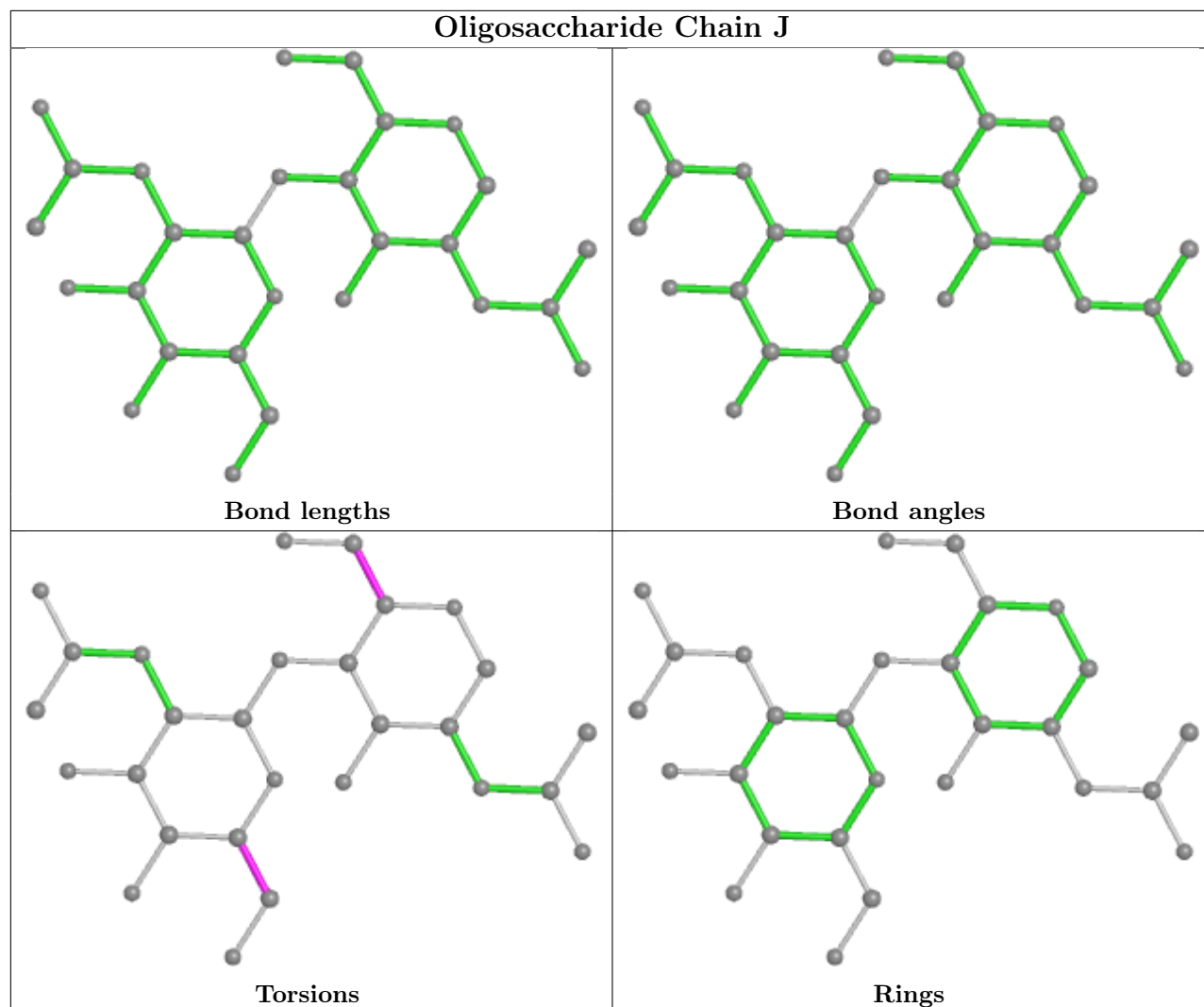
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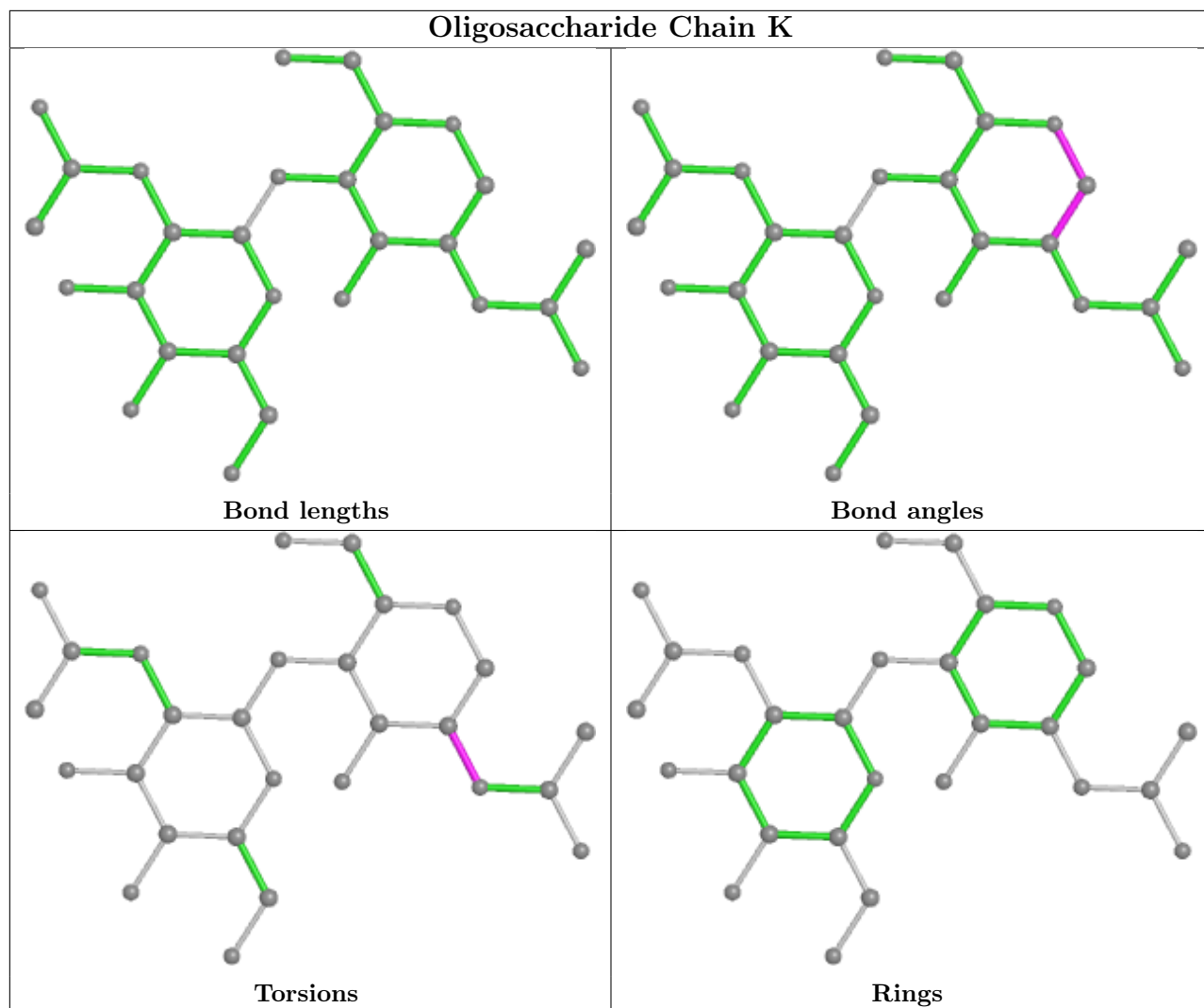
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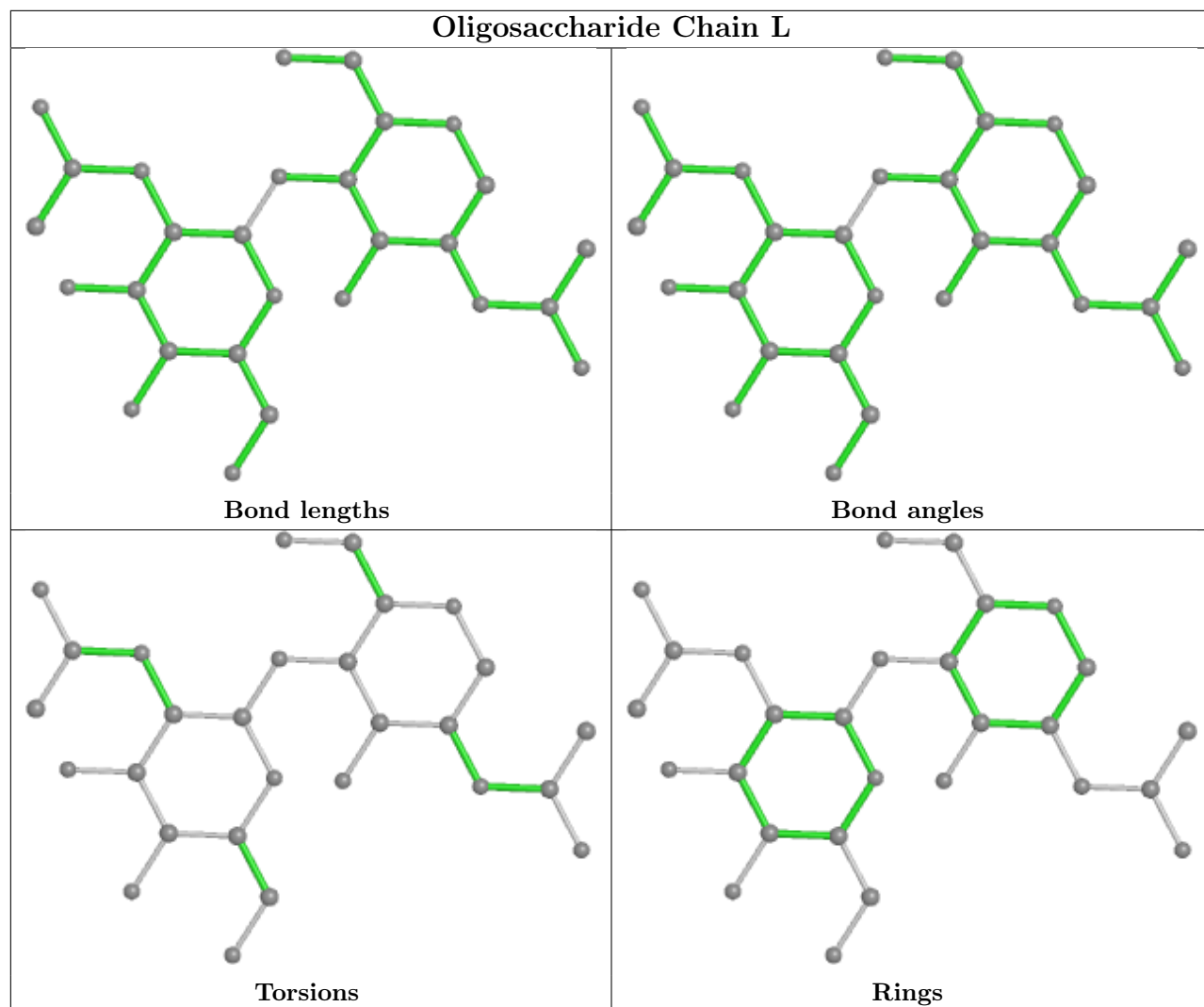
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	2	0
2	Y	1	NAG	1	0
2	Z	2	NAG	2	0
2	M	2	NAG	4	0

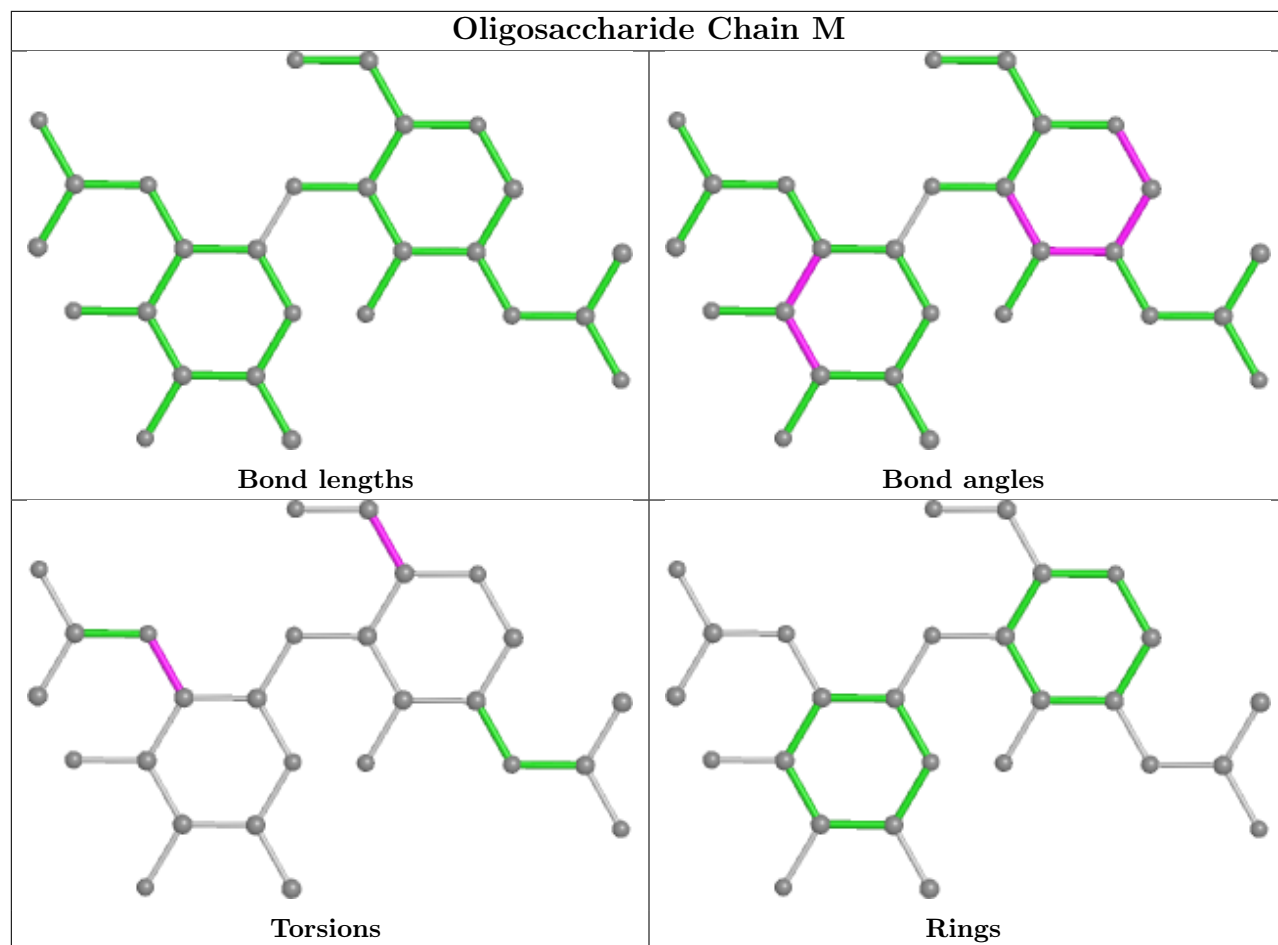
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

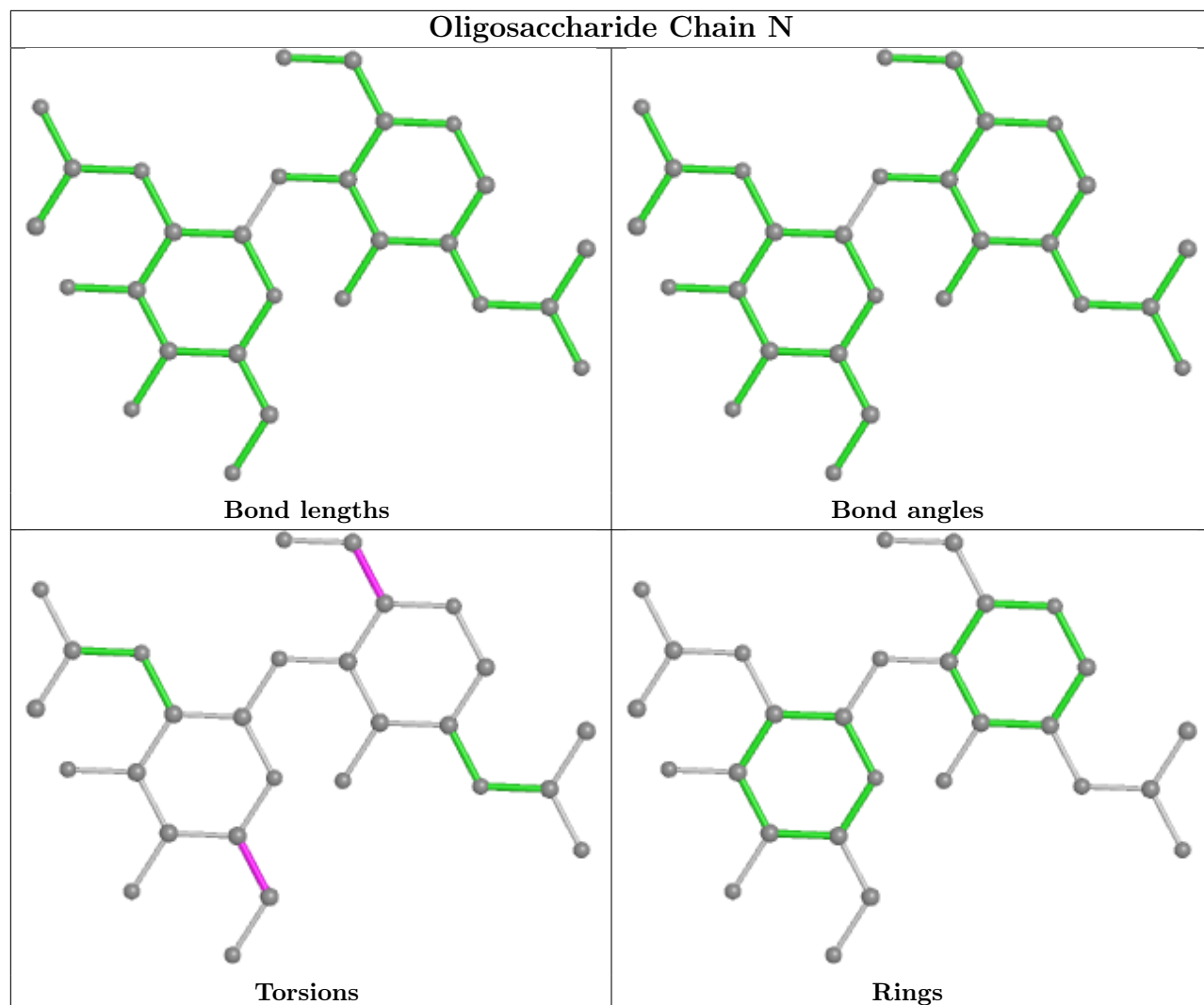


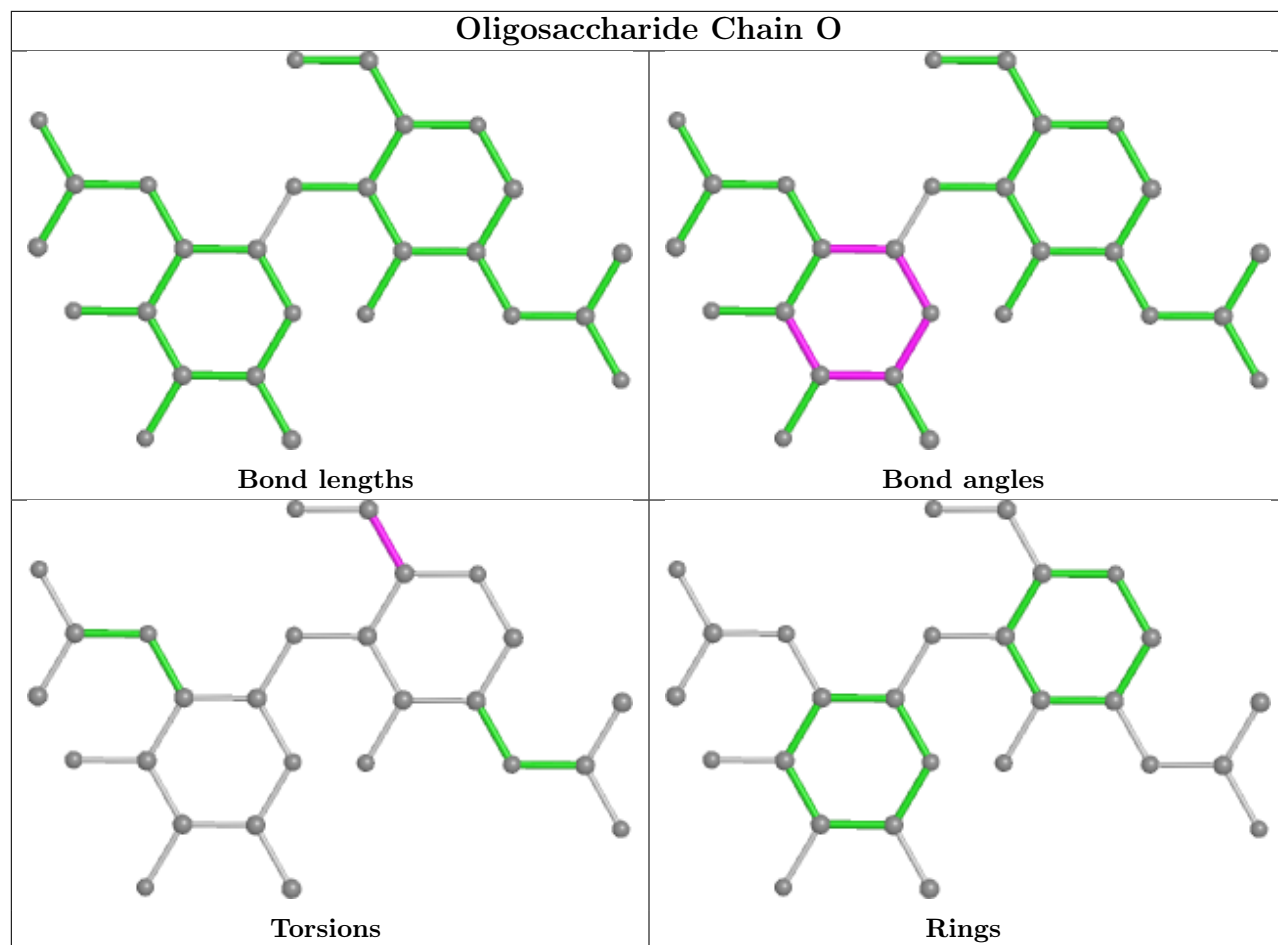


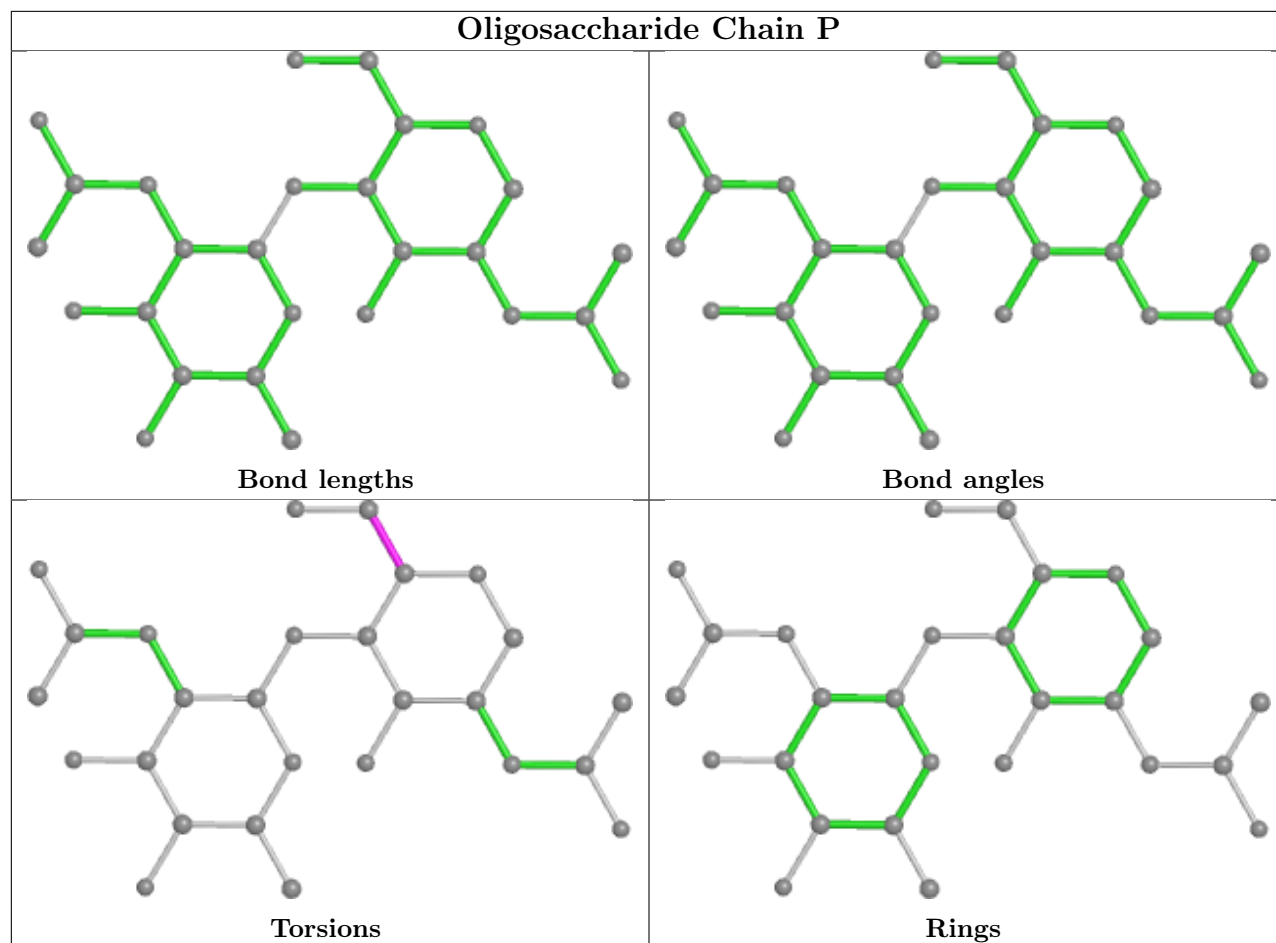


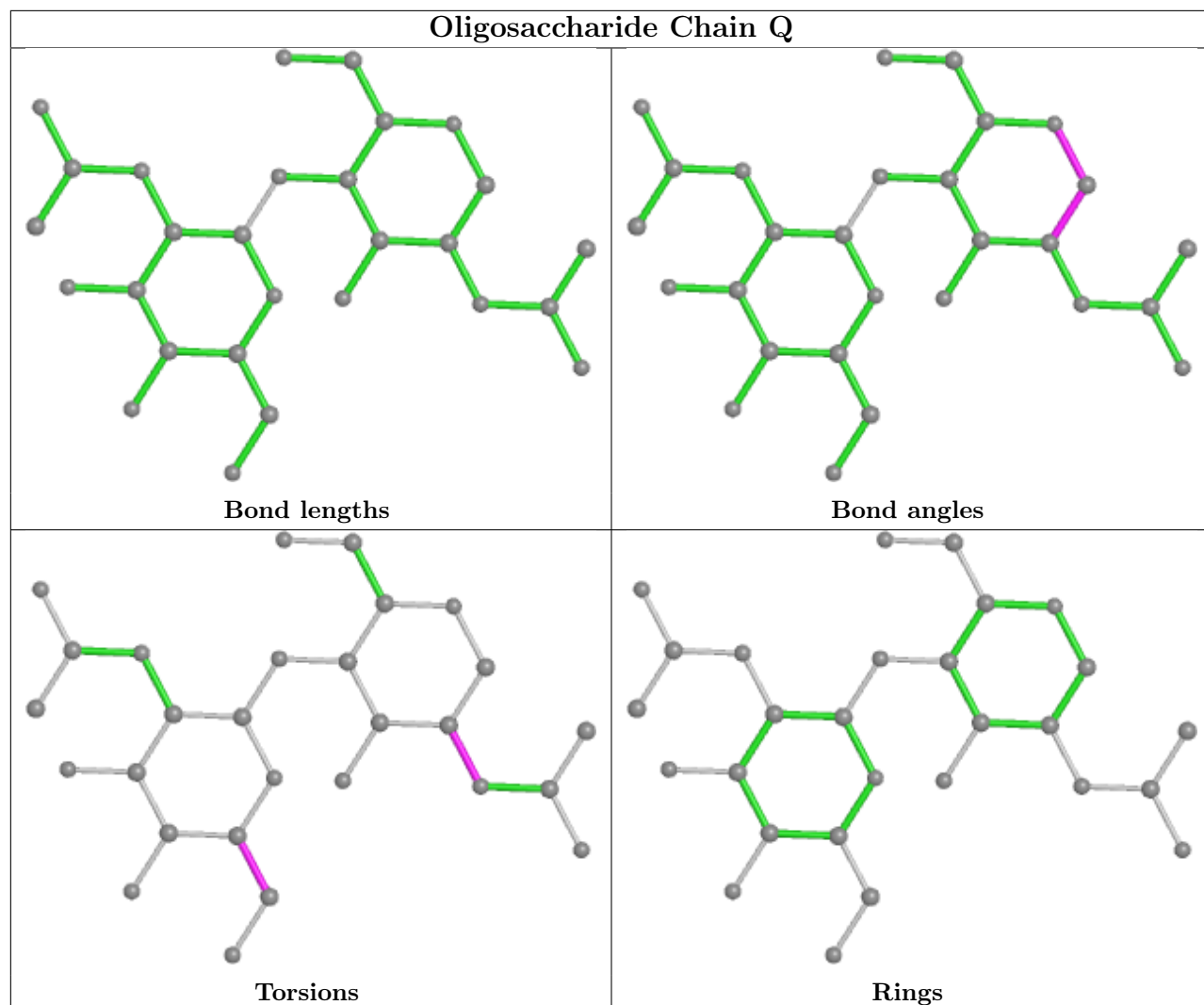


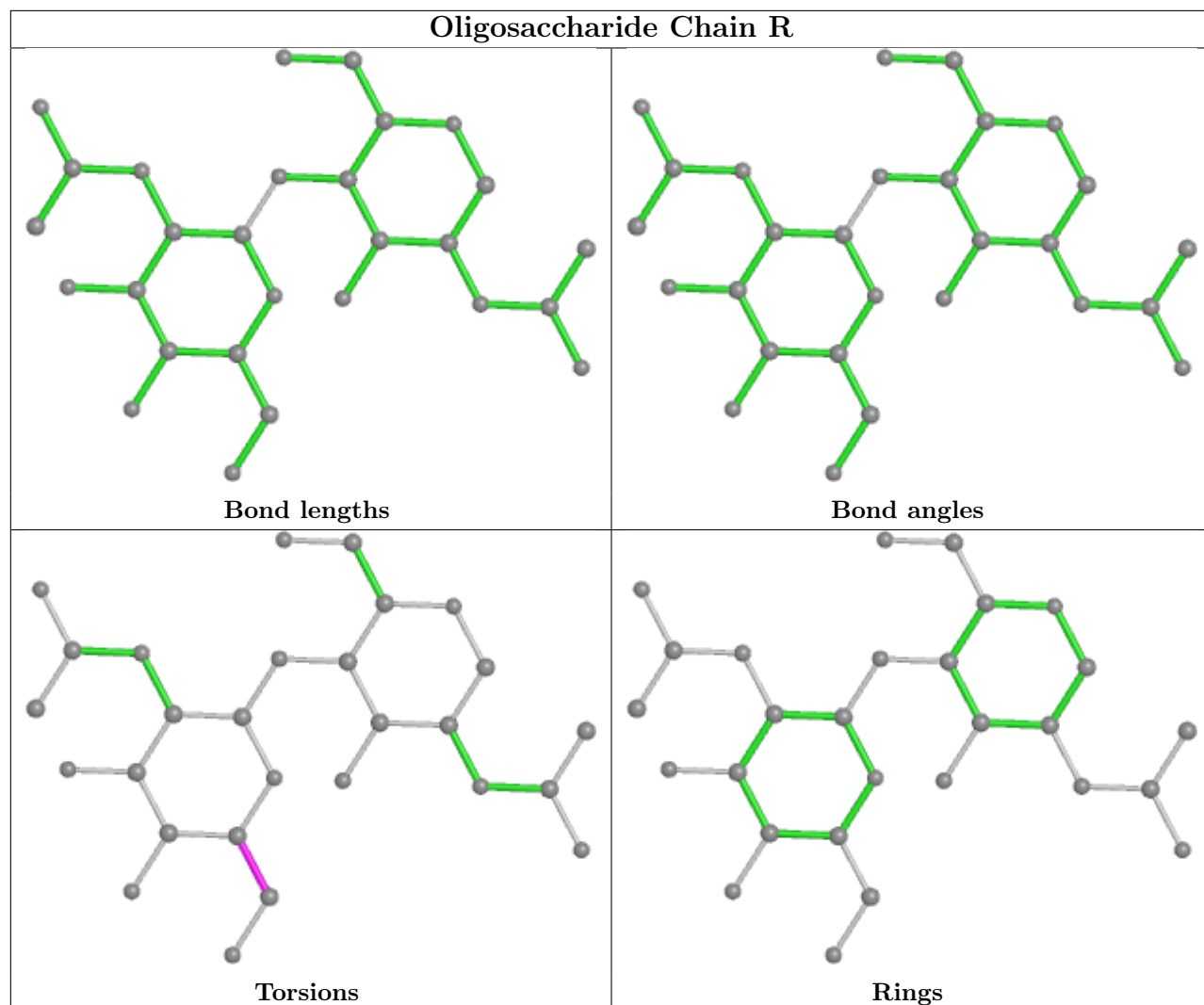


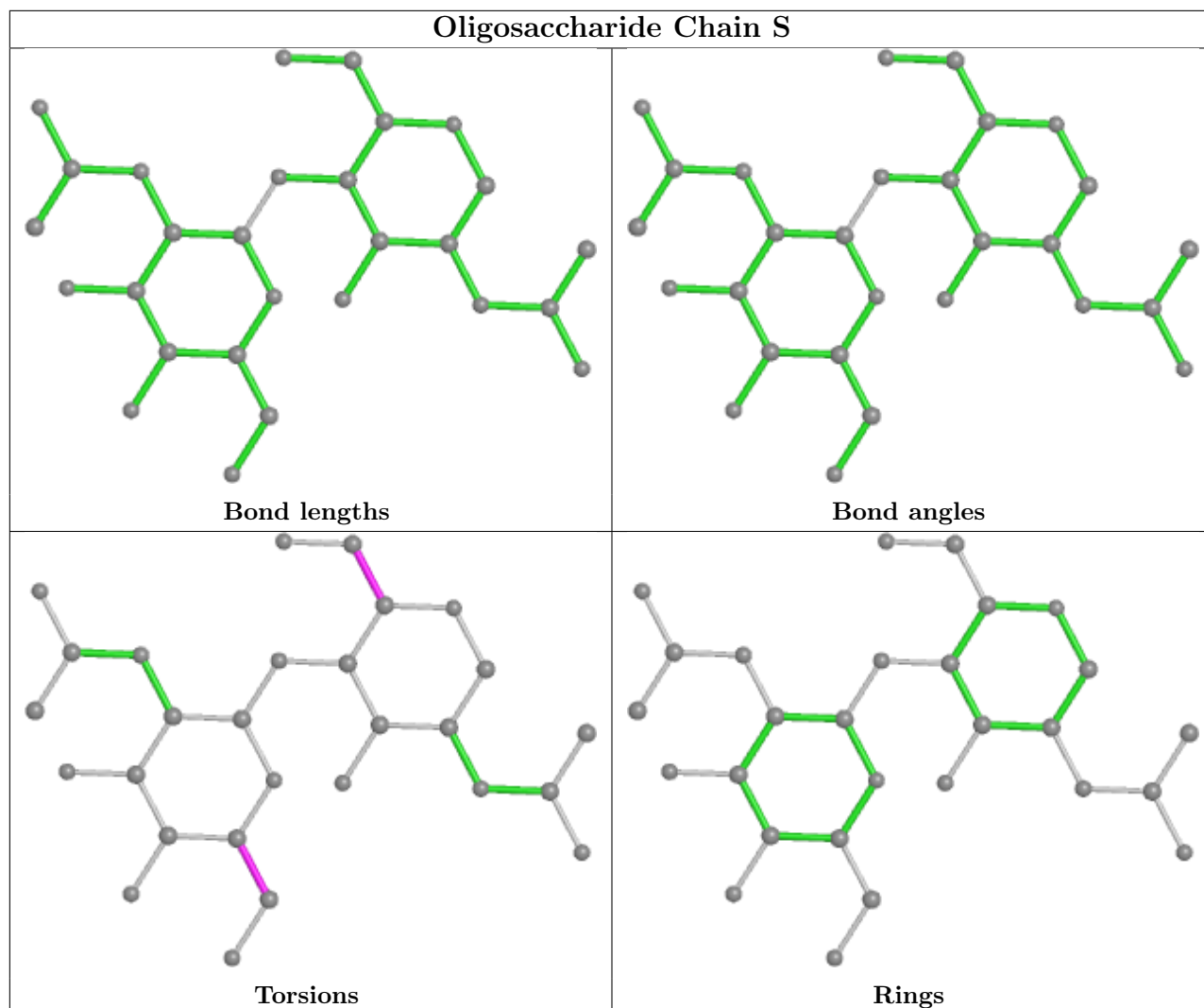


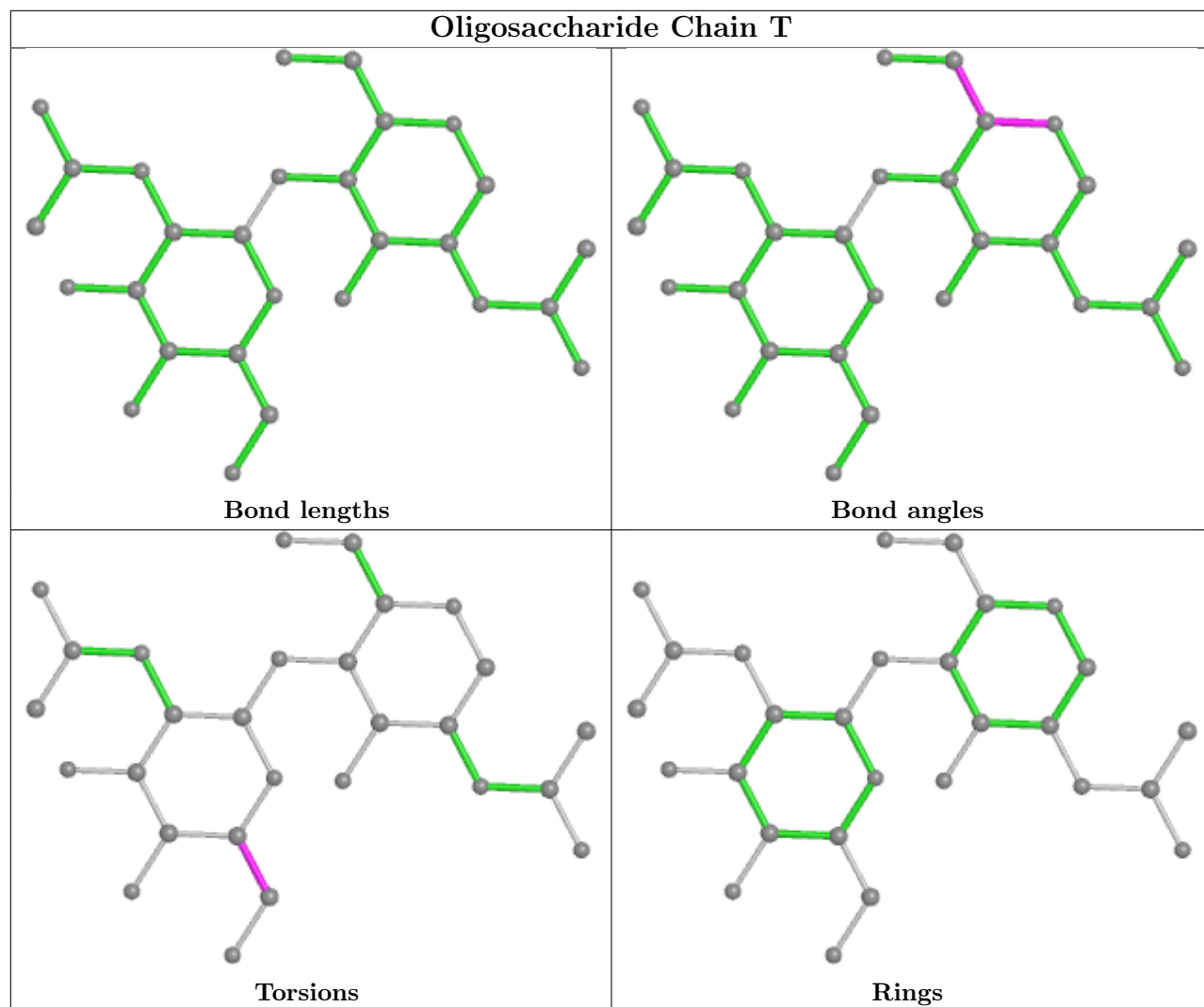


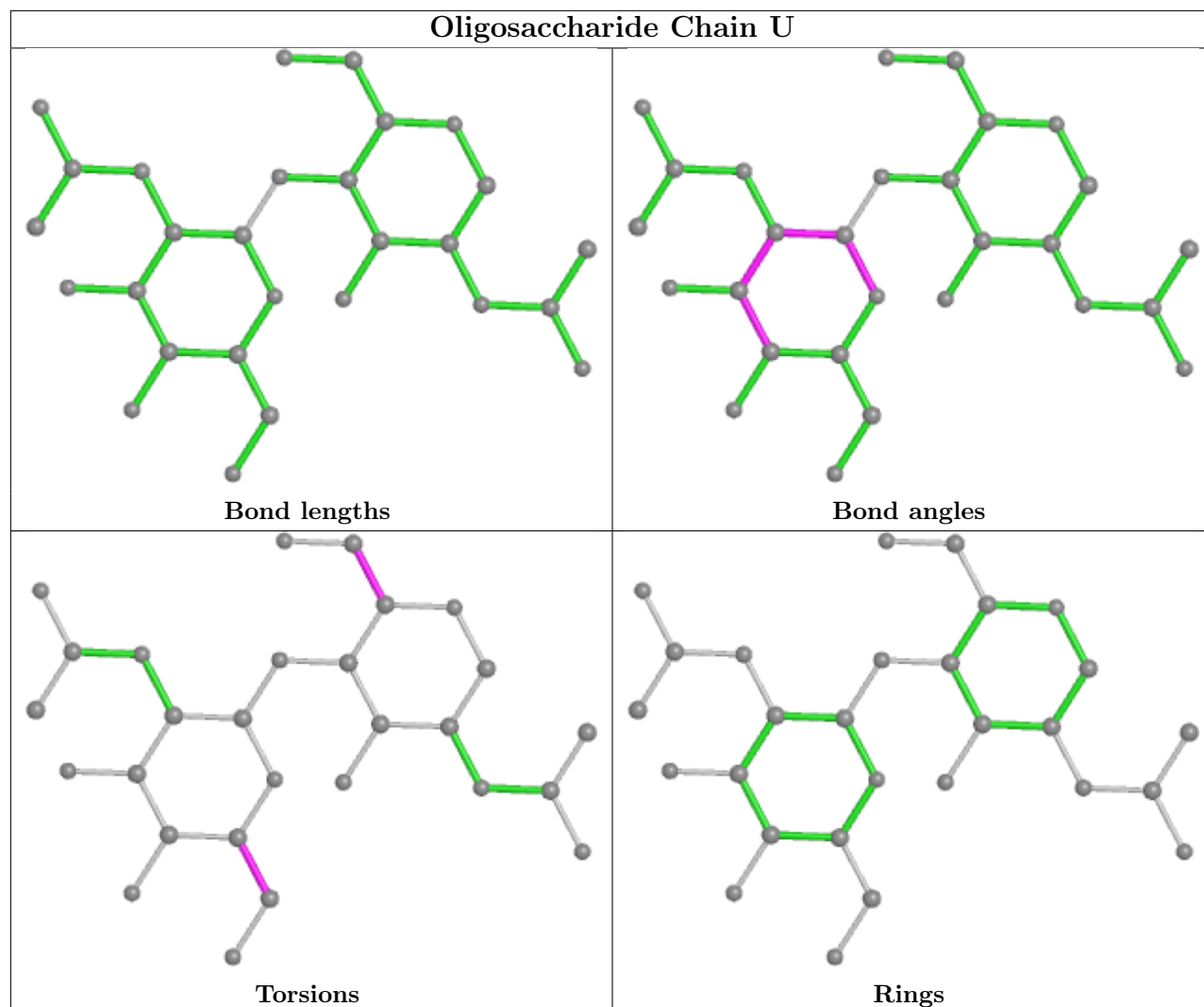


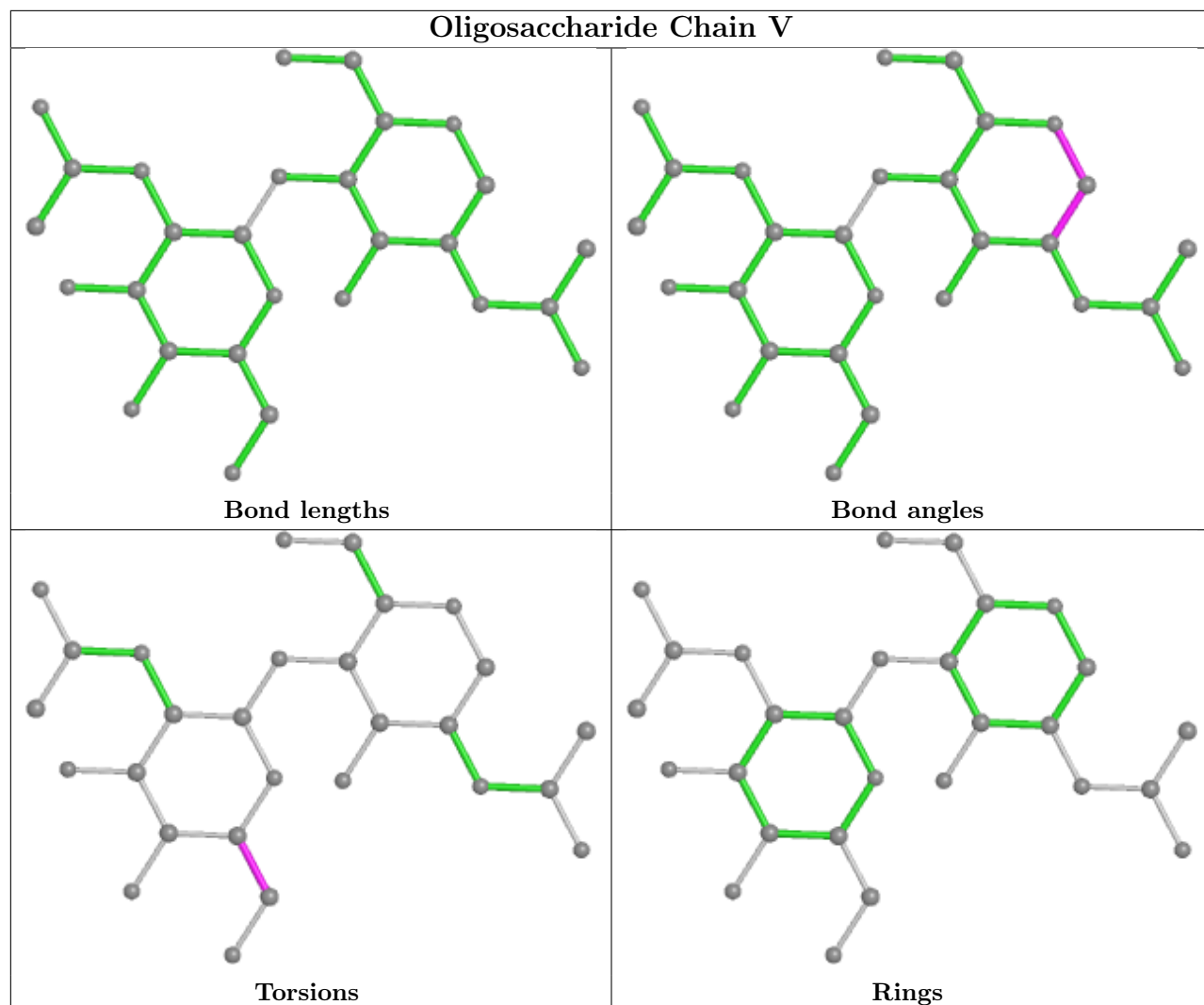


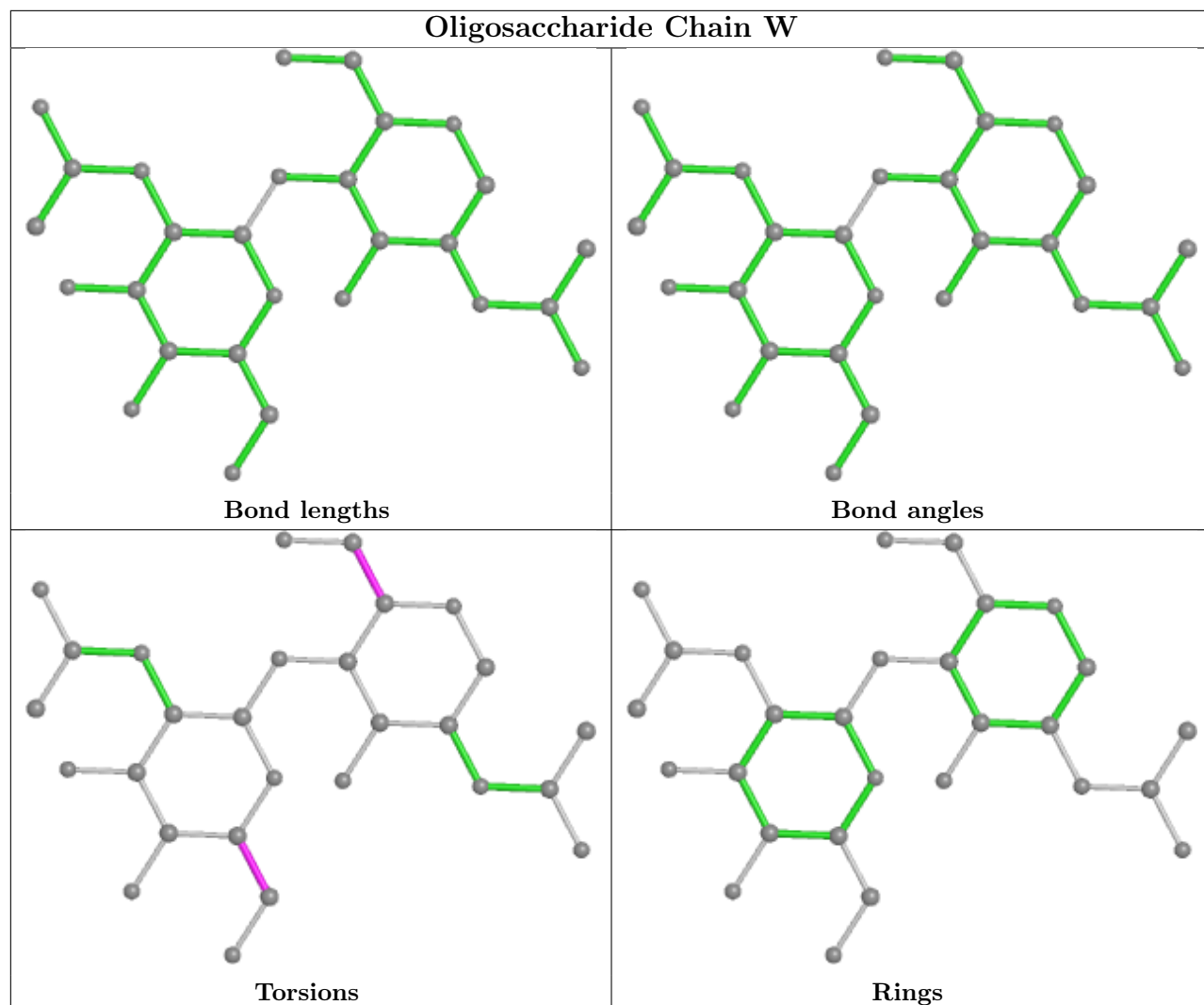


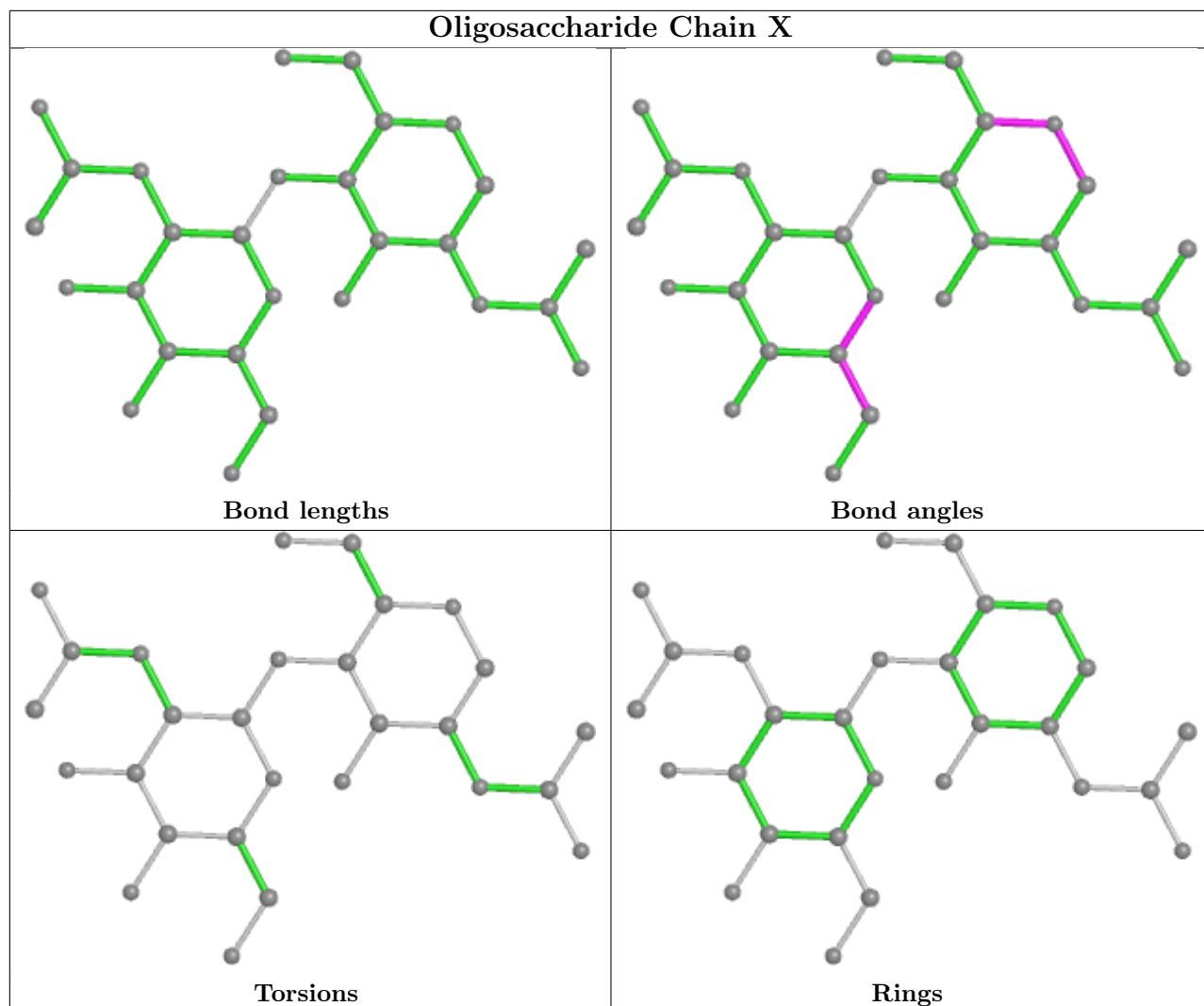


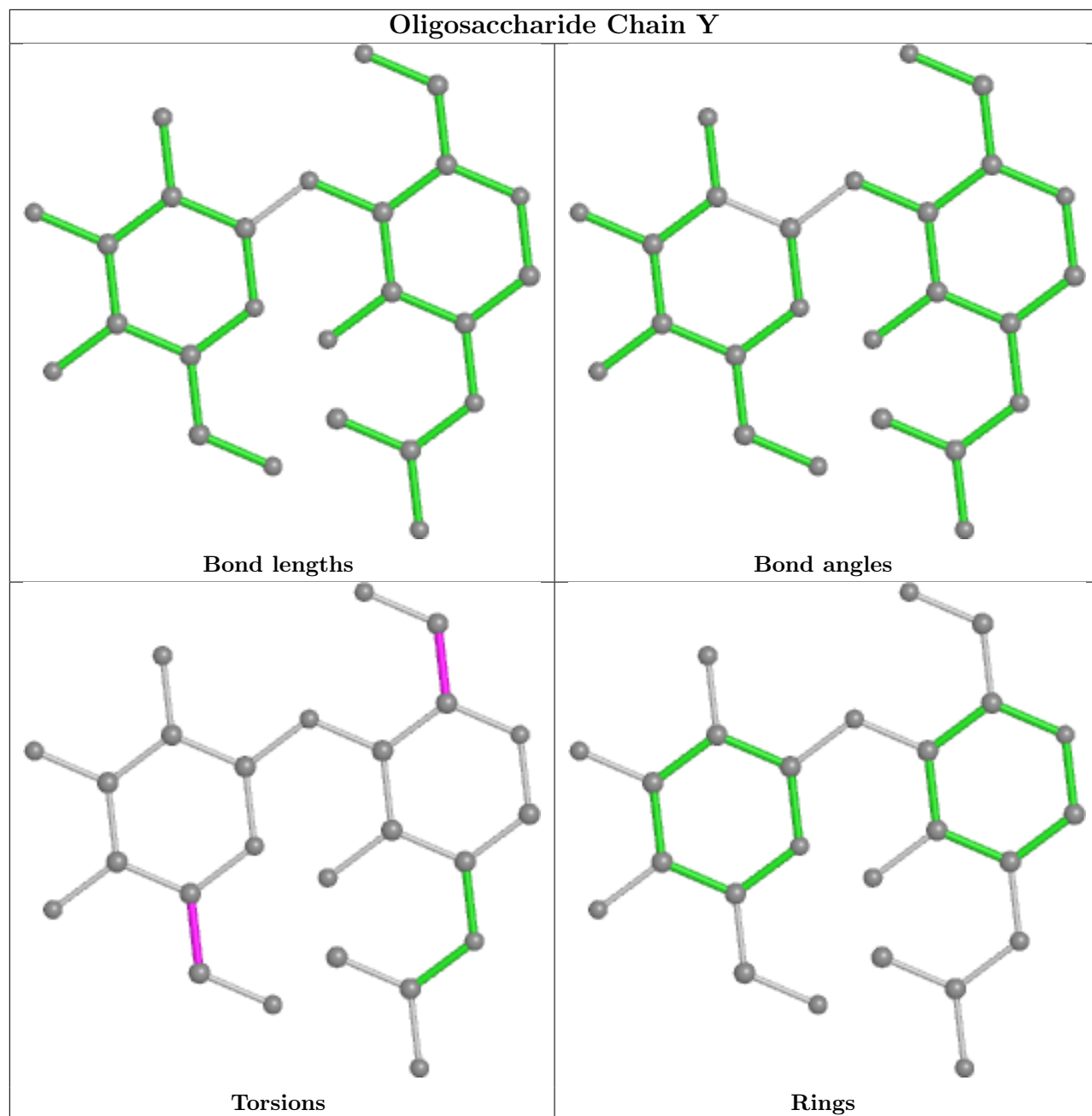


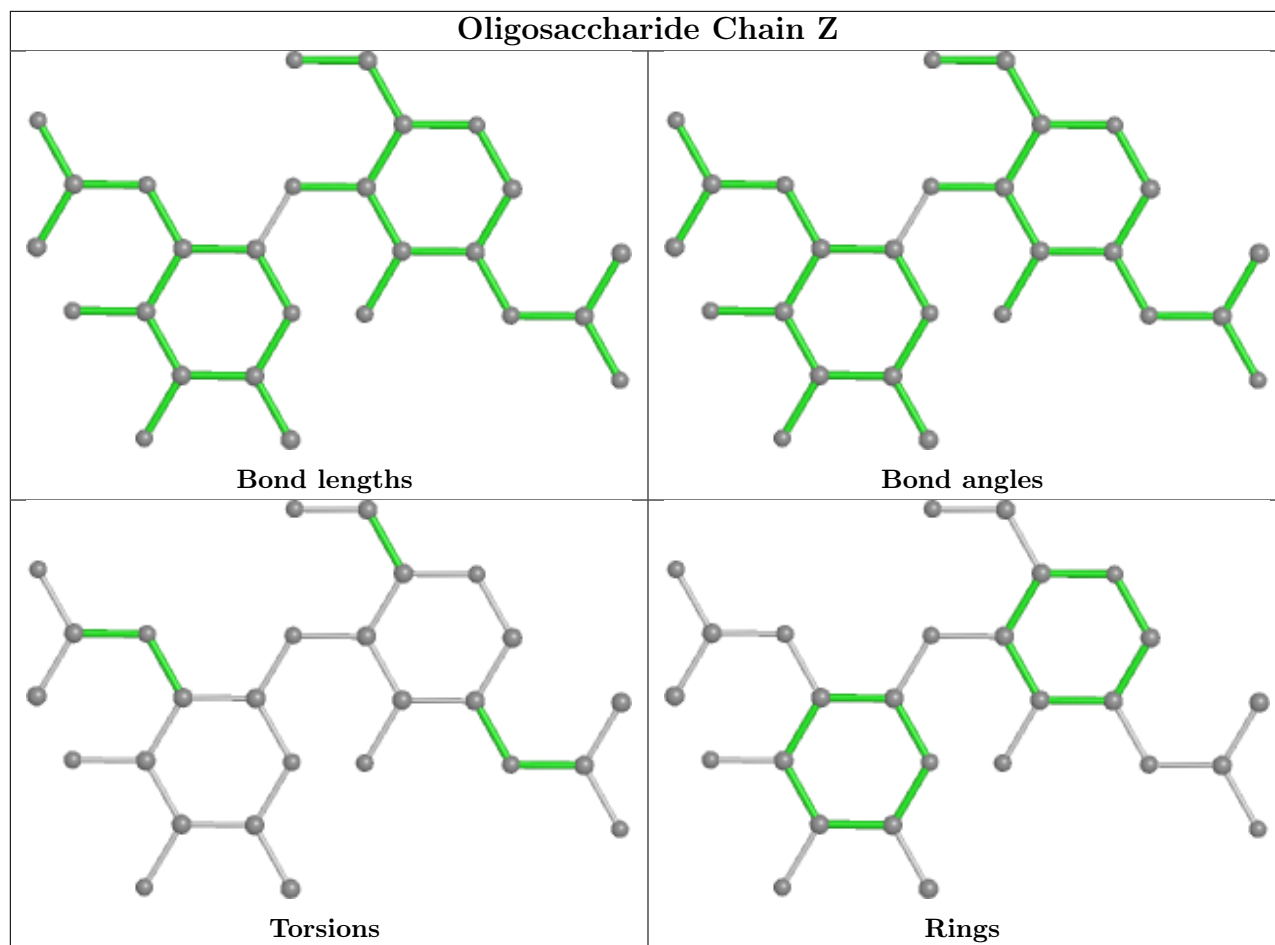












5.6 Ligand geometry [i](#)

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	F	602	1	14,14,15	0.49	0	17,19,21	0.87	0
4	NAG	G	605	1	10,10,15	0.62	0	11,14,21	0.65	0
4	NAG	A	608	1	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
4	NAG	B	607	1	14,14,15	0.54	0	17,19,21	0.92	1 (5%)
4	NAG	C	608	1	14,14,15	0.56	0	17,19,21	0.89	0
4	NAG	G	604	1	14,14,15	0.54	0	17,19,21	0.92	1 (5%)

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	0.51	0	17,19,21	0.71	0
6	PEG	D	609	-	4,4,6	0.59	0	3,3,5	0.22	0
4	NAG	H	606	1	14,14,15	0.48	0	17,19,21	0.84	0
4	NAG	D	608	1	14,14,15	0.51	0	17,19,21	1.37	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	F	602	1	-	0/6/23/26	0/1/1/1
4	NAG	G	605	1	-	-	0/1/1/1
4	NAG	A	608	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	G	604	1	-	2/6/23/26	0/1/1/1
4	NAG	F	605	1	-	2/6/23/26	0/1/1/1
6	PEG	D	609	-	-	2/2/2/4	-
4	NAG	H	606	1	-	4/6/23/26	0/1/1/1
4	NAG	D	608	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	608	NAG	C1-O5-C5	4.36	118.10	112.19
4	G	604	NAG	C1-O5-C5	2.30	115.31	112.19
4	B	607	NAG	C1-O5-C5	2.20	115.17	112.19
4	A	608	NAG	O5-C5-C6	2.10	110.50	107.20

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
4	F	605	NAG	O5-C5-C6-O6
4	H	606	NAG	C8-C7-N2-C2
4	H	606	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	F	605	NAG	C4-C5-C6-O6
4	H	606	NAG	O5-C5-C6-O6
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%)	-0.20	1 (0%) 95 94	26, 48, 70, 100	0
1	B	480/510 (94%)	-0.18	2 (0%) 92 91	22, 41, 71, 101	0
1	C	483/510 (94%)	-0.10	7 (1%) 75 73	28, 46, 75, 105	0
1	D	479/510 (93%)	-0.25	2 (0%) 92 91	26, 42, 67, 114	0
1	E	482/510 (94%)	0.41	36 (7%) 14 13	54, 83, 119, 135	0
1	F	477/510 (93%)	0.22	22 (4%) 32 31	53, 75, 99, 126	0
1	G	478/510 (93%)	0.38	35 (7%) 15 13	44, 77, 122, 160	0
1	H	481/510 (94%)	0.69	52 (10%) 5 5	62, 91, 128, 142	0
All	All	3843/4080 (94%)	0.12	157 (4%) 37 36	22, 63, 111, 160	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	184	GLY	6.7
1	E	349	LEU	5.6
1	G	231	ALA	4.9
1	E	354	ALA	4.8
1	F	217	PRO	4.7
1	G	191	GLY	4.6
1	E	420	PRO	4.5
1	E	230	PRO	4.4
1	G	370	VAL	4.3
1	H	418	GLY	4.2
1	H	329	PRO	4.2
1	H	470	LYS	4.1
1	H	467	GLN	4.1
1	H	466	ASP	4.0
1	B	502	LEU	4.0
1	H	416	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	370	VAL	3.9
1	H	463	MET	3.8
1	H	266	THR	3.8
1	H	361	VAL	3.8
1	B	200	GLY	3.7
1	E	352	LEU	3.7
1	F	203	GLY	3.6
1	E	418	GLY	3.6
1	G	115	GLY	3.6
1	E	353	GLU	3.5
1	H	455	PRO	3.5
1	E	325	TRP	3.5
1	A	203	GLY	3.5
1	G	186	SER	3.4
1	E	224	TYR	3.3
1	H	412	LEU	3.3
1	G	234	ALA	3.3
1	E	312	TYR	3.2
1	G	200	GLY	3.2
1	H	328	ILE	3.2
1	H	44	ALA	3.1
1	F	237	ALA	3.1
1	H	326	PHE	3.1
1	H	469	ALA	3.1
1	G	366	SER	3.1
1	H	454	ASP	3.0
1	H	299	PRO	3.0
1	H	465	ARG	3.0
1	G	367	HIS	3.0
1	F	24	ASN	3.0
1	G	90	GLY	3.0
1	G	114	ALA	3.0
1	C	479	TRP	3.0
1	H	203	GLY	2.9
1	E	493	PRO	2.9
1	G	72	PRO	2.9
1	G	157	LEU	2.9
1	G	188	PRO	2.8
1	G	88	MET	2.8
1	H	218	LEU	2.8
1	H	471	TRP	2.8
1	G	197	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	459	GLN	2.8
1	C	185	HIS	2.8
1	H	417	ALA	2.8
1	H	219	ASP	2.8
1	H	67	VAL	2.7
1	F	168	ASP	2.7
1	E	403	TYR	2.7
1	H	215	TYR	2.7
1	G	259	ASP	2.7
1	H	186	SER	2.6
1	E	491	LEU	2.6
1	E	322	ILE	2.6
1	E	463	MET	2.6
1	G	430	TYR	2.6
1	H	110	LEU	2.6
1	G	201	GLU	2.6
1	D	370	VAL	2.6
1	H	114	ALA	2.6
1	E	445	PRO	2.6
1	H	231	ALA	2.5
1	F	95	VAL	2.5
1	H	298	SER	2.5
1	E	350	PRO	2.5
1	H	320	PRO	2.5
1	G	185	HIS	2.5
1	H	98	PHE	2.5
1	E	458	ALA	2.5
1	F	153	THR	2.5
1	E	91	LEU	2.5
1	G	202	SER	2.5
1	C	478	PRO	2.5
1	F	406	PRO	2.5
1	E	473	TRP	2.4
1	G	368	HIS	2.4
1	H	453	THR	2.4
1	G	238	ALA	2.4
1	H	373	SER	2.4
1	H	161	LYS	2.4
1	E	326	PHE	2.4
1	F	232	ALA	2.4
1	G	218	LEU	2.4
1	E	370	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	90	GLY	2.4
1	G	180	PRO	2.4
1	H	216	ASP	2.4
1	H	202	SER	2.4
1	H	45	ILE	2.3
1	H	366	SER	2.3
1	G	373	SER	2.3
1	E	457	PHE	2.3
1	F	91	LEU	2.3
1	E	68	SER	2.3
1	H	479	TRP	2.3
1	E	384	PHE	2.3
1	G	193	PHE	2.3
1	H	384	PHE	2.3
1	G	230	PRO	2.3
1	H	171	PHE	2.3
1	E	406	PRO	2.2
1	C	186	SER	2.2
1	H	323	LEU	2.2
1	F	165	THR	2.2
1	E	357	LEU	2.2
1	E	348	LEU	2.2
1	E	168	ASP	2.2
1	E	444	ASP	2.2
1	F	216	ASP	2.2
1	H	90	GLY	2.2
1	F	134	PHE	2.2
1	C	491	LEU	2.2
1	F	214	ALA	2.2
1	F	22	PRO	2.1
1	H	357	LEU	2.1
1	G	126	VAL	2.1
1	C	366	SER	2.1
1	G	241	THR	2.1
1	E	100	SER	2.1
1	F	209	ASP	2.1
1	G	96	HIS	2.1
1	F	187	GLN	2.1
1	H	419	GLN	2.1
1	C	480	VAL	2.1
1	D	366	SER	2.1
1	E	442	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	492	SER	2.1
1	H	272	SER	2.1
1	E	419	GLN	2.1
1	F	170	PRO	2.0
1	G	67	VAL	2.0
1	F	202	SER	2.0
1	E	448	THR	2.0
1	G	203	GLY	2.0
1	G	410	ASP	2.0
1	H	170	PRO	2.0
1	H	46	ALA	2.0
1	H	92	HIS	2.0
1	H	91	LEU	2.0
1	F	162	PHE	2.0
1	F	171	PHE	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	0.24	72,75,80,83	0
1	FGP	E	70	11/12	0.88	0.22	68,80,139,144	0
1	FGP	F	70	11/12	0.91	0.17	61,72,131,141	0
1	FGP	D	70	11/12	0.93	0.16	29,40,93,95	0
1	FGP	B	70	11/12	0.94	0.16	26,34,85,101	0
1	FGP	C	70	11/12	0.94	0.17	32,40,91,115	0
1	FGP	A	70	11/12	0.94	0.16	33,50,105,123	0
1	FGP	H	70	7/12	0.94	0.22	66,68,70,75	0

6.3 Carbohydrates [i](#)

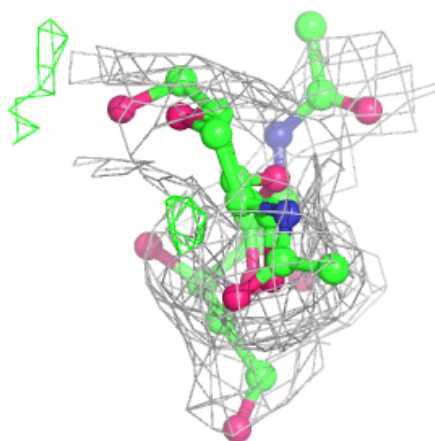
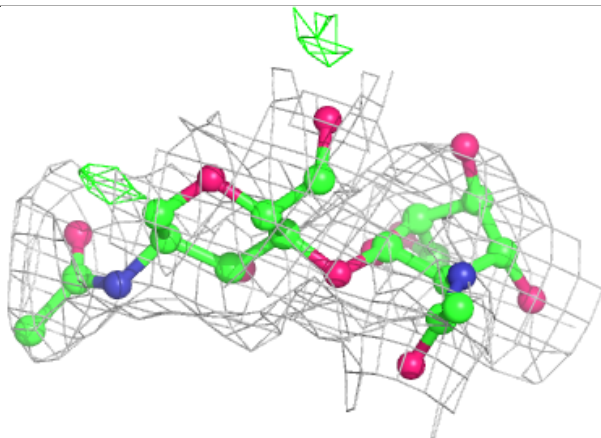
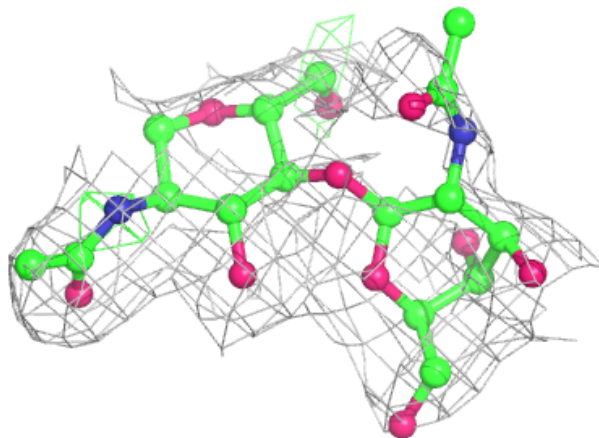
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	K	2	14/15	0.74	0.25	74,102,124,126	0
2	NAG	U	2	14/15	0.74	0.25	71,119,139,145	0
2	NAG	a	2	14/15	0.75	0.35	86,132,149,150	0
2	NAG	R	2	14/15	0.77	0.36	71,104,136,136	0
2	NAG	I	1	14/15	0.78	0.18	60,98,132,137	0
2	NAG	Q	1	14/15	0.78	0.23	71,112,124,129	0
2	NAG	R	1	14/15	0.78	0.17	48,80,128,145	0
2	NAG	I	2	14/15	0.79	0.29	78,106,134,140	0
2	NAG	Q	2	14/15	0.79	0.29	80,116,146,150	0
2	NAG	a	1	14/15	0.81	0.28	76,127,145,153	0
2	NAG	O	1	14/15	0.82	0.15	55,78,105,130	0
2	NAG	L	2	14/15	0.83	0.23	73,97,111,114	0
2	NAG	O	2	13/15	0.83	0.26	84,105,126,132	0
2	NAG	U	1	14/15	0.83	0.17	80,128,152,152	0
2	NAG	W	2	14/15	0.84	0.17	58,74,92,96	0
2	NAG	Z	2	13/15	0.86	0.31	69,98,115,115	0
2	NAG	S	2	14/15	0.86	0.17	53,76,115,118	0
2	NAG	J	2	14/15	0.86	0.18	47,83,104,116	0
2	NAG	L	1	14/15	0.87	0.13	49,64,88,90	0
2	NAG	W	1	14/15	0.87	0.14	44,78,94,95	0
2	NAG	X	1	14/15	0.88	0.18	58,73,85,86	0
2	NAG	Y	1	14/15	0.88	0.15	52,80,105,114	0
2	NAG	M	2	13/15	0.88	0.21	55,103,128,139	0
2	NAG	T	2	14/15	0.88	0.17	72,101,118,120	0
2	NAG	N	2	14/15	0.88	0.23	70,87,99,104	0
2	NAG	Y	2	11/15	0.89	0.15	80,116,138,142	0
2	NAG	K	1	14/15	0.89	0.13	54,72,94,97	0
2	NAG	X	2	14/15	0.90	0.26	60,75,94,100	0
2	NAG	P	2	13/15	0.90	0.21	60,92,106,120	0
2	NAG	M	1	14/15	0.90	0.20	44,65,85,107	0
2	NAG	V	2	14/15	0.92	0.14	56,77,85,90	0
2	NAG	Z	1	14/15	0.93	0.16	47,64,74,77	0
2	NAG	V	1	14/15	0.94	0.13	49,63,77,79	0
2	NAG	N	1	14/15	0.94	0.07	48,63,78,81	0
2	NAG	J	1	14/15	0.94	0.12	36,48,61,70	0
2	NAG	T	1	14/15	0.94	0.13	56,65,92,100	0
2	NAG	S	1	14/15	0.96	0.10	36,43,61,69	0
2	NAG	P	1	14/15	0.96	0.12	39,49,67,68	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.

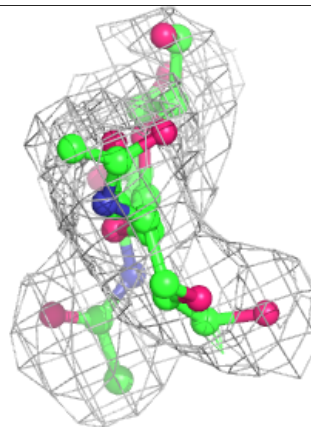
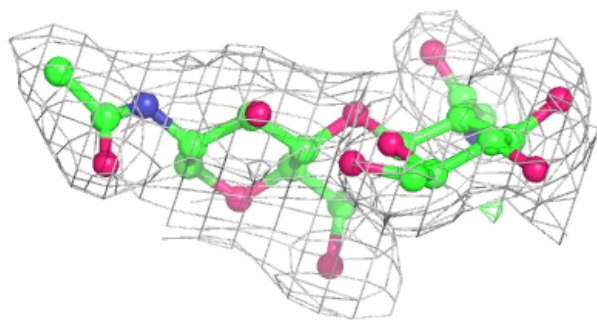
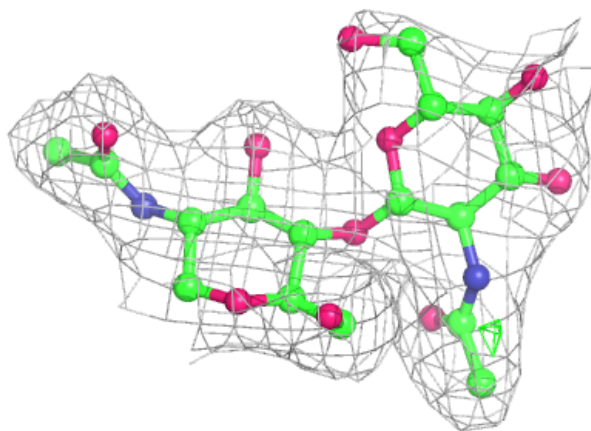
Electron density around Chain I:

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



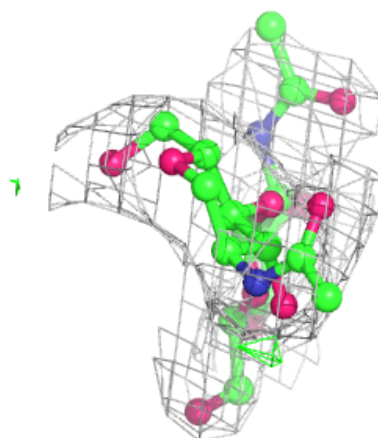
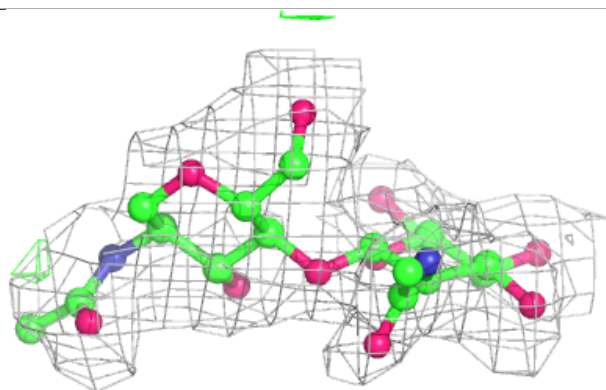
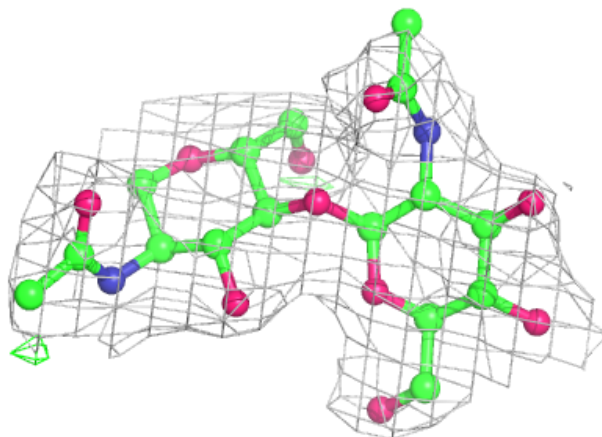
Electron density around Chain J:

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



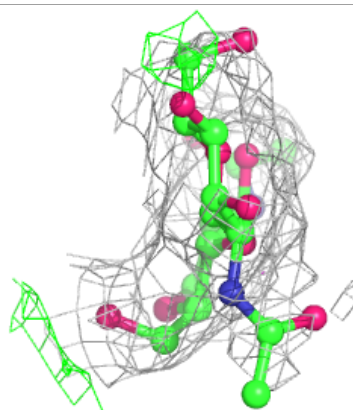
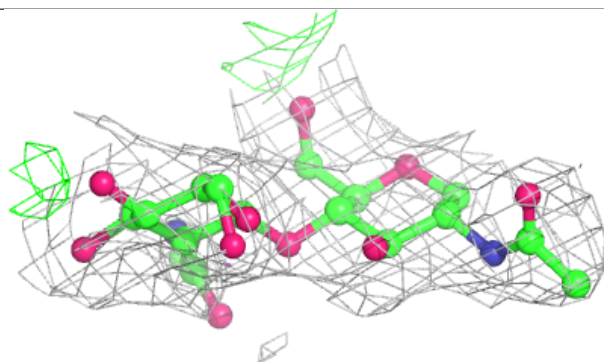
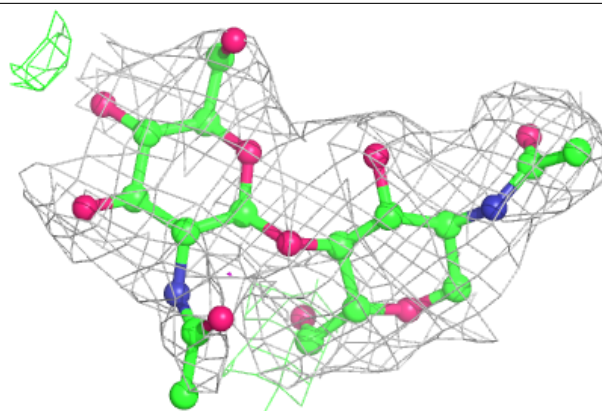
Electron density around Chain K:

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

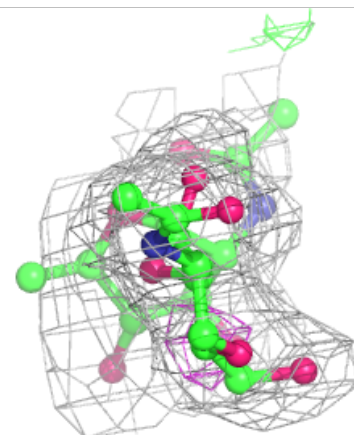
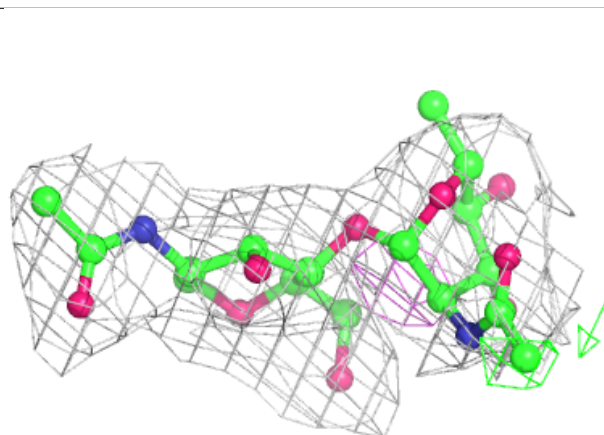
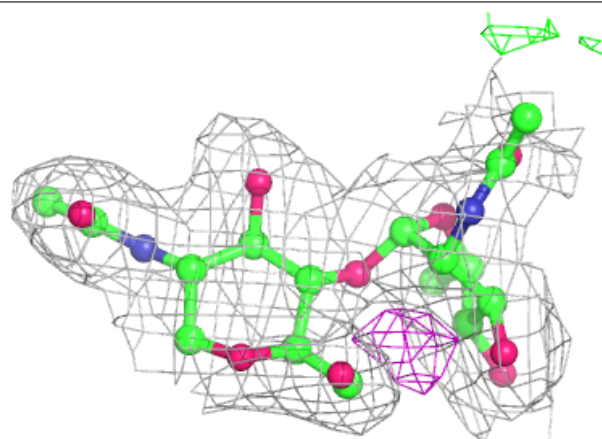


Electron density around Chain L:

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

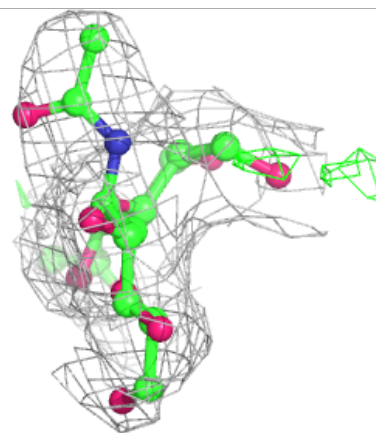
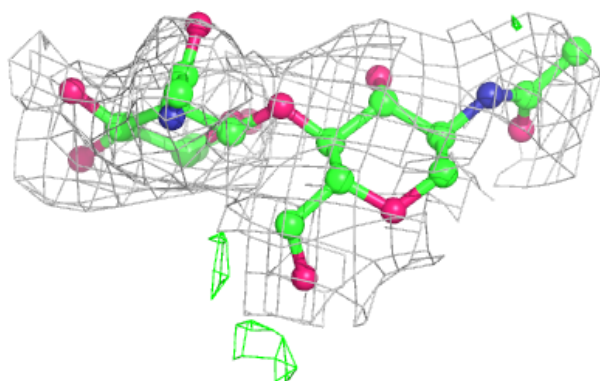
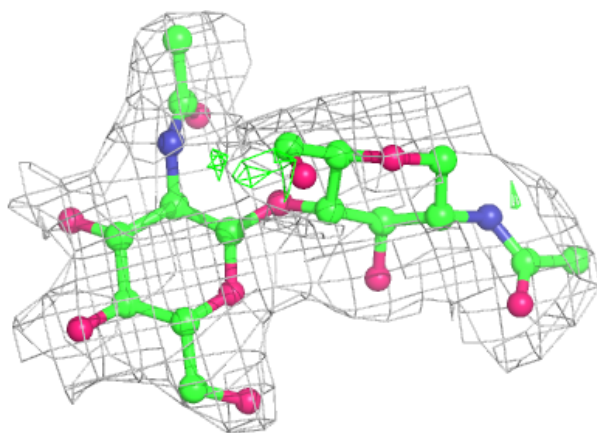
**Electron density around Chain M:**

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



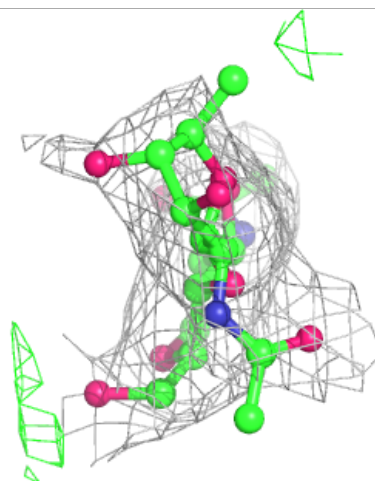
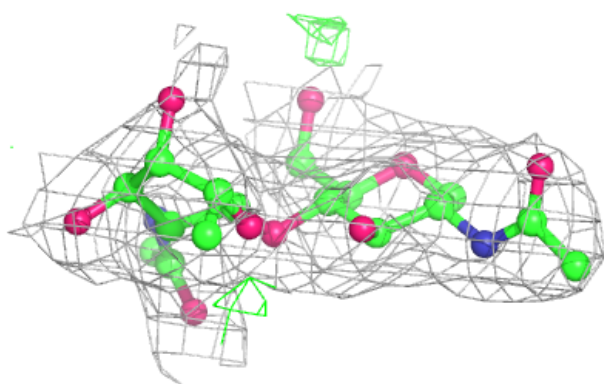
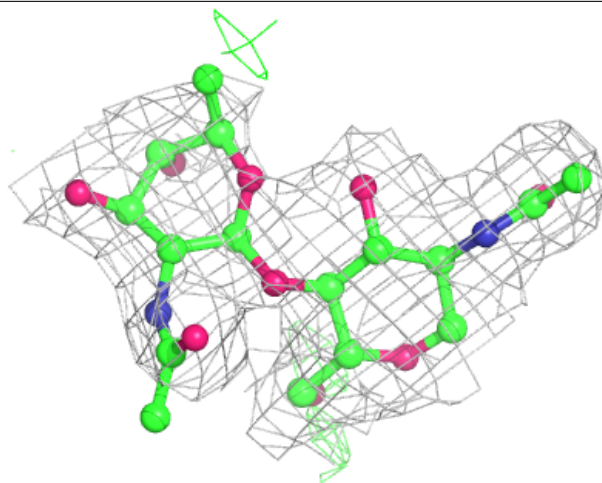
Electron density around Chain N:

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



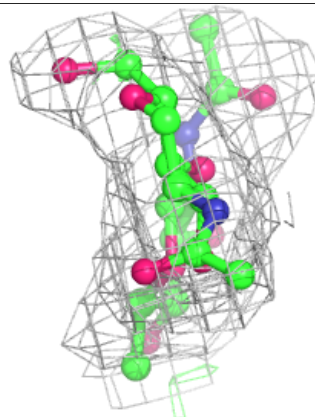
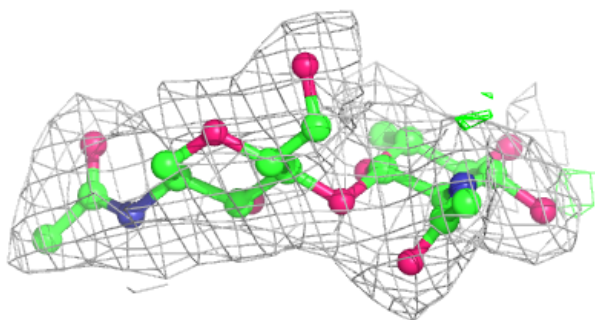
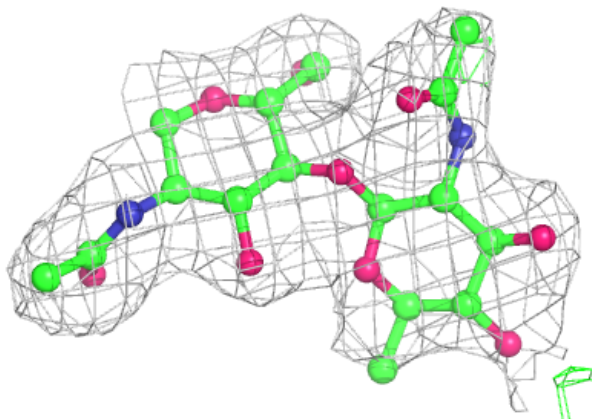
Electron density around Chain O:

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



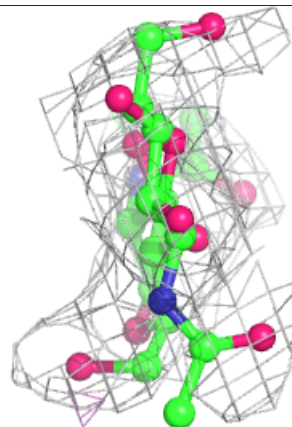
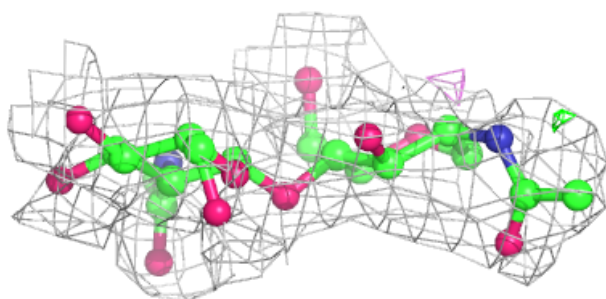
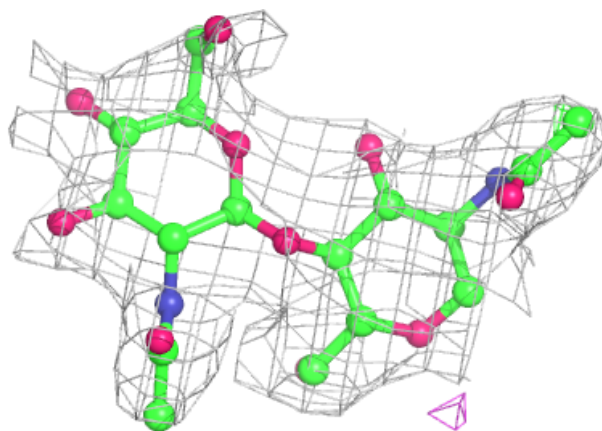
Electron density around Chain P:

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



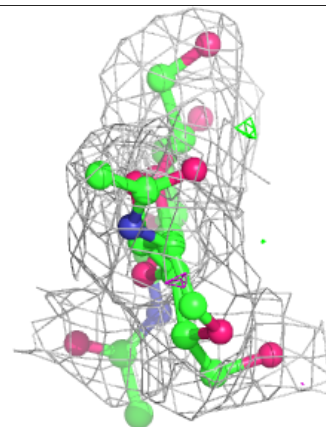
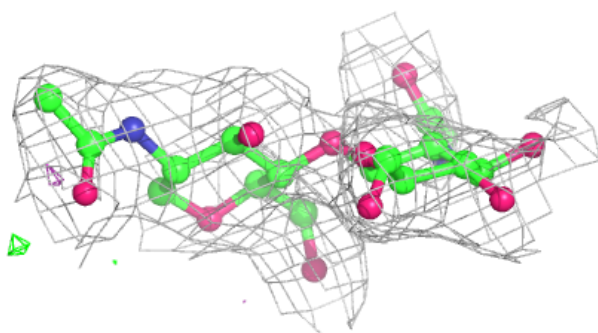
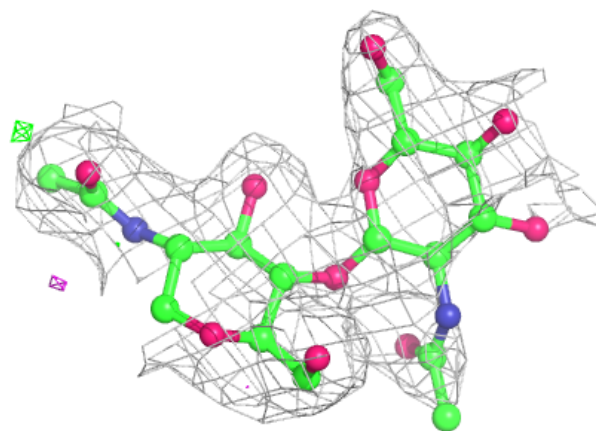
Electron density around Chain Q:

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



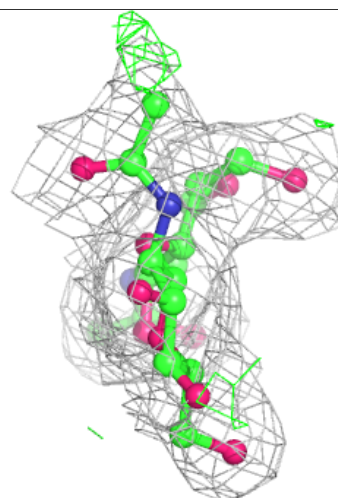
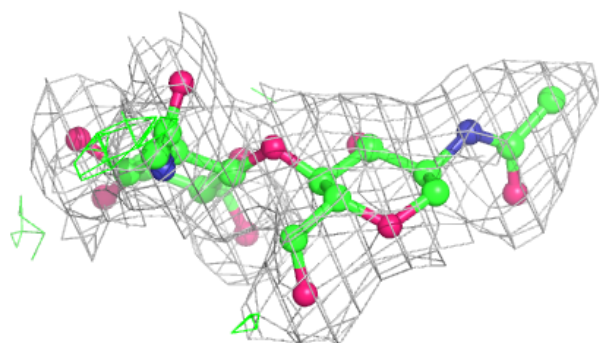
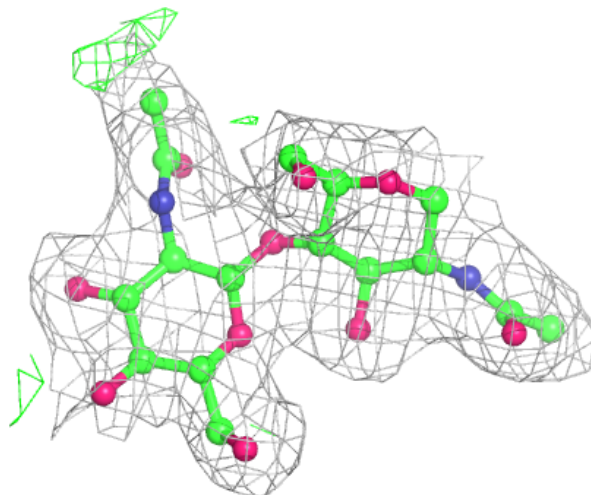
Electron density around Chain R:

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



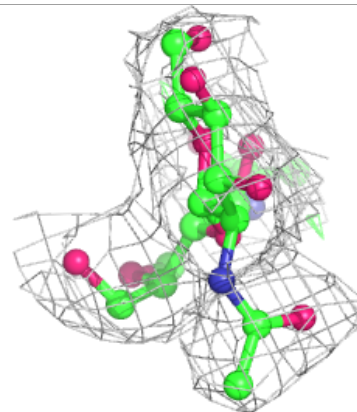
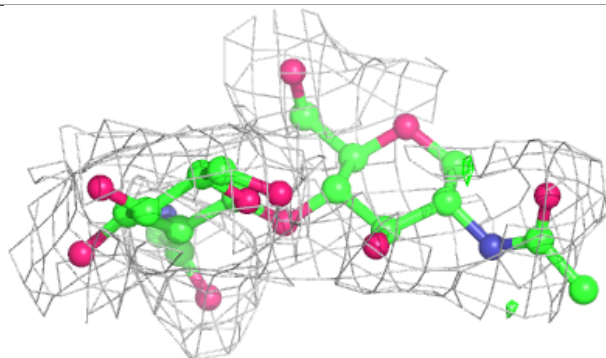
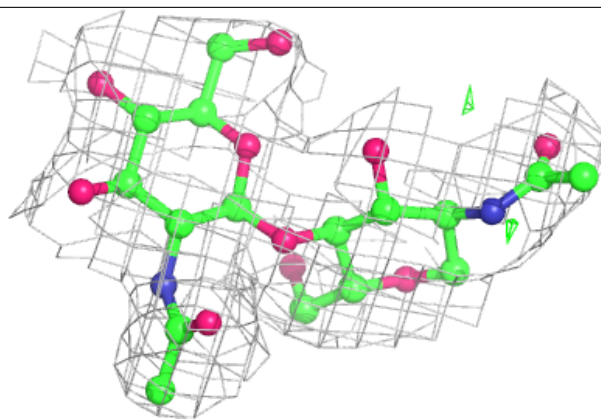
Electron density around Chain S:

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



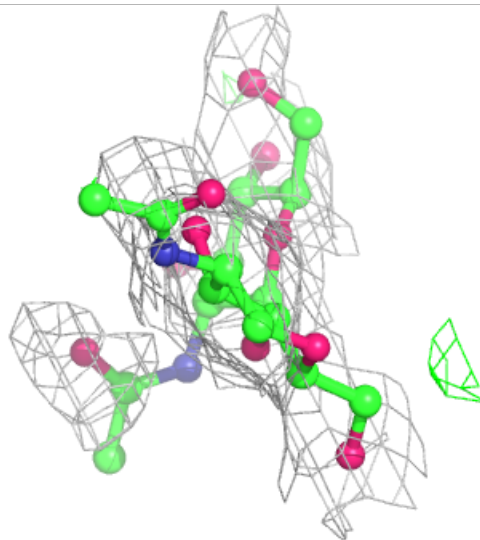
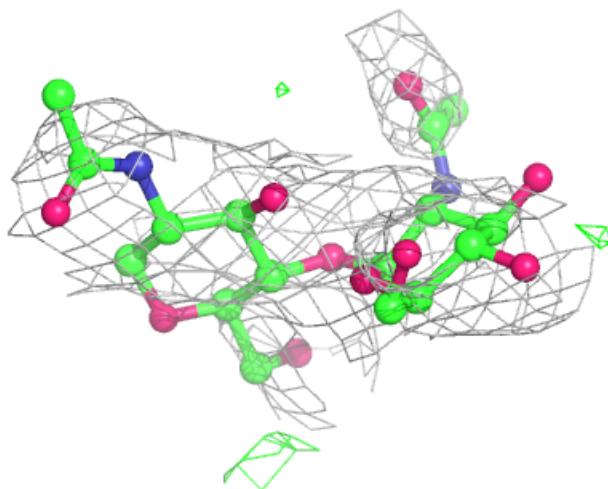
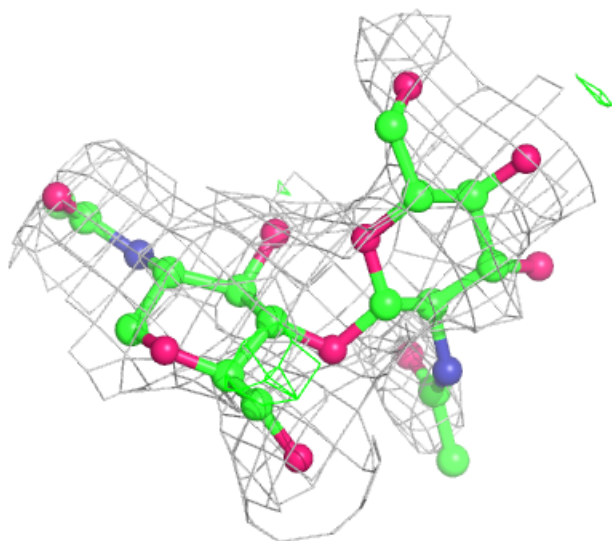
Electron density around Chain T:

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



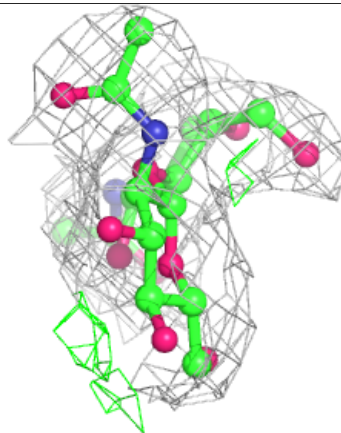
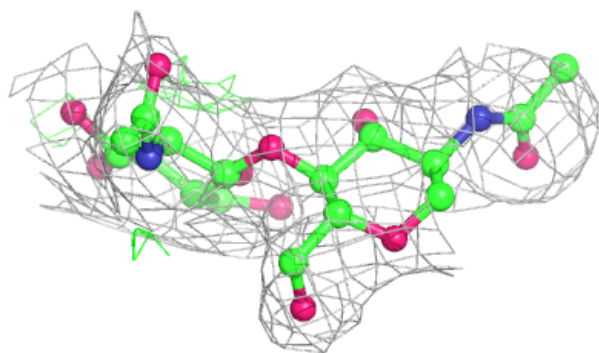
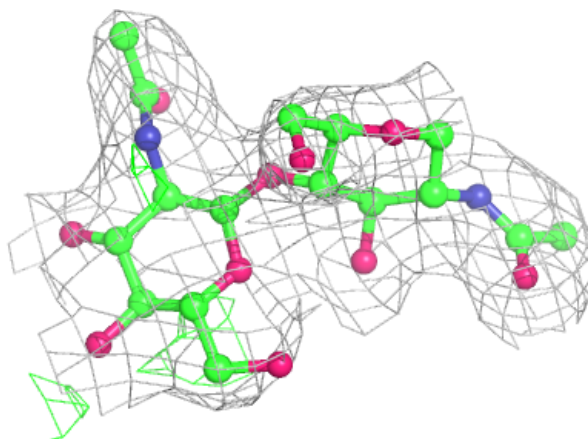
Electron density around Chain U:

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

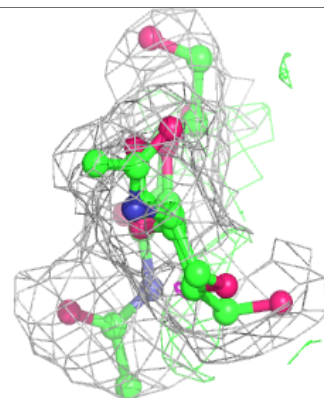
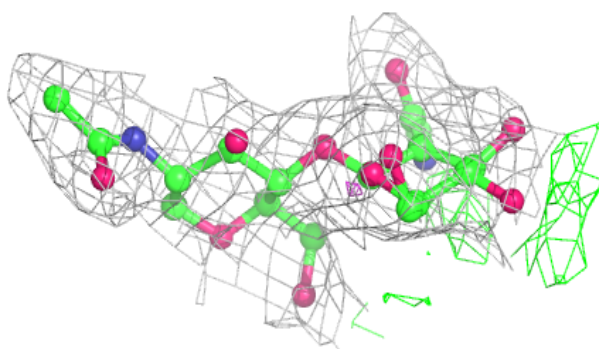
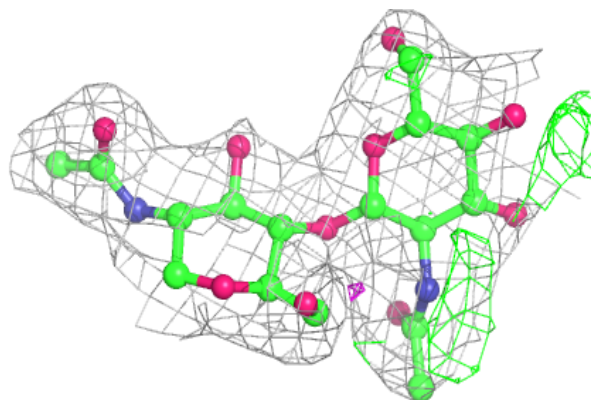


Electron density around Chain V:

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

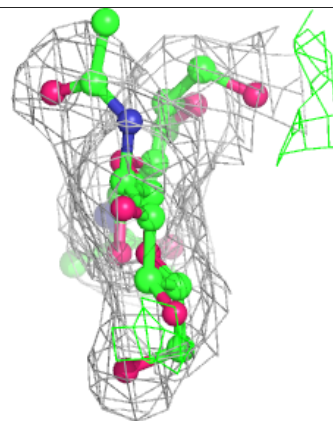
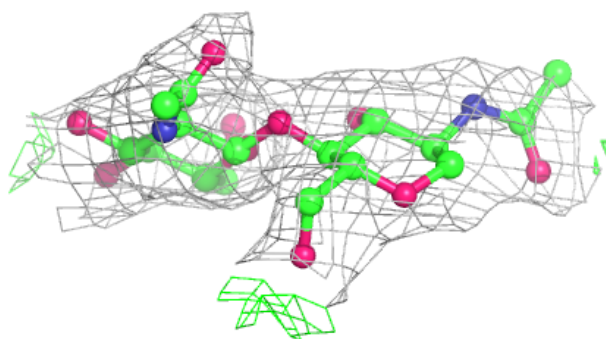
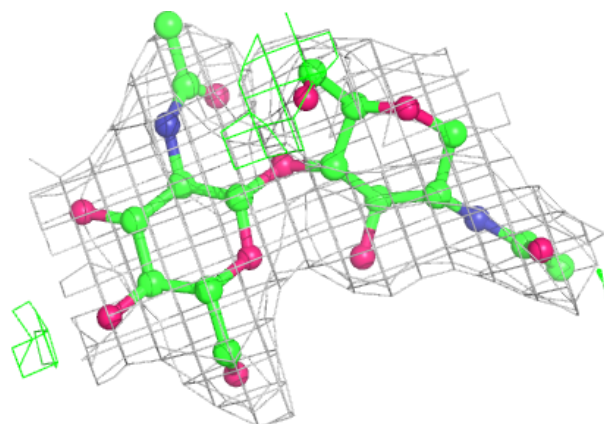
**Electron density around Chain W:**

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

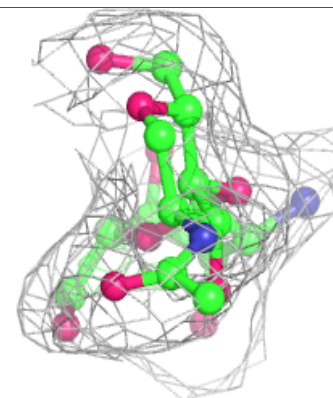
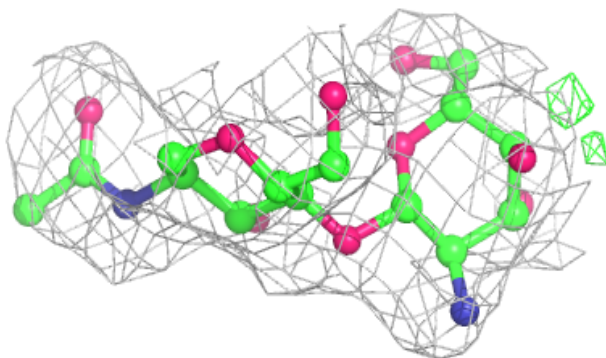
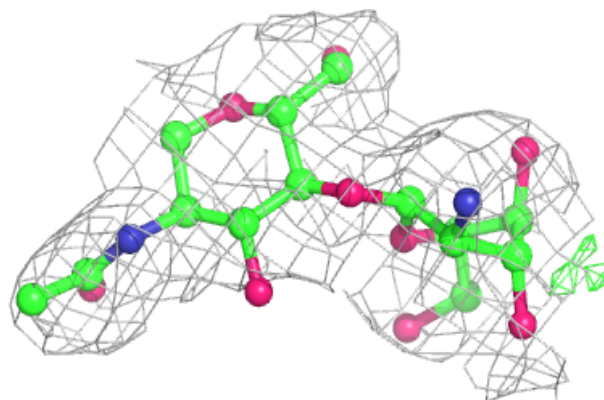


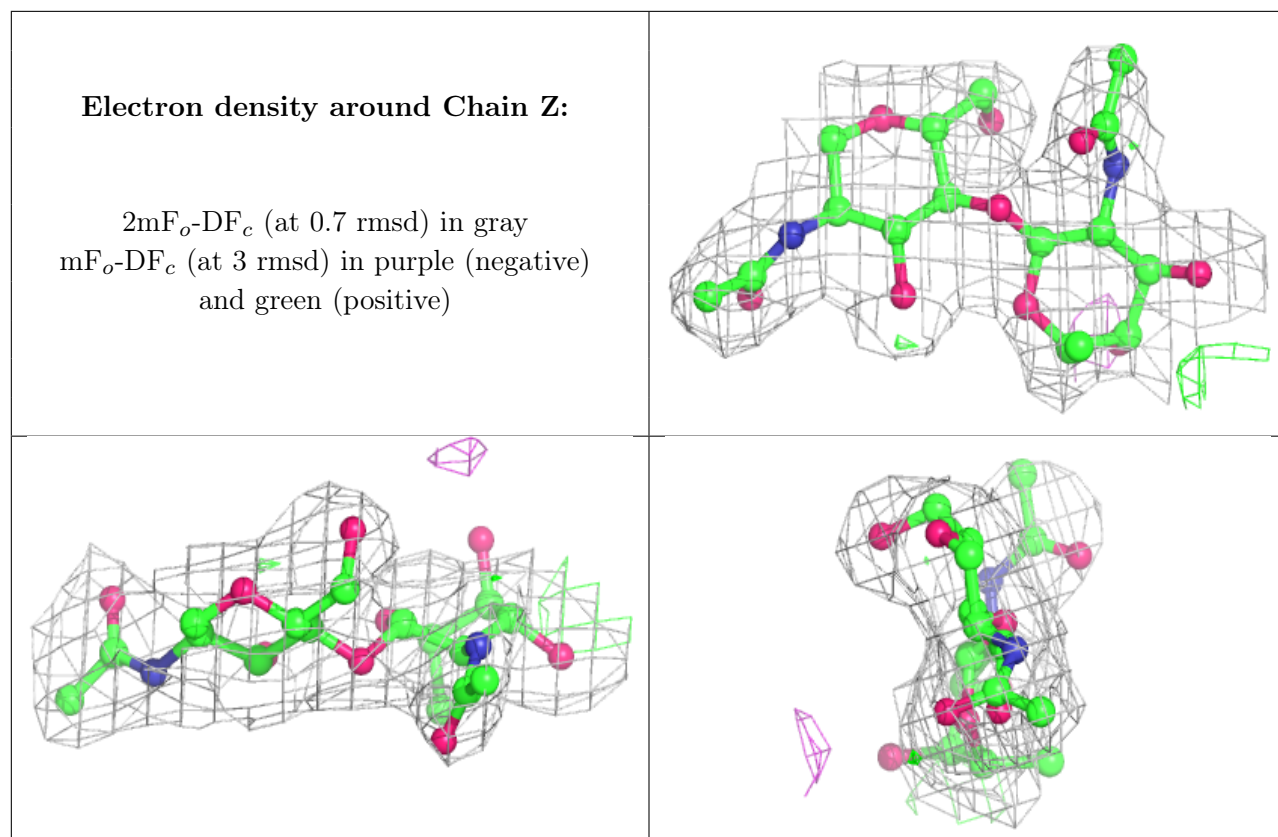
Electron density around Chain X:

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

**Electron density around Chain Y:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	608	14/15	0.75	0.26	73,114,126,128	0
4	NAG	G	604	14/15	0.79	0.21	61,83,117,120	0
4	NAG	G	605	10/15	0.79	0.19	72,88,104,107	0
3	CA	G	601	1/1	0.81	0.10	107,107,107,107	0
4	NAG	C	608	14/15	0.83	0.29	56,79,108,112	0
4	NAG	F	602	14/15	0.85	0.13	63,87,110,118	0
3	CA	F	601	1/1	0.86	0.06	73,73,73,73	0
4	NAG	D	608	14/15	0.87	0.12	37,62,87,91	0
4	NAG	B	607	14/15	0.87	0.16	50,71,89,101	0
4	NAG	H	606	14/15	0.88	0.23	81,99,115,117	0
6	PEG	D	609	5/7	0.90	0.22	27,33,49,54	0
4	NAG	F	605	14/15	0.91	0.18	77,105,120,129	0
3	CA	H	601	1/1	0.96	0.05	75,75,75,75	0
3	CA	C	601	1/1	0.97	0.04	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	600	1/1	0.97	0.06	52,52,52,52	0
3	CA	D	601	1/1	0.98	0.06	43,43,43,43	0
3	CA	E	600	1/1	0.98	0.05	69,69,69,69	0
5	CL	A	609	1/1	0.98	0.11	43,43,43,43	0
5	CL	C	609	1/1	0.98	0.37	64,64,64,64	0
3	CA	A	601	1/1	0.98	0.05	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.