



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 06:43 PM EDT

PDB ID : 9B7I / pdb\_00009b7i  
Title : Crystal structure of the H3 hemagglutinin COBRA J4  
Authors : Dzimianski, J.V.; DuBois, R.M.  
Deposited on : 2024-03-27  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

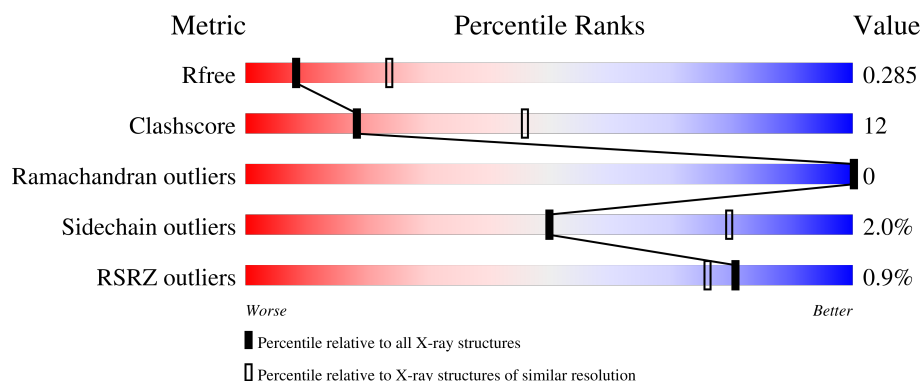
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 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	323	
1	B	323	
1	C	323	
1	D	323	
1	E	323	


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Mol	Chain	Length	Quality of chain
1	F	323	
2	a	181	
2	b	181	
2	c	181	
2	d	181	
2	e	181	
2	f	181	
3	G	4	
3	K	4	
3	O	4	
4	H	4	
4	I	4	
4	T	4	
4	X	4	
5	J	3	
5	L	3	
5	P	3	
5	R	3	
5	S	3	
6	M	5	
6	N	5	
6	U	5	
6	V	5	
7	Q	2	
7	W	2	

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Mol	Chain	Length	Quality of chain
7	Y	2	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2487	1557	443	475	12			
1	B	319	Total	C	N	O	S	0	0	0
			2496	1563	445	476	12			
1	C	318	Total	C	N	O	S	0	0	0
			2487	1557	443	475	12			
1	D	317	Total	C	N	O	S	0	0	0
			2479	1553	441	473	12			
1	E	316	Total	C	N	O	S	0	0	0
			2473	1550	440	471	12			
1	F	318	Total	C	N	O	S	0	0	0
			2487	1557	443	475	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	TYR	PHE	conflict	UNP A0A5J6A4B5
A	225	ASP	ASN	conflict	UNP A0A5J6A4B5
B	159	TYR	PHE	conflict	UNP A0A5J6A4B5
B	225	ASP	ASN	conflict	UNP A0A5J6A4B5
C	159	TYR	PHE	conflict	UNP A0A5J6A4B5
C	225	ASP	ASN	conflict	UNP A0A5J6A4B5
D	159	TYR	PHE	conflict	UNP A0A5J6A4B5
D	225	ASP	ASN	conflict	UNP A0A5J6A4B5
E	159	TYR	PHE	conflict	UNP A0A5J6A4B5
E	225	ASP	ASN	conflict	UNP A0A5J6A4B5
F	159	TYR	PHE	conflict	UNP A0A5J6A4B5
F	225	ASP	ASN	conflict	UNP A0A5J6A4B5

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	172	Total	C	N	O	S	0	0	0
			1388	863	246	273	6			
2	b	171	Total	C	N	O	S	0	0	0
			1379	858	244	271	6			
2	c	172	Total	C	N	O	S	0	0	0
			1388	863	246	273	6			
2	d	170	Total	C	N	O	S	0	0	0
			1372	853	243	270	6			
2	e	171	Total	C	N	O	S	0	0	0
			1379	858	244	271	6			
2	f	172	Total	C	N	O	S	0	0	0
			1388	863	246	273	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	508	VAL	LYS	conflict	UNP A0A5J6UNG5
a	509	PRO	SER	conflict	UNP A0A5J6UNG5
a	510	ARG	GLY	conflict	UNP A0A5J6UNG5
b	508	VAL	LYS	conflict	UNP A0A5J6UNG5
b	509	PRO	SER	conflict	UNP A0A5J6UNG5
b	510	ARG	GLY	conflict	UNP A0A5J6UNG5
c	508	VAL	LYS	conflict	UNP A0A5J6UNG5
c	509	PRO	SER	conflict	UNP A0A5J6UNG5
c	510	ARG	GLY	conflict	UNP A0A5J6UNG5
d	508	VAL	LYS	conflict	UNP A0A5J6UNG5
d	509	PRO	SER	conflict	UNP A0A5J6UNG5
d	510	ARG	GLY	conflict	UNP A0A5J6UNG5
e	508	VAL	LYS	conflict	UNP A0A5J6UNG5
e	509	PRO	SER	conflict	UNP A0A5J6UNG5
e	510	ARG	GLY	conflict	UNP A0A5J6UNG5
f	508	VAL	LYS	conflict	UNP A0A5J6UNG5
f	509	PRO	SER	conflict	UNP A0A5J6UNG5
f	510	ARG	GLY	conflict	UNP A0A5J6UNG5

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



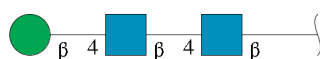
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



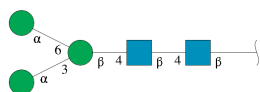
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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
7	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

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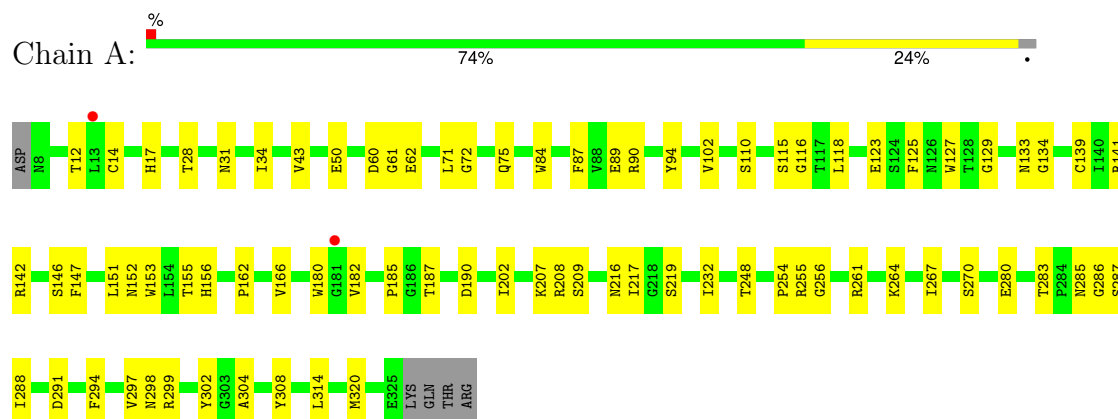
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	a	1	Total	C	N	O	0	0
			14	8	1	5		
8	c	1	Total	C	N	O	0	0
			14	8	1	5		
8	d	1	Total	C	N	O	0	0
			14	8	1	5		
8	f	1	Total	C	N	O	0	0
			14	8	1	5		

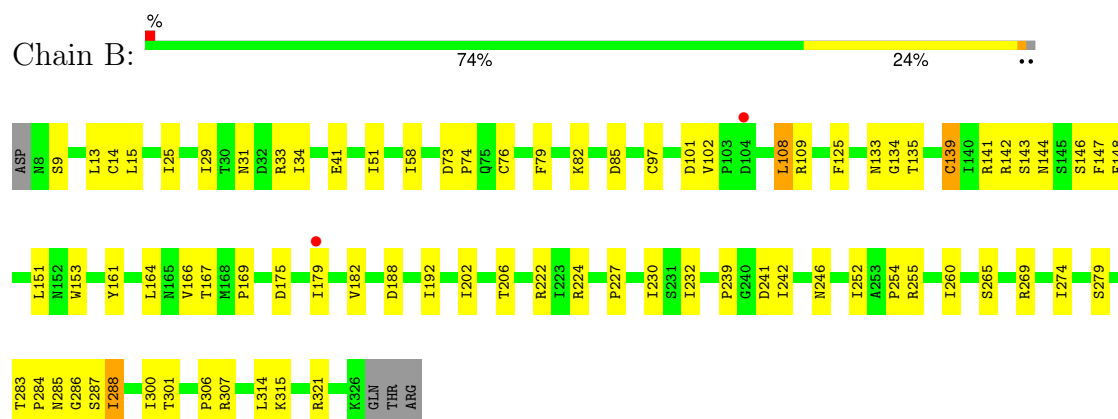
### 3 Residue-property plots

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

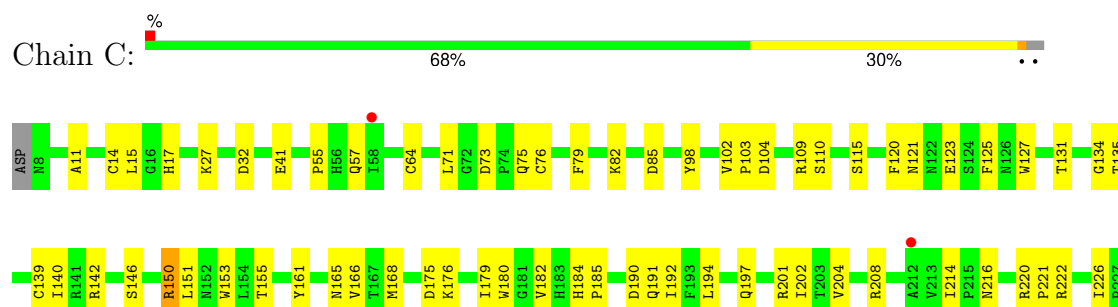
#### • Molecule 1: Hemagglutinin HA1



#### • Molecule 1: Hemagglutinin HA1

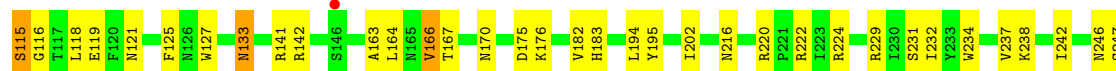
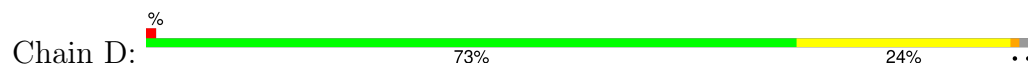


#### • Molecule 1: Hemagglutinin HA1

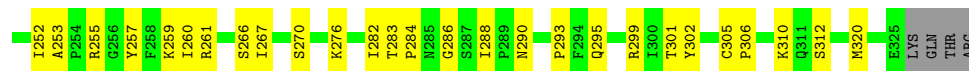




• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1

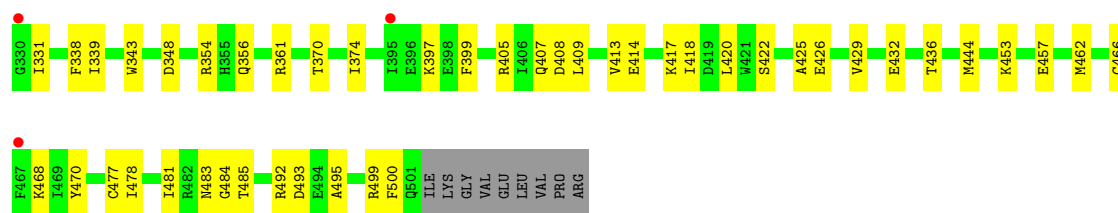


• Molecule 1: Hemagglutinin HA1

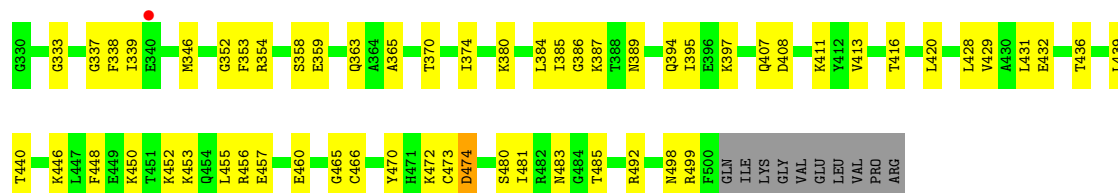


• Molecule 2: Hemagglutinin HA2

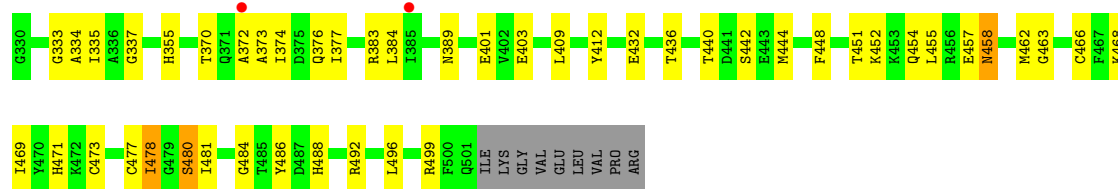




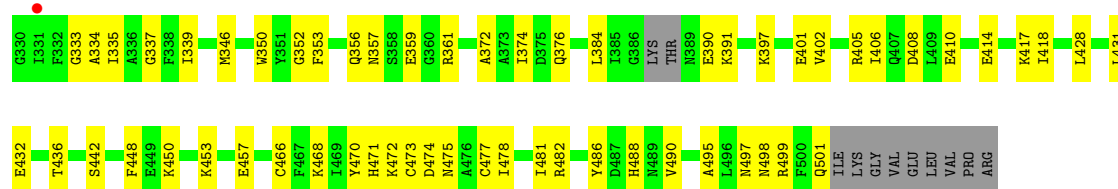
• Molecule 2: Hemagglutinin HA2



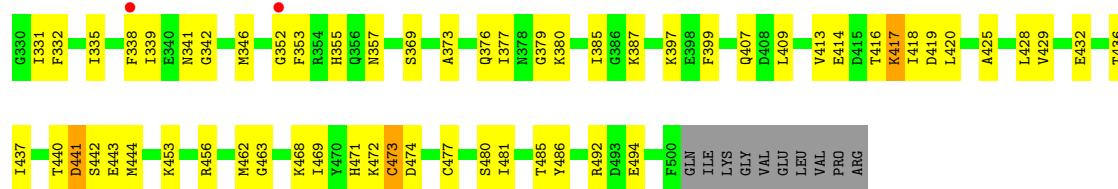
• Molecule 2: Hemagglutinin HA2



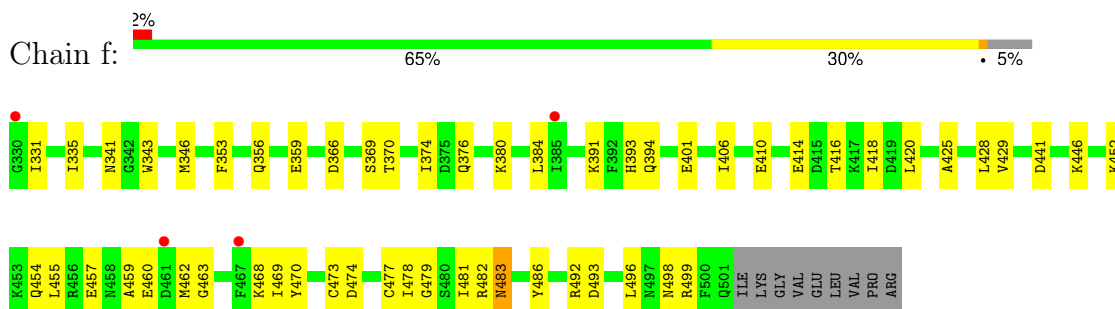
• Molecule 2: Hemagglutinin HA2



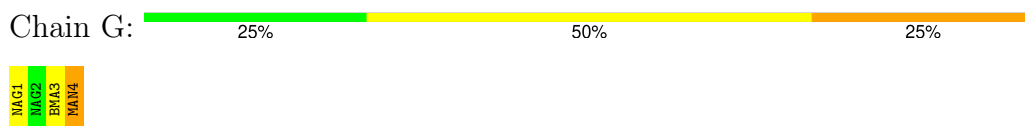
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



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



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



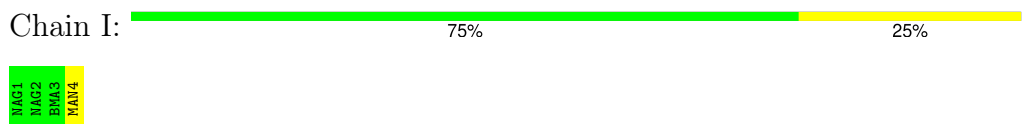
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain T:  75% 25%



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

Chain X:  50% 50%



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

Chain J:  100%



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

Chain L:  33% 67%



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

Chain P:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain M: 



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

Chain N: 



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

Chain U: 



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

Chain V: 




- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.74Å 105.30Å 109.68Å 71.61° 73.38° 87.07°	Depositor
Resolution (Å)	49.92 – 2.90 49.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (49.92-2.90) 87.5 (49.92-2.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.228 , 0.285 0.228 , 0.285	Depositor DCC
$R_{free}$ test set	3797 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.10	0/2543	0.28	0/3457
1	B	0.12	0/2552	0.30	0/3468
1	C	0.13	0/2543	0.31	0/3457
1	D	0.13	0/2535	0.30	0/3446
1	E	0.16	0/2529	0.33	0/3438
1	F	0.16	0/2543	0.34	0/3457
2	a	0.09	0/1412	0.26	0/1895
2	b	0.13	0/1403	0.31	0/1883
2	c	0.12	0/1412	0.28	0/1895
2	d	0.13	0/1395	0.34	0/1871
2	e	0.15	0/1403	0.35	0/1883
2	f	0.13	0/1412	0.31	0/1895
All	All	0.13	0/23682	0.31	0/32045

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2487	0	2437	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2496	0	2454	58	0
1	C	2487	0	2440	71	0
1	D	2479	0	2435	59	0
1	E	2473	0	2427	70	0
1	F	2487	0	2440	59	0
2	a	1388	0	1314	40	0
2	b	1379	0	1308	43	0
2	c	1388	0	1315	42	0
2	d	1372	0	1294	52	0
2	e	1379	0	1308	46	0
2	f	1388	0	1315	53	0
3	G	50	0	43	2	0
3	K	50	0	43	4	0
3	O	50	0	43	2	0
4	H	50	0	43	1	0
4	I	50	0	43	0	0
4	T	50	0	43	0	0
4	X	50	0	43	1	0
5	J	39	0	34	0	0
5	L	39	0	34	2	0
5	P	39	0	34	2	0
5	R	39	0	34	0	0
5	S	39	0	34	0	0
6	M	61	0	52	1	0
6	N	61	0	52	1	0
6	U	61	0	52	1	0
6	V	61	0	52	0	0
7	Q	28	0	25	1	0
7	W	28	0	25	2	0
7	Y	28	0	25	1	0
8	A	56	0	52	0	0
8	B	28	0	26	0	0
8	C	42	0	39	0	0
8	D	14	0	13	0	0
8	E	42	0	39	0	0
8	F	14	0	13	0	0
8	a	14	0	13	0	0
8	c	14	0	13	1	0
8	d	14	0	13	0	0
8	f	14	0	13	1	0
All	All	24328	0	23475	567	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 12.

All (567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:492:ARG:HG2	2:f:496:LEU:HD11	1.43	1.00
1:E:13:LEU:HD11	2:e:353:PHE:HB3	1.54	0.88
1:C:175:ASP:HB2	1:C:260:ILE:HD11	1.56	0.88
1:B:222:ARG:HE	1:B:227:PRO:HG3	1.38	0.87
2:d:472:LYS:HE2	2:d:472:LYS:HA	1.56	0.86
1:E:96:ASN:O	1:E:96:ASN:ND2	2.08	0.84
1:E:259:LYS:HE3	1:E:261:ARG:HH21	1.46	0.81
3:O:1:NAG:H81	5:P:2:NAG:H82	1.62	0.81
2:d:356:GLN:OE1	2:d:361:ARG:HG3	1.81	0.80
1:D:42:LEU:HD11	1:D:316:LEU:HB2	1.64	0.78
1:D:222:ARG:HD2	7:W:2:NAG:H3	1.66	0.77
1:D:176:LYS:HB2	1:D:237:VAL:HG22	1.66	0.77
2:b:474:ASP:N	2:b:474:ASP:OD1	2.18	0.76
2:a:457:GLU:HB2	2:a:492:ARG:HH12	1.50	0.76
1:F:13:LEU:HD11	2:f:353:PHE:HB3	1.69	0.75
1:B:148:PHE:HB2	1:B:151:LEU:HB2	1.69	0.74
2:b:457:GLU:HG3	2:b:499:ARG:HH12	1.52	0.74
2:d:481:ILE:HG12	2:d:486:TYR:HD2	1.52	0.74
1:B:222:ARG:HD2	4:H:2:NAG:H2	1.68	0.74
1:C:182:VAL:HB	1:C:202:ILE:HD11	1.67	0.74
1:E:237:VAL:HG13	1:E:241:ASP:HB3	1.71	0.73
2:b:387:LYS:HZ2	2:b:389:ASN:HA	1.55	0.72
2:d:333:GLY:HA3	2:f:446:LYS:HD3	1.72	0.72
1:C:120:PHE:CD2	1:C:150:ARG:HG3	2.25	0.72
1:D:102:VAL:HG22	1:D:232:ILE:HB	1.72	0.71
2:e:462:MET:HE2	2:e:468:LYS:HB2	1.71	0.71
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.73	0.70
2:b:384:LEU:HD11	2:b:428:LEU:HD21	1.71	0.70
2:d:474:ASP:N	2:d:477:CYS:SG	2.64	0.70
1:C:27:LYS:NZ	1:C:32:ASP:OD1	2.23	0.69
1:E:206:THR:HG23	1:E:208:ARG:H	1.57	0.69
2:d:453:LYS:HD3	2:e:463:GLY:HA3	1.73	0.69
1:B:161:TYR:HE1	1:B:164:LEU:HD11	1.59	0.68
2:c:462:MET:HE2	2:c:468:LYS:HB2	1.75	0.67
1:E:79:PHE:HA	1:E:82:LYS:HD2	1.75	0.67
2:f:492:ARG:HG3	2:f:492:ARG:HH11	1.58	0.67
1:C:98:TYR:HH	1:C:228:SER:HG	1.43	0.66
1:F:182:VAL:HB	1:F:202:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:NH2	2:b:389:ASN:OD1	2.27	0.66
1:D:167:THR:HG21	3:O:1:NAG:H62	1.76	0.66
1:F:176:LYS:HD3	1:F:257:TYR:CG	2.31	0.66
2:f:414:GLU:O	2:f:418:ILE:HG13	1.96	0.65
1:A:308:TYR:HD2	2:a:418:ILE:HD12	1.61	0.65
1:D:163:ALA:HB1	5:P:1:NAG:H2	1.77	0.65
1:E:98:TYR:N	1:E:224:ARG:HH12	1.95	0.65
2:c:481:ILE:HG13	2:c:486:TYR:HD2	1.59	0.65
1:D:104:ASP:HB3	1:D:234:TRP:HH2	1.62	0.64
1:D:202:ILE:HG23	1:D:247:SER:HB2	1.79	0.64
1:F:99:PRO:HB2	1:F:229:ARG:HD2	1.80	0.64
2:d:346:MET:HE1	2:d:352:GLY:HA3	1.80	0.64
2:a:417:LYS:HB2	2:b:416:THR:HG21	1.79	0.64
2:f:462:MET:HE2	2:f:468:LYS:HG3	1.80	0.64
1:B:146:SER:OG	1:B:147:PHE:N	2.30	0.64
2:e:346:MET:HE1	2:e:352:GLY:HA3	1.79	0.63
2:b:457:GLU:HG3	2:b:499:ARG:NH1	2.12	0.63
2:d:472:LYS:HA	2:d:472:LYS:CE	2.29	0.63
2:d:391:LYS:NZ	2:e:419:ASP:OD2	2.32	0.63
2:e:369:SER:HB2	2:e:443:GLU:HG3	1.79	0.63
1:A:288:ILE:HG21	1:A:297:VAL:HG11	1.81	0.62
1:D:288:ILE:HG21	1:D:297:VAL:HG21	1.80	0.62
1:F:169:PRO:HA	1:F:242:ILE:HA	1.80	0.62
2:a:483:ASN:ND2	2:a:485:THR:OG1	2.32	0.62
1:E:34:ILE:HG21	2:e:437:ILE:HD11	1.82	0.62
1:B:97:CYS:O	1:B:224:ARG:NH1	2.33	0.61
1:D:29:ILE:HG21	2:d:431:LEU:HD22	1.83	0.61
1:F:13:LEU:HD22	2:f:481:ILE:HD12	1.82	0.61
2:d:417:LYS:HB2	2:e:416:THR:HG21	1.83	0.61
1:F:325:GLU:OE2	2:f:341:ASN:ND2	2.34	0.61
1:C:208:ARG:HE	1:C:238:LYS:HD2	1.66	0.60
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.83	0.60
1:A:299:ARG:HE	2:a:414:GLU:HG2	1.65	0.60
1:B:79:PHE:HA	1:B:82:LYS:HD2	1.82	0.60
1:C:151:LEU:HD21	1:C:179:ILE:HG22	1.82	0.60
1:B:182:VAL:HG22	1:B:202:ILE:HG13	1.84	0.60
1:D:297:VAL:HA	7:Q:1:NAG:H82	1.82	0.60
2:c:477:CYS:HA	2:c:480:SER:HB3	1.84	0.60
1:D:12:THR:OG1	2:d:356:GLN:HG2	2.01	0.60
1:D:16:GLY:HA2	2:d:339:ILE:HD12	1.83	0.60
1:A:75:GLN:NE2	1:A:94:TYR:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.84	0.60
1:F:136:SER:HB2	1:F:153:TRP:HZ3	1.67	0.59
1:F:314:LEU:HG	2:f:429:VAL:HG11	1.83	0.59
2:a:339:ILE:HD13	2:a:444:MET:HE3	1.83	0.59
1:C:180:TRP:HB3	1:C:254:PRO:HD3	1.83	0.59
2:a:413:VAL:HG11	2:b:413:VAL:HG22	1.84	0.59
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.83	0.59
1:C:17:HIS:CE1	2:c:335:ILE:HG23	2.38	0.59
2:e:409:LEU:O	2:e:413:VAL:HG23	2.03	0.59
2:d:339:ILE:HG22	2:d:339:ILE:O	2.02	0.59
1:C:109:ARG:NH2	1:C:269:ARG:HE	2.01	0.59
1:D:18:HIS:HE2	1:D:37:THR:HG21	1.68	0.58
1:A:182:VAL:HG22	1:A:202:ILE:HG13	1.85	0.58
2:c:334:ALA:HB1	2:c:444:MET:HG2	1.85	0.58
2:b:352:GLY:HA3	2:b:365:ALA:HA	1.85	0.58
2:d:357:ASN:ND2	2:d:475:ASN:OD1	2.30	0.58
1:B:148:PHE:CD2	1:B:151:LEU:HD12	2.38	0.58
2:a:370:THR:O	2:a:374:ILE:HG13	2.03	0.58
1:F:160:LYS:HG3	1:F:162:PRO:HD3	1.86	0.58
2:a:492:ARG:HG3	2:a:492:ARG:HH11	1.68	0.58
1:E:310:LYS:HE2	1:E:310:LYS:HA	1.86	0.58
1:E:57:GLN:H	1:E:85:ASP:HB2	1.69	0.57
1:C:55:PRO:HG3	1:C:280:GLU:OE1	2.04	0.57
1:E:204:VAL:HG22	1:E:245:ILE:HG23	1.86	0.56
1:F:32:ASP:OD1	1:F:32:ASP:N	2.34	0.56
2:b:436:THR:O	2:b:440:THR:HG23	2.04	0.56
1:F:11:ALA:HB3	2:f:469:ILE:CG1	2.35	0.56
2:c:486:TYR:HE1	2:c:488:HIS:HA	1.70	0.56
2:e:414:GLU:O	2:e:418:ILE:HG13	2.05	0.56
2:f:478:ILE:HD12	2:f:479:GLY:N	2.20	0.56
1:B:135:THR:HG22	1:B:146:SER:HA	1.86	0.56
1:A:125:PHE:HB3	1:A:166:VAL:HG11	1.87	0.56
1:B:34:ILE:HD11	1:B:321:ARG:HD2	1.88	0.56
2:d:457:GLU:O	2:d:499:ARG:NH1	2.38	0.56
1:C:110:SER:OG	2:a:408:ASP:OD2	2.22	0.56
2:c:454:GLN:NE2	2:c:484:GLY:HA2	2.21	0.56
1:B:175:ASP:OD1	1:B:239:PRO:HD3	2.06	0.56
1:F:166:VAL:HG12	1:F:245:ILE:HB	1.87	0.56
1:C:123:GLU:HB2	1:C:256:GLY:HA2	1.87	0.56
1:D:13:LEU:HD11	2:d:353:PHE:HB3	1.86	0.56
2:a:409:LEU:O	2:a:413:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:C	1:A:216:ASN:HD22	2.14	0.55
1:D:115:SER:HG	1:D:261:ARG:H	1.54	0.55
1:F:141:ARG:HH12	1:F:149:SER:HB3	1.71	0.55
2:f:353:PHE:HD2	2:f:482:ARG:HG2	1.71	0.55
2:e:335:ILE:HG12	2:e:444:MET:HE2	1.88	0.55
1:C:185:PRO:HG2	1:C:191:GLN:HB2	1.88	0.55
2:d:414:GLU:O	2:d:418:ILE:HG13	2.06	0.55
2:e:492:ARG:NH1	2:f:499:ARG:O	2.40	0.55
1:F:138:ALA:HB2	1:F:226:ILE:HG13	1.89	0.55
1:B:169:PRO:HA	1:B:242:ILE:HA	1.88	0.54
2:a:432:GLU:O	2:a:436:THR:OG1	2.21	0.54
2:c:370:THR:O	2:c:374:ILE:HG13	2.07	0.54
1:B:151:LEU:HD22	1:B:252:ILE:CG2	2.37	0.54
1:D:57:GLN:H	1:D:85:ASP:HB2	1.71	0.54
1:D:299:ARG:HD3	2:d:397:LYS:HB3	1.89	0.54
2:f:353:PHE:CD2	2:f:482:ARG:HG2	2.42	0.54
1:A:71:LEU:HD22	1:A:151:LEU:HD11	1.88	0.54
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.72	0.54
1:B:246:ASN:CG	3:K:1:NAG:HN2	2.16	0.54
1:B:188:ASP:O	1:B:192:ILE:HD12	2.08	0.54
1:B:283:THR:HB	1:B:286:GLY:O	2.07	0.54
1:C:307:ARG:NH2	2:c:389:ASN:HD22	2.05	0.53
1:D:183:HIS:ND1	1:D:195:TYR:OH	2.36	0.53
1:A:17:HIS:HB2	1:A:320:MET:HE1	1.90	0.53
1:A:216:ASN:HD22	1:A:217:ILE:N	2.07	0.53
1:C:71:LEU:O	1:C:150:ARG:HB2	2.08	0.53
1:C:266:SER:OG	1:C:267:ILE:N	2.41	0.53
2:e:399:PHE:CD2	2:e:407:GLN:HG3	2.44	0.53
1:E:185:PRO:HG2	1:E:191:GLN:HB2	1.90	0.53
1:D:18:HIS:ND1	2:d:350:TRP:HA	2.24	0.53
2:d:481:ILE:HG12	2:d:486:TYR:CD2	2.40	0.53
2:e:339:ILE:HG22	2:e:339:ILE:O	2.09	0.53
2:e:481:ILE:HG12	2:e:486:TYR:CD2	2.44	0.53
2:c:432:GLU:O	2:c:436:THR:OG1	2.26	0.53
2:e:456:ARG:NH2	2:f:460:GLU:OE1	2.33	0.53
1:E:66:LEU:HD21	1:E:112:VAL:HB	1.90	0.52
2:b:338:PHE:CD1	2:b:339:ILE:HG13	2.44	0.52
2:f:492:ARG:HG3	2:f:492:ARG:NH1	2.23	0.52
1:E:206:THR:HA	1:F:221:PRO:HG2	1.91	0.52
2:a:500:PHE:HD1	2:c:496:LEU:HD13	1.74	0.52
1:A:31:ASN:HD22	1:A:34:ILE:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:335:ILE:HD12	2:c:335:ILE:H	1.74	0.52
2:e:480:SER:HB2	2:e:485:THR:O	2.08	0.52
1:B:13:LEU:HD11	2:b:353:PHE:HB3	1.92	0.52
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.91	0.52
1:E:120:PHE:HD1	1:E:257:TYR:O	1.92	0.52
2:d:486:TYR:HE1	2:d:488:HIS:HA	1.74	0.52
2:f:478:ILE:O	2:f:482:ARG:HG3	2.10	0.52
1:A:62:GLU:OE1	1:A:62:GLU:N	2.43	0.52
1:A:129:GLY:HA3	1:A:162:PRO:HG2	1.92	0.52
2:e:469:ILE:HG22	2:e:471:HIS:H	1.74	0.52
1:C:161:TYR:O	1:C:197:GLN:NE2	2.42	0.52
1:F:110:SER:OG	2:d:408:ASP:OD2	2.26	0.52
1:B:29:ILE:HD11	2:b:431:LEU:HG	1.92	0.52
2:b:446:LYS:O	2:b:450:LYS:HG3	2.10	0.52
1:F:124:SER:OG	8:c:601:NAG:O7	2.24	0.51
1:C:280:GLU:HB3	1:C:304:ALA:HB3	1.92	0.51
1:E:164:LEU:O	1:E:246:ASN:HA	2.10	0.51
2:b:456:ARG:HB3	2:b:456:ARG:NH1	2.26	0.51
1:D:17:HIS:HD2	1:D:18:HIS:O	1.94	0.51
2:c:458:ASN:OD1	2:c:458:ASN:N	2.43	0.51
2:e:472:LYS:HG3	2:e:494:GLU:OE2	2.11	0.51
2:f:470:TYR:HB3	2:f:498:ASN:HB3	1.92	0.51
2:f:496:LEU:HD12	2:f:496:LEU:H	1.76	0.51
1:D:119:GLU:OE2	1:D:261:ARG:NH2	2.43	0.51
1:E:290:ASN:O	2:e:387:LYS:NZ	2.39	0.51
2:a:399:PHE:CD2	2:a:407:GLN:HG3	2.46	0.51
2:a:492:ARG:HG3	2:a:492:ARG:NH1	2.25	0.51
2:a:499:ARG:NH2	2:c:457:GLU:OE2	2.44	0.51
2:e:376:GLN:O	2:e:380:LYS:HG3	2.10	0.51
1:A:180:TRP:HB3	1:A:254:PRO:HD3	1.93	0.51
1:F:191:GLN:OE1	1:F:250:ASN:ND2	2.31	0.51
1:D:167:THR:HB	1:D:242:ILE:HD11	1.93	0.51
2:d:477:CYS:O	2:d:481:ILE:HG13	2.11	0.51
1:C:14:CYS:HA	2:c:466:CYS:HA	1.92	0.50
1:C:121:ASN:HB2	1:C:257:TYR:CZ	2.47	0.50
1:C:190:ASP:O	1:C:194:LEU:HD12	2.12	0.50
1:A:283:THR:HG22	1:A:286:GLY:O	2.11	0.50
1:B:283:THR:HG23	1:B:284:PRO:HD2	1.93	0.50
2:a:426:GLU:HG3	2:c:383:ARG:HH12	1.77	0.50
2:f:343:TRP:HE3	2:f:346:MET:HE2	1.77	0.50
3:K:1:NAG:H62	3:K:2:NAG:O5	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:HE3	1:F:223:ILE:HG22	1.94	0.50
2:c:454:GLN:HE22	2:c:484:GLY:HA2	1.76	0.50
1:E:138:ALA:HB1	1:E:224:ARG:HD2	1.92	0.50
1:F:67:ILE:O	1:F:71:LEU:HD22	2.12	0.50
1:A:248:THR:HG23	3:G:1:NAG:HN2	1.77	0.50
1:B:167:THR:OG1	5:L:1:NAG:H62	2.12	0.49
1:B:230:ILE:HD13	1:B:252:ILE:HG12	1.94	0.49
1:B:283:THR:HG22	1:B:285:ASN:H	1.77	0.49
2:a:409:LEU:HD21	2:c:409:LEU:HD23	1.93	0.49
1:B:125:PHE:HD2	1:B:166:VAL:HG11	1.77	0.49
1:E:230:ILE:HD13	1:E:252:ILE:HG13	1.94	0.49
1:E:283:THR:OG1	1:E:286:GLY:O	2.24	0.49
1:F:187:THR:OG1	1:F:190:ASP:HB2	2.13	0.49
1:B:169:PRO:HB3	1:B:242:ILE:HG22	1.94	0.49
2:a:492:ARG:NH2	2:b:460:GLU:OE2	2.45	0.49
2:e:357:ASN:HB2	2:e:473:CYS:O	2.12	0.49
1:E:194:LEU:HB2	1:E:195:TYR:CD1	2.48	0.49
1:F:70:LEU:HD22	1:F:112:VAL:HG21	1.95	0.49
2:f:366:ASP:OD2	2:f:369:SER:OG	2.27	0.49
1:A:123:GLU:HG3	1:A:256:GLY:HA2	1.95	0.49
1:D:95:SER:O	1:D:224:ARG:NH1	2.46	0.49
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.48	0.49
1:D:125:PHE:HB2	1:D:127:TRP:CE2	2.48	0.49
1:F:221:PRO:O	1:F:229:ARG:NH2	2.45	0.49
2:f:459:ALA:HB2	2:f:469:ILE:HG22	1.94	0.49
1:E:115:SER:OG	1:E:260:ILE:HG13	2.13	0.49
1:B:288:ILE:HD11	1:B:306:PRO:HD2	1.95	0.49
1:B:300:ILE:HG12	2:b:397:LYS:HD2	1.95	0.49
1:C:120:PHE:HE1	1:C:257:TYR:N	2.11	0.49
1:D:182:VAL:HG12	1:D:231:SER:HB2	1.95	0.49
2:b:385:ILE:HG13	2:b:386:GLY:H	1.78	0.49
2:e:425:ALA:O	2:e:429:VAL:HG13	2.13	0.49
1:B:58:ILE:HG21	1:B:274:ILE:HD12	1.94	0.48
1:B:144:ASN:OD1	1:B:144:ASN:N	2.45	0.48
1:D:17:HIS:ND1	2:d:335:ILE:HD13	2.28	0.48
2:b:387:LYS:NZ	2:b:389:ASN:HA	2.27	0.48
1:B:9:SER:HB2	2:b:472:LYS:HG3	1.95	0.48
2:d:334:ALA:O	2:d:339:ILE:HB	2.13	0.48
2:d:406:ILE:HD11	2:f:406:ILE:HD12	1.95	0.48
2:f:376:GLN:O	2:f:380:LYS:HG3	2.13	0.48
2:c:373:ALA:O	2:c:377:ILE:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:425:ALA:O	2:f:429:VAL:HG12	2.13	0.48
2:f:457:GLU:O	2:f:499:ARG:NH1	2.46	0.48
2:a:478:ILE:H	2:a:478:ILE:HD12	1.79	0.48
1:B:164:LEU:O	1:B:246:ASN:HA	2.12	0.48
1:C:115:SER:OG	1:C:260:ILE:HA	2.13	0.48
1:C:222:ARG:HD3	5:L:2:NAG:H2	1.95	0.48
1:E:127:TRP:CZ3	1:E:166:VAL:HG21	2.48	0.48
1:E:293:PRO:HB3	2:e:385:ILE:HB	1.95	0.48
1:B:151:LEU:HD22	1:B:252:ILE:HG22	1.96	0.48
1:C:191:GLN:OE1	1:C:250:ASN:ND2	2.36	0.48
1:D:24:THR:HG21	1:D:39:ALA:HB3	1.96	0.48
1:D:61:GLY:HA2	1:D:79:PHE:HE2	1.79	0.48
1:D:164:LEU:O	1:D:246:ASN:HA	2.14	0.48
2:a:462:MET:HE2	2:a:468:LYS:HB2	1.96	0.48
1:C:184:HIS:HD1	1:C:216:ASN:H	1.60	0.48
1:D:268:MET:HE3	1:D:268:MET:HB2	1.74	0.48
1:A:125:PHE:HB2	1:A:127:TRP:CE2	2.49	0.48
2:b:370:THR:O	2:b:374:ILE:HG13	2.14	0.48
1:B:241:ASP:OD1	1:B:242:ILE:N	2.47	0.47
1:D:18:HIS:C	1:D:18:HIS:CD2	2.92	0.47
1:E:139:CYS:HB3	1:E:146:SER:O	2.14	0.47
2:a:425:ALA:O	2:a:429:VAL:HG22	2.14	0.47
2:b:470:TYR:HB3	2:b:498:ASN:HB3	1.96	0.47
2:d:410:GLU:HG2	2:e:409:LEU:HD13	1.94	0.47
1:C:202:ILE:HG22	1:C:247:SER:HB2	1.96	0.47
1:C:268:MET:HE2	1:C:300:ILE:HG22	1.96	0.47
1:E:266:SER:OG	1:E:267:ILE:N	2.48	0.47
2:a:483:ASN:OD1	2:a:484:GLY:N	2.46	0.47
1:D:35:GLU:OE2	1:D:322:ASN:ND2	2.38	0.47
1:D:268:MET:HE2	1:D:300:ILE:HG22	1.96	0.47
1:E:193:PHE:HD1	1:E:193:PHE:C	2.23	0.47
1:E:125:PHE:HE1	1:E:168:MET:HB2	1.80	0.47
2:a:470:TYR:O	2:a:495:ALA:HA	2.14	0.47
1:F:30:THR:O	2:e:379:GLY:HA3	2.15	0.47
2:e:474:ASP:N	2:e:477:CYS:SG	2.87	0.47
1:A:71:LEU:HD11	1:A:232:ILE:HG13	1.95	0.47
1:C:15:LEU:HD12	2:c:448:PHE:HA	1.97	0.47
1:E:64:CYS:HB2	1:E:79:PHE:HE2	1.79	0.47
1:E:151:LEU:O	1:E:255:ARG:NH1	2.48	0.47
1:E:194:LEU:HB2	1:E:195:TYR:CE1	2.49	0.47
1:E:84:TRP:HZ2	1:E:113:ALA:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:407:GLN:HG2	2:b:411:LYS:HE2	1.97	0.47
2:b:453:LYS:HD3	2:c:463:GLY:HA2	1.97	0.47
2:c:481:ILE:HG13	2:c:486:TYR:CD2	2.47	0.47
2:f:335:ILE:N	2:f:441:ASP:OD1	2.46	0.47
1:B:25:ILE:HG21	1:B:33:ARG:HG2	1.97	0.47
1:C:41:GLU:OE1	1:C:313:THR:OG1	2.32	0.47
1:C:125:PHE:CZ	1:C:254:PRO:HG2	2.50	0.47
1:C:201:ARG:N	1:C:248:THR:OG1	2.47	0.47
1:D:63:ASN:HA	1:D:93:ALA:HA	1.96	0.47
1:E:73:ASP:HB3	1:E:76:CYS:SG	2.55	0.47
2:f:492:ARG:O	2:f:496:LEU:HD12	2.15	0.47
1:A:14:CYS:HA	2:a:466:CYS:HA	1.97	0.47
1:C:79:PHE:HA	1:C:82:LYS:HD2	1.96	0.47
1:E:193:PHE:C	1:E:193:PHE:CD1	2.92	0.47
1:C:291:ASP:OD1	1:C:291:ASP:N	2.48	0.46
1:D:319:GLY:HA2	2:d:350:TRP:CH2	2.50	0.46
1:F:117:THR:OG1	1:F:119:GLU:OE1	2.22	0.46
1:C:216:ASN:O	1:C:220:ARG:NH2	2.34	0.46
1:E:97:CYS:HA	1:E:139:CYS:HA	1.97	0.46
1:E:127:TRP:CZ3	1:E:166:VAL:HG11	2.50	0.46
1:C:64:CYS:SG	1:C:75:GLN:HG3	2.55	0.46
1:C:104:ASP:HB3	1:C:234:TRP:HH2	1.79	0.46
1:C:120:PHE:HD2	1:C:150:ARG:HG3	1.75	0.46
2:d:468:LYS:HE2	2:d:470:TYR:CZ	2.49	0.46
1:F:43:VAL:HG22	1:F:294:PHE:HB2	1.97	0.46
2:b:436:THR:HA	2:b:439:LEU:HD23	1.97	0.46
1:A:43:VAL:HG22	1:A:294:PHE:HB2	1.97	0.46
1:E:208:ARG:CZ	1:E:208:ARG:HB3	2.45	0.46
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.98	0.46
1:D:141:ARG:HG2	1:D:142:ARG:HD2	1.98	0.46
1:D:175:ASP:OD1	1:D:238:LYS:HA	2.14	0.46
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.98	0.46
1:E:121:ASN:HB2	1:E:257:TYR:CZ	2.50	0.46
2:d:474:ASP:O	2:d:478:ILE:HG12	2.16	0.46
2:b:395:ILE:HG21	2:c:409:LEU:HD12	1.97	0.46
2:e:477:CYS:HA	2:e:480:SER:HB3	1.98	0.46
1:B:206:THR:C	1:C:221:PRO:HG2	2.41	0.46
2:a:405:ARG:HH22	2:c:403:GLU:CD	2.24	0.46
2:a:418:ILE:O	2:a:422:SER:OG	2.29	0.46
2:b:380:LYS:NZ	2:b:432:GLU:O	2.49	0.46
2:e:373:ALA:O	2:e:377:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:O	1:A:287:SER:N	2.43	0.45
1:C:131:THR:HG1	1:C:155:THR:HG1	1.62	0.45
1:D:99:PRO:HB2	1:D:229:ARG:HD2	1.98	0.45
2:c:355:HIS:ND1	2:c:478:ILE:HG21	2.30	0.45
1:D:127:TRP:CZ3	1:D:166:VAL:HG21	2.51	0.45
2:f:391:LYS:HD3	2:f:394:GLN:HE21	1.81	0.45
2:c:471:HIS:NE2	2:c:486:TYR:OH	2.49	0.45
1:B:41:GLU:HG2	1:B:315:LYS:HD3	1.97	0.45
2:f:380:LYS:O	2:f:384:LEU:HG	2.16	0.45
1:B:14:CYS:HA	2:b:466:CYS:HA	1.98	0.45
1:D:121:ASN:HB2	1:D:257:TYR:CE1	2.51	0.45
1:C:125:PHE:CZ	1:C:168:MET:HE1	2.52	0.45
1:D:84:TRP:HZ3	1:D:118:LEU:HG	1.81	0.45
1:E:133:ASN:HA	1:E:255:ARG:NH2	2.31	0.45
2:b:354:ARG:NH2	2:b:363:GLN:OE1	2.45	0.45
2:d:448:PHE:CD1	2:d:448:PHE:C	2.94	0.45
2:d:450:LYS:NZ	2:d:453:LYS:HE3	2.32	0.45
2:f:452:LYS:HE3	2:f:452:LYS:HB3	1.72	0.45
1:B:31:ASN:ND2	1:B:33:ARG:O	2.50	0.45
1:C:103:PRO:HD2	1:C:232:ILE:O	2.17	0.45
1:E:270:SER:HB2	1:E:284:PRO:HA	1.98	0.45
2:e:436:THR:O	2:e:440:THR:HG23	2.17	0.45
1:B:133:ASN:CG	1:B:255:ARG:HH22	2.25	0.45
1:F:11:ALA:HB3	2:f:469:ILE:HD11	1.98	0.45
2:e:355:HIS:HD2	2:e:355:HIS:O	2.00	0.45
1:C:142:ARG:HA	1:C:142:ARG:HD3	1.61	0.45
1:C:201:ARG:NH1	1:C:214:ILE:HD11	2.31	0.45
1:E:168:MET:HE3	1:E:169:PRO:HD2	1.99	0.45
2:f:483:ASN:ND2	8:f:601:NAG:O7	2.49	0.45
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.52	0.45
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.99	0.45
2:d:384:LEU:HD11	2:d:428:LEU:HD11	1.99	0.45
1:A:283:THR:OG1	1:A:298:ASN:HB3	2.17	0.44
1:E:220:ARG:HD3	1:E:229:ARG:HD2	1.99	0.44
2:c:333:GLY:O	2:c:337:GLY:HA3	2.18	0.44
2:d:481:ILE:HG13	2:d:481:ILE:H	1.61	0.44
3:K:1:NAG:H4	3:K:2:NAG:H2	1.78	0.44
1:C:135:THR:HG22	1:C:146:SER:HA	1.99	0.44
1:C:182:VAL:HG12	1:C:233:TYR:HE1	1.81	0.44
1:C:283:THR:HG21	1:C:288:ILE:HD13	1.99	0.44
2:a:361:ARG:HB2	2:a:361:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:359:GLU:OE2	2:d:474:ASP:HB3	2.17	0.44
2:d:478:ILE:O	2:d:482:ARG:HG3	2.18	0.44
1:D:18:HIS:NE2	1:D:37:THR:HG21	2.31	0.44
1:D:170:ASN:HB2	1:D:176:LYS:HD2	1.99	0.44
1:C:304:ALA:HA	2:c:389:ASN:O	2.18	0.44
1:F:18:HIS:NE2	1:F:320:MET:HE3	2.32	0.44
1:F:283:THR:OG1	1:F:286:GLY:O	2.29	0.44
2:d:432:GLU:O	2:d:436:THR:OG1	2.27	0.44
1:E:33:ARG:O	1:E:34:ILE:HD13	2.18	0.44
1:A:152:ASN:HB2	1:A:255:ARG:HG2	2.00	0.44
1:C:316:LEU:HD22	2:c:384:LEU:HD22	2.00	0.44
2:c:452:LYS:HE2	2:c:452:LYS:HB3	1.82	0.44
2:e:417:LYS:HB2	2:f:416:THR:HG21	1.98	0.44
2:f:479:GLY:O	2:f:483:ASN:HB2	2.18	0.44
1:A:283:THR:HG23	1:A:285:ASN:H	1.82	0.44
1:B:314:LEU:HD13	2:b:429:VAL:HG21	1.99	0.44
1:E:182:VAL:HG21	1:E:213:VAL:HB	2.00	0.44
2:a:420:LEU:HD13	2:b:420:LEU:HD13	1.99	0.44
2:b:480:SER:HB2	2:b:485:THR:O	2.18	0.44
2:c:377:ILE:HD12	2:c:377:ILE:H	1.83	0.44
1:A:133:ASN:OD1	1:A:255:ARG:NH1	2.51	0.44
2:c:373:ALA:O	2:c:376:GLN:N	2.49	0.44
1:B:109:ARG:HH12	1:B:269:ARG:HE	1.66	0.43
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.18	0.43
1:D:27:LYS:HG3	1:D:32:ASP:HA	2.00	0.43
1:E:170:ASN:CG	1:E:176:LYS:HE2	2.42	0.43
1:B:51:ILE:HB	1:B:274:ILE:HD13	2.00	0.43
1:F:11:ALA:HB3	2:f:469:ILE:HG12	1.99	0.43
1:F:40:THR:HB	4:X:1:NAG:H62	1.99	0.43
1:F:82:LYS:HD3	1:F:82:LYS:HA	1.70	0.43
1:F:161:TYR:O	1:F:197:GLN:NE2	2.51	0.43
1:C:311:GLN:HB2	1:C:314:LEU:HD21	1.99	0.43
1:D:107:SER:O	1:D:111:LEU:HG	2.18	0.43
2:b:346:MET:HE1	2:b:352:GLY:N	2.33	0.43
2:c:436:THR:O	2:c:440:THR:HG23	2.18	0.43
2:f:370:THR:O	2:f:374:ILE:HG13	2.17	0.43
2:f:359:GLU:OE2	2:f:474:ASP:HB2	2.17	0.43
2:a:343:TRP:CZ3	2:a:354:ARG:HG3	2.54	0.43
2:b:339:ILE:HG12	2:b:465:GLY:HA3	2.00	0.43
1:A:299:ARG:HH21	2:a:414:GLU:HG3	1.84	0.43
1:B:141:ARG:H	1:B:146:SER:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ARG:HG3	1:E:146:SER:HB2	2.00	0.43
1:E:282:ILE:HD12	1:E:302:TYR:HD2	1.83	0.43
1:A:115:SER:HA	1:A:261:ARG:O	2.19	0.43
2:b:455:LEU:HD21	2:b:481:ILE:HG12	2.00	0.43
1:A:72:GLY:O	1:A:141:ARG:NH2	2.52	0.43
1:E:299:ARG:O	2:e:397:LYS:NZ	2.37	0.43
1:F:54:SER:HB3	1:F:278:LYS:HG3	2.01	0.43
1:A:31:ASN:ND2	1:A:34:ILE:HD13	2.34	0.43
1:E:295:GLN:HG2	1:E:306:PRO:HB2	2.00	0.43
1:F:67:ILE:HD13	1:F:67:ILE:HA	1.87	0.43
2:d:471:HIS:HE1	2:d:473:CYS:SG	2.42	0.43
2:f:384:LEU:HD22	2:f:428:LEU:HD21	2.01	0.43
1:A:299:ARG:HD3	2:a:397:LYS:HB3	2.01	0.42
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.89	0.42
1:E:288:ILE:HD12	1:E:288:ILE:O	2.18	0.42
1:F:121:ASN:HB2	1:F:257:TYR:CZ	2.53	0.42
2:c:457:GLU:O	2:c:499:ARG:NH1	2.51	0.42
1:B:175:ASP:HB3	1:B:260:ILE:HD11	2.01	0.42
1:C:176:LYS:HE3	1:C:257:TYR:CG	2.54	0.42
1:F:111:LEU:HD12	1:F:111:LEU:HA	1.82	0.42
2:c:492:ARG:HG3	2:c:492:ARG:HH11	1.83	0.42
2:e:428:LEU:O	2:e:432:GLU:HG2	2.19	0.42
1:B:139:CYS:O	1:B:146:SER:N	2.49	0.42
1:D:81:ASN:HA	1:D:118:LEU:O	2.19	0.42
1:E:120:PHE:CD1	1:E:257:TYR:O	2.72	0.42
1:E:208:ARG:CZ	2:f:401:GLU:OE2	2.67	0.42
1:F:176:LYS:HD3	1:F:257:TYR:CD2	2.53	0.42
2:e:477:CYS:O	2:e:481:ILE:HG13	2.19	0.42
1:A:34:ILE:HD12	1:A:34:ILE:HA	1.94	0.42
1:B:134:GLY:HA3	1:B:153:TRP:HB3	2.00	0.42
1:E:19:ALA:HB2	2:e:342:GLY:HA3	2.01	0.42
2:e:339:ILE:O	2:e:341:ASN:N	2.47	0.42
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.01	0.42
1:C:120:PHE:CE2	1:C:150:ARG:HG3	2.55	0.42
1:C:121:ASN:HB2	1:C:257:TYR:CE1	2.53	0.42
1:C:180:TRP:CH2	1:C:233:TYR:HB2	2.54	0.42
1:E:222:ARG:HD3	1:E:225:ASP:HA	2.01	0.42
2:e:399:PHE:CE2	2:e:407:GLN:HG3	2.54	0.42
1:B:74:PRO:HD3	1:B:139:CYS:SG	2.58	0.42
1:D:44:GLN:O	1:D:296:ASN:N	2.51	0.42
1:D:133:ASN:HA	1:D:255:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ALA:N	2:d:390:GLU:HG3	2.34	0.42
1:F:182:VAL:HG11	1:F:213:VAL:HG11	2.01	0.42
1:F:208:ARG:NE	2:d:401:GLU:OE1	2.53	0.42
1:B:85:ASP:O	1:B:265:SER:HA	2.19	0.42
1:B:279:SER:OG	1:B:287:SER:HB3	2.19	0.42
1:F:141:ARG:HG2	1:F:142:ARG:HG2	2.02	0.42
1:F:151:LEU:HD21	1:F:179:ILE:HG22	2.02	0.42
1:F:160:LYS:HB2	1:F:160:LYS:HE3	1.84	0.42
2:e:453:LYS:HD3	2:f:463:GLY:HA2	2.01	0.42
2:e:485:THR:O	2:e:485:THR:OG1	2.32	0.42
2:f:473:CYS:HB3	2:f:477:CYS:HB3	1.86	0.42
1:D:14:CYS:HA	2:d:466:CYS:HA	2.02	0.42
1:F:66:LEU:HD21	1:F:112:VAL:HB	2.02	0.42
1:A:139:CYS:HB3	1:A:146:SER:O	2.20	0.42
1:A:187:THR:HG23	1:A:190:ASP:H	1.85	0.42
1:B:161:TYR:CE1	1:B:164:LEU:HD11	2.47	0.42
1:D:104:ASP:HB3	1:D:234:TRP:CH2	2.48	0.42
1:D:216:ASN:HD22	1:F:212:ALA:HB3	1.85	0.42
1:E:222:ARG:HH11	1:E:225:ASP:H	1.68	0.42
2:b:394:GLN:HB3	2:c:412:TYR:CE2	2.55	0.42
2:f:455:LEU:HD23	2:f:486:TYR:CE2	2.55	0.42
1:A:264:LYS:O	1:A:302:TYR:OH	2.33	0.42
1:C:120:PHE:HE1	1:C:256:GLY:C	2.27	0.42
1:D:79:PHE:CD1	1:D:79:PHE:N	2.88	0.42
1:E:288:ILE:HD12	1:E:288:ILE:C	2.45	0.42
1:F:291:ASP:OD1	1:F:292:LYS:N	2.53	0.42
2:a:493:ASP:N	2:a:493:ASP:OD1	2.51	0.42
1:A:314:LEU:HG	2:a:429:VAL:HG21	2.02	0.41
1:C:288:ILE:HG21	1:C:297:VAL:HG21	2.01	0.41
1:E:118:LEU:HD23	1:E:118:LEU:HA	1.88	0.41
1:E:163:ALA:CB	6:U:1:NAG:H4	2.50	0.41
1:A:90:ARG:NH1	1:A:270:SER:O	2.43	0.41
1:A:110:SER:OG	2:b:408:ASP:OD2	2.32	0.41
1:B:179:ILE:O	1:B:254:PRO:HB3	2.20	0.41
2:a:361:ARG:HB2	2:a:361:ARG:HH11	1.84	0.41
2:b:452:LYS:NZ	2:b:456:ARG:O	2.53	0.41
1:A:60:ASP:OD1	1:A:61:GLY:N	2.52	0.41
1:A:207:LYS:HE3	1:A:207:LYS:HB3	1.69	0.41
1:B:73:ASP:HB3	1:B:76:CYS:SG	2.60	0.41
1:D:220:ARG:HB3	1:D:229:ARG:NH2	2.36	0.41
1:E:301:THR:HB	1:E:305:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:338:PHE:CD2	2:a:339:ILE:HG13	2.55	0.41
2:b:333:GLY:O	2:b:337:GLY:HA3	2.20	0.41
2:c:451:THR:O	2:c:455:LEU:HG	2.20	0.41
1:A:12:THR:OG1	2:a:356:GLN:HB3	2.20	0.41
1:A:280:GLU:HB3	1:A:304:ALA:HB3	2.02	0.41
1:C:166:VAL:HG22	1:C:245:ILE:HB	2.02	0.41
1:E:276:LYS:HD2	1:E:276:LYS:N	2.36	0.41
1:F:285:ASN:HD22	7:Y:1:NAG:H83	1.85	0.41
3:G:3:BMA:H3	3:G:4:MAN:H2	1.76	0.41
1:A:185:PRO:HD2	1:A:217:ILE:HG13	2.02	0.41
1:A:291:ASP:OD1	1:A:291:ASP:N	2.53	0.41
1:D:194:LEU:HD23	1:D:194:LEU:HA	1.93	0.41
1:F:8:ASN:CG	1:F:9:SER:H	2.28	0.41
2:e:481:ILE:HG13	2:e:481:ILE:H	1.58	0.41
3:K:1:NAG:O7	3:K:1:NAG:O3	2.35	0.41
1:E:60:ASP:OD1	1:E:90:ARG:NE	2.54	0.41
1:E:97:CYS:C	1:E:224:ARG:HH12	2.28	0.41
1:F:276:LYS:O	1:F:276:LYS:HG2	2.20	0.41
2:d:450:LYS:O	2:d:453:LYS:HG3	2.20	0.41
1:E:27:LYS:HG2	1:E:32:ASP:O	2.21	0.41
2:b:358:SER:O	2:b:359:GLU:HB2	2.20	0.41
2:c:492:ARG:HG3	2:c:492:ARG:NH1	2.36	0.41
2:d:350:TRP:CE2	2:d:374:ILE:HD11	2.56	0.41
2:f:492:ARG:HG2	2:f:496:LEU:CD1	2.31	0.41
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.56	0.41
1:E:170:ASN:ND2	1:E:176:LYS:HE2	2.35	0.41
1:E:320:MET:HB3	1:E:320:MET:HE2	1.74	0.41
1:F:84:TRP:HH2	1:F:112:VAL:HG12	1.85	0.41
2:d:333:GLY:O	2:d:337:GLY:HA3	2.21	0.41
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.56	0.41
1:B:102:VAL:HG11	1:B:108:LEU:HD12	2.02	0.41
1:C:11:ALA:HB3	2:c:469:ILE:HB	2.02	0.41
1:C:57:GLN:N	1:C:85:ASP:HB2	2.36	0.41
1:C:73:ASP:HB3	1:C:76:CYS:SG	2.61	0.41
1:C:176:LYS:HB3	1:C:257:TYR:HB2	2.02	0.41
1:E:115:SER:HA	1:E:261:ARG:O	2.20	0.41
1:E:127:TRP:CZ2	1:E:253:ALA:HB1	2.56	0.41
1:F:20:VAL:O	1:F:322:ASN:ND2	2.52	0.41
1:F:114:SER:HB2	2:f:393:HIS:CD2	2.56	0.41
1:F:202:ILE:HG22	1:F:247:SER:HB2	2.02	0.41
2:c:486:TYR:CE1	2:c:488:HIS:HA	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:372:ALA:O	2:d:376:GLN:HG3	2.21	0.41
2:d:442:SER:OG	2:e:331:ILE:O	2.36	0.41
2:d:497:ASN:HA	2:d:501:GLN:HG2	2.03	0.41
2:e:332:PHE:HD2	2:e:441:ASP:HB3	1.86	0.41
2:f:493:ASP:HA	2:f:496:LEU:HD13	2.02	0.41
6:N:3:BMA:H62	6:N:5:MAN:H2	1.78	0.41
1:D:222:ARG:HB2	7:W:2:NAG:O4	2.21	0.41
1:F:268:MET:HE3	1:F:268:MET:HB2	1.83	0.41
2:f:462:MET:CE	2:f:468:LYS:HG3	2.48	0.41
1:C:165:ASN:HB2	6:M:1:NAG:O5	2.21	0.40
2:a:453:LYS:HA	2:a:453:LYS:HD3	1.71	0.40
2:e:420:LEU:HD13	2:f:420:LEU:HD13	2.03	0.40
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.40
1:E:83:LYS:NZ	1:E:261:ARG:HH12	2.19	0.40
1:F:12:THR:OG1	2:f:356:GLN:HB3	2.21	0.40
1:F:125:PHE:HB2	1:F:127:TRP:NE1	2.35	0.40
1:F:276:LYS:H	1:F:276:LYS:HD3	1.86	0.40
2:c:372:ALA:O	2:c:376:GLN:HG3	2.21	0.40
2:d:470:TYR:HB3	2:d:498:ASN:HB3	2.03	0.40
2:e:442:SER:HB2	2:f:331:ILE:O	2.21	0.40
1:B:141:ARG:HG2	1:B:142:ARG:HG2	2.04	0.40
1:C:98:TYR:CE1	1:C:226:ILE:HD13	2.57	0.40
1:C:192:ILE:HD13	1:C:192:ILE:HA	1.86	0.40
1:D:9:SER:N	2:d:472:LYS:HE3	2.36	0.40
1:F:27:LYS:HG2	1:F:32:ASP:HA	2.02	0.40
2:a:477:CYS:O	2:a:481:ILE:HG13	2.22	0.40
2:b:370:THR:HG22	2:b:374:ILE:HD11	2.02	0.40
2:b:492:ARG:HA	2:b:492:ARG:HD3	1.99	0.40
2:e:339:ILE:HG21	2:e:444:MET:HE3	2.03	0.40
1:A:155:THR:HG22	1:A:156:HIS:N	2.37	0.40
1:B:15:LEU:HD22	2:b:448:PHE:HA	2.04	0.40
2:d:405:ARG:NH2	2:f:410:GLU:OE1	2.53	0.40
2:f:455:LEU:HD23	2:f:455:LEU:HA	1.86	0.40
1:C:125:PHE:HB2	1:C:127:TRP:NE1	2.36	0.40
2:a:331:ILE:O	2:c:442:SER:HB2	2.22	0.40
2:d:495:ALA:O	2:d:499:ARG:HG3	2.21	0.40
2:f:478:ILE:HD12	2:f:479:GLY:H	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/323 (98%)	301 (95%)	15 (5%)	0	100	100
1	B	317/323 (98%)	307 (97%)	10 (3%)	0	100	100
1	C	316/323 (98%)	304 (96%)	12 (4%)	0	100	100
1	D	315/323 (98%)	305 (97%)	10 (3%)	0	100	100
1	E	314/323 (97%)	301 (96%)	13 (4%)	0	100	100
1	F	316/323 (98%)	311 (98%)	5 (2%)	0	100	100
2	a	170/181 (94%)	165 (97%)	5 (3%)	0	100	100
2	b	169/181 (93%)	160 (95%)	9 (5%)	0	100	100
2	c	170/181 (94%)	165 (97%)	5 (3%)	0	100	100
2	d	166/181 (92%)	159 (96%)	7 (4%)	0	100	100
2	e	169/181 (93%)	154 (91%)	15 (9%)	0	100	100
2	f	170/181 (94%)	159 (94%)	11 (6%)	0	100	100
All	All	2908/3024 (96%)	2791 (96%)	117 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	282/287 (98%)	278 (99%)	4 (1%)	62	86
1	B	283/287 (99%)	277 (98%)	6 (2%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	282/287 (98%)	278 (99%)	4 (1%)	62	86
1	D	281/287 (98%)	275 (98%)	6 (2%)	48	78
1	E	280/287 (98%)	275 (98%)	5 (2%)	54	82
1	F	282/287 (98%)	272 (96%)	10 (4%)	31	66
2	a	145/153 (95%)	144 (99%)	1 (1%)	81	94
2	b	144/153 (94%)	141 (98%)	3 (2%)	48	78
2	c	145/153 (95%)	140 (97%)	5 (3%)	32	67
2	d	143/153 (94%)	141 (99%)	2 (1%)	62	86
2	e	144/153 (94%)	140 (97%)	4 (3%)	38	73
2	f	145/153 (95%)	143 (99%)	2 (1%)	62	86
All	All	2556/2640 (97%)	2504 (98%)	52 (2%)	50	79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	208	ARG
1	A	209	SER
1	A	219	SER
1	B	101	ASP
1	B	108	LEU
1	B	139	CYS
1	B	143	SER
1	B	288	ILE
1	B	301	THR
1	C	139	CYS
1	C	140	ILE
1	C	150	ARG
1	C	314	LEU
1	D	59	LEU
1	D	110	SER
1	D	115	SER
1	D	133	ASN
1	D	166	VAL
1	D	274	ILE
1	E	96	ASN
1	E	117	THR
1	E	137	SER

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Mol	Chain	Res	Type
1	E	144	ASN
1	E	312	SER
1	F	20	VAL
1	F	31	ASN
1	F	71	LEU
1	F	101	ASP
1	F	118	LEU
1	F	167	THR
1	F	190	ASP
1	F	265	SER
1	F	312	SER
1	F	314	LEU
2	a	348	ASP
2	b	473	CYS
2	b	474	ASP
2	b	483	ASN
2	c	401	GLU
2	c	458	ASN
2	c	473	CYS
2	c	478	ILE
2	c	480	SER
2	d	402	VAL
2	d	490	VAL
2	e	338	PHE
2	e	417	LYS
2	e	441	ASP
2	e	473	CYS
2	f	454	GLN
2	f	483	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	B	38	ASN
1	B	45	ASN
1	B	81	ASN
1	B	122	ASN
1	C	75	GLN
1	C	121	ASN
1	C	122	ASN
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	197	GLN
1	D	57	GLN
1	D	121	ASN
1	D	122	ASN
1	E	211	GLN
1	F	63	ASN
1	F	197	GLN
1	F	211	GLN
2	a	371	GLN
2	a	376	GLN
2	a	394	GLN
2	a	458	ASN
2	b	475	ASN
2	b	488	HIS
2	b	489	ASN
2	b	498	ASN
2	c	376	GLN
2	c	382	ASN
2	c	434	GLN
2	c	435	HIS
2	d	488	HIS
2	e	407	GLN
2	e	488	HIS
2	e	498	ASN
2	f	471	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

69 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	1	3,1	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.55	0
3	BMA	G	3	3	11,11,12	0.50	0	15,15,17	0.66	0
3	MAN	G	4	3	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.22	0	17,19,21	0.53	0
4	NAG	H	2	4	14,14,15	0.21	0	17,19,21	0.49	0
4	BMA	H	3	4	11,11,12	0.45	0	15,15,17	0.98	1 (6%)
4	MAN	H	4	4	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
4	NAG	I	1	1,4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.44	0
4	BMA	I	3	4	11,11,12	0.55	0	15,15,17	0.72	0
4	MAN	I	4	4	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
5	NAG	J	1	5,1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	J	2	5	14,14,15	0.26	0	17,19,21	0.46	0
5	BMA	J	3	5	11,11,12	0.68	0	15,15,17	0.63	0
3	NAG	K	1	3,1	14,14,15	0.68	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	K	2	3	14,14,15	0.64	1 (7%)	17,19,21	0.75	1 (5%)
3	BMA	K	3	3	11,11,12	0.93	0	15,15,17	1.03	2 (13%)
3	MAN	K	4	3	11,11,12	0.87	1 (9%)	15,15,17	0.92	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.19	0	17,19,21	0.68	0
5	NAG	L	2	5	14,14,15	0.28	0	17,19,21	0.52	0
5	BMA	L	3	5	11,11,12	0.60	0	15,15,17	0.78	0
6	NAG	M	1	6,1	14,14,15	0.20	0	17,19,21	0.57	0
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.45	0
6	BMA	M	3	6	11,11,12	0.63	0	15,15,17	0.86	0
6	MAN	M	4	6	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
6	MAN	M	5	6	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.26	0	17,19,21	0.46	0
6	NAG	N	2	6	14,14,15	0.20	0	17,19,21	0.47	0
6	BMA	N	3	6	11,11,12	0.45	0	15,15,17	0.63	0
6	MAN	N	4	6	11,11,12	0.53	0	15,15,17	0.94	1 (6%)
6	MAN	N	5	6	11,11,12	0.61	0	15,15,17	0.82	0
3	NAG	O	1	3,1	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.18	0	17,19,21	0.51	0
3	BMA	O	3	3	11,11,12	0.56	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	O	4	3	11,11,12	0.67	0	15,15,17	0.86	1 (6%)
5	NAG	P	1	5,1	14,14,15	0.31	0	17,19,21	0.72	0
5	NAG	P	2	5	14,14,15	0.31	0	17,19,21	0.59	0
5	BMA	P	3	5	11,11,12	1.00	1 (9%)	15,15,17	1.08	2 (13%)
7	NAG	Q	1	1,7	14,14,15	0.25	0	17,19,21	0.47	0
7	NAG	Q	2	7	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	R	1	5,1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	R	2	5	14,14,15	0.34	0	17,19,21	0.51	0
5	BMA	R	3	5	11,11,12	0.64	0	15,15,17	0.62	0
5	NAG	S	1	5,1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	S	2	5	14,14,15	0.31	0	17,19,21	0.44	0
5	BMA	S	3	5	11,11,12	0.59	0	15,15,17	0.68	0
4	NAG	T	1	1,4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	T	2	4	14,14,15	0.31	0	17,19,21	0.50	0
4	BMA	T	3	4	11,11,12	0.63	0	15,15,17	0.61	0
4	MAN	T	4	4	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
6	NAG	U	1	6,1	14,14,15	0.19	0	17,19,21	0.63	0
6	NAG	U	2	6	14,14,15	0.27	0	17,19,21	0.40	0
6	BMA	U	3	6	11,11,12	0.60	0	15,15,17	0.74	0
6	MAN	U	4	6	11,11,12	0.72	0	15,15,17	1.13	2 (13%)
6	MAN	U	5	6	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
6	NAG	V	1	6,1	14,14,15	0.39	0	17,19,21	0.67	0
6	NAG	V	2	6	14,14,15	0.32	0	17,19,21	0.89	0
6	BMA	V	3	6	11,11,12	0.79	0	15,15,17	1.04	1 (6%)
6	MAN	V	4	6	11,11,12	0.65	0	15,15,17	0.77	0
6	MAN	V	5	6	11,11,12	0.64	0	15,15,17	1.11	2 (13%)
7	NAG	W	1	1,7	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
7	NAG	W	2	7	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
4	NAG	X	1	1,4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	X	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	BMA	X	3	4	11,11,12	0.57	0	15,15,17	0.80	0
4	MAN	X	4	4	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
7	NAG	Y	1	1,7	14,14,15	0.25	0	17,19,21	0.44	0
7	NAG	Y	2	7	14,14,15	0.26	0	17,19,21	0.43	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
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	1/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	2/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1
6	MAN	M	4	6	-	2/2/19/22	0/1/1/1
6	MAN	M	5	6	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	1/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	3	BMA	C1-C2	2.57	1.58	1.52
3	K	1	NAG	O5-C1	-2.22	1.40	1.43
3	K	2	NAG	C1-C2	2.06	1.55	1.52
3	K	4	MAN	O5-C1	-2.04	1.40	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	4	MAN	C1-O5-C5	3.56	116.96	112.19
7	W	1	NAG	C1-O5-C5	3.27	116.56	112.19
6	U	4	MAN	C1-O5-C5	3.25	116.54	112.19
6	V	5	MAN	C1-O5-C5	3.03	116.25	112.19
6	U	5	MAN	C1-O5-C5	2.97	116.16	112.19
4	H	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	H	3	BMA	C1-O5-C5	2.86	116.02	112.19
6	N	4	MAN	C1-O5-C5	2.76	115.88	112.19
4	X	4	MAN	C1-O5-C5	2.74	115.86	112.19
5	P	3	BMA	O2-C2-C3	-2.56	104.85	110.15
4	I	4	MAN	C1-O5-C5	2.54	115.59	112.19
3	K	1	NAG	C2-N2-C7	2.48	126.23	122.90
6	M	5	MAN	C1-O5-C5	2.47	115.49	112.19
3	K	3	BMA	C1-O5-C5	2.42	115.44	112.19
6	V	5	MAN	O2-C2-C3	-2.37	105.24	110.15
3	K	4	MAN	O2-C2-C3	-2.36	105.25	110.15
3	G	4	MAN	C1-O5-C5	2.27	115.22	112.19
6	U	4	MAN	O2-C2-C3	-2.19	105.62	110.15
6	M	4	MAN	O2-C2-C3	-2.18	105.64	110.15
4	T	4	MAN	O2-C2-C3	-2.18	105.64	110.15
6	U	5	MAN	O2-C2-C3	-2.17	105.66	110.15
6	V	3	BMA	C1-O5-C5	2.16	115.08	112.19
4	X	4	MAN	O2-C2-C3	-2.15	105.70	110.15
3	O	4	MAN	O2-C2-C3	-2.13	105.74	110.15
6	M	5	MAN	O2-C2-C3	-2.13	105.74	110.15
4	I	4	MAN	O2-C2-C3	-2.11	105.77	110.15
3	O	3	BMA	C1-O5-C5	2.11	115.01	112.19
5	P	3	BMA	C1-C2-C3	-2.10	106.59	109.64
4	H	4	MAN	O2-C2-C3	-2.09	105.81	110.15
3	K	3	BMA	O3-C3-C4	2.07	115.27	110.38
3	K	2	NAG	C1-O5-C5	2.02	114.90	112.19
7	W	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	3	BMA	C4-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	X	3	BMA	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
7	Q	2	NAG	C8-C7-N2-C2
7	Q	2	NAG	O7-C7-N2-C2
7	Y	1	NAG	C8-C7-N2-C2
7	Y	1	NAG	O7-C7-N2-C2
6	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6

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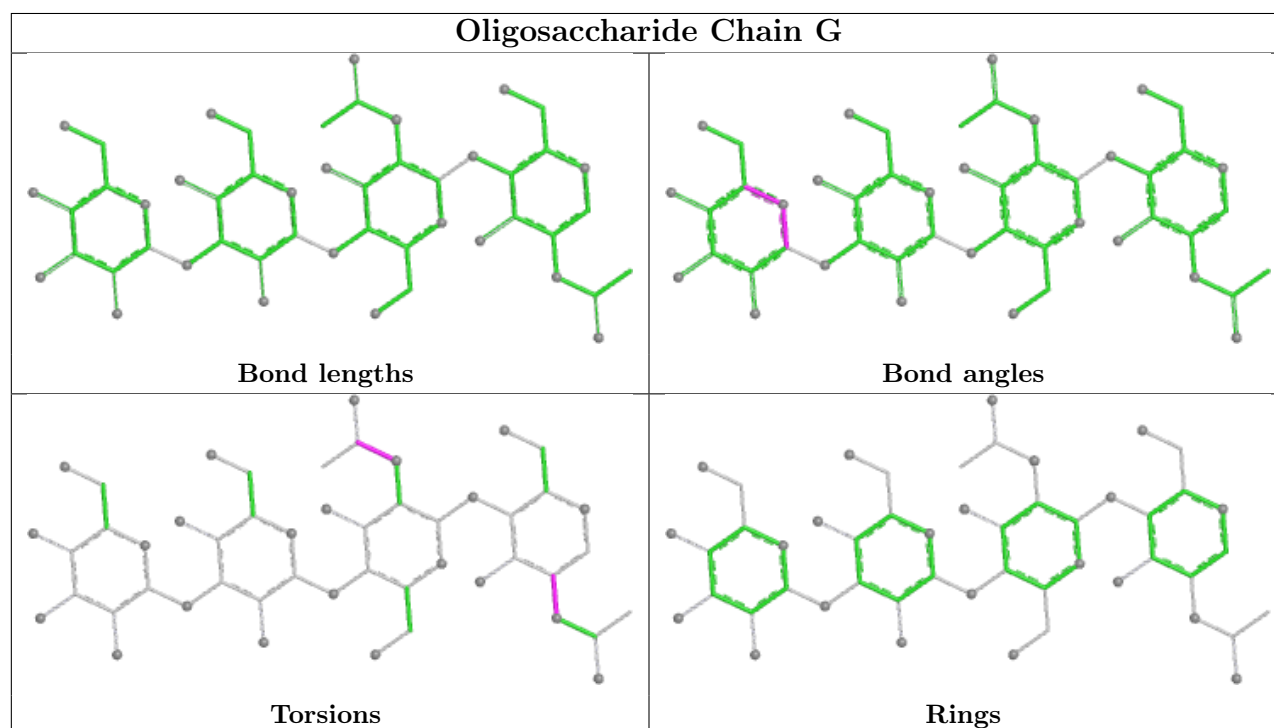
Mol	Chain	Res	Type	Atoms
6	M	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
6	M	4	MAN	C4-C5-C6-O6
3	K	4	MAN	C4-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	M	4	MAN	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
6	M	1	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7
3	K	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
6	M	1	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
7	W	1	NAG	C3-C2-N2-C7
5	P	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7
7	W	1	NAG	C1-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
6	M	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6

There are no ring outliers.

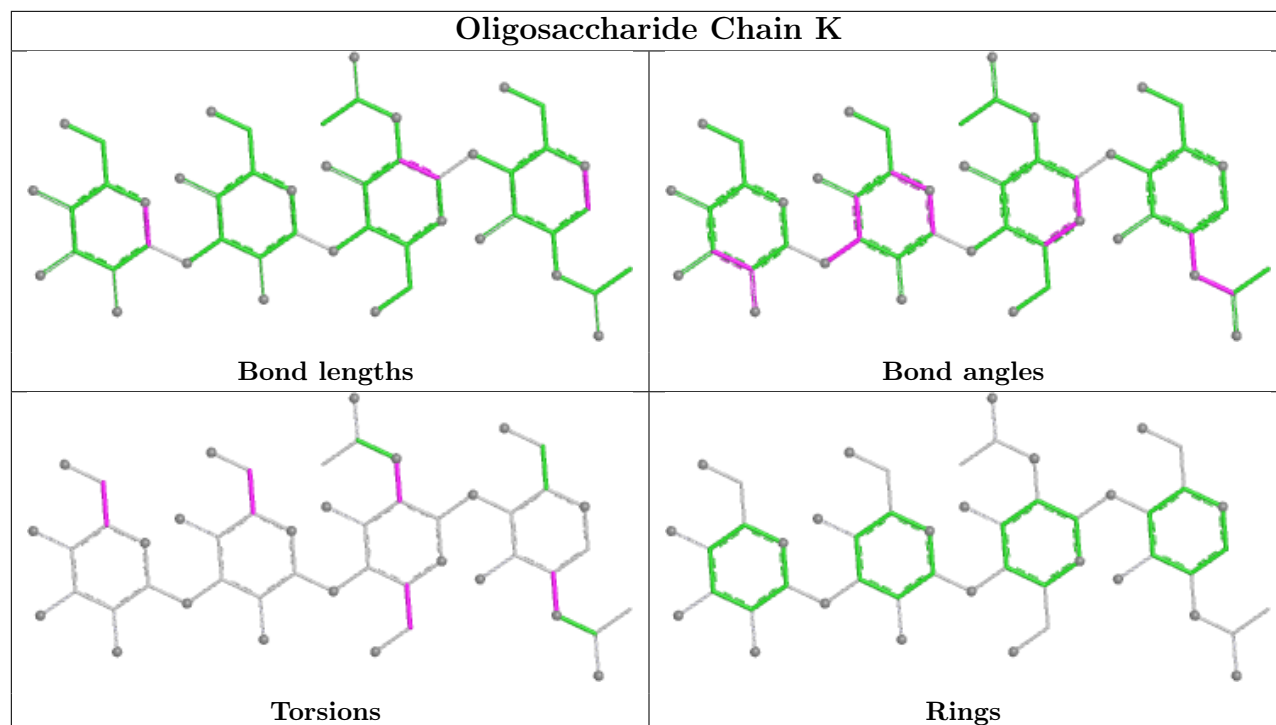
19 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
6	U	1	NAG	1	0
4	H	2	NAG	1	0
3	G	3	BMA	1	0
3	K	2	NAG	2	0
5	P	1	NAG	1	0
3	G	4	MAN	1	0
6	N	3	BMA	1	0
5	L	1	NAG	1	0
3	K	1	NAG	4	0
4	X	1	NAG	1	0
3	O	1	NAG	2	0
5	P	2	NAG	1	0
7	Q	1	NAG	1	0
7	Y	1	NAG	1	0
5	L	2	NAG	1	0
6	M	1	NAG	1	0
6	N	5	MAN	1	0
7	W	2	NAG	2	0

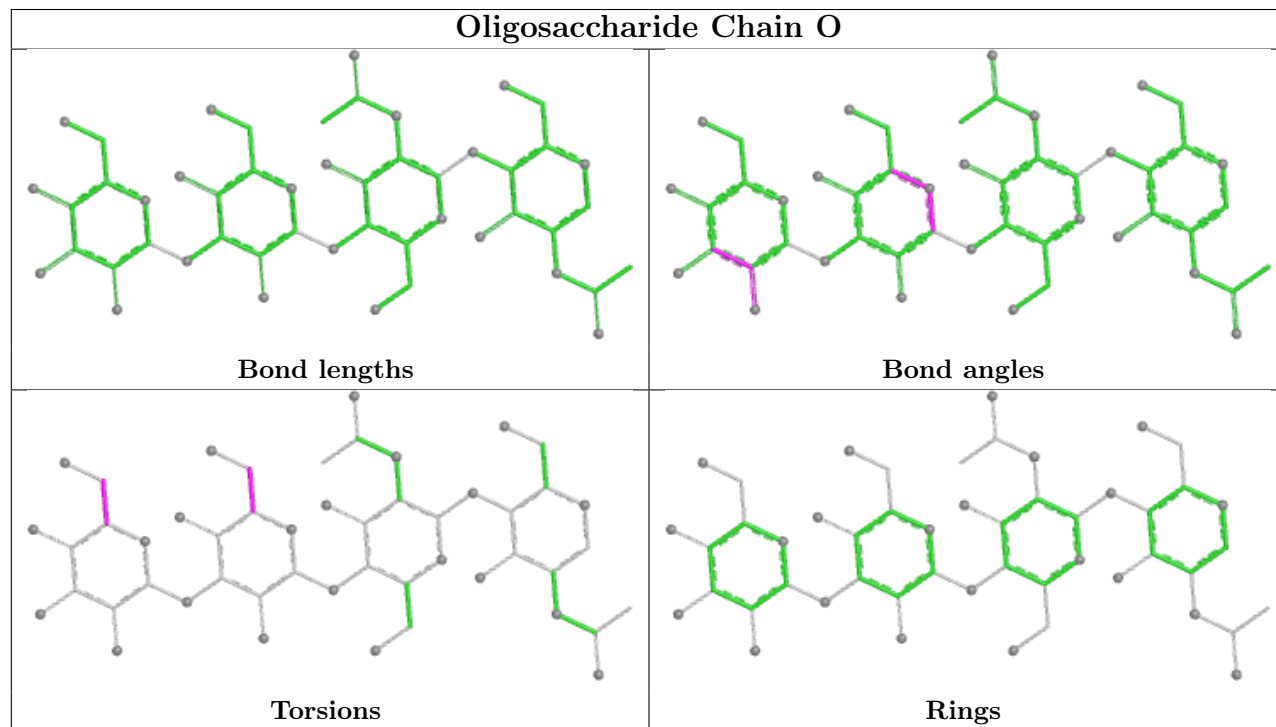
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



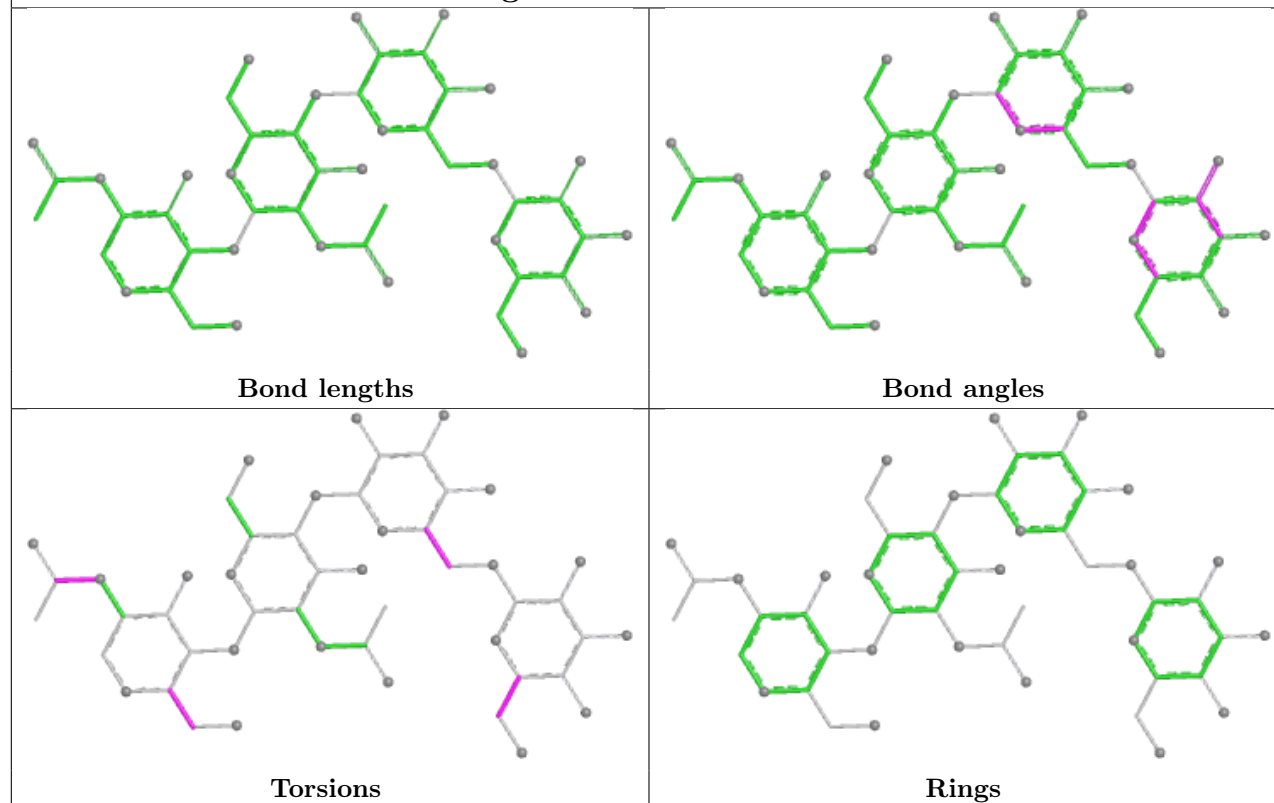
## Oligosaccharide Chain K



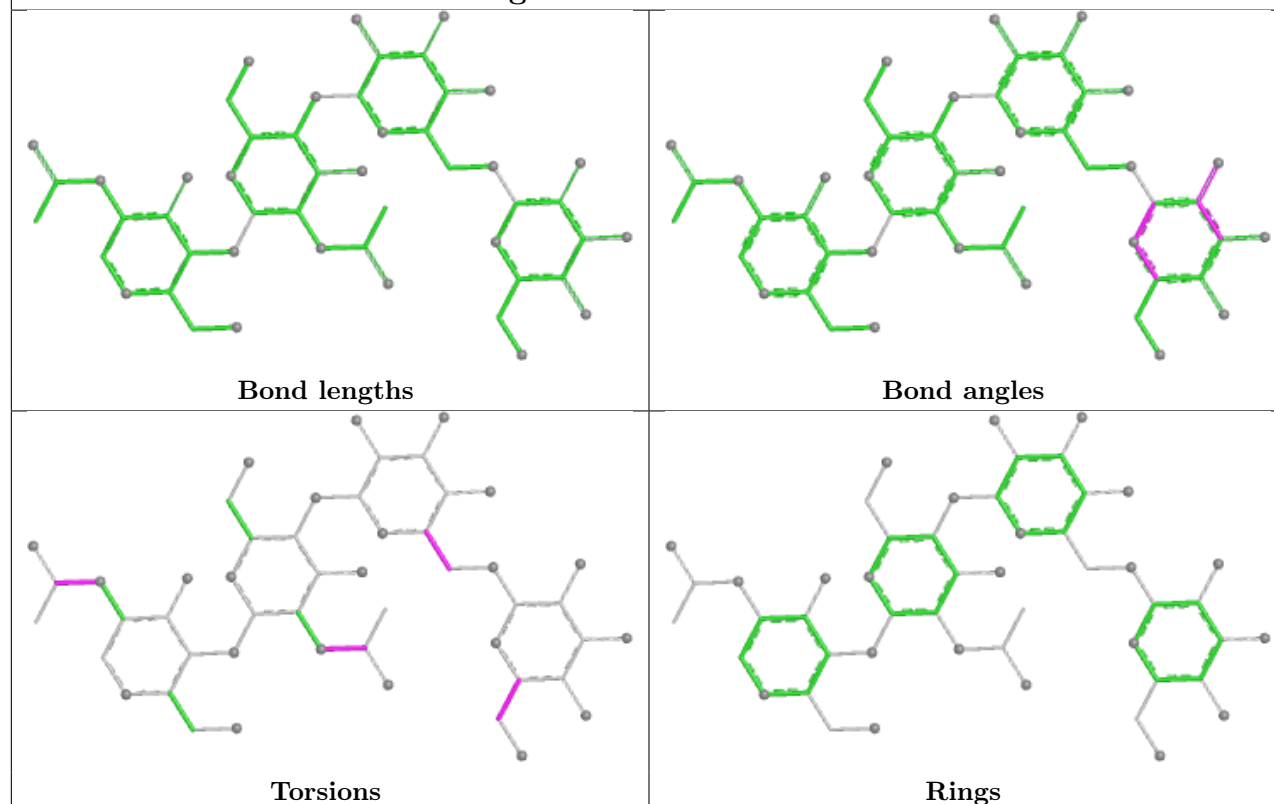
## Oligosaccharide Chain O



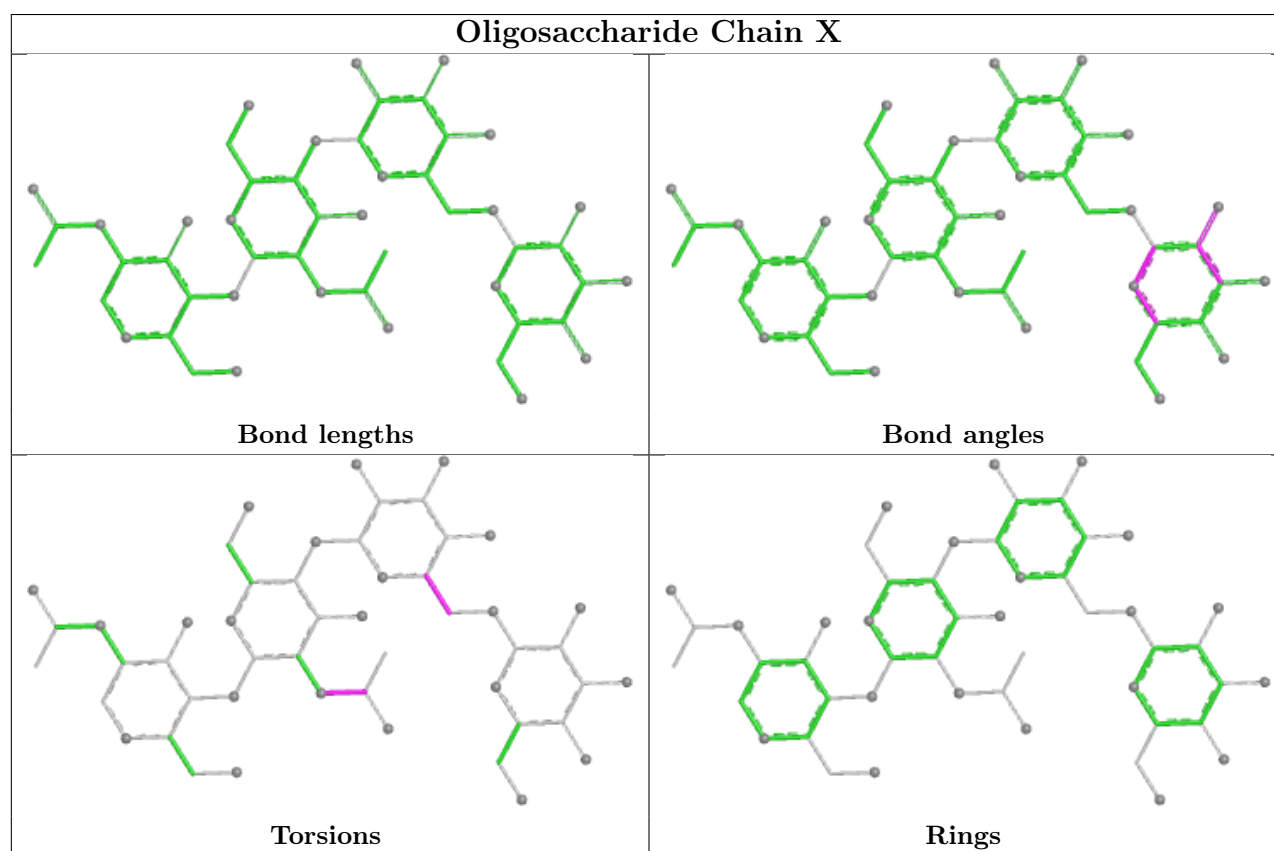
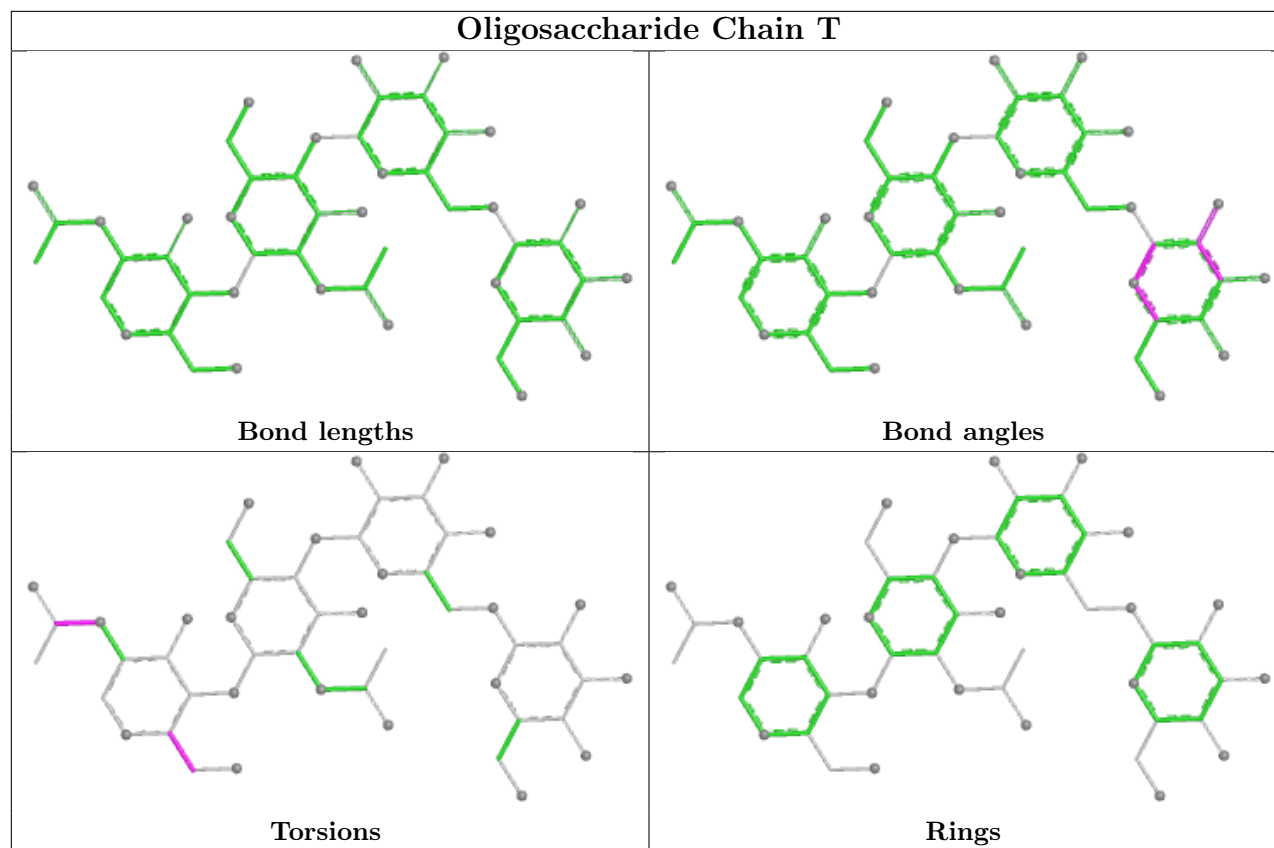
## Oligosaccharide Chain H

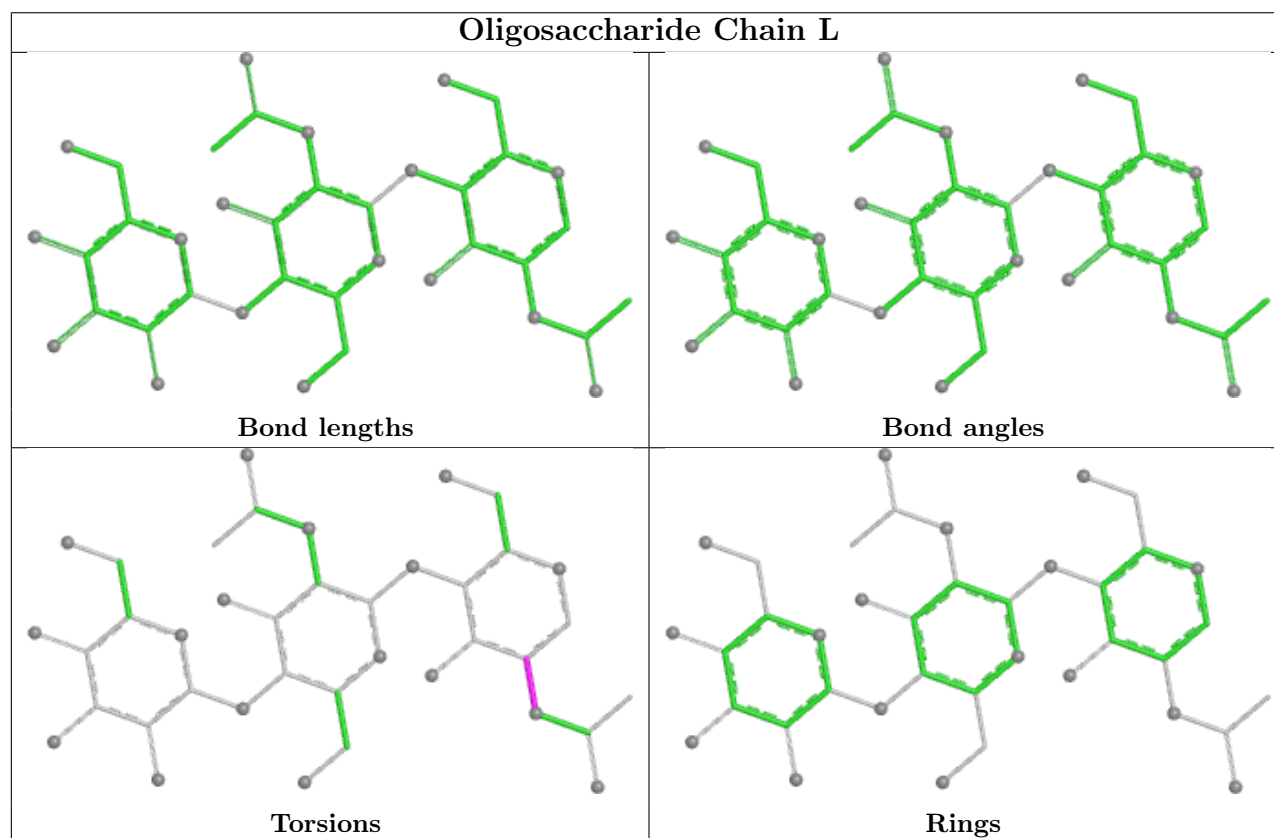
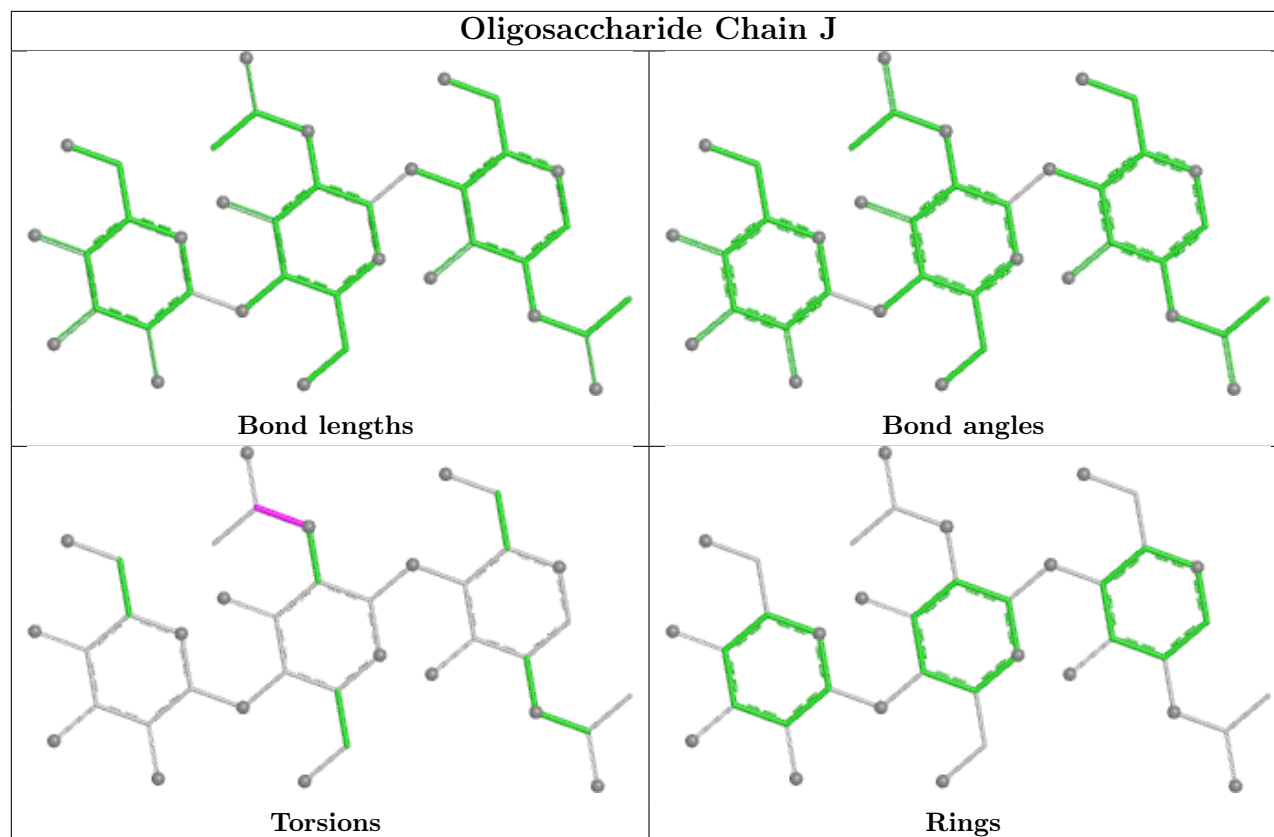


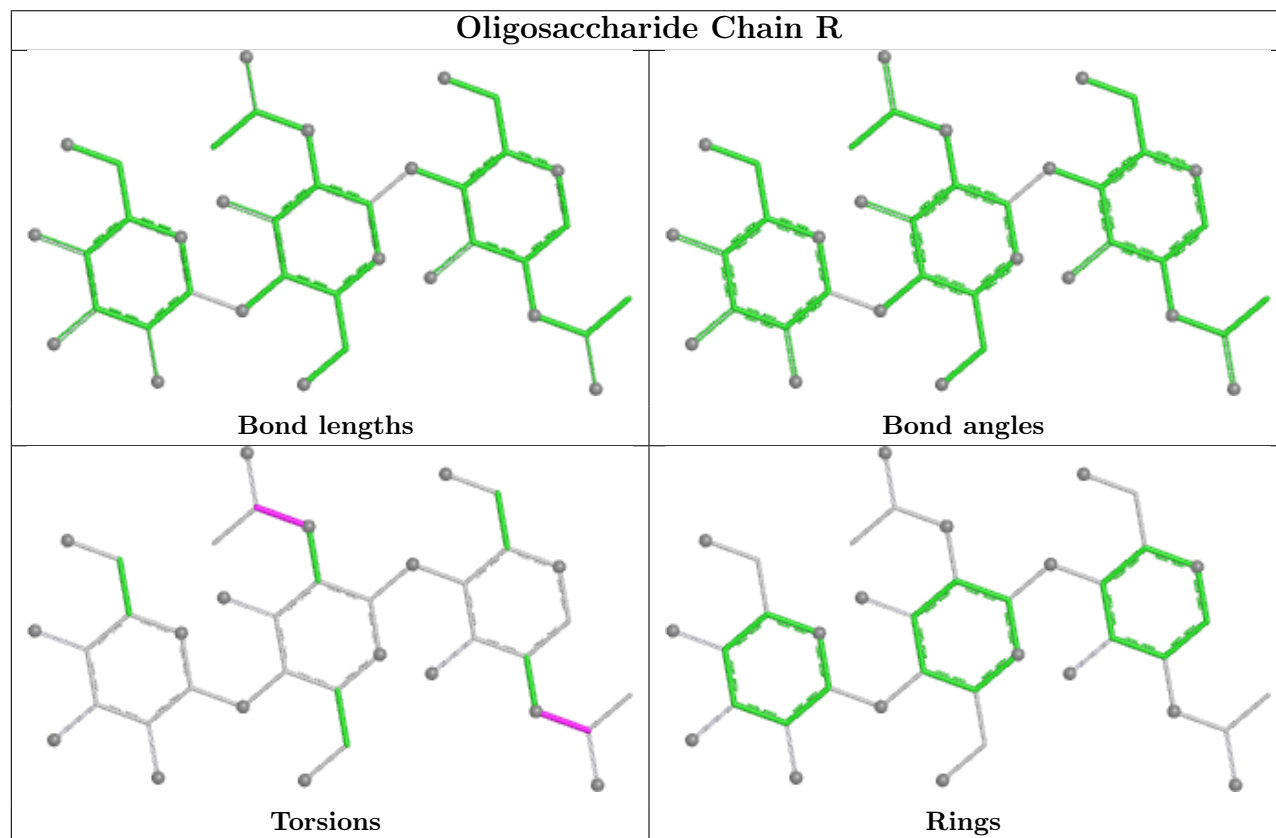
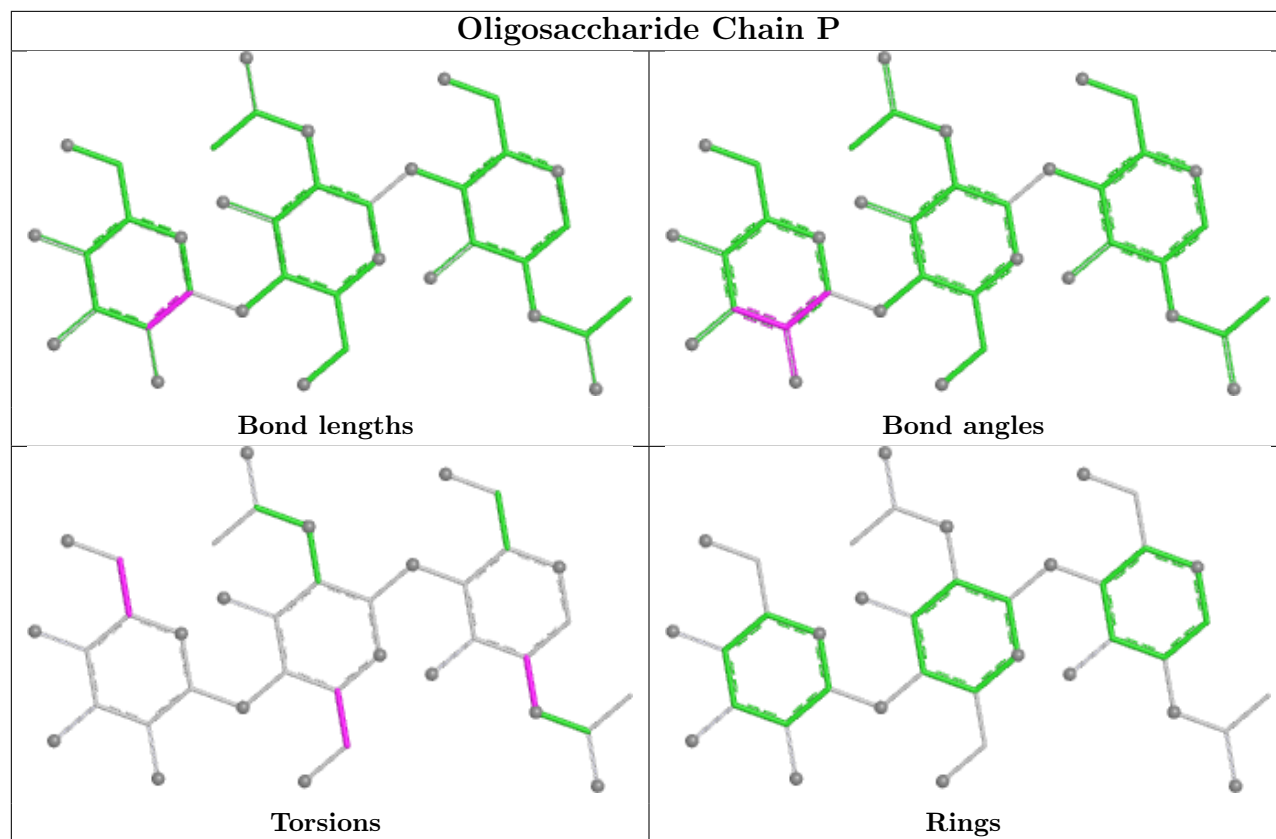
## Oligosaccharide Chain I

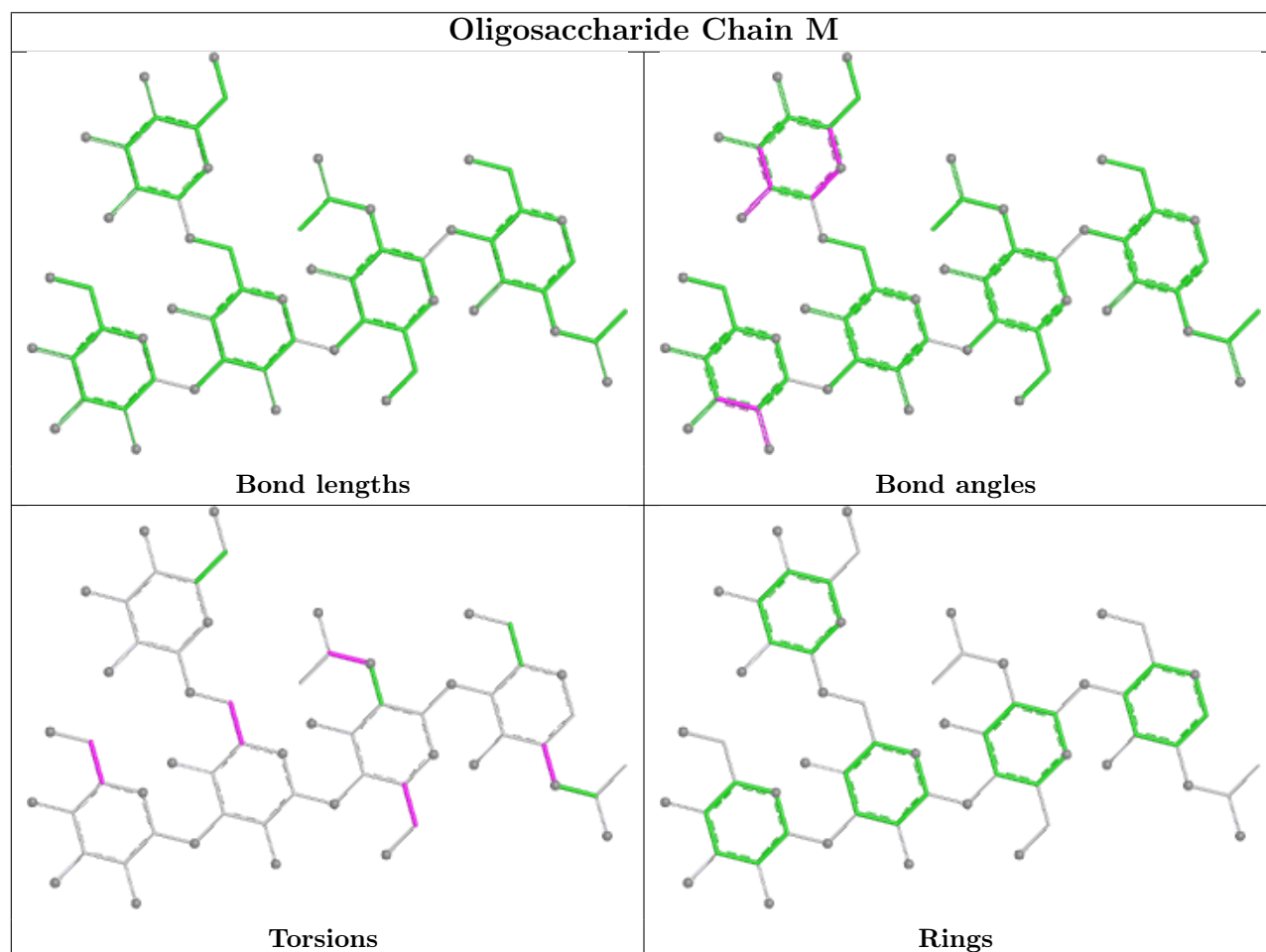
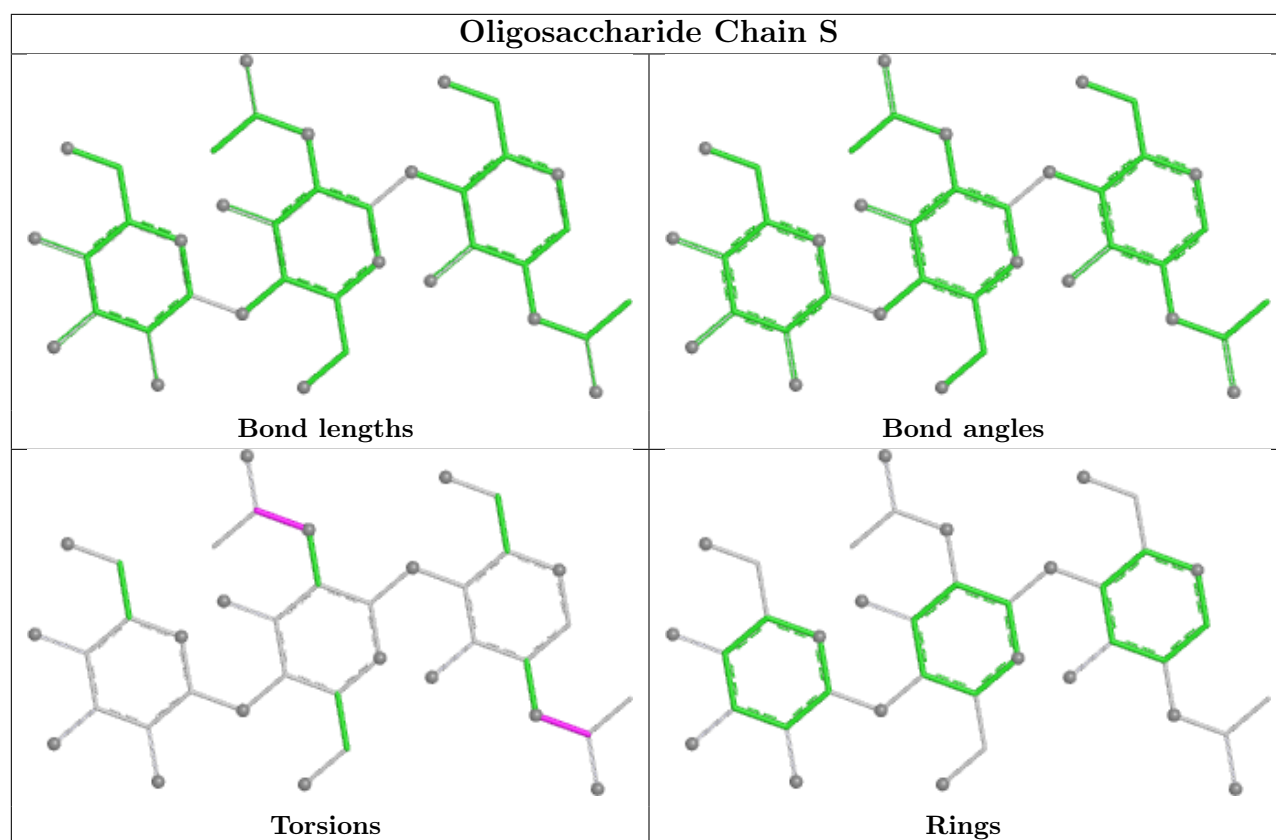


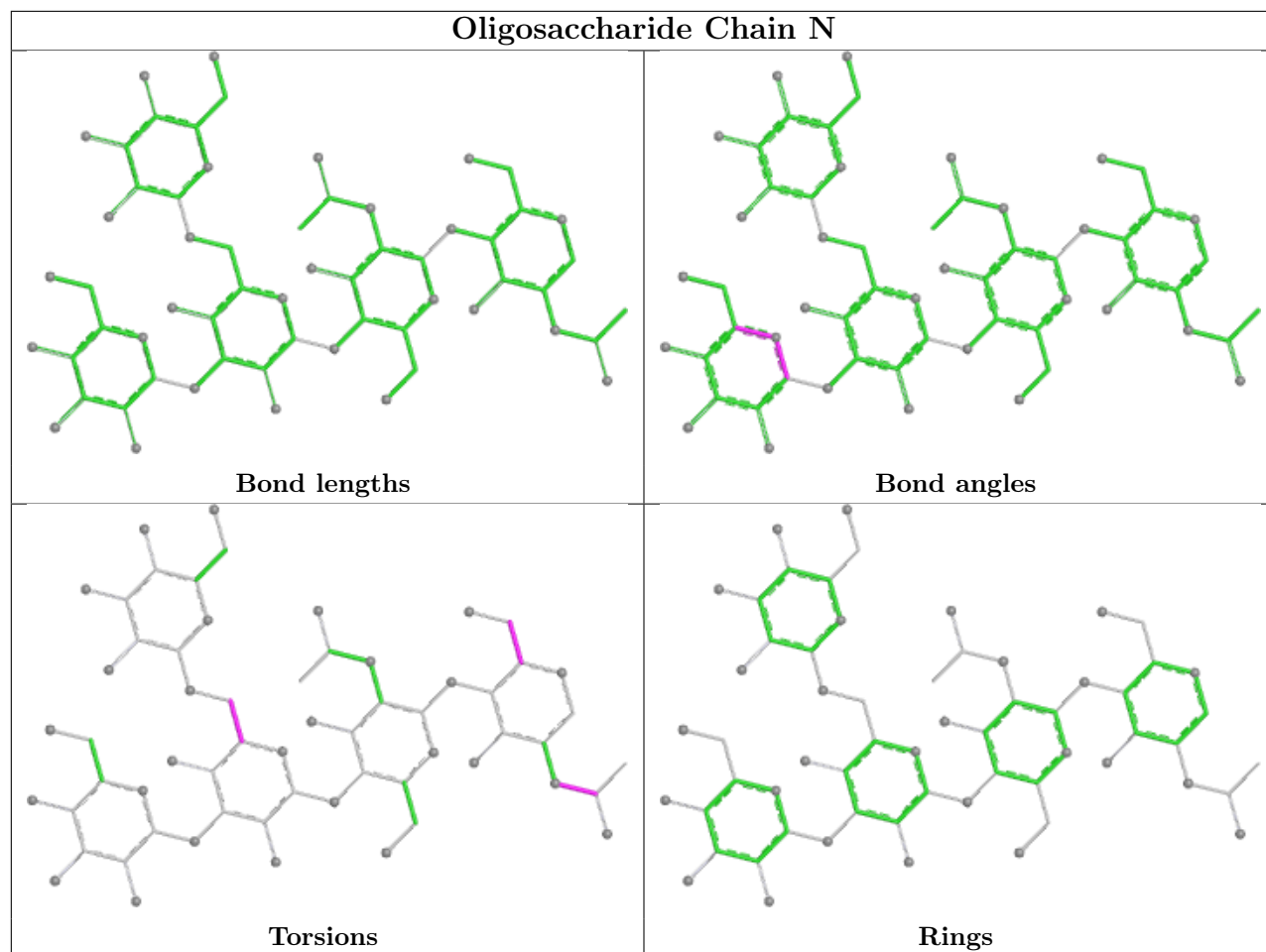


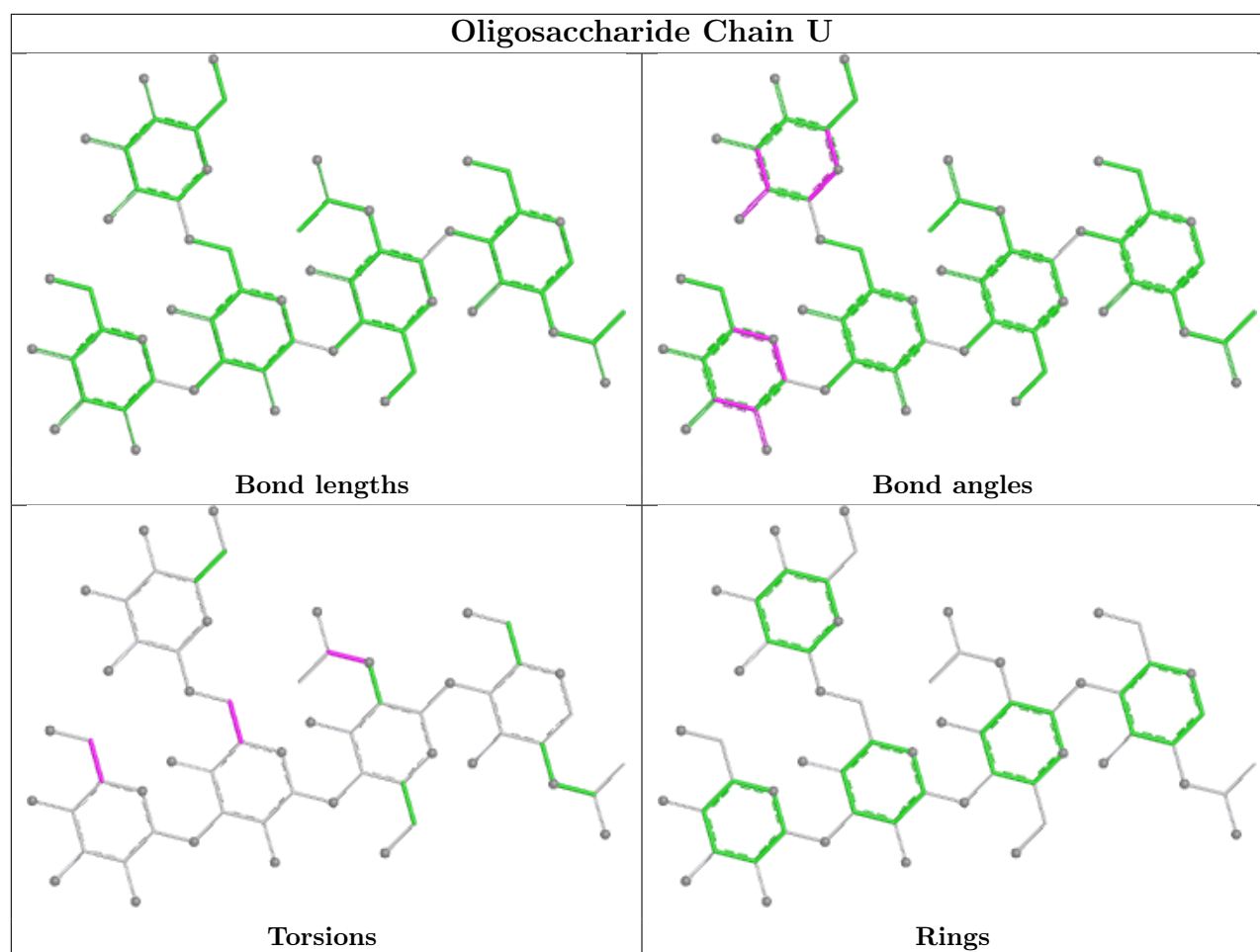


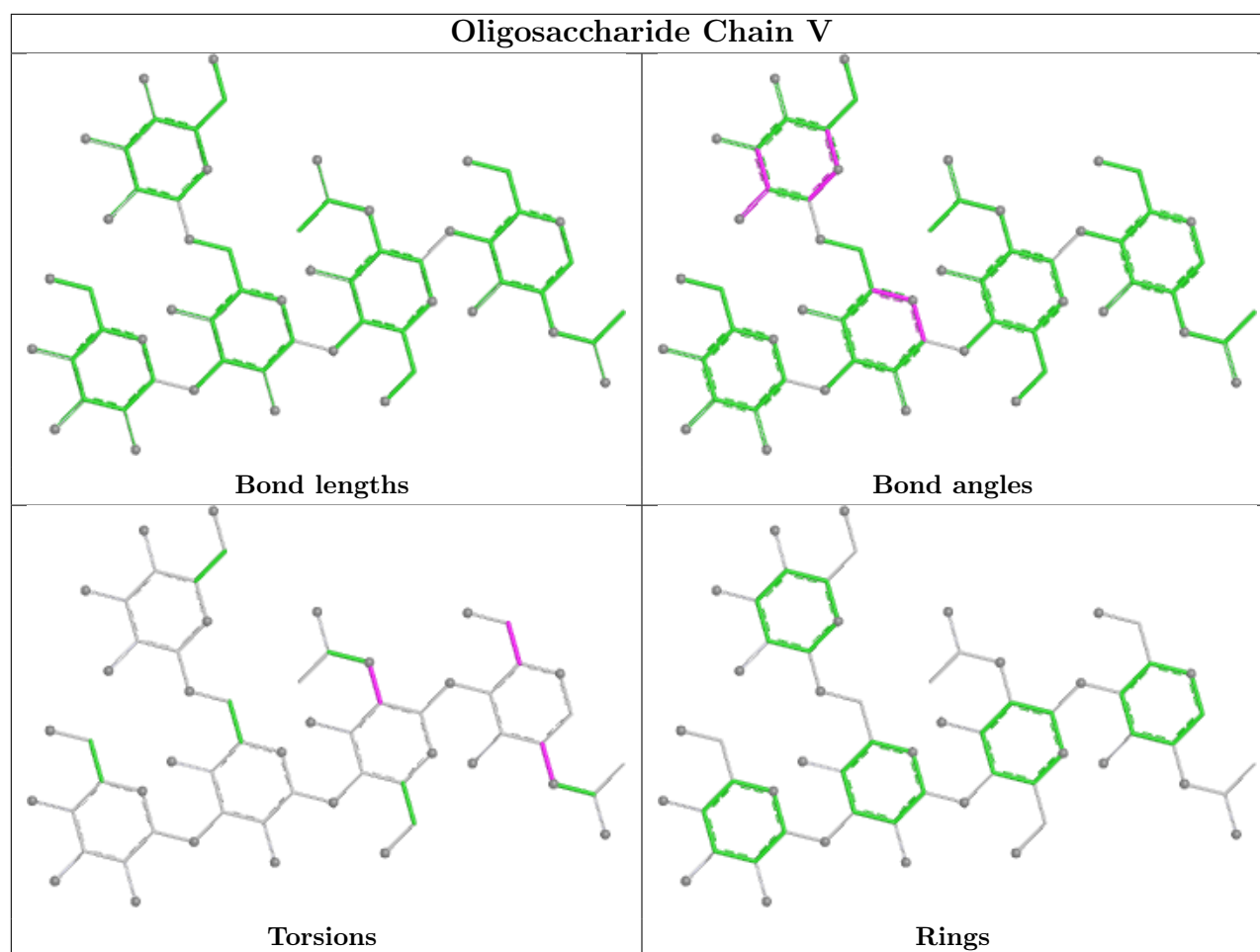


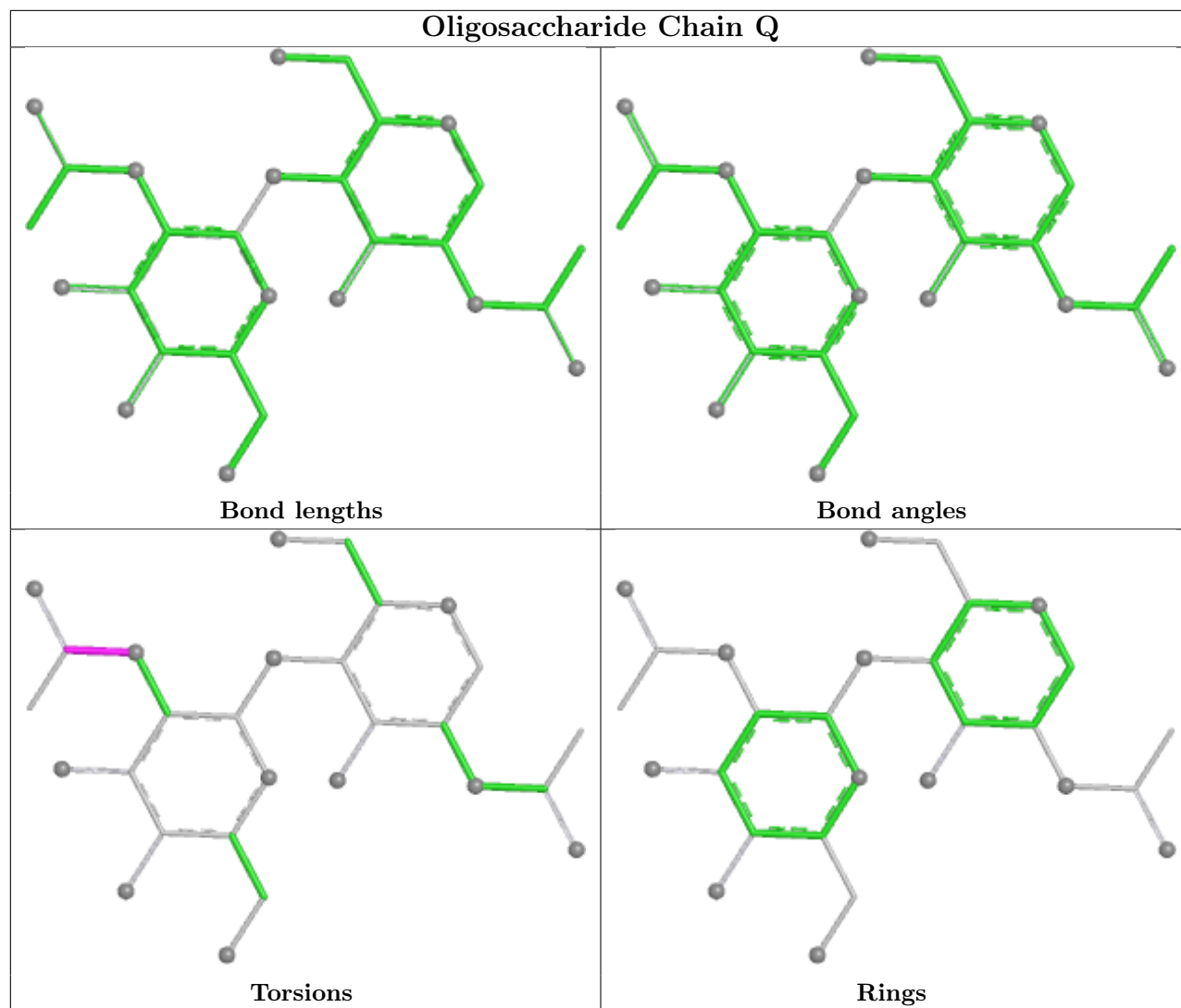




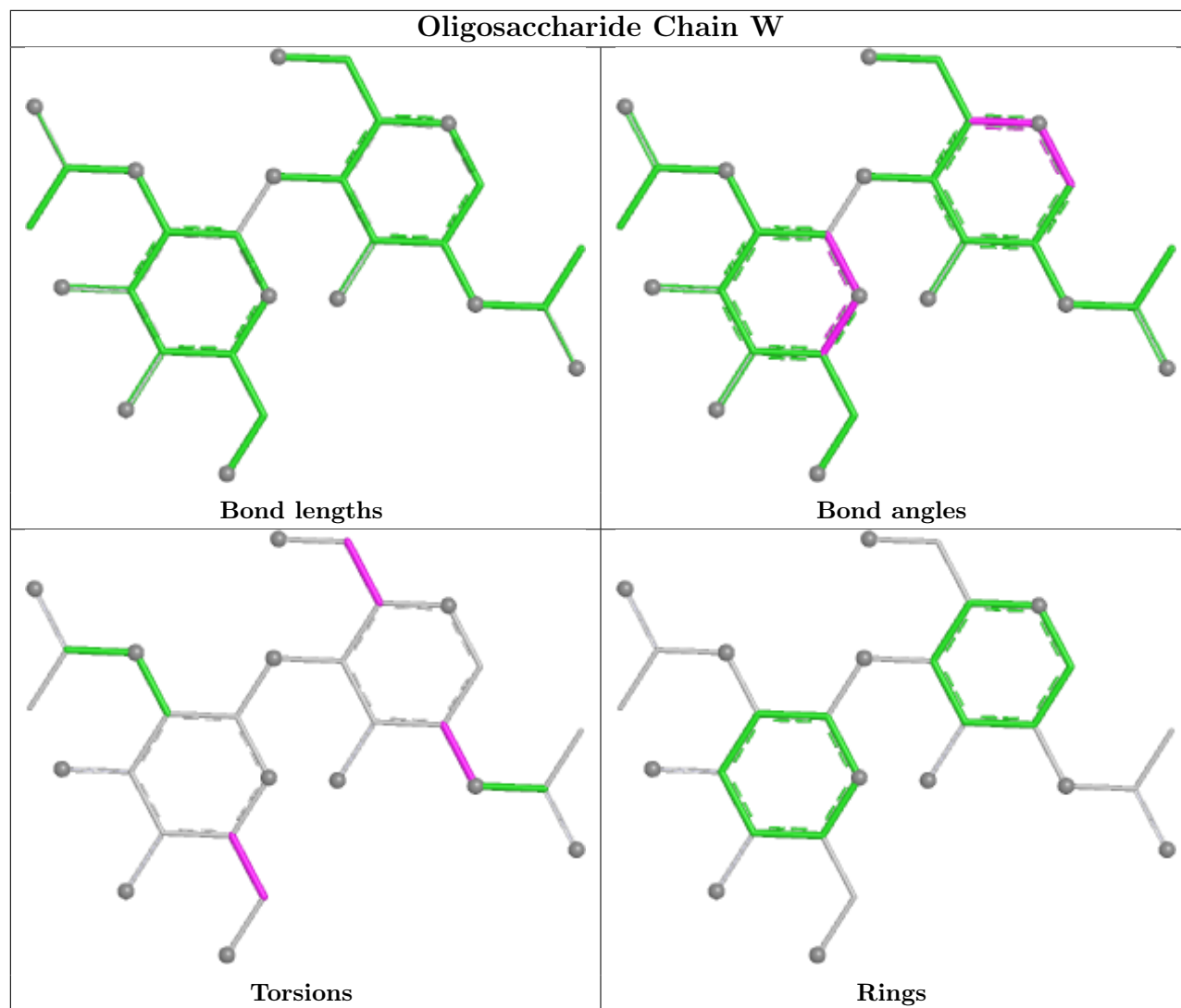


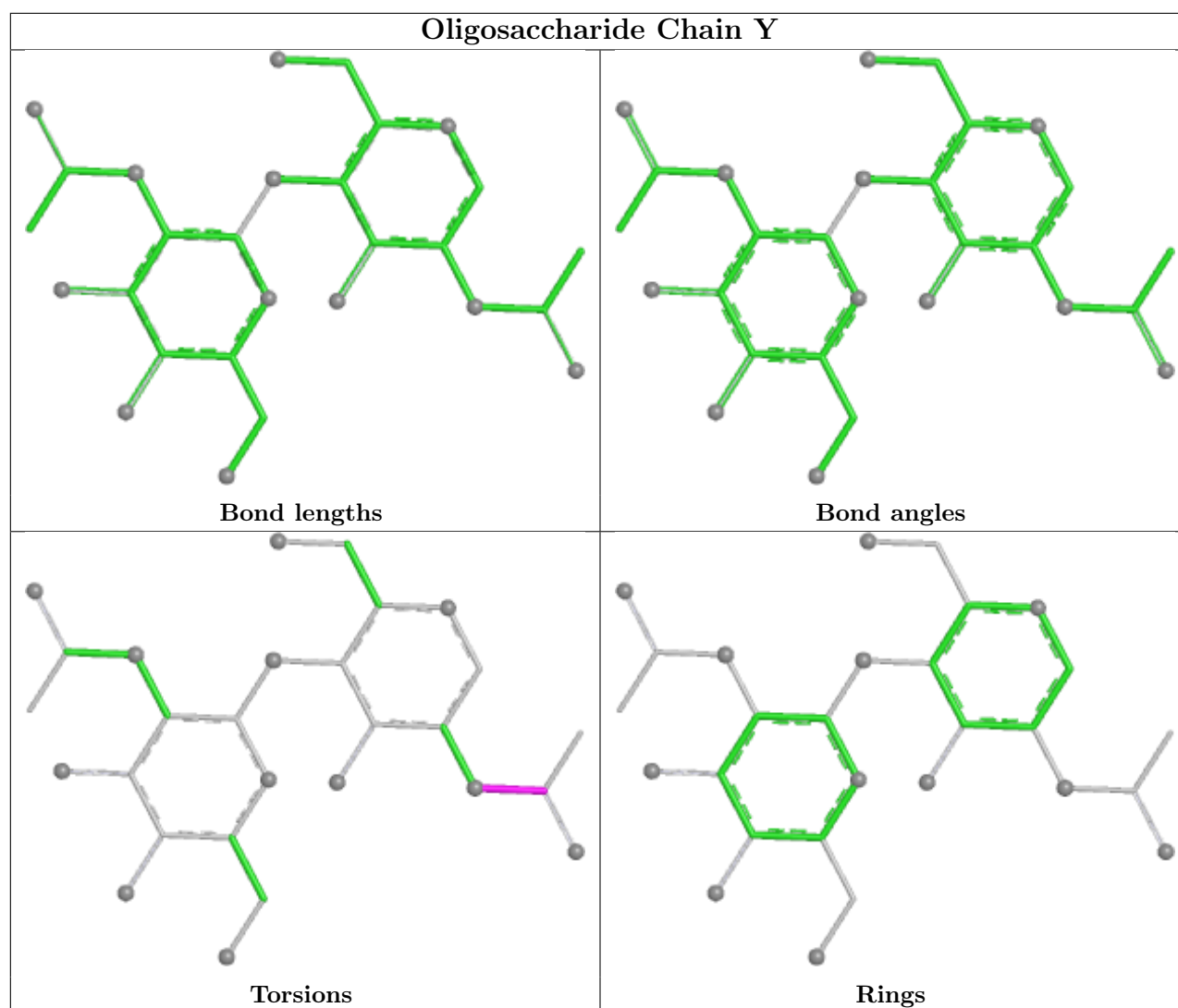












## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	A	401	1	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	C	401	1	14,14,15	0.19	0	17,19,21	0.41	0
8	NAG	a	601	2	14,14,15	0.29	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	f	601	2	14,14,15	0.64	1 (7%)	17,19,21	0.65	0
8	NAG	E	1003	1	14,14,15	0.28	0	17,19,21	0.41	0
8	NAG	d	601	2	14,14,15	0.20	0	17,19,21	0.50	0
8	NAG	A	402	1	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	C	402	1	14,14,15	0.19	0	17,19,21	0.49	0
8	NAG	D	401	1	14,14,15	0.18	0	17,19,21	0.39	0
8	NAG	B	402	1	14,14,15	0.29	0	17,19,21	0.45	0
8	NAG	F	401	1	14,14,15	0.33	0	17,19,21	0.45	0
8	NAG	C	403	1	14,14,15	0.25	0	17,19,21	0.50	0
8	NAG	c	601	2	14,14,15	0.27	0	17,19,21	0.43	0
8	NAG	A	403	1	14,14,15	0.41	0	17,19,21	0.47	0
8	NAG	E	1002	1	14,14,15	0.26	0	17,19,21	0.56	0
8	NAG	B	401	1	14,14,15	0.19	0	17,19,21	0.40	0
8	NAG	A	404	1	14,14,15	0.44	0	17,19,21	0.54	0
8	NAG	E	1001	1	14,14,15	0.24	0	17,19,21	0.55	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
8	NAG	A	401	1	-	0/6/23/26	0/1/1/1
8	NAG	C	401	1	-	2/6/23/26	0/1/1/1
8	NAG	a	601	2	-	2/6/23/26	0/1/1/1
8	NAG	f	601	2	-	1/6/23/26	0/1/1/1
8	NAG	E	1003	1	-	2/6/23/26	0/1/1/1
8	NAG	d	601	2	-	2/6/23/26	0/1/1/1
8	NAG	A	402	1	-	1/6/23/26	0/1/1/1
8	NAG	C	402	1	-	3/6/23/26	0/1/1/1
8	NAG	D	401	1	-	3/6/23/26	0/1/1/1
8	NAG	B	402	1	-	2/6/23/26	0/1/1/1
8	NAG	F	401	1	-	1/6/23/26	0/1/1/1
8	NAG	C	403	1	-	1/6/23/26	0/1/1/1
8	NAG	c	601	2	-	0/6/23/26	0/1/1/1
8	NAG	A	403	1	-	2/6/23/26	0/1/1/1
8	NAG	E	1002	1	-	4/6/23/26	0/1/1/1
8	NAG	B	401	1	-	3/6/23/26	0/1/1/1
8	NAG	A	404	1	-	3/6/23/26	0/1/1/1
8	NAG	E	1001	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	601	NAG	C1-C2	2.26	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	1002	NAG	O5-C5-C6-O6
8	a	601	NAG	O5-C5-C6-O6
8	E	1002	NAG	C4-C5-C6-O6
8	A	403	NAG	C8-C7-N2-C2
8	A	403	NAG	O7-C7-N2-C2
8	B	401	NAG	C8-C7-N2-C2
8	B	401	NAG	O7-C7-N2-C2
8	B	402	NAG	C8-C7-N2-C2
8	B	402	NAG	O7-C7-N2-C2
8	C	401	NAG	C8-C7-N2-C2
8	C	401	NAG	O7-C7-N2-C2
8	C	402	NAG	C8-C7-N2-C2
8	C	402	NAG	O7-C7-N2-C2
8	D	401	NAG	C8-C7-N2-C2
8	D	401	NAG	O7-C7-N2-C2
8	E	1002	NAG	C8-C7-N2-C2
8	E	1002	NAG	O7-C7-N2-C2
8	E	1003	NAG	C8-C7-N2-C2
8	E	1003	NAG	O7-C7-N2-C2
8	A	404	NAG	O5-C5-C6-O6
8	B	401	NAG	O5-C5-C6-O6
8	a	601	NAG	C4-C5-C6-O6
8	A	402	NAG	O5-C5-C6-O6
8	F	401	NAG	O5-C5-C6-O6
8	C	403	NAG	O5-C5-C6-O6
8	D	401	NAG	O5-C5-C6-O6
8	C	402	NAG	O5-C5-C6-O6
8	E	1001	NAG	O5-C5-C6-O6
8	E	1001	NAG	C1-C2-N2-C7
8	A	404	NAG	C4-C5-C6-O6
8	d	601	NAG	C4-C5-C6-O6
8	f	601	NAG	C1-C2-N2-C7
8	A	404	NAG	C3-C2-N2-C7
8	E	1001	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	d	601	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	f	601	NAG	1	0
8	c	601	NAG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	318/323 (98%)	-0.02	2 (0%) 85 82	36, 55, 77, 99	0
1	B	319/323 (98%)	0.02	2 (0%) 85 82	40, 63, 85, 99	0
1	C	318/323 (98%)	0.10	2 (0%) 85 82	43, 67, 88, 105	0
1	D	317/323 (98%)	-0.07	2 (0%) 85 82	35, 60, 81, 106	0
1	E	316/323 (97%)	0.08	2 (0%) 85 82	44, 67, 88, 105	0
1	F	318/323 (98%)	0.01	3 (0%) 81 76	42, 61, 84, 101	0
2	a	172/181 (95%)	0.00	3 (1%) 69 63	40, 61, 83, 99	0
2	b	171/181 (94%)	-0.00	1 (0%) 85 82	37, 63, 85, 101	0
2	c	172/181 (95%)	0.12	2 (1%) 76 71	36, 68, 90, 110	0
2	d	170/181 (93%)	0.15	1 (0%) 85 82	37, 82, 113, 127	0
2	e	171/181 (94%)	0.08	2 (1%) 76 71	40, 75, 103, 121	0
2	f	172/181 (95%)	0.18	4 (2%) 61 54	39, 71, 98, 116	0
All	All	2934/3024 (97%)	0.04	26 (0%) 81 76	35, 64, 92, 127	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	13	LEU	6.2
2	f	467	PHE	3.2
1	B	104	ASP	3.0
1	A	13	LEU	2.8
2	a	467	PHE	2.7
2	b	340	GLU	2.5
2	a	330	GLY	2.5
2	c	385	ILE	2.5
1	F	213	VAL	2.5
2	c	372	ALA	2.5
2	f	330	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	181	GLY	2.4
1	D	146	SER	2.4
1	B	179	ILE	2.4
1	E	10	THR	2.4
1	E	158	ASN	2.3
2	f	385	ILE	2.2
1	C	58	ILE	2.2
2	e	338	PHE	2.2
1	D	321	ARG	2.1
1	C	212	ALA	2.1
1	F	81	ASN	2.1
2	a	395	ILE	2.1
2	f	461	ASP	2.0
2	e	352	GLY	2.0
2	d	331	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	404	14/15	0.34	0.13	94,108,114,116	0
8	NAG	C	403	14/15	0.44	0.16	77,101,109,109	0
8	NAG	E	1002	14/15	0.47	0.13	99,113,118,119	0
8	NAG	E	1003	14/15	0.53	0.12	83,107,114,114	0
8	NAG	d	601	14/15	0.53	0.17	85,99,107,107	0
8	NAG	C	402	14/15	0.55	0.14	75,101,117,117	0
8	NAG	A	403	14/15	0.56	0.12	93,105,110,113	0
8	NAG	B	401	14/15	0.57	0.14	78,85,94,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	c	601	14/15	0.59	0.15	76,92,102,105	0
8	NAG	A	402	14/15	0.59	0.12	83,93,101,106	0
8	NAG	E	1001	14/15	0.65	0.12	76,85,97,100	0
8	NAG	D	401	14/15	0.66	0.11	70,78,85,87	0
8	NAG	F	401	14/15	0.66	0.10	58,96,105,105	0
8	NAG	f	601	14/15	0.69	0.15	97,104,110,112	0
8	NAG	A	401	14/15	0.72	0.12	65,74,82,87	0
8	NAG	B	402	14/15	0.78	0.10	55,70,80,84	0
8	NAG	C	401	14/15	0.82	0.11	80,99,115,118	0
8	NAG	a	601	14/15	0.86	0.09	66,81,96,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.