



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 6D96 / pdb_00006d96
Title : Structure of influenza neuraminidase from strain A/BrevigMission/1/1918(H1N1) expressed in HEK-293E cells
Authors : Campbell, A.C.; Krause, K.L.; Tanner, J.J.
Deposited on : 2018-04-27
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

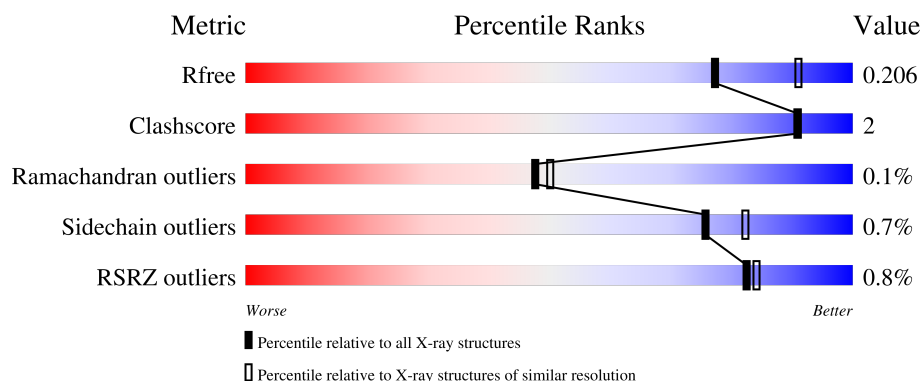
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	404	% 91% 5% .
1	B	404	% 91% 5% .
1	C	404	92% . .
1	D	404	% 90% 5% .
1	E	404	91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	404	% 89% 7% .
1	G	404	92% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25633 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	1	0
			2963	1854	509	577	23			
1	B	386	Total	C	N	O	S	0	1	0
			2971	1861	509	577	24			
1	C	386	Total	C	N	O	S	0	1	0
			2973	1862	511	577	23			
1	D	386	Total	C	N	O	S	0	2	0
			2975	1863	510	578	24			
1	E	386	Total	C	N	O	S	0	2	0
			2977	1864	510	578	25			
1	F	386	Total	C	N	O	S	0	1	0
			2966	1857	509	576	24			
1	G	386	Total	C	N	O	S	0	1	0
			2966	1857	509	576	24			
1	H	386	Total	C	N	O	S	0	0	0
			2967	1858	510	576	23			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	HIS	-	expression tag	UNP Q9IGQ6
A	67	HIS	-	expression tag	UNP Q9IGQ6
A	68	HIS	-	expression tag	UNP Q9IGQ6
A	69	HIS	-	expression tag	UNP Q9IGQ6
A	70	HIS	-	expression tag	UNP Q9IGQ6
A	71	HIS	-	expression tag	UNP Q9IGQ6
A	72	SER	-	expression tag	UNP Q9IGQ6
A	73	LEU	-	expression tag	UNP Q9IGQ6
A	74	VAL	-	expression tag	UNP Q9IGQ6
A	75	PRO	-	expression tag	UNP Q9IGQ6
A	76	ARG	-	expression tag	UNP Q9IGQ6
A	77	GLY	-	expression tag	UNP Q9IGQ6
A	78	SER	-	expression tag	UNP Q9IGQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	79	PRO	-	expression tag	UNP Q9IGQ6
A	80	SER	-	expression tag	UNP Q9IGQ6
A	81	ARG	-	expression tag	UNP Q9IGQ6
B	66	HIS	-	expression tag	UNP Q9IGQ6
B	67	HIS	-	expression tag	UNP Q9IGQ6
B	68	HIS	-	expression tag	UNP Q9IGQ6
B	69	HIS	-	expression tag	UNP Q9IGQ6
B	70	HIS	-	expression tag	UNP Q9IGQ6
B	71	HIS	-	expression tag	UNP Q9IGQ6
B	72	SER	-	expression tag	UNP Q9IGQ6
B	73	LEU	-	expression tag	UNP Q9IGQ6
B	74	VAL	-	expression tag	UNP Q9IGQ6
B	75	PRO	-	expression tag	UNP Q9IGQ6
B	76	ARG	-	expression tag	UNP Q9IGQ6
B	77	GLY	-	expression tag	UNP Q9IGQ6
B	78	SER	-	expression tag	UNP Q9IGQ6
B	79	PRO	-	expression tag	UNP Q9IGQ6
B	80	SER	-	expression tag	UNP Q9IGQ6
B	81	ARG	-	expression tag	UNP Q9IGQ6
C	66	HIS	-	expression tag	UNP Q9IGQ6
C	67	HIS	-	expression tag	UNP Q9IGQ6
C	68	HIS	-	expression tag	UNP Q9IGQ6
C	69	HIS	-	expression tag	UNP Q9IGQ6
C	70	HIS	-	expression tag	UNP Q9IGQ6
C	71	HIS	-	expression tag	UNP Q9IGQ6
C	72	SER	-	expression tag	UNP Q9IGQ6
C	73	LEU	-	expression tag	UNP Q9IGQ6
C	74	VAL	-	expression tag	UNP Q9IGQ6
C	75	PRO	-	expression tag	UNP Q9IGQ6
C	76	ARG	-	expression tag	UNP Q9IGQ6
C	77	GLY	-	expression tag	UNP Q9IGQ6
C	78	SER	-	expression tag	UNP Q9IGQ6
C	79	PRO	-	expression tag	UNP Q9IGQ6
C	80	SER	-	expression tag	UNP Q9IGQ6
C	81	ARG	-	expression tag	UNP Q9IGQ6
D	66	HIS	-	expression tag	UNP Q9IGQ6
D	67	HIS	-	expression tag	UNP Q9IGQ6
D	68	HIS	-	expression tag	UNP Q9IGQ6
D	69	HIS	-	expression tag	UNP Q9IGQ6
D	70	HIS	-	expression tag	UNP Q9IGQ6
D	71	HIS	-	expression tag	UNP Q9IGQ6
D	72	SER	-	expression tag	UNP Q9IGQ6

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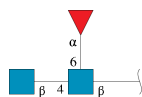
Chain	Residue	Modelled	Actual	Comment	Reference
D	73	LEU	-	expression tag	UNP Q9IGQ6
D	74	VAL	-	expression tag	UNP Q9IGQ6
D	75	PRO	-	expression tag	UNP Q9IGQ6
D	76	ARG	-	expression tag	UNP Q9IGQ6
D	77	GLY	-	expression tag	UNP Q9IGQ6
D	78	SER	-	expression tag	UNP Q9IGQ6
D	79	PRO	-	expression tag	UNP Q9IGQ6
D	80	SER	-	expression tag	UNP Q9IGQ6
D	81	ARG	-	expression tag	UNP Q9IGQ6
E	66	HIS	-	expression tag	UNP Q9IGQ6
E	67	HIS	-	expression tag	UNP Q9IGQ6
E	68	HIS	-	expression tag	UNP Q9IGQ6
E	69	HIS	-	expression tag	UNP Q9IGQ6
E	70	HIS	-	expression tag	UNP Q9IGQ6
E	71	HIS	-	expression tag	UNP Q9IGQ6
E	72	SER	-	expression tag	UNP Q9IGQ6
E	73	LEU	-	expression tag	UNP Q9IGQ6
E	74	VAL	-	expression tag	UNP Q9IGQ6
E	75	PRO	-	expression tag	UNP Q9IGQ6
E	76	ARG	-	expression tag	UNP Q9IGQ6
E	77	GLY	-	expression tag	UNP Q9IGQ6
E	78	SER	-	expression tag	UNP Q9IGQ6
E	79	PRO	-	expression tag	UNP Q9IGQ6
E	80	SER	-	expression tag	UNP Q9IGQ6
E	81	ARG	-	expression tag	UNP Q9IGQ6
F	66	HIS	-	expression tag	UNP Q9IGQ6
F	67	HIS	-	expression tag	UNP Q9IGQ6
F	68	HIS	-	expression tag	UNP Q9IGQ6
F	69	HIS	-	expression tag	UNP Q9IGQ6
F	70	HIS	-	expression tag	UNP Q9IGQ6
F	71	HIS	-	expression tag	UNP Q9IGQ6
F	72	SER	-	expression tag	UNP Q9IGQ6
F	73	LEU	-	expression tag	UNP Q9IGQ6
F	74	VAL	-	expression tag	UNP Q9IGQ6
F	75	PRO	-	expression tag	UNP Q9IGQ6
F	76	ARG	-	expression tag	UNP Q9IGQ6
F	77	GLY	-	expression tag	UNP Q9IGQ6
F	78	SER	-	expression tag	UNP Q9IGQ6
F	79	PRO	-	expression tag	UNP Q9IGQ6
F	80	SER	-	expression tag	UNP Q9IGQ6
F	81	ARG	-	expression tag	UNP Q9IGQ6
G	66	HIS	-	expression tag	UNP Q9IGQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	67	HIS	-	expression tag	UNP Q9IGQ6
G	68	HIS	-	expression tag	UNP Q9IGQ6
G	69	HIS	-	expression tag	UNP Q9IGQ6
G	70	HIS	-	expression tag	UNP Q9IGQ6
G	71	HIS	-	expression tag	UNP Q9IGQ6
G	72	SER	-	expression tag	UNP Q9IGQ6
G	73	LEU	-	expression tag	UNP Q9IGQ6
G	74	VAL	-	expression tag	UNP Q9IGQ6
G	75	PRO	-	expression tag	UNP Q9IGQ6
G	76	ARG	-	expression tag	UNP Q9IGQ6
G	77	GLY	-	expression tag	UNP Q9IGQ6
G	78	SER	-	expression tag	UNP Q9IGQ6
G	79	PRO	-	expression tag	UNP Q9IGQ6
G	80	SER	-	expression tag	UNP Q9IGQ6
G	81	ARG	-	expression tag	UNP Q9IGQ6
H	66	HIS	-	expression tag	UNP Q9IGQ6
H	67	HIS	-	expression tag	UNP Q9IGQ6
H	68	HIS	-	expression tag	UNP Q9IGQ6
H	69	HIS	-	expression tag	UNP Q9IGQ6
H	70	HIS	-	expression tag	UNP Q9IGQ6
H	71	HIS	-	expression tag	UNP Q9IGQ6
H	72	SER	-	expression tag	UNP Q9IGQ6
H	73	LEU	-	expression tag	UNP Q9IGQ6
H	74	VAL	-	expression tag	UNP Q9IGQ6
H	75	PRO	-	expression tag	UNP Q9IGQ6
H	76	ARG	-	expression tag	UNP Q9IGQ6
H	77	GLY	-	expression tag	UNP Q9IGQ6
H	78	SER	-	expression tag	UNP Q9IGQ6
H	79	PRO	-	expression tag	UNP Q9IGQ6
H	80	SER	-	expression tag	UNP Q9IGQ6
H	81	ARG	-	expression tag	UNP Q9IGQ6

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

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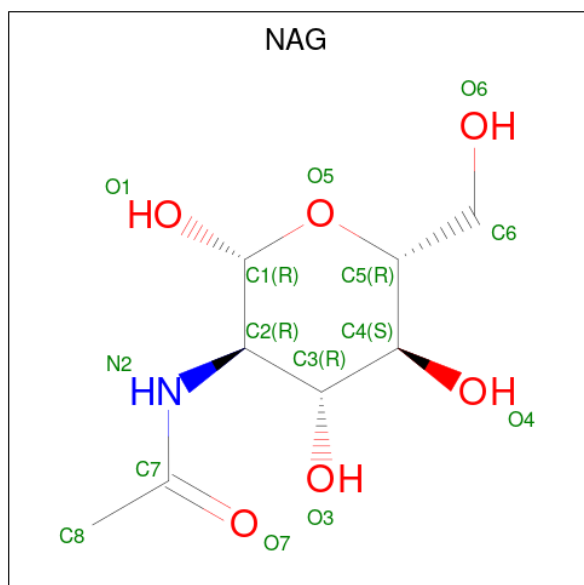
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	L	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	N	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	O	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	M	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

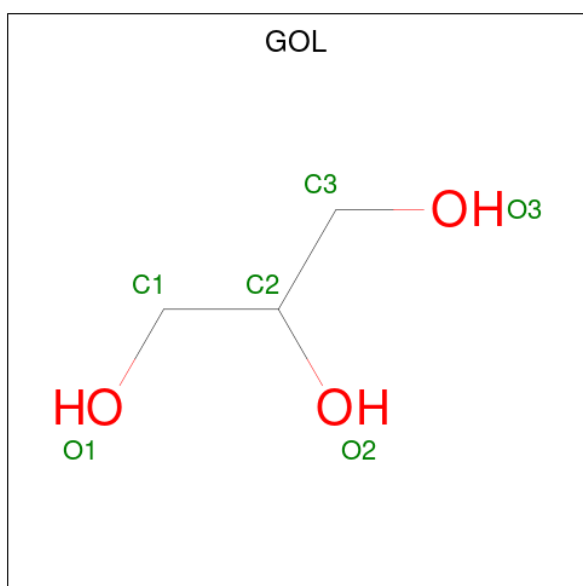
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Ca 3 3	0	0
5	B	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	E	3	Total	Ca	0	0
			3	3		
5	F	2	Total	Ca	0	0
			2	2		
5	G	2	Total	Ca	0	0
			2	2		
5	H	2	Total	Ca	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

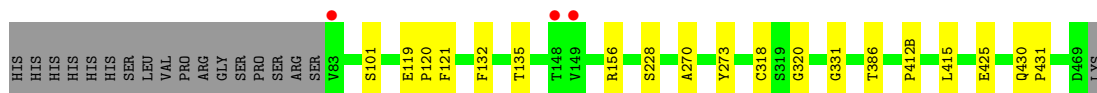
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	168	Total 168	O 168	0	0
7	B	190	Total 190	O 190	0	0
7	C	181	Total 181	O 181	0	0
7	D	143	Total 143	O 143	0	0
7	E	180	Total 180	O 180	0	0
7	F	166	Total 166	O 166	0	0
7	G	175	Total 175	O 175	0	0
7	H	142	Total 142	O 142	0	0

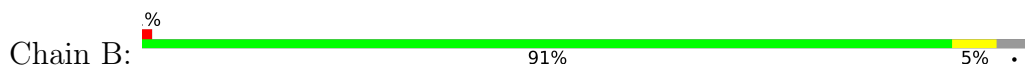
3 Residue-property plots

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

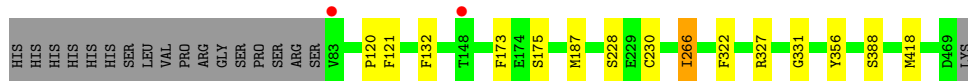
- Molecule 1: Neuraminidase



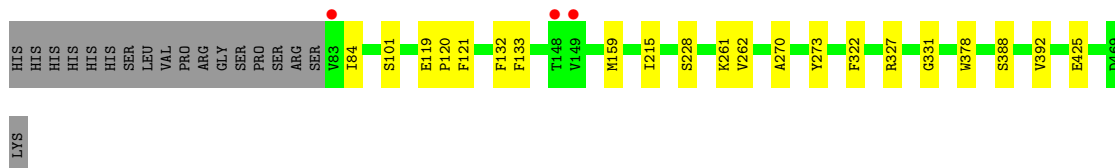
- Molecule 1: Neuraminidase



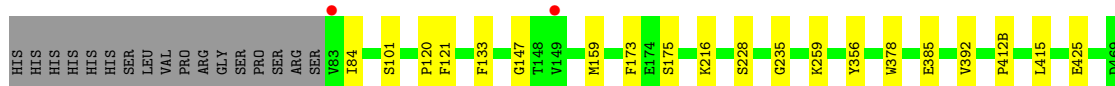
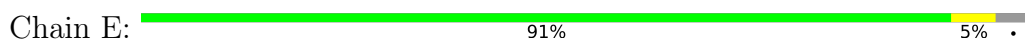
- Molecule 1: Neuraminidase



- Molecule 1: Neuraminidase



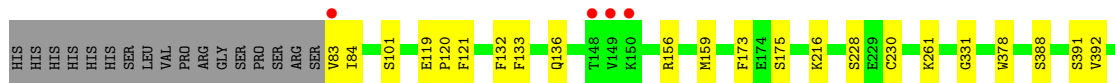
- Molecule 1: Neuraminidase



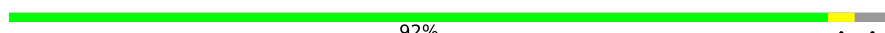
LYS

- Molecule 1: Neuraminidase

Chain F:  89% 7%



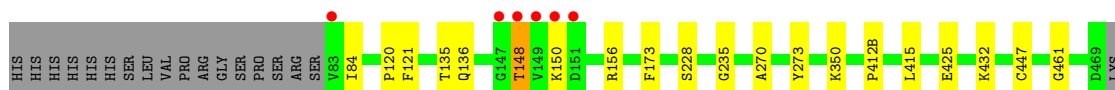
- Molecule 1: Neuraminidase

Chain G:  92%

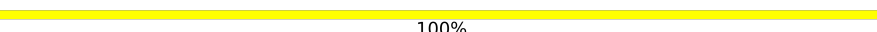


- Molecule 1: Neuraminidase

Chain H:  91% 5%



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

Chain I:  100%



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

Chain J:  67% 33%



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

Chain L:  33% 67%



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

Chain N:  67% 33%

MAG1
MAG2
FUC3

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

Chain O:  33% 67%

MAG1
MAG2
FUC3

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
FUC2

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.68Å 148.19Å 127.17Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	38.96 – 2.15 38.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.96-2.15) 99.0 (38.96-2.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.186 , 0.215 0.176 , 0.206	Depositor DCC
R_{free} test set	7244 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25633	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, FUC, 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	0.36	1/3047 (0.0%)	0.57	0/4146
1	B	0.36	0/3055	0.56	0/4153
1	C	0.36	0/3057	0.55	0/4157
1	D	0.35	1/3062 (0.0%)	0.54	0/4163
1	E	0.35	0/3064	0.58	0/4165
1	F	0.36	1/3050 (0.0%)	0.56	0/4148
1	G	0.34	0/3050	0.56	0/4148
1	H	0.33	0/3048	0.57	0/4144
All	All	0.35	3/24433 (0.0%)	0.56	0/33224

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	119	GLU	C-N	-7.21	1.17	1.33
1	A	119	GLU	C-N	-5.40	1.21	1.33
1	D	119	GLU	C-N	-5.29	1.21	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2963	0	2764	10	0
1	B	2971	0	2790	11	0
1	C	2973	0	2793	9	0
1	D	2975	0	2794	11	0
1	E	2977	0	2797	12	0
1	F	2966	0	2779	14	0
1	G	2966	0	2779	8	0
1	H	2967	0	2785	11	0
2	I	38	0	34	0	0
2	J	38	0	34	0	0
2	L	38	0	34	1	0
2	N	38	0	34	0	0
2	O	38	0	34	0	0
3	K	24	0	22	1	0
3	M	24	0	22	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
4	E	28	0	26	0	0
4	F	28	0	26	0	0
4	G	28	0	26	0	0
4	H	28	0	26	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	1	0
6	D	6	0	8	0	0
6	E	6	0	8	2	0
6	G	6	0	8	0	0
6	H	6	0	8	0	0
7	A	168	0	0	0	0
7	B	190	0	0	1	0
7	C	181	0	0	0	0
7	D	143	0	0	0	0
7	E	180	0	0	0	0
7	F	166	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	175	0	0	0	0
7	H	142	0	0	0	0
All	All	25633	0	22764	78	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 2.

All (78) 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:C:356:TYR:CD2	6:C:508:GOL:H11	2.39	0.57
1:H:84:ILE:HD12	1:H:235:GLY:HA2	1.89	0.55
2:L:2:NAG:H5	2:L:3:FUC:H61	1.89	0.54
1:E:173:PHE:CZ	1:F:101:SER:HA	2.45	0.51
1:A:430[A]:GLN:OE1	1:A:431:PRO:HA	2.10	0.51
1:B:318:CYS:HG	1:B:336:CYS:HG	1.58	0.50
1:F:136:GLN:NE2	1:F:156:ARG:HD2	2.27	0.50
1:H:136:GLN:HG3	1:H:148:THR:HG22	1.93	0.50
1:F:121:PHE:CG	1:F:228:SER:HA	2.47	0.49
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.94	0.49
1:D:331:GLY:O	1:D:388:SER:HB3	2.13	0.49
1:G:116:VAL:HG21	1:G:145:SER:HB2	1.95	0.48
1:H:412(B):PRO:HB3	1:H:415:LEU:O	2.13	0.48
1:E:120:PRO:HD2	1:E:425:GLU:HB2	1.96	0.48
1:D:215:ILE:HD11	1:D:262:VAL:HG21	1.96	0.47
1:D:133:PHE:CZ	1:D:159:MET:HB2	2.50	0.47
1:F:120:PRO:HA	1:F:132:PHE:O	2.15	0.47
1:D:270:ALA:HB1	1:D:273:TYR:HB2	1.96	0.47
1:B:120:PRO:HD2	1:B:425:GLU:HB2	1.96	0.47
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.96	0.46
1:E:216:LYS:HE2	1:F:453:THR:O	2.16	0.46
1:E:412(B):PRO:HB3	1:E:415:LEU:O	2.15	0.46
1:C:120:PRO:HA	1:C:132:PHE:O	2.16	0.45
1:A:121:PHE:CG	1:A:228:SER:HA	2.50	0.45
1:G:322:PHE:HB2	1:G:327:ARG:HD2	1.99	0.45
1:E:356:TYR:CD2	6:E:508:GOL:H12	2.52	0.45
1:B:133:PHE:CZ	1:B:159:MET:HB2	2.52	0.45
1:A:120:PRO:HD2	1:A:425:GLU:HB2	1.99	0.45
1:B:121:PHE:CG	1:B:228:SER:HA	2.50	0.45
1:D:120:PRO:HA	1:D:132:PHE:O	2.17	0.45
1:D:121:PHE:CG	1:D:228:SER:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:PHE:CG	1:E:228:SER:HA	2.53	0.44
1:G:418:MET:HE2	1:G:418:MET:HB2	1.88	0.44
1:G:120:PRO:HD2	1:G:425:GLU:HB2	1.99	0.44
1:A:120:PRO:HA	1:A:132:PHE:O	2.18	0.44
1:D:120:PRO:HD2	1:D:425:GLU:HB2	2.00	0.44
1:F:412(B):PRO:HB3	1:F:415:LEU:O	2.18	0.44
1:H:228:SER:HB3	1:H:350:LYS:HE2	1.99	0.44
1:H:135:THR:O	1:H:156:ARG:HA	2.18	0.44
1:F:216:LYS:HE2	1:G:453:THR:O	2.18	0.43
1:F:84:ILE:HD13	1:F:84:ILE:HA	1.91	0.43
1:H:121:PHE:CG	1:H:228:SER:HA	2.54	0.43
1:A:318:CYS:O	1:A:386:THR:HA	2.19	0.43
1:E:356:TYR:CE2	6:E:508:GOL:H12	2.54	0.43
1:C:331:GLY:O	1:C:388:SER:HB3	2.18	0.43
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.19	0.42
1:B:270:ALA:HB1	1:B:273:TYR:HB2	2.01	0.42
1:C:266:ILE:HD13	1:C:266:ILE:HA	1.89	0.42
1:G:155:TYR:CE1	1:H:461:GLY:HA3	2.54	0.42
1:E:378:TRP:HB3	1:E:392:VAL:HB	2.00	0.42
1:C:173:PHE:CZ	1:D:101:SER:HA	2.54	0.42
1:E:84:ILE:HD12	1:E:235:GLY:HA2	2.01	0.41
1:F:173:PHE:CZ	1:G:101:SER:HA	2.55	0.41
1:F:331:GLY:O	1:F:388:SER:HB3	2.20	0.41
1:F:378:TRP:HB3	1:F:392:VAL:HB	2.03	0.41
1:E:101:SER:HA	1:H:173:PHE:CZ	2.55	0.41
1:E:133:PHE:CZ	1:E:159:MET:HB2	2.55	0.41
1:F:133:PHE:CZ	1:F:159:MET:HB2	2.56	0.41
1:H:120:PRO:HD2	1:H:425:GLU:HB2	2.03	0.41
1:H:270:ALA:HB1	1:H:273:TYR:HB2	2.02	0.41
3:K:1:NAG:H62	3:K:2:FUC:H2	1.95	0.41
1:C:121:PHE:CG	1:C:228:SER:HA	2.56	0.41
1:A:101:SER:HA	1:B:173:PHE:CZ	2.56	0.41
1:A:135:THR:O	1:A:156:ARG:HA	2.21	0.41
1:C:322:PHE:HB2	1:C:327:ARG:HD2	2.02	0.41
1:C:418:MET:HE2	1:C:418:MET:HB2	1.97	0.41
1:D:84:ILE:HD13	1:D:84:ILE:HA	1.93	0.41
1:E:216:LYS:HD2	1:F:452:ASP:HB3	2.03	0.41
1:F:120:PRO:HD2	1:F:425:GLU:HB2	2.03	0.41
1:B:84:ILE:HD13	1:B:84:ILE:HA	1.89	0.41
1:B:150:LYS:HG2	7:B:758:HOH:O	2.21	0.41
1:B:194:ILE:HG12	1:B:203:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:PHE:HB2	1:D:327:ARG:HD2	2.04	0.40
1:B:412(B):PRO:HB3	1:B:415:LEU:O	2.22	0.40
1:C:187:MET:HE2	1:C:187:MET:HB3	1.81	0.40
1:D:378:TRP:HB3	1:D:392:VAL:HB	2.04	0.40
1:G:211:ILE:HD12	1:H:447:CYS:HB2	2.03	0.40
1:A:320:GLY:HA3	1:A:331:GLY:O	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	385/404 (95%)	367 (95%)	18 (5%)	0	100	100
1	B	385/404 (95%)	369 (96%)	16 (4%)	0	100	100
1	C	385/404 (95%)	368 (96%)	17 (4%)	0	100	100
1	D	386/404 (96%)	367 (95%)	19 (5%)	0	100	100
1	E	386/404 (96%)	368 (95%)	17 (4%)	1 (0%)	36	34
1	F	385/404 (95%)	365 (95%)	20 (5%)	0	100	100
1	G	385/404 (95%)	369 (96%)	16 (4%)	0	100	100
1	H	384/404 (95%)	366 (95%)	17 (4%)	1 (0%)	36	34
All	All	3081/3232 (95%)	2939 (95%)	140 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	147	GLY
1	H	148	THR

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	328/348 (94%)	328 (100%)	0	100	100
1	B	331/348 (95%)	329 (99%)	2 (1%)	78	84
1	C	331/348 (95%)	328 (99%)	3 (1%)	70	77
1	D	332/348 (95%)	331 (100%)	1 (0%)	86	91
1	E	333/348 (96%)	330 (99%)	3 (1%)	70	77
1	F	330/348 (95%)	325 (98%)	5 (2%)	57	64
1	G	330/348 (95%)	327 (99%)	3 (1%)	70	77
1	H	330/348 (95%)	328 (99%)	2 (1%)	78	84
All	All	2645/2784 (95%)	2626 (99%)	19 (1%)	76	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	VAL
1	B	230	CYS
1	C	175	SER
1	C	230	CYS
1	C	266	ILE
1	D	261	LYS
1	E	175	SER
1	E	259	LYS
1	E	385	GLU
1	F	83	VAL
1	F	175	SER
1	F	230	CYS
1	F	261	LYS
1	F	391	SER
1	G	83	VAL
1	G	117	ILE
1	G	230	CYS
1	H	150	LYS
1	H	432	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	C	136	GLN
1	C	309	ASN
1	C	329	ASN
1	D	325	ASN
1	E	136	GLN
1	E	344	ASN
1	E	435	ASN
1	F	430	GLN
1	H	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 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	0.86	2 (14%)	17,19,21	0.67	0
2	NAG	I	2	2	14,14,15	0.86	2 (14%)	17,19,21	0.49	0
2	FUC	I	3	2	10,10,11	1.19	1 (10%)	14,14,16	1.38	3 (21%)
2	NAG	J	1	1,2	14,14,15	0.47	0	17,19,21	0.62	0
2	NAG	J	2	2	14,14,15	0.41	0	17,19,21	0.53	0
2	FUC	J	3	2	10,10,11	0.93	1 (10%)	14,14,16	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	1,3	14,14,15	0.38	0	17,19,21	1.54	3 (17%)
3	FUC	K	2	3	10,10,11	1.75	2 (20%)	14,14,16	1.56	3 (21%)
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	0.69	0
2	NAG	L	2	2	14,14,15	0.37	0	17,19,21	0.53	0
2	FUC	L	3	2	10,10,11	0.94	0	14,14,16	1.07	0
3	NAG	M	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	0.55	0
3	FUC	M	2	3	10,10,11	1.26	1 (10%)	14,14,16	1.38	3 (21%)
2	NAG	N	1	1,2	14,14,15	0.76	1 (7%)	17,19,21	0.62	0
2	NAG	N	2	2	14,14,15	0.45	0	17,19,21	0.48	0
2	FUC	N	3	2	10,10,11	0.92	0	14,14,16	0.93	0
2	NAG	O	1	1,2	14,14,15	0.41	0	17,19,21	0.40	0
2	NAG	O	2	2	14,14,15	0.84	1 (7%)	17,19,21	0.53	0
2	FUC	O	3	2	10,10,11	1.18	1 (10%)	14,14,16	1.58	3 (21%)

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	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	FUC	I	3	2	-	-	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	FUC	J	3	2	-	-	0/1/1/1
3	NAG	K	1	1,3	-	6/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	FUC	L	3	2	-	-	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	M	2	3	-	-	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	FUC	N	3	2	-	-	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	FUC	O	3	2	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	FUC	C2-C3	3.65	1.58	1.52
3	K	2	FUC	C4-C3	3.07	1.60	1.52
2	O	2	NAG	C1-C2	2.70	1.56	1.52
3	M	1	NAG	C1-C2	2.55	1.55	1.52
2	O	3	FUC	C4-C3	2.51	1.58	1.52
2	N	1	NAG	O5-C1	-2.48	1.39	1.43
2	I	2	NAG	O5-C1	2.39	1.47	1.43
2	I	1	NAG	O5-C1	-2.29	1.39	1.43
3	M	2	FUC	O5-C1	-2.16	1.40	1.43
2	I	3	FUC	C1-C2	2.15	1.57	1.52
2	J	3	FUC	C1-C2	2.07	1.57	1.52
2	I	1	NAG	C1-C2	2.05	1.55	1.52
2	I	2	NAG	C1-C2	2.03	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C2-N2-C7	4.64	129.12	122.90
2	O	3	FUC	C3-C4-C5	3.36	114.92	109.81
2	O	3	FUC	O5-C5-C4	2.99	114.94	109.55
3	K	2	FUC	C1-O5-C5	2.98	119.99	112.97
3	K	1	NAG	C1-O5-C5	2.78	115.91	112.19
3	K	2	FUC	O5-C5-C4	2.69	114.39	109.55
3	M	2	FUC	C3-C4-C5	2.61	113.78	109.81
2	O	3	FUC	C2-C3-C4	2.39	115.07	110.86
2	I	3	FUC	C1-O5-C5	2.38	118.57	112.97
3	K	2	FUC	C2-C3-C4	2.37	115.03	110.86
3	M	2	FUC	C2-C3-C4	2.29	114.89	110.86
2	I	3	FUC	O2-C2-C1	2.19	114.25	109.22
2	I	3	FUC	O5-C5-C4	2.15	113.42	109.55
3	K	1	NAG	C1-C2-N2	2.14	113.80	110.43
3	M	2	FUC	O2-C2-C1	2.02	113.84	109.22

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6

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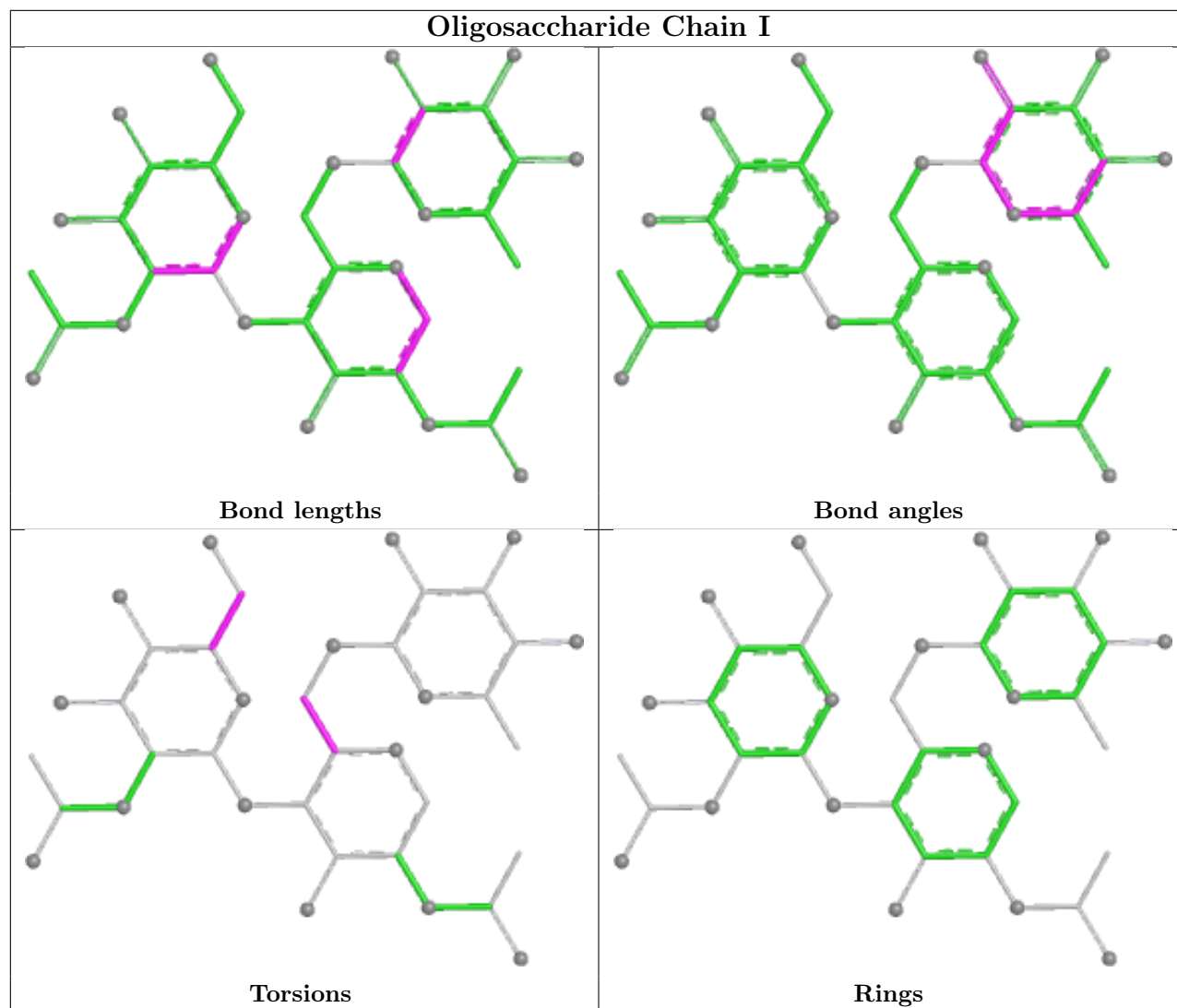
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7

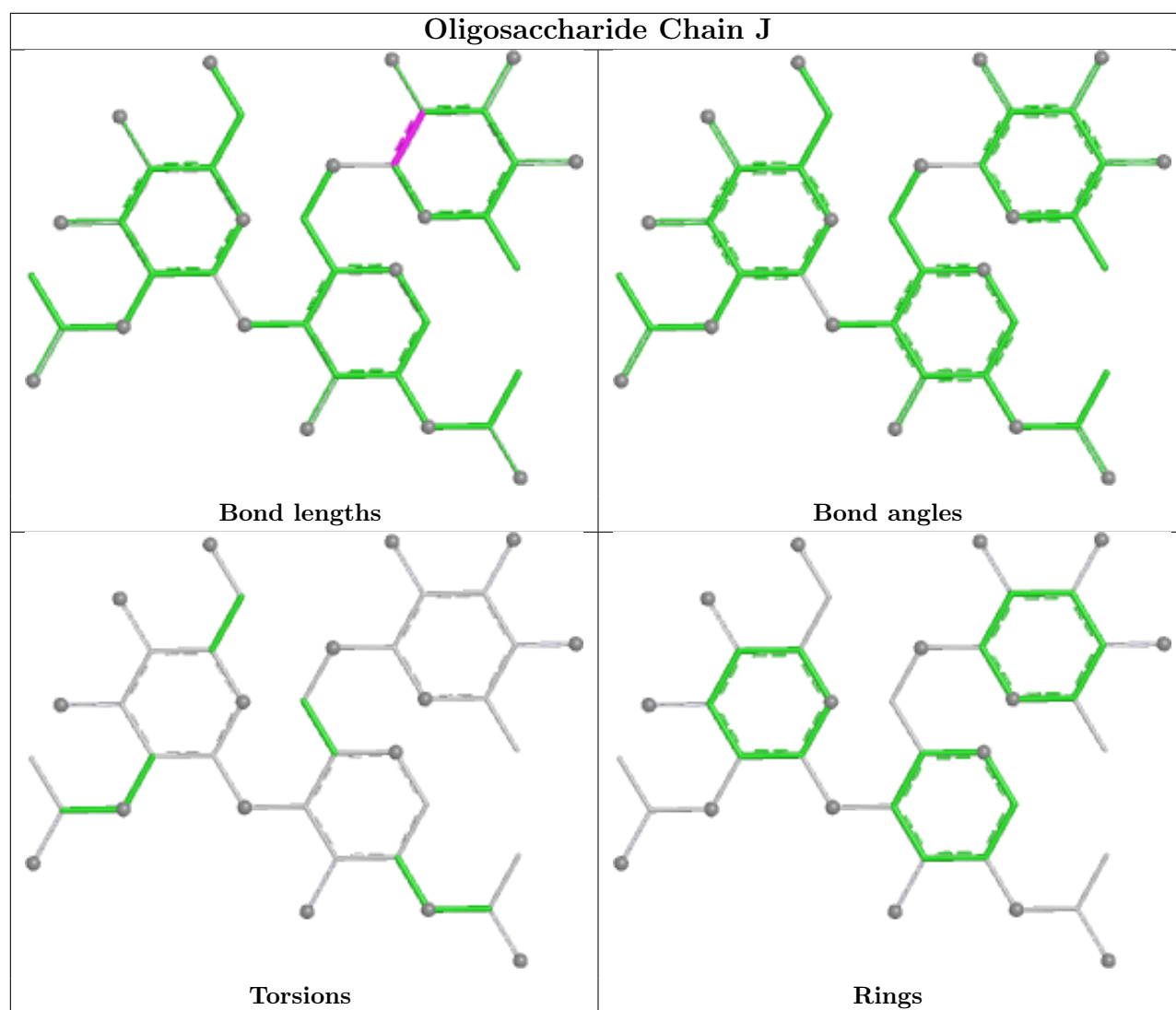
There are no ring outliers.

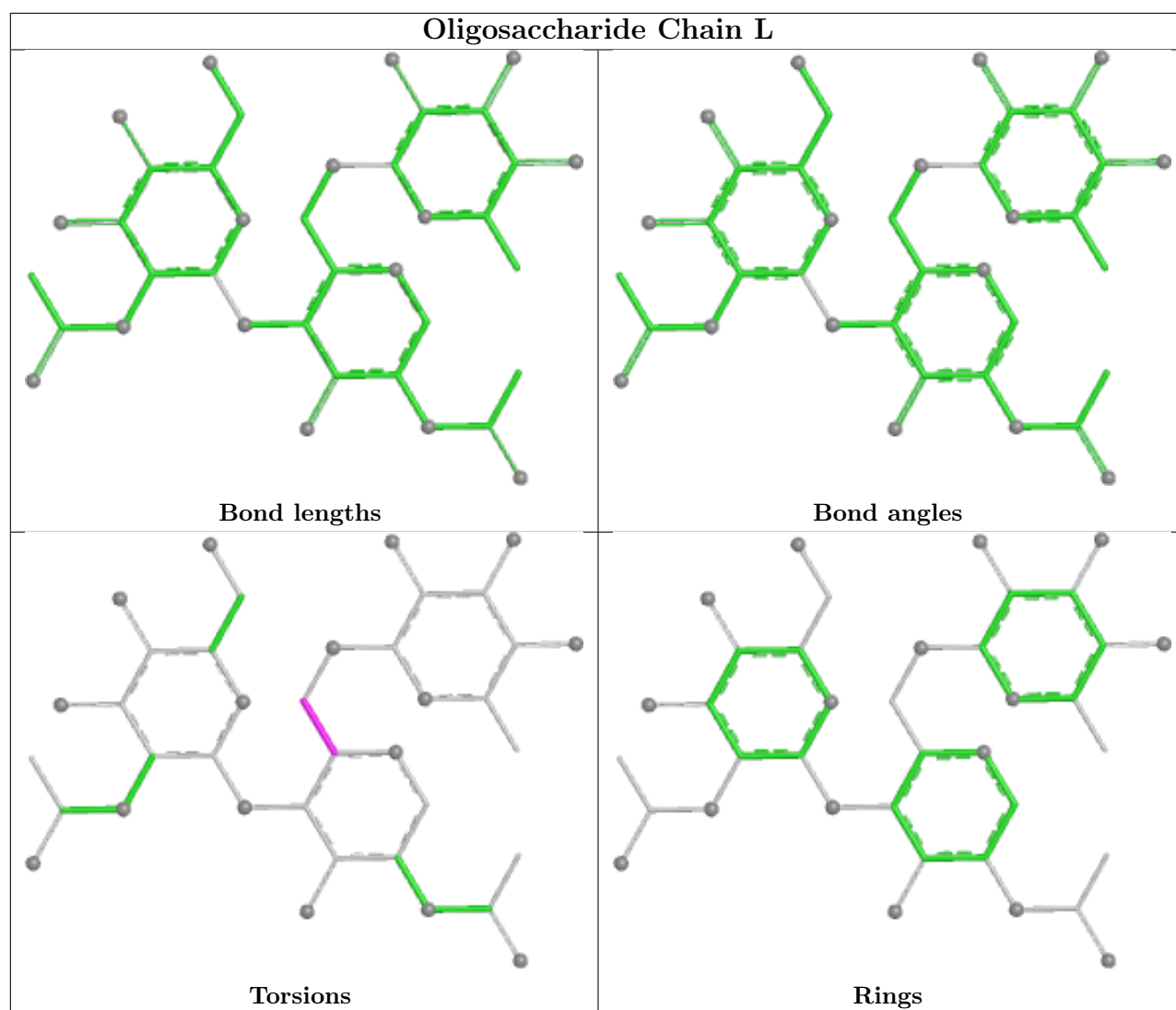
4 monomers are involved in 2 short contacts:

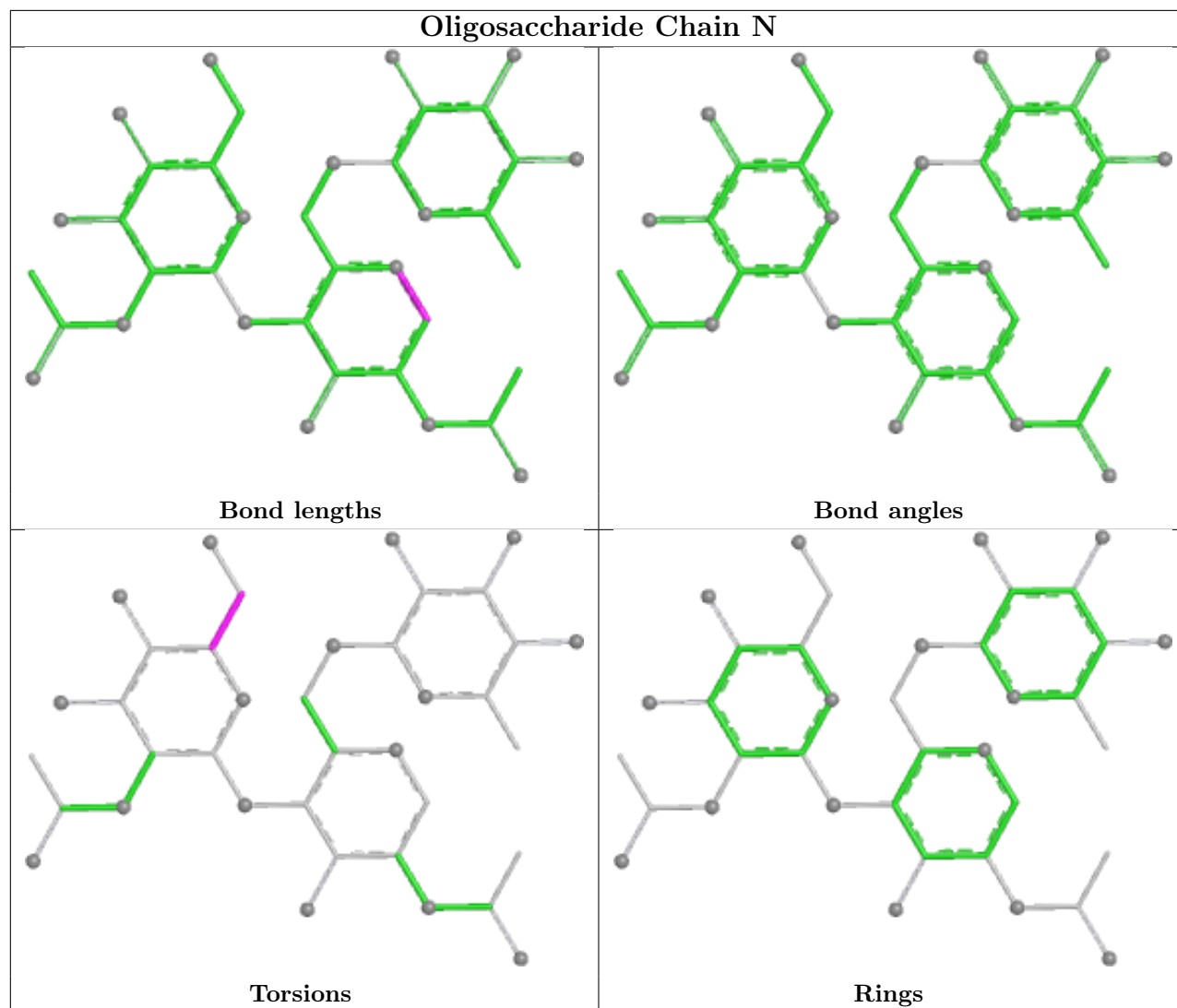
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2	FUC	1	0
3	K	1	NAG	1	0
2	L	2	NAG	1	0
2	L	3	FUC	1	0

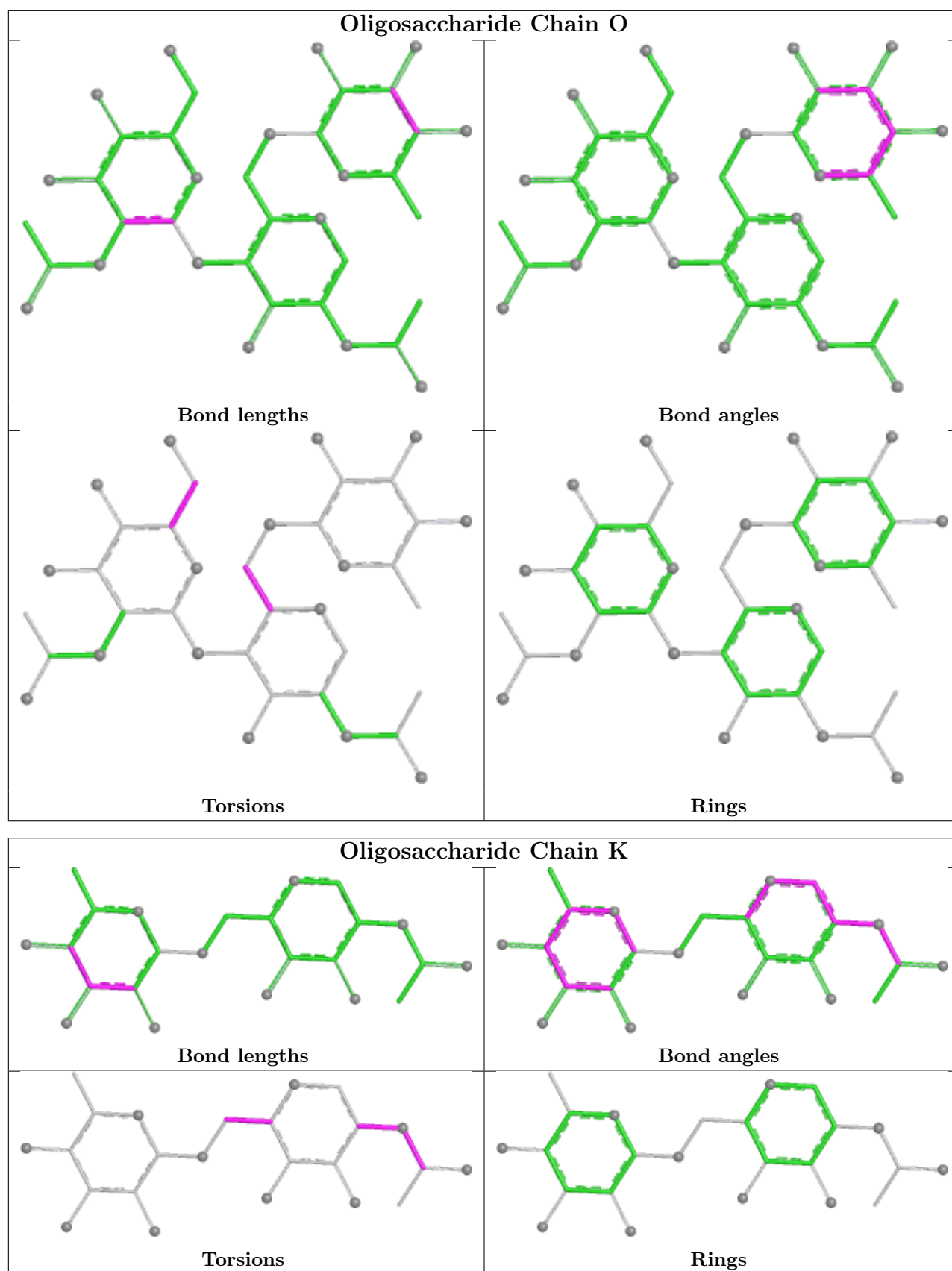
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

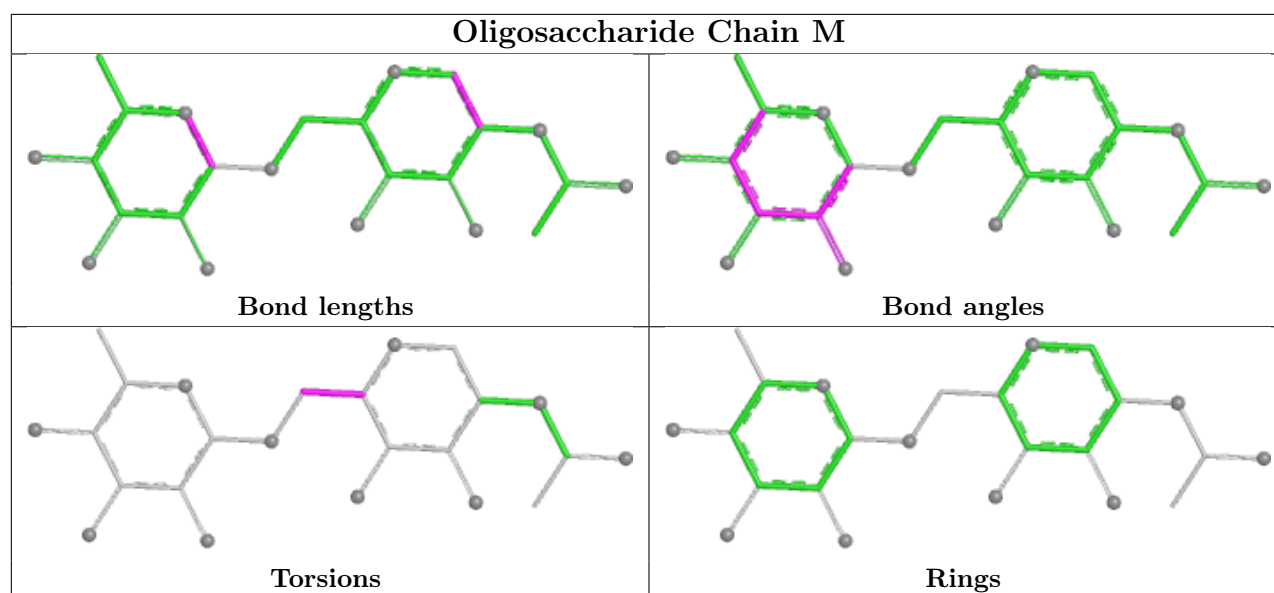












5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 18 are monoatomic - leaving 23 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	A	503	1	14,14,15	0.61	0	17,19,21	1.35	3 (17%)
6	GOL	D	507	-	5,5,5	0.42	0	5,5,5	0.41	0
6	GOL	A	506	-	5,5,5	0.31	0	5,5,5	0.35	0
4	NAG	A	502	1	14,14,15	0.94	1 (7%)	17,19,21	0.70	1 (5%)
4	NAG	A	501	1	14,14,15	1.52	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	E	501	1	14,14,15	0.84	2 (14%)	17,19,21	0.84	1 (5%)
4	NAG	D	502	1	14,14,15	0.51	0	17,19,21	0.45	0
4	NAG	G	505	1	14,14,15	0.94	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	C	501	1	14,14,15	0.85	1 (7%)	17,19,21	0.86	1 (5%)
6	GOL	G	508	-	5,5,5	0.31	0	5,5,5	0.80	0
4	NAG	H	505	1	14,14,15	0.96	2 (14%)	17,19,21	0.62	1 (5%)
4	NAG	F	504	1	14,14,15	0.47	0	17,19,21	0.47	0
4	NAG	E	502	1	14,14,15	0.86	1 (7%)	17,19,21	0.95	1 (5%)
6	GOL	E	508	-	5,5,5	0.39	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	H	508	-	5,5,5	0.39	0	5,5,5	0.37	0
4	NAG	G	501	1	14,14,15	0.56	0	17,19,21	0.75	1 (5%)
6	GOL	C	508	-	5,5,5	0.36	0	5,5,5	0.78	0
4	NAG	C	505	1	14,14,15	0.84	1 (7%)	17,19,21	0.81	1 (5%)
4	NAG	B	501	1	14,14,15	0.87	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	D	501	1	14,14,15	0.85	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	B	505	1	14,14,15	0.77	1 (7%)	17,19,21	0.77	0
4	NAG	F	501	1	14,14,15	0.43	0	17,19,21	1.50	1 (5%)
4	NAG	H	504	1	14,14,15	0.85	1 (7%)	17,19,21	0.72	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	A	503	1	-	3/6/23/26	0/1/1/1
6	GOL	D	507	-	-	2/4/4/4	-
6	GOL	A	506	-	-	4/4/4/4	-
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	E	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	502	1	-	2/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	C	501	1	-	3/6/23/26	0/1/1/1
6	GOL	G	508	-	-	2/4/4/4	-
4	NAG	H	505	1	-	1/6/23/26	0/1/1/1
4	NAG	F	504	1	-	1/6/23/26	0/1/1/1
4	NAG	E	502	1	-	4/6/23/26	0/1/1/1
6	GOL	E	508	-	-	2/4/4/4	-
6	GOL	H	508	-	-	2/4/4/4	-
4	NAG	G	501	1	-	1/6/23/26	0/1/1/1
6	GOL	C	508	-	-	4/4/4/4	-
4	NAG	C	505	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	505	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	501	1	-	2/6/23/26	0/1/1/1
4	NAG	H	504	1	-	3/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	O5-C1	5.27	1.52	1.43
4	A	502	NAG	O5-C1	3.20	1.49	1.43
4	G	505	NAG	O5-C1	3.18	1.49	1.43
4	E	502	NAG	O5-C1	2.90	1.48	1.43
4	C	505	NAG	O5-C1	2.87	1.48	1.43
4	D	501	NAG	O5-C1	2.74	1.48	1.43
4	C	501	NAG	O5-C1	2.71	1.48	1.43
4	H	505	NAG	O5-C1	2.65	1.48	1.43
4	H	504	NAG	O5-C1	2.51	1.47	1.43
4	B	505	NAG	O5-C1	2.50	1.47	1.43
4	B	501	NAG	O5-C1	2.33	1.47	1.43
4	H	505	NAG	C1-C2	2.30	1.55	1.52
4	E	501	NAG	O5-C1	2.20	1.47	1.43
4	E	501	NAG	C1-C2	2.14	1.55	1.52
4	B	501	NAG	C1-C2	2.14	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	NAG	C1-O5-C5	5.66	119.77	112.19
4	E	502	NAG	C1-O5-C5	3.59	116.99	112.19
4	D	501	NAG	C1-O5-C5	3.43	116.78	112.19
4	B	501	NAG	C1-O5-C5	3.38	116.72	112.19
4	A	501	NAG	C1-O5-C5	3.16	116.42	112.19
4	A	503	NAG	C3-C4-C5	3.13	115.91	110.23
4	G	505	NAG	C1-O5-C5	3.06	116.28	112.19
4	C	501	NAG	C1-O5-C5	3.03	116.24	112.19
4	A	503	NAG	C4-C3-C2	2.69	114.95	111.02
4	G	501	NAG	C1-O5-C5	2.65	115.74	112.19
4	E	501	NAG	C1-O5-C5	2.58	115.64	112.19
4	C	505	NAG	C1-O5-C5	2.52	115.56	112.19
4	H	504	NAG	C1-O5-C5	2.38	115.38	112.19
4	A	502	NAG	C1-O5-C5	2.38	115.38	112.19
4	H	505	NAG	C1-O5-C5	2.09	114.99	112.19
4	A	503	NAG	C2-N2-C7	2.07	125.67	122.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	NAG	C1-C2-N2-C7
6	C	508	GOL	O1-C1-C2-C3
6	E	508	GOL	O1-C1-C2-O2
6	E	508	GOL	O1-C1-C2-C3
6	G	508	GOL	O1-C1-C2-C3
4	C	501	NAG	C4-C5-C6-O6
4	A	503	NAG	O5-C5-C6-O6
4	B	501	NAG	C4-C5-C6-O6
4	D	502	NAG	C4-C5-C6-O6
4	D	501	NAG	O5-C5-C6-O6
4	E	502	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	E	501	NAG	C4-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	A	503	NAG	C4-C5-C6-O6
4	E	502	NAG	C4-C5-C6-O6
4	H	504	NAG	C4-C5-C6-O6
4	E	502	NAG	C8-C7-N2-C2
4	E	502	NAG	O7-C7-N2-C2
4	D	502	NAG	O5-C5-C6-O6
6	C	508	GOL	O1-C1-C2-O2
4	H	505	NAG	O5-C5-C6-O6
4	E	501	NAG	O5-C5-C6-O6
4	H	504	NAG	O5-C5-C6-O6
6	A	506	GOL	O1-C1-C2-C3
6	C	508	GOL	C1-C2-C3-O3
6	D	507	GOL	O1-C1-C2-C3
4	D	501	NAG	C4-C5-C6-O6
4	F	501	NAG	O5-C5-C6-O6
4	C	505	NAG	O5-C5-C6-O6
6	G	508	GOL	O1-C1-C2-O2
4	G	501	NAG	O5-C5-C6-O6
6	C	508	GOL	O2-C2-C3-O3
6	D	507	GOL	O1-C1-C2-O2
6	A	506	GOL	O1-C1-C2-O2
6	H	508	GOL	O1-C1-C2-C3
4	B	505	NAG	C4-C5-C6-O6
6	A	506	GOL	O2-C2-C3-O3
6	A	506	GOL	C1-C2-C3-O3
4	B	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C1-C2-N2-C7
4	B	505	NAG	C1-C2-N2-C7
4	C	501	NAG	C1-C2-N2-C7
4	C	505	NAG	C1-C2-N2-C7
4	F	501	NAG	C1-C2-N2-C7
4	F	504	NAG	C1-C2-N2-C7
4	H	504	NAG	C1-C2-N2-C7
6	H	508	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	508	GOL	2	0
6	C	508	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	119:GLU	C	120:PRO	N	1.17

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	386/404 (95%)	-0.48	3 (0%) 82 84	15, 23, 35, 57	1 (0%)
1	B	386/404 (95%)	-0.42	3 (0%) 82 84	14, 24, 36, 55	1 (0%)
1	C	386/404 (95%)	-0.47	2 (0%) 87 89	15, 23, 36, 59	1 (0%)
1	D	386/404 (95%)	-0.35	3 (0%) 82 84	14, 27, 39, 65	2 (0%)
1	E	386/404 (95%)	-0.45	2 (0%) 87 89	14, 23, 36, 50	2 (0%)
1	F	386/404 (95%)	-0.43	4 (1%) 79 82	13, 24, 39, 58	1 (0%)
1	G	386/404 (95%)	-0.46	2 (0%) 87 89	15, 24, 37, 55	1 (0%)
1	H	386/404 (95%)	-0.29	6 (1%) 70 74	16, 27, 41, 64	0
All	All	3088/3232 (95%)	-0.42	25 (0%) 82 84	13, 24, 38, 65	9 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	VAL	4.5
1	H	83	VAL	4.5
1	H	150	LYS	4.4
1	B	83	VAL	4.3
1	C	83	VAL	4.3
1	H	149	VAL	4.1
1	F	83	VAL	4.1
1	E	83	VAL	3.9
1	D	83	VAL	3.8
1	H	151	ASP	3.7
1	G	83	VAL	3.6
1	H	148	THR	3.4
1	C	148	THR	3.2
1	B	149	VAL	3.2
1	A	148	THR	3.2
1	A	149	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	149	VAL	3.0
1	D	148	THR	3.0
1	F	148	THR	2.8
1	D	149	VAL	2.6
1	F	150	LYS	2.6
1	G	149	VAL	2.4
1	B	148	THR	2.3
1	H	147	GLY	2.3
1	E	149	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

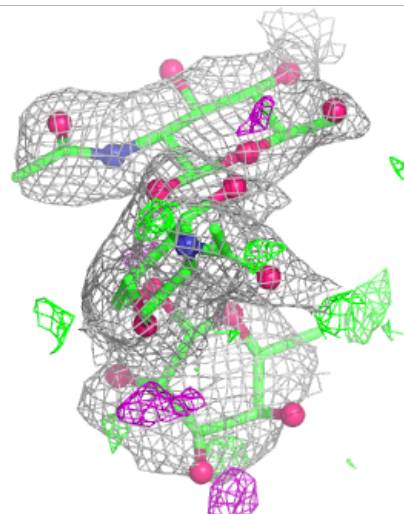
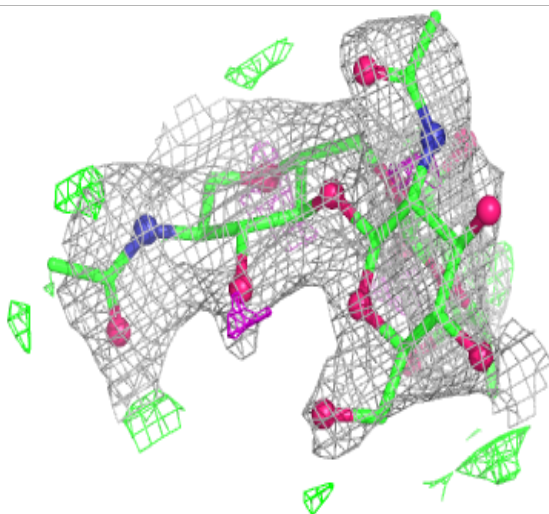
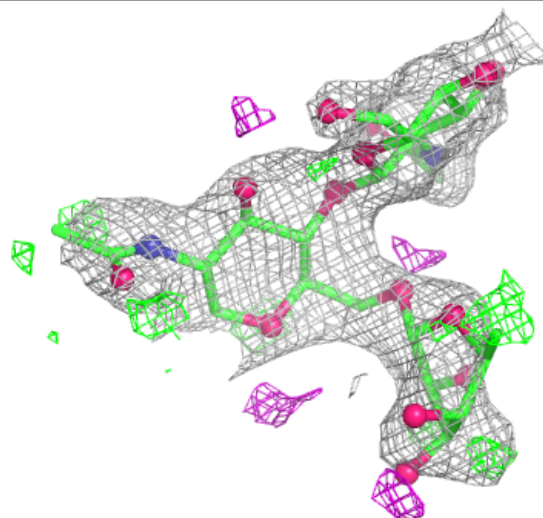
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	I	3	10/11	0.59	0.23	70,75,78,79	0
3	NAG	K	1	14/15	0.61	0.17	55,63,74,78	0
3	FUC	K	2	10/11	0.61	0.20	76,80,83,83	0
2	NAG	O	2	14/15	0.63	0.17	66,75,80,80	0
2	NAG	N	2	14/15	0.68	0.19	72,76,81,82	0
2	NAG	I	2	14/15	0.68	0.15	65,74,77,78	0
3	FUC	M	2	10/11	0.70	0.20	72,76,79,84	0
2	FUC	O	3	10/11	0.73	0.16	64,69,70,72	0
2	NAG	L	2	14/15	0.73	0.15	70,76,80,82	0
3	NAG	M	1	14/15	0.76	0.16	49,60,66,72	0
2	NAG	J	2	14/15	0.76	0.13	65,73,75,76	0
2	NAG	I	1	14/15	0.77	0.15	48,59,69,71	0
2	FUC	L	3	10/11	0.78	0.16	64,71,72,72	0
2	FUC	J	3	10/11	0.81	0.14	61,64,65,65	0
2	NAG	L	1	14/15	0.82	0.13	49,59,73,73	0
2	NAG	J	1	14/15	0.82	0.13	45,54,63,70	0
2	NAG	O	1	14/15	0.83	0.13	48,58,70,71	0
2	FUC	N	3	10/11	0.84	0.13	53,56,58,58	0
2	NAG	N	1	14/15	0.92	0.10	39,48,57,66	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.

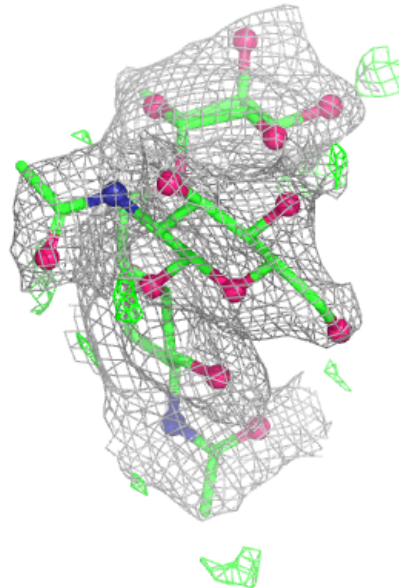
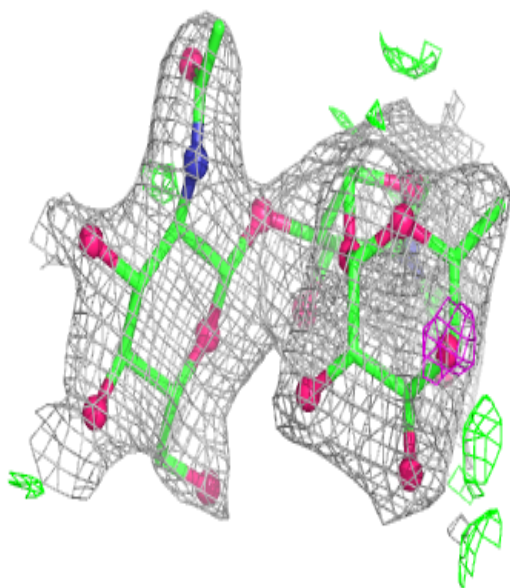
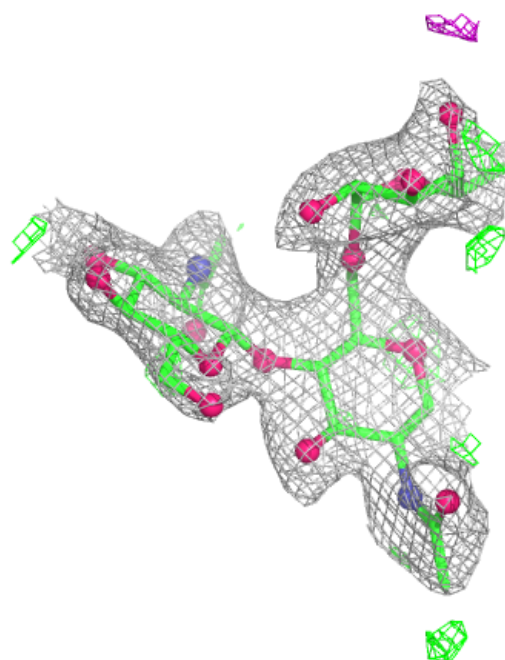
Electron density around Chain I:

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



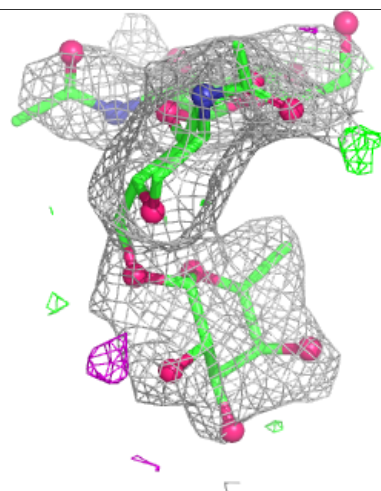
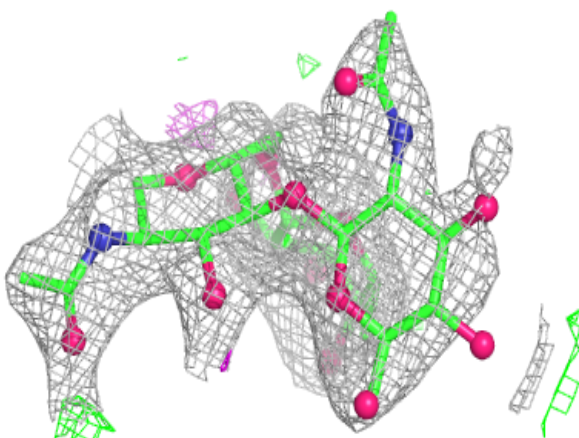
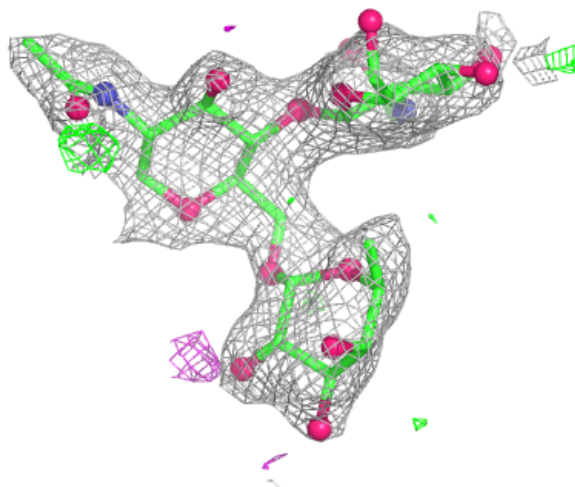
Electron density around Chain J:

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



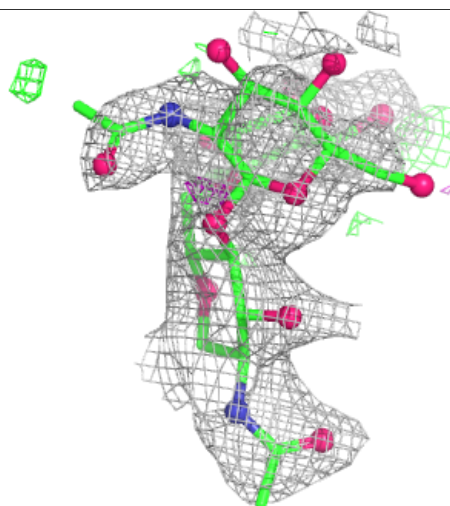
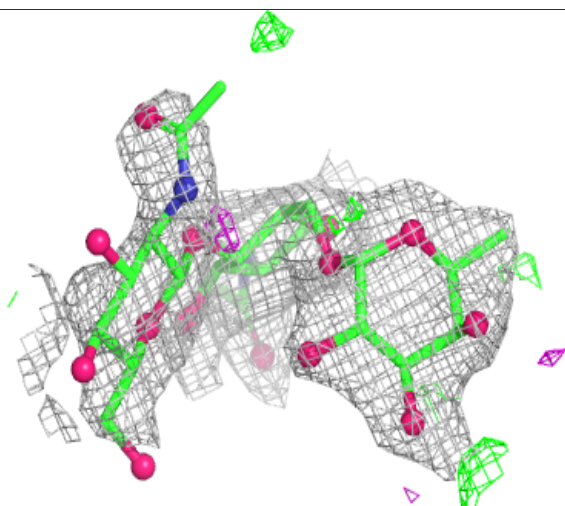
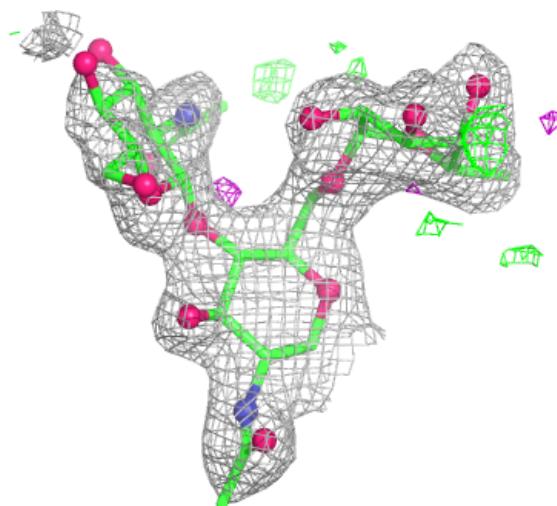
Electron density around Chain L:

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



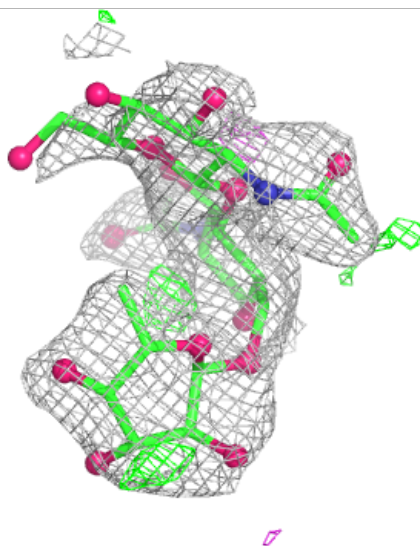
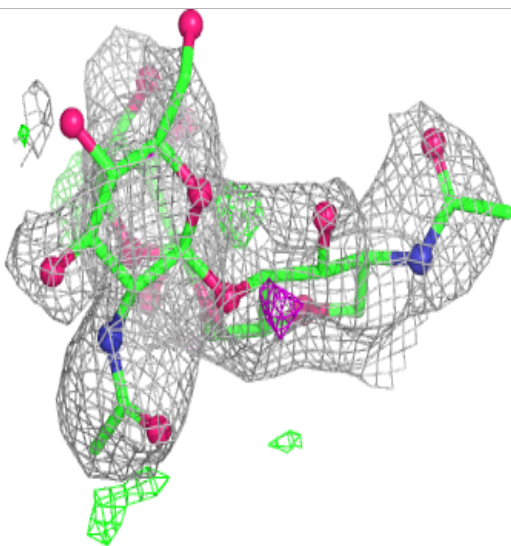
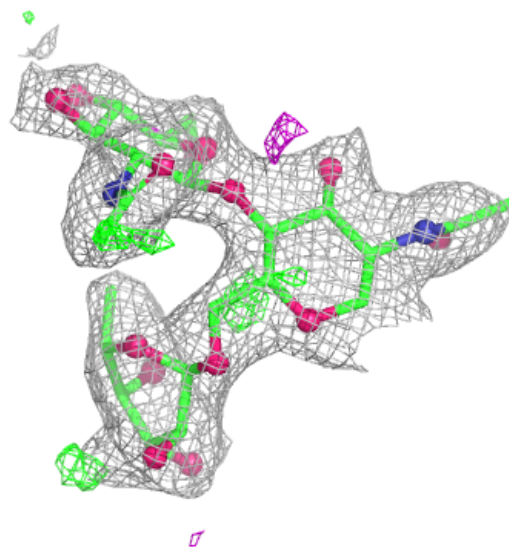
Electron density around Chain N:

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



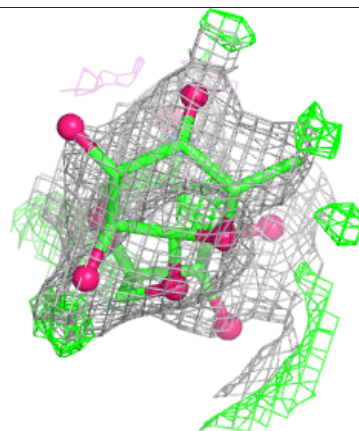
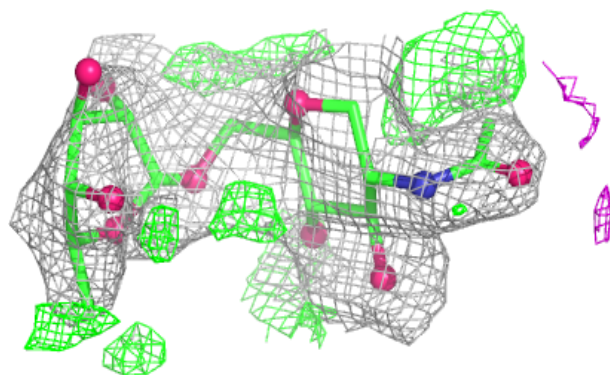
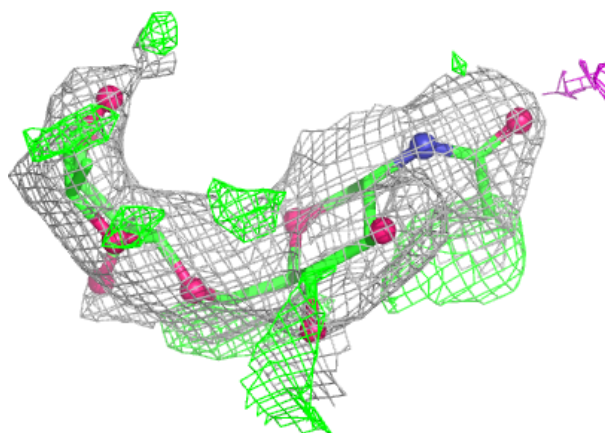
Electron density around Chain O:

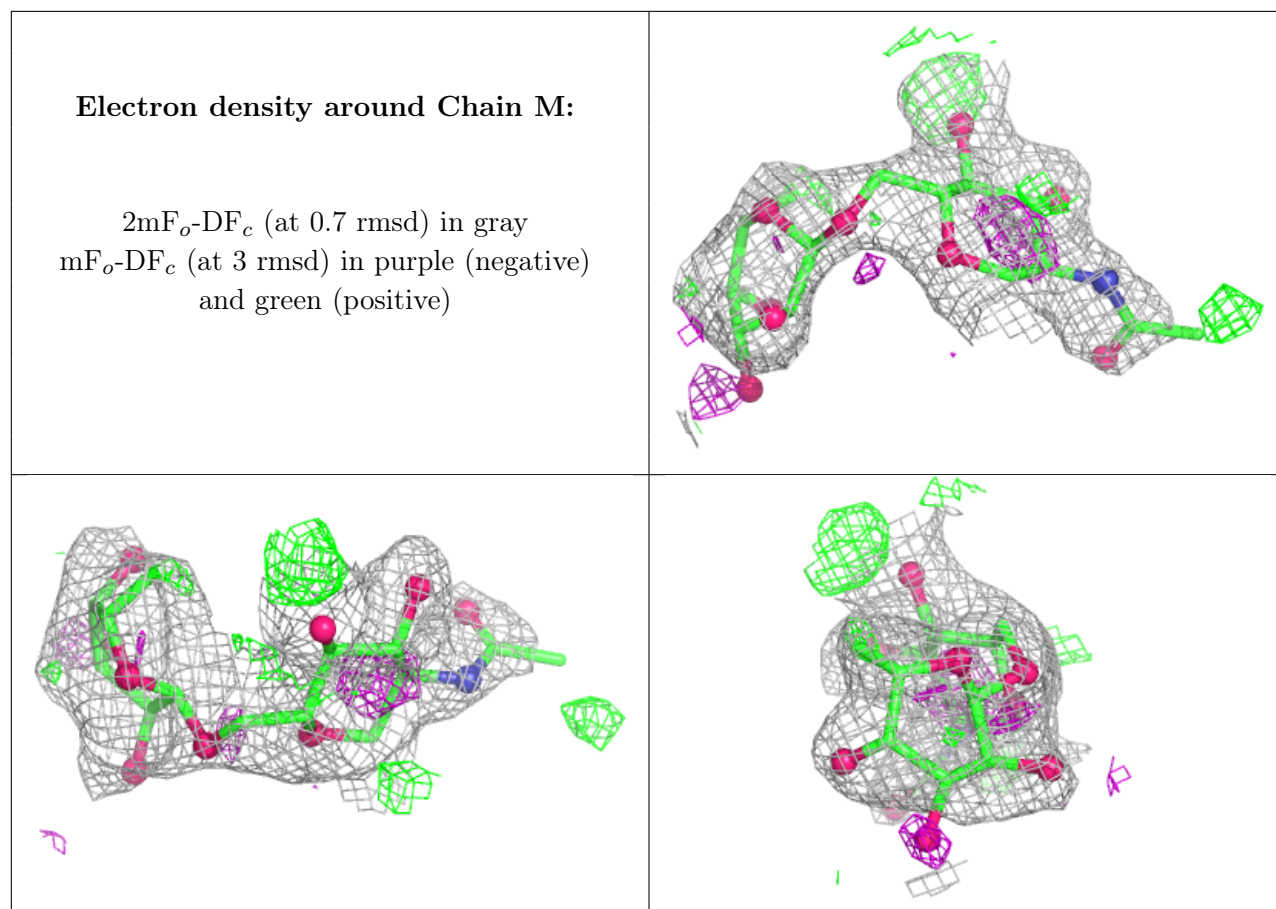
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	504	14/15	0.53	0.22	61,68,74,76	0
4	NAG	E	502	14/15	0.57	0.18	57,66,69,71	0
4	NAG	A	502	14/15	0.60	0.21	65,76,82,84	0
4	NAG	A	503	14/15	0.60	0.21	57,66,71,73	0
4	NAG	H	505	14/15	0.61	0.19	58,68,72,73	0
4	NAG	C	505	14/15	0.63	0.18	62,76,80,80	0
4	NAG	B	505	14/15	0.67	0.17	53,61,68,69	0
4	NAG	G	501	14/15	0.68	0.16	55,63,72,72	0
4	NAG	G	505	14/15	0.72	0.17	50,60,63,63	0
4	NAG	D	502	14/15	0.72	0.15	58,65,71,71	0
4	NAG	A	501	14/15	0.74	0.16	45,50,55,55	0
4	NAG	B	501	14/15	0.74	0.17	51,59,69,74	0
4	NAG	E	501	14/15	0.77	0.16	47,54,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	501	14/15	0.77	0.15	49,54,62,63	0
4	NAG	C	501	14/15	0.81	0.15	47,54,64,66	0
4	NAG	H	504	14/15	0.82	0.14	51,57,66,67	0
4	NAG	D	501	14/15	0.82	0.14	47,58,65,65	0
6	GOL	D	507	6/6	0.88	0.14	44,48,53,56	0
6	GOL	G	508	6/6	0.90	0.10	35,38,38,40	0
6	GOL	E	508	6/6	0.92	0.12	39,47,50,53	0
6	GOL	A	506	6/6	0.92	0.13	41,43,50,54	0
6	GOL	C	508	6/6	0.93	0.11	41,44,44,47	0
6	GOL	H	508	6/6	0.93	0.11	44,47,48,48	0
5	CA	E	509	1/1	0.95	0.08	69,69,69,69	1
5	CA	A	507	1/1	0.96	0.08	60,60,60,60	0
5	CA	F	506	1/1	0.98	0.03	29,29,29,29	0
5	CA	H	506	1/1	0.98	0.03	25,25,25,25	0
5	CA	B	507	1/1	0.99	0.02	23,23,23,23	0
5	CA	G	506	1/1	0.99	0.03	25,25,25,25	0
5	CA	C	506	1/1	0.99	0.02	21,21,21,21	0
5	CA	H	507	1/1	0.99	0.04	34,34,34,34	0
5	CA	C	507	1/1	0.99	0.03	23,23,23,23	0
5	CA	D	506	1/1	0.99	0.03	35,35,35,35	0
5	CA	E	506	1/1	0.99	0.02	20,20,20,20	0
5	CA	E	507	1/1	0.99	0.02	26,26,26,26	0
5	CA	B	506	1/1	0.99	0.02	20,20,20,20	0
5	CA	F	505	1/1	0.99	0.02	21,21,21,21	0
5	CA	A	504	1/1	1.00	0.02	16,16,16,16	0
5	CA	D	505	1/1	1.00	0.01	27,27,27,27	0
5	CA	A	505	1/1	1.00	0.02	28,28,28,28	0
5	CA	G	507	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.