



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 01:15 PM EDT

PDB ID : 4GEZ
Title : Structure of a neuraminidase-like protein from A/bat/Guatemala/164/2009
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on : 2012-08-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

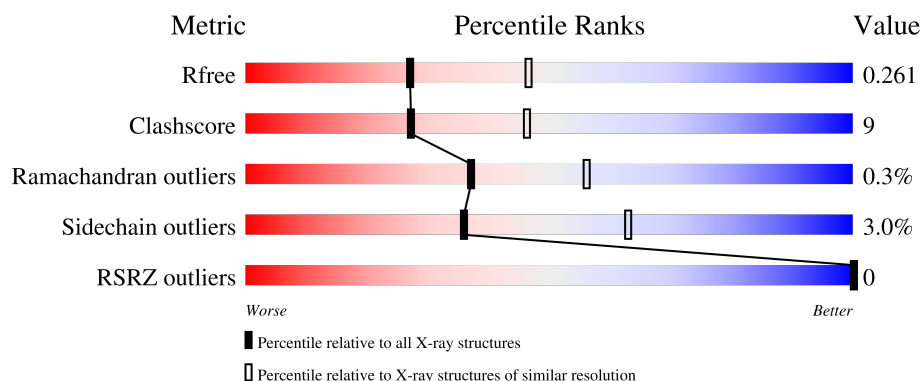
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




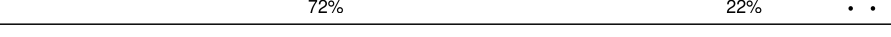

The reported resolution of this entry is 2.50 Å.

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.





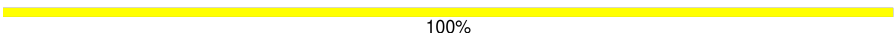

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	378	
1	B	378	
1	C	378	
1	D	378	
1	E	378	

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Mol	Chain	Length	Quality of chain
1	F	378	 79%16% . .
1	G	378	 75%20% . .
1	H	378	 79%17% . .
1	I	378	 79%16% . .
1	J	378	 71%24% . .
1	K	378	 71%24% . .
1	L	378	 71%25% . .
2	M	2	 50%50%
2	O	2	 100%
2	Q	2	 100%
3	N	3	 33%67%
3	P	3	 33%67%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35035 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	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	B	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	C	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	D	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	E	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	F	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	G	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	H	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	I	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	J	363	Total	C	N	O	S	0	0	0
			2832	1784	484	544	20			
1	K	364	Total	C	N	O	S	0	0	0
			2846	1795	486	545	20			
1	L	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	expression tag	UNP H6QM85
A	66	SER	-	expression tag	UNP H6QM85
A	67	GLY	-	expression tag	UNP H6QM85
A	68	ASP	-	expression tag	UNP H6QM85
A	69	SER	-	expression tag	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP H6QM85
A	71	SER	-	expression tag	UNP H6QM85
A	72	PRO	-	expression tag	UNP H6QM85
A	73	GLY	-	expression tag	UNP H6QM85
B	65	GLY	-	expression tag	UNP H6QM85
B	66	SER	-	expression tag	UNP H6QM85
B	67	GLY	-	expression tag	UNP H6QM85
B	68	ASP	-	expression tag	UNP H6QM85
B	69	SER	-	expression tag	UNP H6QM85
B	70	GLY	-	expression tag	UNP H6QM85
B	71	SER	-	expression tag	UNP H6QM85
B	72	PRO	-	expression tag	UNP H6QM85
B	73	GLY	-	expression tag	UNP H6QM85
C	65	GLY	-	expression tag	UNP H6QM85
C	66	SER	-	expression tag	UNP H6QM85
C	67	GLY	-	expression tag	UNP H6QM85
C	68	ASP	-	expression tag	UNP H6QM85
C	69	SER	-	expression tag	UNP H6QM85
C	70	GLY	-	expression tag	UNP H6QM85
C	71	SER	-	expression tag	UNP H6QM85
C	72	PRO	-	expression tag	UNP H6QM85
C	73	GLY	-	expression tag	UNP H6QM85
D	65	GLY	-	expression tag	UNP H6QM85
D	66	SER	-	expression tag	UNP H6QM85
D	67	GLY	-	expression tag	UNP H6QM85
D	68	ASP	-	expression tag	UNP H6QM85
D	69	SER	-	expression tag	UNP H6QM85
D	70	GLY	-	expression tag	UNP H6QM85
D	71	SER	-	expression tag	UNP H6QM85
D	72	PRO	-	expression tag	UNP H6QM85
D	73	GLY	-	expression tag	UNP H6QM85
E	65	GLY	-	expression tag	UNP H6QM85
E	66	SER	-	expression tag	UNP H6QM85
E	67	GLY	-	expression tag	UNP H6QM85
E	68	ASP	-	expression tag	UNP H6QM85
E	69	SER	-	expression tag	UNP H6QM85
E	70	GLY	-	expression tag	UNP H6QM85
E	71	SER	-	expression tag	UNP H6QM85
E	72	PRO	-	expression tag	UNP H6QM85
E	73	GLY	-	expression tag	UNP H6QM85
F	65	GLY	-	expression tag	UNP H6QM85
F	66	SER	-	expression tag	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	GLY	-	expression tag	UNP H6QM85
F	68	ASP	-	expression tag	UNP H6QM85
F	69	SER	-	expression tag	UNP H6QM85
F	70	GLY	-	expression tag	UNP H6QM85
F	71	SER	-	expression tag	UNP H6QM85
F	72	PRO	-	expression tag	UNP H6QM85
F	73	GLY	-	expression tag	UNP H6QM85
G	65	GLY	-	expression tag	UNP H6QM85
G	66	SER	-	expression tag	UNP H6QM85
G	67	GLY	-	expression tag	UNP H6QM85
G	68	ASP	-	expression tag	UNP H6QM85
G	69	SER	-	expression tag	UNP H6QM85
G	70	GLY	-	expression tag	UNP H6QM85
G	71	SER	-	expression tag	UNP H6QM85
G	72	PRO	-	expression tag	UNP H6QM85
G	73	GLY	-	expression tag	UNP H6QM85
H	65	GLY	-	expression tag	UNP H6QM85
H	66	SER	-	expression tag	UNP H6QM85
H	67	GLY	-	expression tag	UNP H6QM85
H	68	ASP	-	expression tag	UNP H6QM85
H	69	SER	-	expression tag	UNP H6QM85
H	70	GLY	-	expression tag	UNP H6QM85
H	71	SER	-	expression tag	UNP H6QM85
H	72	PRO	-	expression tag	UNP H6QM85
H	73	GLY	-	expression tag	UNP H6QM85
I	65	GLY	-	expression tag	UNP H6QM85
I	66	SER	-	expression tag	UNP H6QM85
I	67	GLY	-	expression tag	UNP H6QM85
I	68	ASP	-	expression tag	UNP H6QM85
I	69	SER	-	expression tag	UNP H6QM85
I	70	GLY	-	expression tag	UNP H6QM85
I	71	SER	-	expression tag	UNP H6QM85
I	72	PRO	-	expression tag	UNP H6QM85
I	73	GLY	-	expression tag	UNP H6QM85
J	65	GLY	-	expression tag	UNP H6QM85
J	66	SER	-	expression tag	UNP H6QM85
J	67	GLY	-	expression tag	UNP H6QM85
J	68	ASP	-	expression tag	UNP H6QM85
J	69	SER	-	expression tag	UNP H6QM85
J	70	GLY	-	expression tag	UNP H6QM85
J	71	SER	-	expression tag	UNP H6QM85
J	72	PRO	-	expression tag	UNP H6QM85

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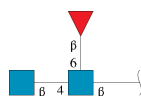
Chain	Residue	Modelled	Actual	Comment	Reference
J	73	GLY	-	expression tag	UNP H6QM85
K	65	GLY	-	expression tag	UNP H6QM85
K	66	SER	-	expression tag	UNP H6QM85
K	67	GLY	-	expression tag	UNP H6QM85
K	68	ASP	-	expression tag	UNP H6QM85
K	69	SER	-	expression tag	UNP H6QM85
K	70	GLY	-	expression tag	UNP H6QM85
K	71	SER	-	expression tag	UNP H6QM85
K	72	PRO	-	expression tag	UNP H6QM85
K	73	GLY	-	expression tag	UNP H6QM85
L	65	GLY	-	expression tag	UNP H6QM85
L	66	SER	-	expression tag	UNP H6QM85
L	67	GLY	-	expression tag	UNP H6QM85
L	68	ASP	-	expression tag	UNP H6QM85
L	69	SER	-	expression tag	UNP H6QM85
L	70	GLY	-	expression tag	UNP H6QM85
L	71	SER	-	expression tag	UNP H6QM85
L	72	PRO	-	expression tag	UNP H6QM85
L	73	GLY	-	expression tag	UNP H6QM85

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



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

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



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

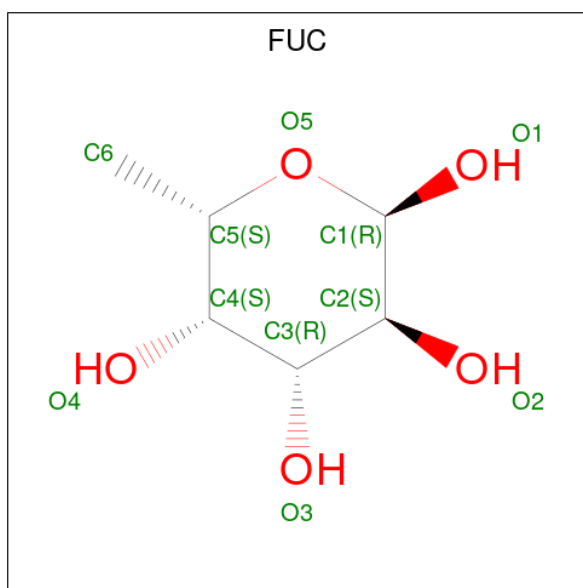
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		
4	H	1	Total	Ca	0	0
			1	1		
4	I	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		
4	K	1	Total	Ca	0	0
			1	1		
4	L	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		
7	B	54	Total	O	0	0
			54	54		
7	C	45	Total	O	0	0
			45	45		
7	D	46	Total	O	0	0
			46	46		
7	E	60	Total	O	0	0
			60	60		
7	F	41	Total	O	0	0
			41	41		
7	G	31	Total	O	0	0
			31	31		
7	H	15	Total	O	0	0
			15	15		
7	I	14	Total	O	0	0
			14	14		
7	J	25	Total	O	0	0
			25	25		

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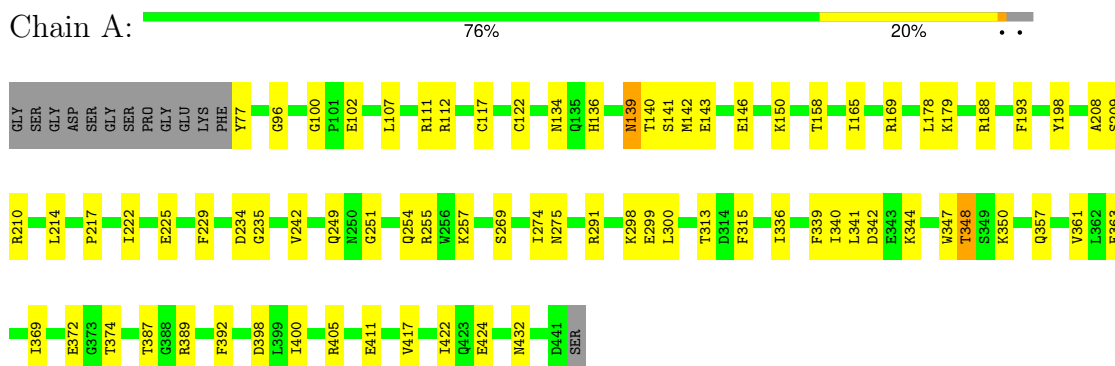
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	17	Total	O	0	0
			17	17		
7	L	8	Total	O	0	0
			8	8		

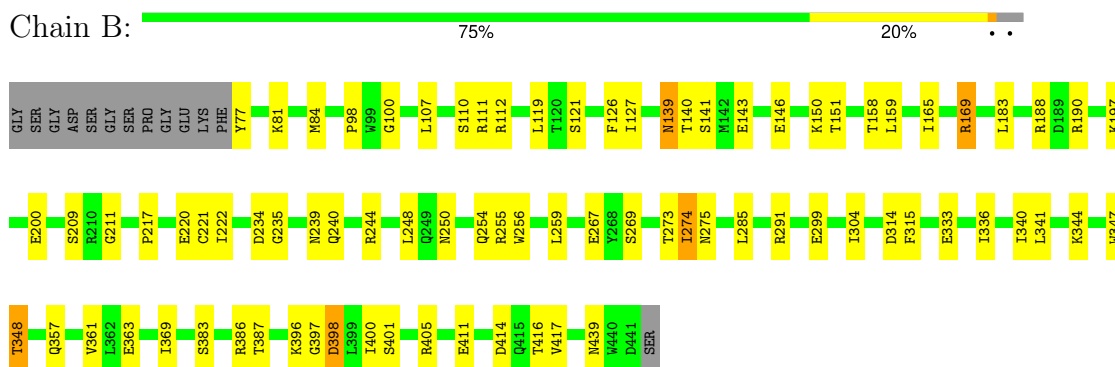
3 Residue-property plots

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.

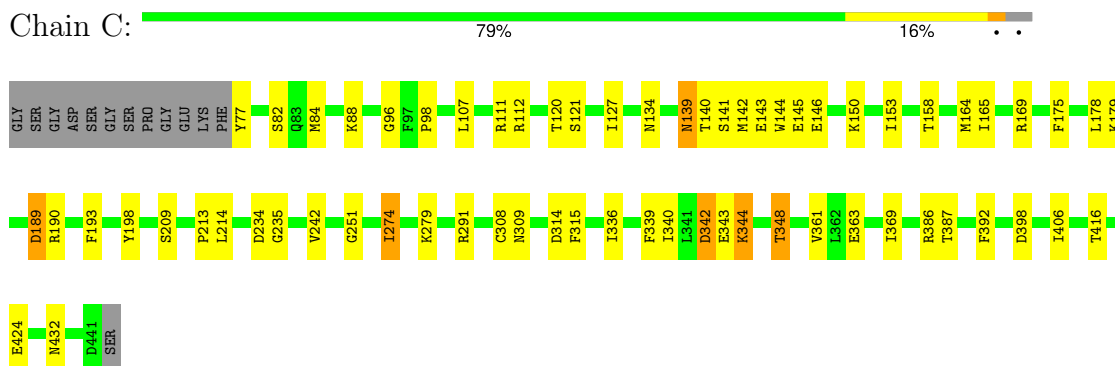
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase

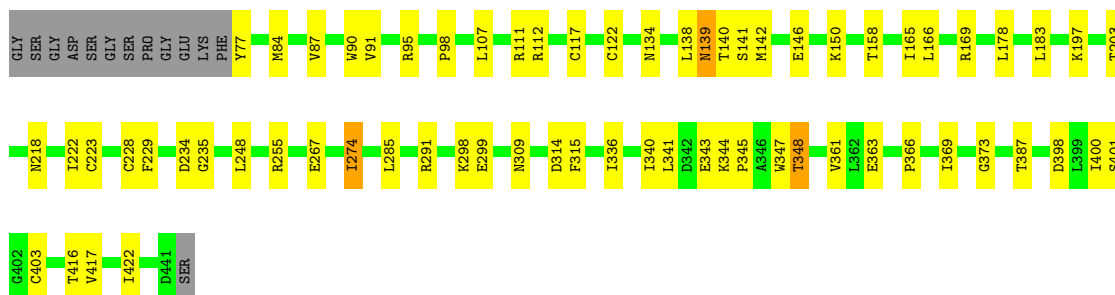


F175	GLY
K179	GLY
R188	ASP
M195	GLY
I196	SER
K197	PRO
Y198	GLY
G199	GLU
E200	LYS
S209	PHE
R210	W78
R219	R79
P217	A80
E220	K81
C221	M84
I222	H87
D234	K88
G235	G89
M239	W90
V242	R95
G251	P98
K257	W99
Q258	G100
L259	L107
K260	R111
T261	R112
S269	A113
T273	C117
I274	C122
K278	F125
K279	F126
R291	N139
F296	T140
L300	S141
N301	E145
D314	E146
F315	K150
I336	T151
F339	T158
I340	I165
I341	R169



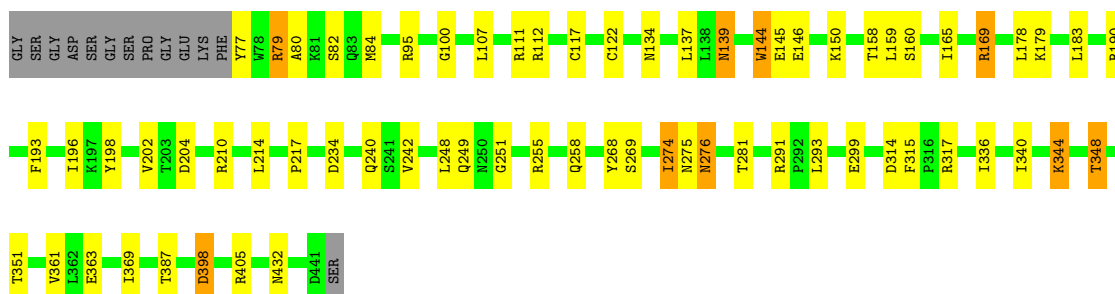
• Molecule 1: Neuraminidase

Chain H: 79% 17%



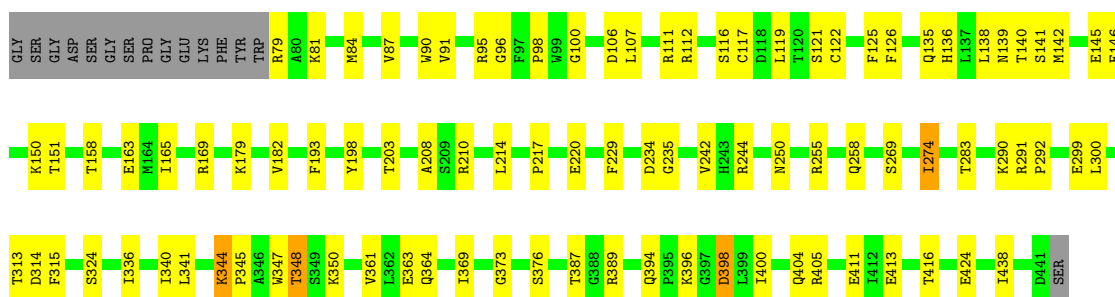
• Molecule 1: Neuraminidase

Chain I: 79% 16%



• Molecule 1: Neuraminidase

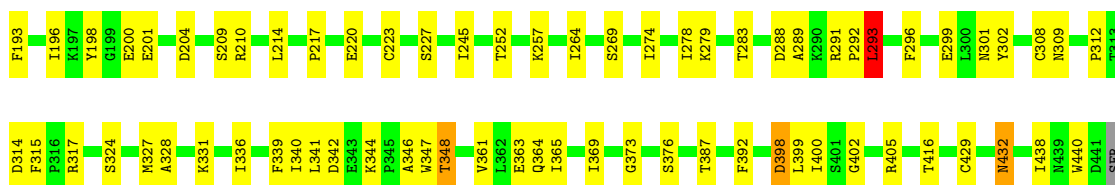
Chain J: 71% 24%



• Molecule 1: Neuraminidase

Chain K: 71% 24%





- Molecule 1: Neuraminidase

Chain L: 71% 25%



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

Chain M: 50% 50%



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

Chain O: 100%



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

Chain Q: 100%



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

Chain N: 33% 67%



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

Chain P:

33%

67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.33Å 113.33Å 114.31Å 81.47° 81.55° 67.72°	Depositor
Resolution (Å)	29.88 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.88-2.50) 91.9 (29.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.218 , 0.262 0.219 , 0.261	Depositor DCC
R_{free} test set	8258 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.369 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35035	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: FUL, NAG, CA, FUC

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	0.30	0/2926	0.53	0/3966
1	B	0.29	0/2926	0.51	0/3966
1	C	0.29	0/2926	0.52	0/3966
1	D	0.29	0/2926	0.53	0/3966
1	E	0.29	0/2926	0.52	0/3966
1	F	0.30	0/2926	0.53	0/3966
1	G	0.29	0/2926	0.52	0/3966
1	H	0.28	0/2926	0.54	0/3966
1	I	0.28	0/2926	0.54	0/3966
1	J	0.27	0/2897	0.52	0/3925
1	K	0.27	0/2913	0.53	1/3948 (0.0%)
1	L	0.27	0/2926	0.53	0/3966
All	All	0.29	0/35070	0.53	1/47533 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	J	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	293	LEU	CA-CB-CG	5.86	128.77	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	LYS	Peptide
1	C	344	LYS	Peptide
1	G	344	LYS	Peptide
1	I	344	LYS	Peptide
1	J	344	LYS	Peptide

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	2858	0	2762	49	2
1	B	2858	0	2764	54	2
1	C	2858	0	2764	51	1
1	D	2858	0	2765	67	0
1	E	2858	0	2763	47	2
1	F	2858	0	2764	43	1
1	G	2858	0	2764	51	1
1	H	2858	0	2764	38	0
1	I	2858	0	2763	51	0
1	J	2832	0	2746	64	0
1	K	2846	0	2755	60	0
1	L	2858	0	2763	60	0
2	M	24	0	22	0	0
2	O	24	0	22	0	1
2	Q	24	0	22	0	0
3	N	38	0	34	2	0
3	P	38	0	34	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	28	0	26	2	0
5	B	14	0	13	2	0
5	C	14	0	13	1	0
5	D	42	0	39	2	0
5	E	14	0	13	1	0
5	F	14	0	13	1	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	2	0
5	K	14	0	13	0	0
5	L	14	0	12	1	0
6	D	10	0	10	0	0
7	A	55	0	0	9	0
7	B	54	0	0	11	0
7	C	45	0	0	12	0
7	D	46	0	0	16	0
7	E	60	0	0	7	0
7	F	41	0	0	6	0
7	G	31	0	0	7	0
7	H	15	0	0	1	0
7	I	14	0	0	9	0
7	J	25	0	0	14	0
7	K	17	0	0	8	0
7	L	8	0	0	1	0
All	All	35035	0	33462	610	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 610 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:D:187:GLY:O	7:D:612:HOH:O	1.83	0.96
1:C:309:ASN:OD1	7:C:645:HOH:O	1.85	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLY:O	7:D:626:HOH:O	1.84	0.93
1:B:314:ASP:OD2	7:B:645:HOH:O	1.87	0.93
1:I:291:ARG:NH2	1:I:336:ILE:O	2.02	0.92

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:OE1	1:G:88:LYS:NZ[1_455]	2.12	0.08
1:A:257:LYS:NZ	1:F:254:GLN:O[1_455]	2.15	0.05
1:B:299:GLU:OE2	2:O:2:FUC:O3[1_545]	2.15	0.05
1:C:88:LYS:NZ	1:E:254:GLN:OE1[1_545]	2.17	0.03
1:B:254:GLN:O	1:E:257:LYS:NZ[1_545]	2.19	0.01

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	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	37	56
1	B	363/378 (96%)	339 (93%)	22 (6%)	2 (1%)	22	39
1	C	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	37	56
1	D	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	37	56
1	E	363/378 (96%)	343 (94%)	19 (5%)	1 (0%)	37	56
1	F	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	37	56
1	G	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	37	56
1	H	363/378 (96%)	341 (94%)	21 (6%)	1 (0%)	37	56
1	I	363/378 (96%)	338 (93%)	24 (7%)	1 (0%)	37	56
1	J	361/378 (96%)	338 (94%)	21 (6%)	2 (1%)	22	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	362/378 (96%)	339 (94%)	22 (6%)	1 (0%)	37 56
1	L	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	37 56
All	All	4353/4536 (96%)	4090 (94%)	249 (6%)	14 (0%)	37 56

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	E	398	ASP
1	F	398	ASP
1	B	398	ASP
1	C	398	ASP

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	318/327 (97%)	310 (98%)	8 (2%)	42 69
1	B	318/327 (97%)	308 (97%)	10 (3%)	35 62
1	C	318/327 (97%)	309 (97%)	9 (3%)	38 65
1	D	318/327 (97%)	307 (96%)	11 (4%)	31 57
1	E	318/327 (97%)	310 (98%)	8 (2%)	42 69
1	F	318/327 (97%)	308 (97%)	10 (3%)	35 62
1	G	318/327 (97%)	304 (96%)	14 (4%)	24 47
1	H	318/327 (97%)	310 (98%)	8 (2%)	42 69
1	I	318/327 (97%)	307 (96%)	11 (4%)	31 57
1	J	316/327 (97%)	308 (98%)	8 (2%)	42 69
1	K	317/327 (97%)	306 (96%)	11 (4%)	31 57
1	L	318/327 (97%)	311 (98%)	7 (2%)	47 73
All	All	3813/3924 (97%)	3698 (97%)	115 (3%)	36 63

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	139	ASN
1	L	274	ILE
1	H	169	ARG
1	L	139	ASN
1	K	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	250	ASN
1	G	136	HIS
1	I	240	GLN
1	C	136	HIS
1	D	260	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 ⓘ

12 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	M	1	1,2	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
2	FUC	M	2	2	10,10,11	0.77	0	14,14,16	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	1,3	14,14,15	0.51	0	17,19,21	1.26	2 (11%)
3	NAG	N	2	3	14,14,15	0.43	0	17,19,21	1.69	4 (23%)
3	FUL	N	3	3	10,10,11	1.55	3 (30%)	14,14,16	1.54	3 (21%)
2	NAG	O	1	1,2	14,14,15	0.70	0	17,19,21	1.53	2 (11%)
2	FUC	O	2	2	10,10,11	0.90	0	14,14,16	0.74	0
3	NAG	P	1	1,3	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
3	NAG	P	2	3	14,14,15	0.51	0	17,19,21	1.54	3 (17%)
3	FUL	P	3	3	10,10,11	1.45	2 (20%)	14,14,16	1.79	4 (28%)
2	NAG	Q	1	1,2	14,14,15	0.52	0	17,19,21	1.92	3 (17%)
2	FUC	Q	2	2	10,10,11	1.11	1 (10%)	14,14,16	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	FUL	N	3	3	-	-	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	FUL	P	3	3	-	-	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	FUL	C4-C5	2.75	1.58	1.52
3	P	3	FUL	C4-C5	2.47	1.58	1.52
2	Q	2	FUC	O5-C1	-2.44	1.39	1.43
3	N	3	FUL	O5-C5	2.37	1.48	1.43
3	N	3	FUL	C4-C3	2.12	1.57	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NAG	C1-O5-C5	6.00	120.23	112.19
3	N	2	NAG	C1-O5-C5	4.21	117.83	112.19
3	P	3	FUL	O5-C5-C4	3.89	116.56	109.55
2	O	1	NAG	C4-C3-C2	3.57	116.25	111.02
3	P	1	NAG	O5-C5-C6	3.50	114.48	107.66

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

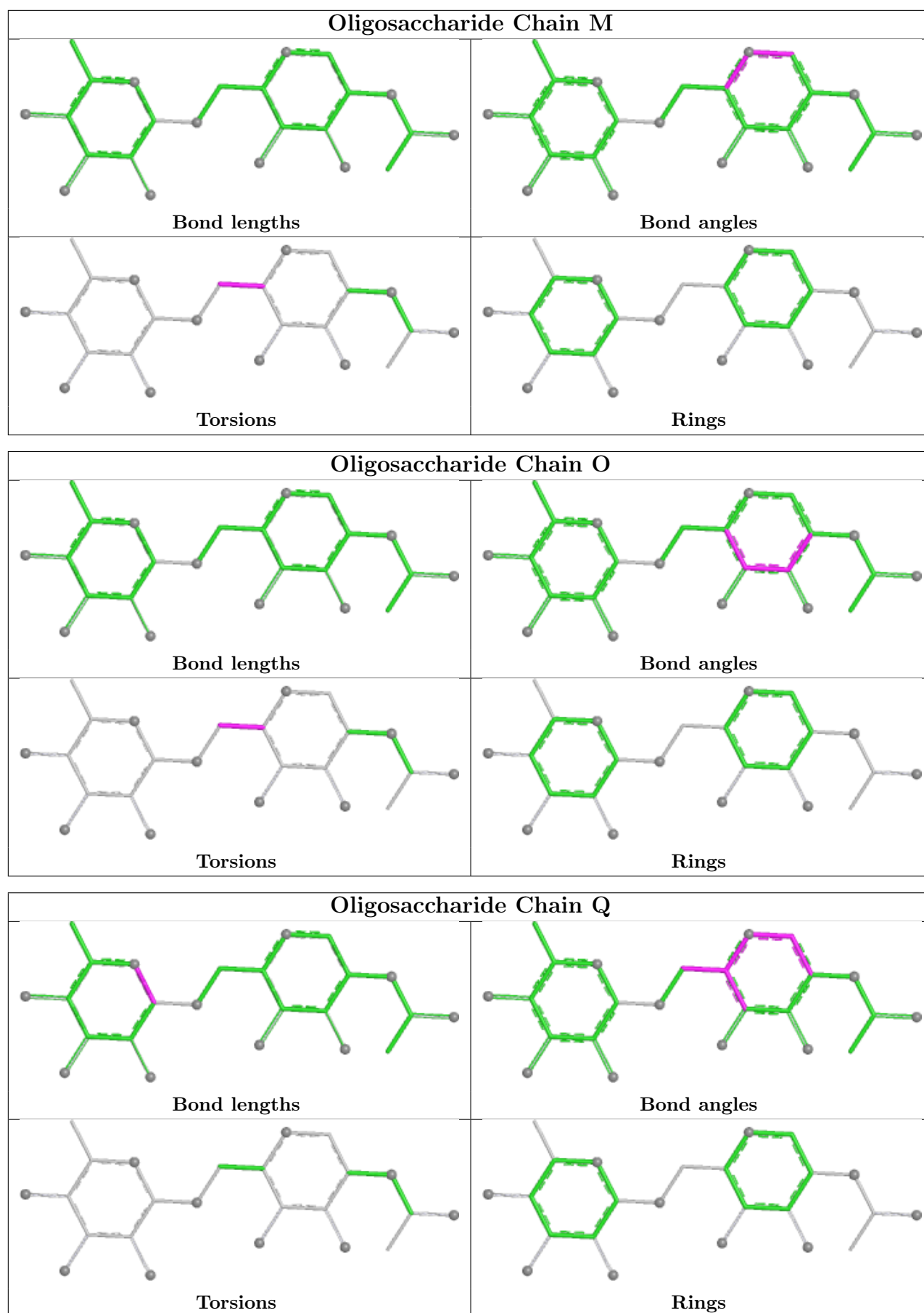
Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	P	1	NAG	O5-C5-C6-O6

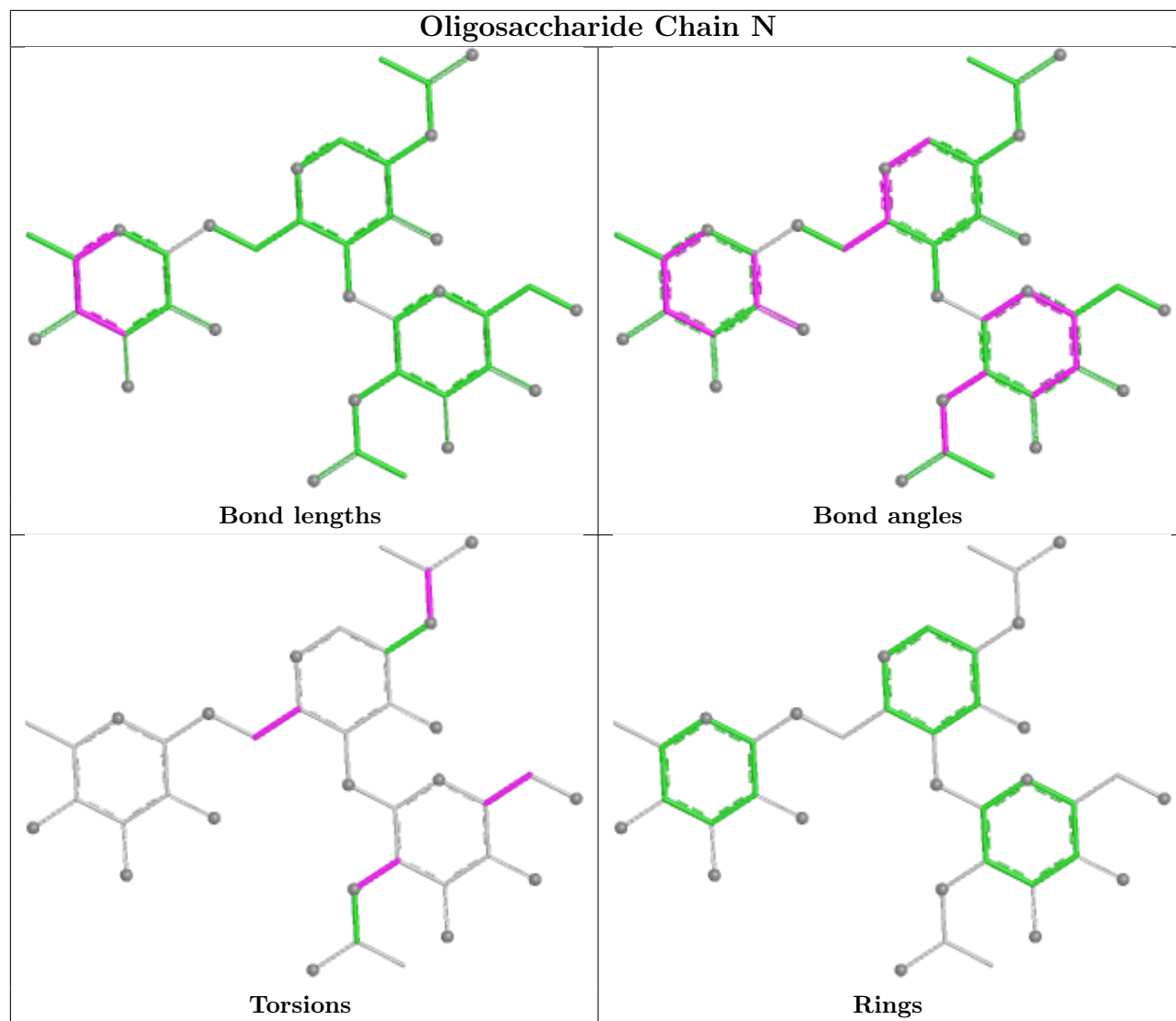
There are no ring outliers.

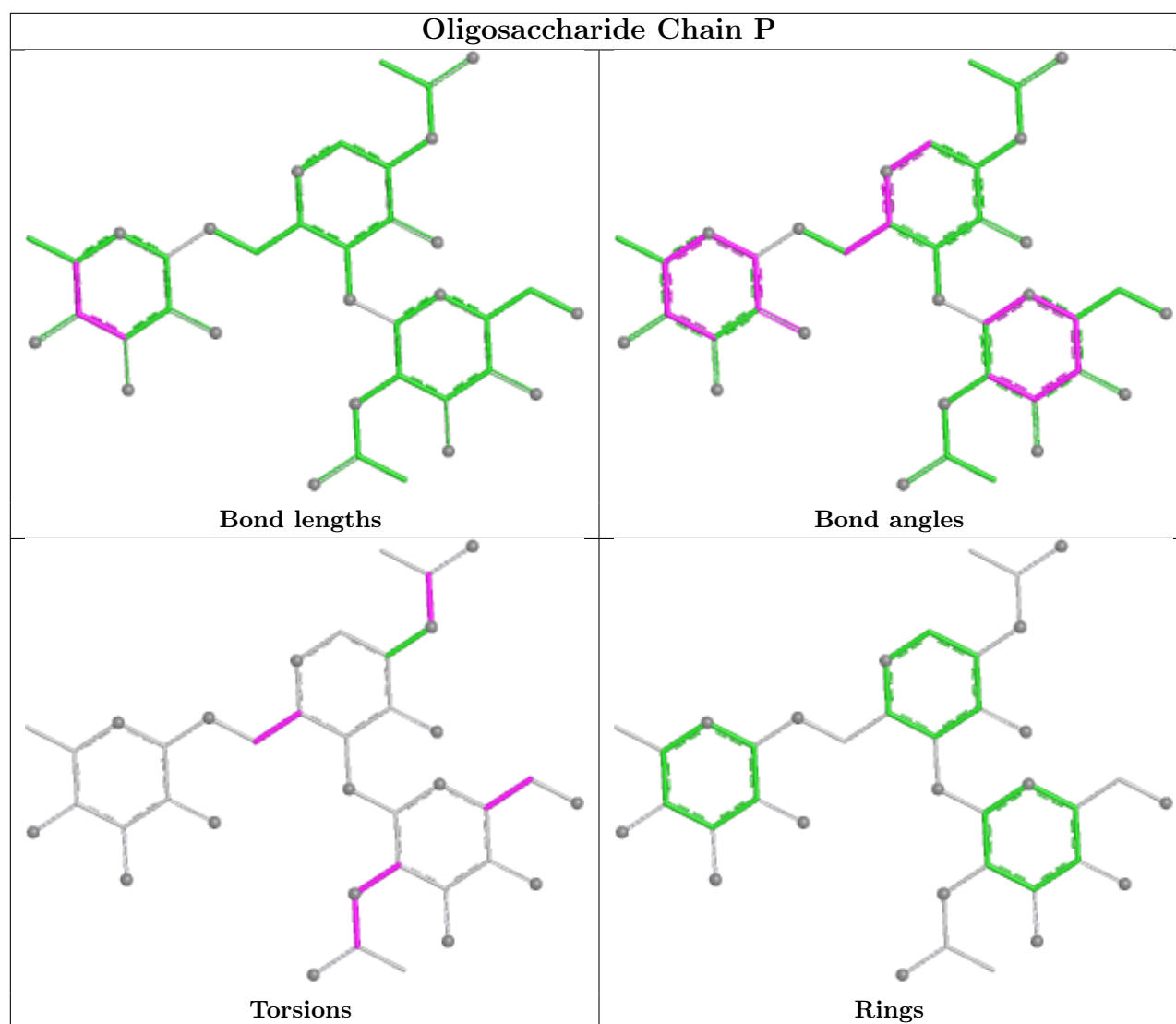
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	3	FUL	1	0
3	N	3	FUL	1	0
2	O	2	FUC	0	1
3	N	2	NAG	1	0
3	P	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z > 2$
5	NAG	E	502	1	14,14,15	0.45	0	17,19,21	0.74	0
5	NAG	D	504	-	14,14,15	0.43	0	17,19,21	4.50	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	502	1	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
6	FUC	D	505	-	10,10,11	1.97	2 (20%)	14,14,16	3.23	3 (21%)
5	NAG	D	503	-	14,14,15	0.63	0	17,19,21	1.58	2 (11%)
5	NAG	D	502	-	14,14,15	0.49	0	17,19,21	1.23	1 (5%)
5	NAG	H	502	1	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	NAG	C	502	1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
5	NAG	B	505	-	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
5	NAG	A	502	1	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
5	NAG	F	505	-	14,14,15	0.50	0	17,19,21	0.66	0
5	NAG	I	502	1	14,14,15	0.52	0	17,19,21	1.40	1 (5%)
5	NAG	L	502	1	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
5	NAG	K	502	1	14,14,15	0.56	0	17,19,21	1.25	3 (17%)
5	NAG	A	503	1	14,14,15	0.44	0	17,19,21	1.65	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	504	-	-	2/6/23/26	0/1/1/1
5	NAG	G	502	1	-	4/6/23/26	0/1/1/1
6	FUC	D	505	-	-	-	0/1/1/1
5	NAG	D	503	-	-	0/6/23/26	0/1/1/1
5	NAG	D	502	-	-	2/6/23/26	0/1/1/1
5	NAG	H	502	1	-	2/6/23/26	0/1/1/1
5	NAG	C	502	1	-	2/6/23/26	0/1/1/1
5	NAG	B	505	-	-	1/6/23/26	0/1/1/1
5	NAG	A	502	1	-	3/6/23/26	0/1/1/1
5	NAG	F	505	-	-	2/6/23/26	0/1/1/1
5	NAG	I	502	1	-	3/6/23/26	0/1/1/1
5	NAG	L	502	1	-	2/6/23/26	0/1/1/1
5	NAG	K	502	1	-	5/6/23/26	0/1/1/1
5	NAG	A	503	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	505	FUC	C2-C3	4.36	1.59	1.52
6	D	505	FUC	C1-C2	3.91	1.61	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	504	NAG	C1-O5-C5	12.78	129.32	112.19
5	D	504	NAG	O5-C1-C2	-12.19	92.44	111.29
6	D	505	FUC	O5-C1-C2	-10.85	84.91	110.79
5	I	502	NAG	C1-O5-C5	4.26	117.90	112.19
5	D	503	NAG	O5-C1-C2	4.19	117.78	111.29

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	C3-C2-N2-C7
5	A	502	NAG	C8-C7-N2-C2
5	A	502	NAG	O7-C7-N2-C2
5	E	502	NAG	C8-C7-N2-C2
5	E	502	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	502	NAG	1	0
5	D	504	NAG	1	0
5	D	503	NAG	1	0
5	D	502	NAG	1	0
5	C	502	NAG	1	0
5	B	505	NAG	2	0
5	F	505	NAG	1	0
5	I	502	NAG	2	0
5	L	502	NAG	1	0
5	A	503	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/378 (96%)	-1.62	0 100 100	10, 33, 79, 133	0
1	B	365/378 (96%)	-1.67	0 100 100	11, 34, 71, 137	0
1	C	365/378 (96%)	-1.65	0 100 100	12, 39, 81, 141	0
1	D	365/378 (96%)	-1.62	0 100 100	11, 38, 88, 148	0
1	E	365/378 (96%)	-1.65	0 100 100	11, 34, 82, 133	0
1	F	365/378 (96%)	-1.65	0 100 100	12, 34, 69, 140	0
1	G	365/378 (96%)	-1.51	0 100 100	14, 46, 93, 135	0
1	H	365/378 (96%)	-1.54	0 100 100	13, 45, 96, 139	0
1	I	365/378 (96%)	-1.44	0 100 100	39, 65, 106, 137	0
1	J	363/378 (96%)	-1.33	0 100 100	47, 75, 104, 146	0
1	K	364/378 (96%)	-1.13	0 100 100	45, 87, 112, 149	0
1	L	365/378 (96%)	-1.07	0 100 100	45, 84, 116, 145	0
All	All	4377/4536 (96%)	-1.49	0 100 100	10, 51, 104, 149	0

There are no RSRZ outliers to report.

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

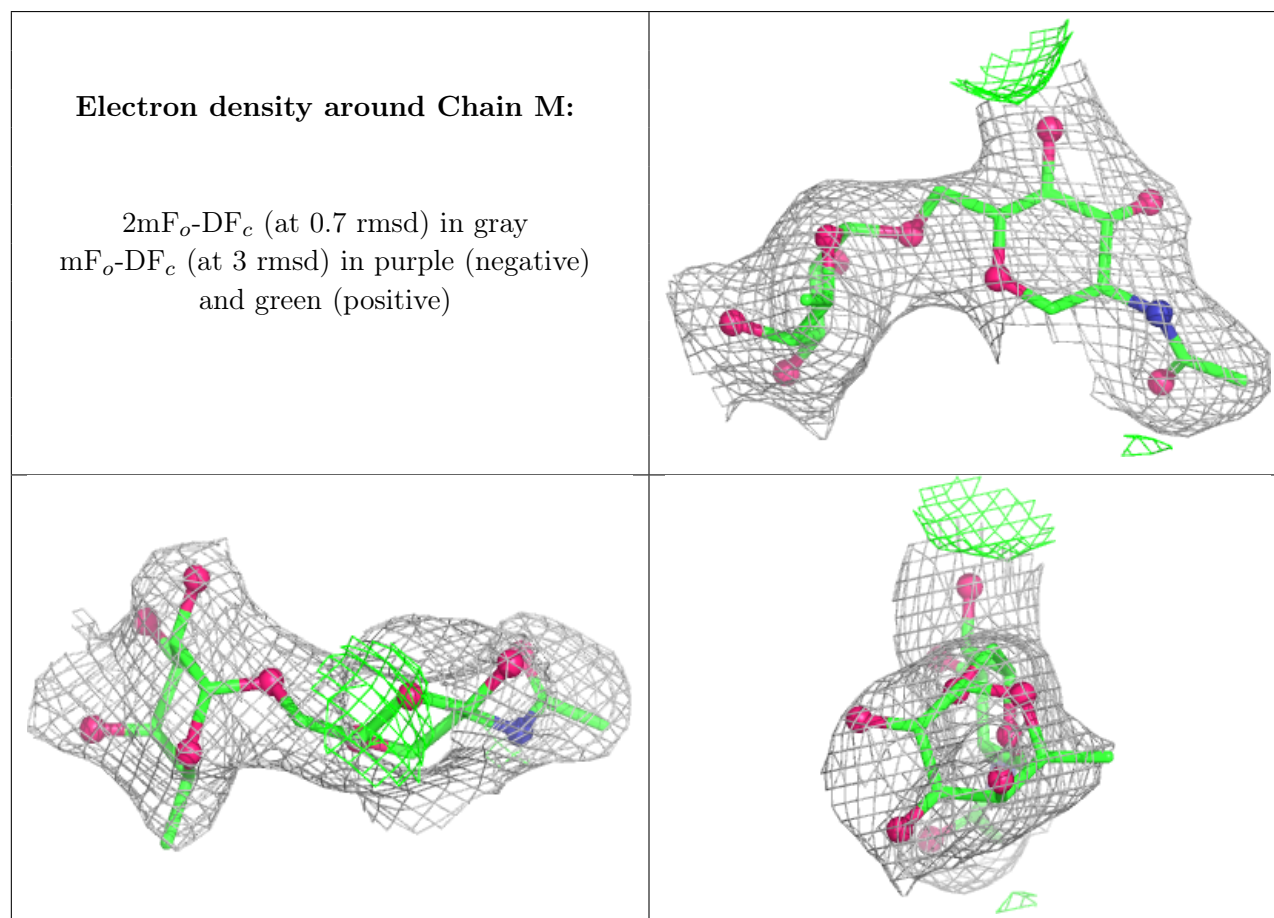
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

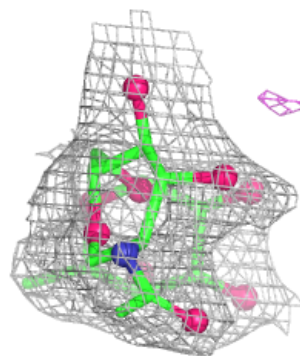
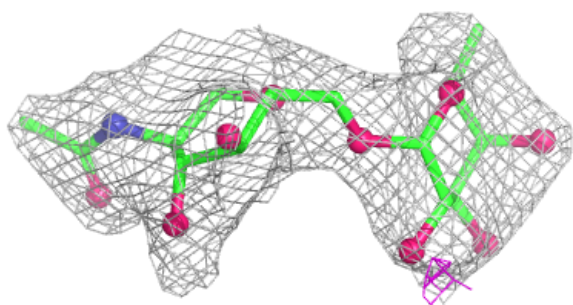
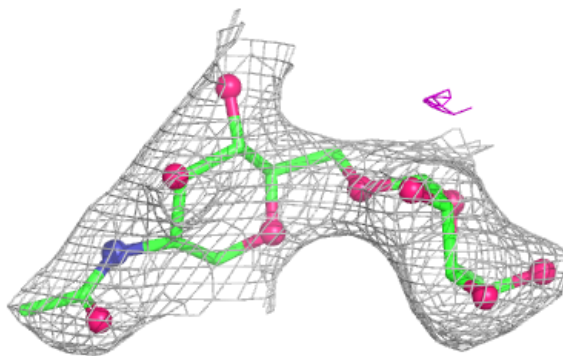
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	N	2	14/15	0.97	0.04	86,92,96,96	0
3	NAG	P	2	14/15	0.97	0.04	89,95,101,102	0
3	FUL	N	3	10/11	0.98	0.05	68,80,83,84	0
3	NAG	P	1	14/15	0.98	0.03	55,67,75,82	0
2	FUC	M	2	10/11	0.98	0.04	26,46,53,63	0
3	FUL	P	3	10/11	0.98	0.04	54,61,69,70	0
3	NAG	N	1	14/15	0.99	0.03	60,69,80,83	0
2	NAG	M	1	14/15	0.99	0.03	38,48,52,52	0
2	NAG	O	1	14/15	0.99	0.03	45,48,54,55	0
2	FUC	O	2	10/11	0.99	0.03	54,57,61,63	0
2	NAG	Q	1	14/15	0.99	0.03	35,55,67,68	0
2	FUC	Q	2	10/11	0.99	0.03	74,79,86,87	0

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

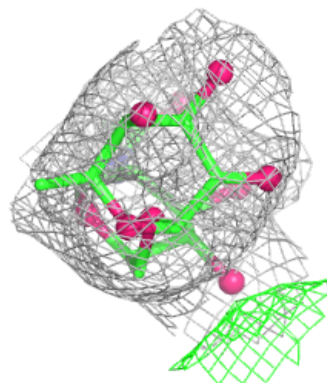
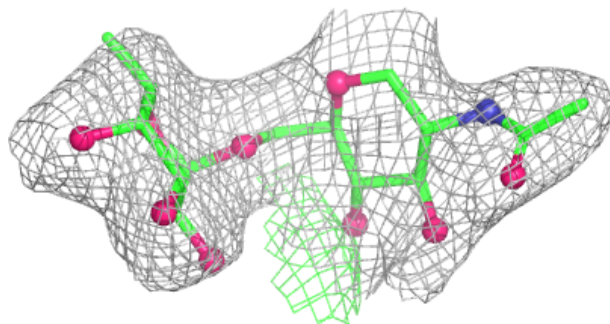
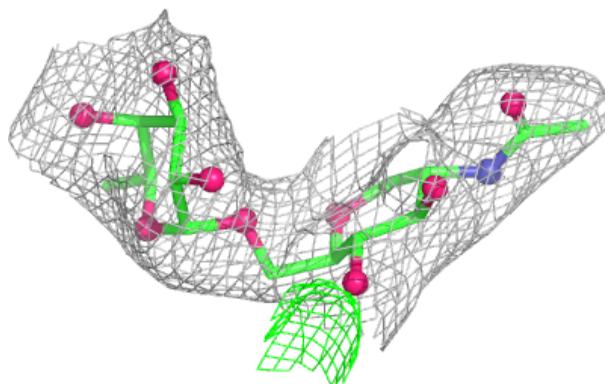


Electron density around Chain O:

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

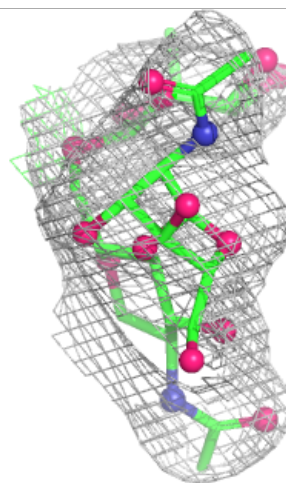
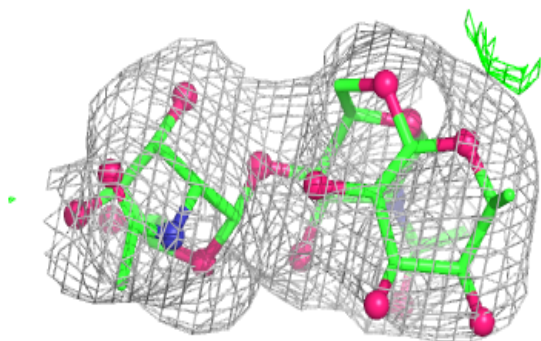
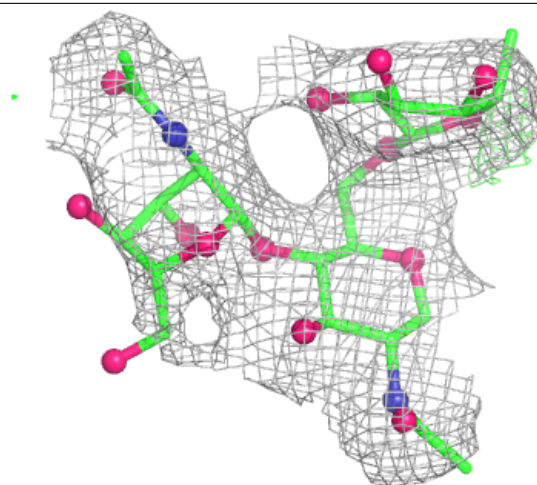
**Electron density around Chain Q:**

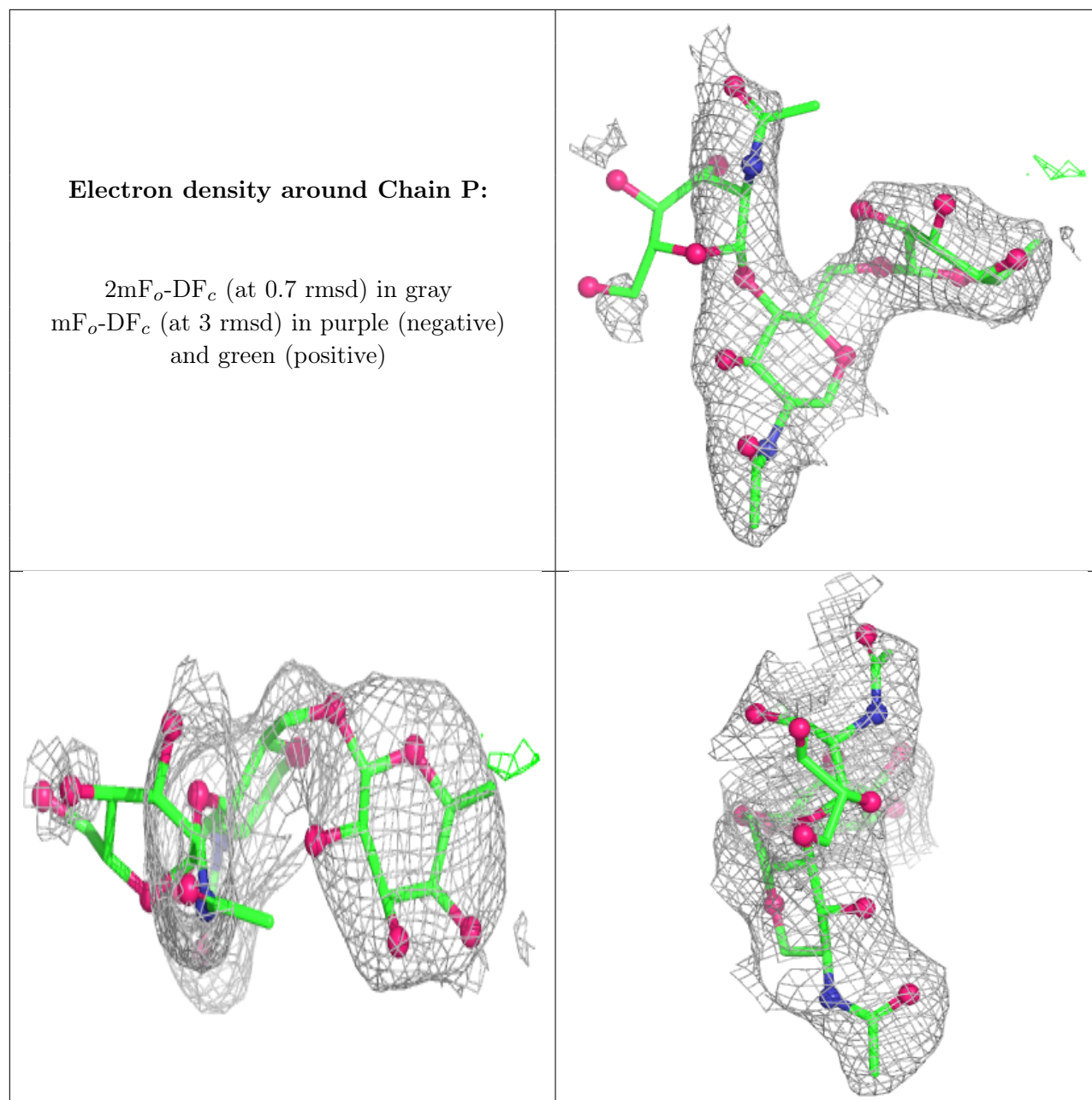
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
5	NAG	K	502	14/15	0.94	0.06	73,86,92,93	0
5	NAG	A	502	14/15	0.95	0.05	82,102,105,105	0
5	NAG	G	502	14/15	0.96	0.04	64,72,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	L	502	14/15	0.96	0.04	75,86,94,96	0
5	NAG	I	502	14/15	0.97	0.04	79,85,89,91	0
5	NAG	E	502	14/15	0.97	0.06	83,97,100,101	0
5	NAG	B	505	14/15	0.97	0.07	64,76,81,83	0
5	NAG	H	502	14/15	0.98	0.03	54,67,82,84	0
5	NAG	D	503	14/15	0.98	0.04	49,73,79,83	0
5	NAG	A	503	14/15	0.98	0.05	83,99,103,104	0
5	NAG	D	502	14/15	0.98	0.03	75,87,90,91	0
5	NAG	F	505	14/15	0.99	0.05	63,81,85,86	0
5	NAG	D	504	14/15	0.99	0.03	30,81,85,85	0
5	NAG	C	502	14/15	0.99	0.03	44,53,61,64	0
6	FUC	D	505	10/11	0.99	0.04	46,59,84,86	0
4	CA	D	501	1/1	1.00	0.01	33,33,33,33	0
4	CA	E	501	1/1	1.00	0.03	41,41,41,41	0
4	CA	F	501	1/1	1.00	0.01	45,45,45,45	0
4	CA	G	501	1/1	1.00	0.02	28,28,28,28	0
4	CA	H	501	1/1	1.00	0.02	37,37,37,37	0
4	CA	I	501	1/1	1.00	0.02	51,51,51,51	0
4	CA	J	501	1/1	1.00	0.01	65,65,65,65	0
4	CA	K	501	1/1	1.00	0.02	51,51,51,51	0
4	CA	L	501	1/1	1.00	0.03	84,84,84,84	0
4	CA	A	501	1/1	1.00	0.01	34,34,34,34	0
4	CA	B	501	1/1	1.00	0.02	42,42,42,42	0
4	CA	C	501	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.