Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 11:16 AM EDT

PDB ID	:	6D96
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 (i) 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 (i)) were used in the production of this report:

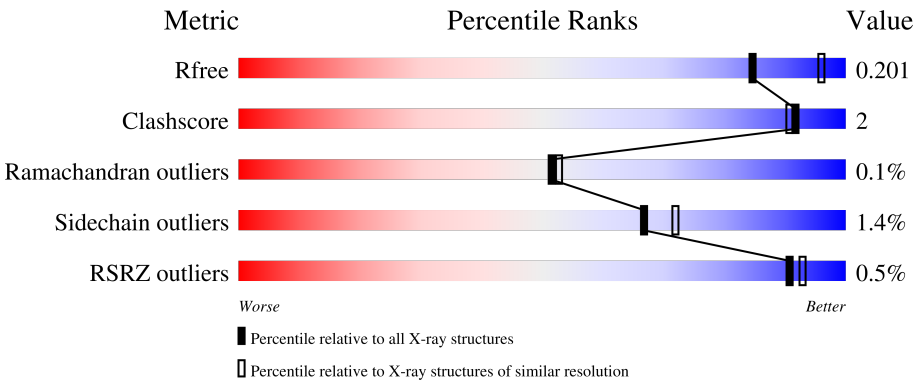
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	90% 5% ·
1	B	404	90% 6% ·
1	C	404	92% · ·
1	D	404	89% 6% ·
1	E	404	90% 5% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	404	% 89% 6%
1	G	404	92%
1	H	404	% 90% 5%
2	I	3	100%
2	J	3	67% 33%
2	L	3	33% 33% 33%
2	N	3	33% 67%
2	O	3	33% 67%
3	K	2	100%
3	M	2	100%

2 Entry composition (i)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

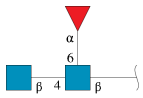
Chain	Residue	Modelled	Actual	Comment	Reference
D	73	LEU	-	expression tag	UNP Q9IGQ6
D	74	VAL	-	expression tag	UNP Q9IGQ6
D	75	PRO	-	expression tag	UNP Q9IGQ6
D	76	ARG	-	expression tag	UNP Q9IGQ6
D	77	GLY	-	expression tag	UNP Q9IGQ6
D	78	SER	-	expression tag	UNP Q9IGQ6
D	79	PRO	-	expression tag	UNP Q9IGQ6
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

Continued on next page...

Continued from previous page...

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
			Total	C	N	O			
2	I	3	38	22	2	14	0	0	0

Continued on next page...

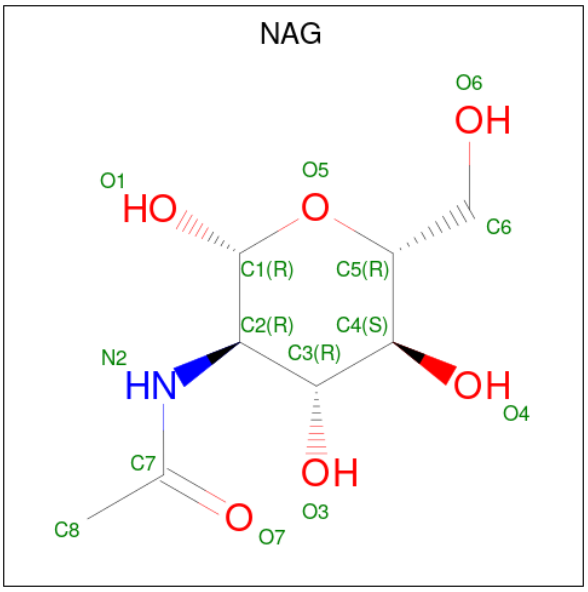
Continued from previous page...

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

- 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
			Total	C	N	O			
3	K	2	24	14	1	9	0	0	0
			Total	C	N	O			
3	M	2	24	14	1	9	0	0	0

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



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

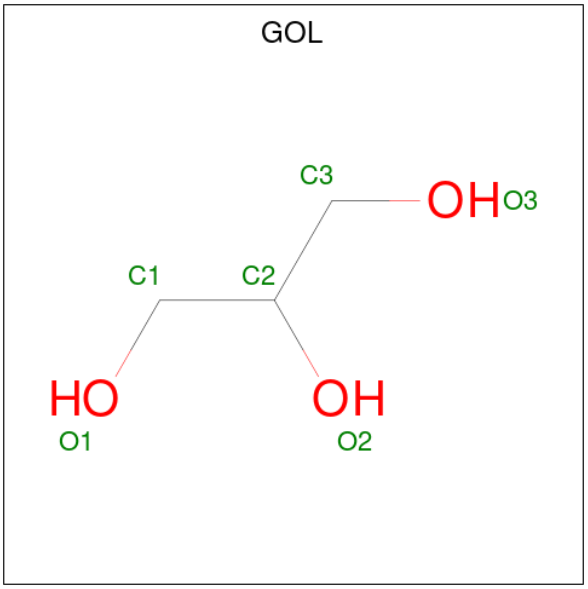
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	3	3	3	0	0
5	B	2	2	2	0	0
5	C	2	2	2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

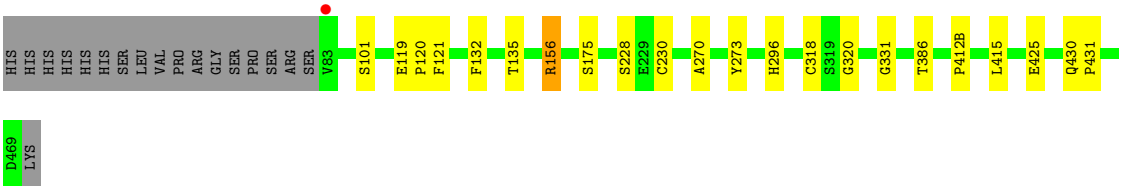
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	168	168	168	0	0
			Total	O		
7	B	190	190	190	0	0
			Total	O		
7	C	181	181	181	0	0
			Total	O		
7	D	143	143	143	0	0
			Total	O		
7	E	180	180	180	0	0
			Total	O		
7	F	166	166	166	0	0
			Total	O		
7	G	175	175	175	0	0
			Total	O		
7	H	142	142	142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

3 Residue-property plots (i)

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

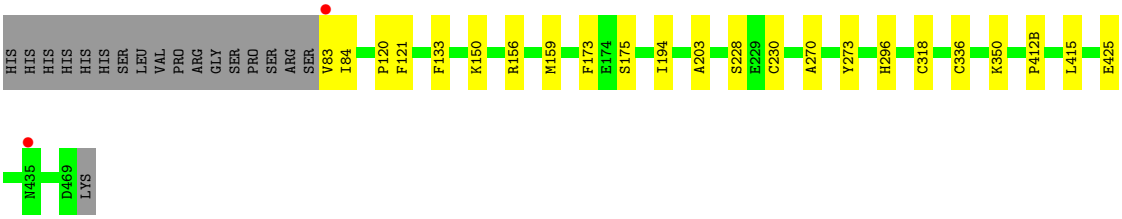
- Molecule 1: Neuraminidase

Chain A:



- Molecule 1: Neuraminidase

Chain B:

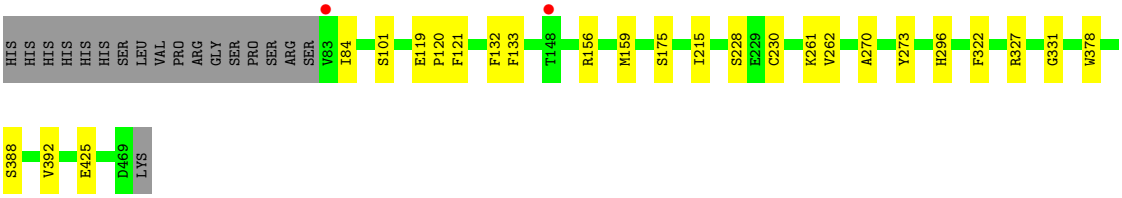


- Molecule 1: Neuraminidase

Chain C:

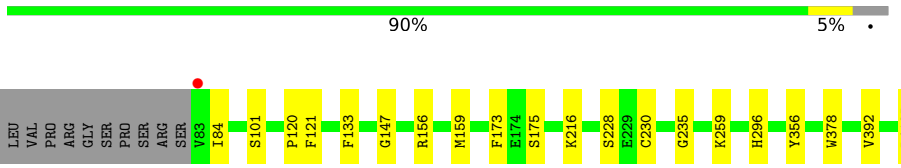
- Molecule 1: Neuraminidase

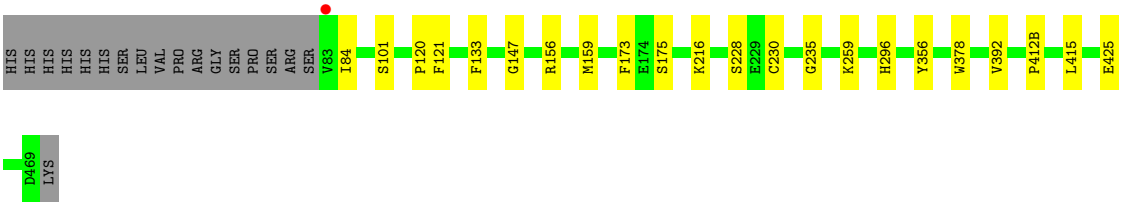
Chain D:



• Molecule 1: Neuraminidase

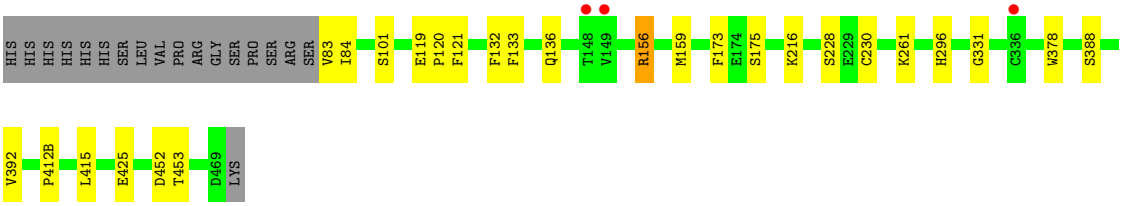
Chain E:





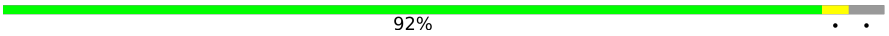
• Molecule 1: Neuraminidase

Chain F:



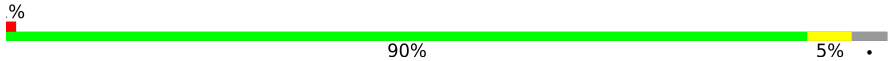
• Molecule 1: Neuraminidase

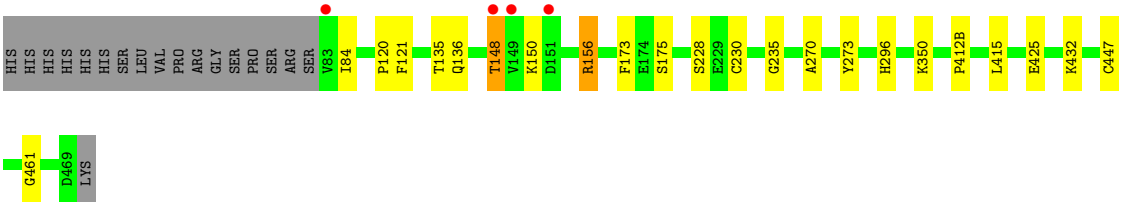
Chain G:



• Molecule 1: Neuraminidase

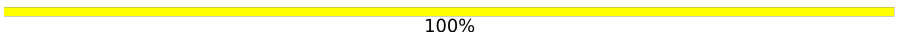
Chain H:





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

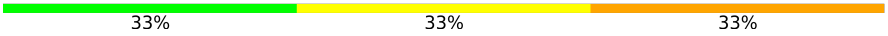
Chain I:



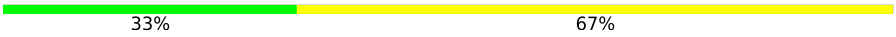
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

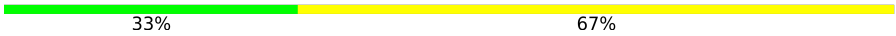
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

• 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: 

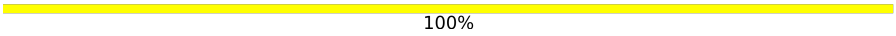
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 

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

Chain K:

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

Chain M: 

4 Data and refinement statistics (i)

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 48.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.96-2.15) 99.0 (48.15-2.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.186 , 0.215 0.169 , 0.201	Depositor DCC
R_{free} test set	7244 reflections (2.98%)	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)	0.34 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, GOL, FUC, 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	0.45	1/3047 (0.0%)	0.61	0/4146
1	B	0.45	0/3055	0.59	0/4153
1	C	0.44	1/3057 (0.0%)	0.59	0/4157
1	D	0.44	1/3062 (0.0%)	0.60	0/4163
1	E	0.43	0/3064	0.61	0/4165
1	F	0.45	1/3050 (0.0%)	0.60	0/4148
1	G	0.43	0/3050	0.59	0/4148
1	H	0.40	0/3048	0.59	0/4144
All	All	0.44	4/24433 (0.0%)	0.60	0/33224

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	119	GLU	C-N	-9.09	1.17	1.34
1	A	119	GLU	C-N	-6.87	1.21	1.34
1	D	119	GLU	C-N	-6.73	1.21	1.34
1	C	119	GLU	C-N	-6.05	1.22	1.34

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	2963	0	2764	10	0
1	B	2971	0	2790	11	0
1	C	2973	0	2793	7	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	7	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

Continued on next page...

Continued from previous page...

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	75	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 (75) 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: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:B:318:CYS:HG	1:B:336:CYS:HG	1.62	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

Continued on next page...

Continued from previous page...

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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	37
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%)	41	37
All	All	3081/3232 (95%)	2939 (95%)	140 (4%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/348 (94%)	324 (99%)	4 (1%)	71	76
1	B	331/348 (95%)	326 (98%)	5 (2%)	65	69
1	C	331/348 (95%)	327 (99%)	4 (1%)	71	76
1	D	332/348 (95%)	327 (98%)	5 (2%)	65	69
1	E	333/348 (96%)	328 (98%)	5 (2%)	65	69
1	F	330/348 (95%)	324 (98%)	6 (2%)	59	63
1	G	330/348 (95%)	327 (99%)	3 (1%)	78	83
1	H	330/348 (95%)	324 (98%)	6 (2%)	59	63
All	All	2645/2784 (95%)	2607 (99%)	38 (1%)	67	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ARG
1	A	175	SER
1	A	230	CYS
1	A	296	HIS
1	B	83	VAL
1	B	156	ARG
1	B	175	SER
1	B	230	CYS
1	B	296	HIS
1	C	156	ARG
1	C	175	SER
1	C	230	CYS
1	C	296	HIS
1	D	156	ARG
1	D	175	SER
1	D	230	CYS
1	D	261	LYS
1	D	296	HIS
1	E	156	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	175	SER
1	E	230	CYS
1	E	259	LYS
1	E	296	HIS
1	F	83	VAL
1	F	156	ARG
1	F	175	SER
1	F	230	CYS
1	F	261	LYS
1	F	296	HIS
1	G	156	ARG
1	G	230	CYS
1	G	296	HIS
1	H	150	LYS
1	H	156	ARG
1	H	175	SER
1	H	230	CYS
1	H	296	HIS
1	H	432	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1 (7%)	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.85	1 (7%)	17,19,21	0.49	0
2	FUC	I	3	2	10,10,11	1.21	1 (10%)	14,14,16	1.53	4 (28%)
2	NAG	J	1	1,2	14,14,15	0.48	0	17,19,21	0.61	0
2	NAG	J	2	2	14,14,15	0.38	0	17,19,21	0.51	0
2	FUC	J	3	2	10,10,11	0.95	1 (10%)	14,14,16	1.05	0
3	NAG	K	1	1,3	14,14,15	0.38	0	17,19,21	1.47	2 (11%)
3	FUC	K	2	3	10,10,11	1.78	2 (20%)	14,14,16	1.65	4 (28%)
2	NAG	L	1	1,2	14,14,15	0.49	0	17,19,21	0.71	0
2	NAG	L	2	2	14,14,15	0.35	0	17,19,21	0.51	0
2	FUC	L	3	2	10,10,11	0.94	1 (10%)	14,14,16	1.15	1 (7%)
3	NAG	M	1	1,3	14,14,15	0.78	1 (7%)	17,19,21	0.55	0
3	FUC	M	2	3	10,10,11	1.30	1 (10%)	14,14,16	1.45	3 (21%)
2	NAG	N	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
2	NAG	N	2	2	14,14,15	0.42	0	17,19,21	0.46	0
2	FUC	N	3	2	10,10,11	0.94	0	14,14,16	1.15	2 (14%)
2	NAG	O	1	1,2	14,14,15	0.39	0	17,19,21	0.39	0
2	NAG	O	2	2	14,14,15	0.79	1 (7%)	17,19,21	0.53	0
2	FUC	O	3	2	10,10,11	1.21	2 (20%)	14,14,16	1.62	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3.78	1.58	1.52
3	K	2	FUC	C4-C3	3.13	1.60	1.52
2	N	1	NAG	O5-C1	-2.62	1.39	1.43
2	O	3	FUC	C4-C3	2.57	1.58	1.52
2	I	2	NAG	O5-C1	2.50	1.47	1.43
2	O	2	NAG	C1-C2	2.46	1.56	1.52
2	I	1	NAG	O5-C1	-2.43	1.39	1.43
3	M	1	NAG	C1-C2	2.33	1.55	1.52
3	M	2	FUC	O5-C1	-2.28	1.40	1.43
2	I	3	FUC	C1-C2	2.26	1.57	1.52
2	J	3	FUC	C1-C2	2.17	1.57	1.52
2	L	3	FUC	C1-C2	2.02	1.56	1.52
2	O	3	FUC	O5-C1	-2.01	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1	NAG	C2-N2-C7	4.36	129.12	122.90
2	O	3	FUC	C3-C4-C5	3.31	114.92	109.77
3	K	2	FUC	C1-O5-C5	3.18	119.99	112.78
2	O	3	FUC	O5-C5-C4	3.02	114.94	109.52
2	N	3	FUC	O5-C1-C2	2.80	115.10	110.77
3	K	1	NAG	C1-O5-C5	2.74	115.91	112.19
3	K	2	FUC	O5-C5-C4	2.72	114.39	109.52
3	M	2	FUC	C3-C4-C5	2.57	113.78	109.77
2	I	3	FUC	C1-O5-C5	2.56	118.57	112.78
2	I	3	FUC	O2-C2-C1	2.49	114.25	109.15
2	O	3	FUC	C2-C3-C4	2.41	115.07	110.89
3	K	2	FUC	C2-C3-C4	2.39	115.03	110.89
3	M	2	FUC	C2-C3-C4	2.31	114.89	110.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	3	FUC	C1-C2-C3	2.30	112.50	109.67
3	M	2	FUC	O2-C2-C1	2.29	113.84	109.15
2	N	3	FUC	C1-C2-C3	2.27	112.45	109.67
3	K	2	FUC	O2-C2-C1	2.24	113.74	109.15
2	I	3	FUC	O5-C5-C4	2.17	113.42	109.52
2	L	3	FUC	C1-O5-C5	2.05	117.43	112.78

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
3	K	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
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	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

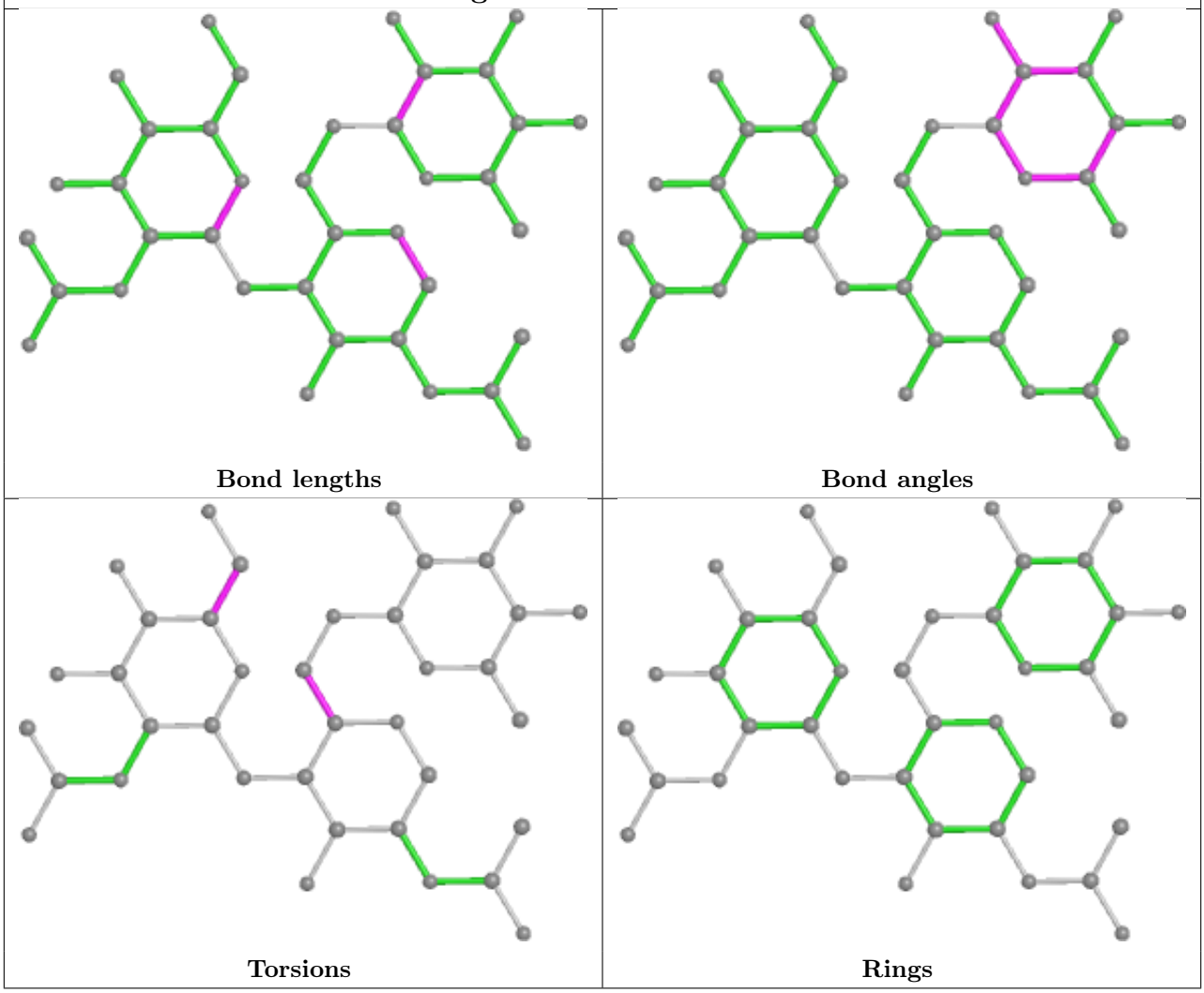
There are no ring outliers.

4 monomers are involved in 2 short contacts:

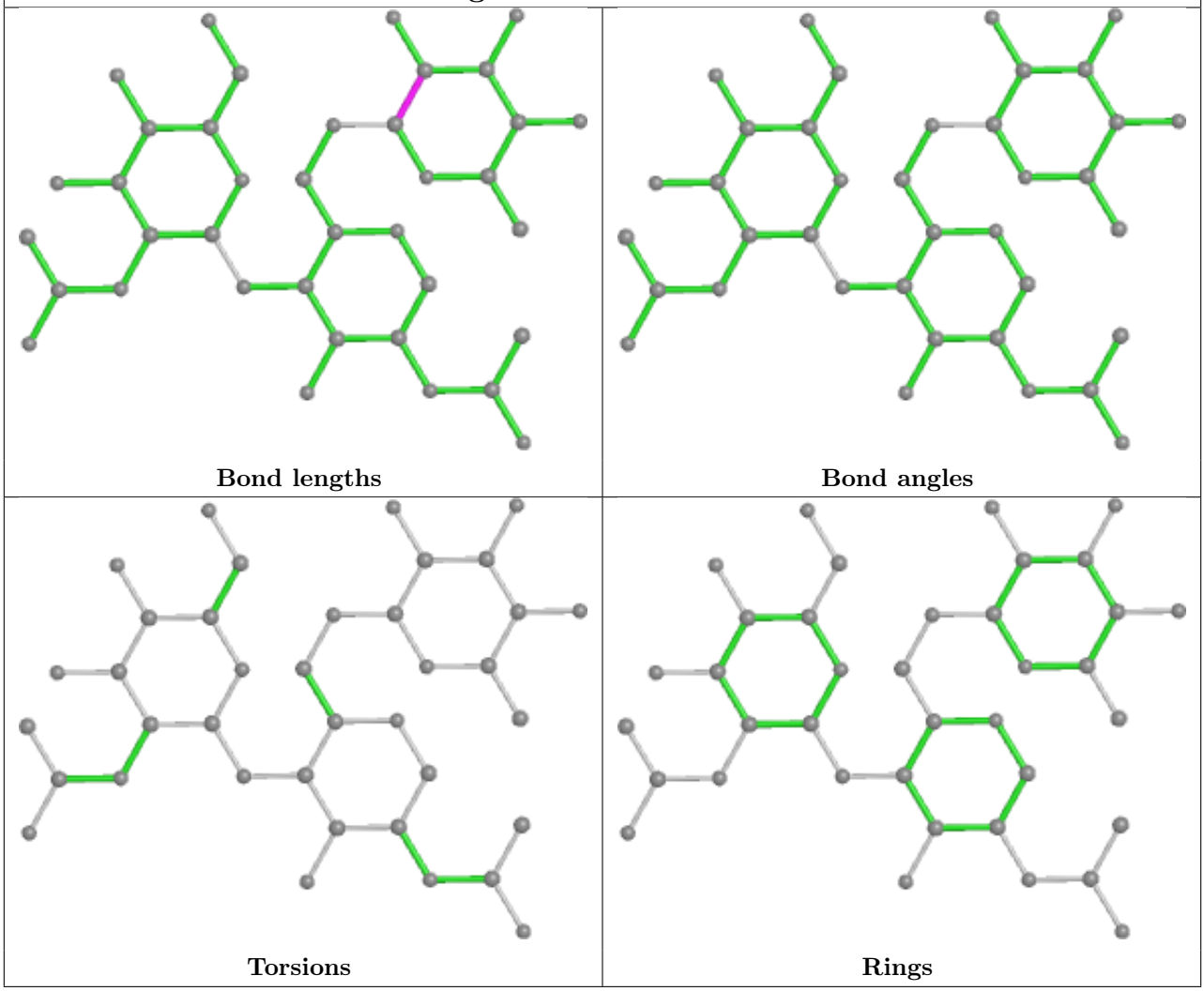
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	1	0
2	L	3	FUC	1	0
3	K	2	FUC	1	0
2	L	2	NAG	1	0

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

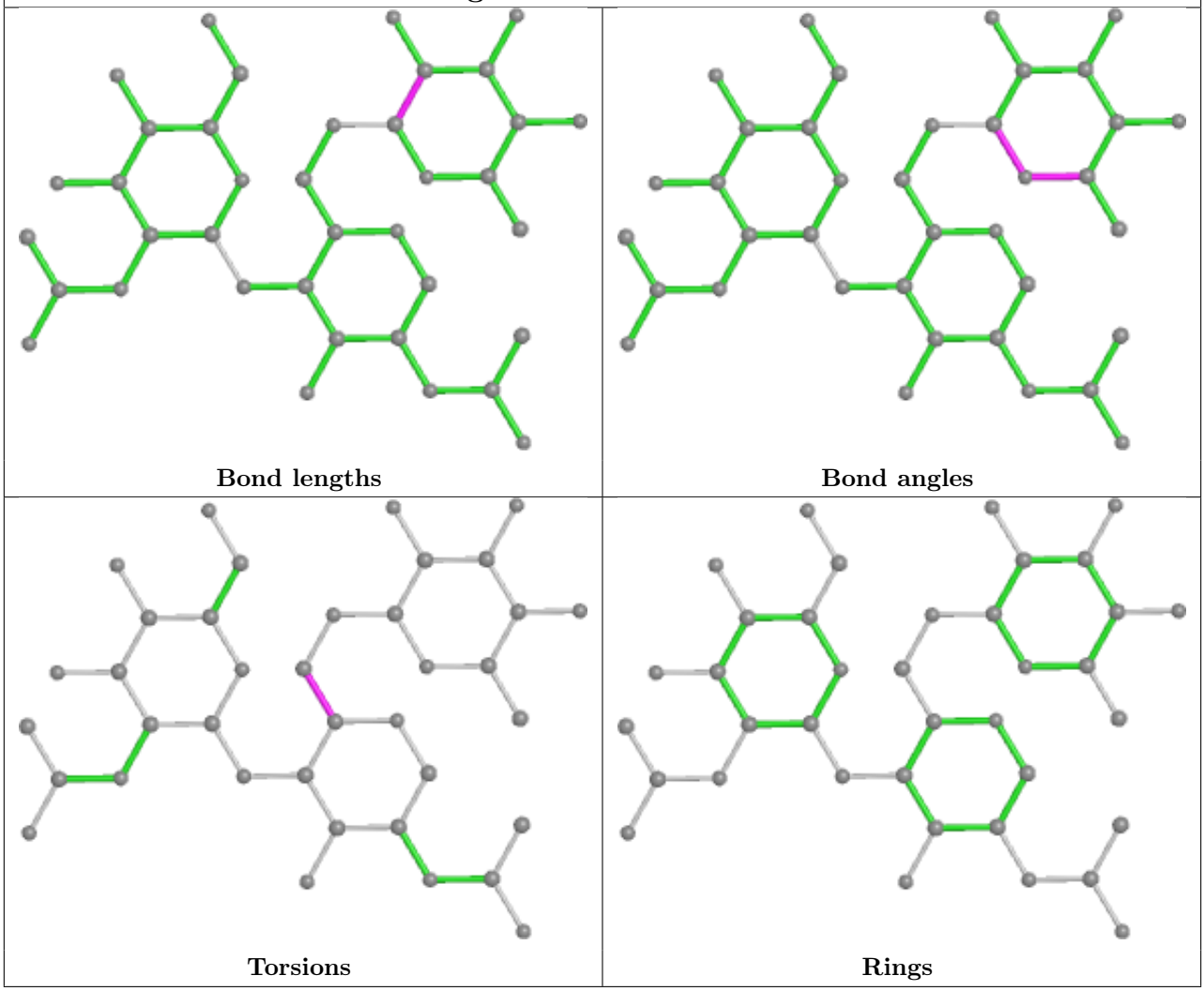
Oligosaccharide Chain I



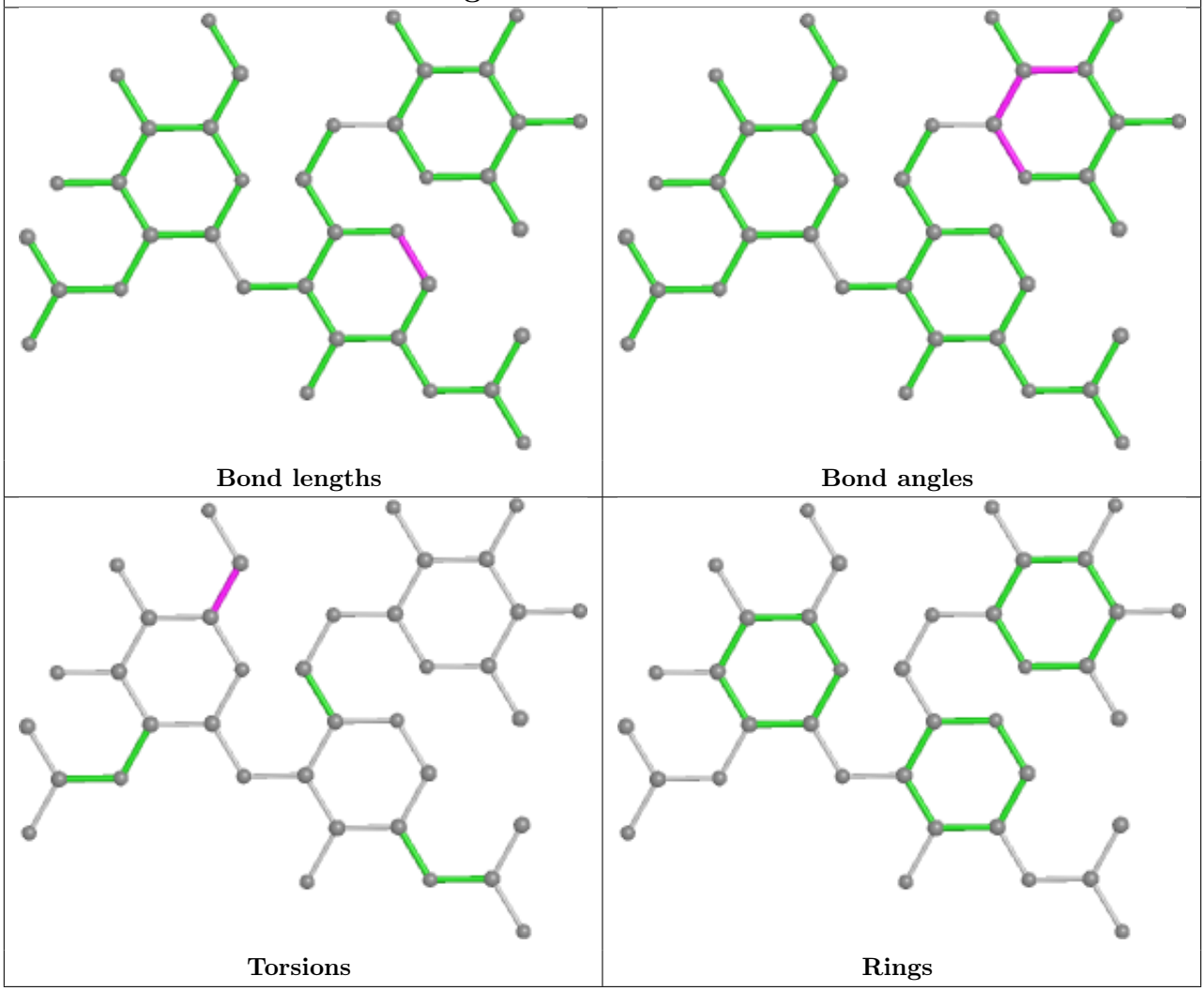
Oligosaccharide Chain J



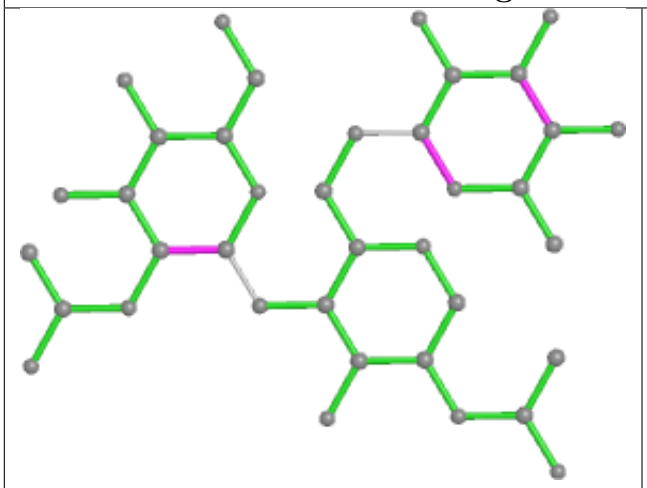
Oligosaccharide Chain L



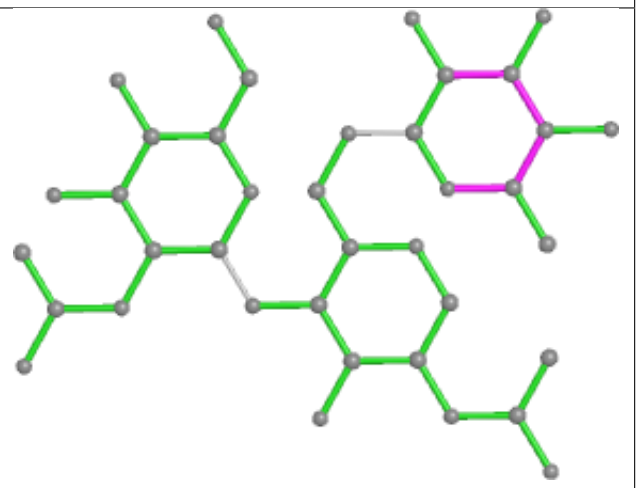
Oligosaccharide Chain N



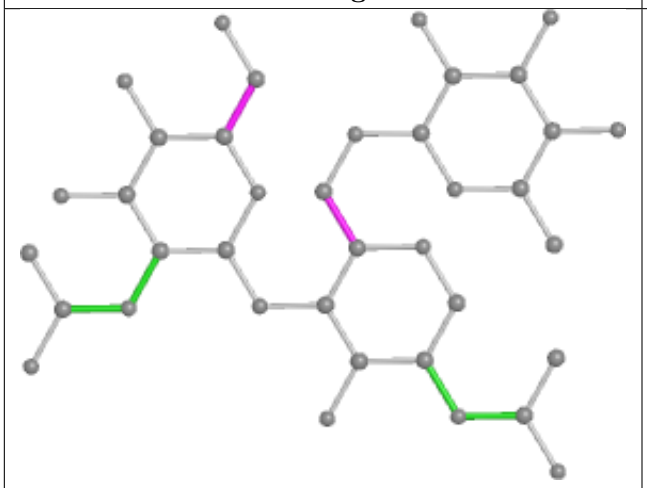
Oligosaccharide Chain O



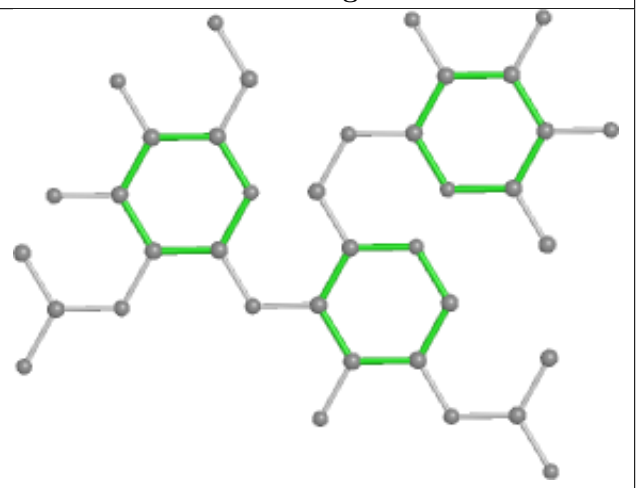
Bond lengths



Bond angles

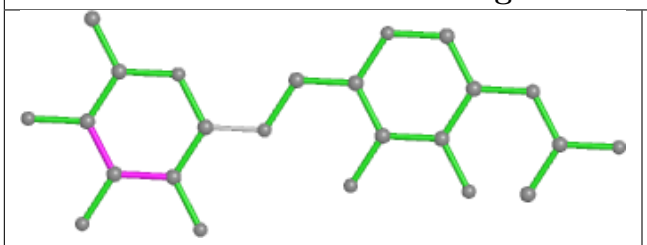


Torsions

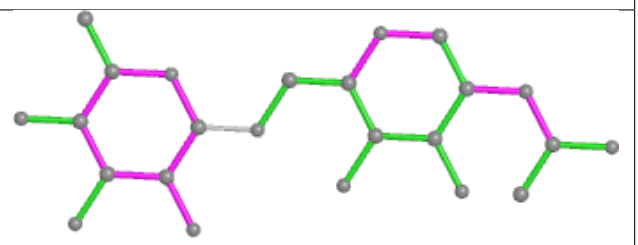


Rings

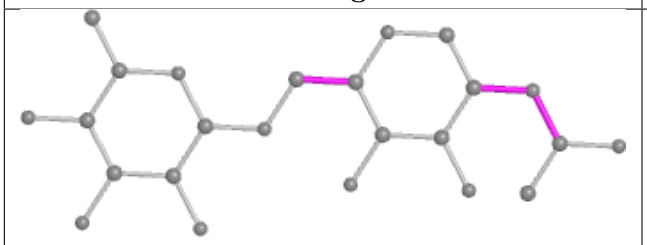
Oligosaccharide Chain K



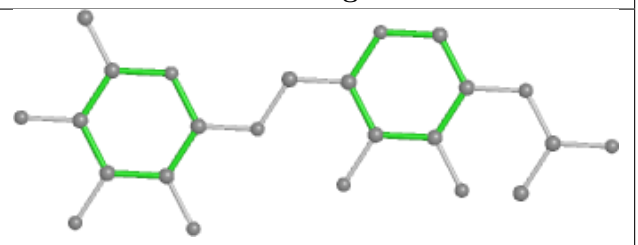
Bond lengths



Bond angles

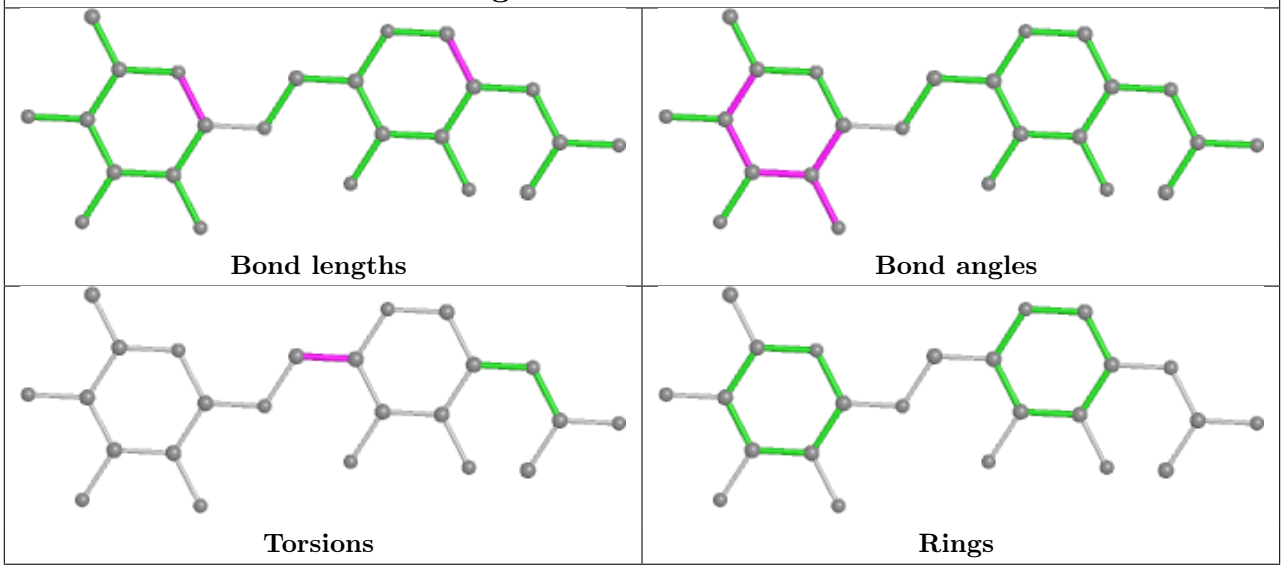


Torsions



Rings

Oligosaccharide Chain M



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	0.62	0	17,19,21	1.33	2 (11%)
4	NAG	F	504	1	14,14,15	0.47	0	17,19,21	0.47	0
4	NAG	C	501	1	14,14,15	0.87	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	F	501	1	14,14,15	0.43	0	17,19,21	1.48	1 (5%)
6	GOL	D	507	-	5,5,5	0.41	0	5,5,5	0.37	0
4	NAG	B	501	1	14,14,15	0.86	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	D	502	1	14,14,15	0.50	0	17,19,21	0.43	0
4	NAG	H	505	1	14,14,15	0.95	2 (14%)	17,19,21	0.61	1 (5%)
4	NAG	C	505	1	14,14,15	0.86	1 (7%)	17,19,21	0.79	1 (5%)
4	NAG	A	502	1	14,14,15	0.97	1 (7%)	17,19,21	0.68	1 (5%)
4	NAG	B	505	1	14,14,15	0.79	1 (7%)	17,19,21	0.75	0
6	GOL	C	508	-	5,5,5	0.36	0	5,5,5	0.73	0
4	NAG	A	501	1	14,14,15	1.57	1 (7%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	502	1	14,14,15	0.89	1 (7%)	17,19,21	0.93	1 (5%)
6	GOL	H	508	-	5,5,5	0.38	0	5,5,5	0.36	0
6	GOL	G	508	-	5,5,5	0.31	0	5,5,5	0.75	0
4	NAG	D	501	1	14,14,15	0.86	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	G	501	1	14,14,15	0.58	1 (7%)	17,19,21	0.73	1 (5%)
4	NAG	H	504	1	14,14,15	0.85	1 (7%)	17,19,21	0.71	1 (5%)
6	GOL	A	506	-	5,5,5	0.31	0	5,5,5	0.32	0
4	NAG	E	501	1	14,14,15	0.82	1 (7%)	17,19,21	0.82	1 (5%)
6	GOL	E	508	-	5,5,5	0.38	0	5,5,5	0.21	0
4	NAG	G	505	1	14,14,15	0.97	1 (7%)	17,19,21	0.84	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
4	NAG	F	504	1	-	0/6/23/26	0/1/1/1
4	NAG	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	F	501	1	-	1/6/23/26	0/1/1/1
6	GOL	D	507	-	-	2/4/4/4	-
4	NAG	B	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	H	505	1	-	1/6/23/26	0/1/1/1
4	NAG	C	505	1	-	1/6/23/26	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	505	1	-	2/6/23/26	0/1/1/1
6	GOL	C	508	-	-	4/4/4/4	-
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	E	502	1	-	4/6/23/26	0/1/1/1
6	GOL	H	508	-	-	1/4/4/4	-
6	GOL	G	508	-	-	2/4/4/4	-
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	1/6/23/26	0/1/1/1
4	NAG	H	504	1	-	2/6/23/26	0/1/1/1
6	GOL	A	506	-	-	4/4/4/4	-
4	NAG	E	501	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	508	-	-	2/4/4/4	-
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	O5-C1	5.53	1.52	1.43
4	A	502	NAG	O5-C1	3.36	1.49	1.43
4	G	505	NAG	O5-C1	3.33	1.49	1.43
4	E	502	NAG	O5-C1	3.03	1.48	1.43
4	C	505	NAG	O5-C1	3.00	1.48	1.43
4	D	501	NAG	O5-C1	2.87	1.48	1.43
4	C	501	NAG	O5-C1	2.84	1.48	1.43
4	H	505	NAG	O5-C1	2.77	1.48	1.43
4	H	504	NAG	O5-C1	2.63	1.47	1.43
4	B	505	NAG	O5-C1	2.61	1.47	1.43
4	B	501	NAG	O5-C1	2.44	1.47	1.43
4	E	501	NAG	O5-C1	2.30	1.47	1.43
4	H	505	NAG	C1-C2	2.11	1.55	1.52
4	G	501	NAG	O5-C1	2.01	1.46	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	501	NAG	C1-O5-C5	5.59	119.77	112.19
4	E	502	NAG	C1-O5-C5	3.54	116.99	112.19
4	D	501	NAG	C1-O5-C5	3.39	116.78	112.19
4	B	501	NAG	C1-O5-C5	3.34	116.72	112.19
4	A	503	NAG	C3-C4-C5	3.18	115.91	110.24
4	A	501	NAG	C1-O5-C5	3.12	116.42	112.19
4	G	505	NAG	C1-O5-C5	3.02	116.28	112.19
4	C	501	NAG	C1-O5-C5	2.99	116.24	112.19
4	A	503	NAG	C4-C3-C2	2.69	114.95	111.02
4	G	501	NAG	C1-O5-C5	2.62	115.74	112.19
4	E	501	NAG	C1-O5-C5	2.55	115.64	112.19
4	C	505	NAG	C1-O5-C5	2.49	115.56	112.19
4	H	504	NAG	C1-O5-C5	2.35	115.38	112.19
4	A	502	NAG	C1-O5-C5	2.35	115.38	112.19
4	H	505	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	508	GOL	1	0
6	E	508	GOL	2	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 (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	386/404 (95%)	-0.48	1 (0%)	94	95	15, 23, 35, 57	0
1	B	386/404 (95%)	-0.41	2 (0%)	91	93	17, 24, 36, 55	0
1	C	386/404 (95%)	-0.44	1 (0%)	94	95	16, 23, 36, 59	0
1	D	386/404 (95%)	-0.40	2 (0%)	91	93	17, 27, 39, 65	0
1	E	386/404 (95%)	-0.42	1 (0%)	94	95	15, 24, 36, 50	0
1	F	386/404 (95%)	-0.39	3 (0%)	86	89	17, 24, 39, 58	0
1	G	386/404 (95%)	-0.43	0	100	100	16, 24, 37, 55	0
1	H	386/404 (95%)	-0.27	4 (1%)	82	86	16, 27, 41, 64	0
All	All	3088/3232 (95%)	-0.41	14 (0%)	91	93	15, 24, 38, 65	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	4.5
1	F	149	VAL	3.4
1	F	148	THR	3.2
1	H	149	VAL	3.2
1	B	83	VAL	3.1
1	A	83	VAL	2.8
1	H	83	VAL	2.7
1	D	148	THR	2.6
1	B	435	ASN	2.1
1	D	83	VAL	2.1
1	F	336	CYS	2.1
1	C	83	VAL	2.0
1	H	148	THR	2.0
1	H	151	ASP	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)

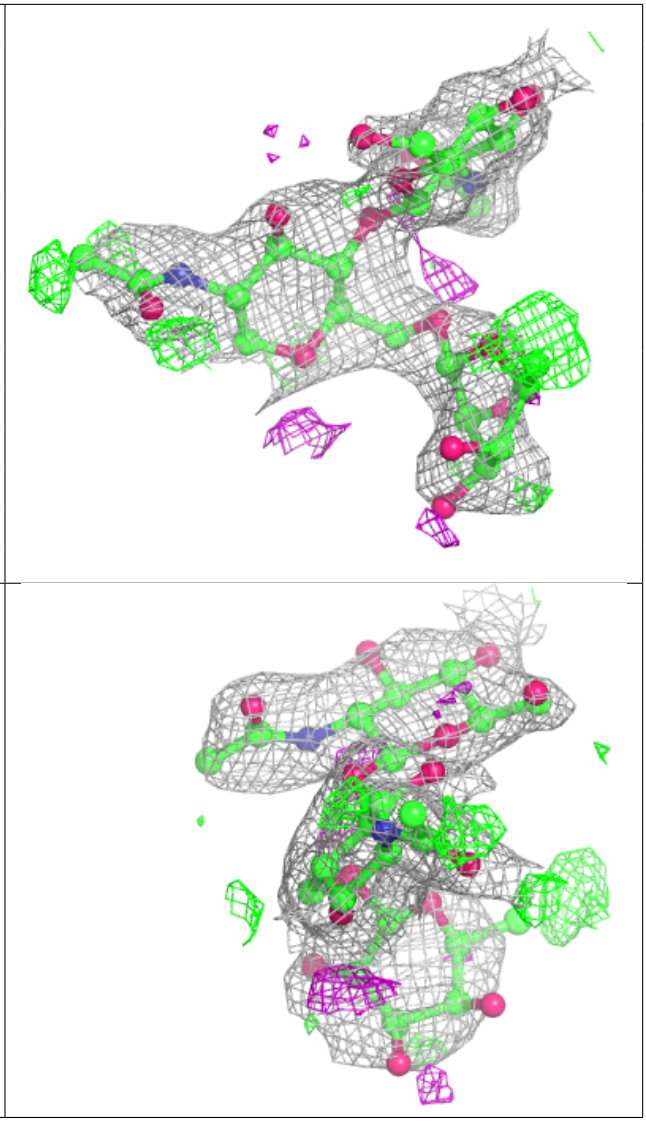
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	O	2	14/15	0.76	0.39	66,75,80,80	0
3	FUC	M	2	10/11	0.77	0.30	72,76,79,84	0
3	NAG	M	1	14/15	0.78	0.35	49,60,66,72	0
2	FUC	I	3	10/11	0.80	0.40	70,75,78,79	0
3	FUC	K	2	10/11	0.81	0.31	76,80,83,83	0
2	NAG	I	1	14/15	0.81	0.22	48,59,69,71	0
3	NAG	K	1	14/15	0.81	0.21	55,63,74,78	0
2	NAG	N	2	14/15	0.82	0.42	72,76,81,82	0
2	FUC	O	3	10/11	0.85	0.31	64,69,70,72	0
2	NAG	L	1	14/15	0.86	0.28	49,59,73,73	0
2	NAG	I	2	14/15	0.86	0.29	65,74,77,78	0
2	NAG	J	1	14/15	0.87	0.22	45,54,63,70	0
2	NAG	J	2	14/15	0.87	0.33	65,73,75,76	0
2	FUC	L	3	10/11	0.88	0.31	64,71,72,72	0
2	NAG	L	2	14/15	0.88	0.42	70,76,80,82	0
2	FUC	J	3	10/11	0.90	0.28	61,64,65,65	0
2	FUC	N	3	10/11	0.90	0.21	53,56,58,58	0
2	NAG	N	1	14/15	0.91	0.26	39,48,57,66	0
2	NAG	O	1	14/15	0.91	0.31	48,58,70,71	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.

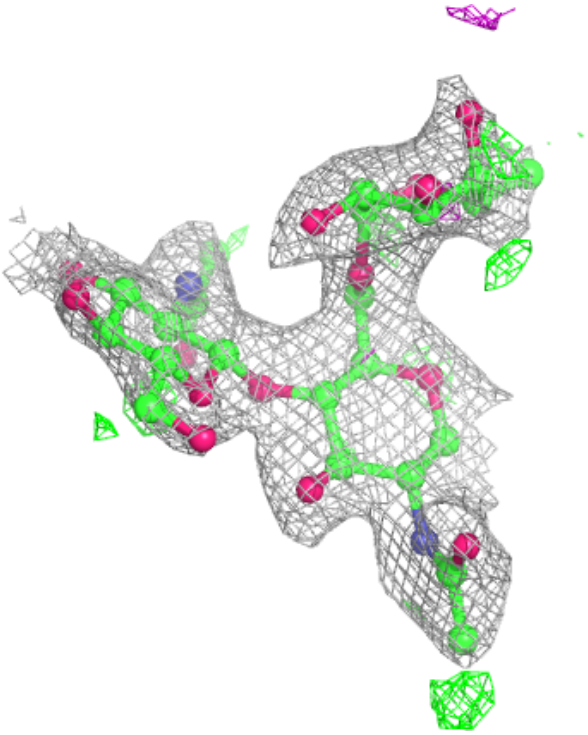
Electron density around Chain I:

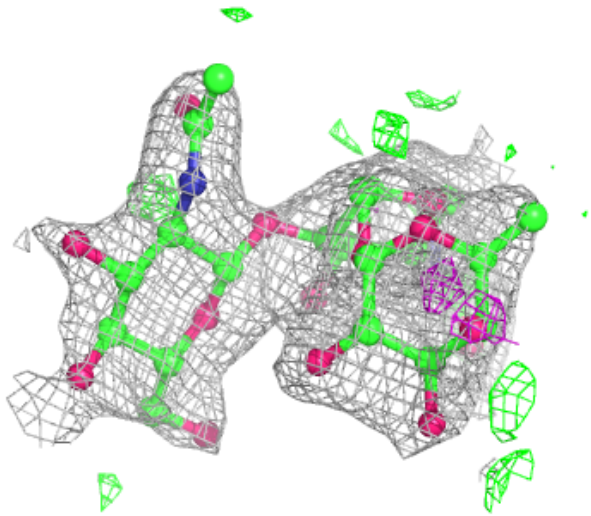
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

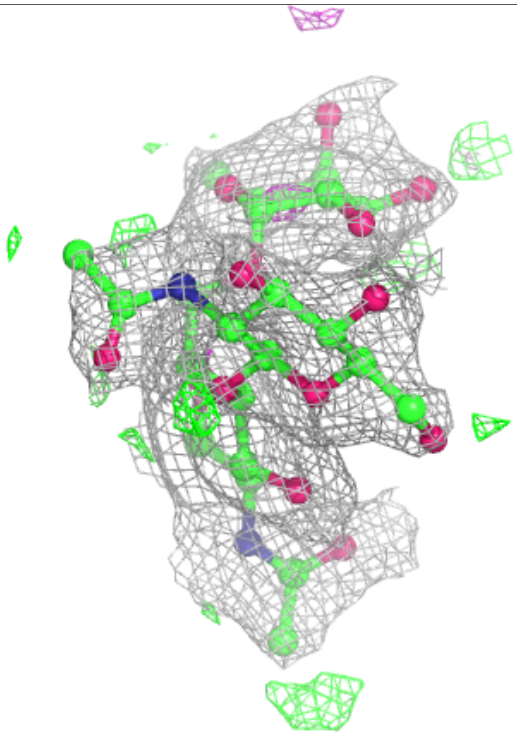


Electron density around Chain J:

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

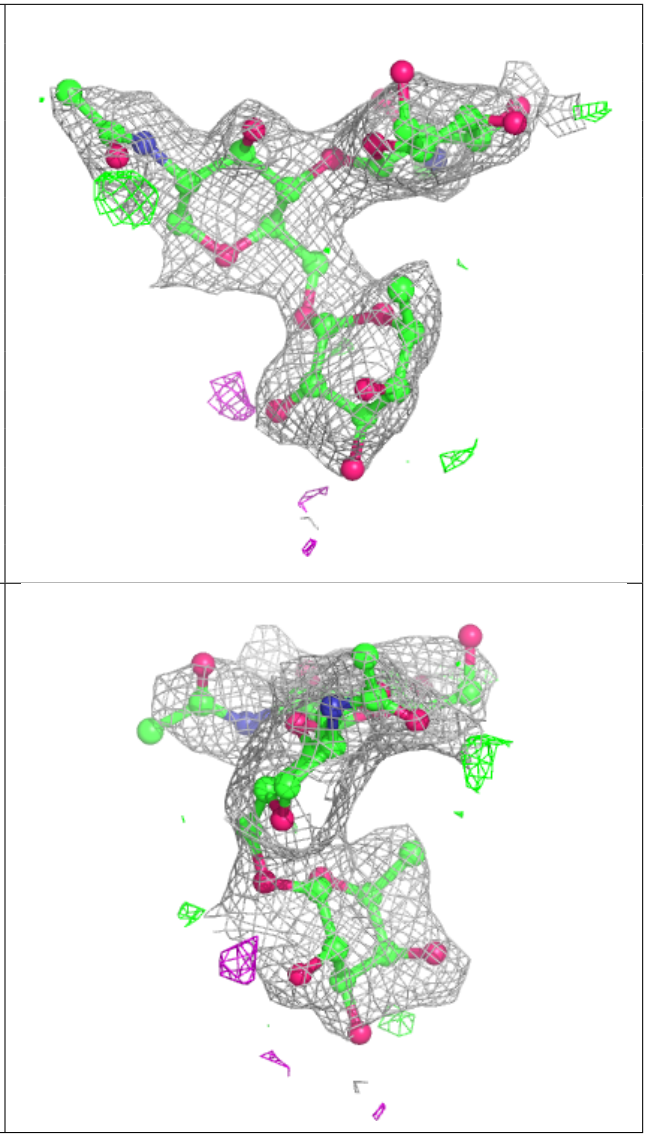






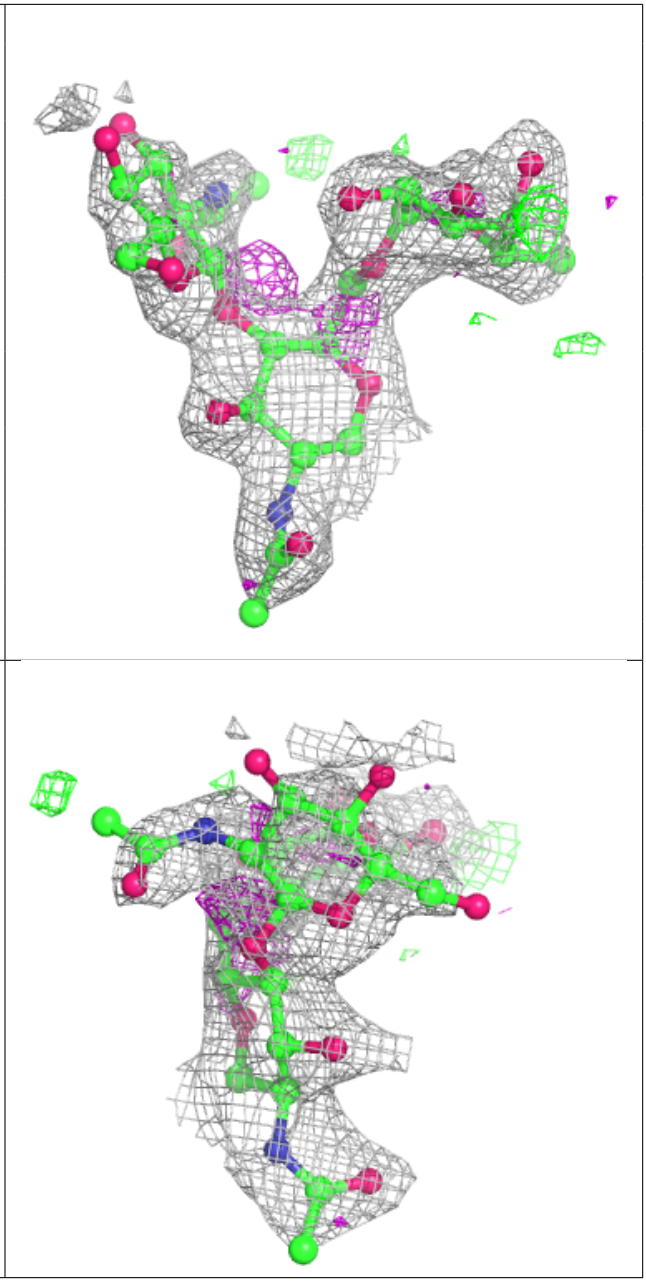
Electron density around Chain L:

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



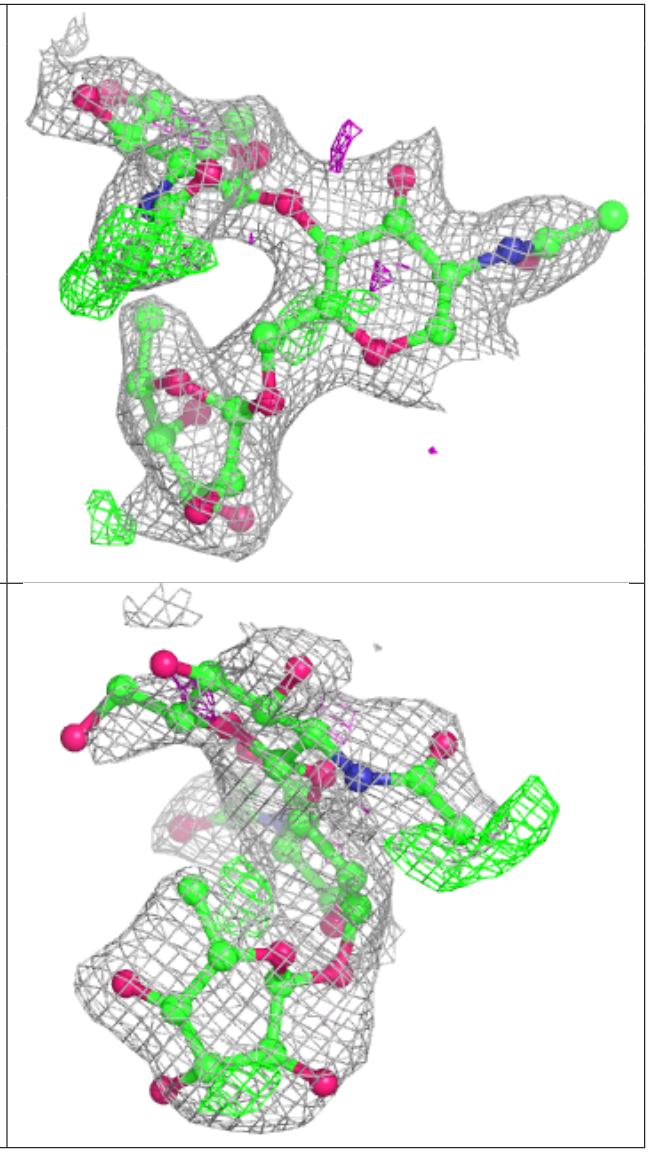
Electron density around Chain N:

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



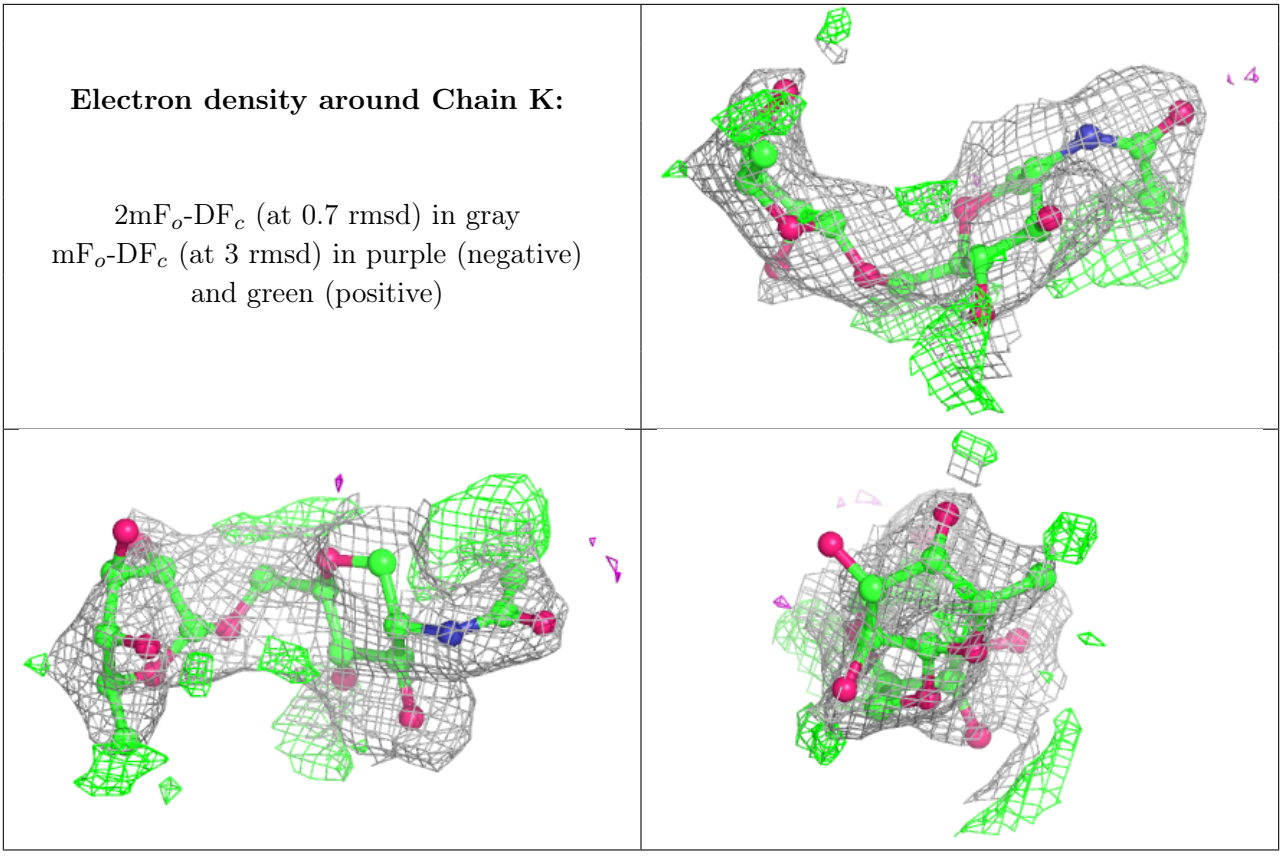
Electron density around Chain O:

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



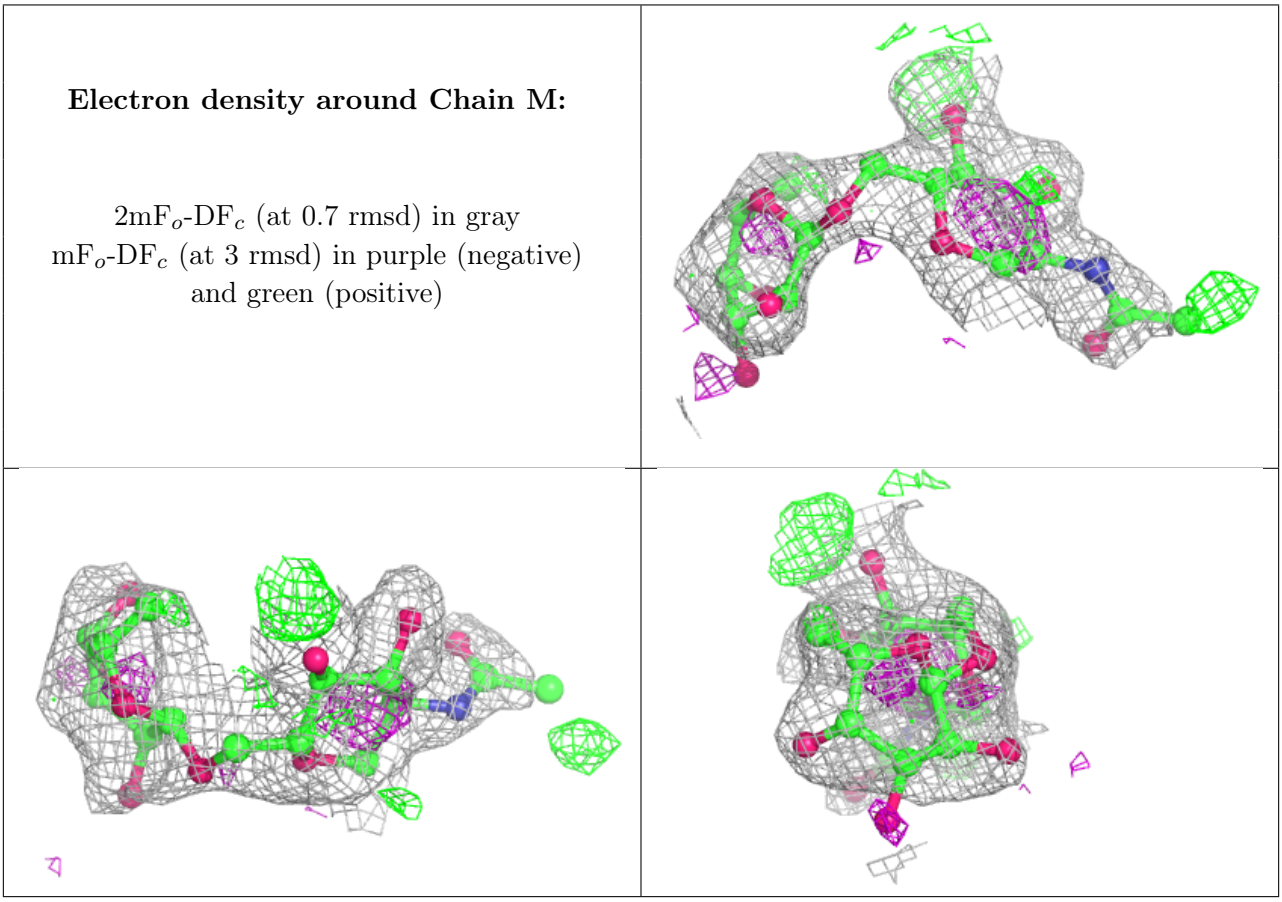
Electron density around Chain K:

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



Electron density around Chain M:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	F	504	14/15	0.64	0.30	61,68,74,76	0
4	NAG	A	502	14/15	0.65	0.35	65,76,82,84	0
4	NAG	E	502	14/15	0.75	0.30	57,66,69,71	0
4	NAG	G	501	14/15	0.76	0.24	55,63,72,72	0
4	NAG	H	505	14/15	0.76	0.29	58,68,72,73	0
4	NAG	A	503	14/15	0.77	0.30	57,66,71,73	0
4	NAG	B	505	14/15	0.79	0.27	53,61,68,69	0
4	NAG	G	505	14/15	0.80	0.25	50,60,63,63	0
4	NAG	E	501	14/15	0.80	0.20	47,54,64,64	0
4	NAG	C	505	14/15	0.82	0.33	62,76,80,80	0
4	NAG	F	501	14/15	0.82	0.24	49,54,62,63	0
4	NAG	A	501	14/15	0.82	0.17	45,50,55,55	0
4	NAG	D	502	14/15	0.83	0.22	58,65,71,71	0
4	NAG	B	501	14/15	0.84	0.25	51,59,69,74	0
4	NAG	H	504	14/15	0.85	0.20	51,57,66,67	0
4	NAG	C	501	14/15	0.87	0.16	47,54,64,66	0
4	NAG	D	501	14/15	0.88	0.19	47,58,65,65	0
6	GOL	D	507	6/6	0.89	0.27	44,48,53,56	0
6	GOL	A	506	6/6	0.90	0.22	41,43,50,54	0
6	GOL	G	508	6/6	0.91	0.13	35,38,38,40	0
6	GOL	H	508	6/6	0.91	0.14	44,47,48,48	0
5	CA	E	509	1/1	0.92	0.12	69,69,69,69	1
6	GOL	E	508	6/6	0.92	0.21	39,47,50,53	0
6	GOL	C	508	6/6	0.93	0.17	41,44,44,47	0
5	CA	A	507	1/1	0.96	0.10	60,60,60,60	0
5	CA	H	506	1/1	0.96	0.07	25,25,25,25	0
5	CA	H	507	1/1	0.98	0.08	34,34,34,34	0
5	CA	F	506	1/1	0.99	0.06	29,29,29,29	0
5	CA	G	506	1/1	0.99	0.08	25,25,25,25	0
5	CA	B	506	1/1	0.99	0.12	20,20,20,20	0
5	CA	B	507	1/1	0.99	0.04	23,23,23,23	0
5	CA	C	506	1/1	0.99	0.07	21,21,21,21	0
5	CA	C	507	1/1	0.99	0.04	23,23,23,23	0
5	CA	D	506	1/1	0.99	0.06	35,35,35,35	0
5	CA	E	506	1/1	0.99	0.08	20,20,20,20	0
5	CA	A	504	1/1	0.99	0.08	16,16,16,16	0
5	CA	F	505	1/1	0.99	0.05	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	D	505	1/1	1.00	0.06	27,27,27,27	0
5	CA	E	507	1/1	1.00	0.09	26,26,26,26	0
5	CA	A	505	1/1	1.00	0.05	28,28,28,28	0
5	CA	G	507	1/1	1.00	0.05	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.