



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 07:27 AM EDT

PDB ID : 4FMI  
Title : Merkel cell polyomavirus VP1 in complex with 3'-sialyllactosamine  
Authors : Neu, U.; Hengel, H.; Stehle, T.  
Deposited on : 2012-06-17  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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
buster-report	:	1.1.7 (2018)
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

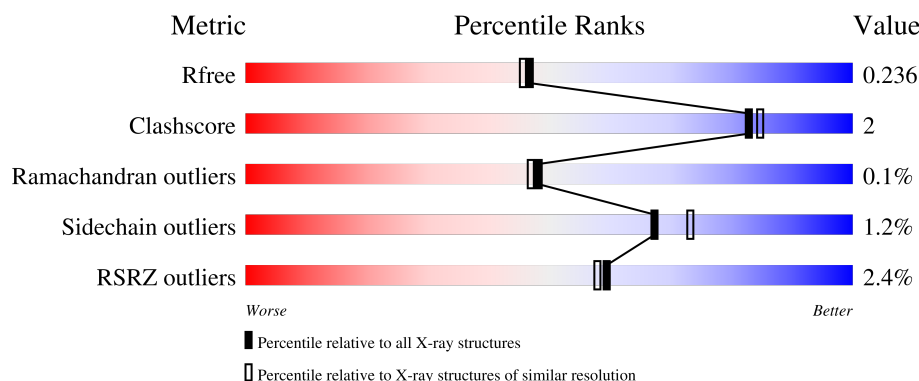
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	289	<div> <div>0%</div> <div>88%</div> <div>6%</div> <div>7%</div> </div>
1	B	289	<div> <div>0%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
1	C	289	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	D	289	<div> <div>0%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	E	289	<div> <div>2%</div> <div>87%</div> <div>6%</div> <div>• 6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	289	
1	G	289	
1	H	289	
1	I	289	
1	J	289	
1	K	289	
1	L	289	
1	M	289	
1	N	289	
1	O	289	
1	P	289	
1	Q	289	
1	R	289	
1	S	289	
1	T	289	
2	U	3	
3	V	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	L	501	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47100 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	3	0
			2127	1359	352	406	10			
1	B	279	Total	C	N	O	S	0	2	0
			2188	1391	362	424	11			
1	C	279	Total	C	N	O	S	0	5	0
			2204	1403	364	426	11			
1	D	270	Total	C	N	O	S	0	4	0
			2134	1362	354	408	10			
1	E	271	Total	C	N	O	S	0	2	0
			2128	1359	354	405	10			
1	F	272	Total	C	N	O	S	0	3	0
			2147	1370	356	411	10			
1	G	274	Total	C	N	O	S	0	4	0
			2159	1377	357	415	10			
1	H	280	Total	C	N	O	S	0	4	0
			2212	1407	368	426	11			
1	I	270	Total	C	N	O	S	0	3	0
			2124	1357	352	405	10			
1	J	271	Total	C	N	O	S	0	2	0
			2131	1360	353	408	10			
1	K	274	Total	C	N	O	S	0	5	0
			2170	1383	359	418	10			
1	L	271	Total	C	N	O	S	0	2	0
			2125	1356	352	407	10			
1	M	278	Total	C	N	O	S	0	0	0
			2171	1383	358	419	11			
1	N	278	Total	C	N	O	S	0	3	0
			2193	1395	362	424	12			
1	O	271	Total	C	N	O	S	0	3	0
			2133	1360	353	410	10			
1	P	273	Total	C	N	O	S	0	4	0
			2160	1376	357	417	10			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	271	Total	C	N	O	S	0	1	0
			2124	1356	352	406	10			
1	R	278	Total	C	N	O	S	0	4	0
			2197	1399	362	425	11			
1	S	271	Total	C	N	O	S	0	2	0
			2128	1358	353	407	10			
1	T	273	Total	C	N	O	S	0	6	0
			2177	1387	363	417	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	expression tag	UNP C0JPK1
A	33	SER	-	expression tag	UNP C0JPK1
A	34	HIS	-	expression tag	UNP C0JPK1
A	35	MET	-	expression tag	UNP C0JPK1
A	36	LEU	-	expression tag	UNP C0JPK1
A	37	GLU	-	expression tag	UNP C0JPK1
B	32	GLY	-	expression tag	UNP C0JPK1
B	33	SER	-	expression tag	UNP C0JPK1
B	34	HIS	-	expression tag	UNP C0JPK1
B	35	MET	-	expression tag	UNP C0JPK1
B	36	LEU	-	expression tag	UNP C0JPK1
B	37	GLU	-	expression tag	UNP C0JPK1
C	32	GLY	-	expression tag	UNP C0JPK1
C	33	SER	-	expression tag	UNP C0JPK1
C	34	HIS	-	expression tag	UNP C0JPK1
C	35	MET	-	expression tag	UNP C0JPK1
C	36	LEU	-	expression tag	UNP C0JPK1
C	37	GLU	-	expression tag	UNP C0JPK1
D	32	GLY	-	expression tag	UNP C0JPK1
D	33	SER	-	expression tag	UNP C0JPK1
D	34	HIS	-	expression tag	UNP C0JPK1
D	35	MET	-	expression tag	UNP C0JPK1
D	36	LEU	-	expression tag	UNP C0JPK1
D	37	GLU	-	expression tag	UNP C0JPK1
E	32	GLY	-	expression tag	UNP C0JPK1
E	33	SER	-	expression tag	UNP C0JPK1
E	34	HIS	-	expression tag	UNP C0JPK1
E	35	MET	-	expression tag	UNP C0JPK1
E	36	LEU	-	expression tag	UNP C0JPK1
E	37	GLU	-	expression tag	UNP C0JPK1
F	32	GLY	-	expression tag	UNP C0JPK1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	33	SER	-	expression tag	UNP C0JPK1
F	34	HIS	-	expression tag	UNP C0JPK1
F	35	MET	-	expression tag	UNP C0JPK1
F	36	LEU	-	expression tag	UNP C0JPK1
F	37	GLU	-	expression tag	UNP C0JPK1
G	32	GLY	-	expression tag	UNP C0JPK1
G	33	SER	-	expression tag	UNP C0JPK1
G	34	HIS	-	expression tag	UNP C0JPK1
G	35	MET	-	expression tag	UNP C0JPK1
G	36	LEU	-	expression tag	UNP C0JPK1
G	37	GLU	-	expression tag	UNP C0JPK1
H	32	GLY	-	expression tag	UNP C0JPK1
H	33	SER	-	expression tag	UNP C0JPK1
H	34	HIS	-	expression tag	UNP C0JPK1
H	35	MET	-	expression tag	UNP C0JPK1
H	36	LEU	-	expression tag	UNP C0JPK1
H	37	GLU	-	expression tag	UNP C0JPK1
I	32	GLY	-	expression tag	UNP C0JPK1
I	33	SER	-	expression tag	UNP C0JPK1
I	34	HIS	-	expression tag	UNP C0JPK1
I	35	MET	-	expression tag	UNP C0JPK1
I	36	LEU	-	expression tag	UNP C0JPK1
I	37	GLU	-	expression tag	UNP C0JPK1
J	32	GLY	-	expression tag	UNP C0JPK1
J	33	SER	-	expression tag	UNP C0JPK1
J	34	HIS	-	expression tag	UNP C0JPK1
J	35	MET	-	expression tag	UNP C0JPK1
J	36	LEU	-	expression tag	UNP C0JPK1
J	37	GLU	-	expression tag	UNP C0JPK1
K	32	GLY	-	expression tag	UNP C0JPK1
K	33	SER	-	expression tag	UNP C0JPK1
K	34	HIS	-	expression tag	UNP C0JPK1
K	35	MET	-	expression tag	UNP C0JPK1
K	36	LEU	-	expression tag	UNP C0JPK1
K	37	GLU	-	expression tag	UNP C0JPK1
L	32	GLY	-	expression tag	UNP C0JPK1
L	33	SER	-	expression tag	UNP C0JPK1
L	34	HIS	-	expression tag	UNP C0JPK1
L	35	MET	-	expression tag	UNP C0JPK1
L	36	LEU	-	expression tag	UNP C0JPK1
L	37	GLU	-	expression tag	UNP C0JPK1
M	32	GLY	-	expression tag	UNP C0JPK1

*Continued on next page...*

*Continued from previous page...*

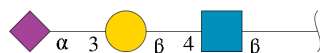
Chain	Residue	Modelled	Actual	Comment	Reference
M	33	SER	-	expression tag	UNP C0JPK1
M	34	HIS	-	expression tag	UNP C0JPK1
M	35	MET	-	expression tag	UNP C0JPK1
M	36	LEU	-	expression tag	UNP C0JPK1
M	37	GLU	-	expression tag	UNP C0JPK1
N	32	GLY	-	expression tag	UNP C0JPK1
N	33	SER	-	expression tag	UNP C0JPK1
N	34	HIS	-	expression tag	UNP C0JPK1
N	35	MET	-	expression tag	UNP C0JPK1
N	36	LEU	-	expression tag	UNP C0JPK1
N	37	GLU	-	expression tag	UNP C0JPK1
O	32	GLY	-	expression tag	UNP C0JPK1
O	33	SER	-	expression tag	UNP C0JPK1
O	34	HIS	-	expression tag	UNP C0JPK1
O	35	MET	-	expression tag	UNP C0JPK1
O	36	LEU	-	expression tag	UNP C0JPK1
O	37	GLU	-	expression tag	UNP C0JPK1
P	32	GLY	-	expression tag	UNP C0JPK1
P	33	SER	-	expression tag	UNP C0JPK1
P	34	HIS	-	expression tag	UNP C0JPK1
P	35	MET	-	expression tag	UNP C0JPK1
P	36	LEU	-	expression tag	UNP C0JPK1
P	37	GLU	-	expression tag	UNP C0JPK1
Q	32	GLY	-	expression tag	UNP C0JPK1
Q	33	SER	-	expression tag	UNP C0JPK1
Q	34	HIS	-	expression tag	UNP C0JPK1
Q	35	MET	-	expression tag	UNP C0JPK1
Q	36	LEU	-	expression tag	UNP C0JPK1
Q	37	GLU	-	expression tag	UNP C0JPK1
R	32	GLY	-	expression tag	UNP C0JPK1
R	33	SER	-	expression tag	UNP C0JPK1
R	34	HIS	-	expression tag	UNP C0JPK1
R	35	MET	-	expression tag	UNP C0JPK1
R	36	LEU	-	expression tag	UNP C0JPK1
R	37	GLU	-	expression tag	UNP C0JPK1
S	32	GLY	-	expression tag	UNP C0JPK1
S	33	SER	-	expression tag	UNP C0JPK1
S	34	HIS	-	expression tag	UNP C0JPK1
S	35	MET	-	expression tag	UNP C0JPK1
S	36	LEU	-	expression tag	UNP C0JPK1
S	37	GLU	-	expression tag	UNP C0JPK1
T	32	GLY	-	expression tag	UNP C0JPK1

*Continued on next page...*

*Continued from previous page...*

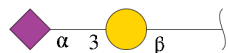
Chain	Residue	Modelled	Actual	Comment	Reference
T	33	SER	-	expression tag	UNP C0JPK1
T	34	HIS	-	expression tag	UNP C0JPK1
T	35	MET	-	expression tag	UNP C0JPK1
T	36	LEU	-	expression tag	UNP C0JPK1
T	37	GLU	-	expression tag	UNP C0JPK1

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



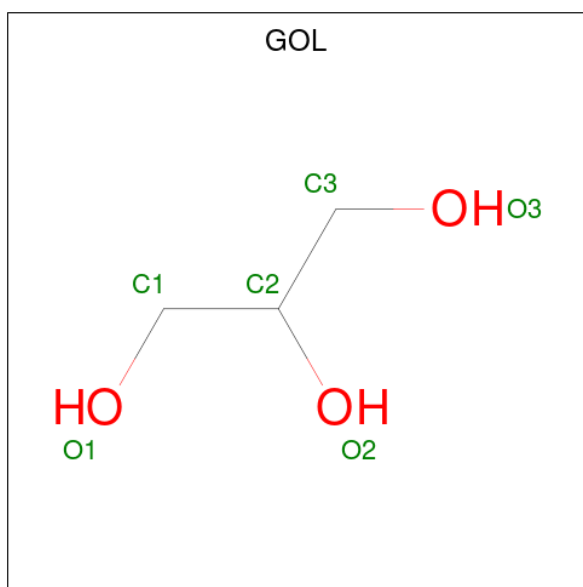
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	V	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0
4	P	1	Total C O 6 3 3	0	0
4	Q	1	Total C O 6 3 3	0	0
4	R	1	Total C O 6 3 3	0	0
4	R	1	Total C O 6 3 3	0	0
4	S	1	Total C O 6 3 3	0	0
4	T	1	Total C O 6 3 3	0	0

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

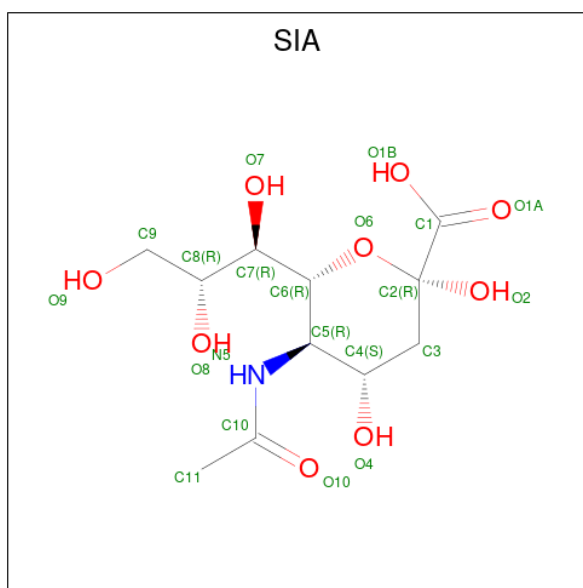
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		
5	K	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		
5	M	1	Total	Cl	0	0
			1	1		
5	N	1	Total	Cl	0	0
			1	1		
5	O	1	Total	Cl	0	0
			1	1		
5	P	1	Total	Cl	0	0
			1	1		
5	Q	1	Total	Cl	0	0
			1	1		
5	R	1	Total	Cl	0	0
			1	1		
5	S	2	Total	Cl	0	0
			2	2		
5	T	1	Total	Cl	0	0
			1	1		

- Molecule 6 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			21	11	1	9		
6	M	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	185	Total	O	0	0
			185	185		
7	B	184	Total	O	0	0
			184	184		
7	C	176	Total	O	0	0
			176	176		
7	D	188	Total	O	0	0
			188	188		
7	E	179	Total	O	0	0
			179	179		
7	F	162	Total	O	0	0
			162	162		
7	G	182	Total	O	0	0
			182	182		
7	H	173	Total	O	0	0
			173	173		
7	I	165	Total	O	0	0
			165	165		
7	J	163	Total	O	0	0
			163	163		
7	K	192	Total	O	0	0
			192	192		
7	L	192	Total	O	0	0
			192	192		
7	M	221	Total	O	0	0
			221	221		
7	N	191	Total	O	0	0
			191	191		
7	O	179	Total	O	0	0
			179	179		
7	P	194	Total	O	0	0
			194	194		
7	Q	184	Total	O	0	0
			184	184		
7	R	210	Total	O	0	0
			210	210		

*Continued on next page...*

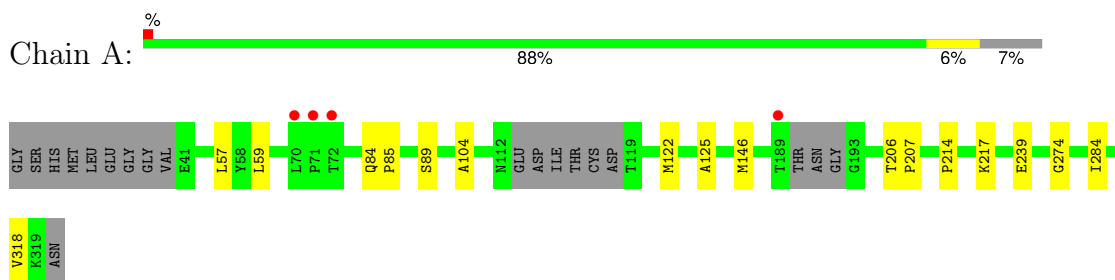
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	S	179	Total 179	O 179	0	0
7	T	178	Total 178	O 178	0	0

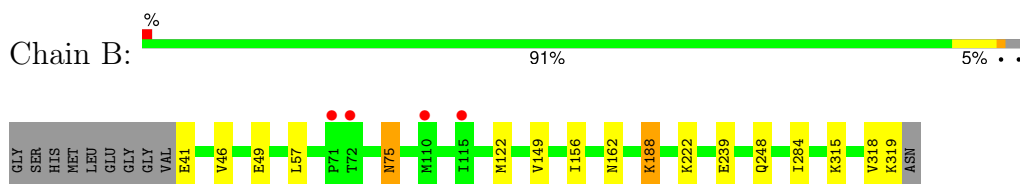
### 3 Residue-property plots [i](#)

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.

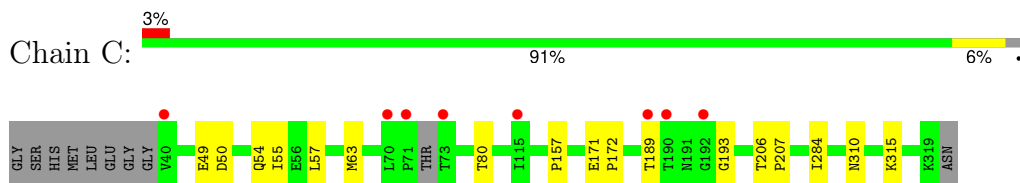
- Molecule 1: VP1



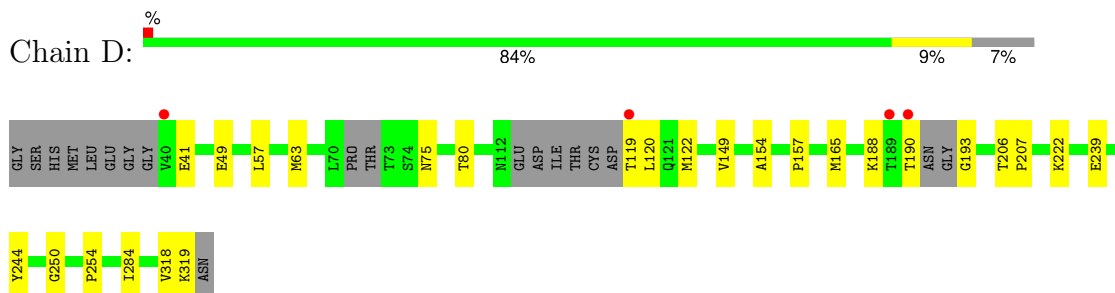
- Molecule 1: VP1



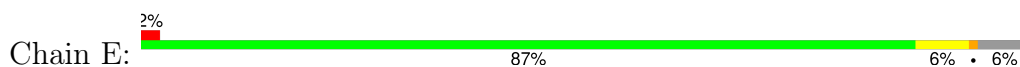
- Molecule 1: VP1

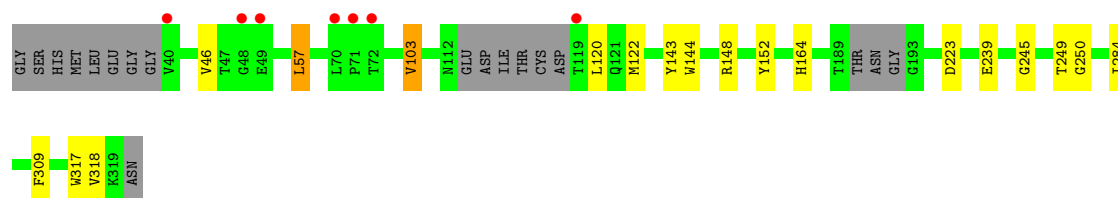


- Molecule 1: VP1

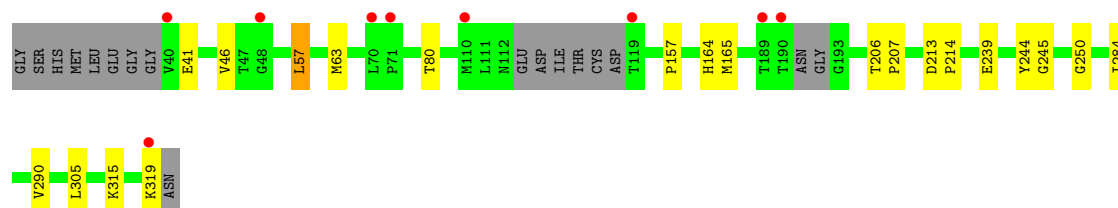
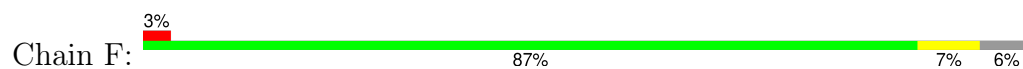


- Molecule 1: VP1

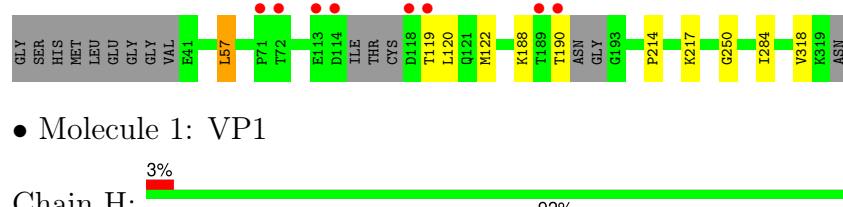




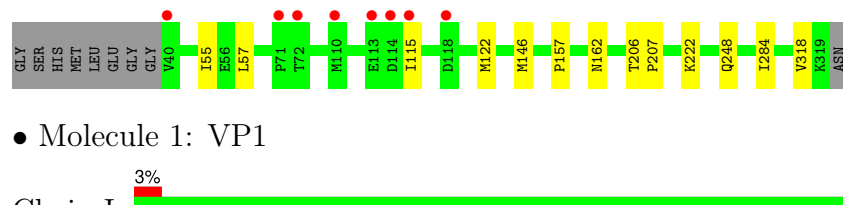
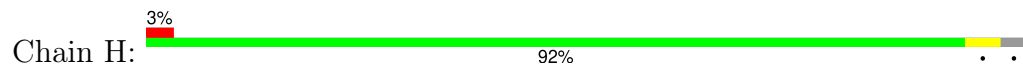
- Molecule 1: VP1



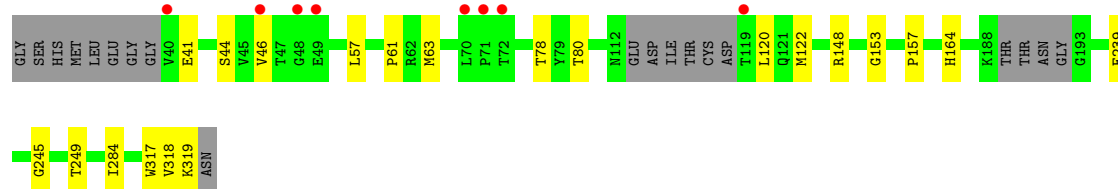
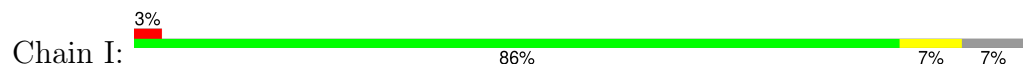
- Molecule 1: VP1



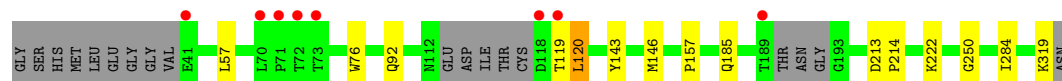
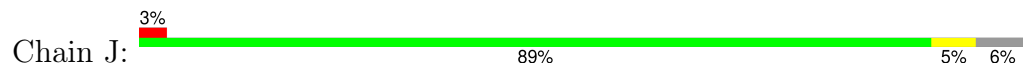
- Molecule 1: VP1



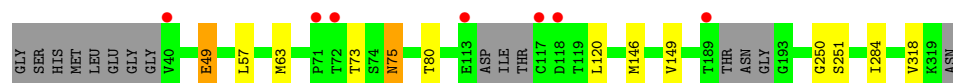
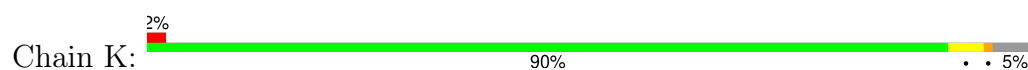
- Molecule 1: VP1



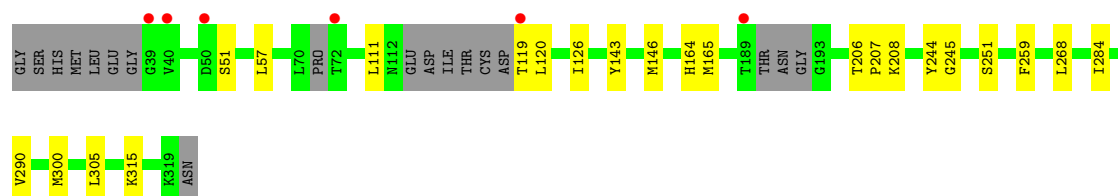
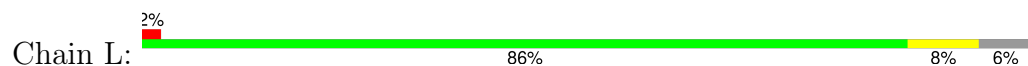
- Molecule 1: VP1



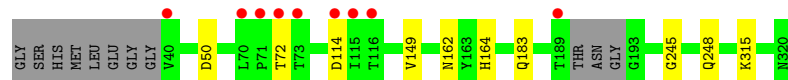
- Molecule 1: VP1



• Molecule 1: VP1



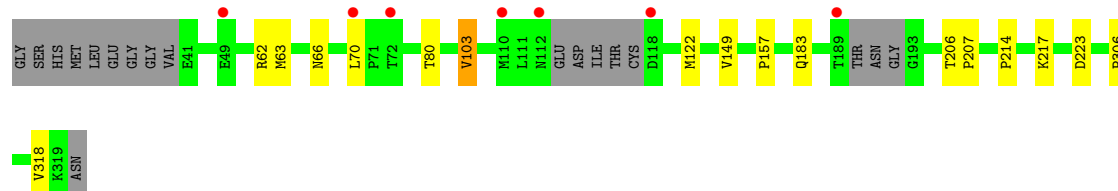
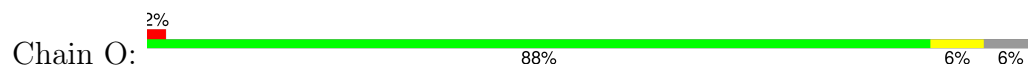
• Molecule 1: VP1



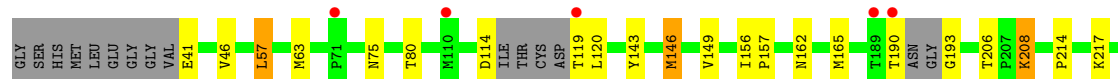
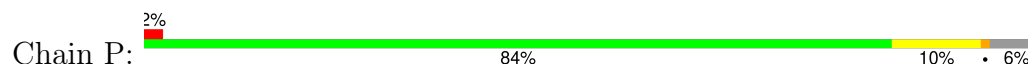
• Molecule 1: VP1

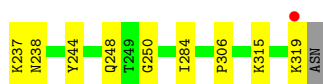


• Molecule 1: VP1

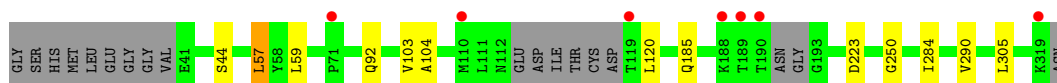
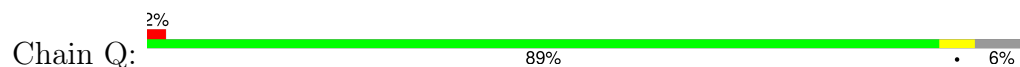


• Molecule 1: VP1





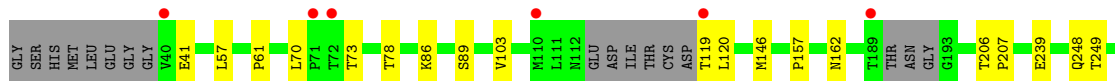
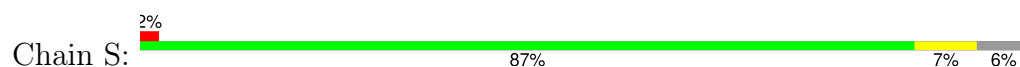
- Molecule 1: VP1



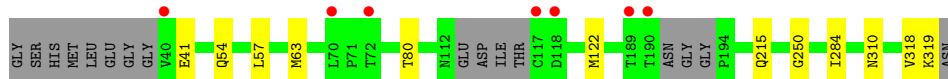
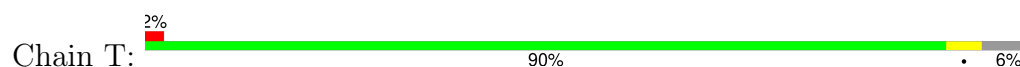
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.04Å 85.70Å 248.73Å 93.02° 100.41° 108.07°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-2.00) 89.6 (50.00-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.196 , 0.236 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	3934 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	47100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7749e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, NAG, GOL, CL

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	0.42	0/2181	0.55	0/2971
1	B	0.41	0/2241	0.55	0/3057
1	C	0.41	0/2262	0.55	0/3084
1	D	0.43	0/2186	0.55	0/2975
1	E	0.43	0/2182	0.56	0/2972
1	F	0.41	0/2198	0.54	0/2995
1	G	0.41	0/2213	0.54	0/3015
1	H	0.41	0/2268	0.53	0/3093
1	I	0.41	0/2175	0.54	0/2963
1	J	0.41	0/2185	0.55	1/2976 (0.0%)
1	K	0.41	0/2224	0.55	0/3030
1	L	0.41	0/2174	0.54	0/2959
1	M	0.42	0/2223	0.56	0/3029
1	N	0.41	0/2245	0.54	0/3058
1	O	0.41	0/2187	0.53	0/2980
1	P	0.41	0/2211	0.56	0/3013
1	Q	0.41	0/2175	0.55	0/2963
1	R	0.43	0/2249	0.56	0/3066
1	S	0.42	0/2179	0.54	0/2969
1	T	0.40	0/2231	0.55	0/3039
All	All	0.41	0/44189	0.55	1/60207 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	120	LEU	CA-CB-CG	5.58	128.13	115.30

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	2127	0	2114	11	0
1	B	2188	0	2160	10	0
1	C	2204	0	2182	10	0
1	D	2134	0	2115	16	0
1	E	2128	0	2116	13	0
1	F	2147	0	2131	13	0
1	G	2159	0	2135	6	0
1	H	2212	0	2190	7	0
1	I	2124	0	2103	12	0
1	J	2131	0	2113	7	0
1	K	2170	0	2142	11	0
1	L	2125	0	2109	15	0
1	M	2171	0	2148	7	0
1	N	2193	0	2165	10	0
1	O	2133	0	2106	10	0
1	P	2160	0	2135	18	0
1	Q	2124	0	2108	7	0
1	R	2197	0	2173	13	0
1	S	2128	0	2108	11	0
1	T	2177	0	2154	9	0
2	U	46	0	40	0	0
3	V	32	0	28	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	1	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	12	0	16	1	0
4	L	18	0	24	5	0
4	M	12	0	16	0	0
4	N	6	0	8	1	0
4	O	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	6	0	8	0	0
4	Q	6	0	8	0	0
4	R	12	0	16	2	0
4	S	6	0	8	0	0
4	T	6	0	8	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	1	0
5	L	1	0	0	1	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	2	0	0	0	0
5	T	1	0	0	1	0
6	E	21	0	18	0	0
6	M	21	0	18	0	0
7	A	185	0	0	0	0
7	B	184	0	0	0	0
7	C	176	0	0	1	0
7	D	188	0	0	0	0
7	E	179	0	0	1	0
7	F	162	0	0	0	0
7	G	182	0	0	0	0
7	H	173	0	0	1	0
7	I	165	0	0	0	0
7	J	163	0	0	0	0
7	K	192	0	0	1	0
7	L	192	0	0	0	0
7	M	221	0	0	1	0
7	N	191	0	0	0	0
7	O	179	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	194	0	0	1	0
7	Q	184	0	0	0	0
7	R	210	0	0	0	0
7	S	179	0	0	2	0
7	T	178	0	0	1	0
All	All	47100	0	43011	197	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.

The worst 5 of 197 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:Q:57:LEU:HD21	1:Q:284:ILE:HD12	1.33	1.10
1:R:57:LEU:HD21	1:R:284:ILE:HD12	1.45	0.98
1:D:57:LEU:HD21	1:D:284:ILE:HD13	1.48	0.94
1:L:57:LEU:HD21	1:L:284:ILE:HD13	1.53	0.91
1:P:57:LEU:HD21	1:P:284:ILE:HD12	1.56	0.85

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	267/289 (92%)	256 (96%)	11 (4%)	0	100	100
1	B	279/289 (96%)	263 (94%)	15 (5%)	1 (0%)	30	27
1	C	280/289 (97%)	268 (96%)	11 (4%)	1 (0%)	30	27
1	D	266/289 (92%)	257 (97%)	9 (3%)	0	100	100
1	E	267/289 (92%)	255 (96%)	12 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	269/289 (93%)	257 (96%)	12 (4%)	0	100	100
1	G	272/289 (94%)	258 (95%)	14 (5%)	0	100	100
1	H	282/289 (98%)	267 (95%)	15 (5%)	0	100	100
1	I	267/289 (92%)	257 (96%)	10 (4%)	0	100	100
1	J	267/289 (92%)	253 (95%)	14 (5%)	0	100	100
1	K	273/289 (94%)	261 (96%)	12 (4%)	0	100	100
1	L	265/289 (92%)	255 (96%)	10 (4%)	0	100	100
1	M	274/289 (95%)	262 (96%)	11 (4%)	1 (0%)	30	27
1	N	277/289 (96%)	264 (95%)	13 (5%)	0	100	100
1	O	268/289 (93%)	256 (96%)	12 (4%)	0	100	100
1	P	271/289 (94%)	259 (96%)	12 (4%)	0	100	100
1	Q	266/289 (92%)	256 (96%)	10 (4%)	0	100	100
1	R	278/289 (96%)	264 (95%)	14 (5%)	0	100	100
1	S	267/289 (92%)	253 (95%)	14 (5%)	0	100	100
1	T	273/289 (94%)	258 (94%)	15 (6%)	0	100	100
All	All	5428/5780 (94%)	5179 (95%)	246 (4%)	3 (0%)	48	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	GLU
1	C	49	GLU
1	M	72	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	241/253 (95%)	239 (99%)	2 (1%)	79	84
1	B	248/253 (98%)	243 (98%)	5 (2%)	50	55

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	251/253 (99%)	250 (100%)	1 (0%)	89	92
1	D	241/253 (95%)	237 (98%)	4 (2%)	56	61
1	E	240/253 (95%)	236 (98%)	4 (2%)	56	61
1	F	243/253 (96%)	241 (99%)	2 (1%)	79	84
1	G	244/253 (96%)	240 (98%)	4 (2%)	58	64
1	H	251/253 (99%)	248 (99%)	3 (1%)	67	73
1	I	239/253 (94%)	237 (99%)	2 (1%)	79	84
1	J	241/253 (95%)	237 (98%)	4 (2%)	56	61
1	K	245/253 (97%)	238 (97%)	7 (3%)	37	39
1	L	240/253 (95%)	238 (99%)	2 (1%)	79	84
1	M	246/253 (97%)	245 (100%)	1 (0%)	89	92
1	N	249/253 (98%)	244 (98%)	5 (2%)	50	55
1	O	241/253 (95%)	239 (99%)	2 (1%)	79	84
1	P	245/253 (97%)	238 (97%)	7 (3%)	37	39
1	Q	240/253 (95%)	238 (99%)	2 (1%)	79	84
1	R	250/253 (99%)	249 (100%)	1 (0%)	89	92
1	S	240/253 (95%)	235 (98%)	5 (2%)	48	53
1	T	246/253 (97%)	246 (100%)	0	100	100
All	All	4881/5060 (96%)	4818 (99%)	63 (1%)	67	71

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	146	MET
1	Q	57	LEU
1	K	120	LEU
1	P	208	LYS
1	S	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	225	ASN
1	L	92	GLN
1	R	183	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	183	GLN
1	Q	183	GLN

### 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 ⓘ

5 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	U	1	2	15,15,15	0.50	0	21,21,21	0.93	0
2	GAL	U	2	2	11,11,12	0.69	0	15,15,17	0.85	1 (6%)
2	SIA	U	3	2	20,20,21	0.80	0	21,28,31	1.15	2 (9%)
3	GAL	V	1	3	12,12,12	0.51	0	17,17,17	0.59	0
3	SIA	V	2	3	20,20,21	0.67	0	21,28,31	0.96	2 (9%)

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	U	1	2	-	0/6/26/26	0/1/1/1
2	GAL	U	2	2	-	1/2/19/22	0/1/1/1
2	SIA	U	3	2	-	0/18/34/38	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	V	1	3	-	0/2/22/22	0/1/1/1
3	SIA	V	2	3	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	SIA	O1B-C1-C2	2.40	118.94	112.71
3	V	2	SIA	O6-C2-C1	2.31	112.08	107.72
2	U	2	GAL	C1-C2-C3	2.25	112.91	109.64
2	U	3	SIA	O1B-C1-C2	2.20	118.44	112.71
2	U	3	SIA	O6-C2-C1	2.16	111.79	107.72

There are no chirality outliers.

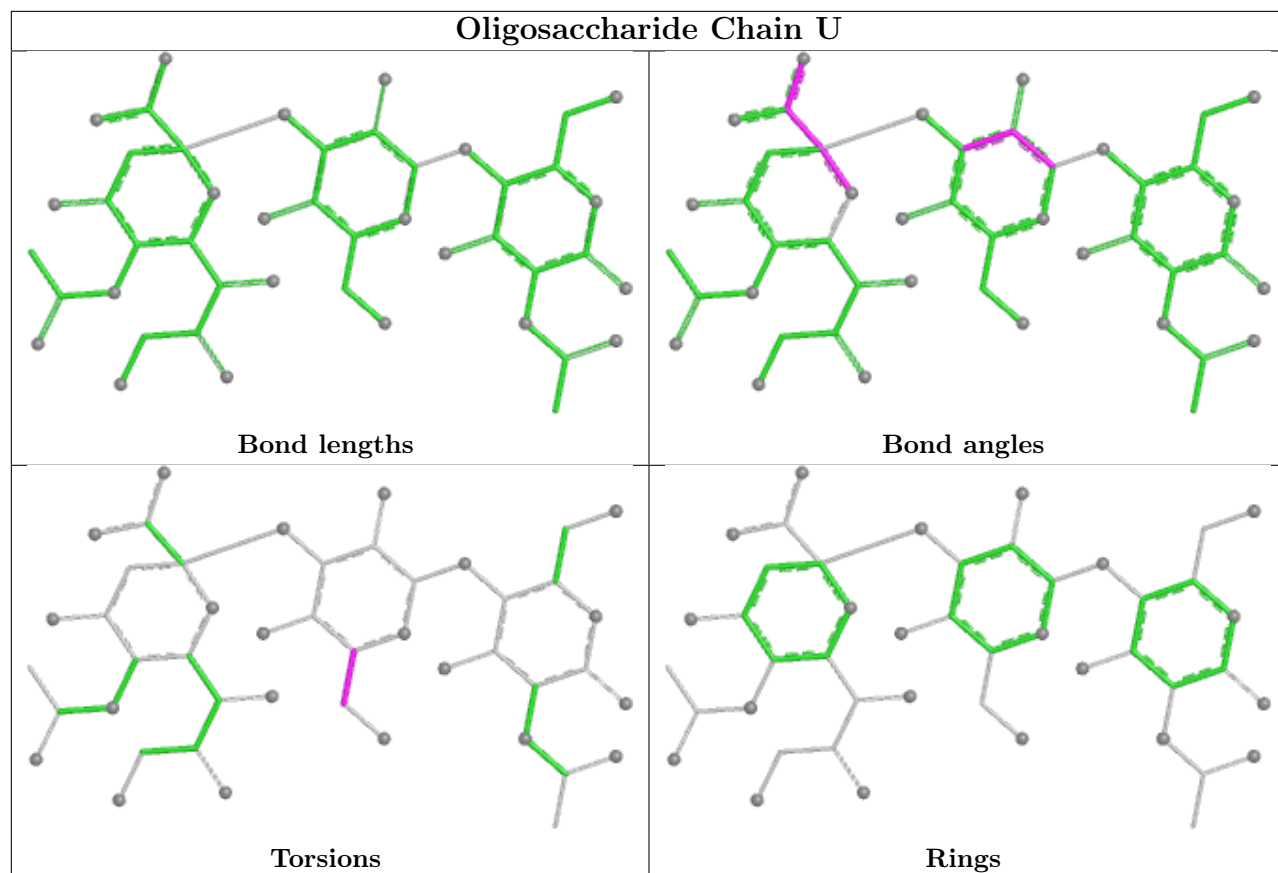
All (3) torsion outliers are listed below:

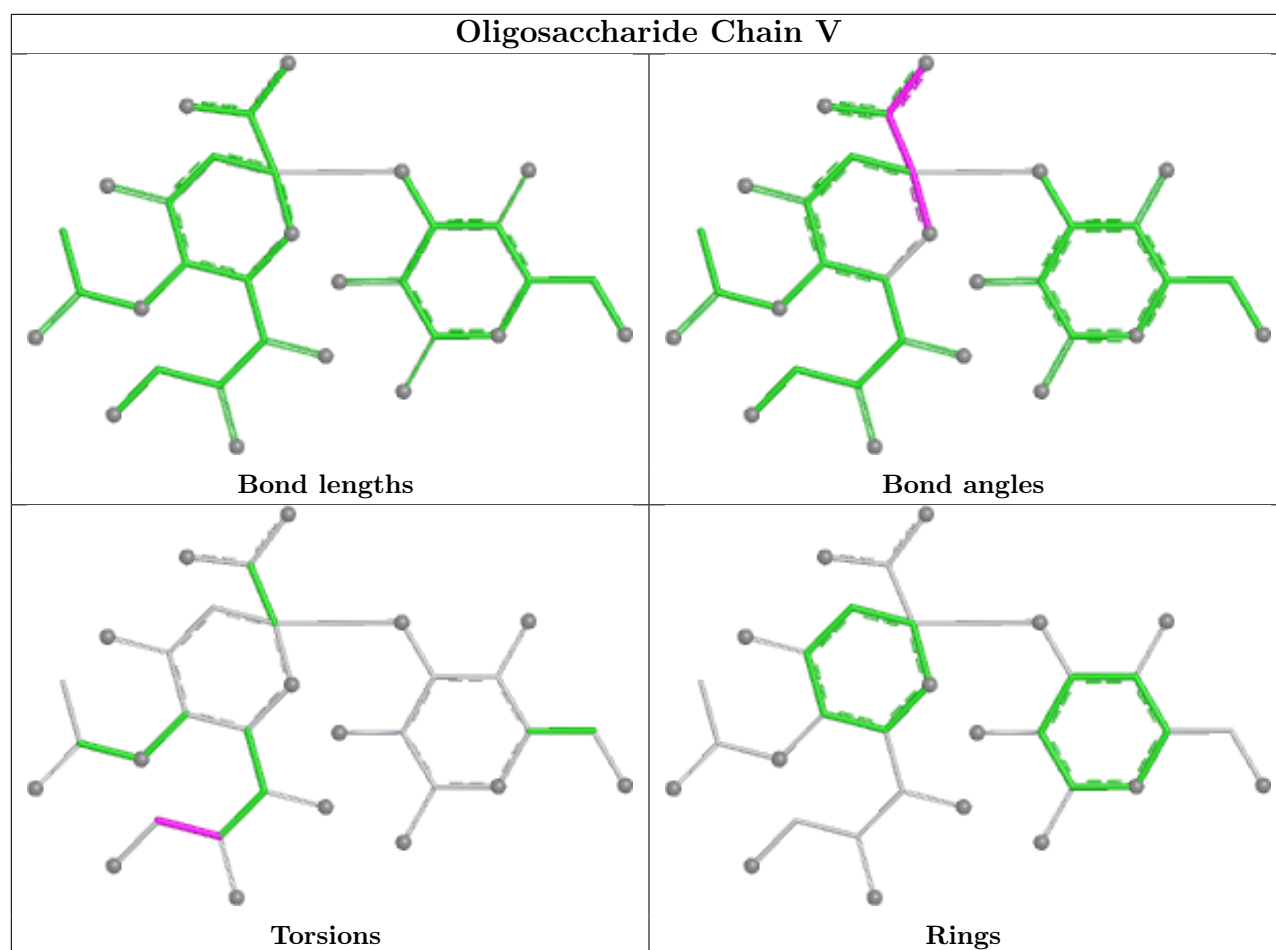
Mol	Chain	Res	Type	Atoms
2	U	2	GAL	O5-C5-C6-O6
3	V	2	SIA	O8-C8-C9-O9
3	V	2	SIA	C7-C8-C9-O9

There are no ring outliers.

No monomer is involved in short contacts.

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 48 ligands modelled in this entry, 21 are monoatomic - leaving 27 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	GOL	C	401	-	5,5,5	0.40	0	5,5,5	0.22	0
4	GOL	L	503	-	5,5,5	0.38	0	5,5,5	0.41	0
4	GOL	N	401	-	5,5,5	0.43	0	5,5,5	0.26	0
4	GOL	Q	401	-	5,5,5	0.52	0	5,5,5	0.82	0
4	GOL	T	403	-	5,5,5	0.47	0	5,5,5	0.33	0
4	GOL	D	401	-	5,5,5	0.47	0	5,5,5	0.40	0
4	GOL	M	403	-	5,5,5	0.41	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	401	-	5,5,5	0.48	0	5,5,5	0.35	0
4	GOL	A	404	-	5,5,5	0.45	0	5,5,5	0.21	0
4	GOL	F	401	-	5,5,5	0.31	0	5,5,5	0.54	0
4	GOL	R	501	-	5,5,5	0.33	0	5,5,5	0.66	0
4	GOL	E	402	-	5,5,5	0.46	0	5,5,5	0.31	0
6	SIA	M	401	-	21,21,21	1.04	2 (9%)	24,31,31	1.13	1 (4%)
4	GOL	K	403	-	5,5,5	0.43	0	5,5,5	0.20	0
4	GOL	K	401	-	5,5,5	0.52	0	5,5,5	0.39	0
4	GOL	R	502	-	5,5,5	0.47	0	5,5,5	0.32	0
6	SIA	E	401	-	21,21,21	0.98	1 (4%)	24,31,31	1.02	1 (4%)
4	GOL	J	401	-	5,5,5	0.45	0	5,5,5	0.30	0
4	GOL	O	401	-	5,5,5	0.44	0	5,5,5	0.62	0
4	GOL	I	401	-	5,5,5	0.42	0	5,5,5	0.20	0
4	GOL	L	502	-	5,5,5	0.49	0	5,5,5	0.38	0
4	GOL	M	402	-	5,5,5	0.52	0	5,5,5	0.55	0
4	GOL	G	401	-	5,5,5	0.47	0	5,5,5	0.52	0
4	GOL	L	501	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	S	401	-	5,5,5	0.39	0	5,5,5	0.47	0
4	GOL	H	401	-	5,5,5	0.42	0	5,5,5	0.19	0
4	GOL	P	401	-	5,5,5	0.44	0	5,5,5	0.28	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
4	GOL	C	401	-	-	2/4/4/4	-
4	GOL	L	503	-	-	4/4/4/4	-
4	GOL	N	401	-	-	2/4/4/4	-
4	GOL	Q	401	-	-	2/4/4/4	-
4	GOL	T	403	-	-	2/4/4/4	-
4	GOL	D	401	-	-	0/4/4/4	-
4	GOL	M	403	-	-	0/4/4/4	-
4	GOL	B	401	-	-	2/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	F	401	-	-	0/4/4/4	-
4	GOL	R	501	-	-	2/4/4/4	-
4	GOL	E	402	-	-	2/4/4/4	-
6	SIA	M	401	-	-	5/20/38/38	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	K	403	-	-	2/4/4/4	-
4	GOL	K	401	-	-	4/4/4/4	-
4	GOL	R	502	-	-	2/4/4/4	-
6	SIA	E	401	-	-	7/20/38/38	0/1/1/1
4	GOL	J	401	-	-	4/4/4/4	-
4	GOL	O	401	-	-	3/4/4/4	-
4	GOL	I	401	-	-	3/4/4/4	-
4	GOL	L	502	-	-	2/4/4/4	-
4	GOL	M	402	-	-	2/4/4/4	-
4	GOL	G	401	-	-	2/4/4/4	-
4	GOL	L	501	-	-	2/4/4/4	-
4	GOL	S	401	-	-	0/4/4/4	-
4	GOL	H	401	-	-	1/4/4/4	-
4	GOL	P	401	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	SIA	O2-C2	3.27	1.44	1.39
6	E	401	SIA	O2-C2	3.18	1.44	1.39
6	M	401	SIA	C3-C2	2.25	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	SIA	O1A-C1-C2	-3.56	117.91	123.85
6	E	401	SIA	O1A-C1-C2	-3.13	118.64	123.85

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	GOL	C1-C2-C3-O3
4	K	401	GOL	O1-C1-C2-C3
4	K	403	GOL	O1-C1-C2-C3
4	L	501	GOL	C1-C2-C3-O3
4	L	503	GOL	C1-C2-C3-O3

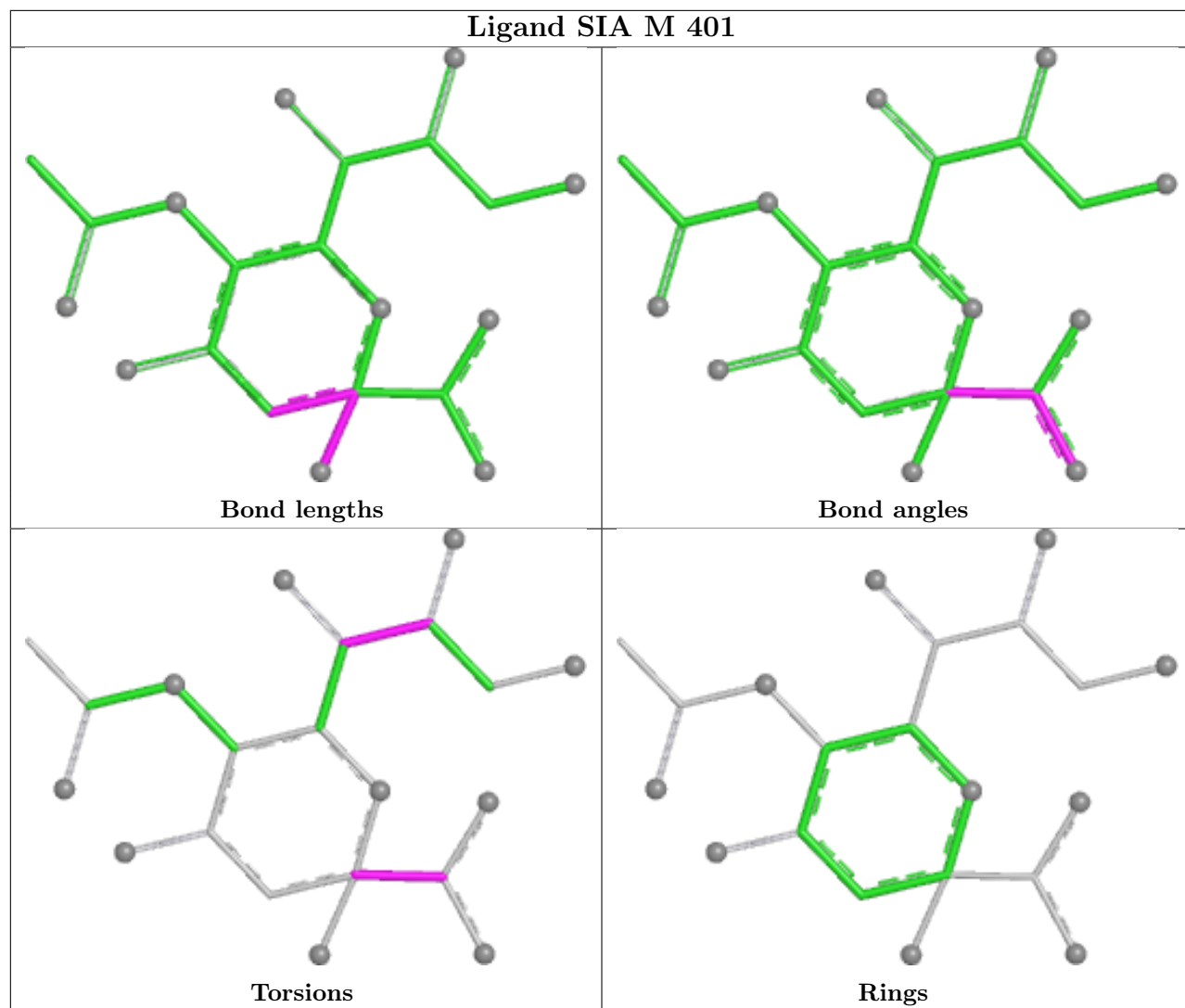
There are no ring outliers.

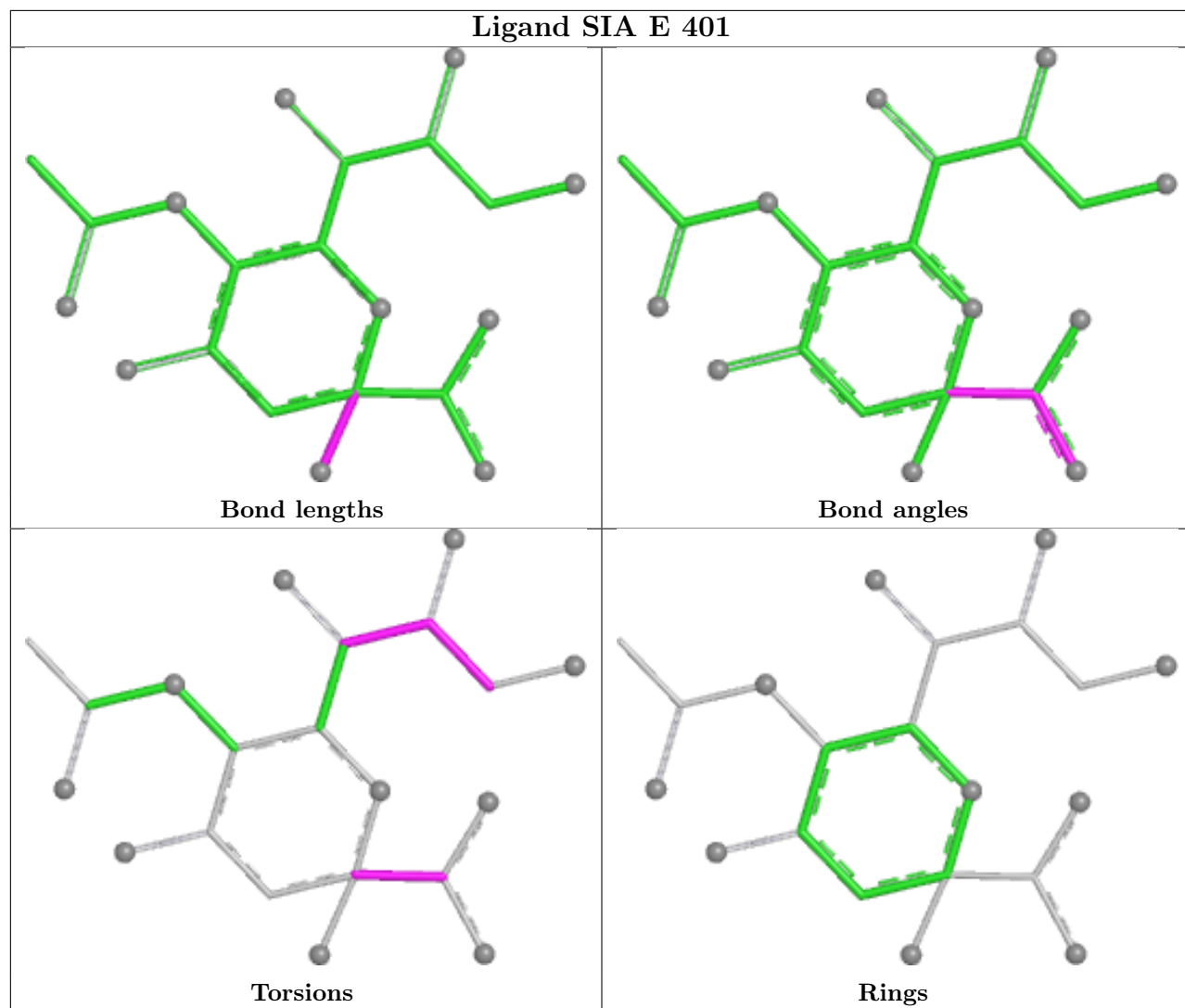
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	401	GOL	1	0
4	T	403	GOL	1	0
4	F	401	GOL	1	0
4	R	501	GOL	2	0
4	K	401	GOL	1	0
4	L	502	GOL	1	0
4	L	501	GOL	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand SIA M 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	270/289 (93%)	-0.18	4 (1%) 71 70	10, 20, 43, 63	3 (1%)
1	B	279/289 (96%)	-0.15	4 (1%) 73 72	12, 22, 46, 65	2 (0%)
1	C	279/289 (96%)	-0.17	8 (2%) 54 52	9, 21, 48, 68	5 (1%)
1	D	270/289 (93%)	-0.24	4 (1%) 71 70	5, 19, 43, 70	4 (1%)
1	E	271/289 (93%)	-0.20	7 (2%) 57 55	10, 19, 43, 82	2 (0%)
1	F	272/289 (94%)	-0.07	9 (3%) 49 47	12, 22, 50, 75	3 (1%)
1	G	274/289 (94%)	-0.10	8 (2%) 54 52	8, 22, 50, 72	4 (1%)
1	H	280/289 (96%)	-0.05	8 (2%) 54 52	12, 23, 51, 72	4 (1%)
1	I	270/289 (93%)	-0.13	8 (2%) 52 51	7, 23, 47, 80	3 (1%)
1	J	271/289 (93%)	-0.08	8 (2%) 52 51	12, 22, 47, 66	2 (0%)
1	K	274/289 (94%)	-0.19	7 (2%) 57 55	6, 21, 48, 76	5 (1%)
1	L	271/289 (93%)	-0.22	6 (2%) 62 60	7, 20, 42, 69	2 (0%)
1	M	278/289 (96%)	-0.19	9 (3%) 50 48	11, 19, 46, 77	0
1	N	278/289 (96%)	-0.16	5 (1%) 67 66	7, 21, 44, 56	3 (1%)
1	O	271/289 (93%)	-0.18	7 (2%) 57 55	6, 22, 45, 66	3 (1%)
1	P	273/289 (94%)	-0.12	6 (2%) 62 60	6, 21, 47, 65	4 (1%)
1	Q	271/289 (93%)	-0.19	7 (2%) 57 55	11, 20, 46, 64	1 (0%)
1	R	278/289 (96%)	-0.25	5 (1%) 67 66	7, 19, 43, 62	4 (1%)
1	S	271/289 (93%)	-0.26	6 (2%) 62 60	10, 20, 45, 68	2 (0%)
1	T	273/289 (94%)	-0.24	7 (2%) 57 55	12, 20, 47, 72	6 (2%)
All	All	5474/5780 (94%)	-0.17	133 (2%) 59 58	5, 21, 47, 82	62 (1%)

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	72	THR	4.7
1	Q	190	THR	4.6
1	K	117	CYS	4.4
1	T	117	CYS	4.2
1	M	72	THR	4.1

## 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](#)

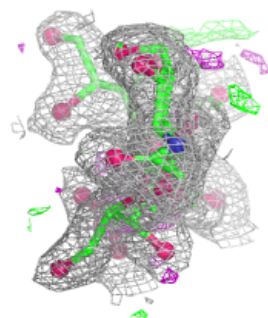
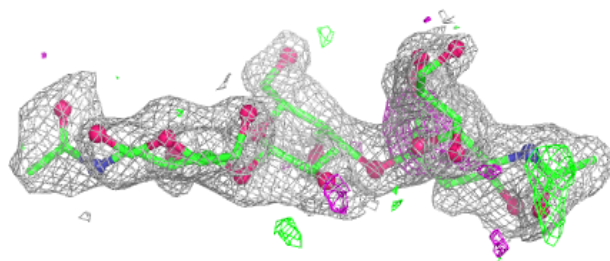
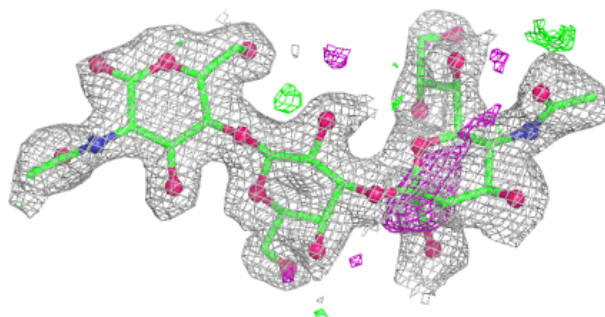
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	V	1	12/12	0.80	0.14	37,43,46,48	12
2	SIA	U	3	20/21	0.85	0.12	19,30,34,34	0
3	SIA	V	2	20/21	0.85	0.13	21,33,38,40	20
2	NAG	U	1	15/15	0.86	0.11	29,33,37,39	0
2	GAL	U	2	11/12	0.91	0.08	28,29,34,38	0

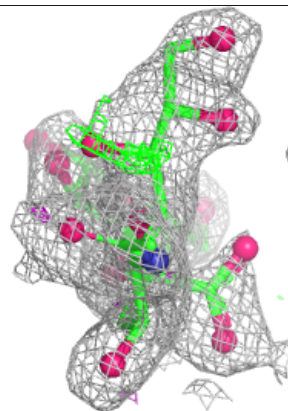
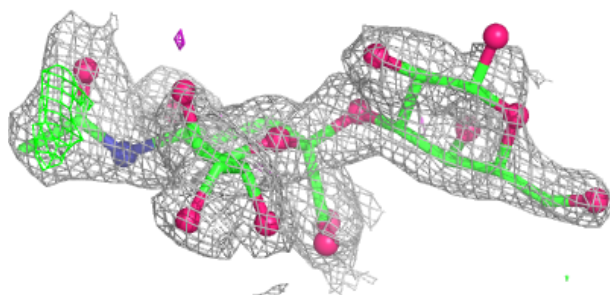
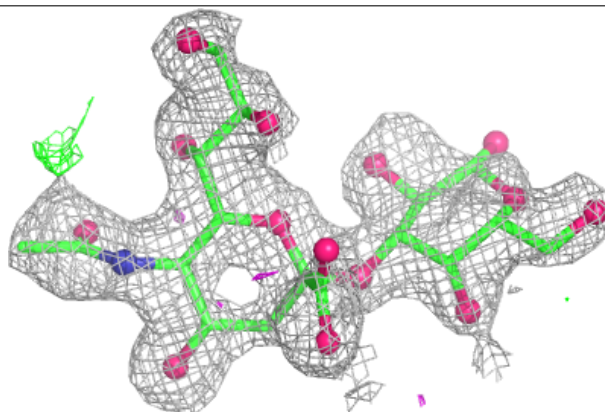
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain U:**

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

**Electron density around Chain V:**

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



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SIA	M	401	21/21	0.83	0.16	22,33,37,42	21
6	SIA	E	401	21/21	0.89	0.11	9,22,31,32	21
4	GOL	A	404	6/6	0.89	0.12	20,36,39,41	0
4	GOL	L	501	6/6	0.90	0.11	21,25,32,35	0
4	GOL	L	503	6/6	0.90	0.15	40,42,43,43	0
4	GOL	M	402	6/6	0.90	0.13	16,21,25,25	6
4	GOL	N	401	6/6	0.90	0.12	25,36,36,37	0
4	GOL	T	403	6/6	0.90	0.11	27,29,31,33	0
4	GOL	C	401	6/6	0.90	0.12	24,34,35,38	0
4	GOL	G	401	6/6	0.90	0.11	24,35,37,39	0
4	GOL	J	401	6/6	0.91	0.10	27,36,37,37	0
4	GOL	K	403	6/6	0.91	0.12	28,39,41,43	0
4	GOL	B	401	6/6	0.91	0.14	22,34,35,36	0
4	GOL	D	401	6/6	0.92	0.11	21,31,33,35	0
4	GOL	F	401	6/6	0.92	0.10	21,33,37,38	0
4	GOL	Q	401	6/6	0.93	0.10	18,28,31,32	0
4	GOL	R	501	6/6	0.93	0.09	8,15,18,29	0
4	GOL	M	403	6/6	0.93	0.11	18,24,29,33	0
4	GOL	K	401	6/6	0.93	0.10	19,27,29,32	0
4	GOL	O	401	6/6	0.93	0.09	22,35,37,37	0
4	GOL	I	401	6/6	0.94	0.10	21,31,34,36	0
4	GOL	P	401	6/6	0.94	0.10	17,31,34,34	0
4	GOL	S	401	6/6	0.94	0.09	21,26,27,28	0
4	GOL	E	402	6/6	0.95	0.10	23,33,37,38	0
4	GOL	R	502	6/6	0.95	0.09	17,28,33,35	0
4	GOL	H	401	6/6	0.95	0.11	18,28,35,37	0
4	GOL	L	502	6/6	0.96	0.10	9,27,31,33	0
5	CL	G	402	1/1	0.98	0.05	20,20,20,20	0
5	CL	I	402	1/1	0.98	0.10	24,24,24,24	0
5	CL	J	402	1/1	0.98	0.09	24,24,24,24	0
5	CL	K	402	1/1	0.98	0.07	22,22,22,22	0
5	CL	L	504	1/1	0.98	0.07	24,24,24,24	0
5	CL	P	402	1/1	0.98	0.08	21,21,21,21	0
5	CL	Q	402	1/1	0.98	0.07	24,24,24,24	0
5	CL	B	402	1/1	0.98	0.10	23,23,23,23	0
5	CL	C	402	1/1	0.98	0.09	21,21,21,21	0
5	CL	A	405	1/1	0.99	0.03	20,20,20,20	0

*Continued on next page...*

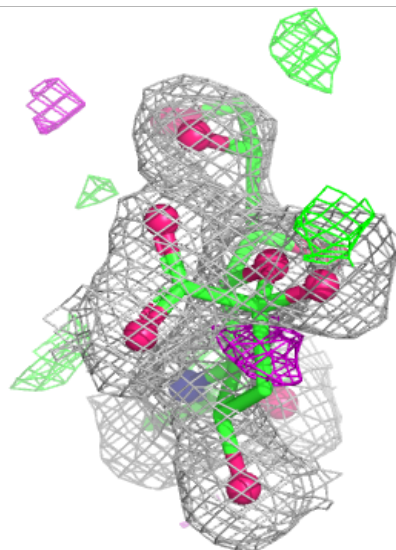
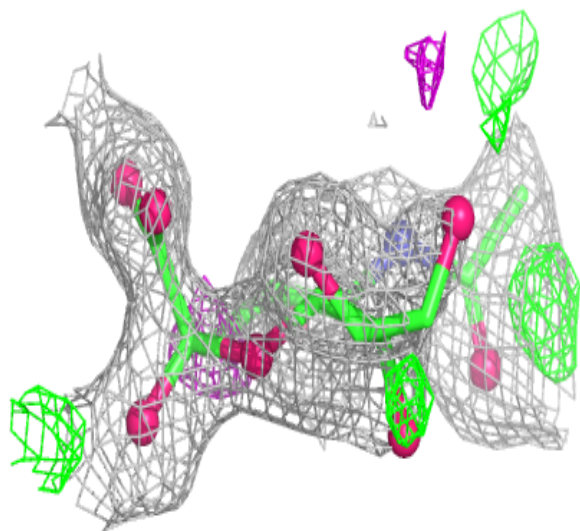
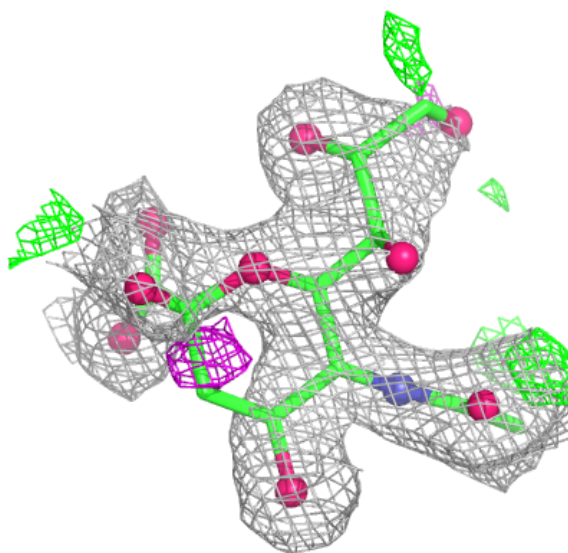
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	M	404	1/1	0.99	0.10	22,22,22,22	0
5	CL	N	402	1/1	0.99	0.05	22,22,22,22	0
5	CL	O	402	1/1	0.99	0.07	20,20,20,20	0
5	CL	H	402	1/1	0.99	0.06	21,21,21,21	0
5	CL	D	402	1/1	0.99	0.05	16,16,16,16	0
5	CL	R	503	1/1	0.99	0.03	21,21,21,21	0
5	CL	S	402	1/1	0.99	0.09	14,14,14,14	0
5	CL	S	403	1/1	0.99	0.10	22,22,22,22	0
5	CL	T	404	1/1	0.99	0.07	19,19,19,19	0
5	CL	E	403	1/1	0.99	0.08	19,19,19,19	0
5	CL	F	402	1/1	0.99	0.04	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

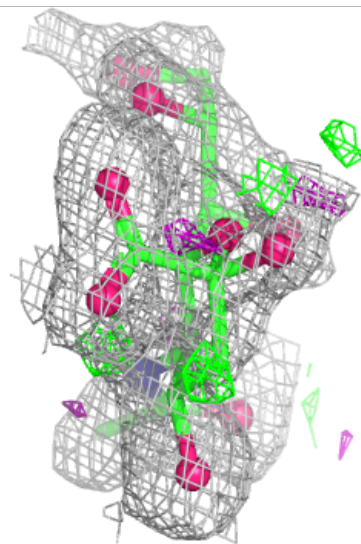
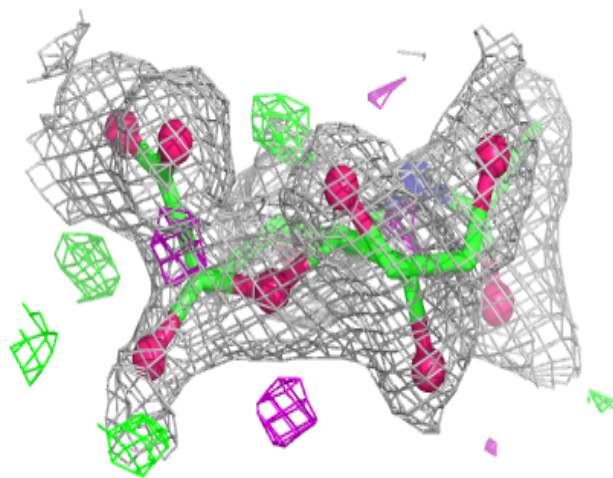
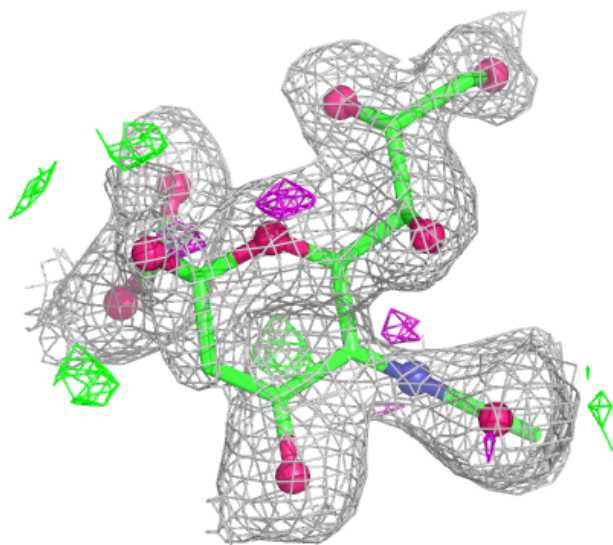
**Electron density around SIA M 401:**

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



**Electron density around SIA E 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.