wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 09:18 AM BST

PDB ID	:	4FMH
Title	:	Merkel Cell Polyomavirus VP1 in complex with Disialyllactose
Authors	:	Neu, U.; Hengel, H.; Stehle, T.
Deposited on	:	2012-06-17
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

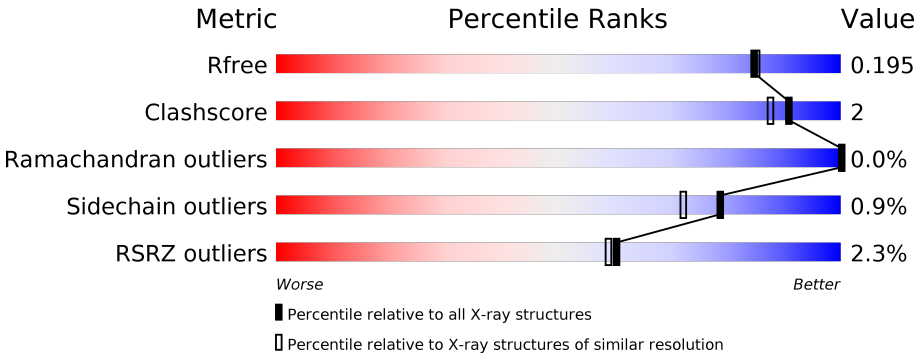
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	289	2% 91% 5%
1	B	289	3% 92%
1	C	289	2% 94%
1	D	289	% 90% 6%
1	E	289	2% 91%
1	F	289	2% 89% 5% 6%

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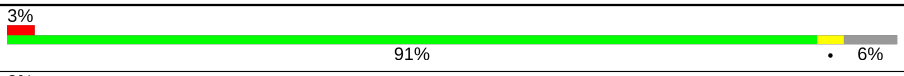
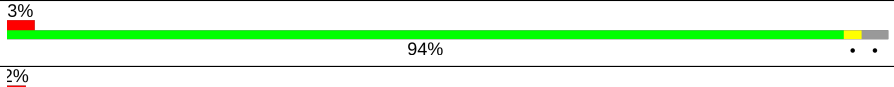
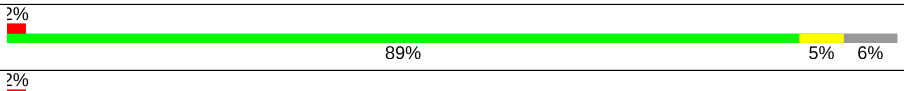
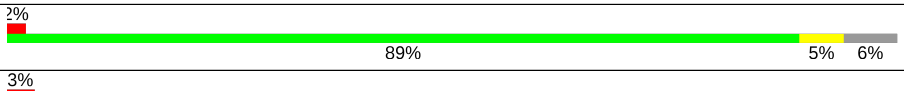
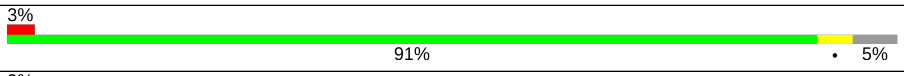
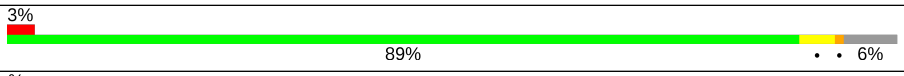
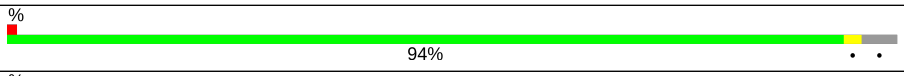
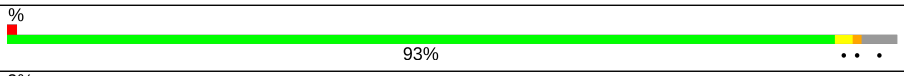
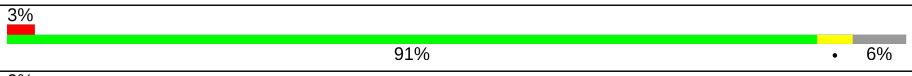
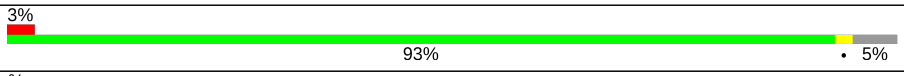
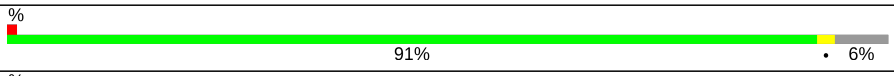
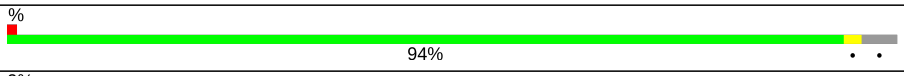
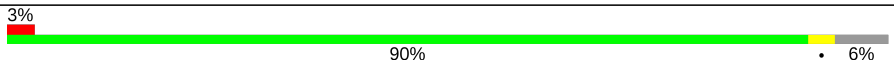
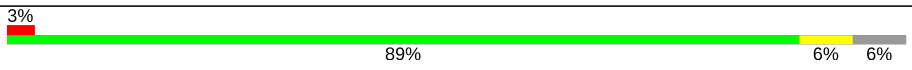
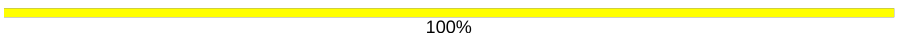
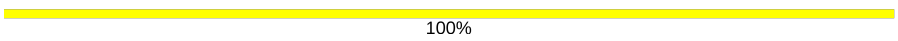
Mol	Chain	Length	Quality of chain
1	G	289	
1	H	289	
1	I	289	
1	J	289	
1	K	289	
1	L	289	
1	M	289	
1	N	289	
1	O	289	
1	P	289	
1	Q	289	
1	R	289	
1	S	289	
1	T	289	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	
2	a	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48934 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	274	Total	C	N	O	S	0	11	0
			2203	1407	364	422	10			
1	B	280	Total	C	N	O	S	0	9	0
			2249	1430	374	434	11			
1	C	280	Total	C	N	O	S	0	10	0
			2247	1431	371	434	11			
1	D	272	Total	C	N	O	S	0	6	0
			2159	1376	359	413	11			
1	E	276	Total	C	N	O	S	0	6	0
			2188	1394	363	421	10			
1	F	272	Total	C	N	O	S	0	8	0
			2177	1388	360	419	10			
1	G	271	Total	C	N	O	S	0	7	0
			2159	1379	357	413	10			
1	H	280	Total	C	N	O	S	0	9	0
			2251	1431	375	434	11			
1	I	271	Total	C	N	O	S	0	8	0
			2167	1382	360	415	10			
1	J	272	Total	C	N	O	S	0	6	0
			2165	1381	359	415	10			
1	K	274	Total	C	N	O	S	0	6	0
			2177	1388	360	419	10			
1	L	272	Total	C	N	O	S	0	8	0
			2175	1389	359	416	11			
1	M	278	Total	C	N	O	S	0	6	0
			2215	1410	365	428	12			
1	N	278	Total	C	N	O	S	0	7	0
			2222	1414	367	429	12			
1	O	273	Total	C	N	O	S	0	6	0
			2173	1384	360	419	10			
1	P	275	Total	C	N	O	S	0	5	0
			2179	1389	360	420	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	271	Total	C	N	O	S	0	4	0
			2145	1370	355	410	10			
1	R	278	Total	C	N	O	S	0	4	0
			2195	1397	362	425	11			
1	S	271	Total	C	N	O	S	0	6	0
			2159	1377	360	412	10			
1	T	273	Total	C	N	O	S	0	8	0
			2189	1394	365	420	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

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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

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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

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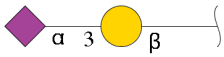
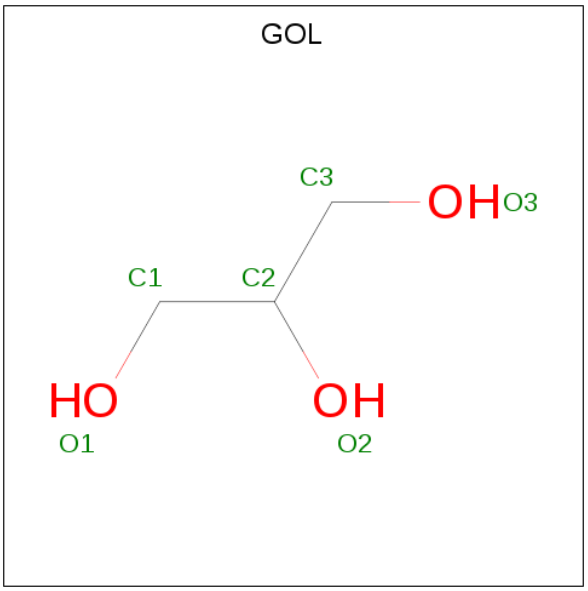
Chain	Residue	Modelled	Actual	Comment	Reference
T	33	SER	-	expression tag	UNP C0JPK1
T	34	HIS	-	expression tag	UNP C0JPK1
T	35	MET	-	expression tag	UNP C0JPK1
T	36	LEU	-	expression tag	UNP C0JPK1
T	37	GLU	-	expression tag	UNP C0JPK1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	V	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	W	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	X	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	Y	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	Z	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	a	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	Q	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	N	1	Total Cl 1 1	0	0
4	O	1	Total Cl 1 1	0	0
4	R	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0
4	S	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	M	1	Total Cl 1 1	0	0

- Molecule 5 is water.

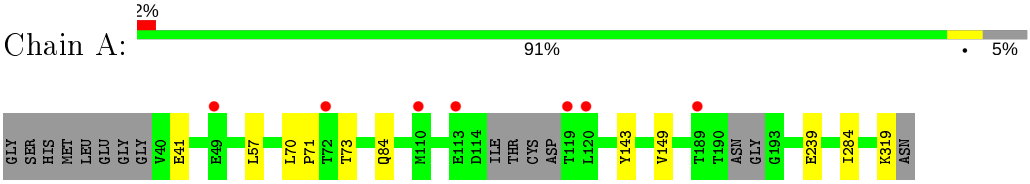
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	214	Total O 214 214	0	0
5	B	235	Total O 235 235	0	0
5	C	232	Total O 232 232	0	0
5	D	239	Total O 239 239	0	0
5	E	229	Total O 229 229	0	0
5	F	210	Total O 210 210	0	0
5	G	217	Total O 217 217	0	0
5	H	231	Total O 231 231	0	0
5	I	216	Total O 216 216	0	0
5	J	197	Total O 197 197	0	0
5	K	225	Total O 225 225	0	0
5	L	237	Total O 237 237	0	0
5	M	257	Total O 257 257	0	0
5	N	239	Total O 239 239	0	0
5	O	231	Total O 231 231	0	0
5	P	239	Total O 239 239	0	0
5	Q	229	Total O 229 229	0	0
5	R	237	Total O 237 237	0	0
5	S	218	Total O 218 218	0	0
5	T	228	Total O 228 228	0	0

3 Residue-property plots

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

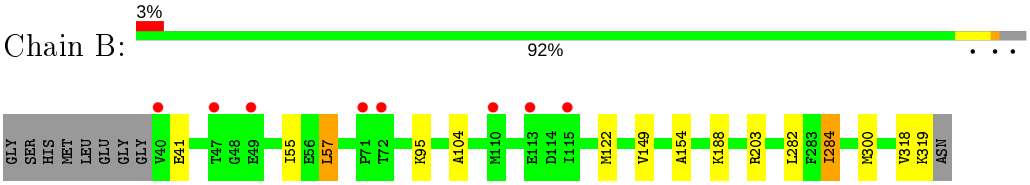
- Molecule 1: VP1

Chain A:



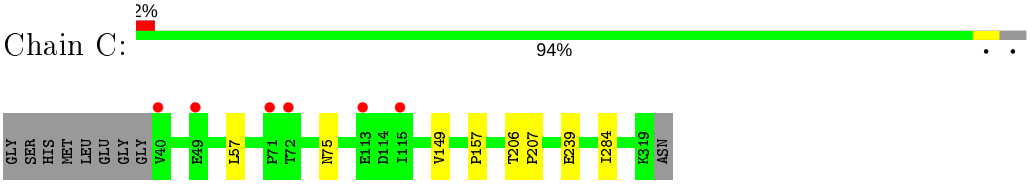
- Molecule 1: VP1

Chain B:



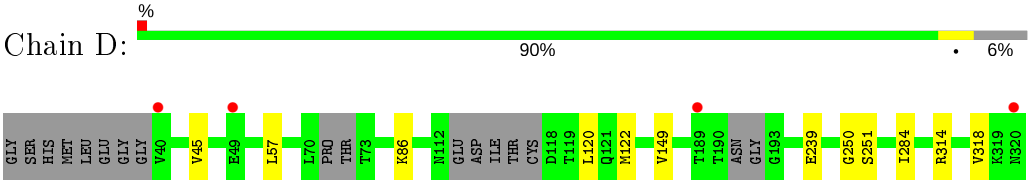
- Molecule 1: VP1

Chain C:



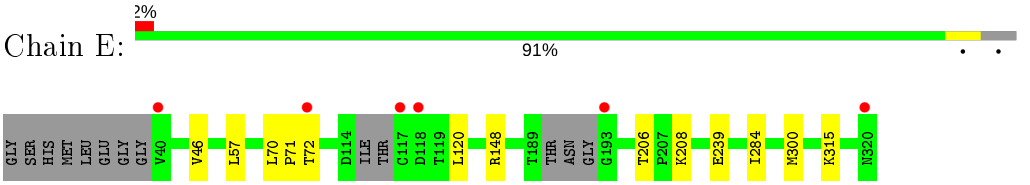
- Molecule 1: VP1

Chain D:



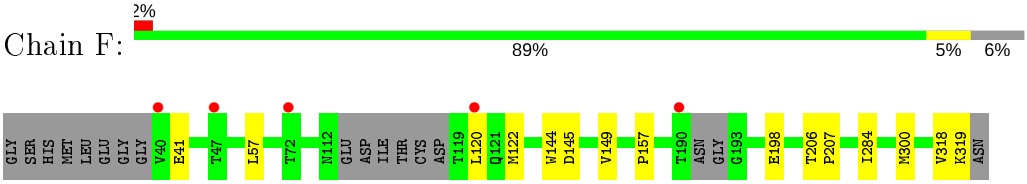
- Molecule 1: VP1

Chain E:



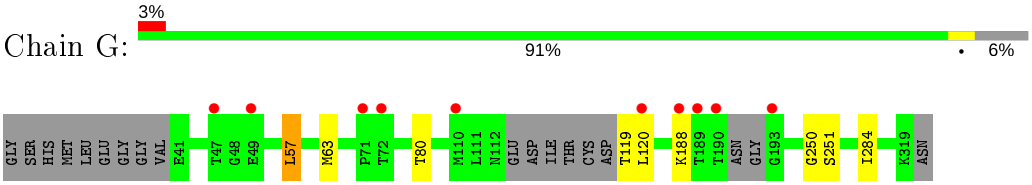
- Molecule 1: VP1

Chain F:



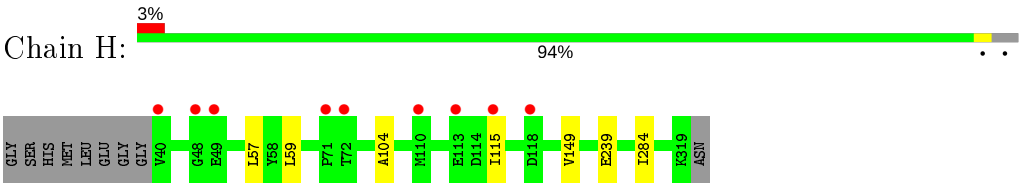
• Molecule 1: VP1

Chain G:



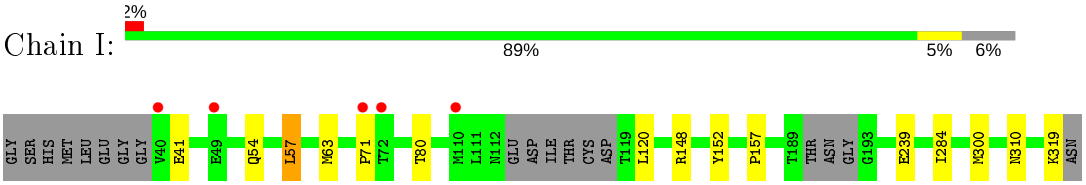
• Molecule 1: VP1

Chain H:



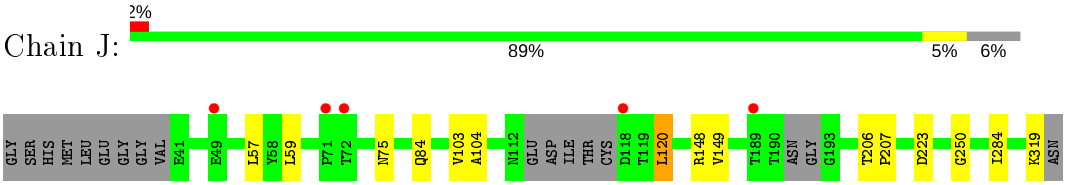
• Molecule 1: VP1

Chain I:



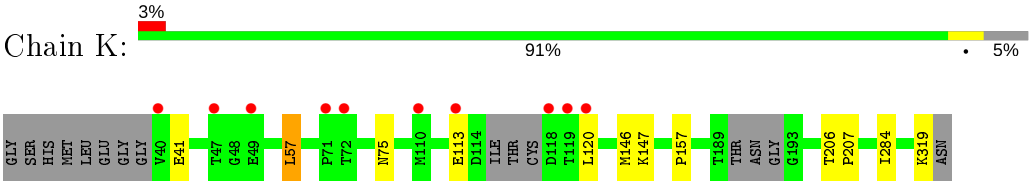
• Molecule 1: VP1

Chain J:



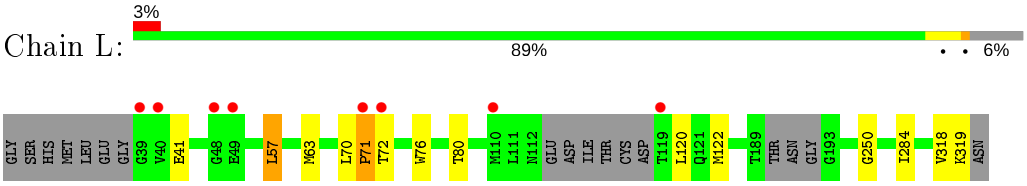
• Molecule 1: VP1

Chain K:



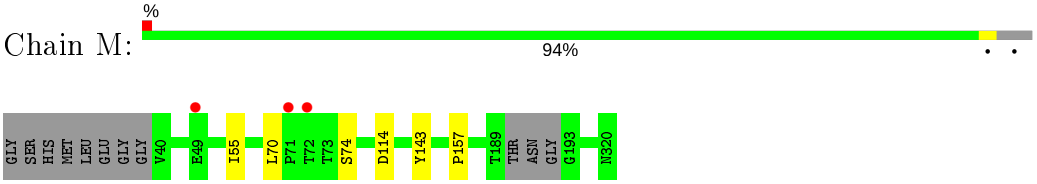
• Molecule 1: VP1

Chain L:



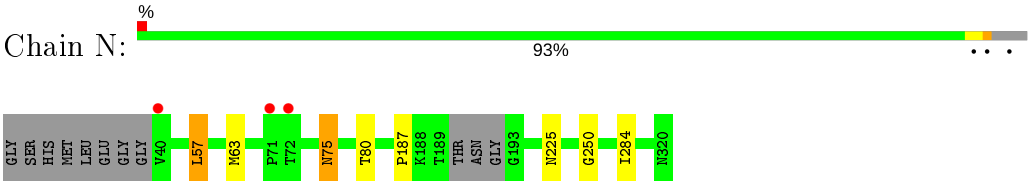
• Molecule 1: VP1

Chain M:



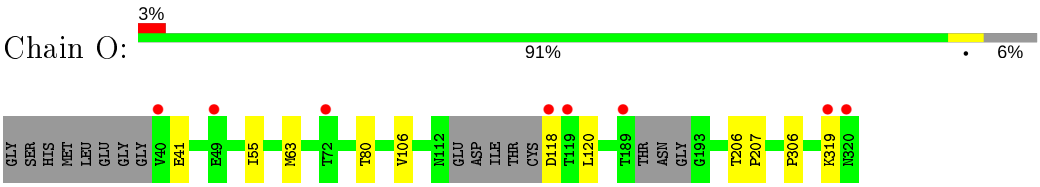
• Molecule 1: VP1

Chain N:



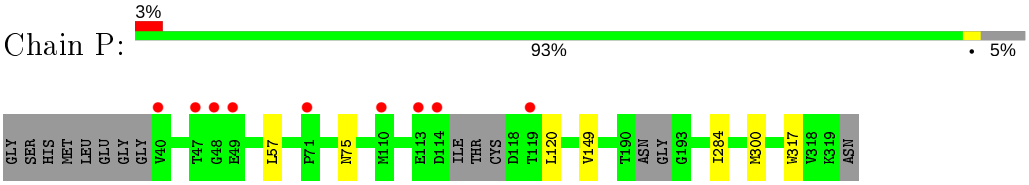
• Molecule 1: VP1

Chain O:



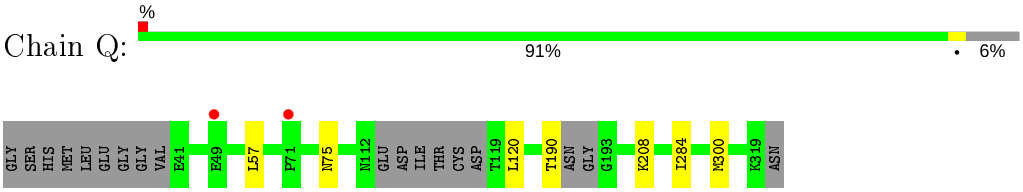
• Molecule 1: VP1

Chain P:



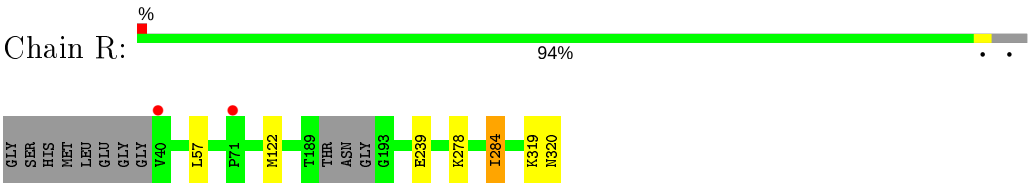
• Molecule 1: VP1

Chain Q:



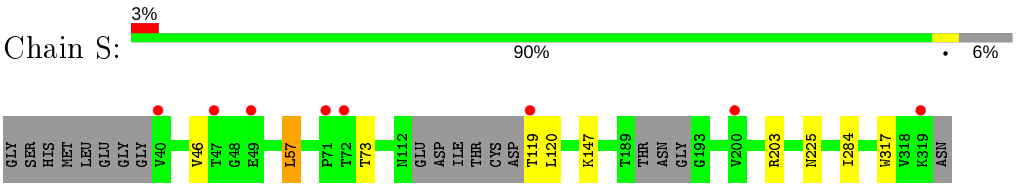
• Molecule 1: VP1

Chain R:



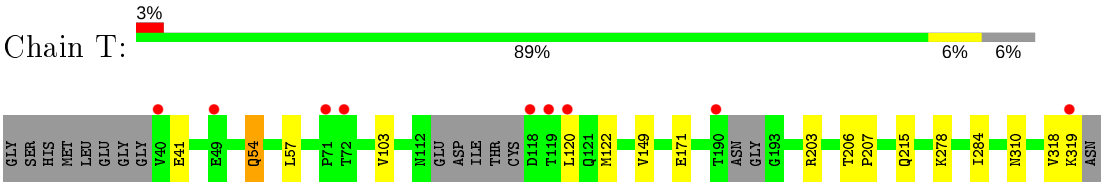
• Molecule 1: VP1

Chain S:



• Molecule 1: VP1

Chain T:



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

Chain U:

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

Chain V:

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

Chain W:

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

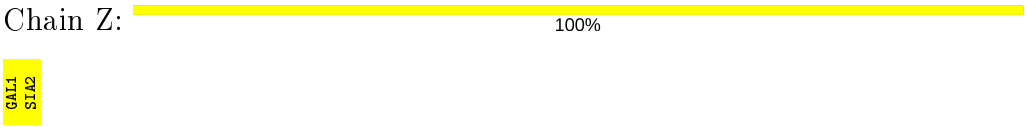
Chain X:

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

Chain Y:

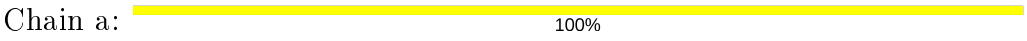
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain Z:



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

Chain a:



GAL1
SIA2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.27Å 85.77Å 248.71Å 92.97° 100.48° 108.05°	Depositor
Resolution (Å)	50.00 – 1.85 48.58 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-1.85) 94.7 (48.58-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.166 , 0.196 0.166 , 0.195	Depositor DCC
R_{free} test set	5310 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	48934	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SIA, GAL, 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	0.40	0/2258	0.54	0/3079
1	B	0.39	0/2305	0.52	0/3144
1	C	0.40	0/2309	0.54	0/3149
1	D	0.42	0/2214	0.55	0/3008
1	E	0.41	0/2243	0.55	0/3057
1	F	0.40	0/2231	0.54	0/3042
1	G	0.39	0/2216	0.52	0/3018
1	H	0.39	0/2307	0.52	0/3146
1	I	0.39	0/2221	0.53	0/3026
1	J	0.39	0/2219	0.54	1/3023 (0.0%)
1	K	0.41	0/2231	0.55	0/3040
1	L	0.41	0/2227	0.52	0/3035
1	M	0.42	0/2267	0.55	0/3089
1	N	0.39	0/2274	0.54	0/3098
1	O	0.40	0/2224	0.54	0/3031
1	P	0.39	0/2230	0.54	0/3040
1	Q	0.39	0/2196	0.54	0/2992
1	R	0.40	0/2247	0.54	0/3063
1	S	0.41	0/2210	0.53	0/3011
1	T	0.39	0/2243	0.54	0/3056
All	All	0.40	0/44872	0.54	1/61147 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	120	LEU	CA-CB-CG	5.10	127.03	115.30

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	2203	0	2179	10	0
1	B	2249	0	2227	15	0
1	C	2247	0	2232	7	0
1	D	2159	0	2132	8	0
1	E	2188	0	2156	7	0
1	F	2177	0	2152	12	0
1	G	2159	0	2150	8	0
1	H	2251	0	2226	5	0
1	I	2167	0	2142	10	0
1	J	2165	0	2142	11	0
1	K	2177	0	2150	8	0
1	L	2175	0	2161	10	0
1	M	2215	0	2190	6	0
1	N	2222	0	2198	6	0
1	O	2173	0	2143	5	0
1	P	2179	0	2154	6	0
1	Q	2145	0	2130	6	0
1	R	2195	0	2166	4	0
1	S	2159	0	2140	7	0
1	T	2189	0	2166	10	0
2	U	32	0	28	0	0
2	V	32	0	28	0	0
2	W	32	0	28	0	0
2	X	32	0	28	0	0
2	Y	32	0	28	0	0
2	Z	32	0	28	0	0
2	a	32	0	28	0	0
3	A	18	0	24	2	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
3	D	18	0	24	1	0
3	E	18	0	24	0	0
3	F	12	0	16	0	0
3	G	12	0	16	0	0
3	H	12	0	16	0	0
3	I	12	0	16	0	0
3	J	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	18	0	24	1	0
3	L	24	0	32	3	0
3	M	24	0	32	1	0
3	N	18	0	24	0	0
3	O	12	0	16	0	0
3	P	18	0	24	0	0
3	Q	18	0	24	0	0
3	R	24	0	32	1	0
3	S	30	0	40	2	0
3	T	12	0	16	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	1	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
5	A	214	0	0	0	0
5	B	235	0	0	2	0
5	C	232	0	0	1	0
5	D	239	0	0	1	0
5	E	229	0	0	2	0
5	F	210	0	0	1	0
5	G	217	0	0	0	0
5	H	231	0	0	0	0
5	I	216	0	0	4	0
5	J	197	0	0	0	0
5	K	225	0	0	1	0
5	L	237	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	257	0	0	1	0
5	N	239	0	0	0	0
5	O	231	0	0	0	0
5	P	239	0	0	2	0
5	Q	229	0	0	0	0
5	R	237	0	0	0	0
5	S	218	0	0	2	0
5	T	228	0	0	1	0
All	All	48934	0	43980	151	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 151 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:B:55[B]:ILE:O	1:B:55[B]:ILE:HD12	1.08	1.23
1:B:55[B]:ILE:O	1:B:55[B]:ILE:CD1	1.97	1.13
1:B:55[B]:ILE:HD12	1:B:55[B]:ILE:C	1.79	1.02
1:I:57:LEU:HD21	1:I:284:ILE:HD12	1.42	1.01
1:D:57:LEU:HD21	1:D:284:ILE:HD12	1.47	0.96

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	279/289 (96%)	264 (95%)	15 (5%)	0	100	100
1	B	287/289 (99%)	276 (96%)	11 (4%)	0	100	100
1	C	288/289 (100%)	277 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	269/289 (93%)	259 (96%)	10 (4%)	0	100	100
1	E	276/289 (96%)	262 (95%)	14 (5%)	0	100	100
1	F	274/289 (95%)	260 (95%)	14 (5%)	0	100	100
1	G	272/289 (94%)	262 (96%)	10 (4%)	0	100	100
1	H	287/289 (99%)	276 (96%)	11 (4%)	0	100	100
1	I	273/289 (94%)	264 (97%)	8 (3%)	1 (0%)	34	19
1	J	272/289 (94%)	262 (96%)	10 (4%)	0	100	100
1	K	274/289 (95%)	262 (96%)	12 (4%)	0	100	100
1	L	274/289 (95%)	259 (94%)	13 (5%)	2 (1%)	22	9
1	M	280/289 (97%)	265 (95%)	15 (5%)	0	100	100
1	N	281/289 (97%)	268 (95%)	13 (5%)	0	100	100
1	O	273/289 (94%)	262 (96%)	11 (4%)	0	100	100
1	P	274/289 (95%)	265 (97%)	9 (3%)	0	100	100
1	Q	269/289 (93%)	257 (96%)	12 (4%)	0	100	100
1	R	278/289 (96%)	267 (96%)	11 (4%)	0	100	100
1	S	271/289 (94%)	257 (95%)	14 (5%)	0	100	100
1	T	275/289 (95%)	262 (95%)	13 (5%)	0	100	100
All	All	5526/5780 (96%)	5286 (96%)	237 (4%)	3 (0%)	100	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	71	PRO
1	L	71[A]	PRO
1	L	71[B]	PRO

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	249/253 (98%)	248 (100%)	1 (0%)	91	89
1	B	256/253 (101%)	252 (98%)	4 (2%)	62	49
1	C	257/253 (102%)	256 (100%)	1 (0%)	91	89
1	D	243/253 (96%)	241 (99%)	2 (1%)	81	76
1	E	246/253 (97%)	242 (98%)	4 (2%)	62	49
1	F	247/253 (98%)	246 (100%)	1 (0%)	91	89
1	G	246/253 (97%)	243 (99%)	3 (1%)	71	62
1	H	256/253 (101%)	254 (99%)	2 (1%)	81	76
1	I	245/253 (97%)	242 (99%)	3 (1%)	71	62
1	J	245/253 (97%)	244 (100%)	1 (0%)	91	89
1	K	246/253 (97%)	241 (98%)	5 (2%)	55	40
1	L	247/253 (98%)	245 (99%)	2 (1%)	81	76
1	M	252/253 (100%)	251 (100%)	1 (0%)	91	89
1	N	253/253 (100%)	248 (98%)	5 (2%)	55	40
1	O	246/253 (97%)	244 (99%)	2 (1%)	81	76
1	P	247/253 (98%)	246 (100%)	1 (0%)	91	89
1	Q	243/253 (96%)	241 (99%)	2 (1%)	81	76
1	R	249/253 (98%)	247 (99%)	2 (1%)	81	76
1	S	244/253 (96%)	240 (98%)	4 (2%)	62	49
1	T	248/253 (98%)	244 (98%)	4 (2%)	62	49
All	All	4965/5060 (98%)	4915 (99%)	50 (1%)	78	69

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	57[A]	LEU
1	L	57	LEU
1	T	54[A]	GLN
1	K	57[B]	LEU
1	K	120	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN

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Mol	Chain	Res	Type
1	A	185	GLN
1	E	183	GLN
1	J	84	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

14 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	GAL	U	1	2	12,12,12	0.51	0	17,17,17	0.69	0
2	SIA	U	2	2	17,20,21	0.55	0	21,28,31	1.22	2 (9%)
2	GAL	V	1	2	12,12,12	0.53	0	17,17,17	0.55	0
2	SIA	V	2	2	17,20,21	0.47	0	21,28,31	1.09	2 (9%)
2	GAL	W	1	2	12,12,12	0.55	0	17,17,17	0.49	0
2	SIA	W	2	2	17,20,21	0.48	0	21,28,31	1.16	2 (9%)
2	GAL	X	1	2	12,12,12	0.55	0	17,17,17	0.60	0
2	SIA	X	2	2	17,20,21	0.41	0	21,28,31	1.26	2 (9%)
2	GAL	Y	1	2	12,12,12	0.51	0	17,17,17	0.51	0
2	SIA	Y	2	2	17,20,21	0.41	0	21,28,31	0.98	1 (4%)
2	GAL	Z	1	2	12,12,12	0.49	0	17,17,17	0.61	1 (5%)
2	SIA	Z	2	2	17,20,21	0.43	0	21,28,31	1.06	1 (4%)
2	GAL	a	1	2	12,12,12	0.55	0	17,17,17	0.96	1 (5%)
2	SIA	a	2	2	17,20,21	0.59	0	21,28,31	1.03	1 (4%)

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	GAL	U	1	2	-	0/2/22/22	0/1/1/1
2	SIA	U	2	2	-	2/14/34/38	0/1/1/1
2	GAL	V	1	2	-	2/2/22/22	0/1/1/1
2	SIA	V	2	2	-	2/14/34/38	0/1/1/1
2	GAL	W	1	2	-	1/2/22/22	0/1/1/1
2	SIA	W	2	2	-	2/14/34/38	0/1/1/1
2	GAL	X	1	2	-	1/2/22/22	0/1/1/1
2	SIA	X	2	2	-	2/14/34/38	0/1/1/1
2	GAL	Y	1	2	-	1/2/22/22	0/1/1/1
2	SIA	Y	2	2	-	2/14/34/38	0/1/1/1
2	GAL	Z	1	2	-	0/2/22/22	0/1/1/1
2	SIA	Z	2	2	-	2/14/34/38	0/1/1/1
2	GAL	a	1	2	-	1/2/22/22	0/1/1/1
2	SIA	a	2	2	-	5/14/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2	SIA	C6-O6-C2	4.20	120.32	111.34
2	U	2	SIA	C6-O6-C2	3.89	119.67	111.34
2	W	2	SIA	C6-O6-C2	3.84	119.56	111.34
2	Z	2	SIA	C6-O6-C2	3.63	119.10	111.34
2	V	2	SIA	C6-O6-C2	3.54	118.92	111.34

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

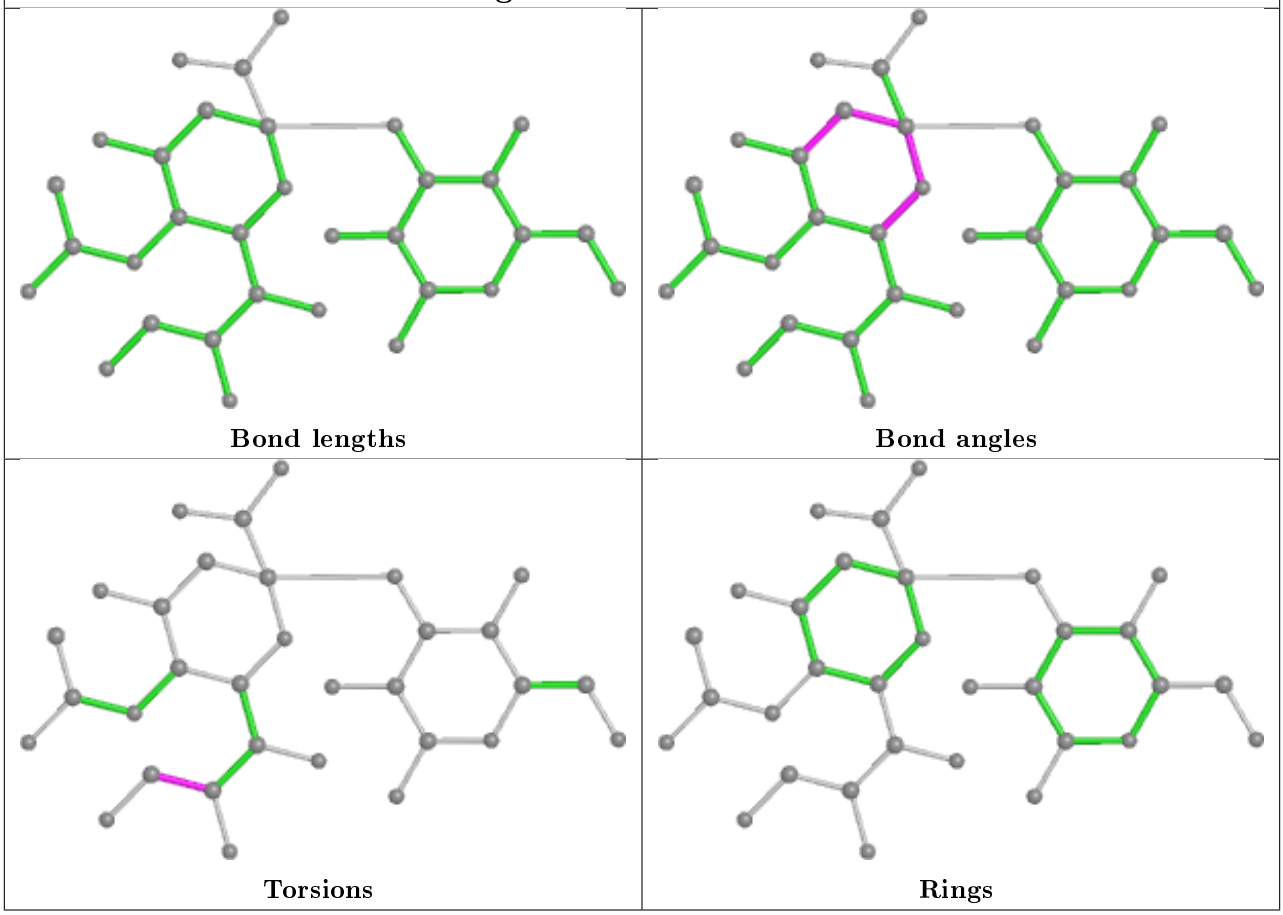
Mol	Chain	Res	Type	Atoms
2	U	2	SIA	C7-C8-C9-O9
2	W	2	SIA	C7-C8-C9-O9
2	V	2	SIA	C7-C8-C9-O9
2	X	2	SIA	C7-C8-C9-O9
2	U	2	SIA	O8-C8-C9-O9

There are no ring outliers.

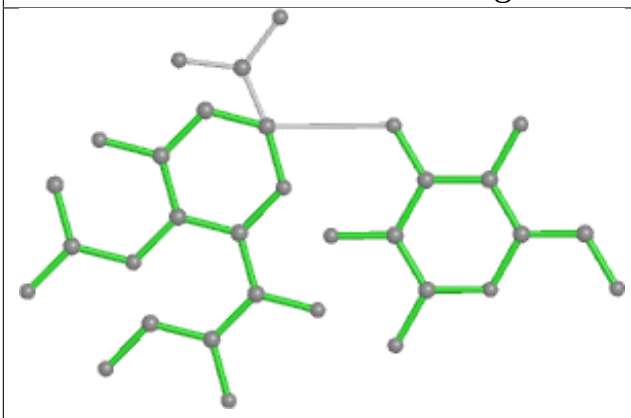
No monomer is involved in short contacts.

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

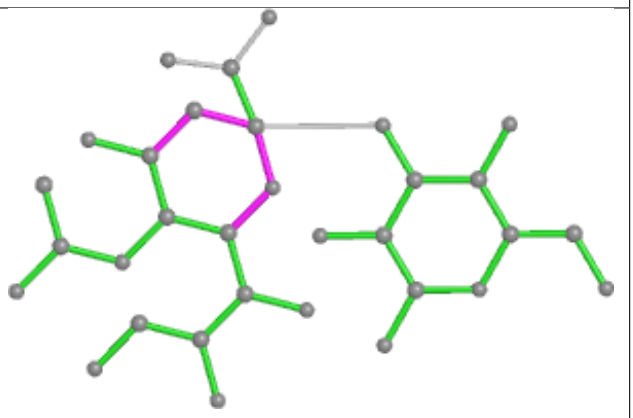
Oligosaccharide Chain U



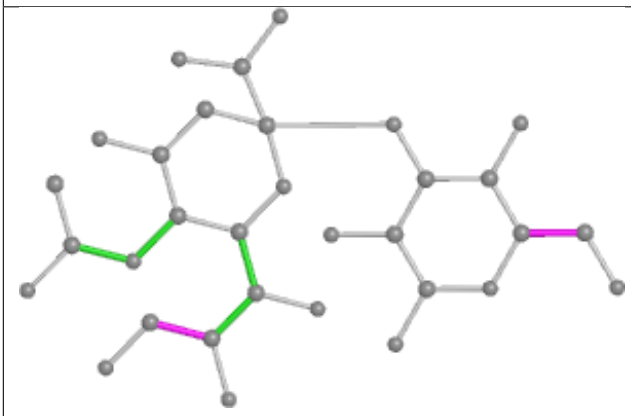
Oligosaccharide Chain V



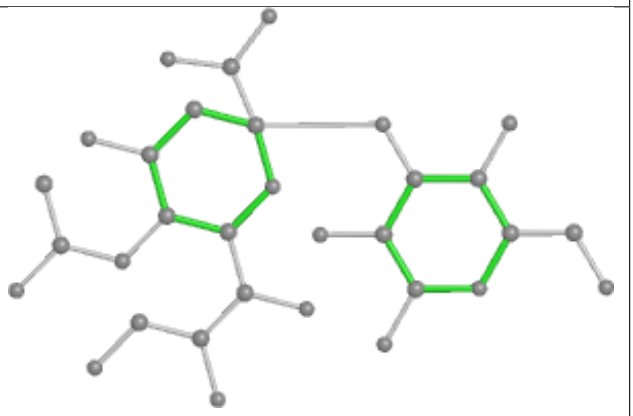
Bond lengths



Bond angles

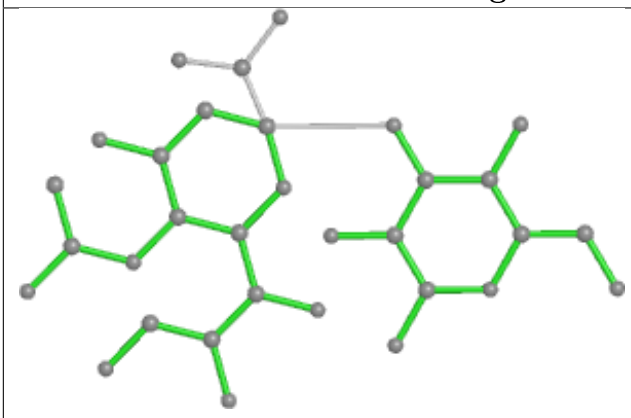


Torsions

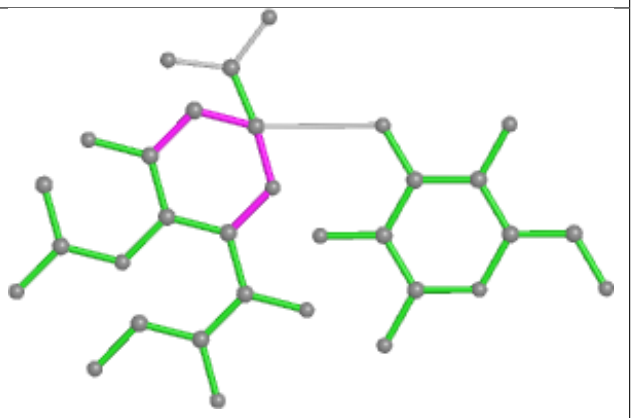


Rings

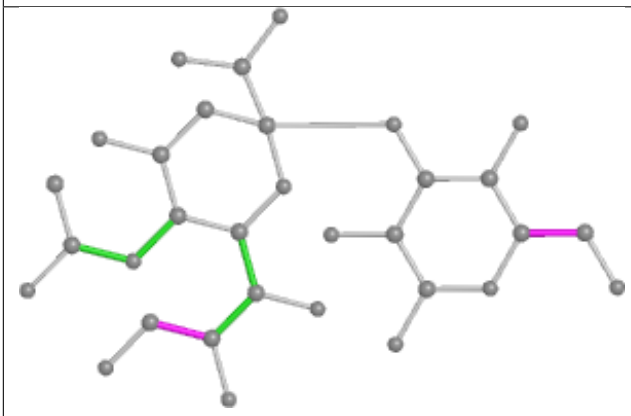
Oligosaccharide Chain W



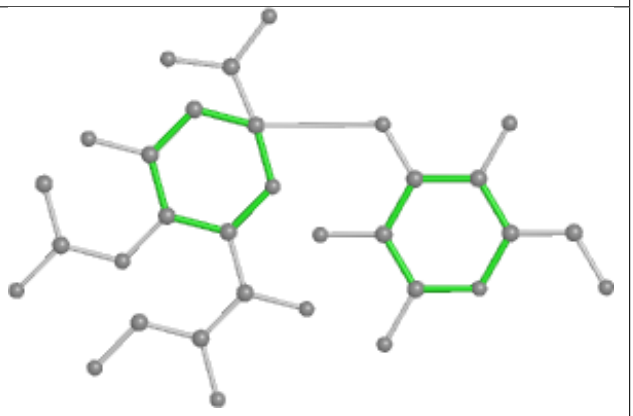
Bond lengths



Bond angles

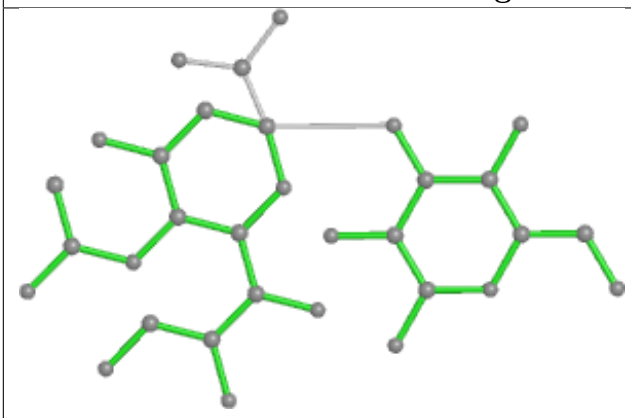


Torsions

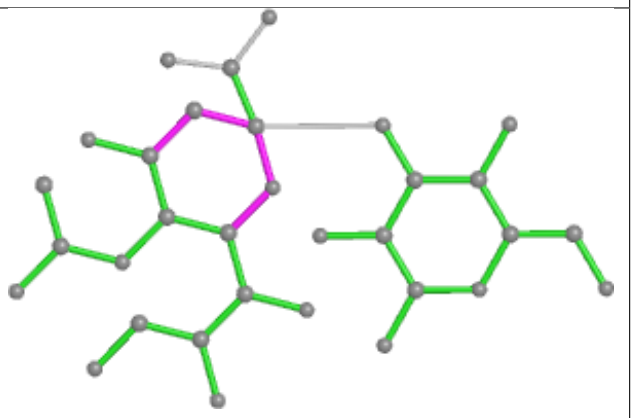


Rings

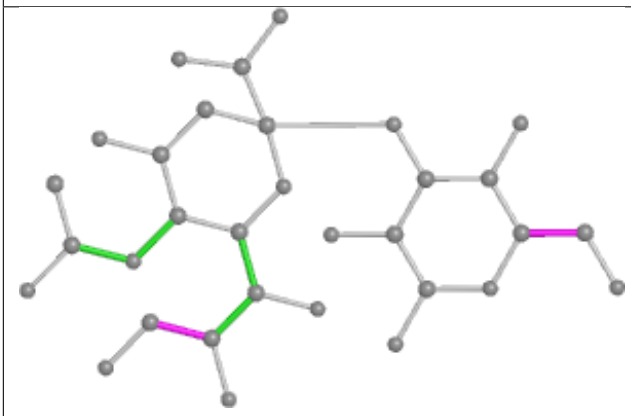
Oligosaccharide Chain X



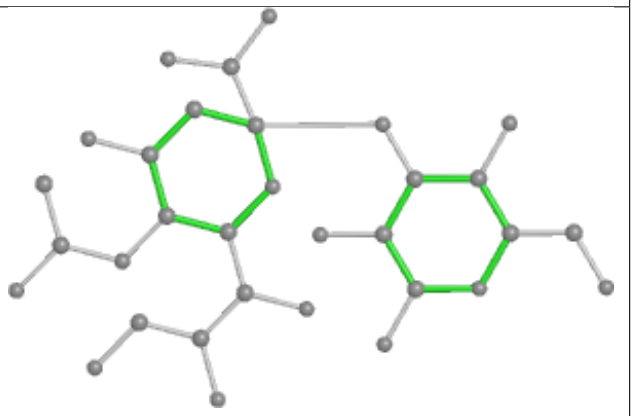
Bond lengths



Bond angles

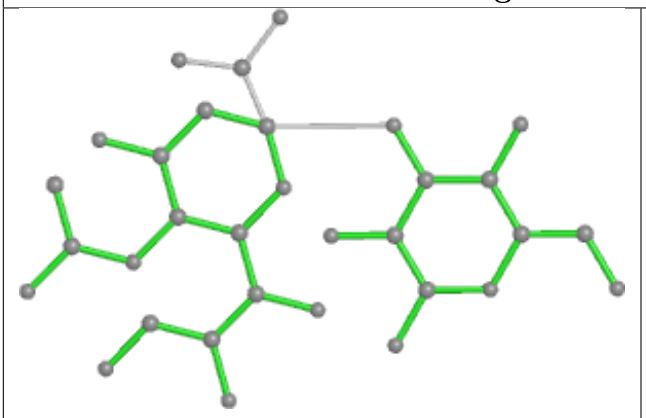


Torsions

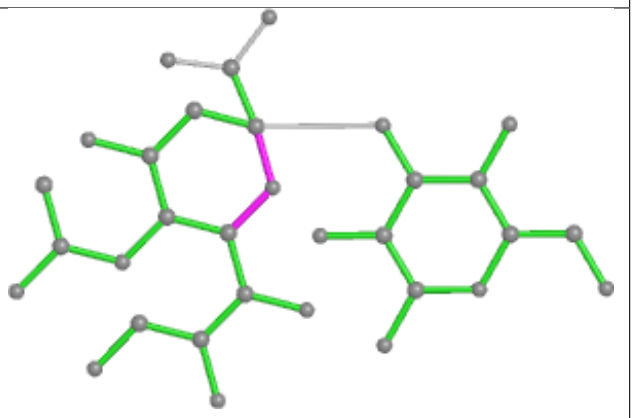


Rings

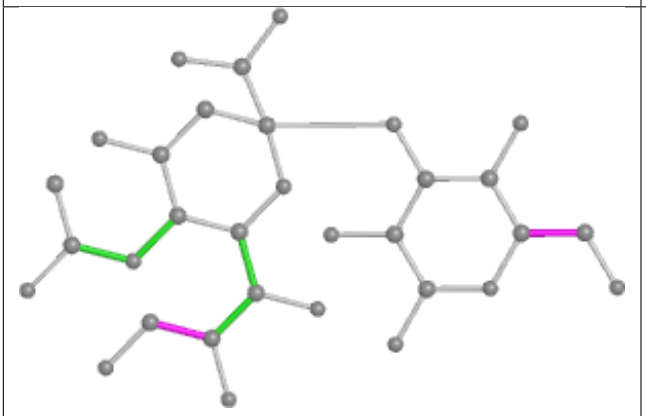
Oligosaccharide Chain Y



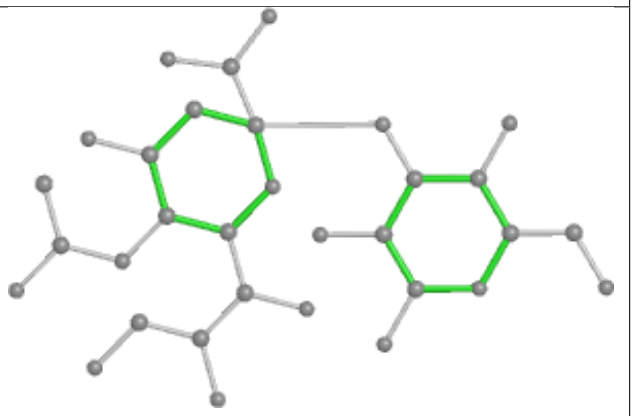
Bond lengths



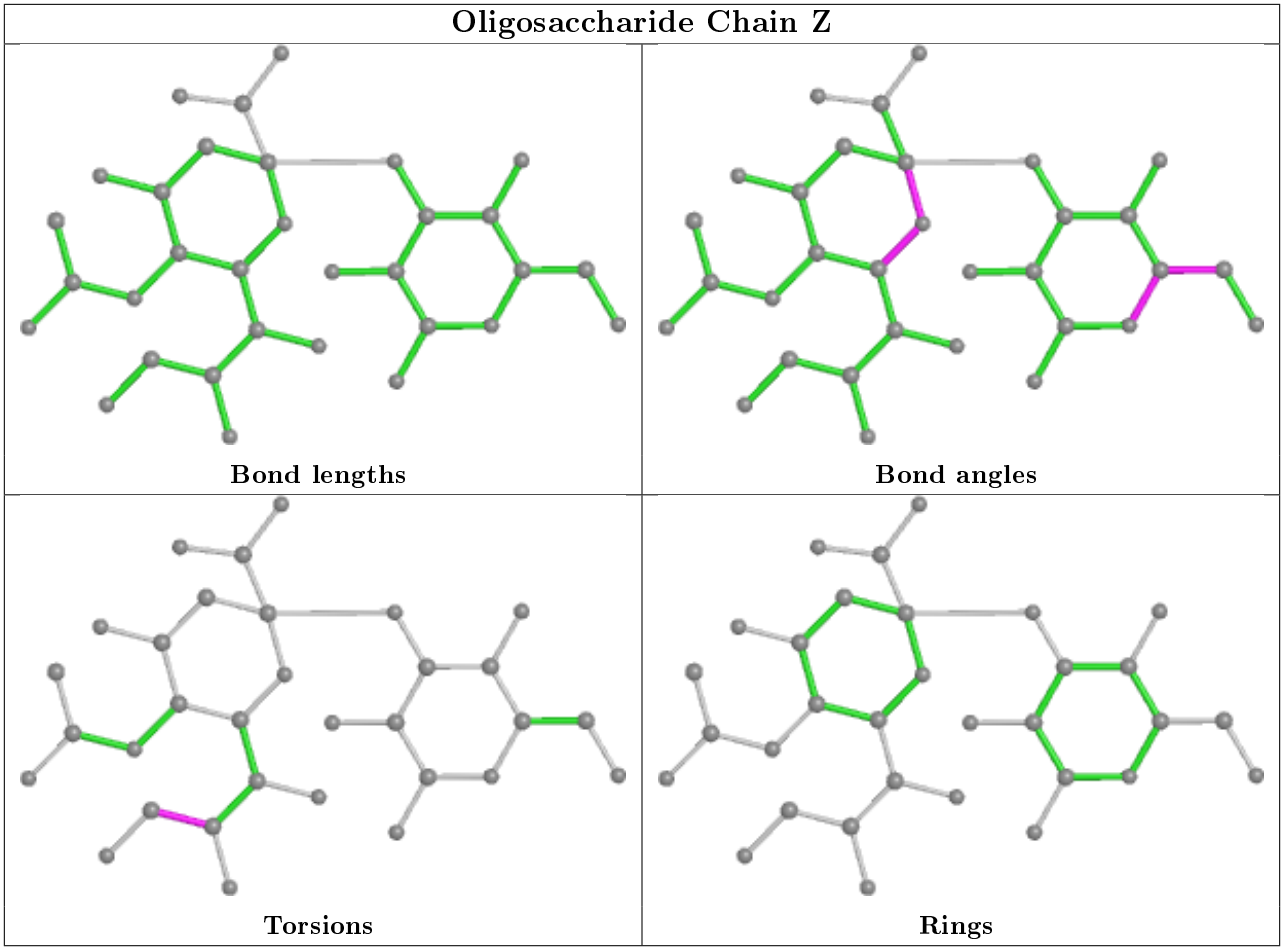
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 76 ligands modelled in this entry, 20 are monoatomic - leaving 56 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	$\#\|Z\| > 2$
3	GOL	O	403	-	5,5,5	0.44	0	5,5,5	0.41	0
3	GOL	D	502	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	H	403	-	5,5,5	0.40	0	5,5,5	0.29	0
3	GOL	G	401	-	5,5,5	0.44	0	5,5,5	0.22	0
3	GOL	E	402	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	F	401	-	5,5,5	0.39	0	5,5,5	0.15	0
3	GOL	Q	403	-	5,5,5	0.37	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	K	406	-	5,5,5	0.35	0	5,5,5	0.43	0
3	GOL	M	406	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	L	503	-	5,5,5	0.44	0	5,5,5	0.42	0
3	GOL	L	504	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	N	401	-	5,5,5	0.43	0	5,5,5	0.33	0
3	GOL	A	502	-	5,5,5	0.39	0	5,5,5	0.20	0
3	GOL	T	404	-	5,5,5	0.40	0	5,5,5	0.46	0
3	GOL	S	503	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	M	403	-	5,5,5	0.46	0	5,5,5	0.57	0
3	GOL	M	404	-	5,5,5	0.44	0	5,5,5	0.27	0
3	GOL	L	501	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	R	504	-	5,5,5	0.31	0	5,5,5	0.37	0
3	GOL	N	403	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	H	404	-	5,5,5	0.41	0	5,5,5	0.46	0
3	GOL	T	403	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	I	402	-	5,5,5	0.38	0	5,5,5	0.40	0
3	GOL	S	501	-	5,5,5	0.54	0	5,5,5	0.80	0
3	GOL	E	401	-	5,5,5	0.40	0	5,5,5	0.28	0
3	GOL	M	405	-	5,5,5	0.40	0	5,5,5	0.20	0
3	GOL	E	403	-	5,5,5	0.39	0	5,5,5	0.36	0
3	GOL	R	502	-	5,5,5	0.45	0	5,5,5	0.32	0
3	GOL	P	401	-	5,5,5	0.43	0	5,5,5	0.34	0
3	GOL	J	402	-	5,5,5	0.39	0	5,5,5	0.46	0
3	GOL	P	402	-	5,5,5	0.42	0	5,5,5	0.23	0
3	GOL	S	502	-	5,5,5	0.48	0	5,5,5	0.34	0
3	GOL	D	503	-	5,5,5	0.37	0	5,5,5	0.41	0
3	GOL	C	402	-	5,5,5	0.40	0	5,5,5	0.54	0
3	GOL	D	501	-	5,5,5	0.40	0	5,5,5	0.54	0
3	GOL	P	403	-	5,5,5	0.33	0	5,5,5	0.30	0
3	GOL	Q	404	-	5,5,5	0.43	0	5,5,5	0.42	0
3	GOL	I	401	-	5,5,5	0.42	0	5,5,5	0.16	0
3	GOL	J	401	-	5,5,5	0.41	0	5,5,5	0.23	0
3	GOL	L	502	-	5,5,5	0.43	0	5,5,5	0.19	0
3	GOL	N	402	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	S	505	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	R	501	-	5,5,5	0.33	0	5,5,5	0.40	0
3	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.35	0
3	GOL	G	402	-	5,5,5	0.37	0	5,5,5	0.46	0
3	GOL	K	403	-	5,5,5	0.41	0	5,5,5	0.31	0
3	GOL	Q	405	-	5,5,5	0.34	0	5,5,5	0.32	0
3	GOL	C	401	-	5,5,5	0.43	0	5,5,5	0.38	0
3	GOL	R	503	-	5,5,5	0.45	0	5,5,5	0.46	0
3	GOL	S	504	-	5,5,5	0.40	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	501	-	5,5,5	0.45	0	5,5,5	0.37	0
3	GOL	F	402	-	5,5,5	0.27	0	5,5,5	0.39	0
3	GOL	K	404	-	5,5,5	0.42	0	5,5,5	0.60	0
3	GOL	O	404	-	5,5,5	0.39	0	5,5,5	0.37	0
3	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.51	0
3	GOL	B	403	-	5,5,5	0.40	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	O	403	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	H	403	-	-	0/4/4/4	-
3	GOL	G	401	-	-	0/4/4/4	-
3	GOL	E	402	-	-	0/4/4/4	-
3	GOL	F	401	-	-	4/4/4/4	-
3	GOL	Q	403	-	-	1/4/4/4	-
3	GOL	K	406	-	-	1/4/4/4	-
3	GOL	M	406	-	-	1/4/4/4	-
3	GOL	L	503	-	-	2/4/4/4	-
3	GOL	L	504	-	-	2/4/4/4	-
3	GOL	N	401	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	T	404	-	-	2/4/4/4	-
3	GOL	S	503	-	-	0/4/4/4	-
3	GOL	M	403	-	-	2/4/4/4	-
3	GOL	M	404	-	-	0/4/4/4	-
3	GOL	L	501	-	-	2/4/4/4	-
3	GOL	R	504	-	-	0/4/4/4	-
3	GOL	N	403	-	-	0/4/4/4	-
3	GOL	H	404	-	-	2/4/4/4	-
3	GOL	T	403	-	-	2/4/4/4	-
3	GOL	I	402	-	-	2/4/4/4	-
3	GOL	S	501	-	-	4/4/4/4	-
3	GOL	E	401	-	-	4/4/4/4	-
3	GOL	M	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	403	-	-	2/4/4/4	-
3	GOL	R	502	-	-	2/4/4/4	-
3	GOL	P	401	-	-	2/4/4/4	-
3	GOL	J	402	-	-	2/4/4/4	-
3	GOL	P	402	-	-	0/4/4/4	-
3	GOL	S	502	-	-	1/4/4/4	-
3	GOL	D	503	-	-	4/4/4/4	-
3	GOL	C	402	-	-	4/4/4/4	-
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	P	403	-	-	2/4/4/4	-
3	GOL	Q	404	-	-	2/4/4/4	-
3	GOL	I	401	-	-	0/4/4/4	-
3	GOL	J	401	-	-	2/4/4/4	-
3	GOL	L	502	-	-	2/4/4/4	-
3	GOL	N	402	-	-	2/4/4/4	-
3	GOL	S	505	-	-	0/4/4/4	-
3	GOL	R	501	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	G	402	-	-	2/4/4/4	-
3	GOL	K	403	-	-	2/4/4/4	-
3	GOL	Q	405	-	-	2/4/4/4	-
3	GOL	C	401	-	-	2/4/4/4	-
3	GOL	R	503	-	-	2/4/4/4	-
3	GOL	S	504	-	-	2/4/4/4	-
3	GOL	A	501	-	-	1/4/4/4	-
3	GOL	F	402	-	-	4/4/4/4	-
3	GOL	K	404	-	-	0/4/4/4	-
3	GOL	O	404	-	-	2/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	503	GOL	O1-C1-C2-O2
3	L	503	GOL	O1-C1-C2-C3
3	M	403	GOL	O1-C1-C2-C3
3	L	501	GOL	C1-C2-C3-O3
3	T	403	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	GOL	1	0
3	M	403	GOL	1	0
3	L	501	GOL	2	0
3	S	501	GOL	1	0
3	J	402	GOL	1	0
3	L	502	GOL	1	0
3	R	501	GOL	1	0
3	S	504	GOL	1	0
3	A	501	GOL	2	0
3	K	404	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	274/289 (94%)	-0.39	7 (2%)	56	54	9, 17, 41, 67	0
1	B	280/289 (96%)	-0.50	8 (2%)	51	50	9, 18, 47, 67	0
1	C	280/289 (96%)	-0.51	6 (2%)	63	63	8, 16, 41, 68	0
1	D	272/289 (94%)	-0.53	4 (1%)	73	74	6, 14, 36, 76	0
1	E	276/289 (95%)	-0.50	6 (2%)	62	61	7, 15, 39, 70	0
1	F	272/289 (94%)	-0.39	5 (1%)	68	68	9, 18, 42, 70	0
1	G	271/289 (93%)	-0.33	10 (3%)	41	39	9, 18, 40, 58	0
1	H	280/289 (96%)	-0.49	9 (3%)	47	45	9, 18, 48, 71	0
1	I	271/289 (93%)	-0.48	5 (1%)	68	68	9, 19, 40, 66	0
1	J	272/289 (94%)	-0.53	5 (1%)	68	68	9, 18, 44, 79	0
1	K	274/289 (94%)	-0.44	10 (3%)	42	40	9, 16, 42, 71	0
1	L	272/289 (94%)	-0.41	8 (2%)	51	50	8, 16, 36, 69	0
1	M	278/289 (96%)	-0.59	3 (1%)	80	81	8, 14, 39, 64	0
1	N	278/289 (96%)	-0.43	3 (1%)	80	81	9, 17, 44, 63	0
1	O	273/289 (94%)	-0.38	8 (2%)	51	50	9, 18, 39, 74	0
1	P	275/289 (95%)	-0.32	9 (3%)	46	44	9, 16, 44, 65	0
1	Q	271/289 (93%)	-0.58	2 (0%)	87	88	8, 15, 38, 65	0
1	R	278/289 (96%)	-0.47	2 (0%)	87	88	8, 15, 39, 58	0
1	S	271/289 (93%)	-0.48	8 (2%)	50	48	9, 15, 39, 69	0
1	T	273/289 (94%)	-0.44	9 (3%)	46	44	8, 16, 41, 69	0
All	All	5491/5780 (95%)	-0.46	127 (2%)	60	59	6, 16, 41, 79	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	40	VAL	6.7
1	O	320	ASN	5.9
1	B	72	THR	5.9
1	F	40	VAL	5.6
1	K	72	THR	5.2

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)

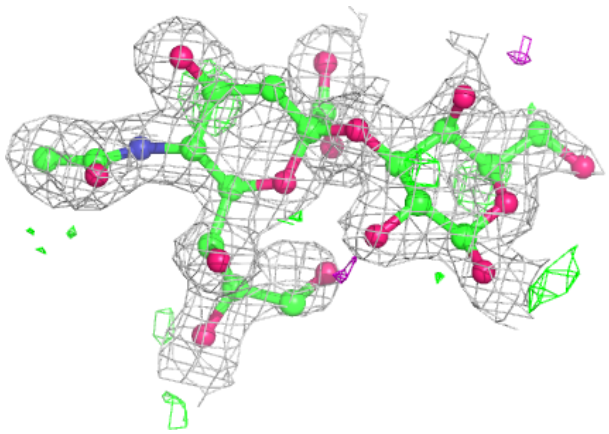
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

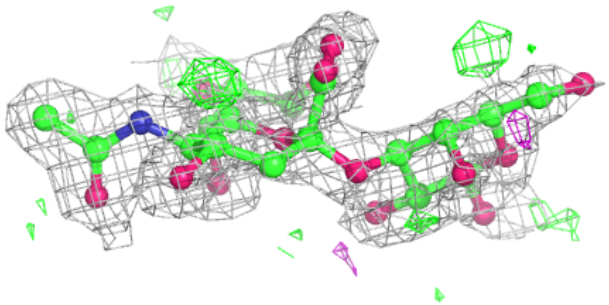
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	X	1	12/12	0.83	0.21	29,38,40,41	12
2	GAL	U	1	12/12	0.85	0.31	29,35,39,40	12
2	SIA	Y	2	20/21	0.85	0.14	15,24,34,35	20
2	SIA	X	2	20/21	0.85	0.15	9,24,30,32	20
2	SIA	W	2	20/21	0.86	0.18	17,24,30,31	20
2	SIA	V	2	20/21	0.86	0.21	16,25,33,36	20
2	GAL	Y	1	12/12	0.86	0.15	26,32,35,36	12
2	SIA	a	2	20/21	0.87	0.18	16,26,37,38	0
2	SIA	Z	2	20/21	0.87	0.17	6,20,29,30	20
2	GAL	Z	1	12/12	0.87	0.20	22,28,30,31	12
2	SIA	U	2	20/21	0.88	0.24	15,26,33,36	20
2	GAL	V	1	12/12	0.89	0.29	30,38,42,45	12
2	GAL	a	1	12/12	0.91	0.23	29,36,39,41	0
2	GAL	W	1	12/12	0.91	0.20	28,36,39,41	12

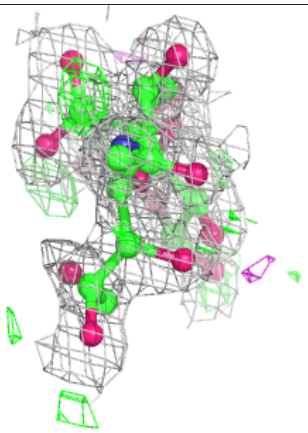
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

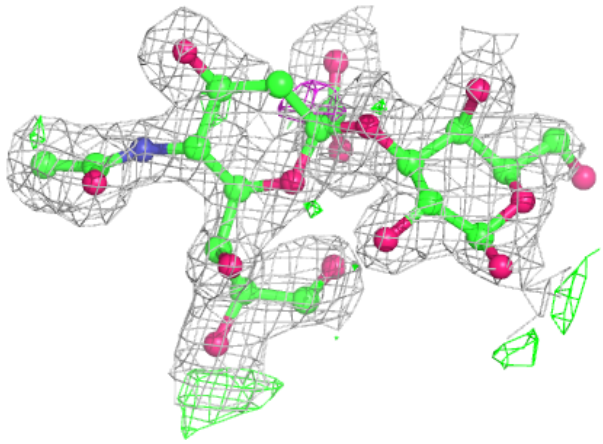


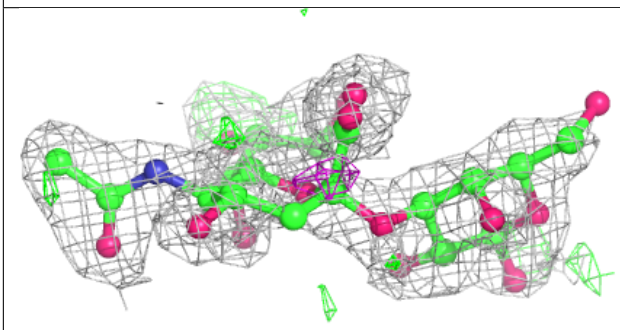


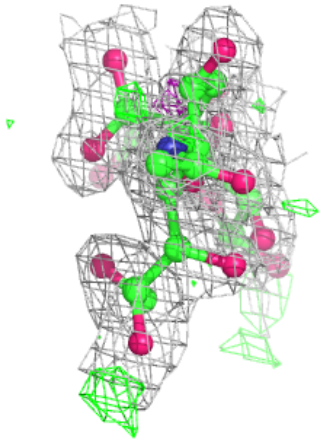


Electron density around Chain V:

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

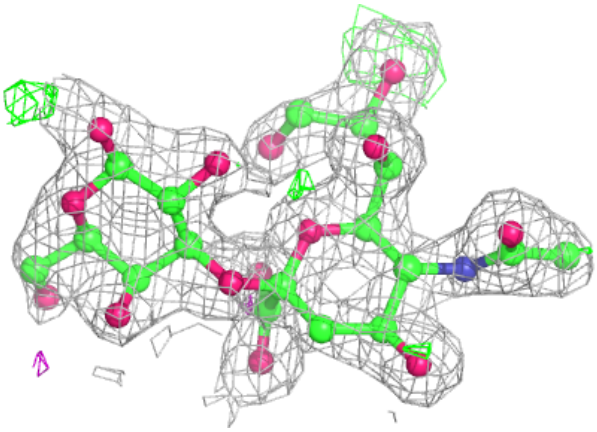


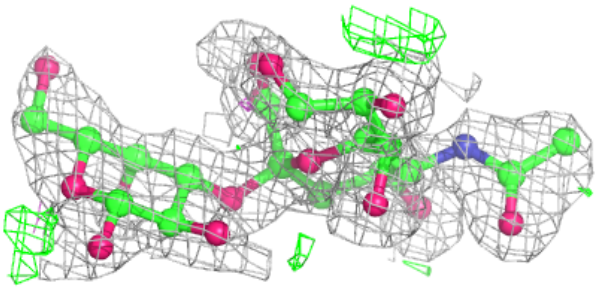




Electron density around Chain W:

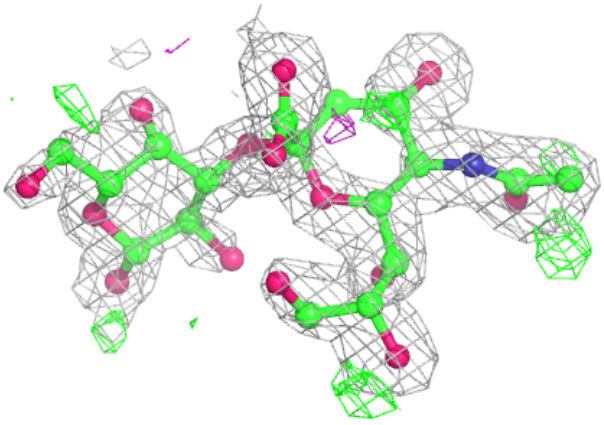
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

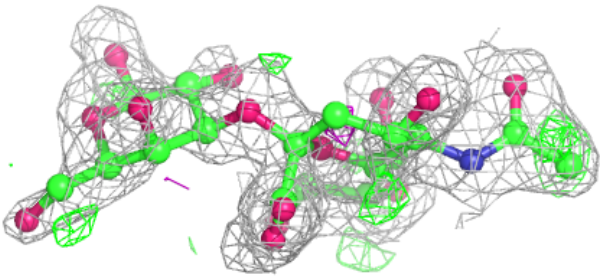




Electron density around Chain X:

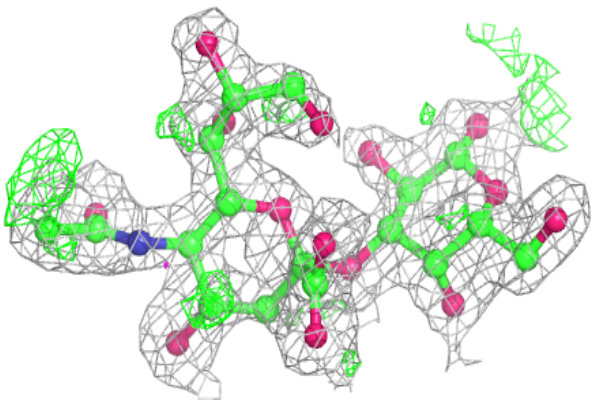
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

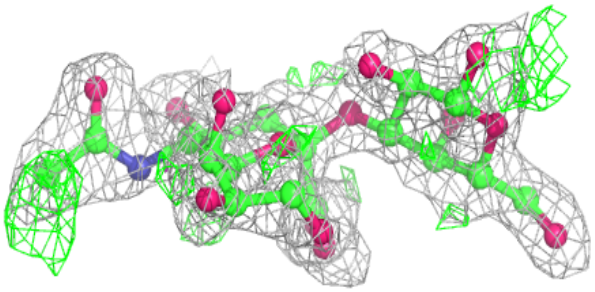


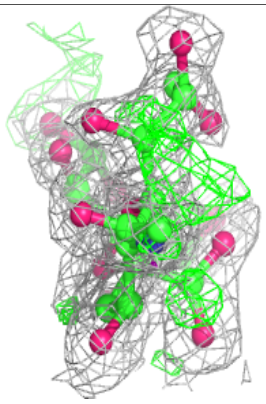


Electron density around Chain Y:

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

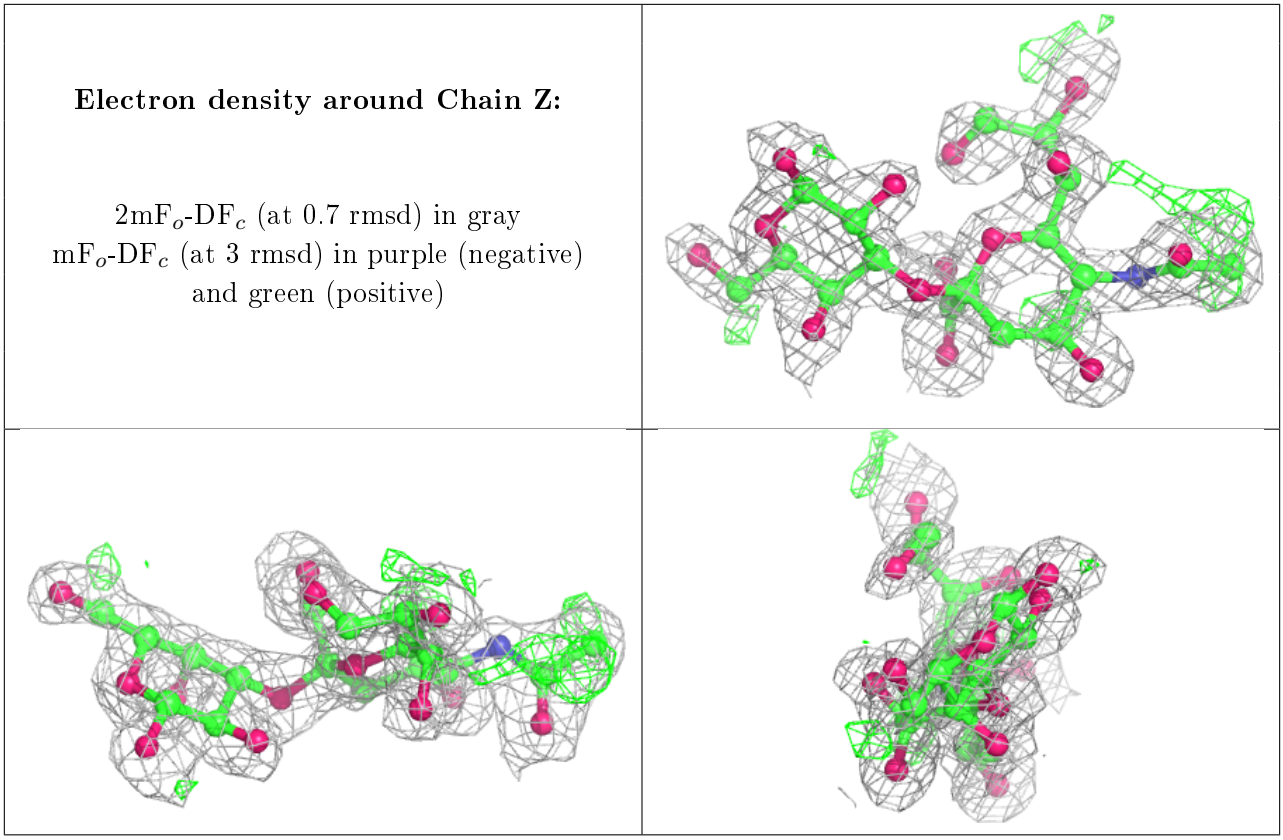






Electron density around Chain Z:

$2mF_o$-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^{th} 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
3	GOL	L	504	6/6	0.75	0.30	34,45,47,51	0
3	GOL	N	402	6/6	0.78	0.26	41,48,49,52	0
3	GOL	J	402	6/6	0.80	0.29	44,49,50,54	0
3	GOL	L	503	6/6	0.82	0.20	43,45,46,46	0
3	GOL	E	403	6/6	0.83	0.24	40,47,51,52	0
3	GOL	R	504	6/6	0.84	0.16	31,38,40,44	0
3	GOL	R	503	6/6	0.85	0.20	40,41,44,45	0
3	GOL	K	404	6/6	0.85	0.24	37,41,42,43	0
3	GOL	O	404	6/6	0.86	0.28	35,42,46,46	0
3	GOL	A	503	6/6	0.86	0.25	26,42,45,49	0
3	GOL	P	402	6/6	0.87	0.17	37,41,42,45	0
3	GOL	Q	404	6/6	0.87	0.16	36,38,40,44	0
3	GOL	B	404	6/6	0.87	0.21	28,39,40,46	0
3	GOL	D	503	6/6	0.88	0.21	28,37,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	P	403	6/6	0.88	0.20	25,40,43,49	0
3	GOL	K	406	6/6	0.88	0.13	26,28,32,39	0
3	GOL	N	403	6/6	0.88	0.12	33,37,39,39	0
3	GOL	T	404	6/6	0.89	0.19	33,35,38,41	0
3	GOL	I	402	6/6	0.89	0.19	45,48,49,50	0
3	GOL	S	501	6/6	0.89	0.17	24,30,32,35	0
3	GOL	G	402	6/6	0.90	0.19	29,37,39,44	0
3	GOL	D	501	6/6	0.90	0.19	19,29,31,33	0
3	GOL	A	501	6/6	0.90	0.15	27,28,32,32	0
3	GOL	E	402	6/6	0.90	0.25	40,44,47,50	0
3	GOL	H	404	6/6	0.90	0.22	33,39,40,42	0
3	GOL	M	405	6/6	0.91	0.13	34,35,38,41	0
3	GOL	M	403	6/6	0.91	0.21	21,28,32,33	0
3	GOL	M	406	6/6	0.91	0.21	22,38,38,45	0
3	GOL	S	503	6/6	0.91	0.19	36,38,43,44	0
3	GOL	R	501	6/6	0.92	0.17	8,16,26,32	0
3	GOL	L	501	6/6	0.92	0.16	16,22,27,36	0
3	GOL	S	504	6/6	0.92	0.27	24,35,37,42	0
3	GOL	F	402	6/6	0.93	0.11	26,29,33,37	0
3	GOL	Q	405	6/6	0.93	0.17	19,36,39,46	0
3	GOL	S	505	6/6	0.93	0.08	24,28,29,30	0
3	GOL	C	402	6/6	0.94	0.19	29,38,39,39	0
3	GOL	J	401	6/6	0.95	0.14	22,32,33,34	0
3	GOL	N	401	6/6	0.95	0.13	12,30,31,31	0
3	GOL	K	403	6/6	0.95	0.11	13,29,32,34	0
3	GOL	T	403	6/6	0.95	0.10	18,29,31,34	0
3	GOL	I	401	6/6	0.95	0.12	15,29,30,31	0
3	GOL	B	403	6/6	0.95	0.08	16,29,32,33	0
3	GOL	A	502	6/6	0.96	0.08	13,26,28,31	0
3	GOL	L	502	6/6	0.96	0.11	15,29,29,32	0
3	GOL	H	403	6/6	0.96	0.08	14,27,30,32	0
3	GOL	O	403	6/6	0.96	0.13	17,29,31,33	0
3	GOL	R	502	6/6	0.96	0.14	13,30,32,34	0
3	GOL	P	401	6/6	0.96	0.11	13,28,30,31	0
3	GOL	Q	403	6/6	0.96	0.11	17,29,32,34	0
3	GOL	D	502	6/6	0.96	0.11	14,29,30,33	0
3	GOL	C	401	6/6	0.97	0.09	11,26,31,32	0
3	GOL	F	401	6/6	0.97	0.11	14,28,31,34	0
3	GOL	S	502	6/6	0.97	0.08	15,26,30,31	0
3	GOL	M	404	6/6	0.97	0.09	16,26,28,29	0
3	GOL	E	401	6/6	0.98	0.10	13,28,31,32	0
3	GOL	G	401	6/6	0.98	0.08	15,28,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	R	505	1/1	0.99	0.03	17,17,17,17	0
4	CL	F	403	1/1	0.99	0.03	21,21,21,21	0
4	CL	J	403	1/1	0.99	0.02	18,18,18,18	0
4	CL	D	504	1/1	0.99	0.03	18,18,18,18	0
4	CL	L	505	1/1	0.99	0.03	19,19,19,19	0
4	CL	G	403	1/1	0.99	0.02	17,17,17,17	0
4	CL	S	506	1/1	1.00	0.03	19,19,19,19	0
4	CL	C	403	1/1	1.00	0.04	22,22,22,22	0
4	CL	N	404	1/1	1.00	0.03	17,17,17,17	0
4	CL	E	404	1/1	1.00	0.04	17,17,17,17	0
4	CL	A	504	1/1	1.00	0.03	17,17,17,17	0
4	CL	K	405	1/1	1.00	0.02	17,17,17,17	0
4	CL	O	405	1/1	1.00	0.03	19,19,19,19	0
4	CL	Q	406	1/1	1.00	0.04	20,20,20,20	0
4	CL	H	405	1/1	1.00	0.02	18,18,18,18	0
4	CL	P	404	1/1	1.00	0.03	19,19,19,19	0
4	CL	B	405	1/1	1.00	0.03	19,19,19,19	0
4	CL	T	405	1/1	1.00	0.03	16,16,16,16	0
4	CL	M	407	1/1	1.00	0.03	18,18,18,18	0
4	CL	I	403	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.