wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 10:50 AM EDT

PDB ID	:	4FMJ
Title	:	Merkel cell polyomavirus VP1 in complex with GD1a oligosaccharide
Authors	:	Neu, U.; Hengel, H.; Stehle, T.
Deposited on	:	2012-06-17
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

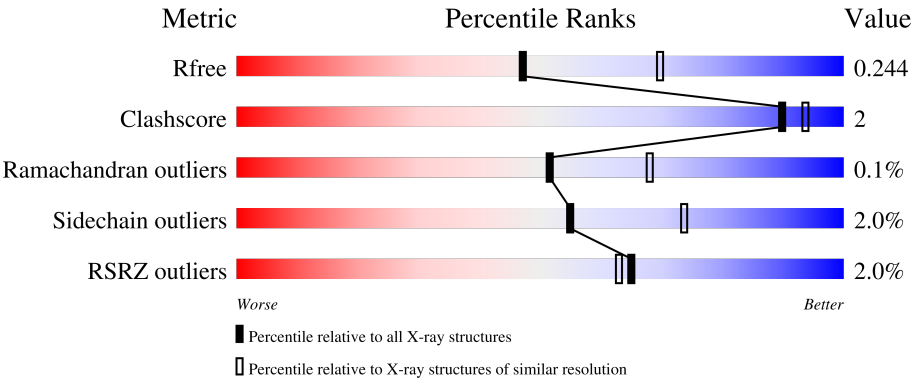
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	289	2% 88% 5% 7%
1	B	289	2% 90% 7% .
1	C	289	2% 89% 7% .
1	D	289	% 88% 6% 6%
1	E	289	% 90% . 6%

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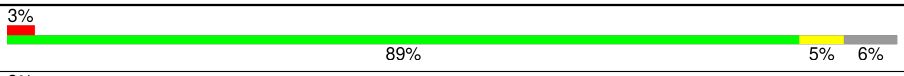
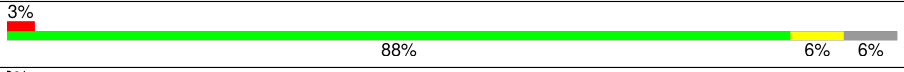
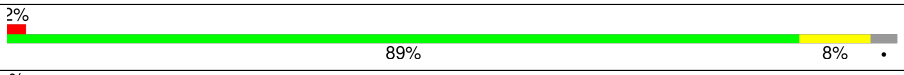
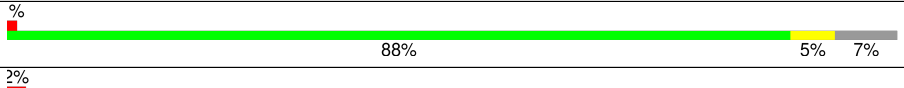
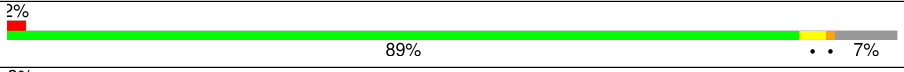
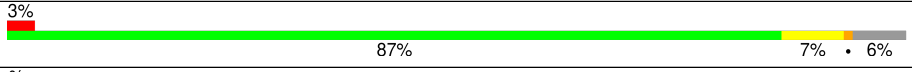
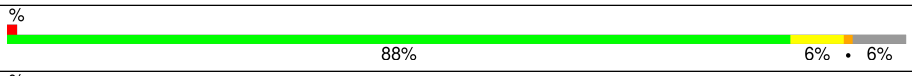
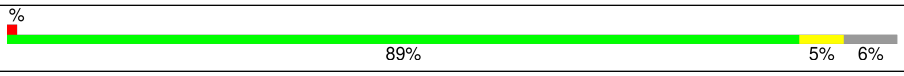
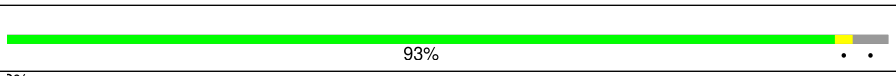
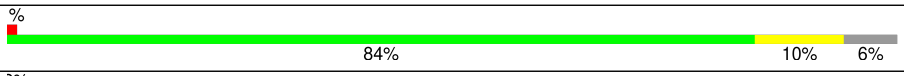
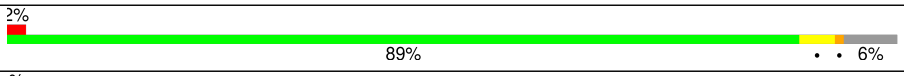
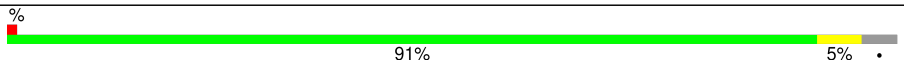
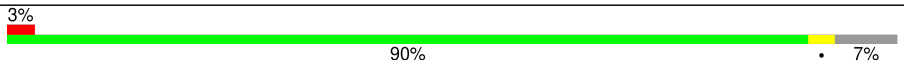
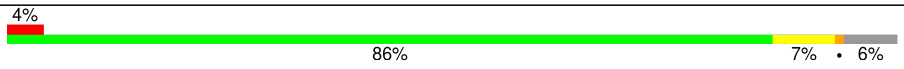
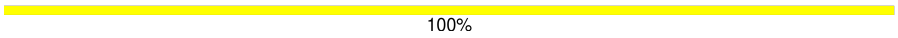
Mol	Chain	Length	Quality of chain
1	F	289	
1	G	289	
1	H	289	
1	I	289	
1	J	289	
1	K	289	
1	L	289	
1	M	289	
1	N	289	
1	O	289	
1	P	289	
1	Q	289	
1	R	289	
1	S	289	
1	T	289	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 44465 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	269	Total	C	N	O	S	0	1	0
			2107	1347	349	401	10			
1	B	280	Total	C	N	O	S	0	1	0
			2186	1392	361	422	11			
1	C	276	Total	C	N	O	S	0	1	0
			2157	1372	357	417	11			
1	D	271	Total	C	N	O	S	0	0	0
			2112	1349	350	403	10			
1	E	272	Total	C	N	O	S	0	0	0
			2122	1355	351	406	10			
1	F	272	Total	C	N	O	S	0	1	0
			2126	1358	351	407	10			
1	G	271	Total	C	N	O	S	0	0	0
			2116	1352	350	404	10			
1	H	280	Total	C	N	O	S	0	1	0
			2184	1390	361	422	11			
1	I	268	Total	C	N	O	S	0	1	0
			2096	1340	348	398	10			
1	J	270	Total	C	N	O	S	0	0	0
			2110	1347	349	404	10			
1	K	273	Total	C	N	O	S	0	0	0
			2131	1360	352	409	10			
1	L	272	Total	C	N	O	S	0	1	0
			2129	1360	352	407	10			
1	M	271	Total	C	N	O	S	0	1	0
			2121	1356	351	404	10			
1	N	278	Total	C	N	O	S	0	0	0
			2171	1383	358	419	11			
1	O	271	Total	C	N	O	S	0	0	0
			2114	1350	349	405	10			
1	P	271	Total	C	N	O	S	0	1	0
			2123	1356	351	406	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	271	Total	C	N	O	S	0	1	0
			2121	1356	351	404	10			
1	R	277	Total	C	N	O	S	0	0	0
			2162	1378	356	417	11			
1	S	270	Total	C	N	O	S	0	0	0
			2109	1348	349	402	10			
1	T	271	Total	C	N	O	S	0	1	0
			2119	1354	351	404	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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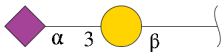
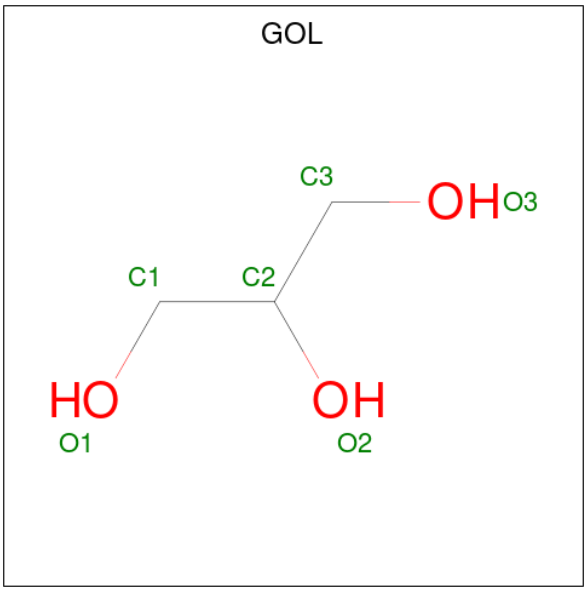
Chain	Residue	Modelled	Actual	Comment	Reference
T	33	SER	-	expression tag	UNP C0JPK1
T	34	HIS	-	expression tag	UNP C0JPK1
T	35	MET	-	expression tag	UNP C0JPK1
T	36	LEU	-	expression tag	UNP C0JPK1
T	37	GLU	-	expression tag	UNP C0JPK1

- 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			

- 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	C	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0
3	Q	1	Total C O 6 3 3	0	0
3	T	1	Total C O 6 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

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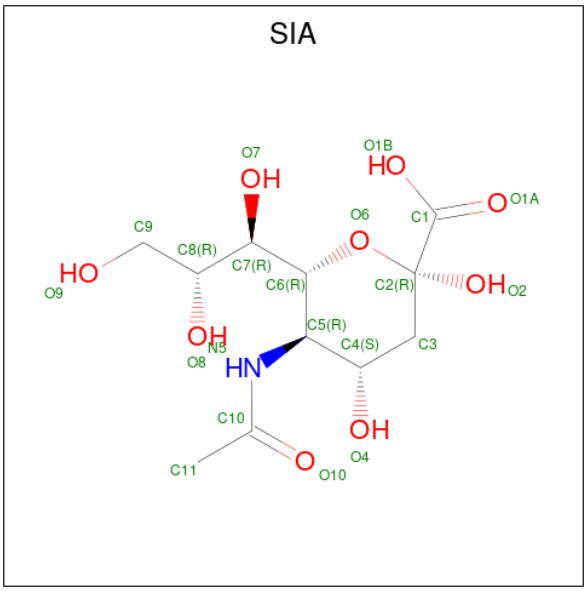
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0
4	M	1	Total Cl 1 1	0	0
4	N	1	Total Cl 1 1	0	0
4	O	1	Total Cl 1 1	0	0
4	P	1	Total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

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C N O 21 11 1 9	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	57	Total O 57 57	0	0
6	B	69	Total O 69 69	0	0
6	C	63	Total O 63 63	0	0
6	D	94	Total O 94 94	0	0
6	E	90	Total O 90 90	0	0
6	F	80	Total O 80 80	0	0
6	G	77	Total O 77 77	0	0
6	H	75	Total O 75 75	0	0
6	I	47	Total O 47 47	0	0
6	J	56	Total O 56 56	0	0
6	K	92	Total O 92 92	0	0

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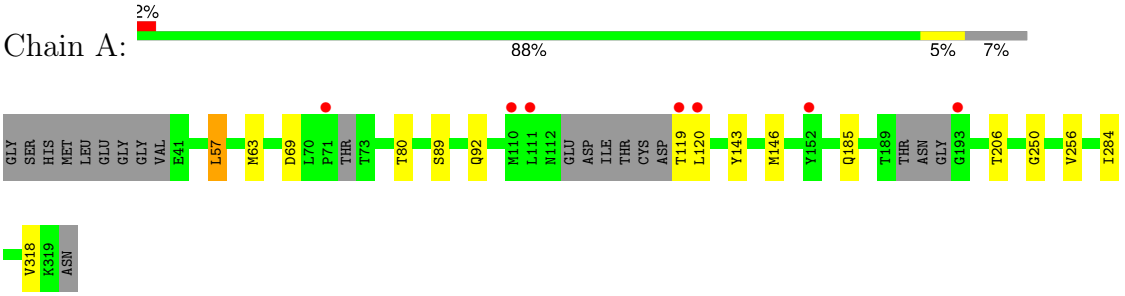
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	104	Total O 104 104	0	0
6	M	101	Total O 101 101	0	0
6	N	109	Total O 109 109	0	0
6	O	89	Total O 89 89	0	0
6	P	87	Total O 87 87	0	0
6	Q	74	Total O 74 74	0	0
6	R	75	Total O 75 75	0	0
6	S	70	Total O 70 70	0	0
6	T	59	Total O 59 59	0	0

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.

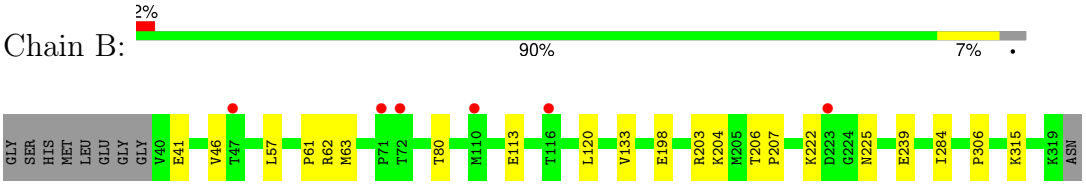
- Molecule 1: VP1

Chain A:



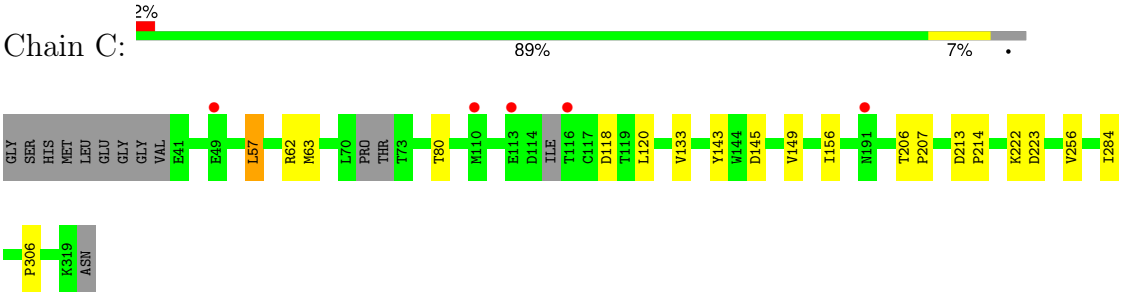
- Molecule 1: VP1

Chain B:



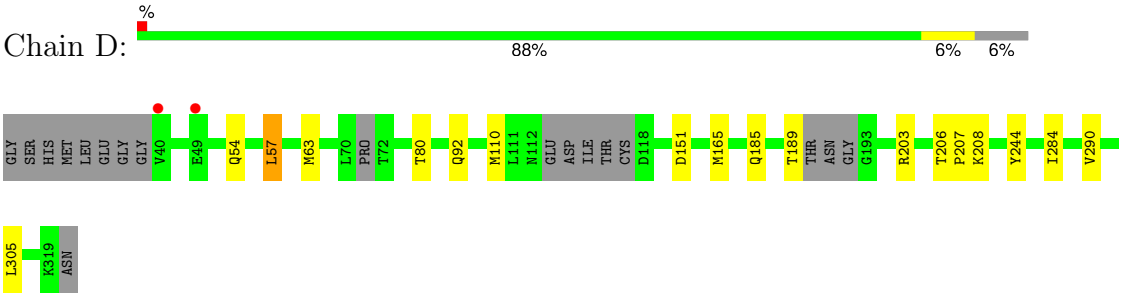
- Molecule 1: VP1

Chain C:



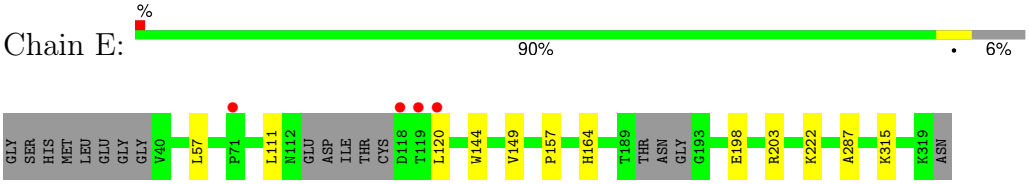
- Molecule 1: VP1

Chain D:



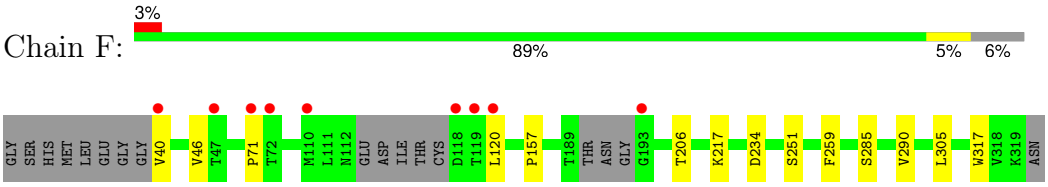
• Molecule 1: VP1

Chain E:



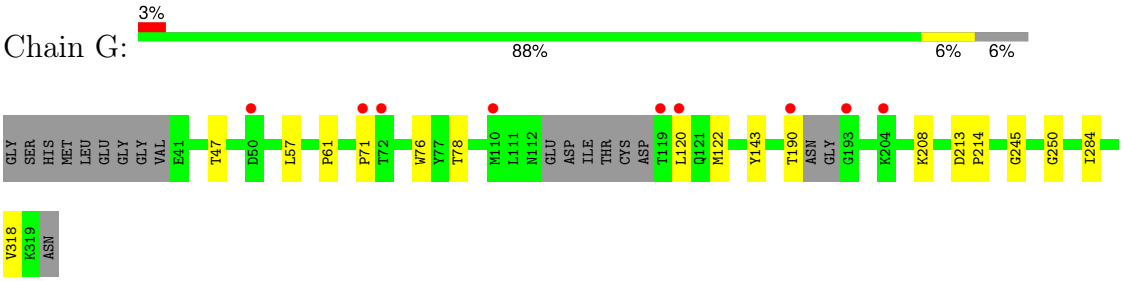
• Molecule 1: VP1

Chain F:



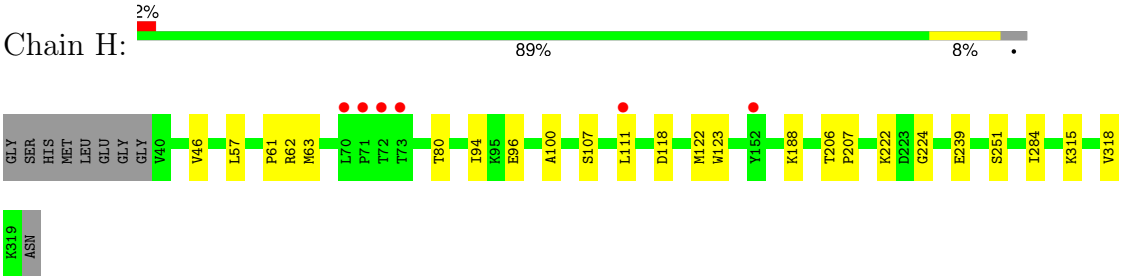
• Molecule 1: VP1

Chain G:



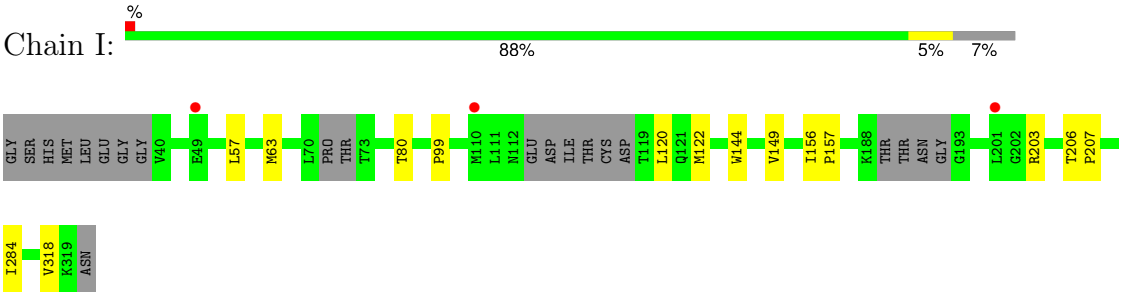
• Molecule 1: VP1

Chain H:



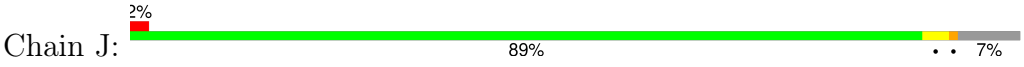
• Molecule 1: VP1

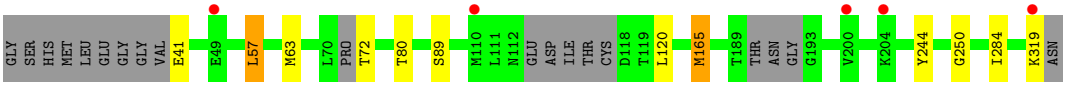
Chain I:



• Molecule 1: VP1

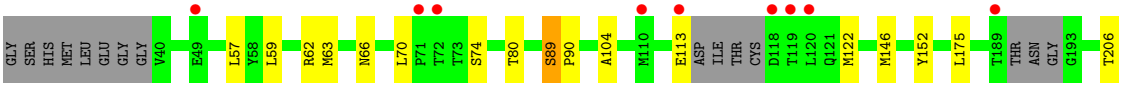
Chain J:





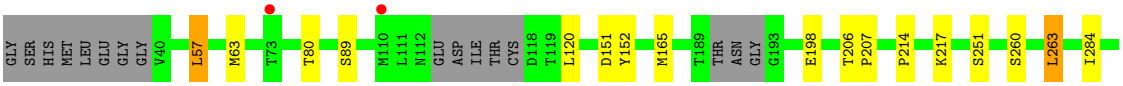
• Molecule 1: VP1

Chain K:



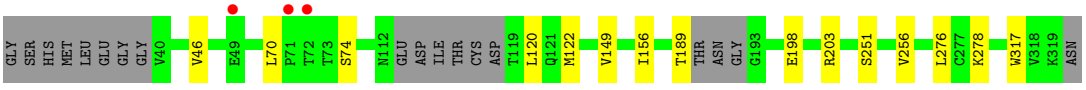
• Molecule 1: VP1

Chain L:



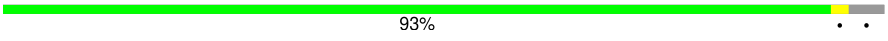
• Molecule 1: VP1

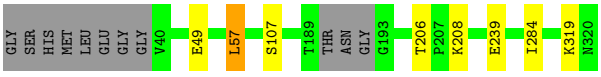
Chain M:



• Molecule 1: VP1

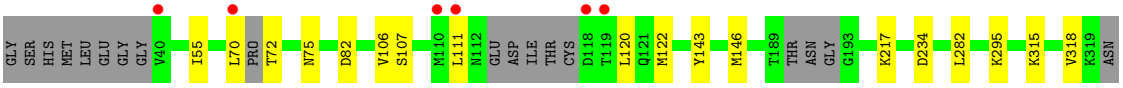
Chain N:





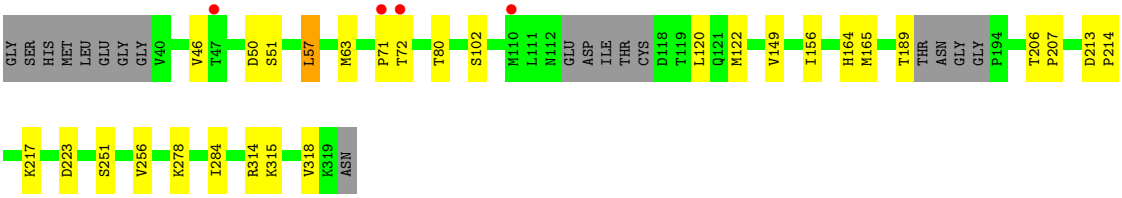
• Molecule 1: VP1

Chain O:

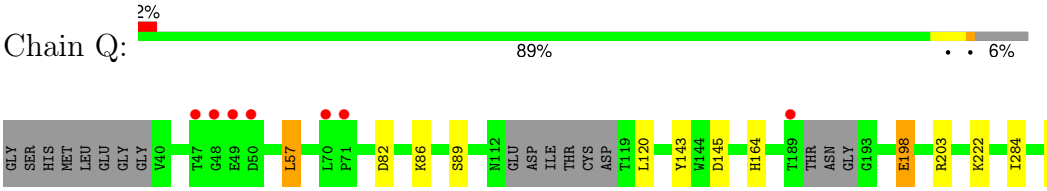


• Molecule 1: VP1

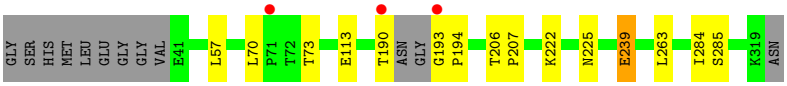
Chain P:



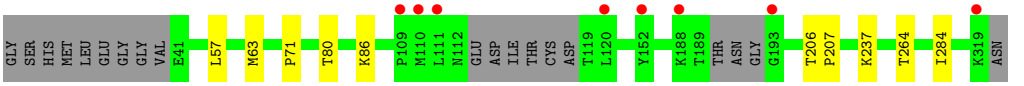
• Molecule 1: VP1



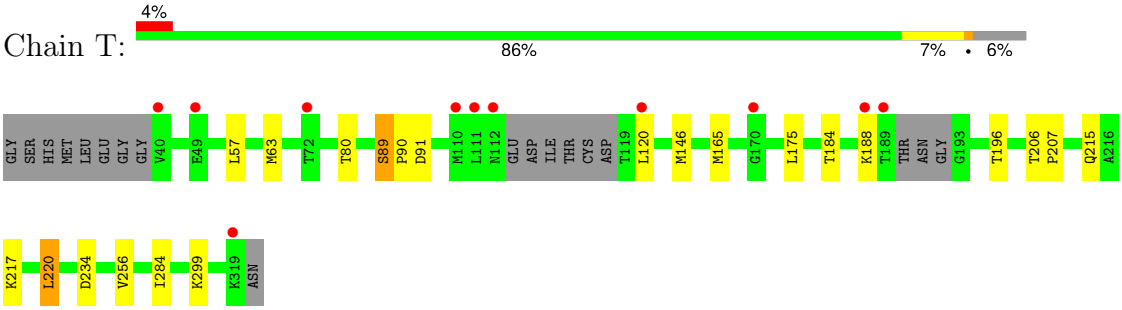
• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 1: VP1

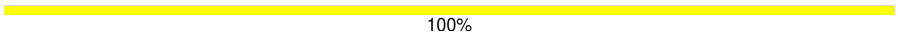


• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

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

• 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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.66Å 130.15Å 165.53Å 98.04° 101.02° 105.81°	Depositor
Resolution (Å)	50.00 – 2.40 47.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-2.40) 97.3 (47.13-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.192 , 0.246 0.193 , 0.244	Depositor DCC
R_{free} test set	6193 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	44465	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 77.40 % 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 8.5663e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.44	0/2160	0.54	0/2940
1	B	0.43	0/2242	0.55	0/3058
1	C	0.44	0/2210	0.53	0/3009
1	D	0.46	0/2161	0.56	0/2941
1	E	0.46	0/2173	0.56	0/2960
1	F	0.45	0/2180	0.55	0/2971
1	G	0.45	0/2167	0.56	0/2952
1	H	0.43	0/2240	0.55	0/3055
1	I	0.42	0/2148	0.52	0/2922
1	J	0.42	0/2159	0.55	0/2938
1	K	0.46	0/2182	0.56	0/2972
1	L	0.48	0/2183	0.57	0/2974
1	M	0.48	0/2175	0.56	0/2963
1	N	0.46	0/2223	0.58	0/3029
1	O	0.47	0/2163	0.58	0/2945
1	P	0.46	0/2177	0.56	0/2965
1	Q	0.45	0/2175	0.55	0/2963
1	R	0.42	0/2214	0.55	0/3018
1	S	0.44	0/2160	0.55	0/2942
1	T	0.45	0/2173	0.56	0/2960
All	All	0.45	0/43665	0.55	0/59477

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2107	0	2094	10	0
1	B	2186	0	2166	8	0
1	C	2157	0	2130	10	0
1	D	2112	0	2092	10	0
1	E	2122	0	2102	5	0
1	F	2126	0	2106	5	0
1	G	2116	0	2103	8	0
1	H	2184	0	2159	11	0
1	I	2096	0	2077	10	0
1	J	2110	0	2092	7	0
1	K	2131	0	2108	13	0
1	L	2129	0	2115	9	0
1	M	2121	0	2111	7	0
1	N	2171	0	2149	3	0
1	O	2114	0	2092	8	0
1	P	2123	0	2106	15	0
1	Q	2121	0	2111	6	0
1	R	2162	0	2141	6	0
1	S	2109	0	2096	3	0
1	T	2119	0	2104	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
3	A	6	0	8	2	0
3	C	6	0	8	1	0
3	K	6	0	8	1	0
3	M	6	0	8	1	0
3	N	6	0	8	0	0
3	P	6	0	8	1	0
3	Q	6	0	8	0	0
3	T	6	0	8	1	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	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	0	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	1	0
4	Q	1	0	0	1	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
5	H	21	0	18	0	0
6	A	57	0	0	0	0
6	B	69	0	0	0	0
6	C	63	0	0	0	0
6	D	94	0	0	0	0
6	E	90	0	0	0	0
6	F	80	0	0	0	0
6	G	77	0	0	0	0
6	H	75	0	0	0	0
6	I	47	0	0	1	0
6	J	56	0	0	0	0
6	K	92	0	0	1	0
6	L	104	0	0	0	0
6	M	101	0	0	0	0
6	N	109	0	0	0	0
6	O	89	0	0	0	0
6	P	87	0	0	0	0
6	Q	74	0	0	0	0
6	R	75	0	0	1	0
6	S	70	0	0	0	0
6	T	59	0	0	2	0
All	All	44465	0	42504	157	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 157 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:H:57:LEU:HD21	1:H:284:ILE:HD13	1.58	0.85
1:L:57:LEU:HD21	1:L:284:ILE:HD12	1.58	0.85
1:P:57:LEU:HD21	1:P:284:ILE:HD13	1.60	0.83
1:B:57:LEU:HD21	1:B:284:ILE:HD13	1.62	0.78
1:G:57:LEU:HD21	1:G:284:ILE:HD13	1.68	0.76

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	262/289 (91%)	248 (95%)	14 (5%)	0	100	100
1	B	279/289 (96%)	264 (95%)	15 (5%)	0	100	100
1	C	271/289 (94%)	257 (95%)	14 (5%)	0	100	100
1	D	263/289 (91%)	253 (96%)	10 (4%)	0	100	100
1	E	266/289 (92%)	248 (93%)	18 (7%)	0	100	100
1	F	267/289 (92%)	253 (95%)	13 (5%)	1 (0%)	34	48
1	G	265/289 (92%)	251 (95%)	13 (5%)	1 (0%)	34	48
1	H	279/289 (96%)	265 (95%)	14 (5%)	0	100	100
1	I	261/289 (90%)	249 (95%)	12 (5%)	0	100	100
1	J	262/289 (91%)	251 (96%)	11 (4%)	0	100	100
1	K	267/289 (92%)	251 (94%)	16 (6%)	0	100	100
1	L	267/289 (92%)	253 (95%)	14 (5%)	0	100	100
1	M	266/289 (92%)	252 (95%)	14 (5%)	0	100	100
1	N	274/289 (95%)	262 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	263/289 (91%)	248 (94%)	15 (6%)	0	100	100
1	P	266/289 (92%)	252 (95%)	13 (5%)	1 (0%)	34	48
1	Q	266/289 (92%)	248 (93%)	18 (7%)	0	100	100
1	R	273/289 (94%)	259 (95%)	14 (5%)	0	100	100
1	S	264/289 (91%)	256 (97%)	7 (3%)	1 (0%)	34	48
1	T	266/289 (92%)	252 (95%)	13 (5%)	1 (0%)	34	48
All	All	5347/5780 (92%)	5072 (95%)	270 (5%)	5 (0%)	51	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	71	PRO
1	G	71	PRO
1	S	71	PRO
1	T	220	LEU
1	P	71	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	238/253 (94%)	234 (98%)	4 (2%)	60	78
1	B	248/253 (98%)	243 (98%)	5 (2%)	55	74
1	C	244/253 (96%)	240 (98%)	4 (2%)	62	79
1	D	237/253 (94%)	231 (98%)	6 (2%)	47	67
1	E	239/253 (94%)	235 (98%)	4 (2%)	60	78
1	F	240/253 (95%)	235 (98%)	5 (2%)	53	72
1	G	239/253 (94%)	235 (98%)	4 (2%)	60	78
1	H	247/253 (98%)	242 (98%)	5 (2%)	55	74
1	I	235/253 (93%)	233 (99%)	2 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	238/253 (94%)	234 (98%)	4 (2%)	60	78
1	K	240/253 (95%)	236 (98%)	4 (2%)	60	78
1	L	241/253 (95%)	234 (97%)	7 (3%)	42	62
1	M	240/253 (95%)	236 (98%)	4 (2%)	60	78
1	N	246/253 (97%)	241 (98%)	5 (2%)	55	74
1	O	238/253 (94%)	235 (99%)	3 (1%)	69	84
1	P	240/253 (95%)	234 (98%)	6 (2%)	47	67
1	Q	240/253 (95%)	234 (98%)	6 (2%)	47	67
1	R	245/253 (97%)	237 (97%)	8 (3%)	38	57
1	S	238/253 (94%)	235 (99%)	3 (1%)	69	84
1	T	239/253 (94%)	233 (98%)	6 (2%)	47	67
All	All	4812/5060 (95%)	4717 (98%)	95 (2%)	55	74

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	278	LYS
1	P	251	SER
1	N	57	LEU
1	O	120	LEU
1	Q	120	LEU

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

Mol	Chain	Res	Type
1	P	183	GLN
1	S	75	ASN
1	T	112	ASN
1	F	54	GLN
1	H	54	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GAL	U	1	2	12,12,12	0.60	0	17,17,17	0.57	0
2	SIA	U	2	2	20,20,21	0.65	0	21,28,31	1.08	1 (4%)
2	GAL	V	1	2	12,12,12	0.60	0	17,17,17	0.58	0
2	SIA	V	2	2	20,20,21	0.67	0	21,28,31	0.87	0
2	GAL	W	1	2	12,12,12	0.58	0	17,17,17	0.89	1 (5%)
2	SIA	W	2	2	20,20,21	0.71	0	21,28,31	1.14	3 (14%)
2	GAL	X	1	2	12,12,12	0.57	0	17,17,17	0.73	0
2	SIA	X	2	2	20,20,21	0.61	0	21,28,31	1.20	3 (14%)
2	GAL	Y	1	2	12,12,12	0.48	0	17,17,17	0.65	0
2	SIA	Y	2	2	20,20,21	0.65	0	21,28,31	1.15	2 (9%)
2	GAL	Z	1	2	12,12,12	0.55	0	17,17,17	0.49	0
2	SIA	Z	2	2	20,20,21	0.68	0	21,28,31	1.09	3 (14%)

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	-	2/2/22/22	0/1/1/1
2	SIA	U	2	2	-	6/18/34/38	0/1/1/1
2	GAL	V	1	2	-	1/2/22/22	0/1/1/1
2	SIA	V	2	2	-	2/18/34/38	0/1/1/1
2	GAL	W	1	2	-	0/2/22/22	0/1/1/1
2	SIA	W	2	2	-	0/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	X	1	2	-	2/2/22/22	0/1/1/1
2	SIA	X	2	2	-	2/18/34/38	0/1/1/1
2	GAL	Y	1	2	-	0/2/22/22	0/1/1/1
2	SIA	Y	2	2	-	5/18/34/38	0/1/1/1
2	GAL	Z	1	2	-	1/2/22/22	0/1/1/1
2	SIA	Z	2	2	-	0/18/34/38	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	O1B-C1-C2	2.72	119.78	112.71
2	W	2	SIA	O1B-C1-C2	2.70	119.74	112.71
2	W	1	GAL	O5-C5-C6	2.64	112.99	106.44
2	Y	2	SIA	O1B-C1-C2	2.64	119.58	112.71
2	Z	2	SIA	O1B-C1-C2	2.51	119.24	112.71

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

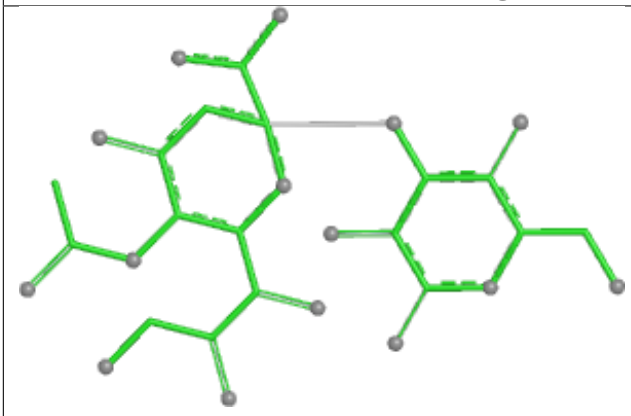
Mol	Chain	Res	Type	Atoms
2	U	2	SIA	C6-C7-C8-C9
2	U	2	SIA	O7-C7-C8-C9
2	V	2	SIA	C7-C8-C9-O9
2	V	2	SIA	O8-C8-C9-O9
2	U	2	SIA	O7-C7-C8-O8

There are no ring outliers.

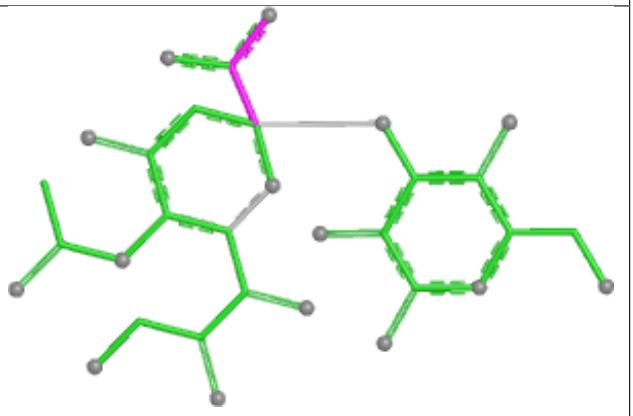
No monomer is involved in short contacts.

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

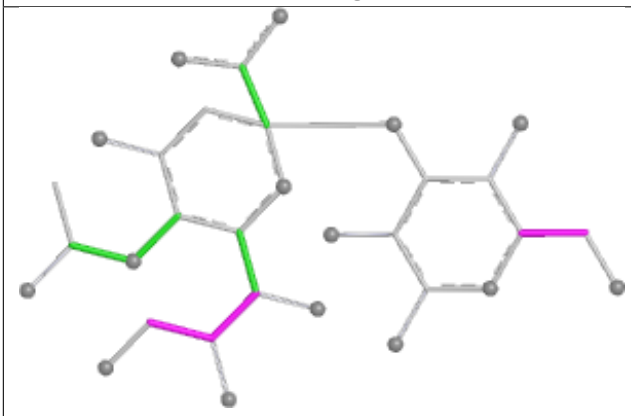
Oligosaccharide Chain U



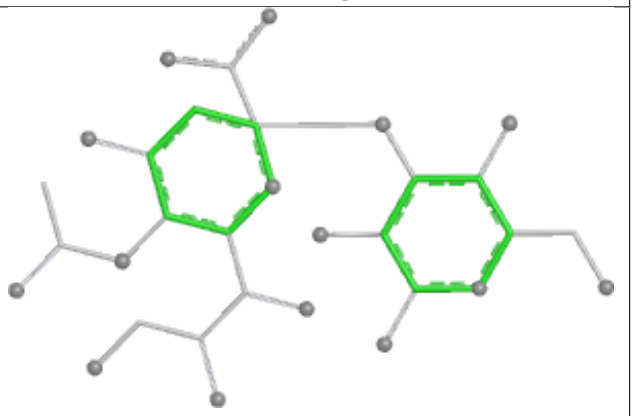
Bond lengths



Bond angles

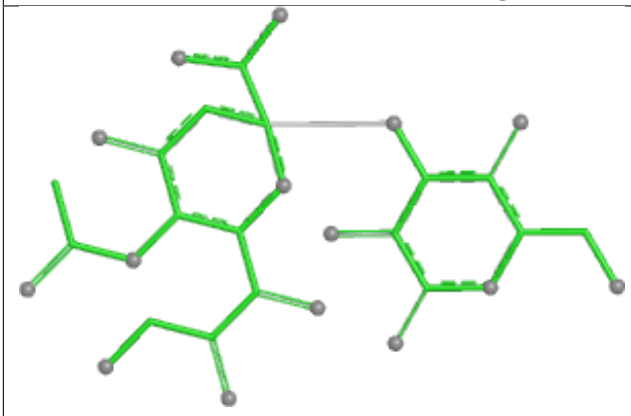


Torsions

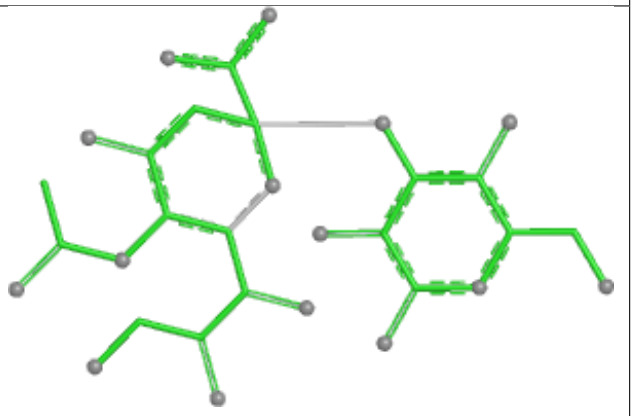


Rings

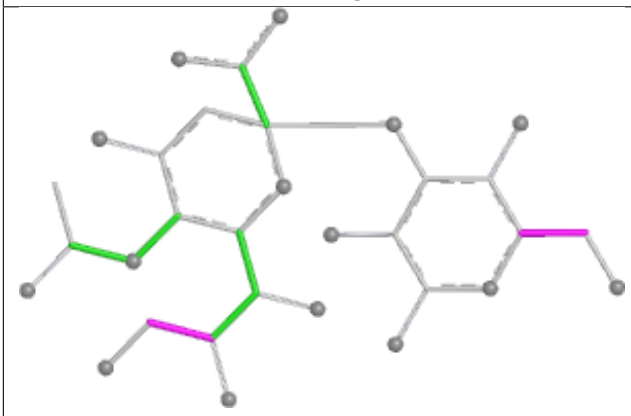
Oligosaccharide Chain V



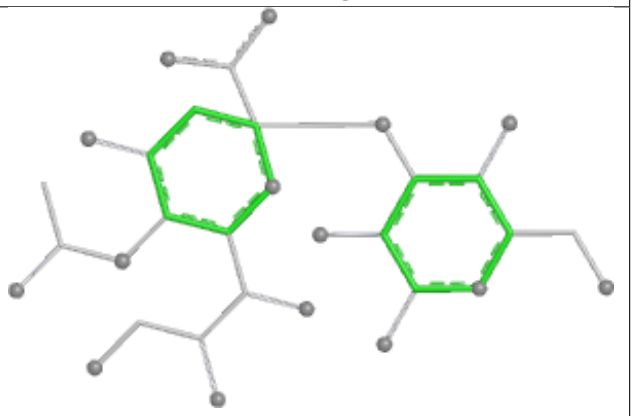
Bond lengths



Bond angles

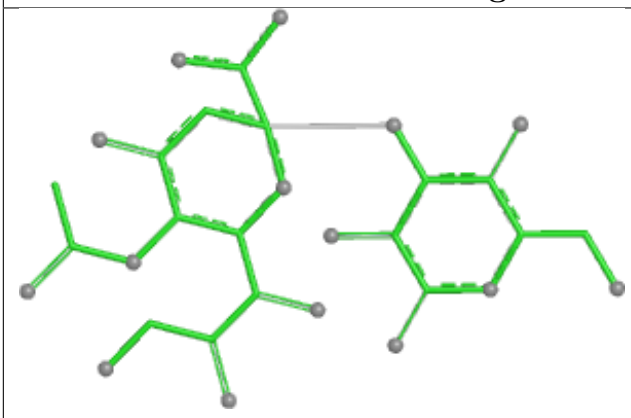


Torsions

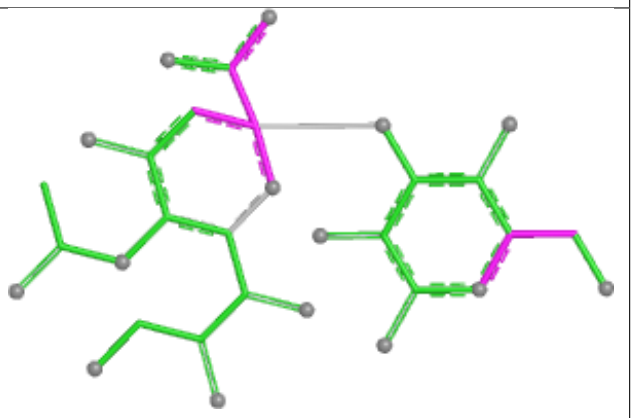


Rings

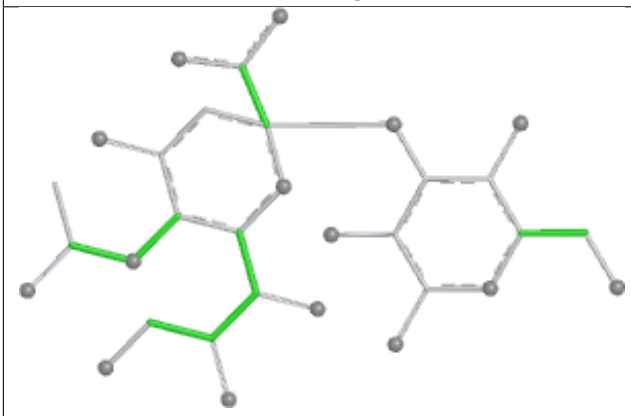
Oligosaccharide Chain W



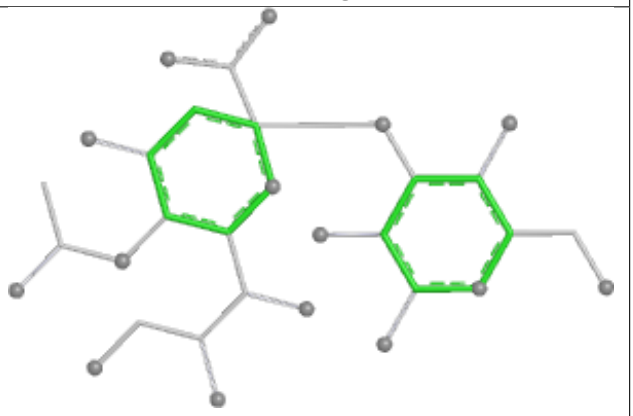
Bond lengths



Bond angles

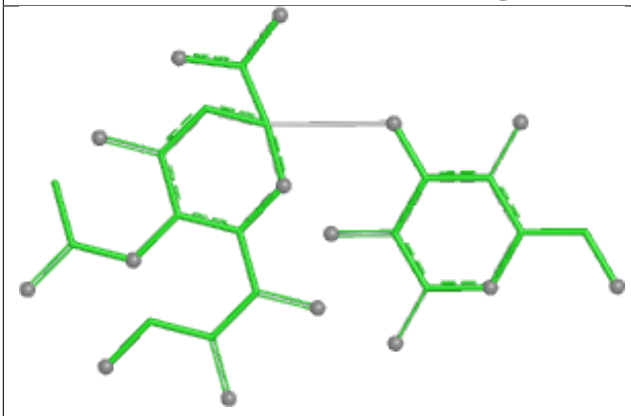


Torsions

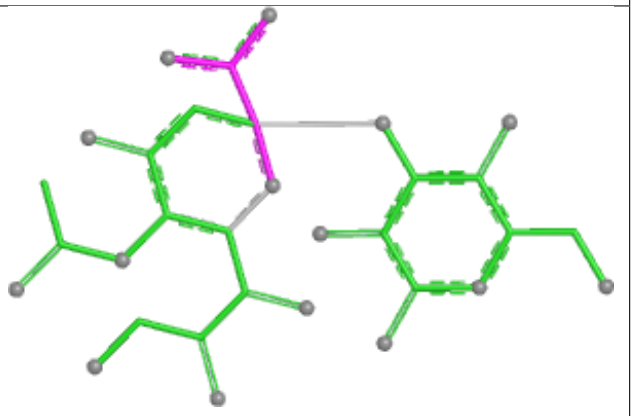


Rings

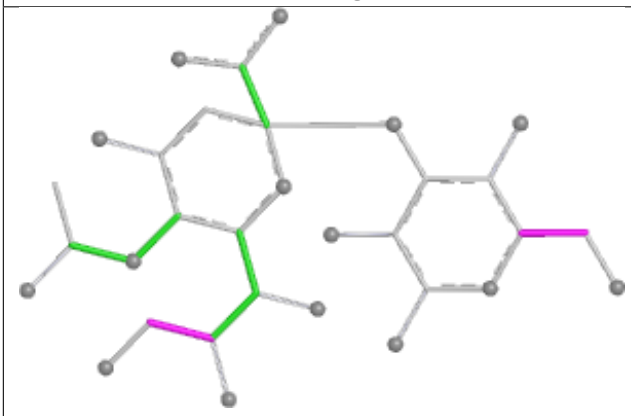
Oligosaccharide Chain X



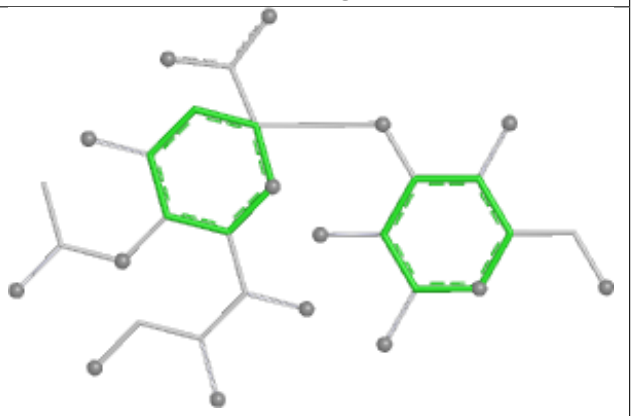
Bond lengths



Bond angles

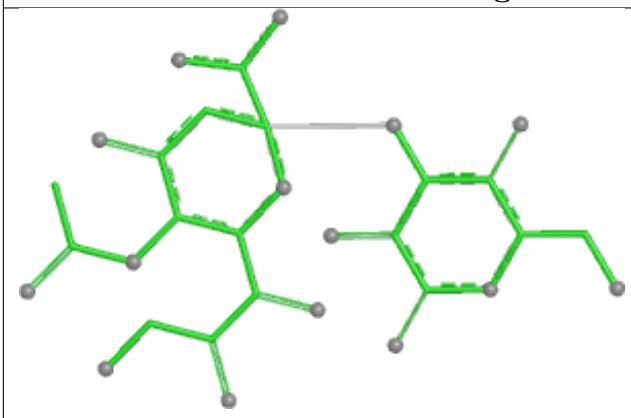


Torsions

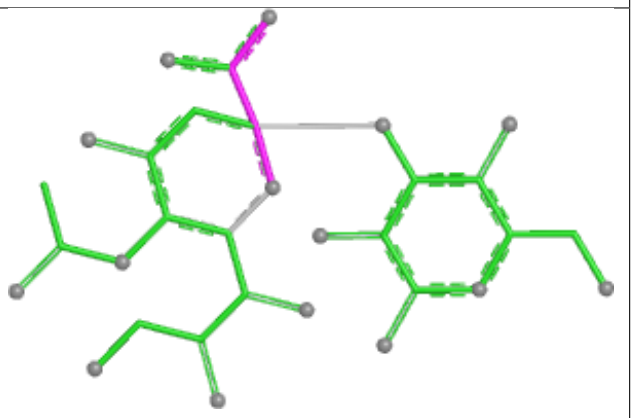


Rings

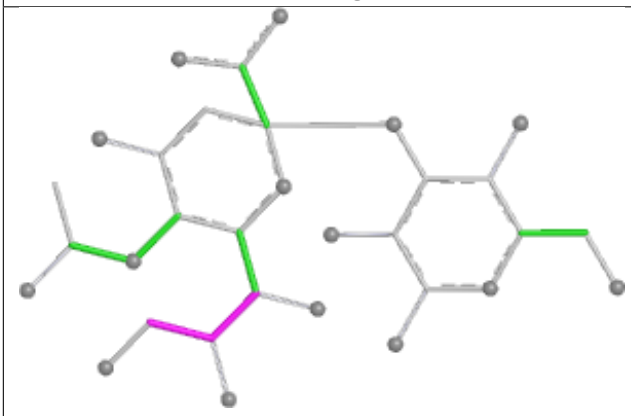
Oligosaccharide Chain Y



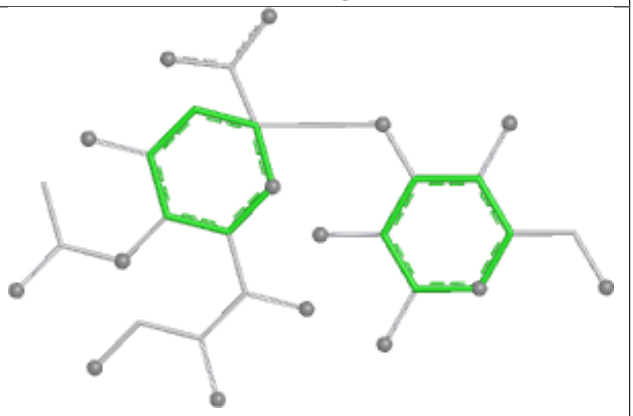
Bond lengths



Bond angles

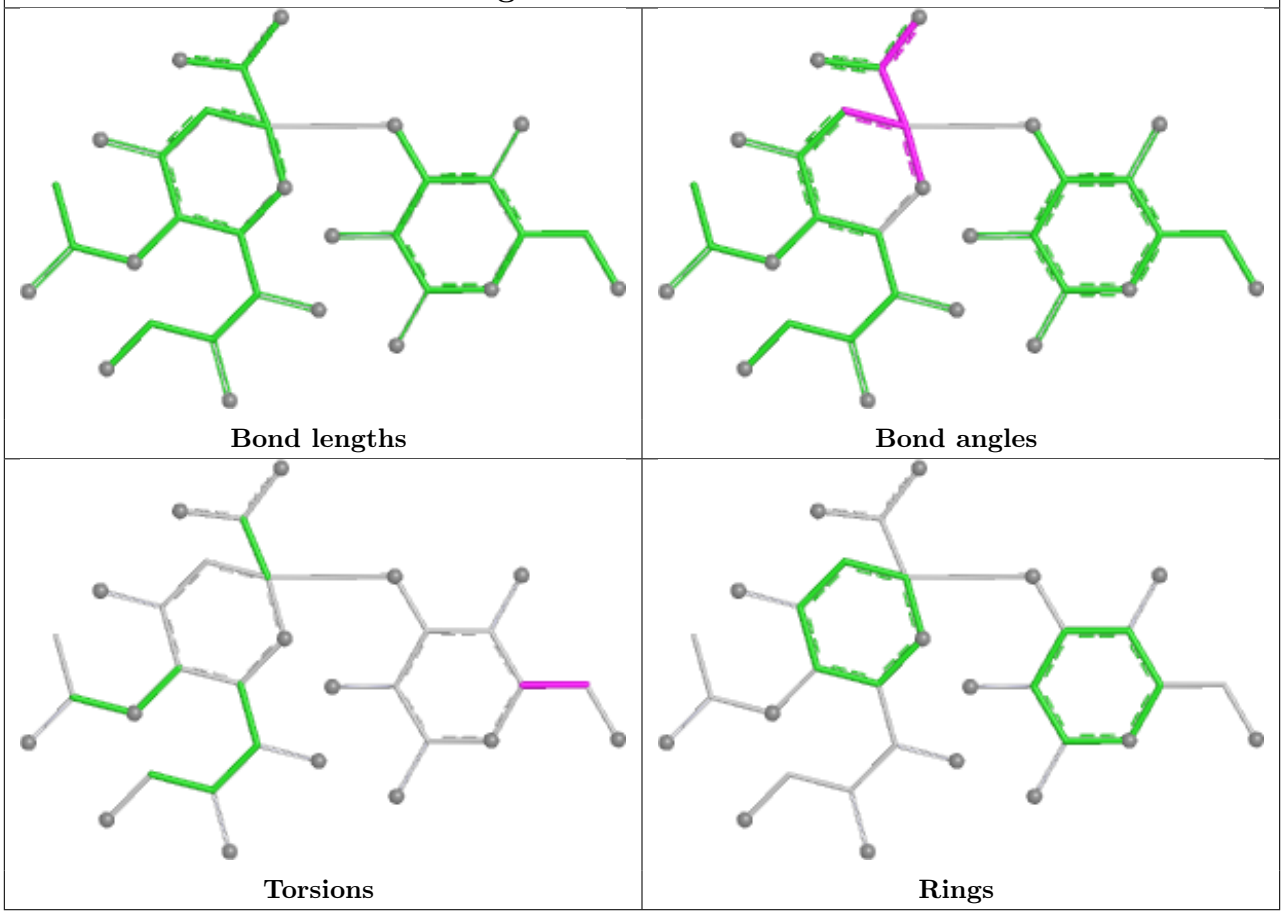


Torsions



Rings

Oligosaccharide Chain Z



5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 20 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SIA	H	401	-	21,21,21	1.01	1 (4%)	24,31,31	1.10	2 (8%)
3	GOL	M	403	-	5,5,5	0.48	0	5,5,5	0.45	0
3	GOL	K	403	-	5,5,5	0.42	0	5,5,5	0.34	0
3	GOL	P	401	-	5,5,5	0.48	0	5,5,5	0.19	0
3	GOL	A	401	-	5,5,5	0.41	0	5,5,5	0.20	0
3	GOL	C	401	-	5,5,5	0.40	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	N	401	-	5,5,5	0.39	0	5,5,5	0.29	0
3	GOL	T	403	-	5,5,5	0.40	0	5,5,5	0.32	0
3	GOL	Q	403	-	5,5,5	0.46	0	5,5,5	0.18	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
5	SIA	H	401	-	-	3/20/38/38	0/1/1/1
3	GOL	M	403	-	-	3/4/4/4	-
3	GOL	K	403	-	-	4/4/4/4	-
3	GOL	P	401	-	-	2/4/4/4	-
3	GOL	A	401	-	-	4/4/4/4	-
3	GOL	C	401	-	-	0/4/4/4	-
3	GOL	N	401	-	-	2/4/4/4	-
3	GOL	T	403	-	-	4/4/4/4	-
3	GOL	Q	403	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	SIA	O2-C2	3.17	1.44	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	401	SIA	O1A-C1-C2	-2.76	119.24	123.85
5	H	401	SIA	C3-C4-C5	2.10	112.97	109.72

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-C3
3	N	401	GOL	O1-C1-C2-O2
3	N	401	GOL	O1-C1-C2-C3
3	P	401	GOL	C1-C2-C3-O3
3	Q	403	GOL	O1-C1-C2-O2

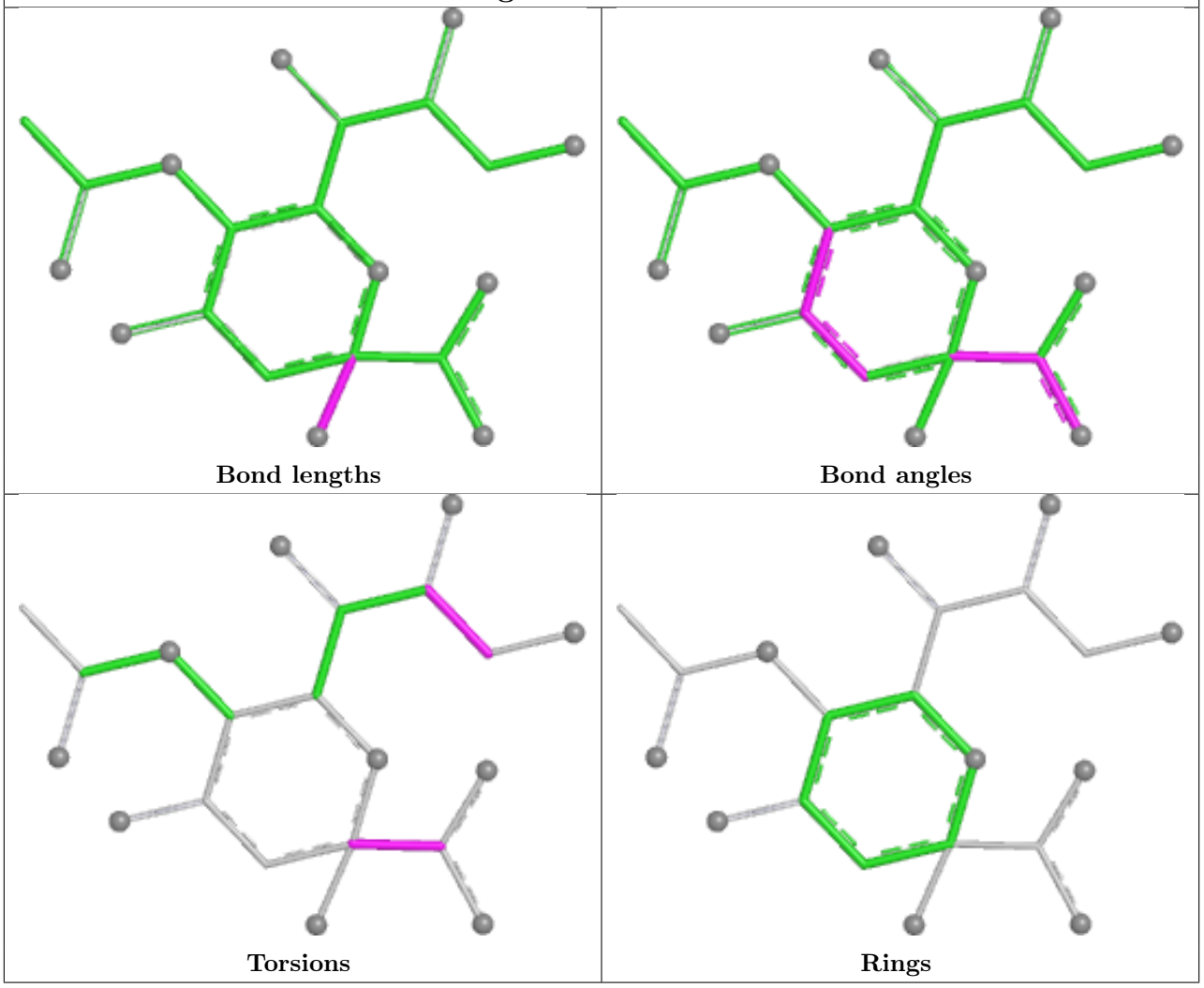
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	403	GOL	1	0
3	K	403	GOL	1	0
3	P	401	GOL	1	0
3	A	401	GOL	2	0
3	C	401	GOL	1	0
3	T	403	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 then 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 H 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	269/289 (93%)	-0.20	7 (2%)	56	54	23, 39, 63, 84	0
1	B	280/289 (96%)	-0.29	6 (2%)	63	61	22, 41, 72, 89	0
1	C	276/289 (95%)	-0.32	5 (1%)	68	66	21, 37, 68, 89	0
1	D	271/289 (93%)	-0.40	2 (0%)	87	86	18, 32, 60, 74	0
1	E	272/289 (94%)	-0.35	4 (1%)	73	72	20, 34, 65, 80	0
1	F	272/289 (94%)	-0.17	9 (3%)	46	45	22, 38, 69, 79	0
1	G	271/289 (93%)	-0.19	9 (3%)	46	45	21, 36, 65, 78	0
1	H	280/289 (96%)	-0.32	6 (2%)	63	61	23, 38, 76, 94	0
1	I	268/289 (92%)	-0.24	3 (1%)	80	79	25, 43, 70, 83	0
1	J	270/289 (93%)	-0.34	5 (1%)	66	64	23, 40, 70, 83	0
1	K	273/289 (94%)	-0.29	10 (3%)	41	41	19, 33, 66, 80	0
1	L	272/289 (94%)	-0.26	2 (0%)	87	86	15, 31, 58, 71	0
1	M	271/289 (93%)	-0.43	3 (1%)	80	79	16, 31, 58, 73	0
1	N	278/289 (96%)	-0.37	0	100	100	16, 31, 61, 70	0
1	O	271/289 (93%)	-0.33	6 (2%)	62	60	19, 32, 62, 81	0
1	P	271/289 (93%)	-0.29	4 (1%)	73	72	17, 32, 64, 83	0
1	Q	271/289 (93%)	-0.32	7 (2%)	56	54	21, 36, 69, 87	0
1	R	277/289 (95%)	-0.33	3 (1%)	80	79	23, 38, 69, 86	0
1	S	270/289 (93%)	-0.29	8 (2%)	50	49	22, 39, 65, 85	0
1	T	271/289 (93%)	-0.23	11 (4%)	37	36	19, 35, 68, 84	0
All	All	5454/5780 (94%)	-0.30	110 (2%)	65	63	15, 36, 66, 94	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	71	PRO	5.0
1	H	72	THR	4.9
1	G	71	PRO	4.8
1	B	72	THR	4.7
1	H	71	PRO	4.7

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)

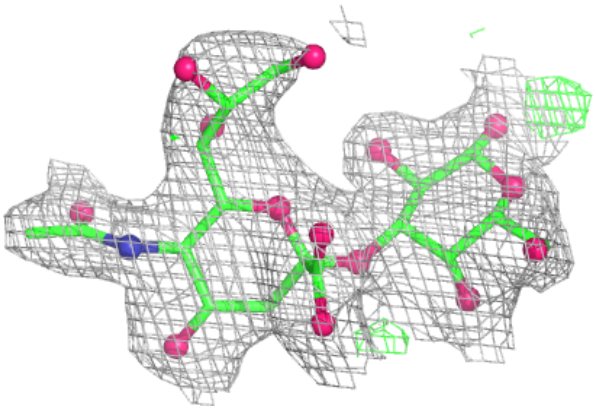
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

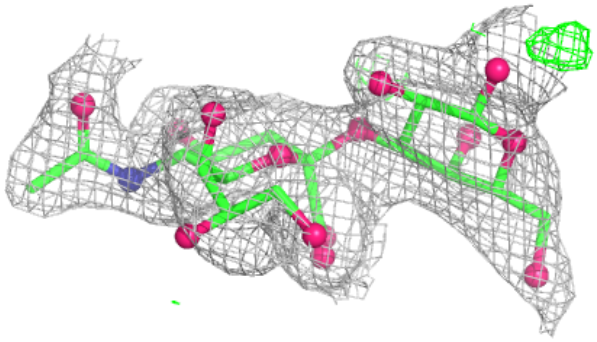
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	W	1	12/12	0.81	0.22	49,53,57,57	12
2	GAL	U	1	12/12	0.82	0.24	64,68,71,73	0
2	GAL	Y	1	12/12	0.83	0.17	47,50,50,51	12
2	GAL	X	1	12/12	0.85	0.23	68,74,76,76	0
2	SIA	Y	2	20/21	0.85	0.20	31,42,50,50	20
2	GAL	V	1	12/12	0.86	0.21	52,59,61,64	0
2	SIA	W	2	20/21	0.88	0.19	35,44,48,48	20
2	SIA	U	2	20/21	0.90	0.23	47,60,74,77	0
2	SIA	V	2	20/21	0.92	0.15	40,48,55,57	0
2	GAL	Z	1	12/12	0.92	0.27	58,63,64,65	0
2	SIA	X	2	20/21	0.93	0.17	56,64,67,67	0
2	SIA	Z	2	20/21	0.93	0.20	37,55,66,69	0

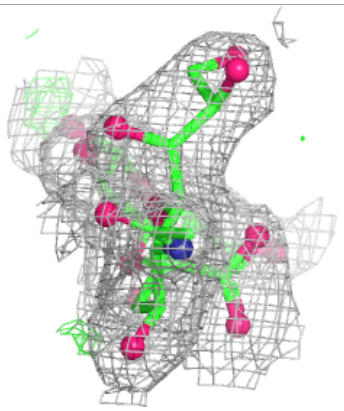
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

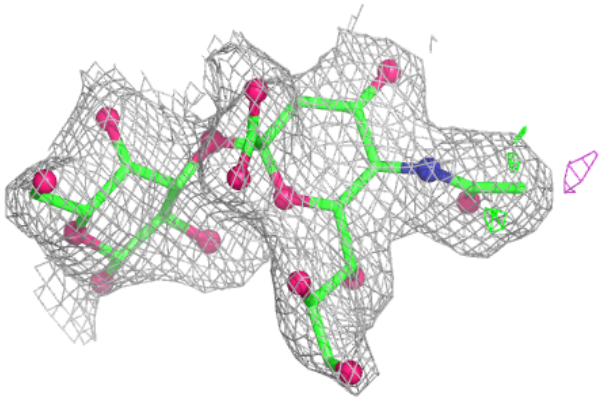


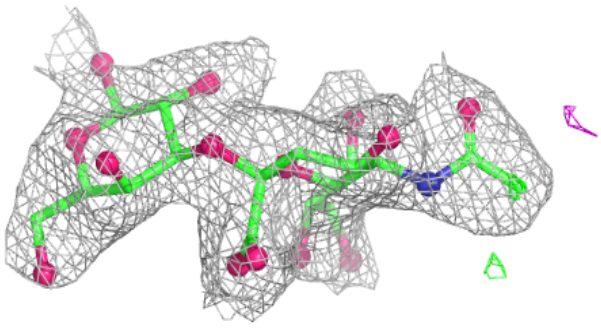


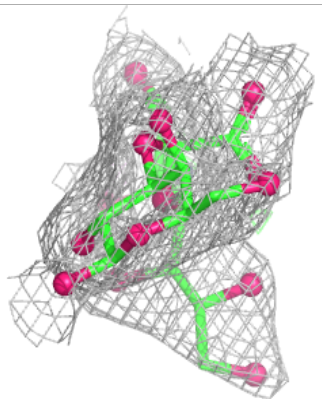


Electron density around Chain V:

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

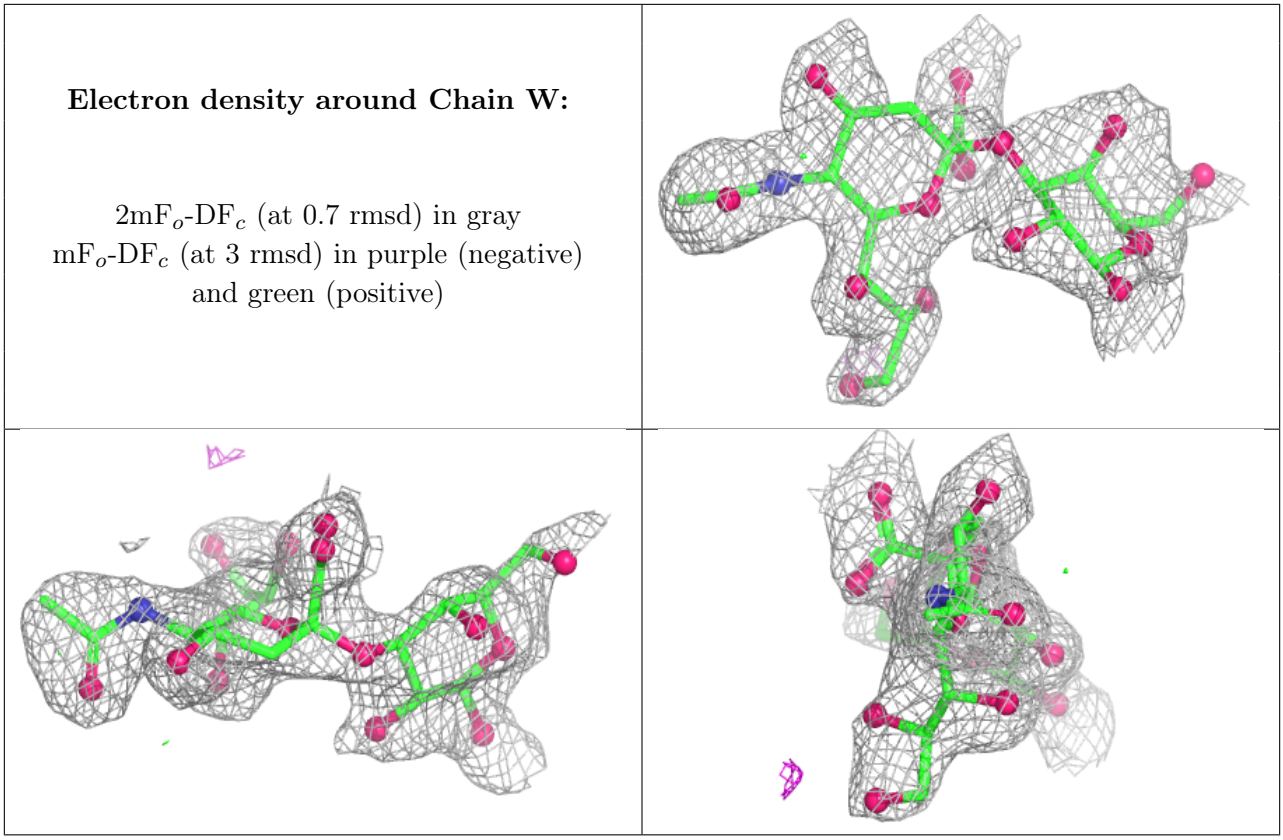






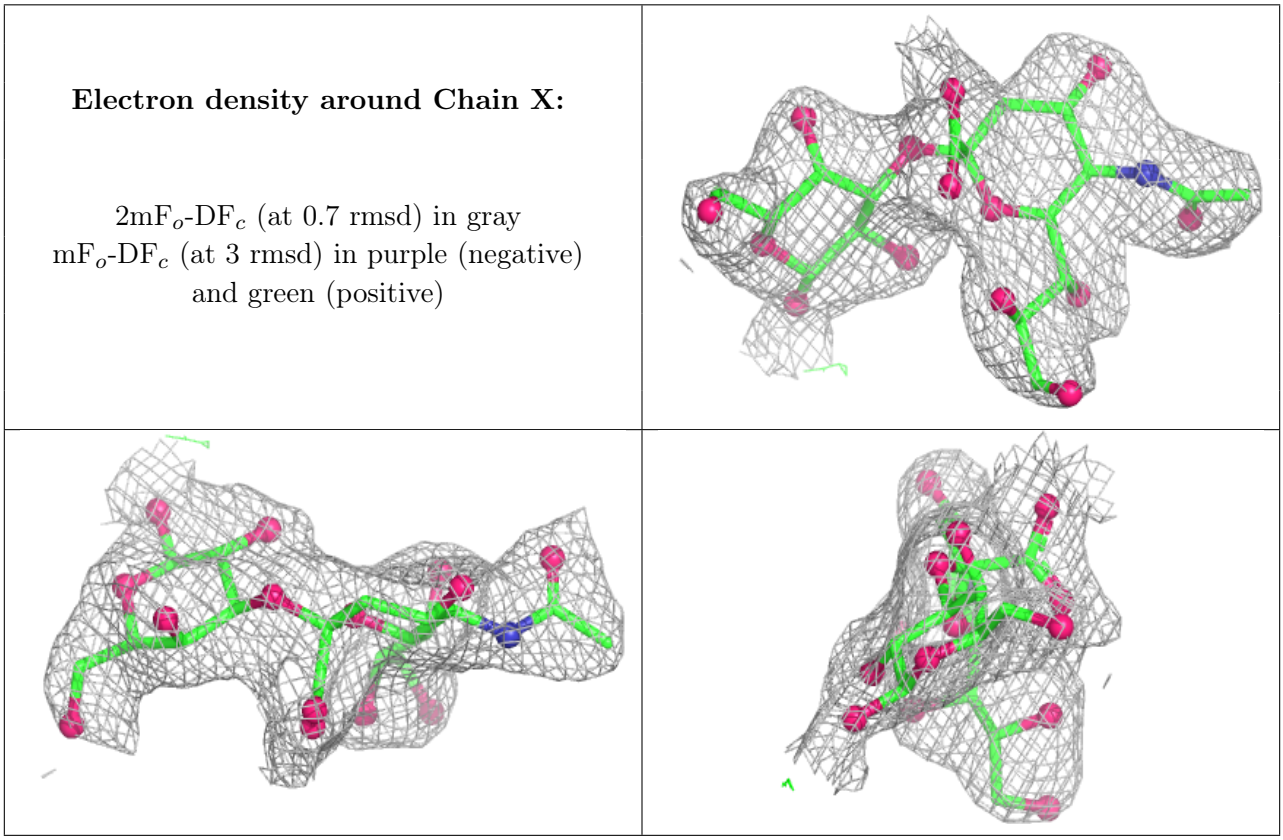
Electron density around Chain W:

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



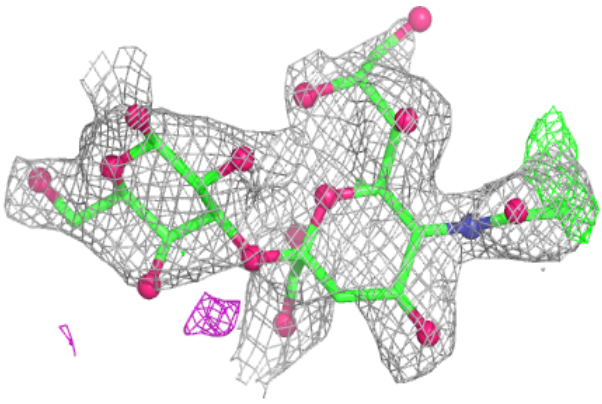
Electron density around Chain X:

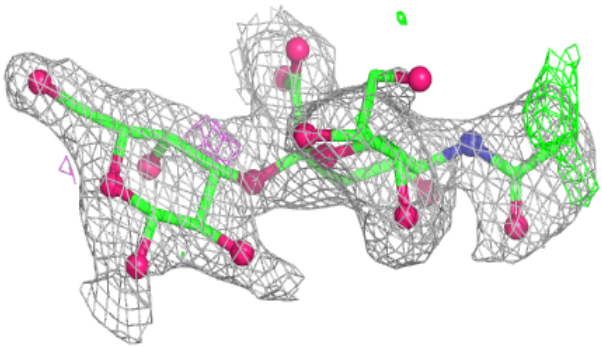
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

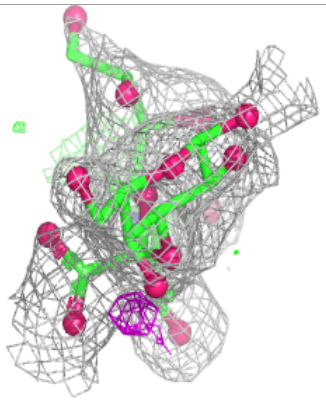


Electron density around Chain Y:

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

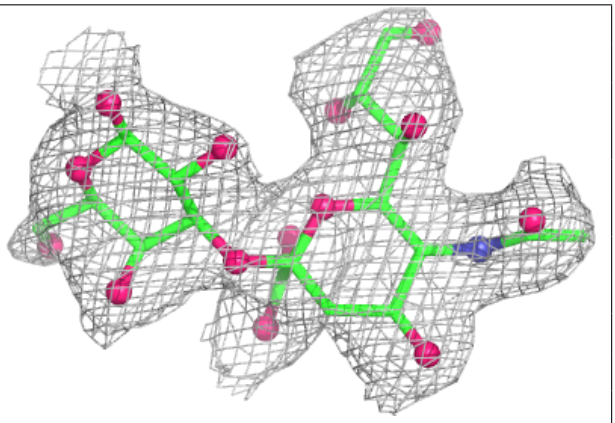


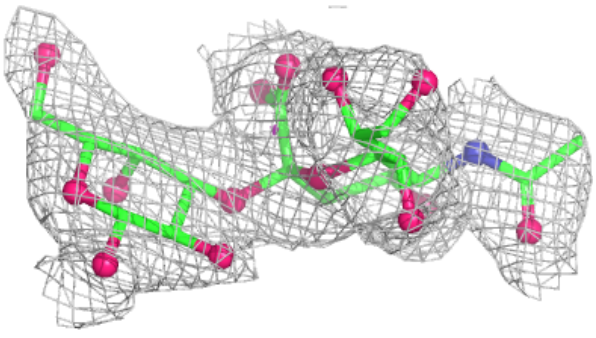


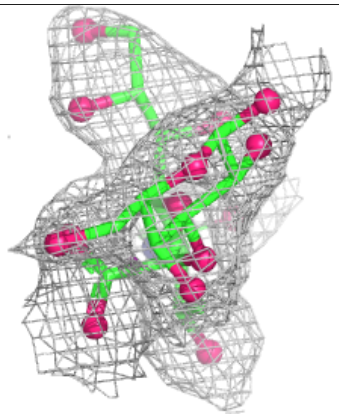


Electron density around Chain Z:

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







6.4 Ligands (i)

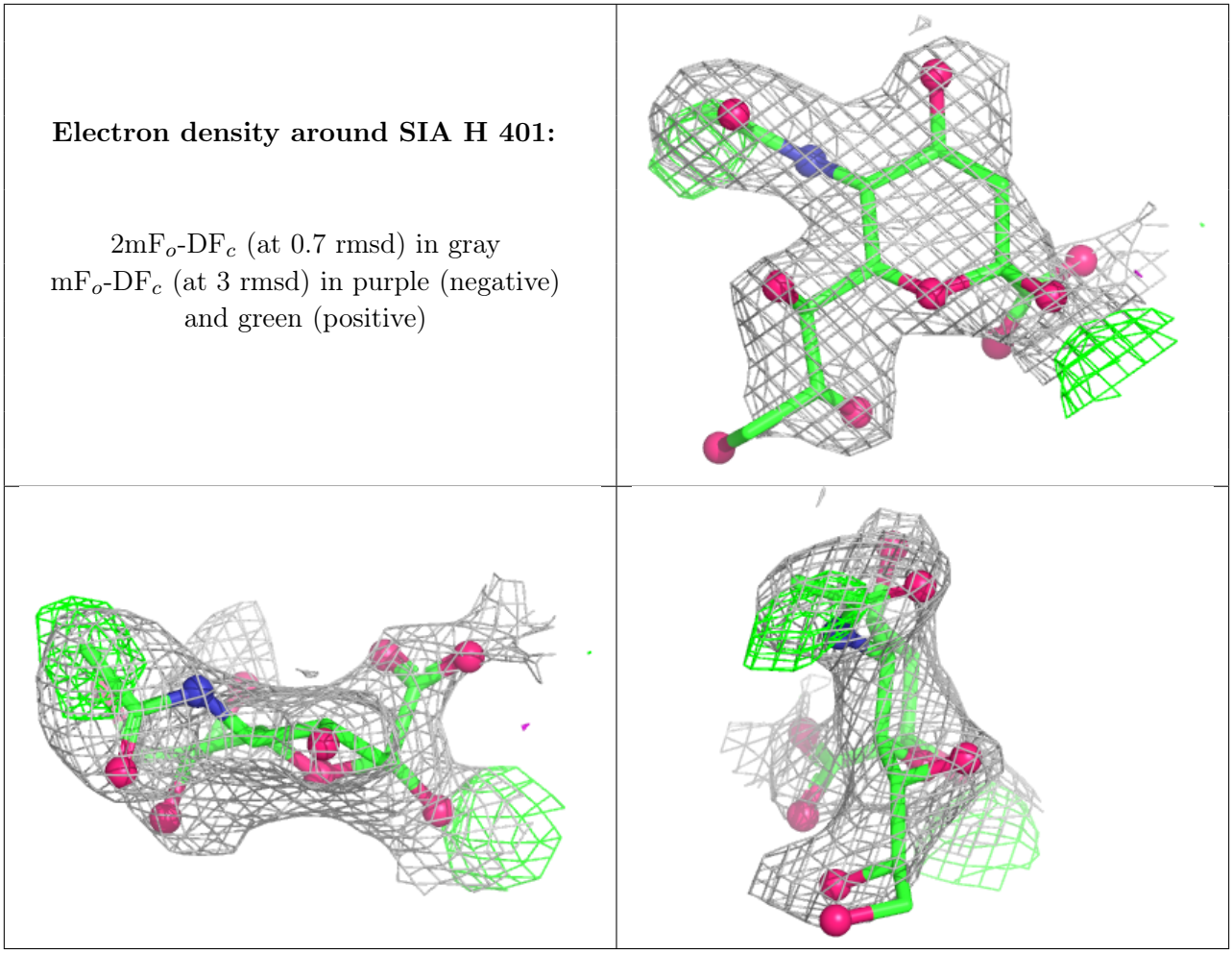
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	SIA	H	401	21/21	0.82	0.33	43,50,53,53	21
3	GOL	C	401	6/6	0.88	0.20	39,43,48,48	0
3	GOL	P	401	6/6	0.90	0.19	36,47,49,51	0
3	GOL	N	401	6/6	0.90	0.20	54,59,59,61	0
3	GOL	K	403	6/6	0.92	0.16	33,39,41,43	0
3	GOL	Q	403	6/6	0.93	0.15	28,39,41,42	0
3	GOL	A	401	6/6	0.93	0.13	39,49,51,52	0
3	GOL	T	403	6/6	0.94	0.15	39,45,47,48	0
3	GOL	M	403	6/6	0.95	0.14	34,41,44,45	0
4	CL	B	601	1/1	0.99	0.07	39,39,39,39	0
4	CL	C	402	1/1	0.99	0.08	38,38,38,38	0
4	CL	F	601	1/1	0.99	0.08	31,31,31,31	0
4	CL	H	402	1/1	0.99	0.06	39,39,39,39	0
4	CL	I	601	1/1	0.99	0.08	43,43,43,43	0
4	CL	J	601	1/1	0.99	0.13	33,33,33,33	0
4	CL	K	404	1/1	0.99	0.07	30,30,30,30	0
4	CL	O	403	1/1	0.99	0.08	25,25,25,25	0
4	CL	P	402	1/1	0.99	0.11	31,31,31,31	0
4	CL	Q	404	1/1	0.99	0.07	33,33,33,33	0
4	CL	T	404	1/1	0.99	0.09	28,28,28,28	0
4	CL	A	402	1/1	0.99	0.10	32,32,32,32	0
4	CL	N	402	1/1	1.00	0.08	26,26,26,26	0
4	CL	D	601	1/1	1.00	0.10	27,27,27,27	0
4	CL	G	601	1/1	1.00	0.07	31,31,31,31	0
4	CL	E	601	1/1	1.00	0.07	22,22,22,22	0
4	CL	R	601	1/1	1.00	0.08	32,32,32,32	0
4	CL	S	403	1/1	1.00	0.09	34,34,34,34	0
4	CL	L	401	1/1	1.00	0.10	28,28,28,28	0
4	CL	M	404	1/1	1.00	0.07	32,32,32,32	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 H 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.