Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 06:03 AM EDT

PDB ID	:	6Y5Y
Title	:	Structure of New Jersey Polyomavirus VP1 in complex with 3'-Sialyllactose
Authors	:	Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on	:	2020-02-26
Resolution	:	1.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

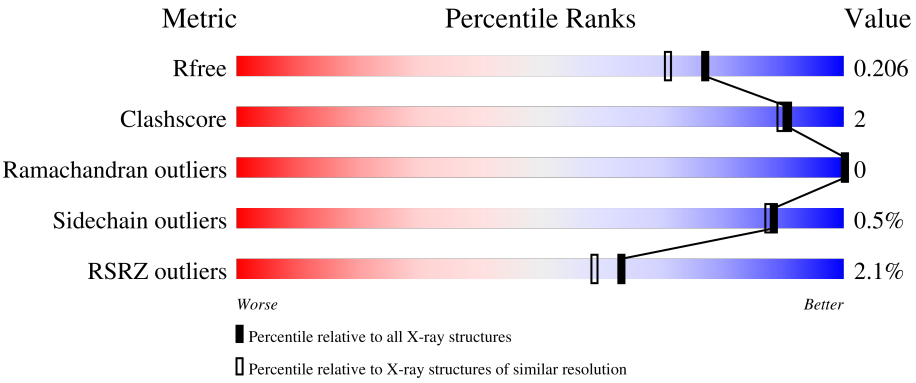
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	311	2% 86% • 10%
1	B	311	2% 88% • 9%
1	C	311	3% 86% • 10%
1	D	311	% 89% • 8%
1	E	311	5% 87% • 10%

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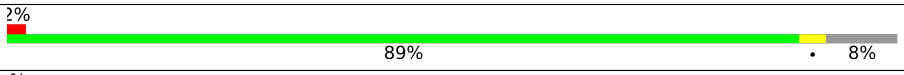
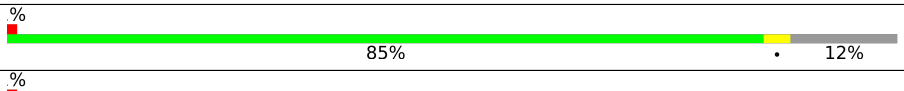
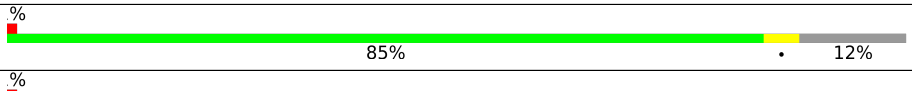
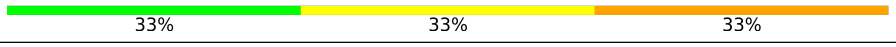
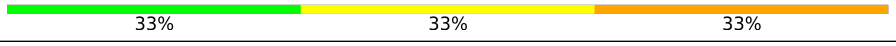
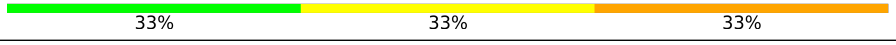
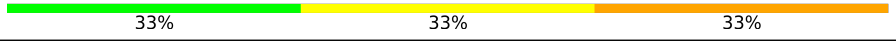
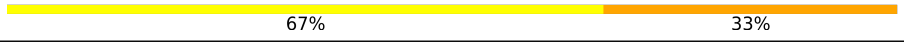
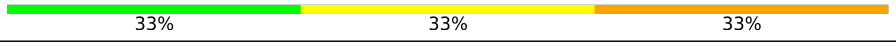
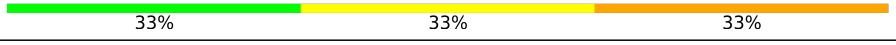
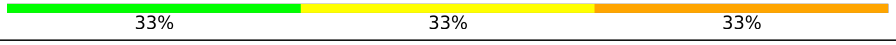
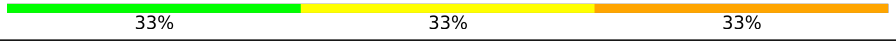
Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	3	
2	M	3	
2	O	3	
2	P	3	
3	L	3	
3	N	3	
3	Q	3	
3	R	3	
3	S	3	
3	T	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25061 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	279	Total	C	N	O	S	0	4	0
			2135	1346	365	410	14			
1	B	283	Total	C	N	O	S	0	5	0
			2179	1376	371	416	16			
1	C	281	Total	C	N	O	S	0	5	0
			2171	1371	368	416	16			
1	D	285	Total	C	N	O	S	0	3	0
			2181	1376	369	420	16			
1	E	281	Total	C	N	O	S	0	5	0
			2163	1368	367	412	16			
1	F	274	Total	C	N	O	S	0	8	0
			2139	1348	364	412	15			
1	G	285	Total	C	N	O	S	0	8	0
			2201	1391	374	420	16			
1	H	274	Total	C	N	O	S	0	8	0
			2135	1348	363	409	15			
1	I	275	Total	C	N	O	S	0	6	0
			2137	1351	361	410	15			
1	J	274	Total	C	N	O	S	0	5	0
			2136	1346	362	412	16			

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP A0A024B5J2
A	13	GLY	-	expression tag	UNP A0A024B5J2
A	14	SER	-	expression tag	UNP A0A024B5J2
A	15	SER	-	expression tag	UNP A0A024B5J2
A	16	HIS	-	expression tag	UNP A0A024B5J2
A	17	HIS	-	expression tag	UNP A0A024B5J2
A	18	HIS	-	expression tag	UNP A0A024B5J2
A	19	HIS	-	expression tag	UNP A0A024B5J2
A	20	HIS	-	expression tag	UNP A0A024B5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	HIS	-	expression tag	UNP A0A024B5J2
A	22	SER	-	expression tag	UNP A0A024B5J2
A	23	SER	-	expression tag	UNP A0A024B5J2
A	24	GLY	-	expression tag	UNP A0A024B5J2
A	25	LEU	-	expression tag	UNP A0A024B5J2
A	26	VAL	-	expression tag	UNP A0A024B5J2
A	27	PRO	-	expression tag	UNP A0A024B5J2
A	28	ARG	-	expression tag	UNP A0A024B5J2
A	29	GLY	-	expression tag	UNP A0A024B5J2
A	30	SER	-	expression tag	UNP A0A024B5J2
A	31	HIS	-	expression tag	UNP A0A024B5J2
A	32	MET	-	expression tag	UNP A0A024B5J2
A	33	LEU	-	expression tag	UNP A0A024B5J2
A	34	ASP	-	expression tag	UNP A0A024B5J2
B	12	MET	-	initiating methionine	UNP A0A024B5J2
B	13	GLY	-	expression tag	UNP A0A024B5J2
B	14	SER	-	expression tag	UNP A0A024B5J2
B	15	SER	-	expression tag	UNP A0A024B5J2
B	16	HIS	-	expression tag	UNP A0A024B5J2
B	17	HIS	-	expression tag	UNP A0A024B5J2
B	18	HIS	-	expression tag	UNP A0A024B5J2
B	19	HIS	-	expression tag	UNP A0A024B5J2
B	20	HIS	-	expression tag	UNP A0A024B5J2
B	21	HIS	-	expression tag	UNP A0A024B5J2
B	22	SER	-	expression tag	UNP A0A024B5J2
B	23	SER	-	expression tag	UNP A0A024B5J2
B	24	GLY	-	expression tag	UNP A0A024B5J2
B	25	LEU	-	expression tag	UNP A0A024B5J2
B	26	VAL	-	expression tag	UNP A0A024B5J2
B	27	PRO	-	expression tag	UNP A0A024B5J2
B	28	ARG	-	expression tag	UNP A0A024B5J2
B	29	GLY	-	expression tag	UNP A0A024B5J2
B	30	SER	-	expression tag	UNP A0A024B5J2
B	31	HIS	-	expression tag	UNP A0A024B5J2
B	32	MET	-	expression tag	UNP A0A024B5J2
B	33	LEU	-	expression tag	UNP A0A024B5J2
B	34	ASP	-	expression tag	UNP A0A024B5J2
C	12	MET	-	initiating methionine	UNP A0A024B5J2
C	13	GLY	-	expression tag	UNP A0A024B5J2
C	14	SER	-	expression tag	UNP A0A024B5J2
C	15	SER	-	expression tag	UNP A0A024B5J2
C	16	HIS	-	expression tag	UNP A0A024B5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	expression tag	UNP A0A024B5J2
C	18	HIS	-	expression tag	UNP A0A024B5J2
C	19	HIS	-	expression tag	UNP A0A024B5J2
C	20	HIS	-	expression tag	UNP A0A024B5J2
C	21	HIS	-	expression tag	UNP A0A024B5J2
C	22	SER	-	expression tag	UNP A0A024B5J2
C	23	SER	-	expression tag	UNP A0A024B5J2
C	24	GLY	-	expression tag	UNP A0A024B5J2
C	25	LEU	-	expression tag	UNP A0A024B5J2
C	26	VAL	-	expression tag	UNP A0A024B5J2
C	27	PRO	-	expression tag	UNP A0A024B5J2
C	28	ARG	-	expression tag	UNP A0A024B5J2
C	29	GLY	-	expression tag	UNP A0A024B5J2
C	30	SER	-	expression tag	UNP A0A024B5J2
C	31	HIS	-	expression tag	UNP A0A024B5J2
C	32	MET	-	expression tag	UNP A0A024B5J2
C	33	LEU	-	expression tag	UNP A0A024B5J2
C	34	ASP	-	expression tag	UNP A0A024B5J2
D	12	MET	-	initiating methionine	UNP A0A024B5J2
D	13	GLY	-	expression tag	UNP A0A024B5J2
D	14	SER	-	expression tag	UNP A0A024B5J2
D	15	SER	-	expression tag	UNP A0A024B5J2
D	16	HIS	-	expression tag	UNP A0A024B5J2
D	17	HIS	-	expression tag	UNP A0A024B5J2
D	18	HIS	-	expression tag	UNP A0A024B5J2
D	19	HIS	-	expression tag	UNP A0A024B5J2
D	20	HIS	-	expression tag	UNP A0A024B5J2
D	21	HIS	-	expression tag	UNP A0A024B5J2
D	22	SER	-	expression tag	UNP A0A024B5J2
D	23	SER	-	expression tag	UNP A0A024B5J2
D	24	GLY	-	expression tag	UNP A0A024B5J2
D	25	LEU	-	expression tag	UNP A0A024B5J2
D	26	VAL	-	expression tag	UNP A0A024B5J2
D	27	PRO	-	expression tag	UNP A0A024B5J2
D	28	ARG	-	expression tag	UNP A0A024B5J2
D	29	GLY	-	expression tag	UNP A0A024B5J2
D	30	SER	-	expression tag	UNP A0A024B5J2
D	31	HIS	-	expression tag	UNP A0A024B5J2
D	32	MET	-	expression tag	UNP A0A024B5J2
D	33	LEU	-	expression tag	UNP A0A024B5J2
D	34	ASP	-	expression tag	UNP A0A024B5J2
E	12	MET	-	initiating methionine	UNP A0A024B5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	13	GLY	-	expression tag	UNP A0A024B5J2
E	14	SER	-	expression tag	UNP A0A024B5J2
E	15	SER	-	expression tag	UNP A0A024B5J2
E	16	HIS	-	expression tag	UNP A0A024B5J2
E	17	HIS	-	expression tag	UNP A0A024B5J2
E	18	HIS	-	expression tag	UNP A0A024B5J2
E	19	HIS	-	expression tag	UNP A0A024B5J2
E	20	HIS	-	expression tag	UNP A0A024B5J2
E	21	HIS	-	expression tag	UNP A0A024B5J2
E	22	SER	-	expression tag	UNP A0A024B5J2
E	23	SER	-	expression tag	UNP A0A024B5J2
E	24	GLY	-	expression tag	UNP A0A024B5J2
E	25	LEU	-	expression tag	UNP A0A024B5J2
E	26	VAL	-	expression tag	UNP A0A024B5J2
E	27	PRO	-	expression tag	UNP A0A024B5J2
E	28	ARG	-	expression tag	UNP A0A024B5J2
E	29	GLY	-	expression tag	UNP A0A024B5J2
E	30	SER	-	expression tag	UNP A0A024B5J2
E	31	HIS	-	expression tag	UNP A0A024B5J2
E	32	MET	-	expression tag	UNP A0A024B5J2
E	33	LEU	-	expression tag	UNP A0A024B5J2
E	34	ASP	-	expression tag	UNP A0A024B5J2
F	12	MET	-	initiating methionine	UNP A0A024B5J2
F	13	GLY	-	expression tag	UNP A0A024B5J2
F	14	SER	-	expression tag	UNP A0A024B5J2
F	15	SER	-	expression tag	UNP A0A024B5J2
F	16	HIS	-	expression tag	UNP A0A024B5J2
F	17	HIS	-	expression tag	UNP A0A024B5J2
F	18	HIS	-	expression tag	UNP A0A024B5J2
F	19	HIS	-	expression tag	UNP A0A024B5J2
F	20	HIS	-	expression tag	UNP A0A024B5J2
F	21	HIS	-	expression tag	UNP A0A024B5J2
F	22	SER	-	expression tag	UNP A0A024B5J2
F	23	SER	-	expression tag	UNP A0A024B5J2
F	24	GLY	-	expression tag	UNP A0A024B5J2
F	25	LEU	-	expression tag	UNP A0A024B5J2
F	26	VAL	-	expression tag	UNP A0A024B5J2
F	27	PRO	-	expression tag	UNP A0A024B5J2
F	28	ARG	-	expression tag	UNP A0A024B5J2
F	29	GLY	-	expression tag	UNP A0A024B5J2
F	30	SER	-	expression tag	UNP A0A024B5J2
F	31	HIS	-	expression tag	UNP A0A024B5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	32	MET	-	expression tag	UNP A0A024B5J2
F	33	LEU	-	expression tag	UNP A0A024B5J2
F	34	ASP	-	expression tag	UNP A0A024B5J2
G	12	MET	-	initiating methionine	UNP A0A024B5J2
G	13	GLY	-	expression tag	UNP A0A024B5J2
G	14	SER	-	expression tag	UNP A0A024B5J2
G	15	SER	-	expression tag	UNP A0A024B5J2
G	16	HIS	-	expression tag	UNP A0A024B5J2
G	17	HIS	-	expression tag	UNP A0A024B5J2
G	18	HIS	-	expression tag	UNP A0A024B5J2
G	19	HIS	-	expression tag	UNP A0A024B5J2
G	20	HIS	-	expression tag	UNP A0A024B5J2
G	21	HIS	-	expression tag	UNP A0A024B5J2
G	22	SER	-	expression tag	UNP A0A024B5J2
G	23	SER	-	expression tag	UNP A0A024B5J2
G	24	GLY	-	expression tag	UNP A0A024B5J2
G	25	LEU	-	expression tag	UNP A0A024B5J2
G	26	VAL	-	expression tag	UNP A0A024B5J2
G	27	PRO	-	expression tag	UNP A0A024B5J2
G	28	ARG	-	expression tag	UNP A0A024B5J2
G	29	GLY	-	expression tag	UNP A0A024B5J2
G	30	SER	-	expression tag	UNP A0A024B5J2
G	31	HIS	-	expression tag	UNP A0A024B5J2
G	32	MET	-	expression tag	UNP A0A024B5J2
G	33	LEU	-	expression tag	UNP A0A024B5J2
G	34	ASP	-	expression tag	UNP A0A024B5J2
H	12	MET	-	initiating methionine	UNP A0A024B5J2
H	13	GLY	-	expression tag	UNP A0A024B5J2
H	14	SER	-	expression tag	UNP A0A024B5J2
H	15	SER	-	expression tag	UNP A0A024B5J2
H	16	HIS	-	expression tag	UNP A0A024B5J2
H	17	HIS	-	expression tag	UNP A0A024B5J2
H	18	HIS	-	expression tag	UNP A0A024B5J2
H	19	HIS	-	expression tag	UNP A0A024B5J2
H	20	HIS	-	expression tag	UNP A0A024B5J2
H	21	HIS	-	expression tag	UNP A0A024B5J2
H	22	SER	-	expression tag	UNP A0A024B5J2
H	23	SER	-	expression tag	UNP A0A024B5J2
H	24	GLY	-	expression tag	UNP A0A024B5J2
H	25	LEU	-	expression tag	UNP A0A024B5J2
H	26	VAL	-	expression tag	UNP A0A024B5J2
H	27	PRO	-	expression tag	UNP A0A024B5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	28	ARG	-	expression tag	UNP A0A024B5J2
H	29	GLY	-	expression tag	UNP A0A024B5J2
H	30	SER	-	expression tag	UNP A0A024B5J2
H	31	HIS	-	expression tag	UNP A0A024B5J2
H	32	MET	-	expression tag	UNP A0A024B5J2
H	33	LEU	-	expression tag	UNP A0A024B5J2
H	34	ASP	-	expression tag	UNP A0A024B5J2
I	12	MET	-	initiating methionine	UNP A0A024B5J2
I	13	GLY	-	expression tag	UNP A0A024B5J2
I	14	SER	-	expression tag	UNP A0A024B5J2
I	15	SER	-	expression tag	UNP A0A024B5J2
I	16	HIS	-	expression tag	UNP A0A024B5J2
I	17	HIS	-	expression tag	UNP A0A024B5J2
I	18	HIS	-	expression tag	UNP A0A024B5J2
I	19	HIS	-	expression tag	UNP A0A024B5J2
I	20	HIS	-	expression tag	UNP A0A024B5J2
I	21	HIS	-	expression tag	UNP A0A024B5J2
I	22	SER	-	expression tag	UNP A0A024B5J2
I	23	SER	-	expression tag	UNP A0A024B5J2
I	24	GLY	-	expression tag	UNP A0A024B5J2
I	25	LEU	-	expression tag	UNP A0A024B5J2
I	26	VAL	-	expression tag	UNP A0A024B5J2
I	27	PRO	-	expression tag	UNP A0A024B5J2
I	28	ARG	-	expression tag	UNP A0A024B5J2
I	29	GLY	-	expression tag	UNP A0A024B5J2
I	30	SER	-	expression tag	UNP A0A024B5J2
I	31	HIS	-	expression tag	UNP A0A024B5J2
I	32	MET	-	expression tag	UNP A0A024B5J2
I	33	LEU	-	expression tag	UNP A0A024B5J2
I	34	ASP	-	expression tag	UNP A0A024B5J2
J	12	MET	-	initiating methionine	UNP A0A024B5J2
J	13	GLY	-	expression tag	UNP A0A024B5J2
J	14	SER	-	expression tag	UNP A0A024B5J2
J	15	SER	-	expression tag	UNP A0A024B5J2
J	16	HIS	-	expression tag	UNP A0A024B5J2
J	17	HIS	-	expression tag	UNP A0A024B5J2
J	18	HIS	-	expression tag	UNP A0A024B5J2
J	19	HIS	-	expression tag	UNP A0A024B5J2
J	20	HIS	-	expression tag	UNP A0A024B5J2
J	21	HIS	-	expression tag	UNP A0A024B5J2
J	22	SER	-	expression tag	UNP A0A024B5J2
J	23	SER	-	expression tag	UNP A0A024B5J2

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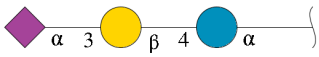
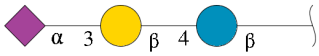
Chain	Residue	Modelled	Actual	Comment	Reference
J	24	GLY	-	expression tag	UNP A0A024B5J2
J	25	LEU	-	expression tag	UNP A0A024B5J2
J	26	VAL	-	expression tag	UNP A0A024B5J2
J	27	PRO	-	expression tag	UNP A0A024B5J2
J	28	ARG	-	expression tag	UNP A0A024B5J2
J	29	GLY	-	expression tag	UNP A0A024B5J2
J	30	SER	-	expression tag	UNP A0A024B5J2
J	31	HIS	-	expression tag	UNP A0A024B5J2
J	32	MET	-	expression tag	UNP A0A024B5J2
J	33	LEU	-	expression tag	UNP A0A024B5J2
J	34	ASP	-	expression tag	UNP A0A024B5J2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	M	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	O	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	P	3	Total	C	N	O	0	0	0
			43	23	1	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	3	Total	C	N	O	0	0	0
			43	23	1	19			
3	N	3	Total	C	N	O	0	0	0
			43	23	1	19			

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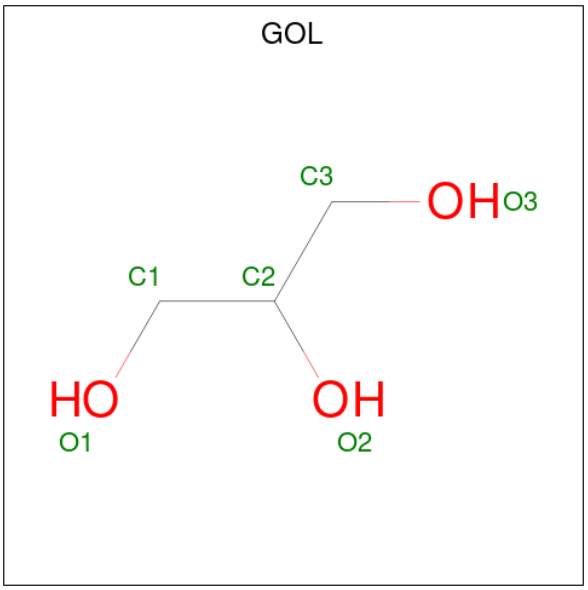
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Q	3	Total C N O 43 23 1 19	0	0	0
3	R	3	Total C N O 43 23 1 19	0	0	0
3	S	3	Total C N O 43 23 1 19	0	0	0
3	T	3	Total C N O 43 23 1 19	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	1
			12	6	6		
4	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 12 6 6	0	1
4	J	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	1	Total Mg 1 1	0	0
5	D	2	Total Mg 2 2	0	0
5	F	2	Total Mg 2 2	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	I	1	Total Mg 1 1	0	0

- Molecule 6 is water.

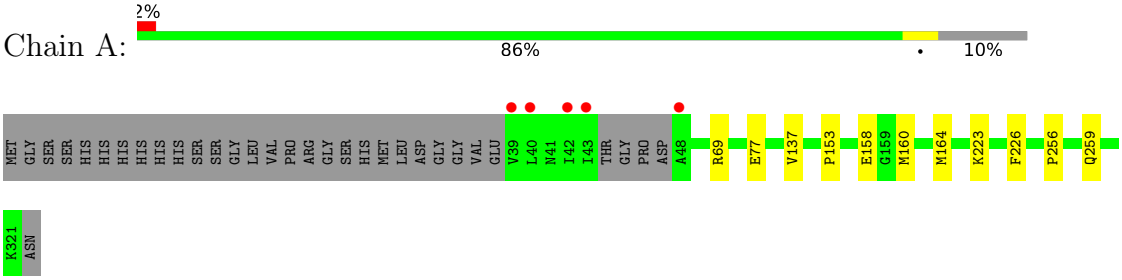
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	249	Total O 250 250	0	1
6	B	280	Total O 283 283	0	3
6	C	275	Total O 277 277	0	2
6	D	242	Total O 244 244	0	2
6	E	233	Total O 233 233	0	0
6	F	295	Total O 298 298	0	3
6	G	340	Total O 344 344	0	4
6	H	272	Total O 274 274	0	2
6	I	298	Total O 300 300	0	2
6	J	293	Total O 295 295	0	2

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.

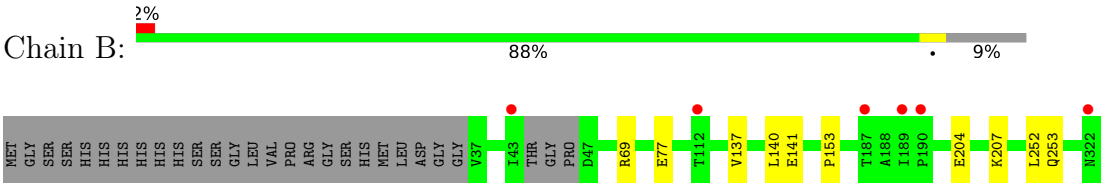
• Molecule 1: VP1

Chain A:



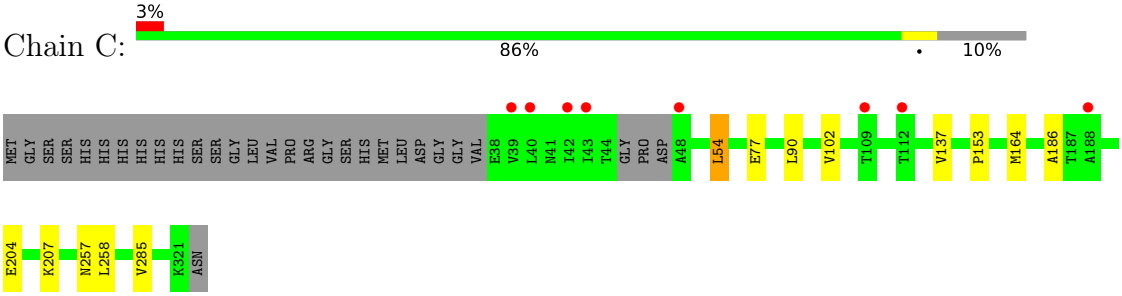
• Molecule 1: VP1

Chain B:



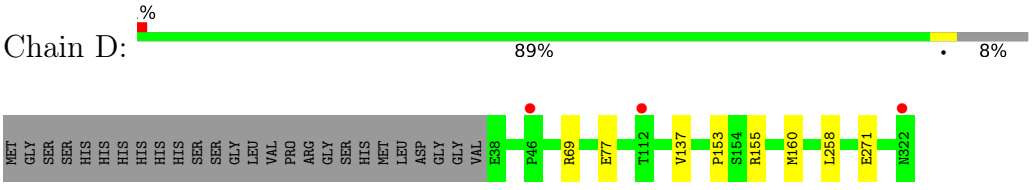
• Molecule 1: VP1

Chain C:



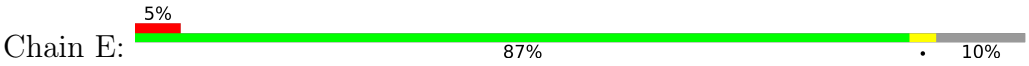
• Molecule 1: VP1

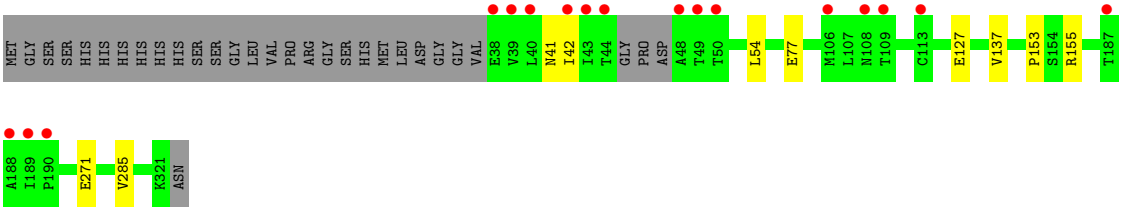
Chain D:



• Molecule 1: VP1

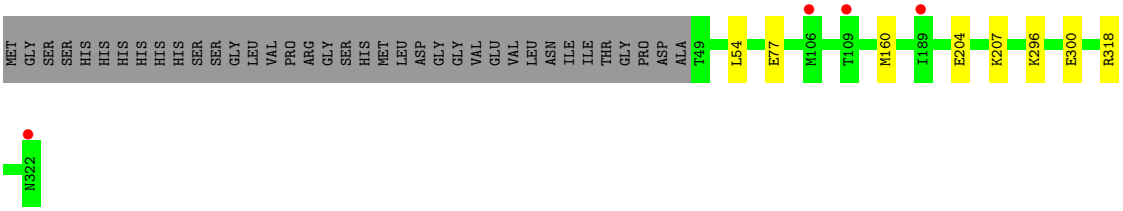
Chain E:





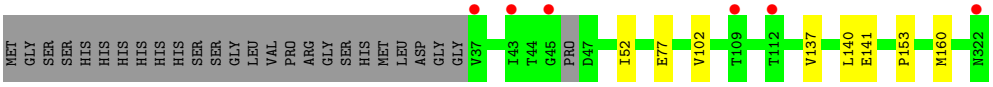
• Molecule 1: VP1

Chain F:



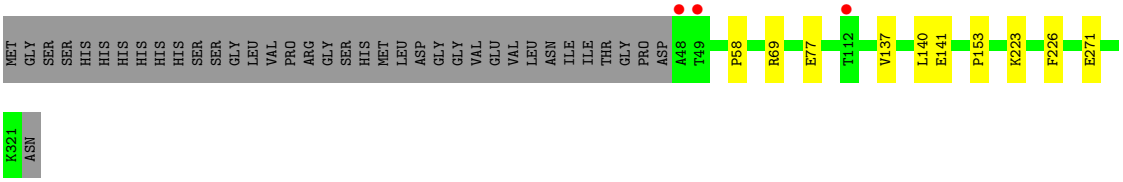
• Molecule 1: VP1

Chain G:



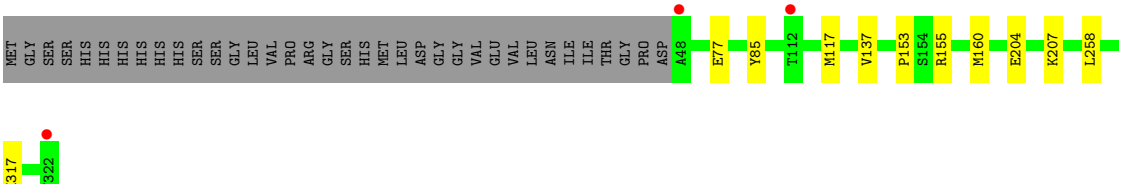
• Molecule 1: VP1

Chain H:



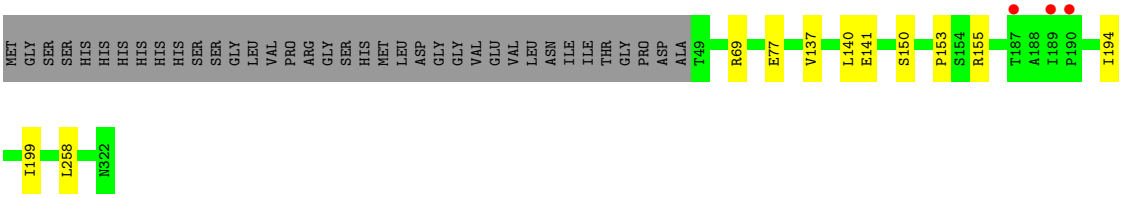
• Molecule 1: VP1

Chain I:



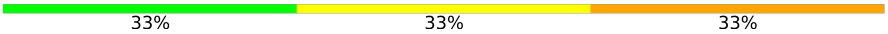
• Molecule 1: VP1

Chain J:



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

Chain K:

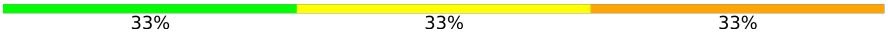


• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain M:

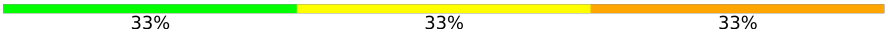
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain O:



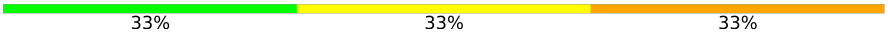
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain P:



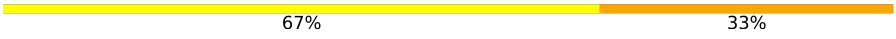
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:



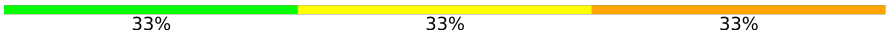
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:



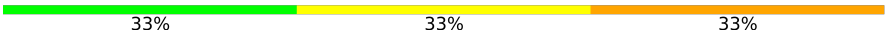
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Q:



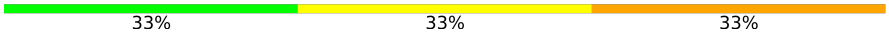
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R:



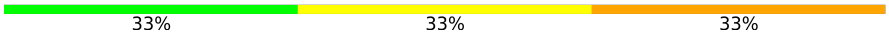
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain S:



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

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.38Å 151.08Å 130.62Å 90.00° 106.56° 90.00°	Depositor
Resolution (Å)	48.20 – 1.80 48.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.20-1.80) 99.8 (48.20-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.166 , 0.206 0.166 , 0.206	Depositor DCC
R_{free} test set	5903 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25061	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: BGC, SIA, GAL, GOL, GLC, MG

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	0.34	0/2188	0.54	0/2976
1	B	0.33	0/2235	0.55	0/3038
1	C	0.35	0/2227	0.56	0/3026
1	D	0.34	0/2236	0.54	0/3041
1	E	0.33	0/2216	0.54	0/3013
1	F	0.37	0/2193	0.56	0/2983
1	G	0.38	0/2257	0.57	0/3072
1	H	0.38	0/2189	0.57	0/2977
1	I	0.35	0/2191	0.56	0/2980
1	J	0.36	0/2187	0.56	0/2971
All	All	0.35	0/22119	0.55	0/30077

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

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	2135	0	2053	7	0
1	B	2179	0	2129	9	0
1	C	2171	0	2119	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2181	0	2112	7	0
1	E	2163	0	2097	8	0
1	F	2139	0	2071	5	0
1	G	2201	0	2132	5	0
1	H	2135	0	2068	7	0
1	I	2137	0	2081	7	0
1	J	2136	0	2078	9	0
2	K	43	0	37	3	0
2	M	43	0	37	1	0
2	O	43	0	37	2	0
2	P	43	0	37	2	0
3	L	43	0	37	3	0
3	N	43	0	37	3	0
3	Q	43	0	37	2	0
3	R	43	0	37	2	0
3	S	43	0	37	2	0
3	T	43	0	37	3	0
4	A	30	0	40	3	0
4	B	30	0	40	1	0
4	C	24	0	32	2	0
4	D	18	0	24	1	0
4	E	24	0	31	1	0
4	F	18	0	24	0	0
4	G	36	0	48	0	0
4	H	18	0	24	0	0
4	I	24	0	32	1	0
4	J	24	0	32	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	A	250	0	0	1	0
6	B	283	0	0	0	0
6	C	277	0	0	0	0
6	D	244	0	0	1	0
6	E	233	0	0	2	0
6	F	298	0	0	0	0
6	G	344	0	0	0	0
6	H	274	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	300	0	0	1	0
6	J	295	0	0	1	0
All	All	25061	0	21637	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (74) 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:E:41:ASN:ND2	1:E:42:ILE:O	2.24	0.70
1:C:258[B]:LEU:HD12	4:C:405:GOL:H11	1.76	0.67
1:F:77:GLU:HG2	2:P:3:SIA:H113	1.77	0.66
1:A:77:GLU:HG2	2:K:3:SIA:H113	1.77	0.66
1:G:77:GLU:HG2	3:Q:3:SIA:H113	1.78	0.65
1:J:77:GLU:HG2	3:T:3:SIA:H113	1.80	0.64
1:I:77:GLU:HG2	3:S:3:SIA:H113	1.82	0.61
1:D:77:GLU:HG2	3:N:3:SIA:H113	1.83	0.61
1:B:77:GLU:HG2	3:L:3:SIA:H113	1.82	0.61
1:G:52:ILE:HG21	1:G:102:VAL:HG11	1.83	0.59
1:D:69:ARG:HH21	3:N:3:SIA:H111	1.68	0.59
1:B:204:GLU:HA	1:B:207:LYS:HD3	1.85	0.58
1:E:77:GLU:HG2	2:O:3:SIA:H113	1.85	0.58
1:J:140[A]:LEU:HG	1:J:141:GLU:HG3	1.87	0.56
1:C:77:GLU:HG2	2:M:3:SIA:H113	1.87	0.56
1:H:77:GLU:HG2	3:R:3:SIA:H113	1.88	0.55
1:C:137:VAL:HB	1:C:153:PRO:HB2	1.90	0.54
1:F:300:GLU:OE1	1:J:150:SER:OG	2.21	0.53
1:F:77:GLU:CG	2:P:3:SIA:H113	2.40	0.52
1:A:77:GLU:CG	2:K:3:SIA:H113	2.40	0.52
1:A:137:VAL:HB	1:A:153:PRO:HB2	1.91	0.52
1:I:137:VAL:HB	1:I:153:PRO:HB2	1.91	0.52
1:B:69:ARG:HH21	3:L:3:SIA:H111	1.74	0.51
1:E:54:LEU:HD11	1:E:285:VAL:HG21	1.92	0.51
1:E:155:ARG:HD2	6:E:531:HOH:O	2.11	0.51
1:H:140[A]:LEU:HG	1:H:141:GLU:HG3	1.93	0.50
1:J:137:VAL:HB	1:J:153:PRO:HB2	1.94	0.50
1:D:137:VAL:HB	1:D:153:PRO:HB2	1.93	0.49
1:C:204:GLU:HA	1:C:207:LYS:HD2	1.95	0.49
1:B:137:VAL:HB	1:B:153:PRO:HB2	1.95	0.48
1:D:258:LEU:HD22	4:D:405:GOL:H11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:VAL:HB	1:G:153:PRO:HB2	1.95	0.48
1:H:69:ARG:HH21	3:R:3:SIA:H111	1.77	0.47
1:F:204:GLU:HA	1:F:207:LYS:HD2	1.96	0.47
1:A:69:ARG:HH11	2:K:3:SIA:H111	1.78	0.47
1:D:271:GLU:H	1:D:271:GLU:CD	2.19	0.47
1:C:54:LEU:HD11	1:C:285:VAL:HG21	1.98	0.46
1:A:259:GLN:NE2	6:A:503:HOH:O	2.42	0.46
1:J:77:GLU:CG	3:T:3:SIA:H113	2.45	0.46
1:H:137:VAL:HB	1:H:153:PRO:HB2	1.98	0.46
1:E:127:GLU:OE1	6:E:501:HOH:O	2.20	0.46
1:D:77:GLU:CG	3:N:3:SIA:H113	2.46	0.46
1:G:77:GLU:CG	3:Q:3:SIA:H113	2.43	0.46
1:J:69:ARG:HH21	3:T:3:SIA:H111	1.81	0.45
4:B:405:GOL:HO3	4:B:406:GOL:HO1	1.64	0.45
1:I:117:MET:HE3	1:I:317:LYS:HB3	1.99	0.45
1:B:77:GLU:CG	3:L:3:SIA:H113	2.47	0.44
1:H:58:PRO:HG3	6:H:618:HOH:O	2.17	0.44
4:A:408:GOL:H32	1:B:252:LEU:H	1.82	0.44
1:A:223:LYS:HE3	1:A:226:PHE:CD1	2.52	0.44
1:C:257:ASN:O	1:C:258[B]:LEU:HD13	2.18	0.44
1:G:140:LEU:HG	1:G:141:GLU:HG3	1.99	0.44
1:E:271:GLU:H	1:E:271:GLU:CD	2.21	0.43
4:A:408:GOL:C3	1:B:252:LEU:H	2.32	0.43
1:E:137:VAL:HB	1:E:153:PRO:HB2	2.01	0.43
1:I:85:TYR:CD2	4:I:404:GOL:H31	2.53	0.43
1:E:77:GLU:CG	2:O:3:SIA:H113	2.49	0.42
1:I:155:ARG:HD2	6:I:543:HOH:O	2.17	0.42
1:I:204:GLU:HA	1:I:207:LYS:HD2	2.00	0.42
1:H:223:LYS:HD3	1:H:226:PHE:CG	2.55	0.42
1:A:158:GLU:HA	1:A:256:PRO:HG3	2.00	0.42
1:F:296:LYS:HB3	1:F:296:LYS:HE2	1.87	0.42
1:J:258[B]:LEU:HD12	4:J:406:GOL:H11	2.00	0.42
1:B:140:LEU:HG	1:B:141:GLU:HG3	2.02	0.41
1:C:54:LEU:HD22	1:C:102:VAL:HG21	2.02	0.41
1:D:155:ARG:HD2	6:D:511:HOH:O	2.20	0.41
4:E:405:GOL:H32	4:E:406:GOL:O3	2.20	0.41
4:A:408:GOL:HO2	1:B:253:GLN:HE21	1.59	0.41
1:I:77:GLU:CG	3:S:3:SIA:H113	2.47	0.41
1:J:194:ILE:HD11	1:J:199:ILE:HD11	2.01	0.41
1:H:271:GLU:H	1:H:271:GLU:CD	2.23	0.41
1:J:155:ARG:HD2	6:J:520:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258[A]:LEU:HD22	4:C:405:GOL:H11	2.04	0.40
1:C:90:LEU:HD23	1:C:186:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/311 (90%)	269 (96%)	10 (4%)	0	100	100
1	B	284/311 (91%)	274 (96%)	10 (4%)	0	100	100
1	C	282/311 (91%)	272 (96%)	10 (4%)	0	100	100
1	D	286/311 (92%)	275 (96%)	11 (4%)	0	100	100
1	E	282/311 (91%)	272 (96%)	10 (4%)	0	100	100
1	F	280/311 (90%)	272 (97%)	8 (3%)	0	100	100
1	G	289/311 (93%)	279 (96%)	10 (4%)	0	100	100
1	H	280/311 (90%)	270 (96%)	10 (4%)	0	100	100
1	I	279/311 (90%)	270 (97%)	9 (3%)	0	100	100
1	J	277/311 (89%)	269 (97%)	8 (3%)	0	100	100
All	All	2818/3110 (91%)	2722 (97%)	96 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	225/261 (86%)	223 (99%)	2 (1%)	78 75
1	B	235/261 (90%)	235 (100%)	0	100 100
1	C	234/261 (90%)	232 (99%)	2 (1%)	78 75
1	D	232/261 (89%)	230 (99%)	2 (1%)	78 75
1	E	229/261 (88%)	229 (100%)	0	100 100
1	F	230/261 (88%)	227 (99%)	3 (1%)	69 62
1	G	234/261 (90%)	233 (100%)	1 (0%)	91 89
1	H	228/261 (87%)	228 (100%)	0	100 100
1	I	229/261 (88%)	226 (99%)	3 (1%)	69 62
1	J	231/261 (88%)	231 (100%)	0	100 100
All	All	2307/2610 (88%)	2294 (99%)	13 (1%)	88 84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	MET
1	A	164	MET
1	C	54	LEU
1	C	164	MET
1	D	160[A]	MET
1	D	160[B]	MET
1	F	54	LEU
1	F	160	MET
1	F	318	ARG
1	G	160	MET
1	I	160	MET
1	I	258[A]	LEU
1	I	258[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	322	ASN
1	E	253	GLN
1	F	253	GLN
1	F	259	GLN

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Mol	Chain	Res	Type
1	G	253	GLN
1	H	259	GLN
1	I	149	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

30 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	GLC	K	1	2	12,12,12	0.57	0	17,17,17	0.66	0
2	GAL	K	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.01	0
2	SIA	K	3	2	20,20,21	2.21	3 (15%)	24,28,31	1.52	6 (25%)
3	BGC	L	1	3	12,12,12	0.50	0	17,17,17	1.00	1 (5%)
3	GAL	L	2	3	11,11,12	0.57	0	15,15,17	0.89	0
3	SIA	L	3	3	20,20,21	2.03	2 (10%)	24,28,31	1.68	6 (25%)
2	GLC	M	1	2	12,12,12	0.62	0	17,17,17	0.71	0
2	GAL	M	2	2	11,11,12	0.79	0	15,15,17	0.83	0
2	SIA	M	3	2	20,20,21	2.02	3 (15%)	24,28,31	1.73	7 (29%)
3	BGC	N	1	3	12,12,12	0.50	0	17,17,17	1.00	2 (11%)
3	GAL	N	2	3	11,11,12	0.88	1 (9%)	15,15,17	0.78	0
3	SIA	N	3	3	20,20,21	2.14	3 (15%)	24,28,31	1.60	6 (25%)
2	GLC	O	1	2	12,12,12	0.55	0	17,17,17	0.53	0
2	GAL	O	2	2	11,11,12	0.61	0	15,15,17	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIA	O	3	2	20,20,21	1.94	2 (10%)	24,28,31	1.56	5 (20%)
2	GLC	P	1	2	12,12,12	0.60	0	17,17,17	0.75	0
2	GAL	P	2	2	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
2	SIA	P	3	2	20,20,21	2.13	2 (10%)	24,28,31	1.65	6 (25%)
3	BGC	Q	1	3	12,12,12	0.55	0	17,17,17	1.17	3 (17%)
3	GAL	Q	2	3	11,11,12	0.85	0	15,15,17	0.83	0
3	SIA	Q	3	3	20,20,21	1.96	3 (15%)	24,28,31	1.37	4 (16%)
3	BGC	R	1	3	12,12,12	0.53	0	17,17,17	0.88	1 (5%)
3	GAL	R	2	3	11,11,12	0.69	0	15,15,17	0.86	0
3	SIA	R	3	3	20,20,21	2.23	3 (15%)	24,28,31	1.51	4 (16%)
3	BGC	S	1	3	12,12,12	0.50	0	17,17,17	0.93	1 (5%)
3	GAL	S	2	3	11,11,12	0.83	0	15,15,17	1.05	0
3	SIA	S	3	3	20,20,21	2.14	2 (10%)	24,28,31	1.73	5 (20%)
3	BGC	T	1	3	12,12,12	0.53	0	17,17,17	1.00	1 (5%)
3	GAL	T	2	3	11,11,12	0.83	0	15,15,17	1.04	0
3	SIA	T	3	3	20,20,21	2.10	3 (15%)	24,28,31	1.60	7 (29%)

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	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	SIA	K	3	2	-	0/18/34/38	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	GAL	L	2	3	-	0/2/19/22	0/1/1/1
3	SIA	L	3	3	-	1/18/34/38	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	SIA	M	3	2	-	1/18/34/38	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	GAL	N	2	3	-	0/2/19/22	0/1/1/1
3	SIA	N	3	3	-	1/18/34/38	0/1/1/1
2	GLC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1
2	SIA	O	3	2	-	0/18/34/38	0/1/1/1
2	GLC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	P	3	2	-	0/18/34/38	0/1/1/1
3	BGC	Q	1	3	-	0/2/22/22	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	0/18/34/38	0/1/1/1
3	BGC	R	1	3	-	0/2/22/22	0/1/1/1
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	1/18/34/38	0/1/1/1
3	BGC	S	1	3	-	0/2/22/22	0/1/1/1
3	GAL	S	2	3	-	0/2/19/22	0/1/1/1
3	SIA	S	3	3	-	0/18/34/38	0/1/1/1
3	BGC	T	1	3	-	0/2/22/22	0/1/1/1
3	GAL	T	2	3	-	0/2/19/22	0/1/1/1
3	SIA	T	3	3	-	0/18/34/38	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3	SIA	C2-C1	8.68	1.60	1.52
2	P	3	SIA	C2-C1	8.55	1.60	1.52
3	R	3	SIA	C2-C1	8.51	1.60	1.52
3	N	3	SIA	C2-C1	8.42	1.59	1.52
3	S	3	SIA	C2-C1	8.31	1.59	1.52
3	T	3	SIA	C2-C1	8.15	1.59	1.52
3	L	3	SIA	C2-C1	7.98	1.59	1.52
2	M	3	SIA	C2-C1	7.91	1.59	1.52
2	O	3	SIA	C2-C1	7.68	1.59	1.52
3	Q	3	SIA	C2-C1	7.40	1.59	1.52
3	S	3	SIA	O6-C2	2.66	1.47	1.43
3	R	3	SIA	O6-C2	2.63	1.47	1.43
3	T	3	SIA	O6-C2	2.57	1.47	1.43
3	L	3	SIA	O6-C2	2.49	1.47	1.43
2	M	3	SIA	O6-C2	2.47	1.47	1.43
3	R	3	SIA	C7-C6	2.43	1.56	1.53
2	P	3	SIA	O6-C2	2.42	1.47	1.43
3	N	3	SIA	O6-C2	2.40	1.47	1.43
2	K	3	SIA	O6-C2	2.40	1.47	1.43
3	Q	3	SIA	O6-C2	2.39	1.46	1.43
3	Q	3	SIA	C7-C6	2.34	1.55	1.53
2	K	2	GAL	O5-C1	-2.31	1.40	1.43
2	O	3	SIA	O6-C2	2.23	1.46	1.43
3	T	3	SIA	C7-C6	2.19	1.55	1.53
3	N	2	GAL	C2-C3	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3	SIA	C7-C6	2.13	1.55	1.53
3	N	3	SIA	C7-C6	2.10	1.55	1.53
2	M	3	SIA	C7-C6	2.04	1.55	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	3	SIA	O1A-C1-C2	-5.08	110.58	122.57
3	L	3	SIA	O1A-C1-C2	-4.34	112.33	122.57
3	S	3	SIA	C6-C5-N5	-3.67	104.81	110.91
3	S	3	SIA	C4-C5-N5	3.59	117.48	110.38
3	T	3	SIA	O1A-C1-C2	-3.37	114.61	122.57
2	P	3	SIA	O1A-C1-C2	-3.32	114.73	122.57
3	Q	3	SIA	C4-C3-C2	3.30	115.73	109.81
3	S	3	SIA	O1A-C1-C2	-3.29	114.79	122.57
3	L	1	BGC	C1-O5-C5	-3.28	107.47	113.66
3	T	1	BGC	C1-O5-C5	-3.26	107.51	113.66
2	P	3	SIA	O6-C2-C3	-3.22	106.03	110.46
3	R	3	SIA	O1A-C1-C2	-3.15	115.14	122.57
2	O	3	SIA	C6-C5-N5	-3.12	105.74	110.91
3	T	3	SIA	C6-C5-N5	-3.08	105.80	110.91
3	N	3	SIA	O1A-C1-C2	-2.99	115.52	122.57
3	N	3	SIA	C6-C5-N5	-2.96	105.99	110.91
3	S	1	BGC	C1-O5-C5	-2.96	108.08	113.66
2	M	3	SIA	O1B-C1-O1A	2.86	130.58	124.09
3	N	3	SIA	C4-C3-C2	2.86	114.94	109.81
3	Q	1	BGC	C1-O5-C5	-2.86	108.27	113.66
2	K	3	SIA	C6-C5-N5	-2.84	106.19	110.91
3	R	3	SIA	C6-C5-N5	-2.83	106.20	110.91
2	K	3	SIA	O6-C2-C3	-2.72	106.71	110.46
2	K	3	SIA	C6-O6-C2	2.66	117.02	111.34
2	K	3	SIA	C4-C5-N5	2.65	115.62	110.38
2	P	3	SIA	C6-C5-N5	-2.54	106.69	110.91
2	O	3	SIA	O1A-C1-C2	-2.52	116.62	122.57
2	O	3	SIA	C6-O6-C2	2.51	116.72	111.34
3	Q	3	SIA	C6-O6-C2	2.50	116.69	111.34
3	Q	3	SIA	O1B-C1-O1A	2.50	129.76	124.09
3	N	3	SIA	O1B-C1-O1A	2.50	129.76	124.09
3	T	3	SIA	C4-C5-N5	2.48	115.29	110.38
2	P	3	SIA	C4-C5-N5	2.47	115.27	110.38
3	L	3	SIA	C4-C3-C2	2.46	114.22	109.81
3	L	3	SIA	C6-C5-N5	-2.46	106.83	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	3	SIA	O1B-C1-O1A	2.45	129.65	124.09
2	P	3	SIA	C4-C3-C2	2.43	114.17	109.81
3	S	3	SIA	C6-O6-C2	2.36	116.39	111.34
3	T	3	SIA	C6-O6-C2	2.36	116.38	111.34
2	M	3	SIA	C4-C3-C2	2.32	113.96	109.81
3	N	1	BGC	C1-O5-C5	-2.31	109.31	113.66
2	K	3	SIA	O1A-C1-C2	-2.30	117.13	122.57
3	T	3	SIA	O6-C2-C3	-2.30	107.30	110.46
3	N	3	SIA	C4-C5-N5	2.30	114.92	110.38
3	Q	1	BGC	C1-C2-C3	-2.29	105.56	110.31
3	Q	3	SIA	C6-C5-N5	-2.29	107.11	110.91
3	N	3	SIA	C6-O6-C2	2.27	116.20	111.34
3	R	3	SIA	O1B-C1-O1A	2.26	129.21	124.09
3	L	3	SIA	O1B-C1-O1A	2.25	129.19	124.09
2	O	3	SIA	C4-C5-N5	2.24	114.81	110.38
3	T	3	SIA	O1B-C1-O1A	2.22	129.13	124.09
2	M	3	SIA	C6-O6-C2	2.20	116.05	111.34
2	P	3	SIA	C3-C4-C5	-2.19	108.82	111.46
3	N	1	BGC	C4-C3-C2	-2.17	107.03	110.82
3	L	3	SIA	C6-O6-C2	2.16	115.97	111.34
3	T	3	SIA	C4-C3-C2	2.15	113.67	109.81
3	R	3	SIA	C6-O6-C2	2.13	115.89	111.34
2	P	2	GAL	C1-O5-C5	2.12	115.06	112.19
2	K	3	SIA	C4-C3-C2	2.11	113.59	109.81
3	S	3	SIA	O1B-C1-O1A	2.11	128.87	124.09
3	Q	1	BGC	O4-C4-C3	-2.07	105.56	110.35
3	L	3	SIA	C4-C5-N5	2.07	114.47	110.38
2	M	3	SIA	C6-C5-N5	-2.07	107.48	110.91
2	O	2	GAL	O2-C2-C3	-2.05	106.02	110.14
2	M	3	SIA	C8-C7-C6	-2.05	109.14	113.03
2	M	3	SIA	O1B-C1-C2	2.03	118.83	113.03
3	R	1	BGC	C1-O5-C5	-2.02	109.85	113.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

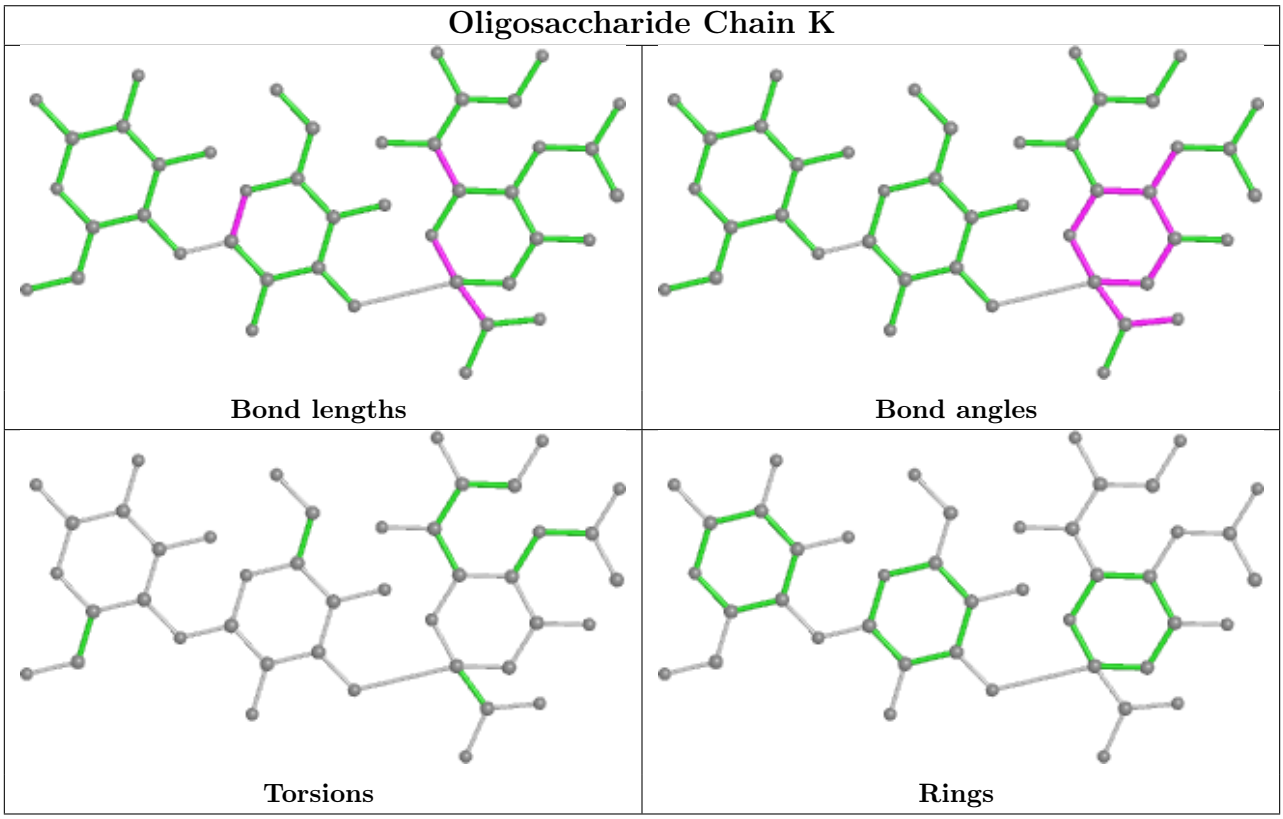
Mol	Chain	Res	Type	Atoms
3	R	3	SIA	O8-C8-C9-O9
2	M	3	SIA	O1B-C1-C2-O6
3	L	3	SIA	O1B-C1-C2-O6
3	N	3	SIA	O1B-C1-C2-O6

There are no ring outliers.

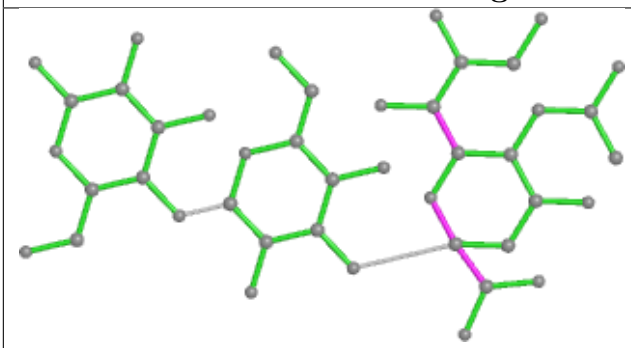
10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	3	SIA	2	0
3	L	3	SIA	3	0
2	K	3	SIA	3	0
3	Q	3	SIA	2	0
3	S	3	SIA	2	0
3	N	3	SIA	3	0
2	P	3	SIA	2	0
2	M	3	SIA	1	0
3	R	3	SIA	2	0
3	T	3	SIA	3	0

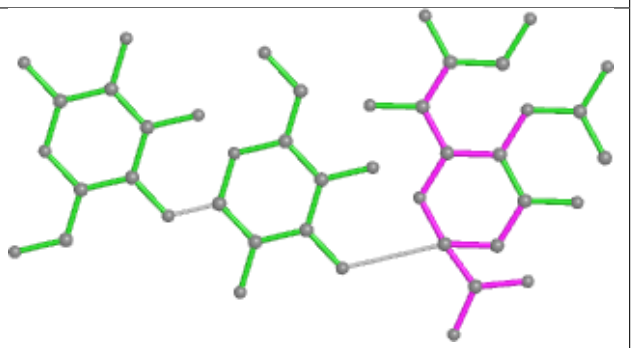
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



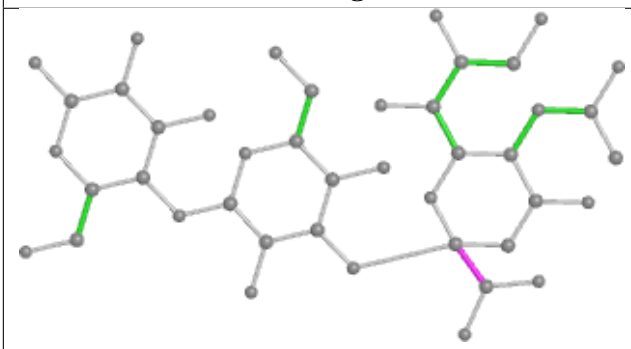
Oligosaccharide Chain M



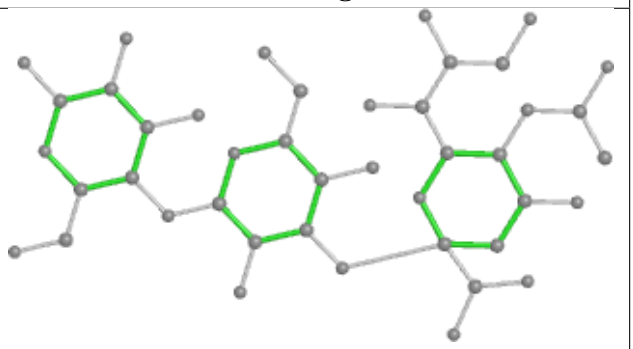
Bond lengths



Bond angles

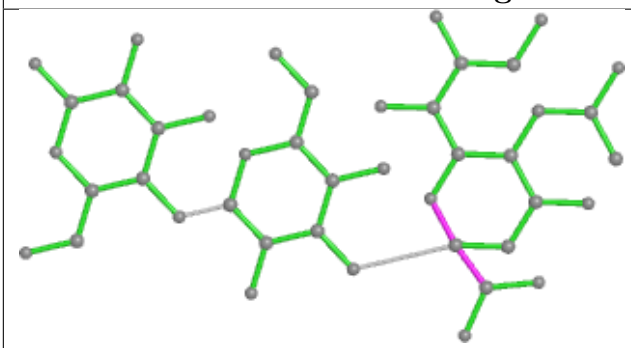


Torsions

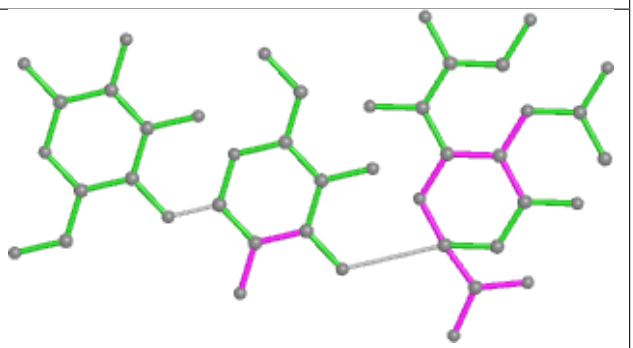


Rings

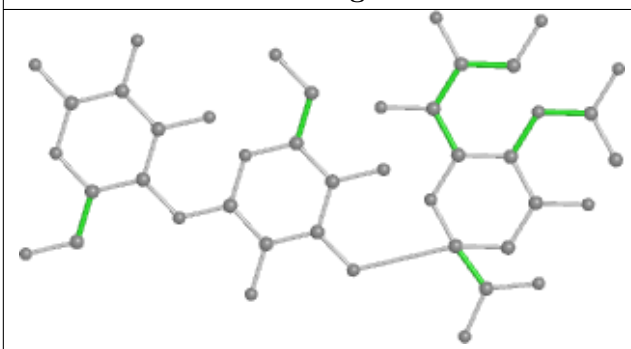
Oligosaccharide Chain O



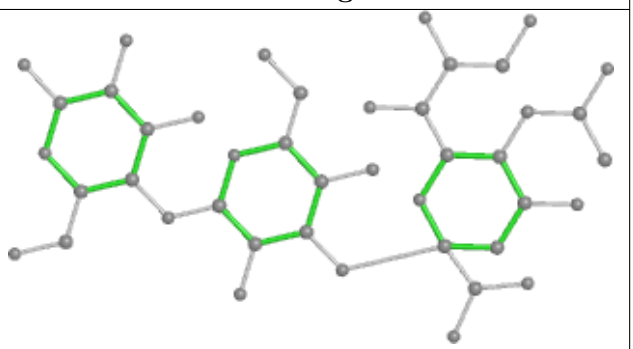
Bond lengths



Bond angles

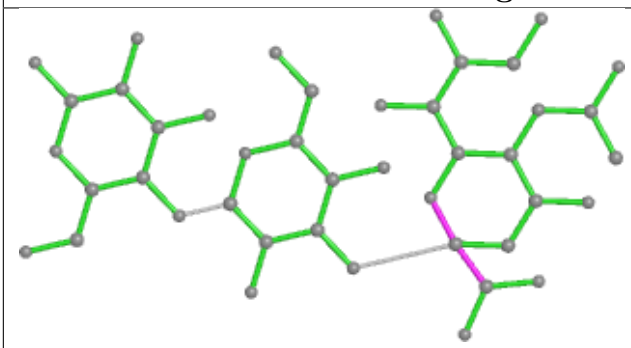


Torsions

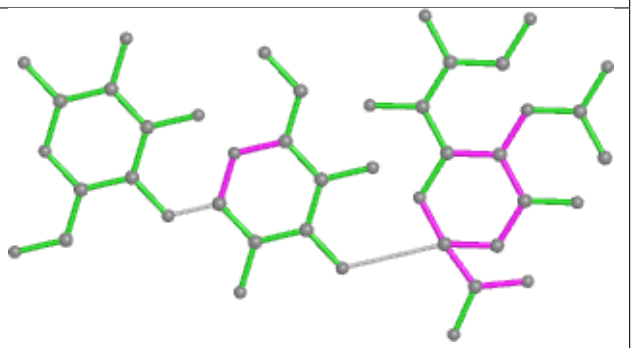


Rings

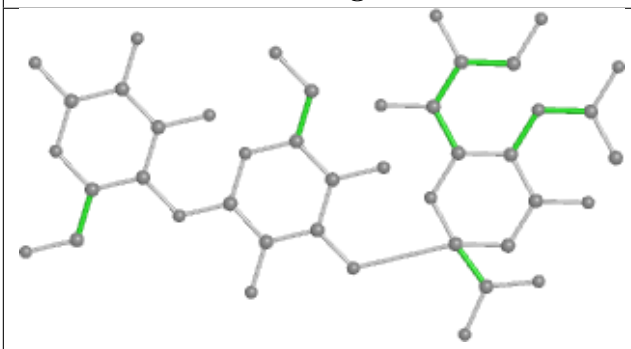
Oligosaccharide Chain P



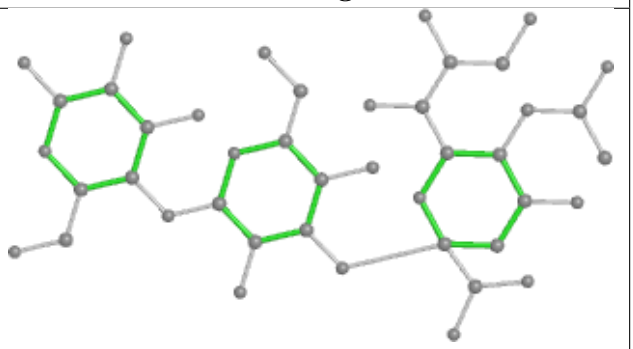
Bond lengths



Bond angles

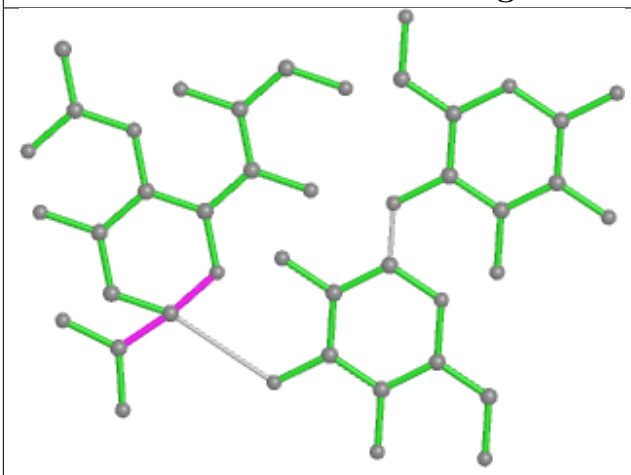


Torsions

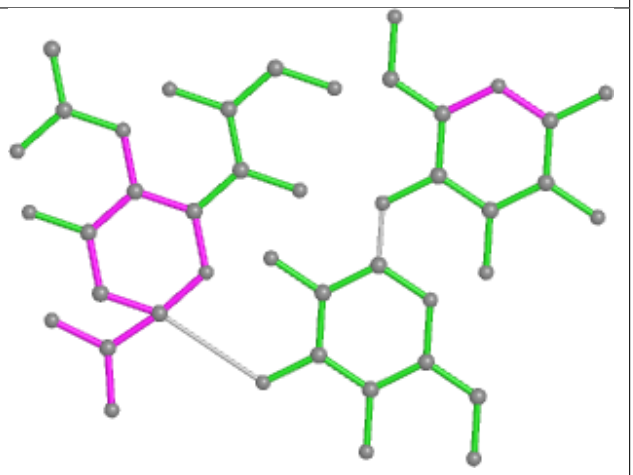


Rings

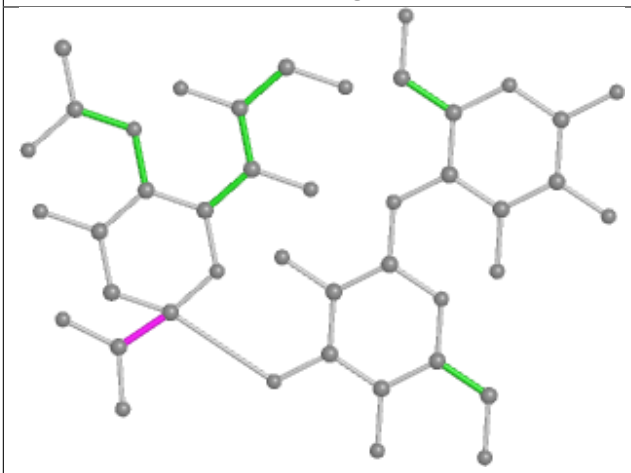
Oligosaccharide Chain L



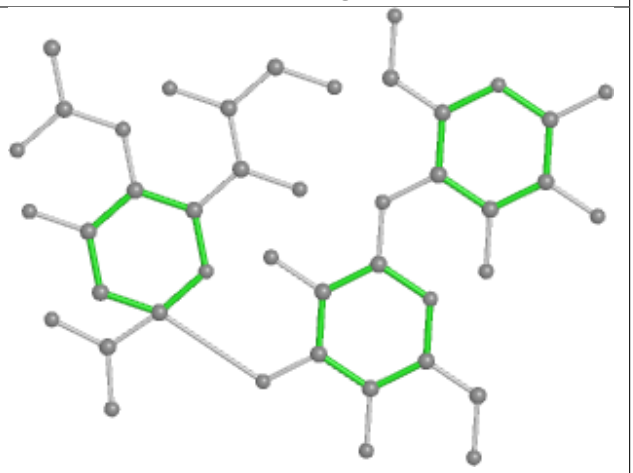
Bond lengths



Bond angles

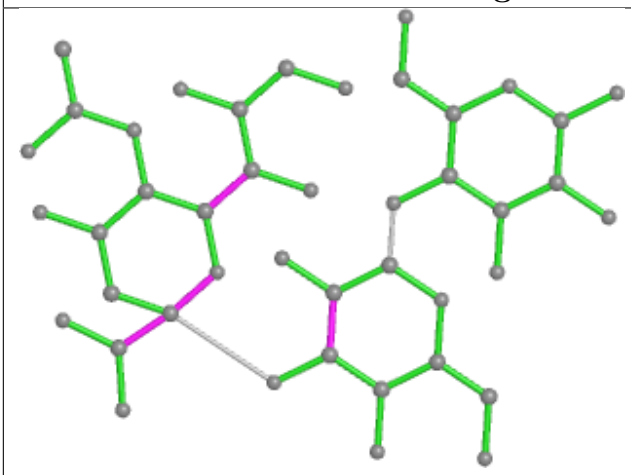


Torsions

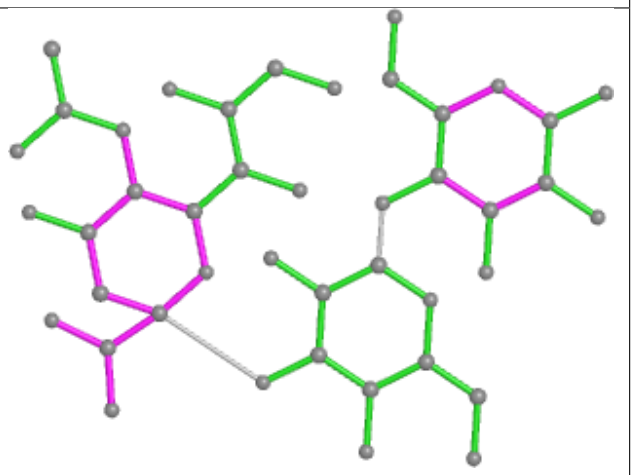


Rings

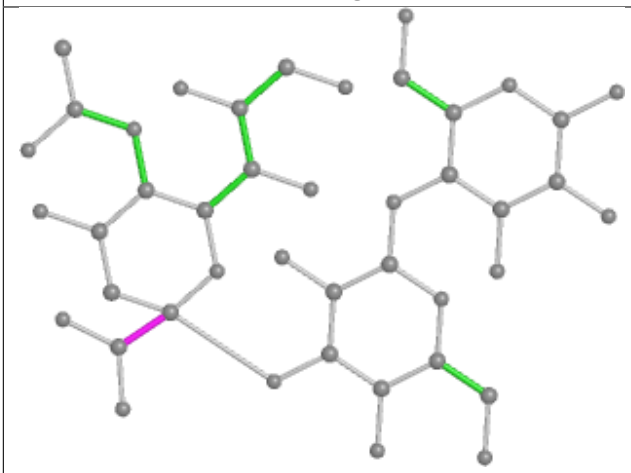
Oligosaccharide Chain N



Bond lengths



Bond angles



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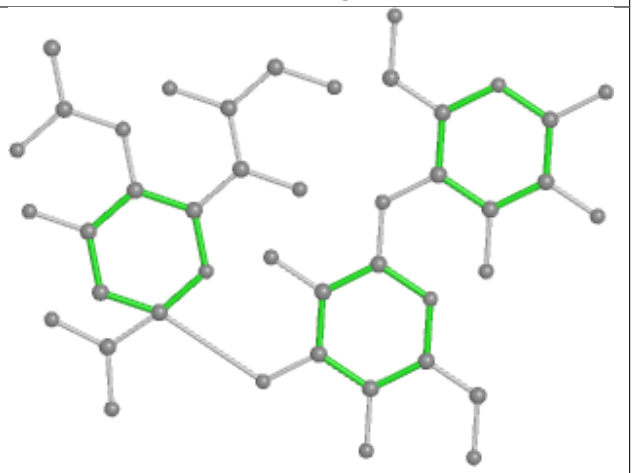
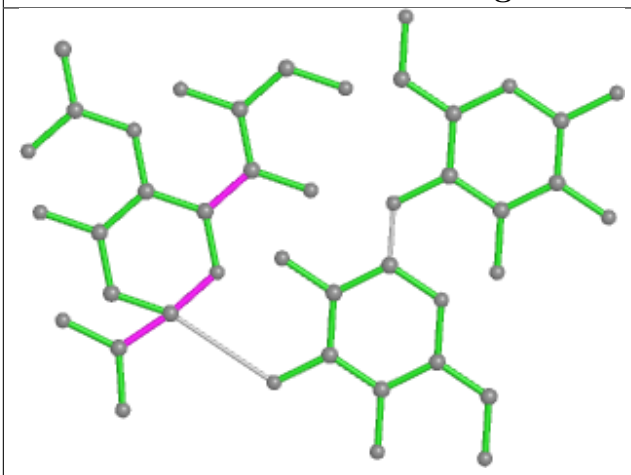
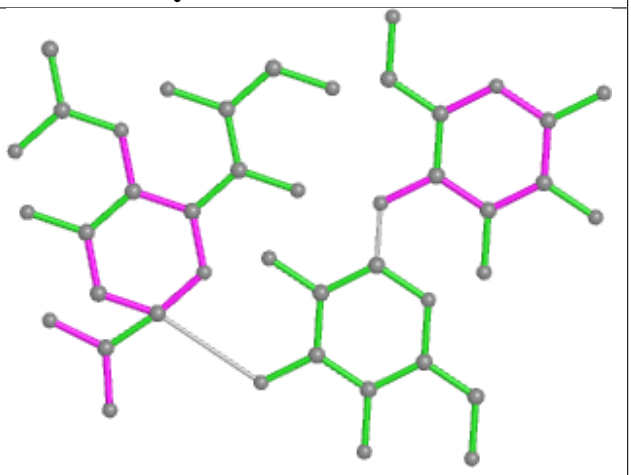


Rings

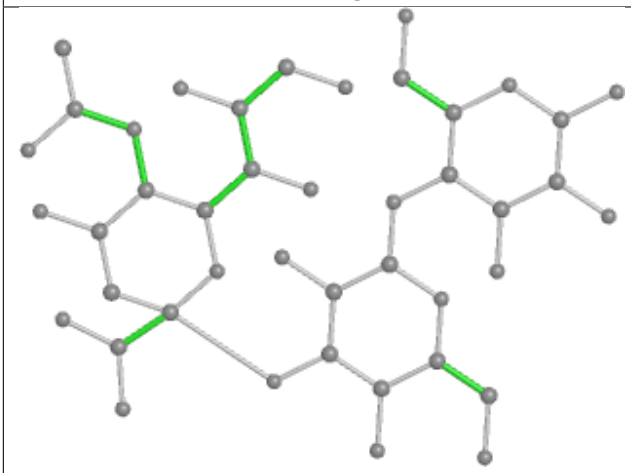
Oligosaccharide Chain Q



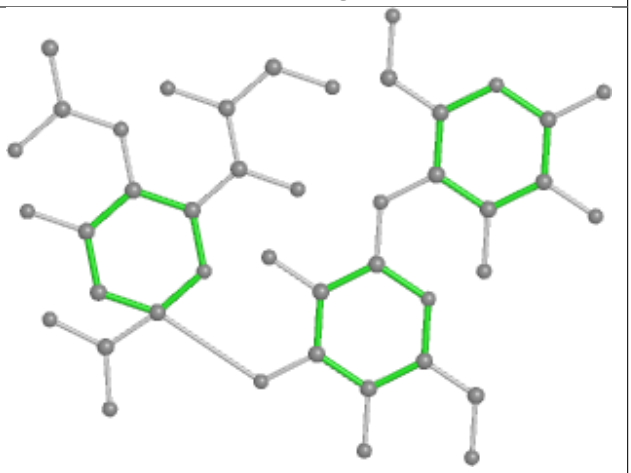
Bond lengths



Bond angles

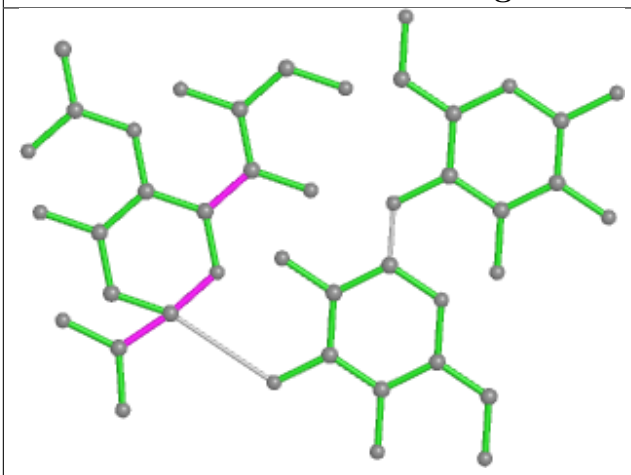


Torsions

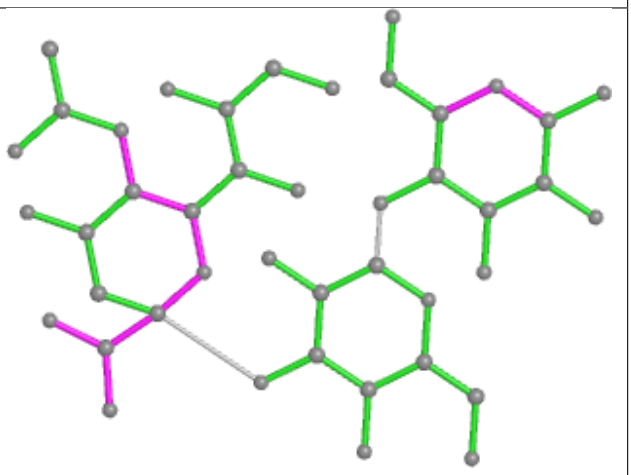


Rings

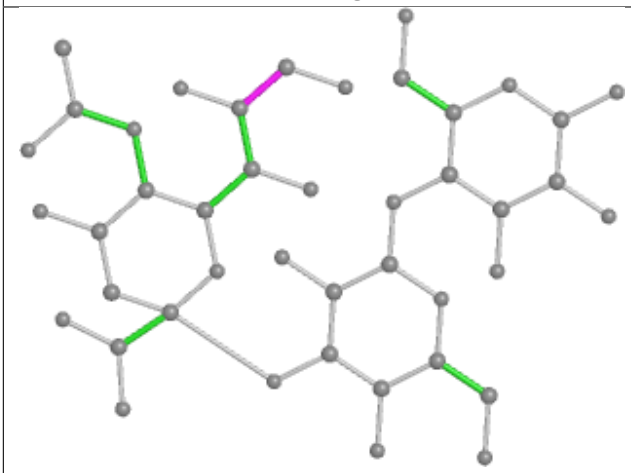
Oligosaccharide Chain R



Bond lengths



Bond angles



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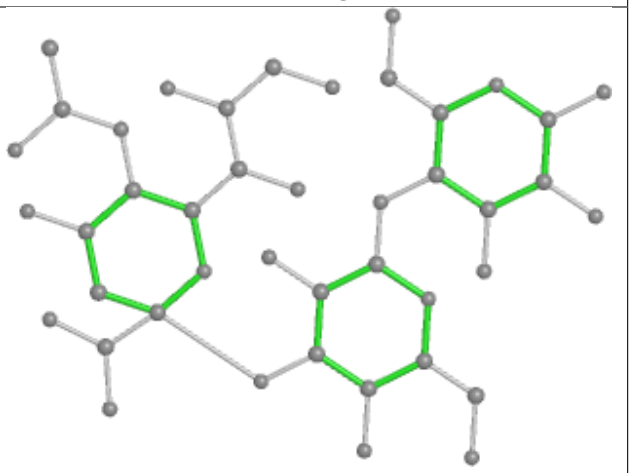
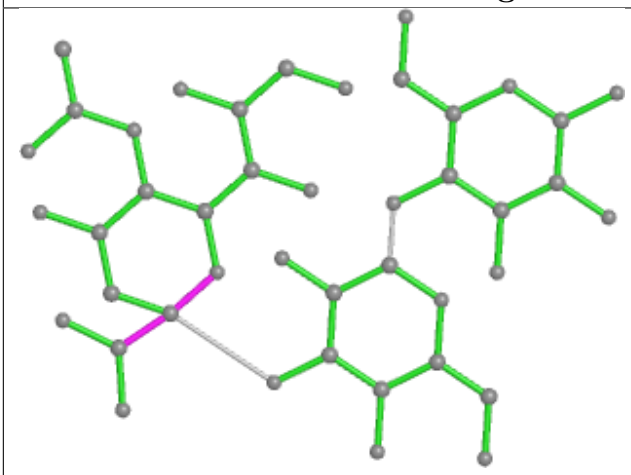
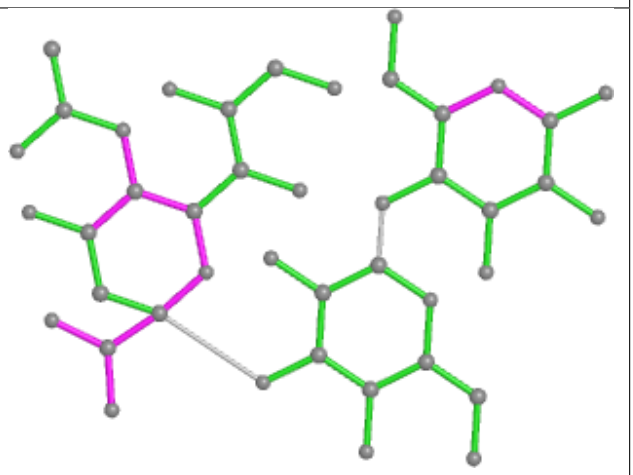


Rings

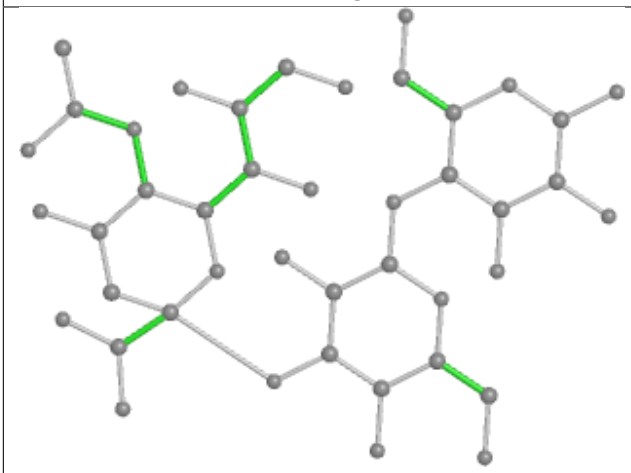
Oligosaccharide Chain S



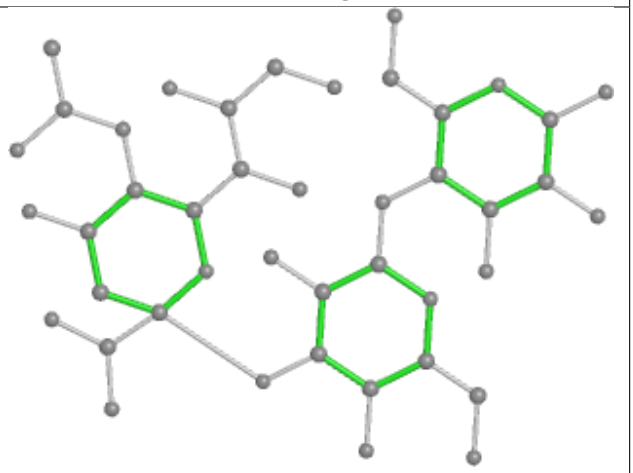
Bond lengths



Bond angles

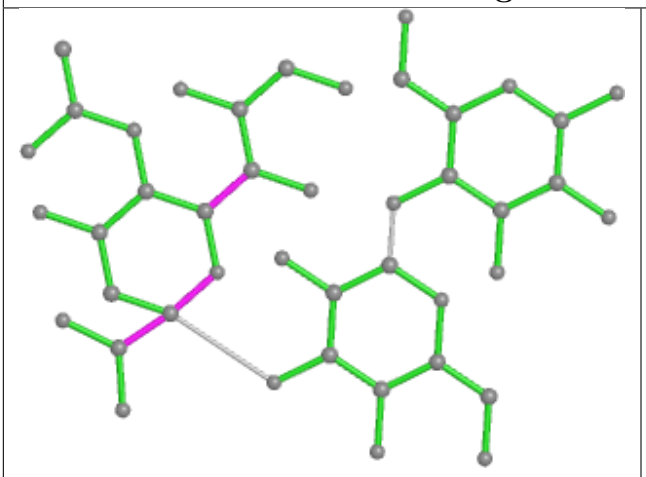


Torsions

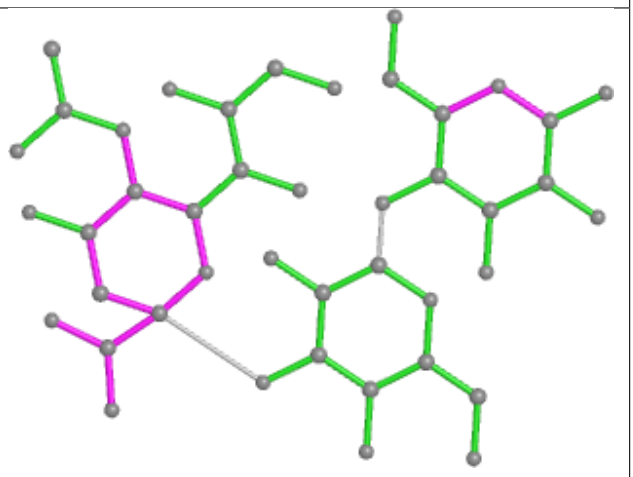


Rings

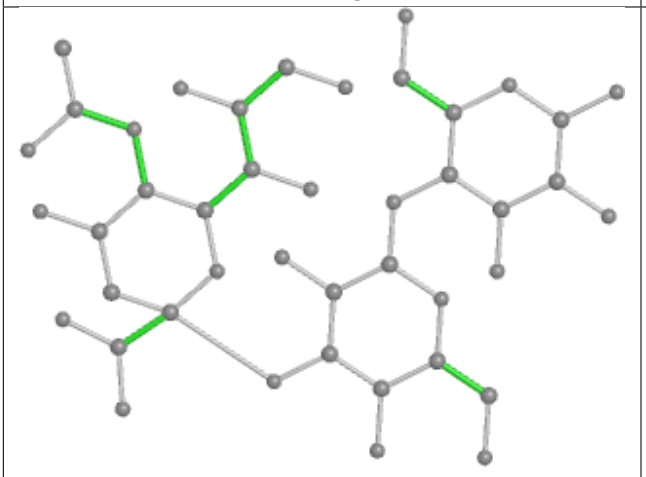
Oligosaccharide Chain T



Bond lengths



Bond angles



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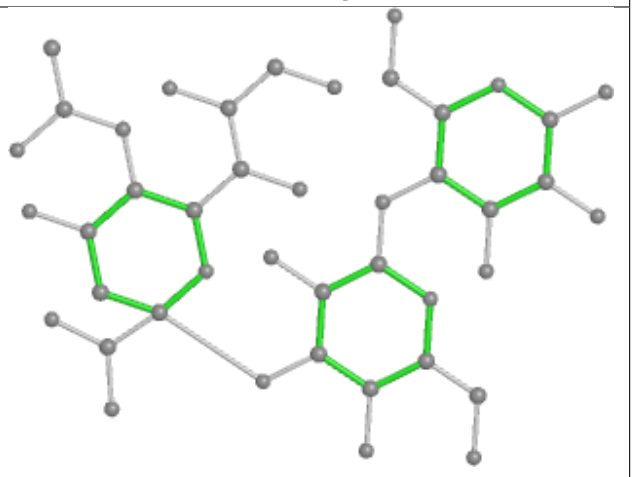

Rings

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 10 are monoatomic - leaving 41 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	408	-	5,5,5	0.97	0	5,5,5	0.99	0
4	GOL	I	405	-	5,5,5	0.68	0	5,5,5	1.07	0
4	GOL	C	407	-	5,5,5	1.01	0	5,5,5	1.02	0
4	GOL	D	407	-	5,5,5	0.97	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	C	404	-	5,5,5	0.89	0	5,5,5	1.08	0
4	GOL	E	407	-	5,5,5	1.02	0	5,5,5	1.02	0
4	GOL	H	404	-	5,5,5	0.72	0	5,5,5	0.95	0
4	GOL	F	405	-	5,5,5	0.85	0	5,5,5	0.99	0
4	GOL	C	406	-	5,5,5	0.75	0	5,5,5	1.13	0
4	GOL	B	404	-	5,5,5	0.79	0	5,5,5	1.02	0
4	GOL	G	405	-	5,5,5	0.99	0	5,5,5	0.80	0
4	GOL	I	406[B]	-	5,5,5	0.88	0	5,5,5	0.94	0
4	GOL	E	406	-	5,5,5	0.84	0	5,5,5	1.01	0
4	GOL	G	404	-	5,5,5	1.04	0	5,5,5	0.90	0
4	GOL	B	408	-	5,5,5	1.07	0	5,5,5	1.00	0
4	GOL	F	404	-	5,5,5	0.91	0	5,5,5	0.85	0
4	GOL	J	407	-	5,5,5	0.88	0	5,5,5	0.95	0
4	GOL	C	405	-	5,5,5	0.99	0	5,5,5	1.02	0
4	GOL	J	404	-	5,5,5	0.98	0	5,5,5	0.90	0
4	GOL	G	406[B]	-	5,5,5	0.92	0	5,5,5	1.06	0
4	GOL	J	406	-	5,5,5	0.73	0	5,5,5	1.06	0
4	GOL	A	406	-	5,5,5	0.84	0	5,5,5	1.12	0
4	GOL	B	406	-	5,5,5	0.65	0	5,5,5	1.01	0
4	GOL	E	405	-	5,5,5	0.87	0	5,5,5	1.28	1 (20%)
4	GOL	B	405	-	5,5,5	0.74	0	5,5,5	1.13	0
4	GOL	D	406	-	5,5,5	0.83	0	5,5,5	0.99	0
4	GOL	E	404	-	5,5,5	0.83	0	5,5,5	0.94	0
4	GOL	I	406[A]	-	5,5,5	0.80	0	5,5,5	0.96	0
4	GOL	A	405	-	5,5,5	0.98	0	5,5,5	1.00	0
4	GOL	F	406	-	5,5,5	0.89	0	5,5,5	0.97	0
4	GOL	G	407	-	5,5,5	0.97	0	5,5,5	0.94	0
4	GOL	A	404	-	5,5,5	1.12	0	5,5,5	0.94	0
4	GOL	J	405	-	5,5,5	1.04	0	5,5,5	0.90	0
4	GOL	A	407	-	5,5,5	0.77	0	5,5,5	0.99	0
4	GOL	B	407	-	5,5,5	0.88	0	5,5,5	0.94	0
4	GOL	H	406	-	5,5,5	0.90	0	5,5,5	0.89	0
4	GOL	I	404	-	5,5,5	0.90	0	5,5,5	1.03	1 (20%)
4	GOL	G	406[A]	-	5,5,5	0.75	0	5,5,5	1.09	0
4	GOL	H	405	-	5,5,5	0.87	0	5,5,5	1.00	0
4	GOL	G	408	-	5,5,5	0.93	0	5,5,5	0.92	0
4	GOL	D	405	-	5,5,5	0.81	0	5,5,5	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	408	-	-	4/4/4/4	-
4	GOL	I	405	-	-	0/4/4/4	-
4	GOL	C	407	-	-	2/4/4/4	-
4	GOL	D	407	-	-	0/4/4/4	-
4	GOL	C	404	-	-	3/4/4/4	-
4	GOL	E	407	-	-	4/4/4/4	-
4	GOL	H	404	-	-	1/4/4/4	-
4	GOL	F	405	-	-	0/4/4/4	-
4	GOL	C	406	-	-	0/4/4/4	-
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	G	405	-	-	0/4/4/4	-
4	GOL	I	406[B]	-	-	4/4/4/4	-
4	GOL	E	406	-	-	4/4/4/4	-
4	GOL	G	404	-	-	0/4/4/4	-
4	GOL	B	408	-	-	2/4/4/4	-
4	GOL	F	404	-	-	0/4/4/4	-
4	GOL	J	407	-	-	0/4/4/4	-
4	GOL	C	405	-	-	2/4/4/4	-
4	GOL	J	404	-	-	0/4/4/4	-
4	GOL	G	406[B]	-	-	0/4/4/4	-
4	GOL	J	406	-	-	0/4/4/4	-
4	GOL	A	406	-	-	0/4/4/4	-
4	GOL	B	406	-	-	2/4/4/4	-
4	GOL	E	405	-	-	1/4/4/4	-
4	GOL	B	405	-	-	0/4/4/4	-
4	GOL	D	406	-	-	2/4/4/4	-
4	GOL	E	404	-	-	0/4/4/4	-
4	GOL	I	406[A]	-	-	4/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-
4	GOL	F	406	-	-	2/4/4/4	-
4	GOL	G	407	-	-	1/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	J	405	-	-	0/4/4/4	-
4	GOL	A	407	-	-	2/4/4/4	-
4	GOL	B	407	-	-	0/4/4/4	-
4	GOL	H	406	-	-	0/4/4/4	-
4	GOL	I	404	-	-	2/4/4/4	-
4	GOL	G	406[A]	-	-	4/4/4/4	-
4	GOL	H	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	408	-	-	0/4/4/4	-
4	GOL	D	405	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	405	GOL	C3-C2-C1	-2.41	102.33	111.70
4	I	404	GOL	C3-C2-C1	-2.03	103.80	111.70

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	407	GOL	O1-C1-C2-C3
4	A	408	GOL	O1-C1-C2-C3
4	A	408	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-C3
4	B	406	GOL	C1-C2-C3-O3
4	C	404	GOL	O1-C1-C2-C3
4	D	406	GOL	C1-C2-C3-O3
4	E	406	GOL	O1-C1-C2-C3
4	E	406	GOL	C1-C2-C3-O3
4	E	407	GOL	C1-C2-C3-O3
4	G	406[A]	GOL	O1-C1-C2-C3
4	I	406[B]	GOL	O1-C1-C2-C3
4	I	406[B]	GOL	C1-C2-C3-O3
4	E	406	GOL	O2-C2-C3-O3
4	E	407	GOL	O1-C1-C2-O2
4	E	407	GOL	O2-C2-C3-O3
4	I	406[B]	GOL	O1-C1-C2-O2
4	A	404	GOL	C1-C2-C3-O3
4	B	408	GOL	C1-C2-C3-O3
4	C	405	GOL	C1-C2-C3-O3
4	E	407	GOL	O1-C1-C2-C3
4	F	406	GOL	C1-C2-C3-O3
4	G	407	GOL	O1-C1-C2-C3
4	I	404	GOL	C1-C2-C3-O3
4	I	406[A]	GOL	O1-C1-C2-C3
4	I	406[A]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	408	GOL	O1-C1-C2-O2
4	A	408	GOL	O2-C2-C3-O3
4	B	406	GOL	O2-C2-C3-O3
4	C	404	GOL	O1-C1-C2-O2
4	G	406[A]	GOL	O1-C1-C2-O2
4	I	406[A]	GOL	O2-C2-C3-O3
4	I	406[B]	GOL	O2-C2-C3-O3
4	C	405	GOL	O2-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3
4	D	406	GOL	O2-C2-C3-O3
4	G	406[A]	GOL	O2-C2-C3-O3
4	I	406[A]	GOL	O1-C1-C2-O2
4	A	407	GOL	O1-C1-C2-O2
4	I	404	GOL	O2-C2-C3-O3
4	C	407	GOL	C1-C2-C3-O3
4	D	405	GOL	C1-C2-C3-O3
4	H	404	GOL	O1-C1-C2-C3
4	E	405	GOL	C1-C2-C3-O3
4	B	408	GOL	O2-C2-C3-O3
4	E	406	GOL	O1-C1-C2-O2
4	D	405	GOL	O2-C2-C3-O3
4	G	406[A]	GOL	C1-C2-C3-O3
4	C	404	GOL	O2-C2-C3-O3
4	C	407	GOL	O2-C2-C3-O3
4	F	406	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	408	GOL	3	0
4	E	406	GOL	1	0
4	C	405	GOL	2	0
4	J	406	GOL	1	0
4	B	406	GOL	1	0
4	E	405	GOL	1	0
4	B	405	GOL	1	0
4	I	404	GOL	1	0
4	D	405	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	279/311 (89%)	-0.46	5 (1%)	68	64	15, 22, 44, 60	0
1	B	283/311 (90%)	-0.48	6 (2%)	63	59	13, 20, 41, 58	0
1	C	281/311 (90%)	-0.51	8 (2%)	53	47	14, 20, 41, 60	0
1	D	285/311 (91%)	-0.57	3 (1%)	80	78	16, 22, 42, 57	0
1	E	281/311 (90%)	-0.26	17 (6%)	21	17	17, 24, 50, 66	0
1	F	274/311 (88%)	-0.55	4 (1%)	73	70	12, 19, 38, 56	0
1	G	285/311 (91%)	-0.55	6 (2%)	63	59	11, 16, 37, 59	0
1	H	274/311 (88%)	-0.59	3 (1%)	80	78	11, 17, 41, 67	0
1	I	275/311 (88%)	-0.53	3 (1%)	80	78	12, 18, 37, 63	0
1	J	274/311 (88%)	-0.55	3 (1%)	80	78	13, 19, 40, 54	0
All	All	2791/3110 (89%)	-0.51	58 (2%)	63	59	11, 20, 42, 67	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	LEU	5.8
1	H	112	THR	5.8
1	A	40	LEU	5.2
1	E	43	ILE	5.1
1	E	42	ILE	4.7
1	I	112	THR	4.6
1	A	43	ILE	4.2
1	E	109	THR	4.1
1	H	48	ALA	4.1
1	E	188	ALA	3.7
1	E	49	THR	3.5
1	B	190	PRO	3.3
1	I	322	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	48	ALA	3.2
1	B	189	ILE	3.2
1	A	48	ALA	3.0
1	C	112	THR	3.0
1	I	48	ALA	3.0
1	F	189	ILE	3.0
1	B	112	THR	3.0
1	E	39	VAL	3.0
1	C	188	ALA	2.9
1	G	37	VAL	2.9
1	C	48	ALA	2.9
1	G	109	THR	2.9
1	C	42	ILE	2.9
1	E	106	MET	2.9
1	B	322	ASN	2.9
1	D	46	PRO	2.9
1	G	112	THR	2.9
1	H	49	THR	2.8
1	A	42	ILE	2.8
1	D	112	THR	2.8
1	E	187	THR	2.7
1	D	322	ASN	2.7
1	E	189	ILE	2.7
1	C	109	THR	2.7
1	J	189	ILE	2.6
1	A	39	VAL	2.6
1	G	322	ASN	2.6
1	E	38	GLU	2.5
1	E	190	PRO	2.5
1	J	187	THR	2.5
1	E	108	ASN	2.4
1	E	44	THR	2.4
1	C	43	ILE	2.4
1	G	43	ILE	2.4
1	F	106	MET	2.4
1	B	43	ILE	2.3
1	E	113	CYS	2.3
1	C	40	LEU	2.3
1	C	39	VAL	2.2
1	F	109	THR	2.1
1	E	50	THR	2.1
1	B	187	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	190	PRO	2.1
1	F	322	ASN	2.0
1	G	45	GLY	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	BGC	R	1	12/12	0.76	0.29	48,53,56,63	0
3	BGC	L	1	12/12	0.79	0.23	40,50,61,68	0
2	GLC	M	1	12/12	0.81	0.25	42,48,64,65	0
2	GLC	O	1	12/12	0.85	0.20	42,55,60,60	0
3	BGC	T	1	12/12	0.86	0.18	33,41,48,51	0
3	BGC	N	1	12/12	0.90	0.21	38,45,53,69	0
2	GAL	M	2	11/12	0.91	0.09	27,31,37,38	0
3	BGC	Q	1	12/12	0.91	0.21	29,42,57,63	0
2	GLC	K	1	12/12	0.92	0.12	26,30,37,43	0
2	GAL	O	2	11/12	0.92	0.09	24,29,35,36	0
3	GAL	R	2	11/12	0.92	0.10	24,31,37,42	0
3	BGC	S	1	12/12	0.92	0.23	31,39,49,61	0
3	GAL	N	2	11/12	0.92	0.10	24,28,33,33	0
3	SIA	N	3	20/21	0.93	0.07	20,27,31,34	0
2	GLC	P	1	12/12	0.94	0.09	19,28,38,42	0
2	SIA	M	3	20/21	0.94	0.08	17,28,36,37	0
2	SIA	O	3	20/21	0.95	0.08	22,27,31,31	0
3	SIA	R	3	20/21	0.95	0.11	20,29,38,40	0
3	GAL	Q	2	11/12	0.95	0.07	15,21,26,29	0
3	GAL	S	2	11/12	0.95	0.08	17,22,26,30	0
2	GAL	K	2	11/12	0.95	0.07	23,26,29,30	0
3	GAL	L	2	11/12	0.96	0.07	21,25,30,31	0
2	GAL	P	2	11/12	0.96	0.06	16,19,21,24	0
2	SIA	K	3	20/21	0.96	0.07	20,26,33,35	0
3	SIA	T	3	20/21	0.96	0.09	19,24,33,35	0

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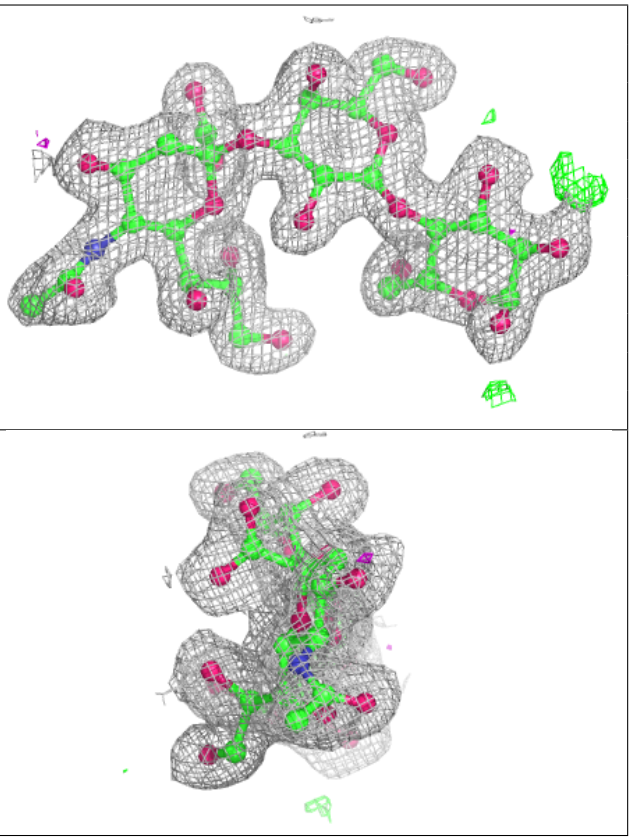
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SIA	S	3	20/21	0.97	0.06	16,20,25,26	0
3	SIA	Q	3	20/21	0.97	0.05	14,17,22,25	0
3	GAL	T	2	11/12	0.97	0.07	24,26,29,29	0
3	SIA	L	3	20/21	0.97	0.09	17,24,28,36	0
2	SIA	P	3	20/21	0.98	0.06	14,20,24,25	0

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.

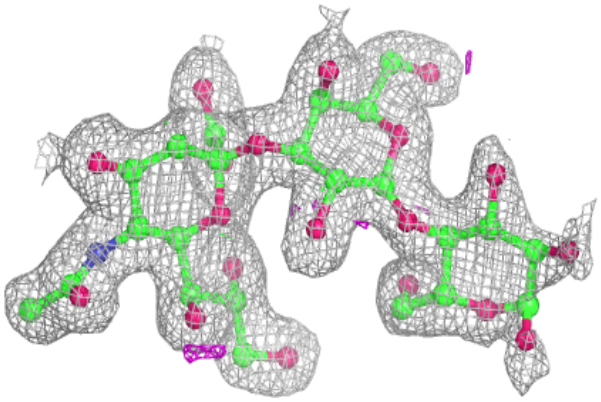
Electron density around Chain K:

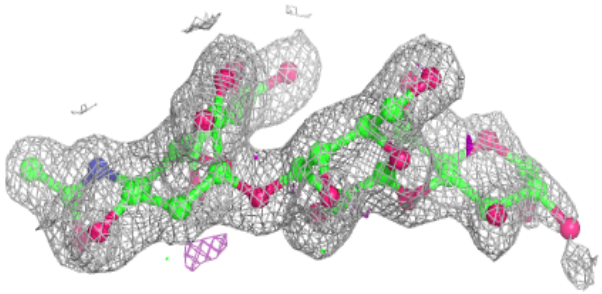
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

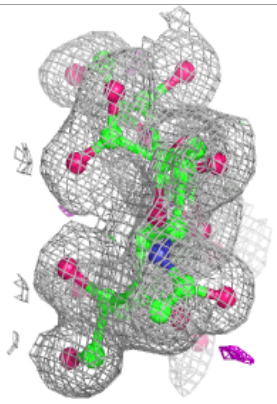


Electron density around Chain M:

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

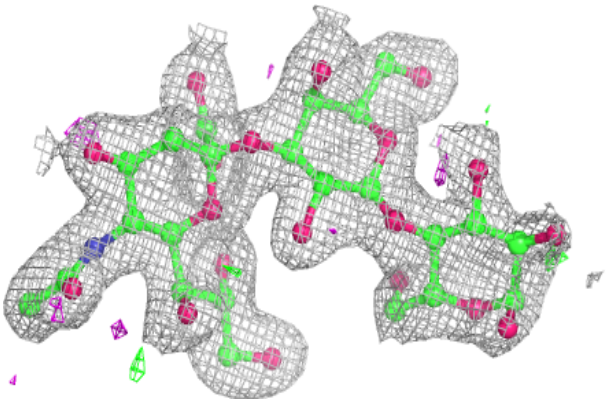


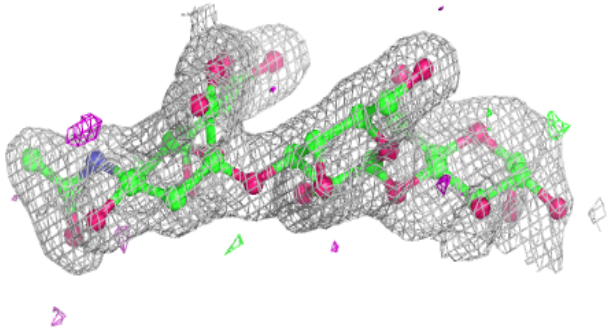


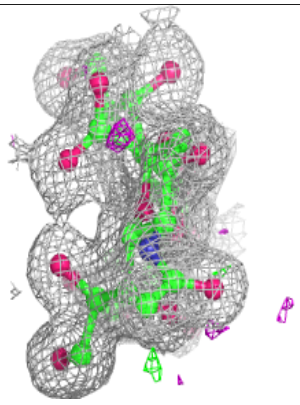


Electron density around Chain O:

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

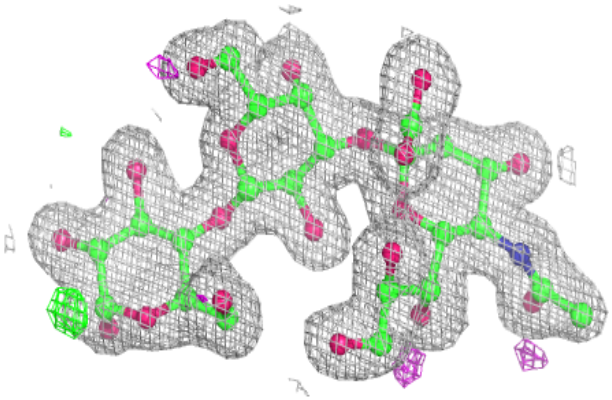


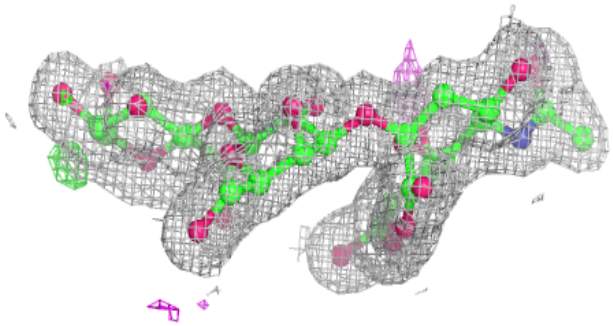


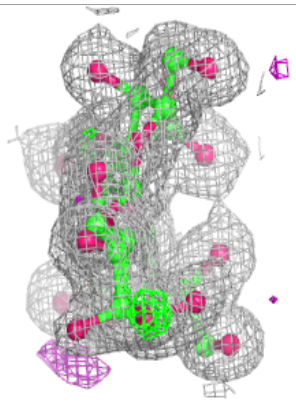


Electron density around Chain P:

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

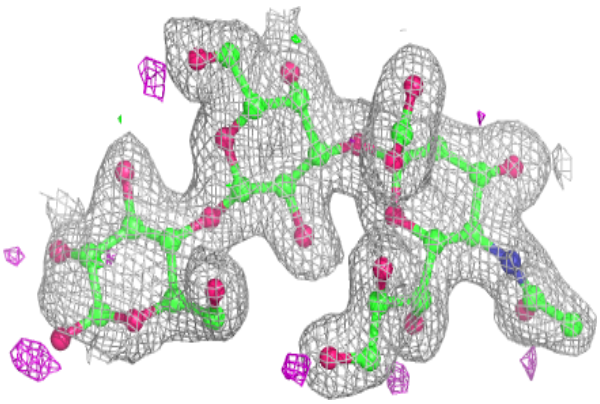


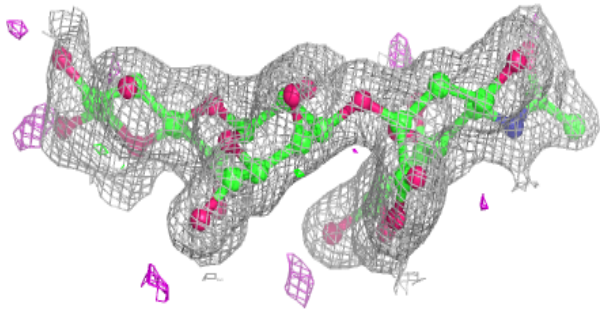


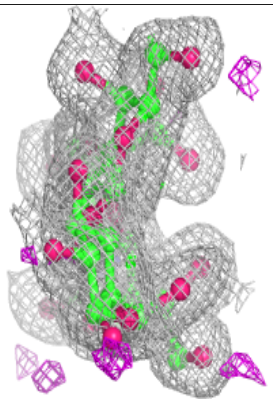


Electron density around Chain L:

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

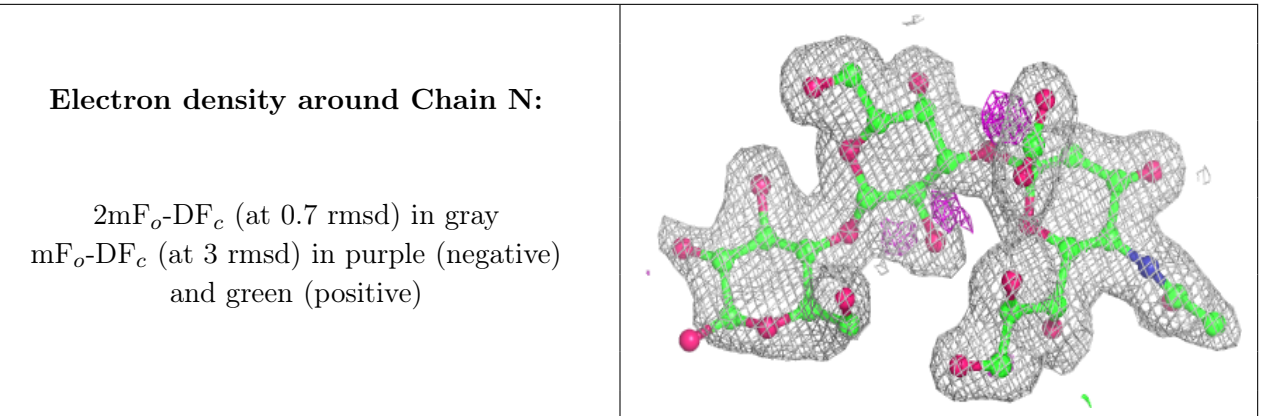


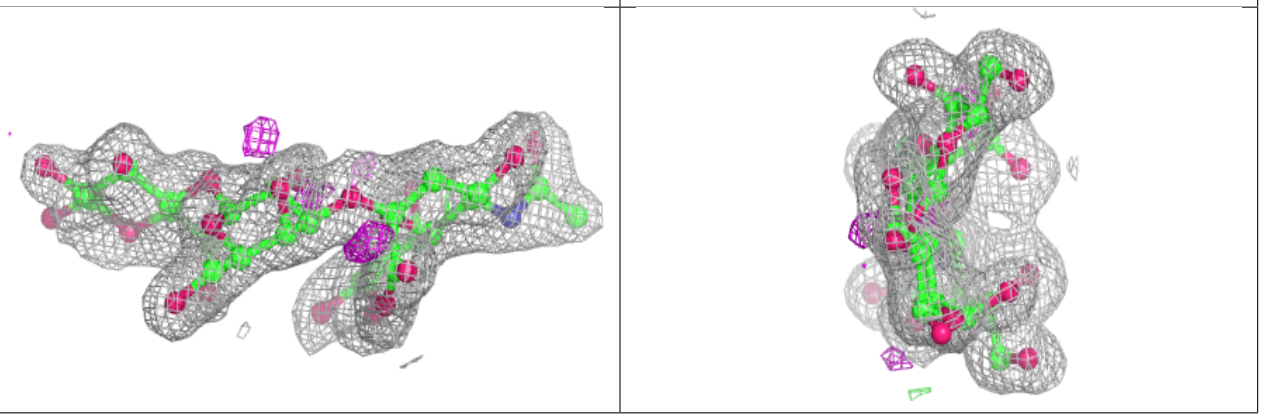




Electron density around Chain N:

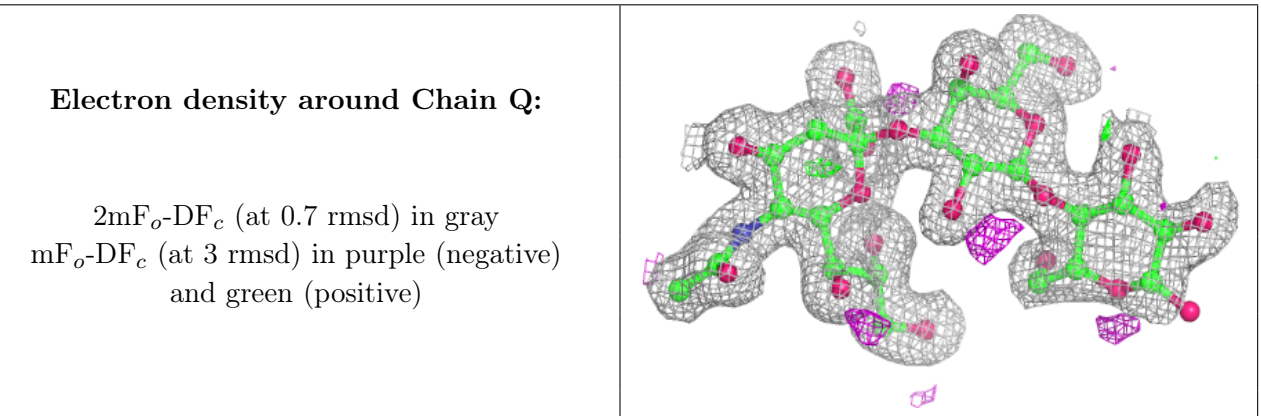
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

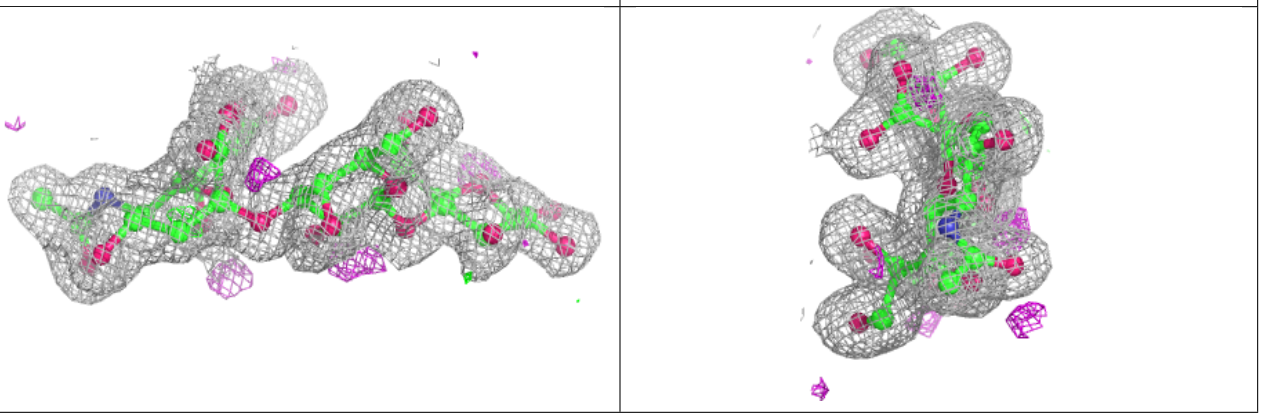




Electron density around Chain Q:

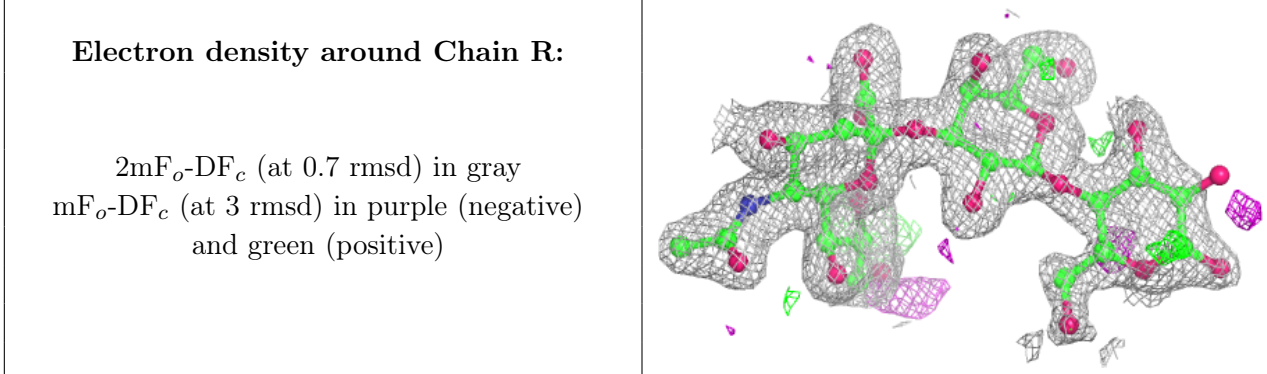
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

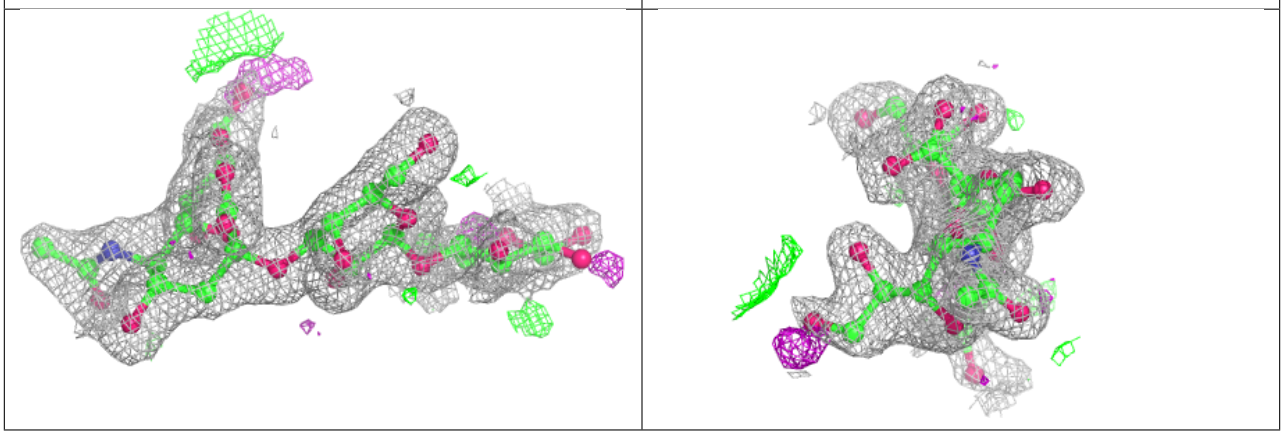




Electron density around Chain R:

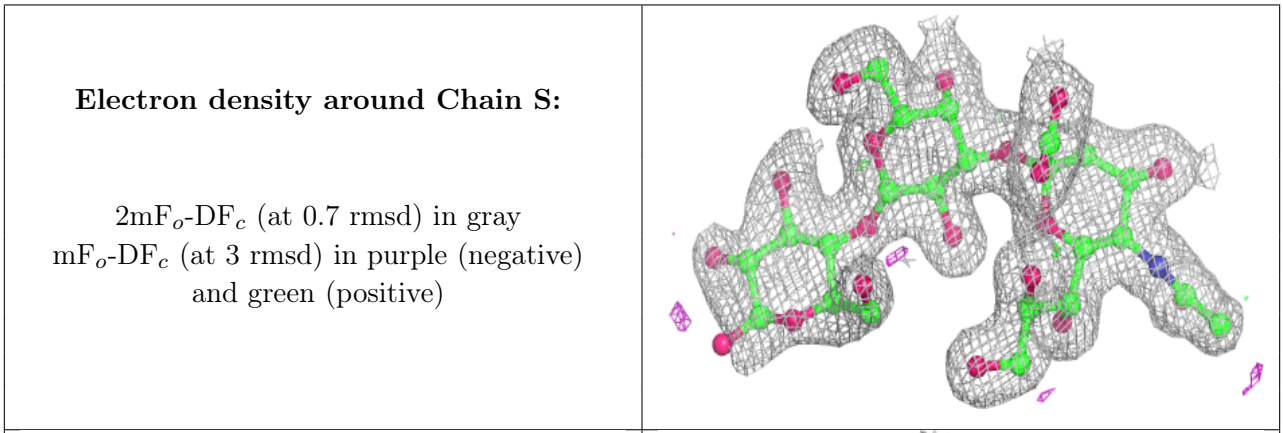
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

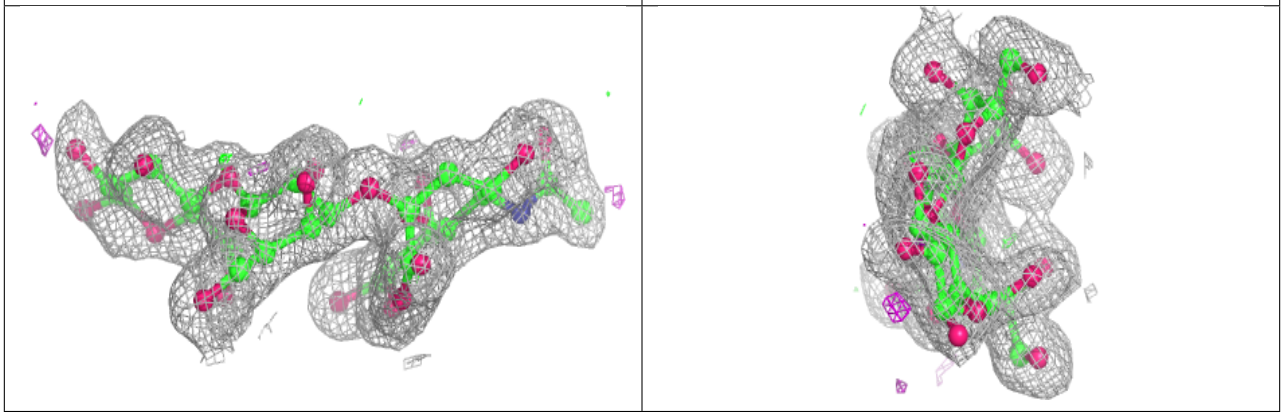


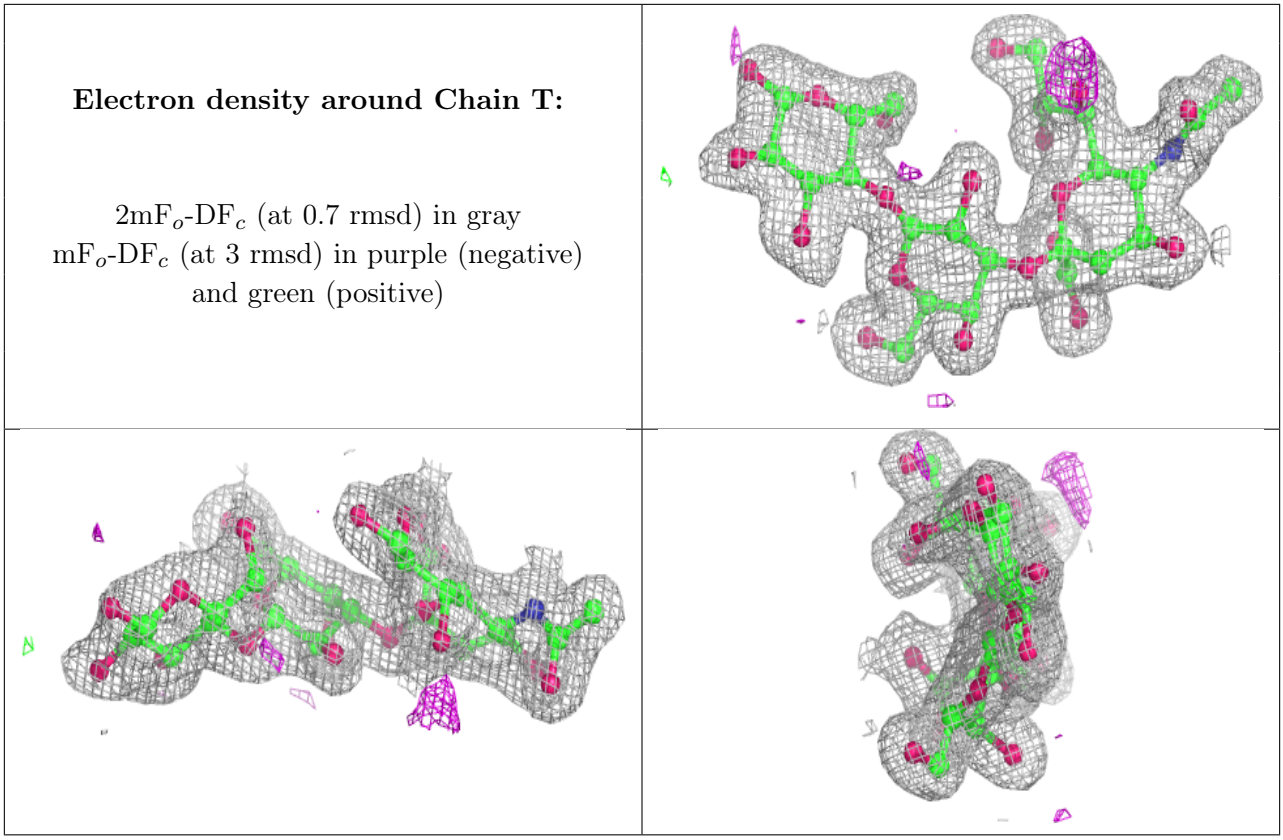


Electron density around Chain S:

$2mF_o$-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
4	GOL	B	408	6/6	0.84	0.31	35,41,44,49	0
4	GOL	C	406	6/6	0.84	0.12	28,31,40,48	0
4	GOL	B	406	6/6	0.85	0.13	25,33,43,44	0
4	GOL	H	405	6/6	0.85	0.13	29,33,37,39	0
4	GOL	D	406	6/6	0.86	0.11	30,32,39,49	0
4	GOL	J	407	6/6	0.87	0.10	32,33,40,42	0
4	GOL	E	406	6/6	0.88	0.10	31,35,44,45	0
4	GOL	C	407	6/6	0.88	0.23	32,37,39,40	0
4	GOL	B	407	6/6	0.88	0.18	29,38,39,49	0
4	GOL	A	407	6/6	0.89	0.11	27,35,43,45	0
4	GOL	I	406[A]	6/6	0.90	0.16	19,23,25,29	6
4	GOL	I	406[B]	6/6	0.90	0.16	21,27,28,31	6
4	GOL	A	405	6/6	0.90	0.12	21,25,37,38	0
4	GOL	E	404	6/6	0.91	0.12	22,24,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	410	1/1	0.91	0.15	48,48,48,48	0
4	GOL	G	407	6/6	0.92	0.23	28,34,38,39	0
4	GOL	G	406[A]	6/6	0.92	0.14	22,23,29,32	6
4	GOL	G	406[B]	6/6	0.92	0.14	22,24,27,31	6
5	MG	F	408	1/1	0.92	0.13	41,41,41,41	0
4	GOL	F	405	6/6	0.93	0.09	28,30,37,40	0
4	GOL	C	405	6/6	0.93	0.11	23,29,31,38	0
4	GOL	B	404	6/6	0.93	0.09	22,28,36,36	0
4	GOL	E	405	6/6	0.93	0.12	26,27,32,37	0
5	MG	D	408	1/1	0.93	0.10	43,43,43,43	0
4	GOL	C	404	6/6	0.93	0.15	18,27,42,46	0
5	MG	I	407	1/1	0.93	0.19	40,40,40,40	0
4	GOL	I	404	6/6	0.94	0.12	17,17,32,39	0
4	GOL	D	407	6/6	0.94	0.10	22,37,38,41	0
4	GOL	A	408	6/6	0.94	0.11	22,35,38,50	0
4	GOL	A	406	6/6	0.94	0.07	25,28,31,34	0
4	GOL	E	407	6/6	0.95	0.10	25,32,41,41	0
4	GOL	I	405	6/6	0.95	0.08	22,27,28,29	0
4	GOL	D	405	6/6	0.95	0.10	28,32,34,35	0
5	MG	F	407	1/1	0.95	0.11	39,39,39,39	0
4	GOL	H	406	6/6	0.95	0.08	19,25,27,28	0
4	GOL	J	405	6/6	0.95	0.10	16,22,31,32	0
4	GOL	J	406	6/6	0.96	0.10	24,28,31,31	0
4	GOL	B	405	6/6	0.96	0.10	23,28,30,33	0
4	GOL	F	404	6/6	0.96	0.09	20,25,29,29	0
5	MG	B	409	1/1	0.96	0.12	36,36,36,36	0
5	MG	D	401	1/1	0.96	0.22	52,52,52,52	0
4	GOL	A	404	6/6	0.96	0.10	24,27,31,34	0
4	GOL	F	406	6/6	0.96	0.08	18,28,35,36	0
4	GOL	J	404	6/6	0.96	0.08	18,22,28,30	0
4	GOL	G	404	6/6	0.96	0.08	15,18,26,29	0
4	GOL	H	404	6/6	0.97	0.06	13,15,20,24	0
4	GOL	G	405	6/6	0.97	0.07	20,22,25,27	0
4	GOL	G	408	6/6	0.97	0.09	16,29,33,34	0
5	MG	G	409	1/1	0.98	0.16	38,38,38,38	0
5	MG	H	407	1/1	0.98	0.23	40,40,40,40	0
5	MG	A	409	1/1	0.98	0.10	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.