Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 01:14 PM EDT

PDB ID	:	6Y64
Title	:	Structure of Sheep Polyomavirus VP1 in complex with 6'-Sialyllactosamine
Authors	:	Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on	:	2020-02-26
Resolution	:	1.60 Å(reported)

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

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

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

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

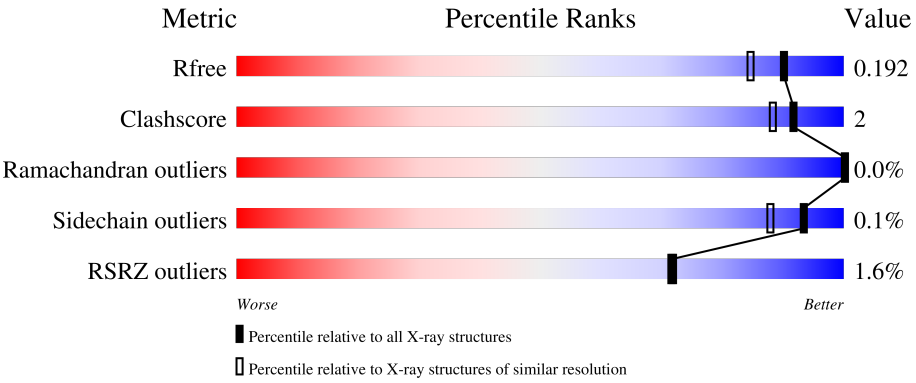
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	293	2% 85% 12%
1	B	293	% 82% 15%
1	C	293	2% 85% 12%
1	D	293	% 82% 15%
1	E	293	86% 12%

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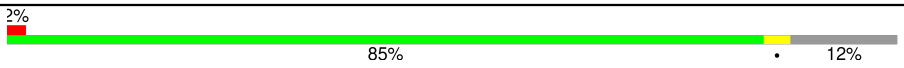
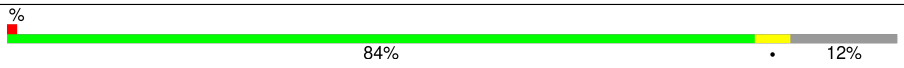
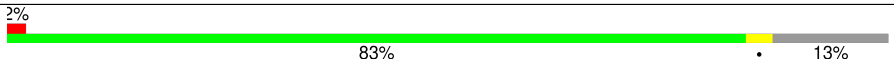
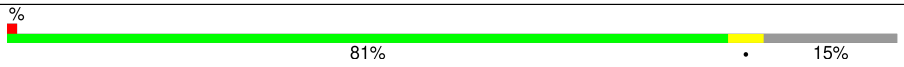
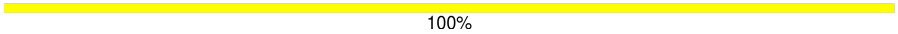
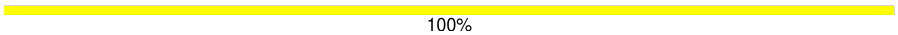
Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	
1	I	293	
1	J	293	
2	K	2	
2	L	2	
2	N	2	
3	M	3	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 22942 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	3	0
			1995	1273	332	375	15			
1	B	250	Total	C	N	O	S	0	2	0
			1950	1247	327	362	14			
1	C	258	Total	C	N	O	S	0	2	0
			1999	1273	332	380	14			
1	D	248	Total	C	N	O	S	0	2	0
			1929	1238	319	359	13			
1	E	258	Total	C	N	O	S	0	4	0
			2012	1282	333	382	15			
1	F	258	Total	C	N	O	S	0	3	0
			2009	1279	333	382	15			
1	G	249	Total	C	N	O	S	0	3	0
			1942	1241	323	365	13			
1	H	257	Total	C	N	O	S	0	3	0
			2006	1279	333	379	15			
1	I	254	Total	C	N	O	S	0	3	0
			1982	1266	328	373	15			
1	J	249	Total	C	N	O	S	0	3	0
			1957	1249	326	368	14			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
A	0	GLY	-	expression tag	UNP A0A0E3ZCF3
A	1	SER	-	expression tag	UNP A0A0E3ZCF3
A	2	SER	-	expression tag	UNP A0A0E3ZCF3
A	3	HIS	-	expression tag	UNP A0A0E3ZCF3
A	4	HIS	-	expression tag	UNP A0A0E3ZCF3
A	5	HIS	-	expression tag	UNP A0A0E3ZCF3
A	6	HIS	-	expression tag	UNP A0A0E3ZCF3
A	7	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP A0A0E3ZCF3
A	9	SER	-	expression tag	UNP A0A0E3ZCF3
A	10	SER	-	expression tag	UNP A0A0E3ZCF3
A	11	GLY	-	expression tag	UNP A0A0E3ZCF3
A	12	LEU	-	expression tag	UNP A0A0E3ZCF3
A	13	VAL	-	expression tag	UNP A0A0E3ZCF3
A	14	PRO	-	expression tag	UNP A0A0E3ZCF3
A	15	ARG	-	expression tag	UNP A0A0E3ZCF3
A	16	GLY	-	expression tag	UNP A0A0E3ZCF3
A	17	SER	-	expression tag	UNP A0A0E3ZCF3
A	18	HIS	-	expression tag	UNP A0A0E3ZCF3
A	19	MET	-	expression tag	UNP A0A0E3ZCF3
A	95	SER	CYS	conflict	UNP A0A0E3ZCF3
B	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
B	0	GLY	-	expression tag	UNP A0A0E3ZCF3
B	1	SER	-	expression tag	UNP A0A0E3ZCF3
B	2	SER	-	expression tag	UNP A0A0E3ZCF3
B	3	HIS	-	expression tag	UNP A0A0E3ZCF3
B	4	HIS	-	expression tag	UNP A0A0E3ZCF3
B	5	HIS	-	expression tag	UNP A0A0E3ZCF3
B	6	HIS	-	expression tag	UNP A0A0E3ZCF3
B	7	HIS	-	expression tag	UNP A0A0E3ZCF3
B	8	HIS	-	expression tag	UNP A0A0E3ZCF3
B	9	SER	-	expression tag	UNP A0A0E3ZCF3
B	10	SER	-	expression tag	UNP A0A0E3ZCF3
B	11	GLY	-	expression tag	UNP A0A0E3ZCF3
B	12	LEU	-	expression tag	UNP A0A0E3ZCF3
B	13	VAL	-	expression tag	UNP A0A0E3ZCF3
B	14	PRO	-	expression tag	UNP A0A0E3ZCF3
B	15	ARG	-	expression tag	UNP A0A0E3ZCF3
B	16	GLY	-	expression tag	UNP A0A0E3ZCF3
B	17	SER	-	expression tag	UNP A0A0E3ZCF3
B	18	HIS	-	expression tag	UNP A0A0E3ZCF3
B	19	MET	-	expression tag	UNP A0A0E3ZCF3
B	95	SER	CYS	conflict	UNP A0A0E3ZCF3
C	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
C	0	GLY	-	expression tag	UNP A0A0E3ZCF3
C	1	SER	-	expression tag	UNP A0A0E3ZCF3
C	2	SER	-	expression tag	UNP A0A0E3ZCF3
C	3	HIS	-	expression tag	UNP A0A0E3ZCF3
C	4	HIS	-	expression tag	UNP A0A0E3ZCF3
C	5	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP A0A0E3ZCF3
C	7	HIS	-	expression tag	UNP A0A0E3ZCF3
C	8	HIS	-	expression tag	UNP A0A0E3ZCF3
C	9	SER	-	expression tag	UNP A0A0E3ZCF3
C	10	SER	-	expression tag	UNP A0A0E3ZCF3
C	11	GLY	-	expression tag	UNP A0A0E3ZCF3
C	12	LEU	-	expression tag	UNP A0A0E3ZCF3
C	13	VAL	-	expression tag	UNP A0A0E3ZCF3
C	14	PRO	-	expression tag	UNP A0A0E3ZCF3
C	15	ARG	-	expression tag	UNP A0A0E3ZCF3
C	16	GLY	-	expression tag	UNP A0A0E3ZCF3
C	17	SER	-	expression tag	UNP A0A0E3ZCF3
C	18	HIS	-	expression tag	UNP A0A0E3ZCF3
C	19	MET	-	expression tag	UNP A0A0E3ZCF3
C	95	SER	CYS	conflict	UNP A0A0E3ZCF3
D	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
D	0	GLY	-	expression tag	UNP A0A0E3ZCF3
D	1	SER	-	expression tag	UNP A0A0E3ZCF3
D	2	SER	-	expression tag	UNP A0A0E3ZCF3
D	3	HIS	-	expression tag	UNP A0A0E3ZCF3
D	4	HIS	-	expression tag	UNP A0A0E3ZCF3
D	5	HIS	-	expression tag	UNP A0A0E3ZCF3
D	6	HIS	-	expression tag	UNP A0A0E3ZCF3
D	7	HIS	-	expression tag	UNP A0A0E3ZCF3
D	8	HIS	-	expression tag	UNP A0A0E3ZCF3
D	9	SER	-	expression tag	UNP A0A0E3ZCF3
D	10	SER	-	expression tag	UNP A0A0E3ZCF3
D	11	GLY	-	expression tag	UNP A0A0E3ZCF3
D	12	LEU	-	expression tag	UNP A0A0E3ZCF3
D	13	VAL	-	expression tag	UNP A0A0E3ZCF3
D	14	PRO	-	expression tag	UNP A0A0E3ZCF3
D	15	ARG	-	expression tag	UNP A0A0E3ZCF3
D	16	GLY	-	expression tag	UNP A0A0E3ZCF3
D	17	SER	-	expression tag	UNP A0A0E3ZCF3
D	18	HIS	-	expression tag	UNP A0A0E3ZCF3
D	19	MET	-	expression tag	UNP A0A0E3ZCF3
D	95	SER	CYS	conflict	UNP A0A0E3ZCF3
E	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
E	0	GLY	-	expression tag	UNP A0A0E3ZCF3
E	1	SER	-	expression tag	UNP A0A0E3ZCF3
E	2	SER	-	expression tag	UNP A0A0E3ZCF3
E	3	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	4	HIS	-	expression tag	UNP A0A0E3ZCF3
E	5	HIS	-	expression tag	UNP A0A0E3ZCF3
E	6	HIS	-	expression tag	UNP A0A0E3ZCF3
E	7	HIS	-	expression tag	UNP A0A0E3ZCF3
E	8	HIS	-	expression tag	UNP A0A0E3ZCF3
E	9	SER	-	expression tag	UNP A0A0E3ZCF3
E	10	SER	-	expression tag	UNP A0A0E3ZCF3
E	11	GLY	-	expression tag	UNP A0A0E3ZCF3
E	12	LEU	-	expression tag	UNP A0A0E3ZCF3
E	13	VAL	-	expression tag	UNP A0A0E3ZCF3
E	14	PRO	-	expression tag	UNP A0A0E3ZCF3
E	15	ARG	-	expression tag	UNP A0A0E3ZCF3
E	16	GLY	-	expression tag	UNP A0A0E3ZCF3
E	17	SER	-	expression tag	UNP A0A0E3ZCF3
E	18	HIS	-	expression tag	UNP A0A0E3ZCF3
E	19	MET	-	expression tag	UNP A0A0E3ZCF3
E	95	SER	CYS	conflict	UNP A0A0E3ZCF3
F	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
F	0	GLY	-	expression tag	UNP A0A0E3ZCF3
F	1	SER	-	expression tag	UNP A0A0E3ZCF3
F	2	SER	-	expression tag	UNP A0A0E3ZCF3
F	3	HIS	-	expression tag	UNP A0A0E3ZCF3
F	4	HIS	-	expression tag	UNP A0A0E3ZCF3
F	5	HIS	-	expression tag	UNP A0A0E3ZCF3
F	6	HIS	-	expression tag	UNP A0A0E3ZCF3
F	7	HIS	-	expression tag	UNP A0A0E3ZCF3
F	8	HIS	-	expression tag	UNP A0A0E3ZCF3
F	9	SER	-	expression tag	UNP A0A0E3ZCF3
F	10	SER	-	expression tag	UNP A0A0E3ZCF3
F	11	GLY	-	expression tag	UNP A0A0E3ZCF3
F	12	LEU	-	expression tag	UNP A0A0E3ZCF3
F	13	VAL	-	expression tag	UNP A0A0E3ZCF3
F	14	PRO	-	expression tag	UNP A0A0E3ZCF3
F	15	ARG	-	expression tag	UNP A0A0E3ZCF3
F	16	GLY	-	expression tag	UNP A0A0E3ZCF3
F	17	SER	-	expression tag	UNP A0A0E3ZCF3
F	18	HIS	-	expression tag	UNP A0A0E3ZCF3
F	19	MET	-	expression tag	UNP A0A0E3ZCF3
F	95	SER	CYS	conflict	UNP A0A0E3ZCF3
G	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
G	0	GLY	-	expression tag	UNP A0A0E3ZCF3
G	1	SER	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	SER	-	expression tag	UNP A0A0E3ZCF3
G	3	HIS	-	expression tag	UNP A0A0E3ZCF3
G	4	HIS	-	expression tag	UNP A0A0E3ZCF3
G	5	HIS	-	expression tag	UNP A0A0E3ZCF3
G	6	HIS	-	expression tag	UNP A0A0E3ZCF3
G	7	HIS	-	expression tag	UNP A0A0E3ZCF3
G	8	HIS	-	expression tag	UNP A0A0E3ZCF3
G	9	SER	-	expression tag	UNP A0A0E3ZCF3
G	10	SER	-	expression tag	UNP A0A0E3ZCF3
G	11	GLY	-	expression tag	UNP A0A0E3ZCF3
G	12	LEU	-	expression tag	UNP A0A0E3ZCF3
G	13	VAL	-	expression tag	UNP A0A0E3ZCF3
G	14	PRO	-	expression tag	UNP A0A0E3ZCF3
G	15	ARG	-	expression tag	UNP A0A0E3ZCF3
G	16	GLY	-	expression tag	UNP A0A0E3ZCF3
G	17	SER	-	expression tag	UNP A0A0E3ZCF3
G	18	HIS	-	expression tag	UNP A0A0E3ZCF3
G	19	MET	-	expression tag	UNP A0A0E3ZCF3
G	95	SER	CYS	conflict	UNP A0A0E3ZCF3
H	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
H	0	GLY	-	expression tag	UNP A0A0E3ZCF3
H	1	SER	-	expression tag	UNP A0A0E3ZCF3
H	2	SER	-	expression tag	UNP A0A0E3ZCF3
H	3	HIS	-	expression tag	UNP A0A0E3ZCF3
H	4	HIS	-	expression tag	UNP A0A0E3ZCF3
H	5	HIS	-	expression tag	UNP A0A0E3ZCF3
H	6	HIS	-	expression tag	UNP A0A0E3ZCF3
H	7	HIS	-	expression tag	UNP A0A0E3ZCF3
H	8	HIS	-	expression tag	UNP A0A0E3ZCF3
H	9	SER	-	expression tag	UNP A0A0E3ZCF3
H	10	SER	-	expression tag	UNP A0A0E3ZCF3
H	11	GLY	-	expression tag	UNP A0A0E3ZCF3
H	12	LEU	-	expression tag	UNP A0A0E3ZCF3
H	13	VAL	-	expression tag	UNP A0A0E3ZCF3
H	14	PRO	-	expression tag	UNP A0A0E3ZCF3
H	15	ARG	-	expression tag	UNP A0A0E3ZCF3
H	16	GLY	-	expression tag	UNP A0A0E3ZCF3
H	17	SER	-	expression tag	UNP A0A0E3ZCF3
H	18	HIS	-	expression tag	UNP A0A0E3ZCF3
H	19	MET	-	expression tag	UNP A0A0E3ZCF3
H	95	SER	CYS	conflict	UNP A0A0E3ZCF3
I	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	expression tag	UNP A0A0E3ZCF3
I	1	SER	-	expression tag	UNP A0A0E3ZCF3
I	2	SER	-	expression tag	UNP A0A0E3ZCF3
I	3	HIS	-	expression tag	UNP A0A0E3ZCF3
I	4	HIS	-	expression tag	UNP A0A0E3ZCF3
I	5	HIS	-	expression tag	UNP A0A0E3ZCF3
I	6	HIS	-	expression tag	UNP A0A0E3ZCF3
I	7	HIS	-	expression tag	UNP A0A0E3ZCF3
I	8	HIS	-	expression tag	UNP A0A0E3ZCF3
I	9	SER	-	expression tag	UNP A0A0E3ZCF3
I	10	SER	-	expression tag	UNP A0A0E3ZCF3
I	11	GLY	-	expression tag	UNP A0A0E3ZCF3
I	12	LEU	-	expression tag	UNP A0A0E3ZCF3
I	13	VAL	-	expression tag	UNP A0A0E3ZCF3
I	14	PRO	-	expression tag	UNP A0A0E3ZCF3
I	15	ARG	-	expression tag	UNP A0A0E3ZCF3
I	16	GLY	-	expression tag	UNP A0A0E3ZCF3
I	17	SER	-	expression tag	UNP A0A0E3ZCF3
I	18	HIS	-	expression tag	UNP A0A0E3ZCF3
I	19	MET	-	expression tag	UNP A0A0E3ZCF3
I	95	SER	CYS	conflict	UNP A0A0E3ZCF3
J	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
J	0	GLY	-	expression tag	UNP A0A0E3ZCF3
J	1	SER	-	expression tag	UNP A0A0E3ZCF3
J	2	SER	-	expression tag	UNP A0A0E3ZCF3
J	3	HIS	-	expression tag	UNP A0A0E3ZCF3
J	4	HIS	-	expression tag	UNP A0A0E3ZCF3
J	5	HIS	-	expression tag	UNP A0A0E3ZCF3
J	6	HIS	-	expression tag	UNP A0A0E3ZCF3
J	7	HIS	-	expression tag	UNP A0A0E3ZCF3
J	8	HIS	-	expression tag	UNP A0A0E3ZCF3
J	9	SER	-	expression tag	UNP A0A0E3ZCF3
J	10	SER	-	expression tag	UNP A0A0E3ZCF3
J	11	GLY	-	expression tag	UNP A0A0E3ZCF3
J	12	LEU	-	expression tag	UNP A0A0E3ZCF3
J	13	VAL	-	expression tag	UNP A0A0E3ZCF3
J	14	PRO	-	expression tag	UNP A0A0E3ZCF3
J	15	ARG	-	expression tag	UNP A0A0E3ZCF3
J	16	GLY	-	expression tag	UNP A0A0E3ZCF3
J	17	SER	-	expression tag	UNP A0A0E3ZCF3
J	18	HIS	-	expression tag	UNP A0A0E3ZCF3
J	19	MET	-	expression tag	UNP A0A0E3ZCF3

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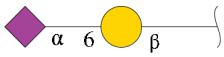
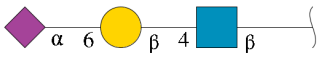
Chain	Residue	Modelled	Actual	Comment	Reference
J	95	SER	CYS	conflict	UNP A0A0E3ZCF3

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



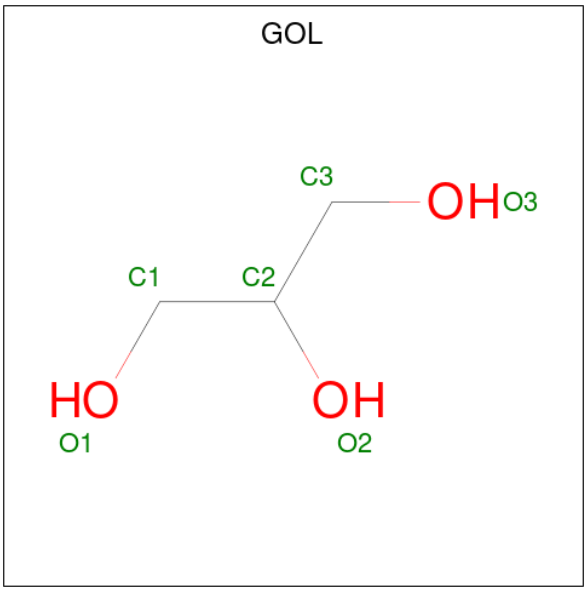
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	L	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	N	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- 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	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	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	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	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	1
			12	6	6		

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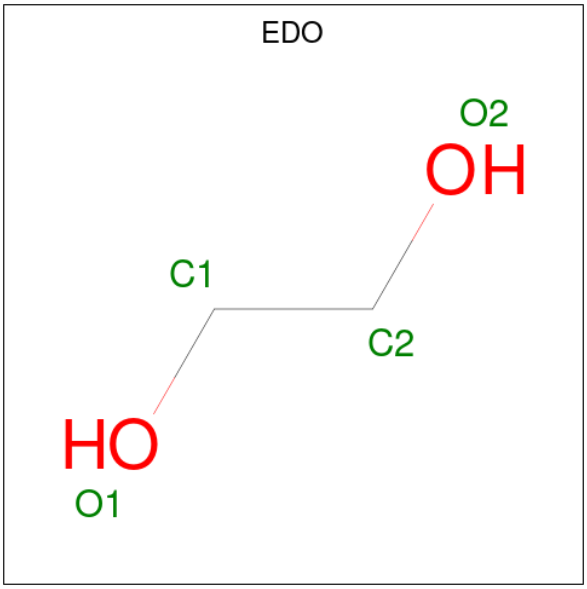
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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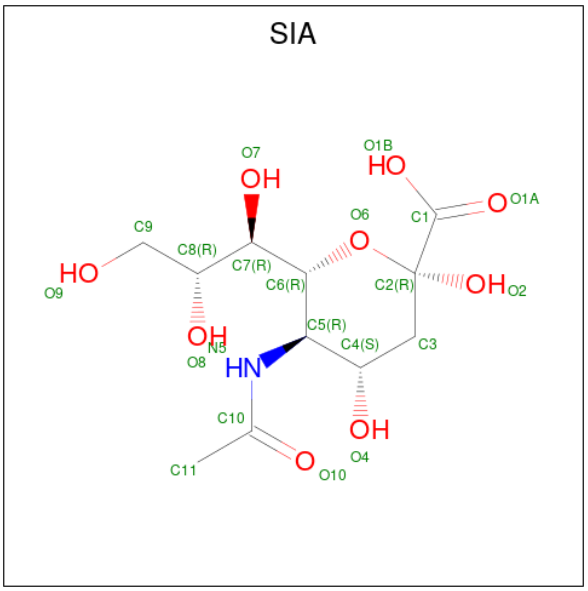
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	I	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	B	1	Total Mg 1 1	0	0
6	C	2	Total Mg 2 2	0	0
6	D	1	Total Mg 1 1	0	0
6	F	3	Total Mg 3 3	0	0
6	G	1	Total Mg 1 1	0	0
6	H	2	Total Mg 2 2	0	0
6	I	2	Total Mg 2 2	0	0

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 21 11 1 9	0	0
7	C	1	Total C N O 21 11 1 9	0	0

- Molecule 8 is water.

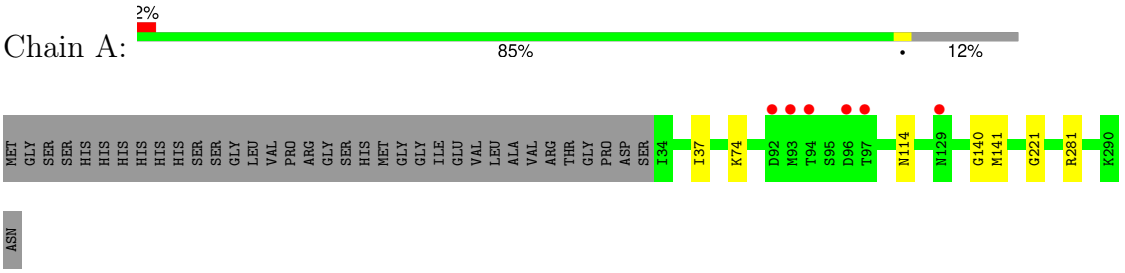
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	273	Total O 277 277	0	4
8	B	280	Total O 281 281	0	1
8	C	273	Total O 275 275	0	2
8	D	270	Total O 273 273	0	3
8	E	270	Total O 275 275	0	5
8	F	244	Total O 248 248	0	4
8	G	275	Total O 279 279	0	4
8	H	292	Total O 293 293	0	1
8	I	291	Total O 299 299	0	8
8	J	285	Total O 289 289	0	4

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.

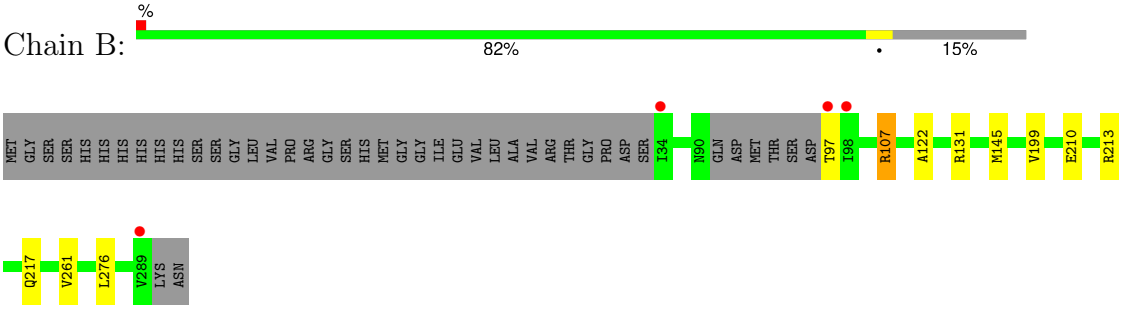
• Molecule 1: Capsid protein VP1

Chain A:



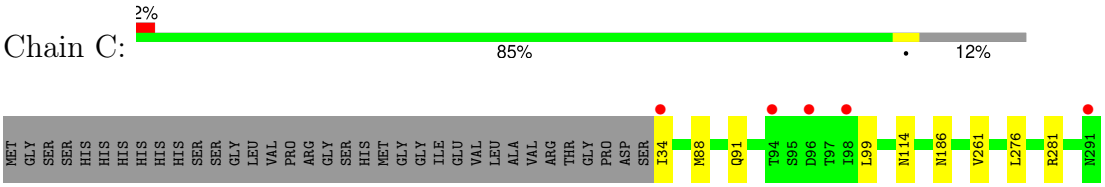
• Molecule 1: Capsid protein VP1

Chain B:



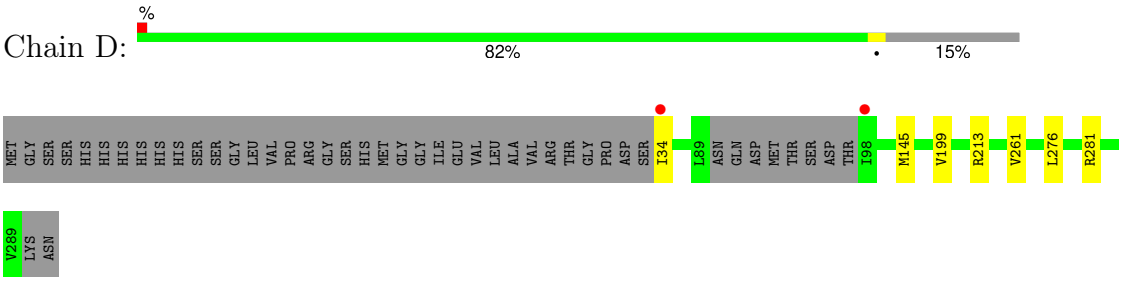
• Molecule 1: Capsid protein VP1

Chain C:



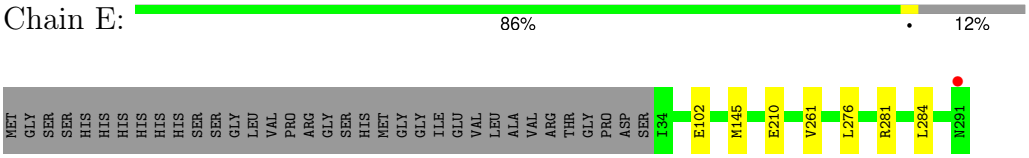
• Molecule 1: Capsid protein VP1

Chain D:



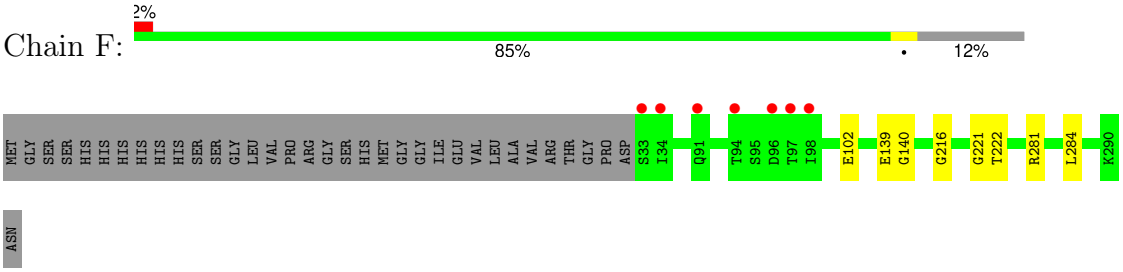
• Molecule 1: Capsid protein VP1

Chain E:



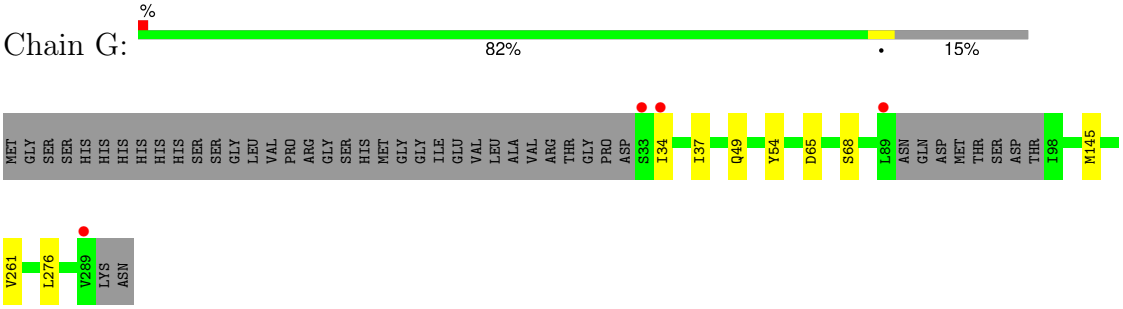
• Molecule 1: Capsid protein VP1

Chain F:



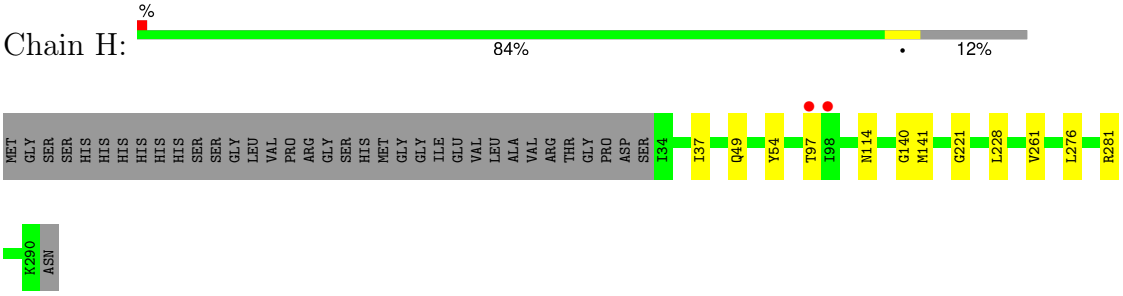
• Molecule 1: Capsid protein VP1

Chain G:



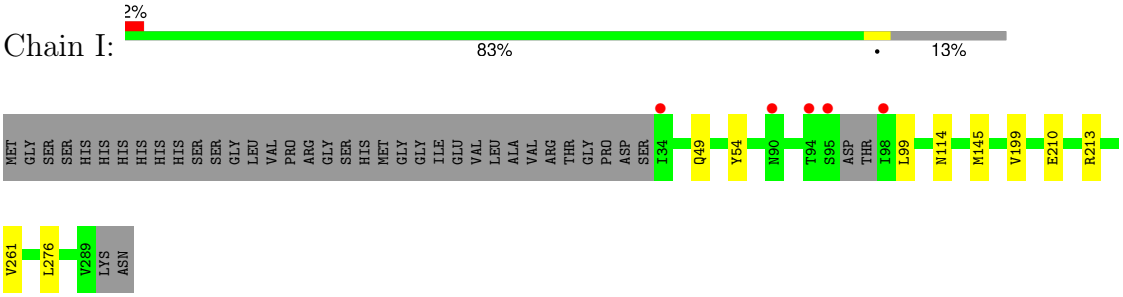
• Molecule 1: Capsid protein VP1

Chain H:



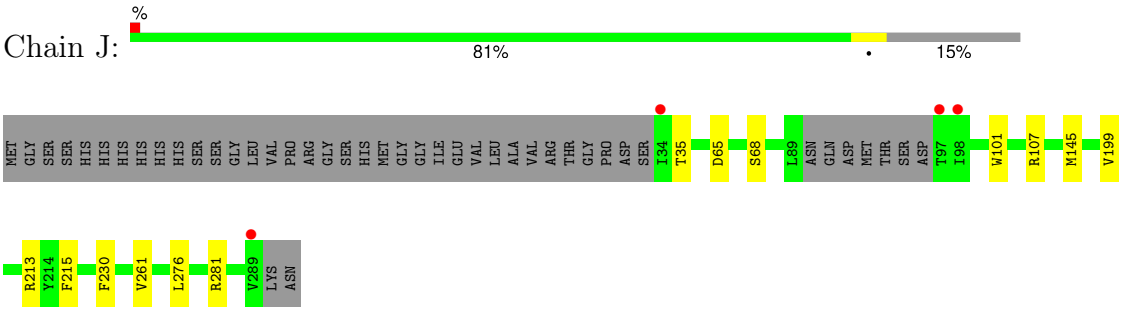
• Molecule 1: Capsid protein VP1

Chain I:



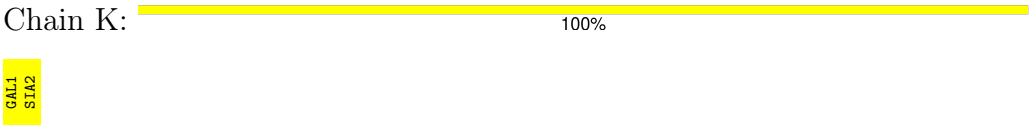
• Molecule 1: Capsid protein VP1

Chain J:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain K:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

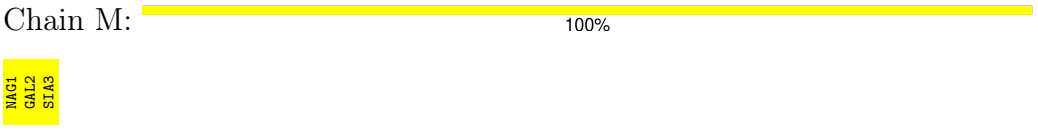
Chain L:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain N:

• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	129.62Å 81.26Å 146.66Å 90.00° 115.52° 90.00°	Depositor
Resolution (Å)	47.47 – 1.60 47.47 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.47-1.60) 96.8 (47.47-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.152 , 0.182 0.163 , 0.192	Depositor DCC
R_{free} test set	3503 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22942	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 20.21 % 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 9.1322e-03.*

[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: SIA, GOL, EDO, GAL, NAG, 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	0.64	0/2047	0.82	0/2782
1	B	0.64	0/2004	0.82	2/2723 (0.1%)
1	C	0.64	0/2057	0.79	1/2799 (0.0%)
1	D	0.63	0/1983	0.81	1/2695 (0.0%)
1	E	0.64	0/2070	0.83	0/2815
1	F	0.63	0/2064	0.81	0/2807
1	G	0.66	0/1996	0.78	0/2713
1	H	0.66	0/2061	0.82	0/2801
1	I	0.64	0/2039	0.83	1/2770 (0.0%)
1	J	0.65	0/2011	0.81	1/2732 (0.0%)
All	All	0.64	0/20332	0.81	6/27637 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	213	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	107	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	C	186	ASN	CB-CA-C	5.49	121.39	110.40
1	I	213	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	213	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	213	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1995	0	1889	6	0
1	B	1950	0	1877	10	0
1	C	1999	0	1903	8	0
1	D	1929	0	1846	5	0
1	E	2012	0	1915	5	0
1	F	2009	0	1908	5	0
1	G	1942	0	1850	5	0
1	H	2006	0	1917	10	0
1	I	1982	0	1898	8	0
1	J	1957	0	1875	10	0
2	K	32	0	28	0	0
2	L	32	0	28	0	0
2	N	32	0	28	0	0
3	M	46	0	40	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	D	12	0	16	0	0
4	E	12	0	16	0	0
4	F	6	0	8	0	0
4	G	12	0	16	0	0
4	H	30	0	40	1	0
4	I	30	0	40	0	0
4	J	6	0	8	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	8	0	12	1	0
5	D	4	0	6	0	0
5	E	8	0	12	0	0
5	F	4	0	6	0	0
5	G	4	0	6	0	0
5	H	4	0	6	0	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3	0	0	0	0
6	G	1	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
7	B	21	0	18	0	0
7	C	21	0	18	0	0
8	A	277	0	0	3	0
8	B	281	0	0	2	0
8	C	275	0	0	4	0
8	D	273	0	0	3	0
8	E	275	0	0	1	0
8	F	248	0	0	2	0
8	G	279	0	0	0	0
8	H	293	0	0	1	0
8	I	299	0	0	1	0
8	J	289	0	0	1	0
All	All	22942	0	19278	64	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 (64) 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:F:281:ARG:NH2	8:F:501:HOH:O	2.01	0.94
1:H:281:ARG:NH1	8:H:501:HOH:O	2.02	0.92
1:C:281:ARG:NH1	8:C:501:HOH:O	2.06	0.89
1:A:281:ARG:NH2	8:A:601:HOH:O	2.05	0.88
5:C:402:EDO:H22	8:C:738:HOH:O	1.74	0.86
1:D:281:ARG:NH2	8:D:501:HOH:O	2.20	0.73
1:J:281:ARG:NH2	8:J:501:HOH:O	2.23	0.71
1:C:99:LEU:HD13	1:H:97:THR:HG21	1.79	0.64
1:C:99:LEU:CD1	1:H:97:THR:HG21	2.31	0.61
1:I:210:GLU:CG	8:I:742:HOH:O	2.49	0.60
1:H:49:GLN:HG2	1:H:54:TYR:CZ	2.37	0.60
1:B:97:THR:HG21	1:I:99:LEU:HD21	1.84	0.58
1:E:281:ARG:NH2	8:E:501:HOH:O	2.36	0.58
1:B:131:ARG:NE	8:B:501:HOH:O	2.36	0.58
8:A:754:HOH:O	1:B:210:GLU:HG3	2.04	0.58
1:B:217:GLN:CG	8:B:740:HOH:O	2.52	0.57
1:H:140:GLY:HA2	1:H:221[A]:GLY:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261[B]:VAL:HG21	1:D:276:LEU:HG	1.90	0.54
1:J:65[B]:ASP:OD1	1:J:68:SER:N	2.42	0.52
1:B:261[B]:VAL:HG21	1:B:276:LEU:HG	1.93	0.50
1:A:140:GLY:HA2	1:A:221[A]:GLY:O	2.12	0.50
1:A:74:LYS:NZ	8:A:607:HOH:O	2.44	0.49
1:E:261[B]:VAL:HG21	1:E:276:LEU:HG	1.95	0.48
1:G:261[A]:VAL:HG21	1:G:276:LEU:HG	1.93	0.48
1:D:145[A]:MET:C	1:D:145[A]:MET:SD	2.92	0.48
1:D:34:ILE:N	8:D:505:HOH:O	2.47	0.48
1:C:91:GLN:OE1	1:C:91:GLN:HA	2.13	0.48
1:H:37:ILE:C	1:H:37:ILE:HD12	2.33	0.48
1:J:35:THR:HG22	1:J:101:TRP:CZ3	2.49	0.47
1:B:145[A]:MET:C	1:B:145[A]:MET:SD	2.93	0.47
1:H:228:LEU:HA	4:H:404[B]:GOL:H32	1.97	0.46
1:B:107:ARG:HH11	1:B:107:ARG:HB3	1.79	0.46
1:G:65[B]:ASP:OD1	1:G:68:SER:OG	2.29	0.45
1:E:145[A]:MET:SD	1:E:145[A]:MET:C	2.95	0.45
1:A:37:ILE:HD12	1:A:37:ILE:C	2.38	0.45
1:C:88:MET:HG2	8:C:560:HOH:O	2.17	0.45
1:I:261[B]:VAL:HG21	1:I:276:LEU:HG	2.00	0.44
1:A:141:MET:O	1:A:141:MET:HG3	2.18	0.44
1:J:145[A]:MET:C	1:J:145[A]:MET:SD	2.96	0.43
1:E:102:GLU:O	1:E:284:LEU:HA	2.18	0.43
1:G:145[A]:MET:C	1:G:145[A]:MET:SD	2.97	0.43
1:J:145[A]:MET:HA	1:J:215:PHE:O	2.18	0.43
1:G:37:ILE:C	1:G:37:ILE:HD12	2.39	0.43
1:J:261[A]:VAL:HG11	1:J:276:LEU:HD12	2.01	0.43
1:F:139:GLU:HG3	8:F:655:HOH:O	2.18	0.43
1:H:261[B]:VAL:HG21	1:H:276:LEU:HG	2.01	0.43
1:H:114:ASN:HB2	1:I:199:VAL:O	2.19	0.42
1:I:145[A]:MET:SD	1:I:145[A]:MET:C	2.97	0.42
1:J:261[B]:VAL:HG21	1:J:276:LEU:HG	2.01	0.42
1:F:216:GLY:HA3	1:J:230:PHE:CZ	2.54	0.42
1:C:34:ILE:N	8:C:709[B]:HOH:O	2.52	0.42
1:C:114:ASN:HB2	1:D:199:VAL:O	2.19	0.42
1:H:141:MET:O	1:H:141:MET:HG3	2.20	0.42
8:D:649:HOH:O	1:E:210:GLU:HG3	2.19	0.42
1:G:49:GLN:HG2	1:G:54:TYR:CZ	2.54	0.42
1:I:49:GLN:HG2	1:I:54:TYR:CZ	2.55	0.42
1:C:261[B]:VAL:HG21	1:C:276:LEU:HG	2.02	0.41
1:B:261[A]:VAL:HG11	1:B:276:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:HB2	1:B:199:VAL:O	2.21	0.41
1:F:102:GLU:O	1:F:284:LEU:HA	2.20	0.41
1:B:97:THR:HG21	1:I:99:LEU:CD2	2.51	0.41
1:F:140:GLY:HA2	1:F:221[A]:GLY:O	2.21	0.41
1:I:114:ASN:HB2	1:J:199:VAL:O	2.20	0.40
1:J:107:ARG:HH11	1:J:107:ARG:HB3	1.85	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	258/293 (88%)	247 (96%)	11 (4%)	0	100	100
1	B	248/293 (85%)	238 (96%)	9 (4%)	1 (0%)	34	15
1	C	258/293 (88%)	248 (96%)	10 (4%)	0	100	100
1	D	246/293 (84%)	238 (97%)	8 (3%)	0	100	100
1	E	260/293 (89%)	249 (96%)	11 (4%)	0	100	100
1	F	259/293 (88%)	248 (96%)	11 (4%)	0	100	100
1	G	248/293 (85%)	240 (97%)	8 (3%)	0	100	100
1	H	258/293 (88%)	249 (96%)	9 (4%)	0	100	100
1	I	253/293 (86%)	243 (96%)	10 (4%)	0	100	100
1	J	248/293 (85%)	239 (96%)	9 (4%)	0	100	100
All	All	2536/2930 (87%)	2439 (96%)	96 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	ALA

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	208/249 (84%)	208 (100%)	0	100 100
1	B	208/249 (84%)	208 (100%)	0	100 100
1	C	214/249 (86%)	214 (100%)	0	100 100
1	D	203/249 (82%)	203 (100%)	0	100 100
1	E	215/249 (86%)	215 (100%)	0	100 100
1	F	214/249 (86%)	213 (100%)	1 (0%)	88 80
1	G	206/249 (83%)	205 (100%)	1 (0%)	88 80
1	H	214/249 (86%)	214 (100%)	0	100 100
1	I	212/249 (85%)	212 (100%)	0	100 100
1	J	210/249 (84%)	210 (100%)	0	100 100
All	All	2104/2490 (84%)	2102 (100%)	2 (0%)	93 88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	222	THR
1	G	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	266	GLN
1	B	175	ASN
1	C	266	GLN
1	D	266	GLN
1	E	266	GLN
1	G	266	GLN
1	H	266	GLN
1	I	186	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

9 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	K	1	2	12,12,12	0.62	0	17,17,17	1.26	1 (5%)
2	SIA	K	2	2	20,20,21	0.74	0	21,28,31	1.61	5 (23%)
2	GAL	L	1	2	12,12,12	0.68	0	17,17,17	0.69	0
2	SIA	L	2	2	20,20,21	0.80	1 (5%)	21,28,31	1.05	1 (4%)
3	NAG	M	1	3	15,15,15	0.46	0	21,21,21	1.14	3 (14%)
3	GAL	M	2	3	11,11,12	0.42	0	15,15,17	1.14	1 (6%)
3	SIA	M	3	3	20,20,21	0.75	0	21,28,31	1.38	4 (19%)
2	GAL	N	1	2	12,12,12	0.57	0	17,17,17	0.85	0
2	SIA	N	2	2	20,20,21	0.63	0	21,28,31	1.41	2 (9%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3	-	1/6/26/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	0/18/34/38	0/1/1/1
2	GAL	N	1	2	-	0/2/22/22	0/1/1/1
2	SIA	N	2	2	-	0/18/34/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	SIA	O1B-C1	-2.01	1.24	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1	GAL	C1-O5-C5	-4.08	105.76	113.65
2	N	2	SIA	O6-C2-C1	3.48	114.30	107.72
3	M	2	GAL	C1-O5-C5	3.41	116.76	112.19
2	K	2	SIA	O10-C10-N5	3.35	127.90	121.98
2	K	2	SIA	C11-C10-N5	-3.34	110.57	116.12
3	M	3	SIA	C8-C7-C6	-3.17	107.09	113.05
2	K	2	SIA	O1B-C1-C2	2.98	120.45	112.71
2	N	2	SIA	O4-C4-C3	-2.96	102.50	109.86
2	K	2	SIA	O1A-C1-C2	-2.74	116.94	122.85
3	M	3	SIA	O10-C10-N5	2.49	126.38	121.98
3	M	3	SIA	C6-C5-N5	-2.49	106.94	110.91
3	M	1	NAG	C1-C2-C3	-2.41	107.26	110.54
2	K	2	SIA	O6-C2-C1	2.33	112.12	107.72
3	M	1	NAG	O5-C1-C2	-2.27	107.23	109.52
3	M	3	SIA	O9-C9-C8	-2.22	106.49	111.16
2	L	2	SIA	O1B-C1-C2	2.02	117.97	112.71
3	M	1	NAG	C1-C2-N2	2.01	113.06	110.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

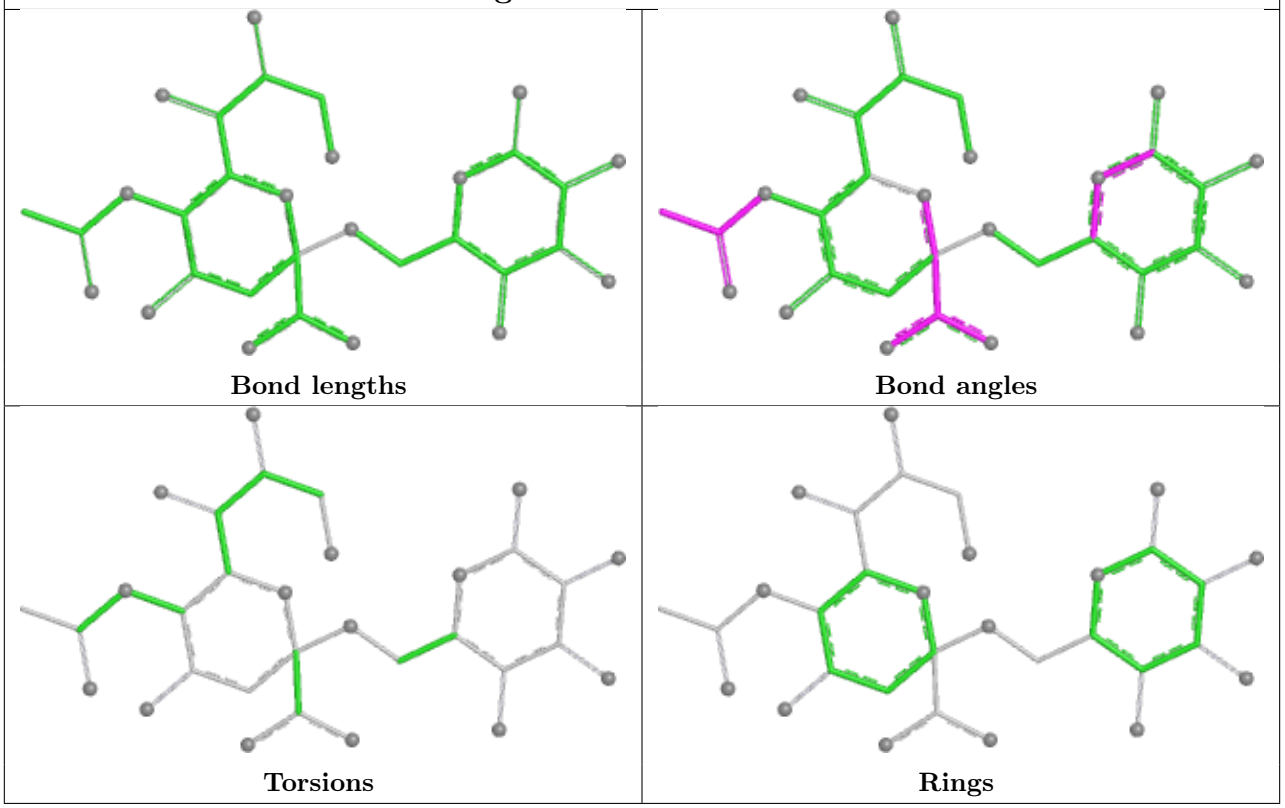
Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O5-C5-C6-O6

There are no ring outliers.

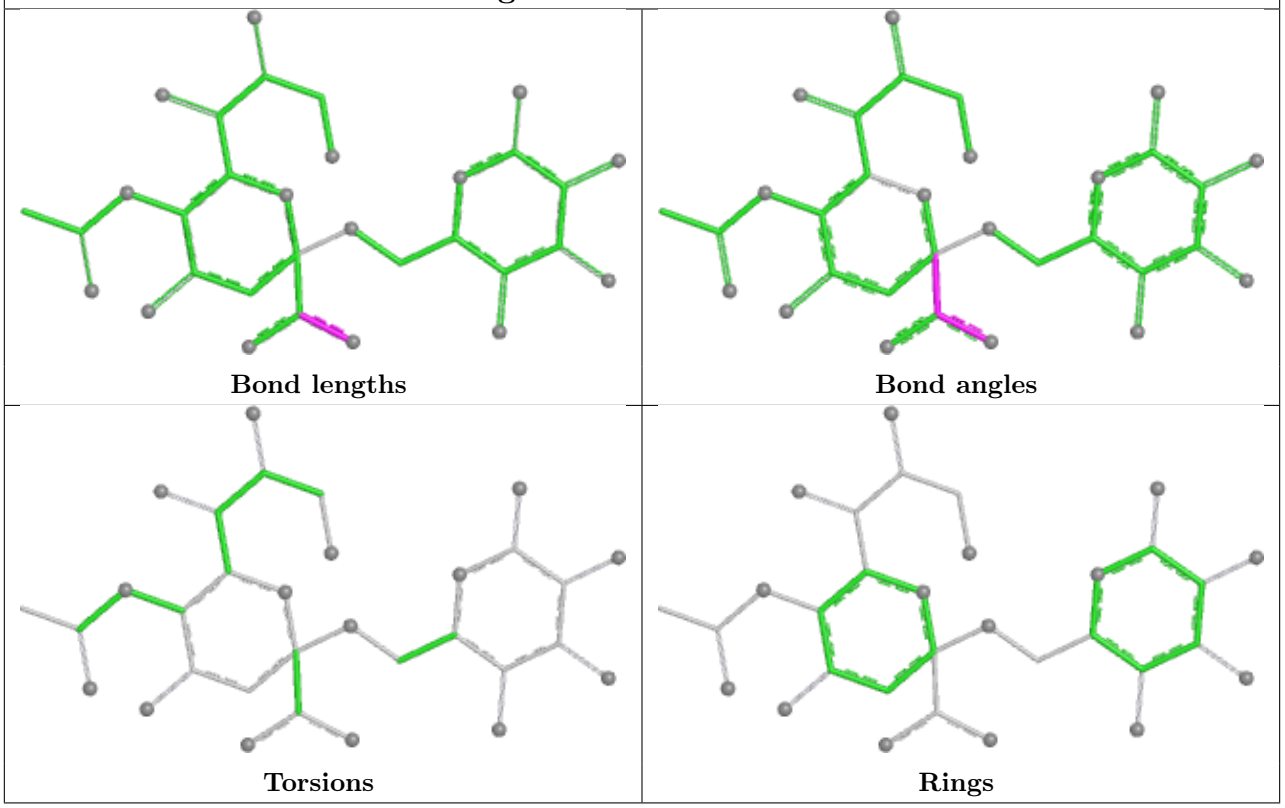
No monomer is involved in short contacts.

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

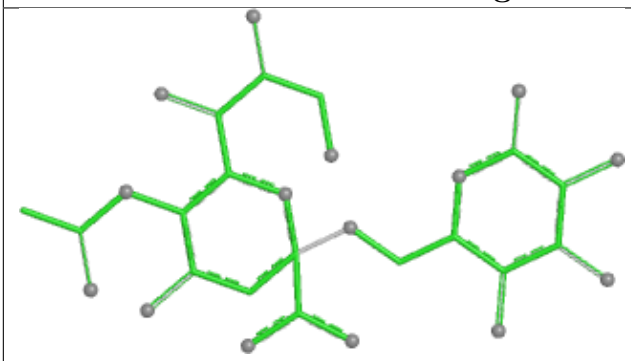
Oligosaccharide Chain K



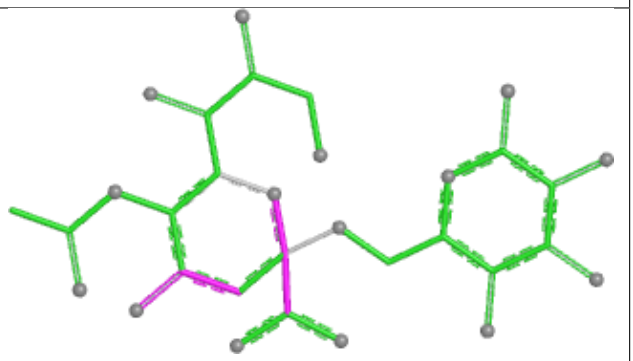
Oligosaccharide Chain L



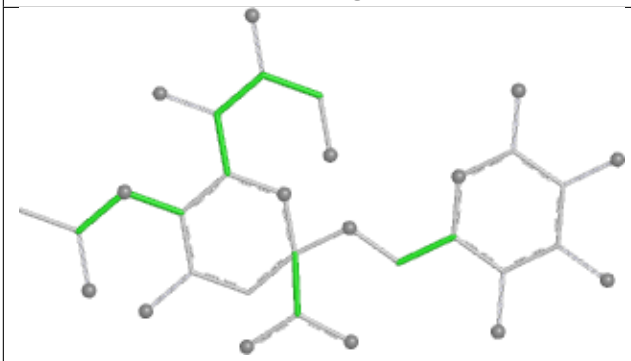
Oligosaccharide Chain N



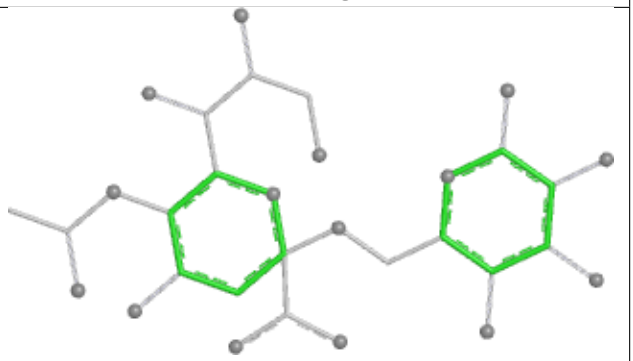
Bond lengths



Bond angles

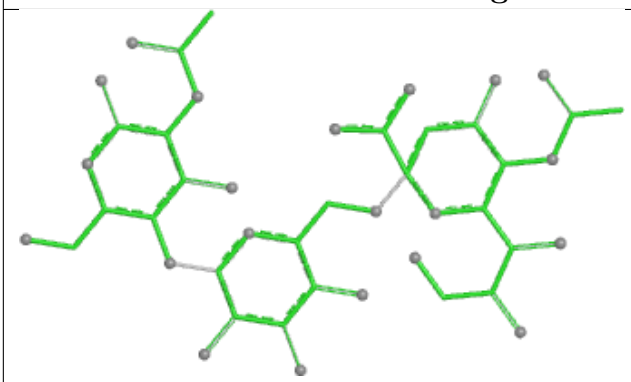


Torsions

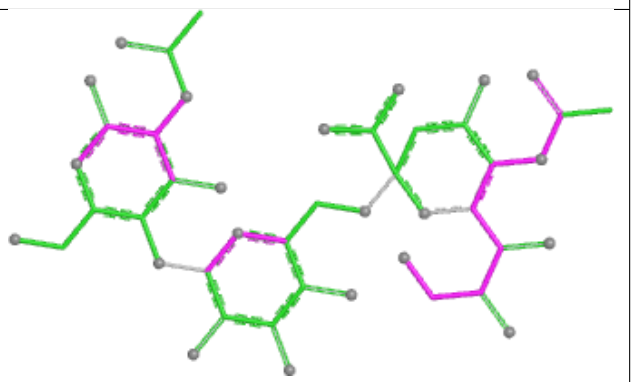


Rings

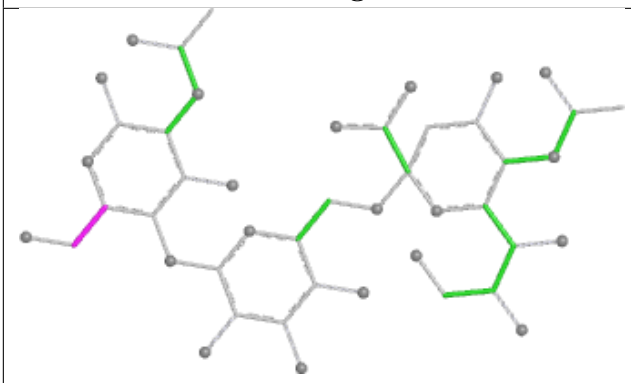
Oligosaccharide Chain M



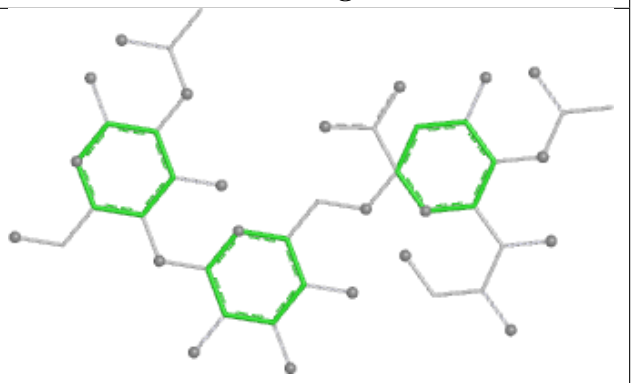
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 14 are monoatomic - leaving 35 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	E	402	-	5,5,5	0.08	0	5,5,5	0.24	0
7	SIA	B	401	-	21,21,21	1.15	1 (4%)	24,31,31	1.52	6 (25%)
4	GOL	I	403	-	5,5,5	0.20	0	5,5,5	0.43	0
4	GOL	H	404[A]	-	5,5,5	0.10	0	5,5,5	0.22	0
4	GOL	F	403	-	5,5,5	0.16	0	5,5,5	0.36	0
4	GOL	E	401	-	5,5,5	0.10	0	5,5,5	0.22	0
5	EDO	G	406	-	3,3,3	0.12	0	2,2,2	0.25	0
4	GOL	G	404	-	5,5,5	0.10	0	5,5,5	0.34	0
4	GOL	G	405	-	5,5,5	0.11	0	5,5,5	0.27	0
4	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.25	0
4	GOL	H	402	-	5,5,5	0.16	0	5,5,5	0.34	0
4	GOL	I	405	-	5,5,5	0.17	0	5,5,5	0.40	0
4	GOL	H	401	-	5,5,5	0.10	0	5,5,5	0.40	0
4	GOL	D	404	-	5,5,5	0.12	0	5,5,5	0.33	0
5	EDO	A	503	-	3,3,3	0.16	0	2,2,2	0.25	0
4	GOL	H	404[B]	-	5,5,5	0.09	0	5,5,5	0.26	0
5	EDO	E	404	-	3,3,3	0.13	0	2,2,2	0.13	0
4	GOL	B	402	-	5,5,5	0.13	0	5,5,5	0.38	0
5	EDO	E	403	-	3,3,3	0.15	0	2,2,2	0.32	0
4	GOL	J	403	-	5,5,5	0.13	0	5,5,5	0.34	0
4	GOL	A	501	-	5,5,5	0.06	0	5,5,5	0.18	0
4	GOL	D	403	-	5,5,5	0.13	0	5,5,5	0.36	0
5	EDO	I	406	-	3,3,3	0.24	0	2,2,2	0.34	0
4	GOL	H	403	-	5,5,5	0.12	0	5,5,5	0.29	0
5	EDO	H	405	-	3,3,3	0.15	0	2,2,2	0.27	0
4	GOL	I	402	-	5,5,5	0.17	0	5,5,5	0.29	0
5	EDO	F	404	-	3,3,3	0.14	0	2,2,2	0.26	0
4	GOL	I	401	-	5,5,5	0.14	0	5,5,5	0.33	0
5	EDO	B	403	-	3,3,3	0.11	0	2,2,2	0.19	0
5	EDO	C	402	-	3,3,3	0.23	0	2,2,2	0.33	0
4	GOL	I	404	-	5,5,5	0.15	0	5,5,5	0.35	0
7	SIA	C	401	-	21,21,21	1.09	1 (4%)	24,31,31	1.18	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	C	403	-	3,3,3	0.19	0	2,2,2	0.33	0
5	EDO	D	405	-	3,3,3	0.07	0	2,2,2	0.26	0
5	EDO	J	404	-	3,3,3	0.14	0	2,2,2	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	402	-	-	0/4/4/4	-
7	SIA	B	401	-	-	3/20/38/38	0/1/1/1
4	GOL	I	403	-	-	0/4/4/4	-
4	GOL	H	404[A]	-	-	2/4/4/4	-
4	GOL	F	403	-	-	2/4/4/4	-
4	GOL	E	401	-	-	0/4/4/4	-
5	EDO	G	406	-	-	1/1/1/1	-
4	GOL	G	404	-	-	2/4/4/4	-
4	GOL	G	405	-	-	0/4/4/4	-
4	GOL	A	502	-	-	4/4/4/4	-
4	GOL	H	402	-	-	0/4/4/4	-
4	GOL	I	405	-	-	2/4/4/4	-
4	GOL	H	401	-	-	0/4/4/4	-
4	GOL	D	404	-	-	2/4/4/4	-
5	EDO	A	503	-	-	1/1/1/1	-
4	GOL	H	404[B]	-	-	2/4/4/4	-
5	EDO	E	404	-	-	0/1/1/1	-
4	GOL	B	402	-	-	2/4/4/4	-
5	EDO	E	403	-	-	1/1/1/1	-
4	GOL	J	403	-	-	0/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	D	403	-	-	0/4/4/4	-
5	EDO	I	406	-	-	1/1/1/1	-
4	GOL	H	403	-	-	2/4/4/4	-
5	EDO	H	405	-	-	1/1/1/1	-
4	GOL	I	402	-	-	0/4/4/4	-
5	EDO	F	404	-	-	1/1/1/1	-
4	GOL	I	401	-	-	0/4/4/4	-
5	EDO	B	403	-	-	1/1/1/1	-
5	EDO	C	402	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	I	404	-	-	2/4/4/4	-
7	SIA	C	401	-	-	1/20/38/38	0/1/1/1
5	EDO	C	403	-	-	1/1/1/1	-
5	EDO	D	405	-	-	1/1/1/1	-
5	EDO	J	404	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	SIA	O2-C2	3.70	1.44	1.39
7	C	401	SIA	O2-C2	3.38	1.44	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	401	SIA	O1A-C1-C2	-3.71	117.65	123.85
7	B	401	SIA	O1A-C1-C2	-3.35	118.26	123.85
7	B	401	SIA	O2-C2-C3	-2.24	106.05	109.44
7	B	401	SIA	C11-C10-N5	-2.21	112.45	116.12
7	B	401	SIA	O4-C4-C3	-2.21	104.84	109.97
7	B	401	SIA	C3-C4-C5	2.07	112.91	109.72
7	B	401	SIA	O10-C10-N5	2.06	125.62	121.98

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	O1-C1-C2-C3
4	H	404[B]	GOL	C1-C2-C3-O3
5	F	404	EDO	O1-C1-C2-O2
4	A	502	GOL	C1-C2-C3-O3
4	D	404	GOL	C1-C2-C3-O3
4	F	403	GOL	C1-C2-C3-O3
4	G	404	GOL	C1-C2-C3-O3
4	H	403	GOL	C1-C2-C3-O3
4	H	404[A]	GOL	C1-C2-C3-O3
4	I	404	GOL	O1-C1-C2-C3
4	A	502	GOL	O1-C1-C2-O2
4	G	404	GOL	O2-C2-C3-O3
4	H	404[B]	GOL	O2-C2-C3-O3
5	C	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	405	EDO	O1-C1-C2-O2
5	E	403	EDO	O1-C1-C2-O2
5	G	406	EDO	O1-C1-C2-O2
5	H	405	EDO	O1-C1-C2-O2
5	J	404	EDO	O1-C1-C2-O2
5	A	503	EDO	O1-C1-C2-O2
7	B	401	SIA	O8-C8-C9-O9
4	H	404[A]	GOL	O2-C2-C3-O3
7	B	401	SIA	C7-C8-C9-O9
5	I	406	EDO	O1-C1-C2-O2
5	B	403	EDO	O1-C1-C2-O2
4	I	404	GOL	O1-C1-C2-O2
4	A	502	GOL	O2-C2-C3-O3
4	F	403	GOL	O2-C2-C3-O3
4	B	402	GOL	C1-C2-C3-O3
4	I	405	GOL	C1-C2-C3-O3
4	D	404	GOL	O2-C2-C3-O3
4	I	405	GOL	O2-C2-C3-O3
7	B	401	SIA	O1B-C1-C2-O6
4	H	403	GOL	O2-C2-C3-O3
7	C	401	SIA	O1B-C1-C2-C3
4	B	402	GOL	O2-C2-C3-O3

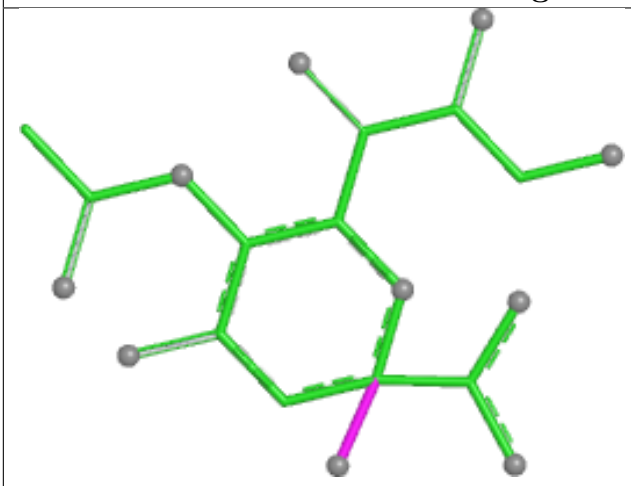
There are no ring outliers.

2 monomers are involved in 2 short contacts:

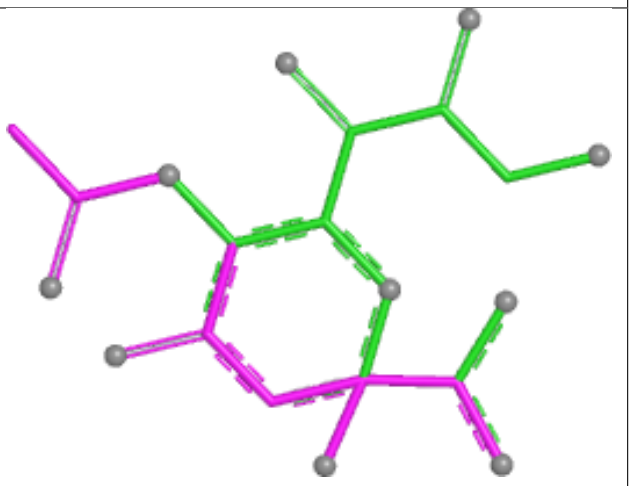
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	404[B]	GOL	1	0
5	C	402	EDO	1	0

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.

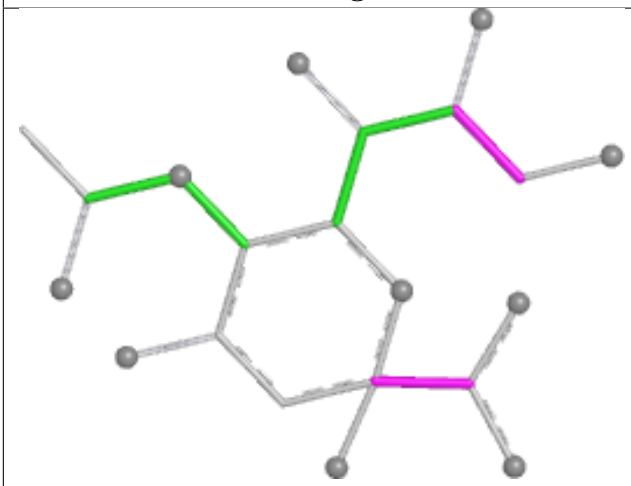
Ligand SIA B 401



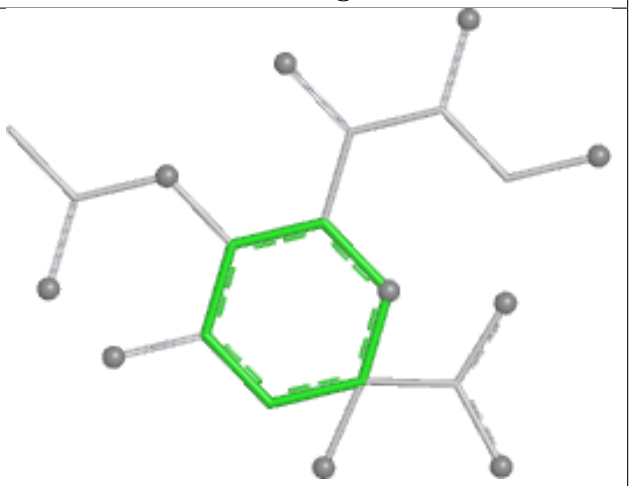
Bond lengths



Bond angles

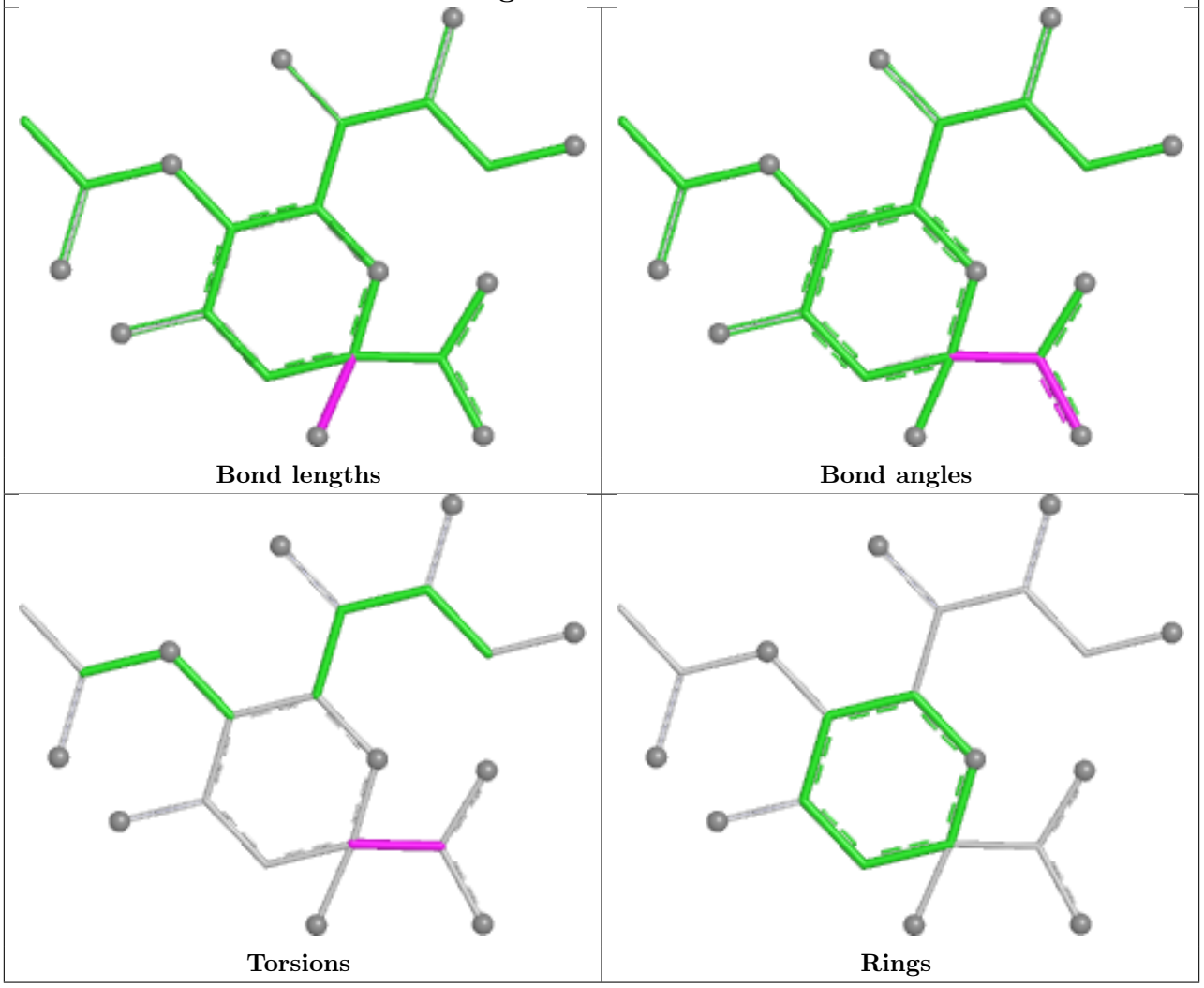


Torsions



Rings

Ligand SIA C 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	257/293 (87%)	-0.36	6 (2%)	60	59	11, 17, 37, 61	0
1	B	250/293 (85%)	-0.38	4 (1%)	72	71	11, 17, 30, 50	0
1	C	258/293 (88%)	-0.37	5 (1%)	66	65	13, 19, 37, 58	0
1	D	248/293 (84%)	-0.44	2 (0%)	86	86	12, 17, 31, 41	0
1	E	258/293 (88%)	-0.43	1 (0%)	92	92	12, 18, 33, 42	0
1	F	258/293 (88%)	-0.33	7 (2%)	54	52	13, 19, 39, 51	0
1	G	249/293 (84%)	-0.42	4 (1%)	72	71	11, 16, 31, 44	0
1	H	257/293 (87%)	-0.54	2 (0%)	86	86	11, 15, 30, 42	0
1	I	254/293 (86%)	-0.42	5 (1%)	65	64	10, 15, 33, 45	0
1	J	249/293 (84%)	-0.39	4 (1%)	72	71	11, 16, 35, 59	0
All	All	2538/2930 (86%)	-0.41	40 (1%)	72	71	10, 17, 34, 61	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	97	THR	4.5
1	A	94	THR	4.0
1	I	94	THR	3.9
1	C	94	THR	3.9
1	I	98	ILE	3.7
1	F	96	ASP	3.6
1	C	291	ASN	3.4
1	I	34	ILE	3.4
1	B	97	THR	3.1
1	F	94	THR	3.1
1	G	34	ILE	3.0
1	I	95	SER	3.0
1	A	129	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	34	ILE	2.9
1	A	93	MET	2.8
1	A	97	THR	2.8
1	C	98	ILE	2.8
1	B	289	VAL	2.8
1	B	34	ILE	2.8
1	I	90	ASN	2.8
1	A	92	ASP	2.7
1	F	34	ILE	2.7
1	A	96	ASP	2.6
1	H	98	ILE	2.6
1	J	34	ILE	2.6
1	D	98	ILE	2.5
1	G	33	SER	2.5
1	E	291	ASN	2.5
1	F	33	SER	2.3
1	C	96	ASP	2.3
1	F	98	ILE	2.3
1	J	289	VAL	2.2
1	B	98	ILE	2.2
1	D	34	ILE	2.2
1	H	97	THR	2.2
1	J	98	ILE	2.1
1	G	289	VAL	2.1
1	F	91	GLN	2.1
1	G	89	LEU	2.0
1	F	97	THR	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
2	GAL	L	1	12/12	0.77	0.25	41,50,51,53	0

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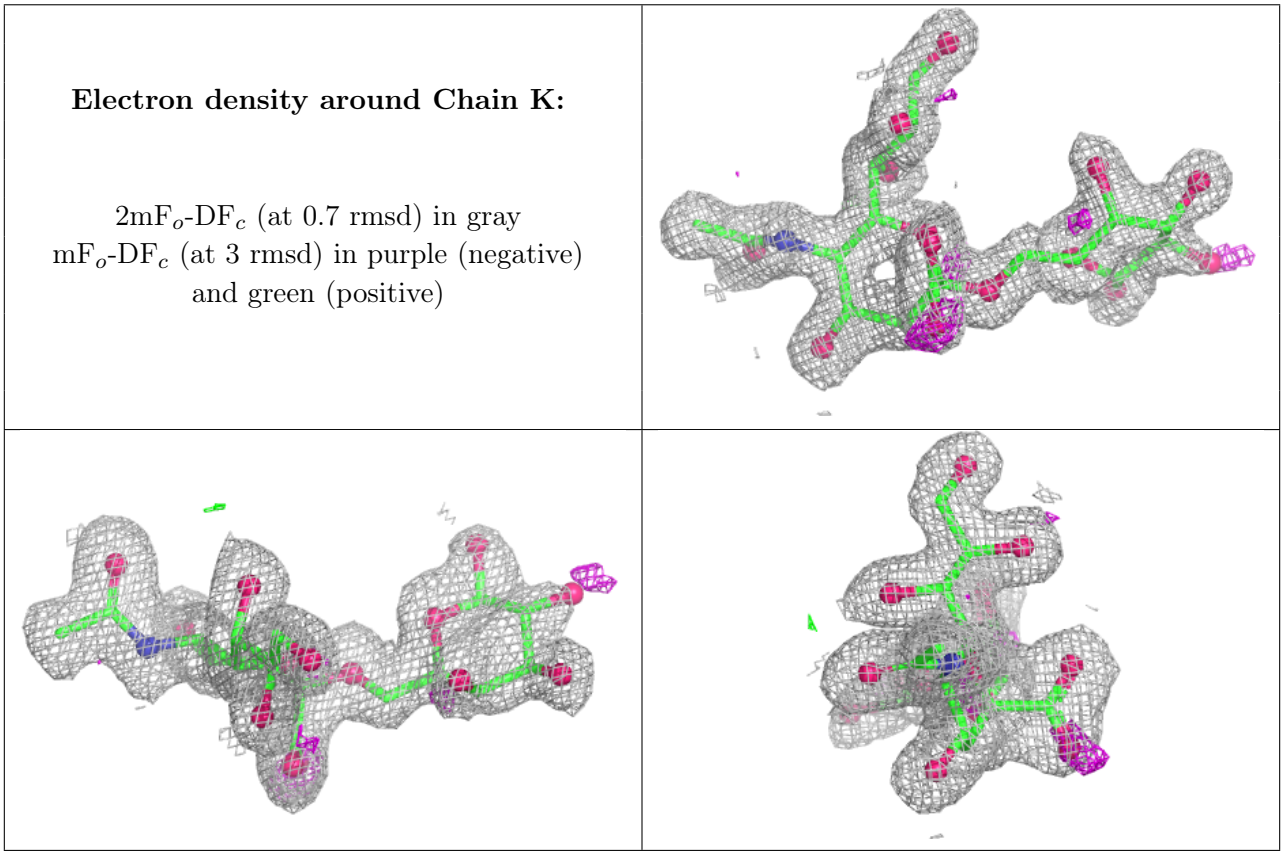
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	K	1	12/12	0.81	0.27	32,42,47,48	0
2	GAL	N	1	12/12	0.81	0.30	32,41,44,45	0
3	NAG	M	1	15/15	0.85	0.28	42,44,48,50	0
3	GAL	M	2	11/12	0.86	0.27	29,40,44,44	0
2	SIA	L	2	20/21	0.87	0.15	24,32,38,39	0
3	SIA	M	3	20/21	0.91	0.17	17,23,31,31	0
2	SIA	N	2	20/21	0.92	0.14	18,25,32,34	0
2	SIA	K	2	20/21	0.92	0.15	20,25,31,32	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.

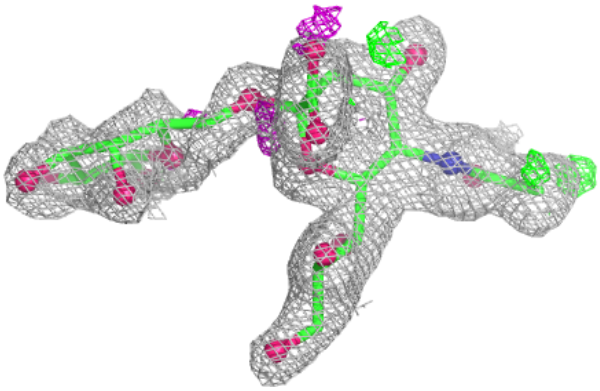
Electron density around Chain K:

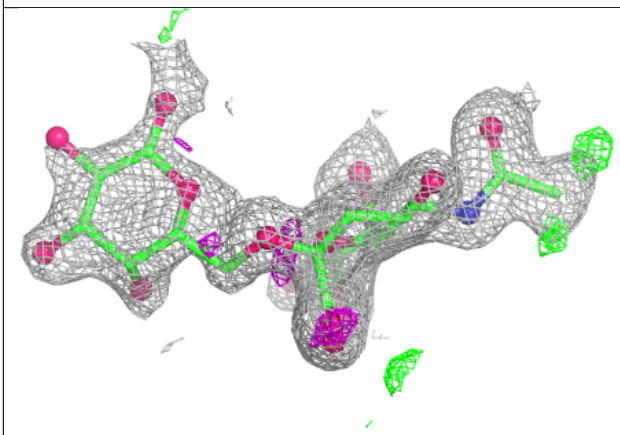
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

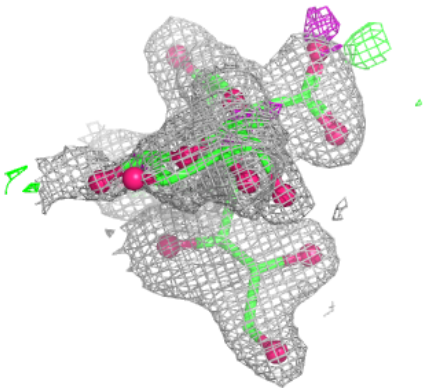


Electron density around Chain L:

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

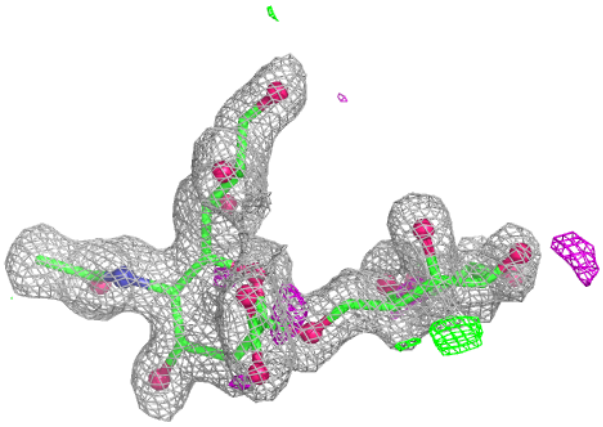


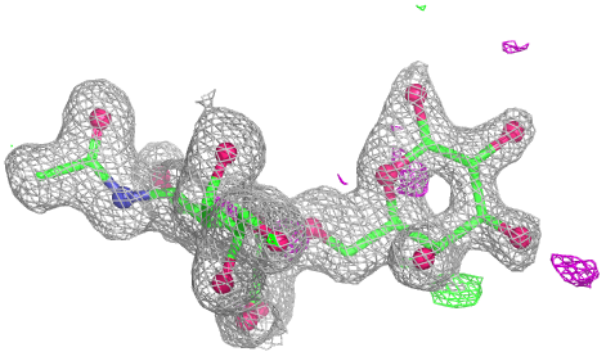


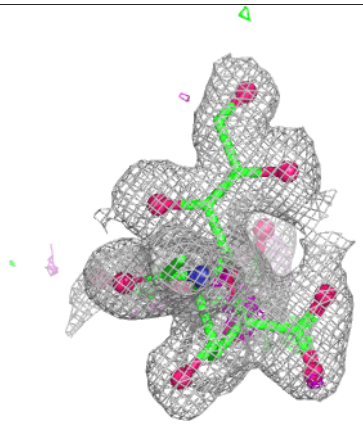


Electron density around Chain N:

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

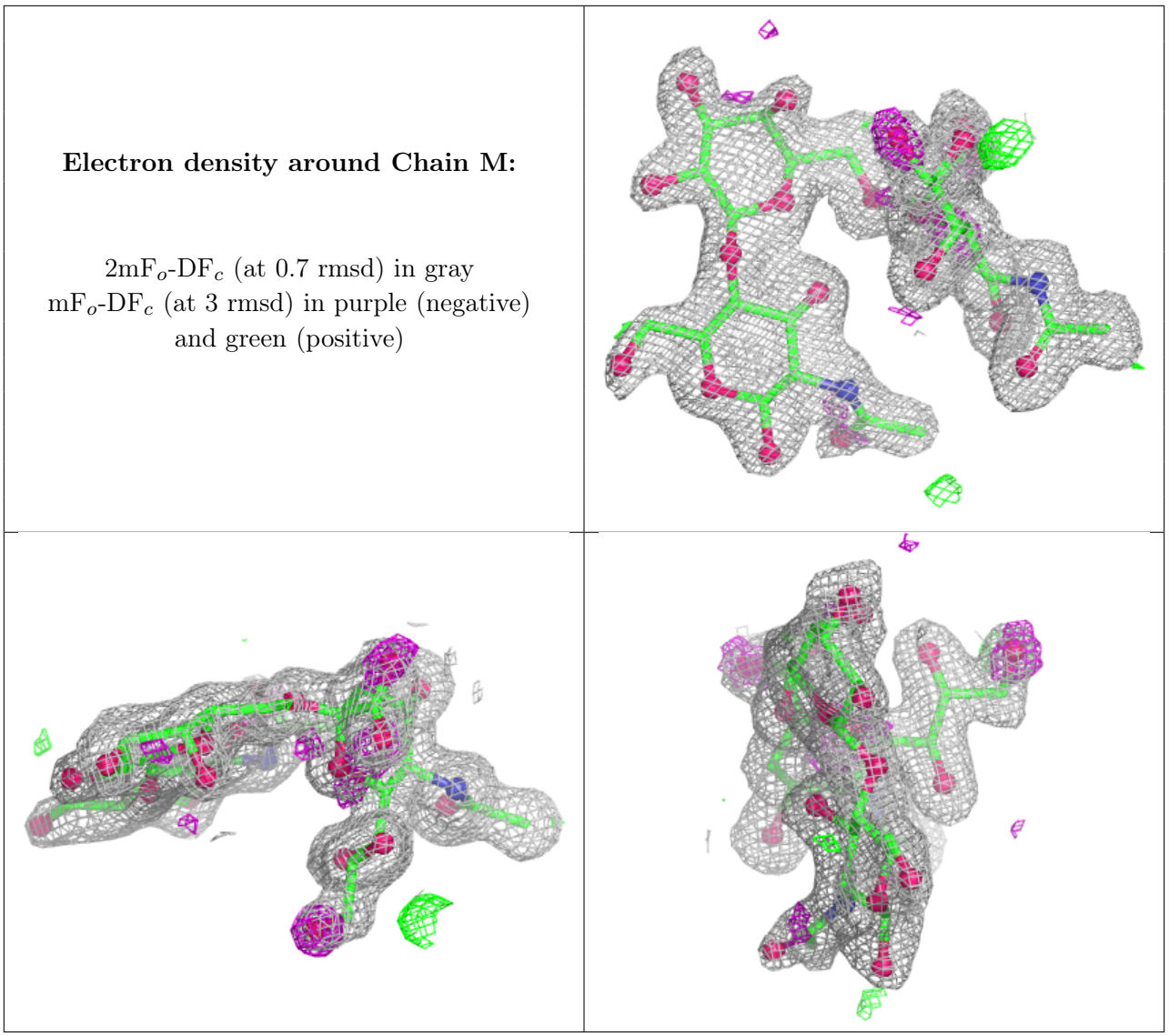






Electron density around Chain M:

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



6.4 Ligands

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	EDO	C	403	4/4	0.75	0.19	39,39,40,40	0
4	GOL	F	403	6/6	0.79	0.13	28,30,31,32	0
5	EDO	A	503	4/4	0.79	0.12	39,39,39,40	0
4	GOL	B	402	6/6	0.79	0.15	29,31,31,35	0
5	EDO	I	406	4/4	0.81	0.14	34,35,36,37	0
5	EDO	E	403	4/4	0.83	0.12	38,38,38,39	0
4	GOL	E	401	6/6	0.83	0.17	33,34,35,35	0

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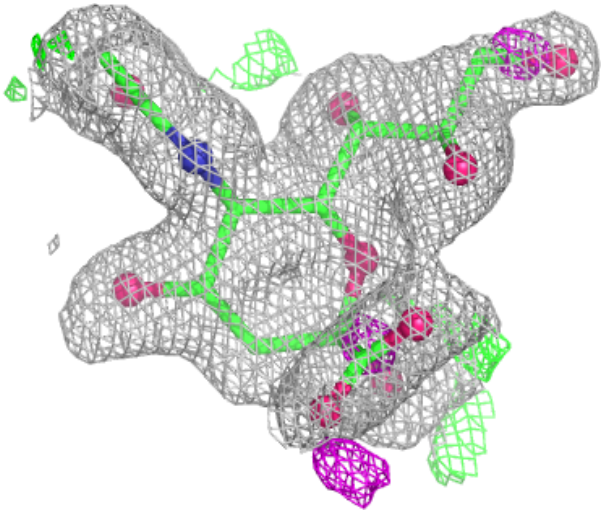
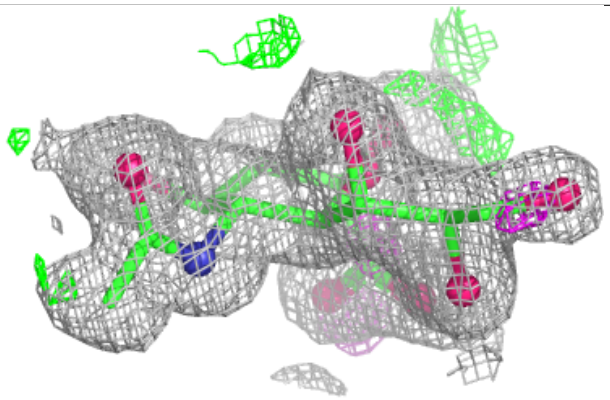
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	H	403	6/6	0.84	0.16	24,31,34,37	0
7	SIA	C	401	21/21	0.84	0.14	22,32,36,38	0
4	GOL	I	404	6/6	0.85	0.12	25,31,35,37	0
4	GOL	D	403	6/6	0.85	0.13	27,29,30,32	0
5	EDO	G	406	4/4	0.86	0.15	39,40,40,42	0
5	EDO	H	405	4/4	0.86	0.09	36,36,37,39	0
4	GOL	G	404	6/6	0.86	0.16	25,31,34,36	0
4	GOL	E	402	6/6	0.86	0.13	32,37,39,42	0
4	GOL	J	403	6/6	0.87	0.11	25,27,28,31	0
4	GOL	D	404	6/6	0.87	0.14	30,38,39,43	0
5	EDO	B	403	4/4	0.87	0.14	35,36,37,39	0
7	SIA	B	401	21/21	0.88	0.17	19,28,34,38	0
4	GOL	G	405	6/6	0.89	0.12	24,27,28,29	0
5	EDO	D	405	4/4	0.89	0.12	40,41,41,41	0
4	GOL	I	401	6/6	0.90	0.11	25,28,30,31	0
4	GOL	I	405	6/6	0.91	0.10	23,26,27,29	0
4	GOL	H	404[B]	6/6	0.91	0.16	30,32,34,36	6
4	GOL	A	502	6/6	0.91	0.11	25,32,36,38	0
4	GOL	H	404[A]	6/6	0.91	0.16	17,17,19,21	6
5	EDO	F	404	4/4	0.92	0.10	38,40,41,44	0
5	EDO	J	404	4/4	0.92	0.10	35,35,36,36	0
4	GOL	A	501	6/6	0.92	0.11	24,26,26,27	0
4	GOL	H	401	6/6	0.92	0.13	21,23,24,27	0
5	EDO	C	402	4/4	0.93	0.09	26,27,27,29	0
4	GOL	H	402	6/6	0.95	0.11	16,21,21,23	0
6	MG	H	407	1/1	0.95	0.33	40,40,40,40	0
6	MG	I	408	1/1	0.95	0.27	41,41,41,41	0
5	EDO	E	404	4/4	0.95	0.06	25,26,26,27	0
4	GOL	I	402	6/6	0.95	0.09	17,19,19,20	0
6	MG	C	404	1/1	0.96	0.17	28,28,28,28	0
4	GOL	I	403	6/6	0.97	0.07	21,23,24,24	0
6	MG	F	405	1/1	0.97	0.14	23,23,23,23	0
6	MG	F	406	1/1	0.97	0.29	37,37,37,37	0
6	MG	F	407	1/1	0.97	0.05	22,22,22,22	0
6	MG	A	504	1/1	0.98	0.11	21,21,21,21	0
6	MG	C	405	1/1	0.98	0.21	28,28,28,28	0
6	MG	A	505	1/1	0.98	0.03	20,20,20,20	0
6	MG	D	406	1/1	0.99	0.03	21,21,21,21	0
6	MG	I	407	1/1	0.99	0.05	19,19,19,19	0
6	MG	B	404	1/1	0.99	0.04	13,13,13,13	0
6	MG	G	407	1/1	0.99	0.07	18,18,18,18	0
6	MG	H	406	1/1	0.99	0.04	21,21,21,21	0

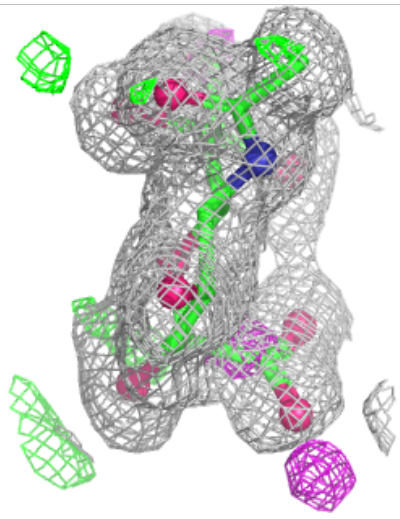
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SIA C 401:

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

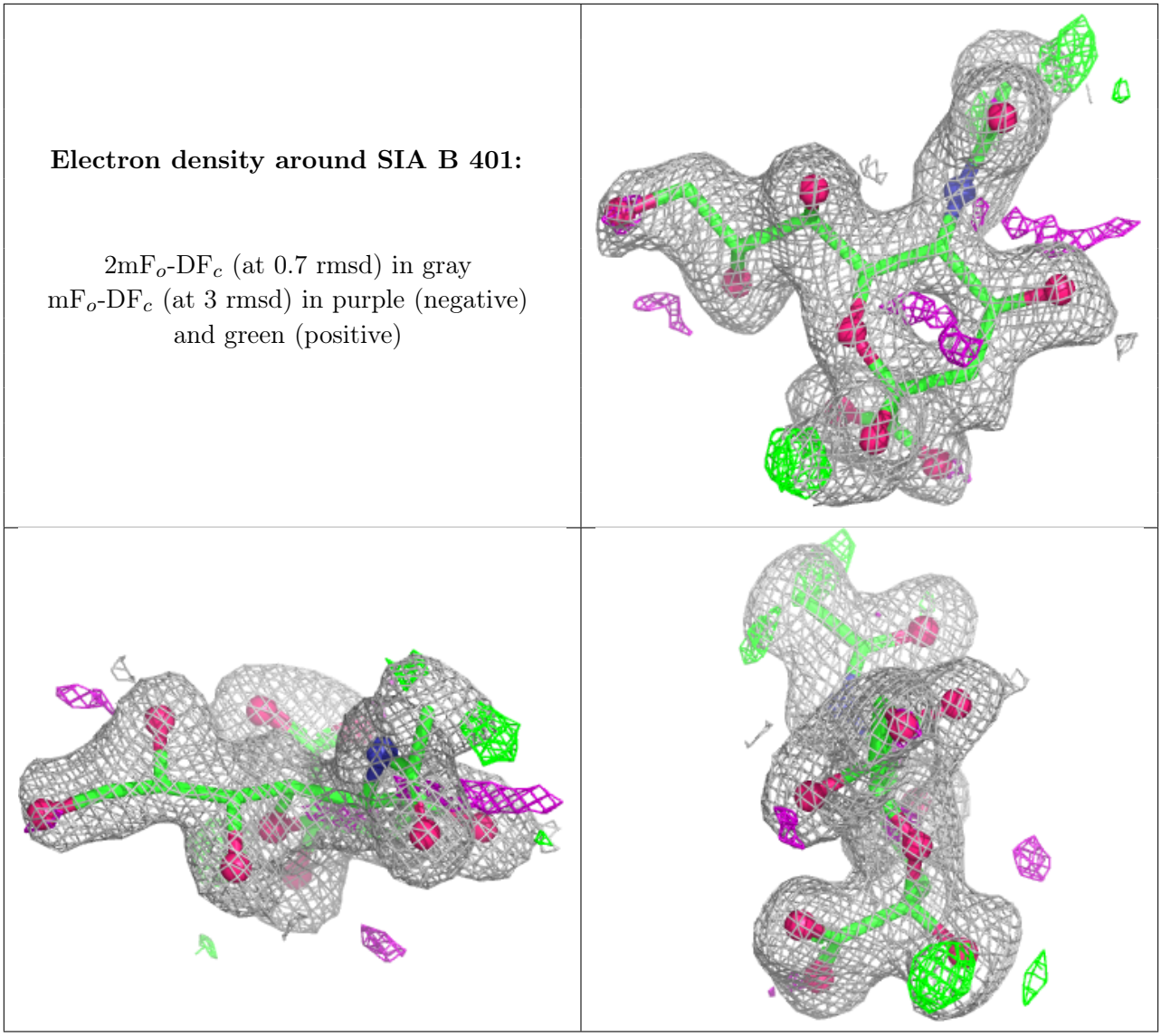






Electron density around SIA B 401:

$2mF_o$-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

There are no such residues in this entry.