



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:03 AM UTC

PDB ID : 6Y64 / pdb_00006y64
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

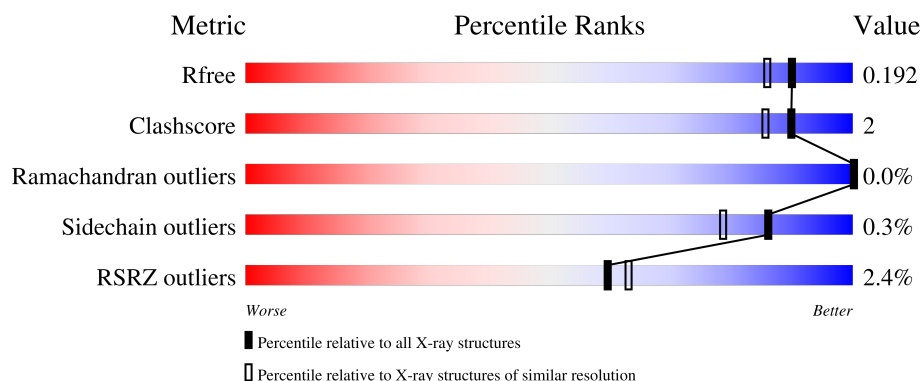
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



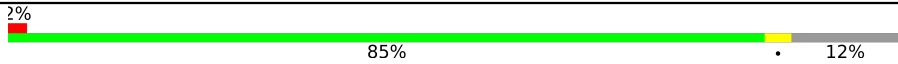
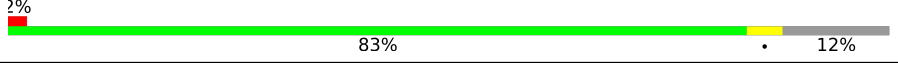
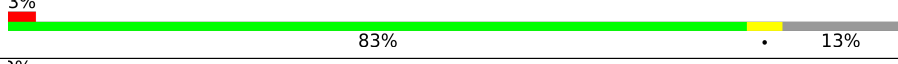
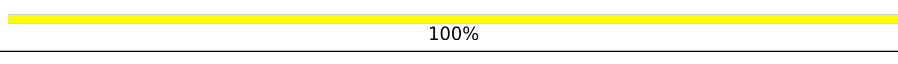
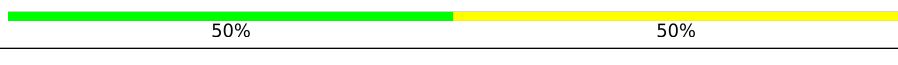
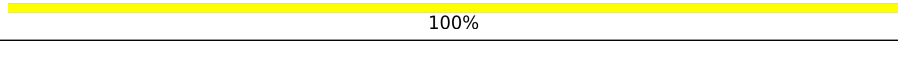
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	293	3% 85% 12%
1	B	293	2% 82% 15%
1	C	293	3% 85% 12%
1	D	293	2% 82% 15%
1	E	293	0% 84% 12%

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

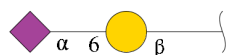
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	expression tag	UNP A0A0E3ZCF3
I	1	SER	-	expression tag	UNP A0A0E3ZCF3
I	2	SER	-	expression tag	UNP A0A0E3ZCF3
I	3	HIS	-	expression tag	UNP A0A0E3ZCF3
I	4	HIS	-	expression tag	UNP A0A0E3ZCF3
I	5	HIS	-	expression tag	UNP A0A0E3ZCF3
I	6	HIS	-	expression 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

Continued on next page...

Continued from previous page...

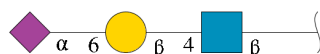
Chain	Residue	Modelled	Actual	Comment	Reference
J	95	SER	CYS	conflict	UNP A0A0E3ZCF3

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



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-galactopyranose-(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 (CCD ID: GOL) (formula: C₃H₈O₃).



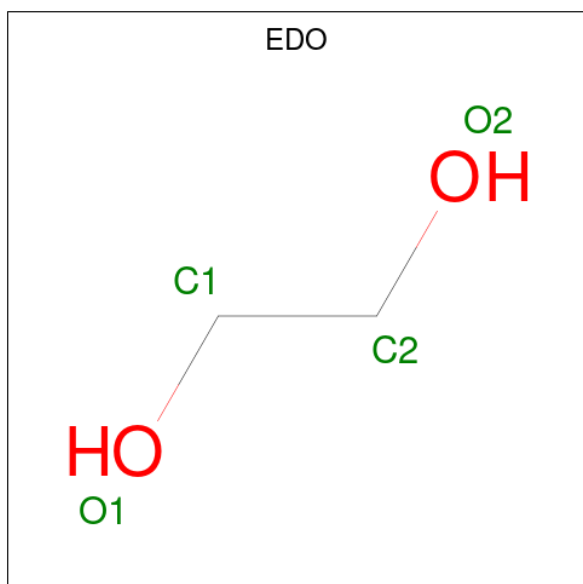
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

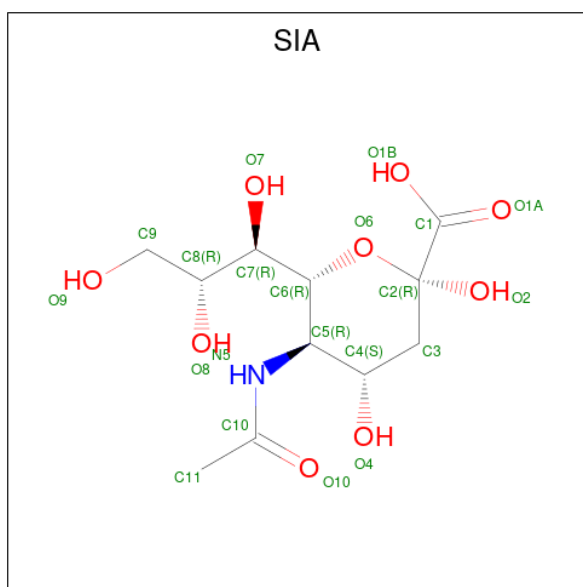
Continued from previous page...

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 (CCD ID: 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 (CCD ID: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

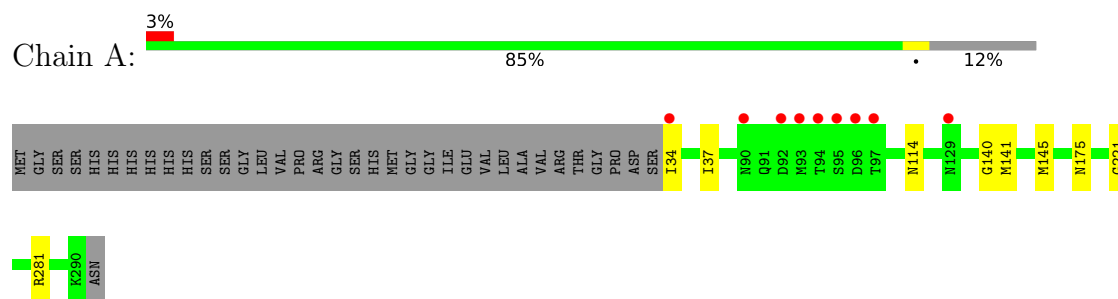
- Molecule 8 is water.

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

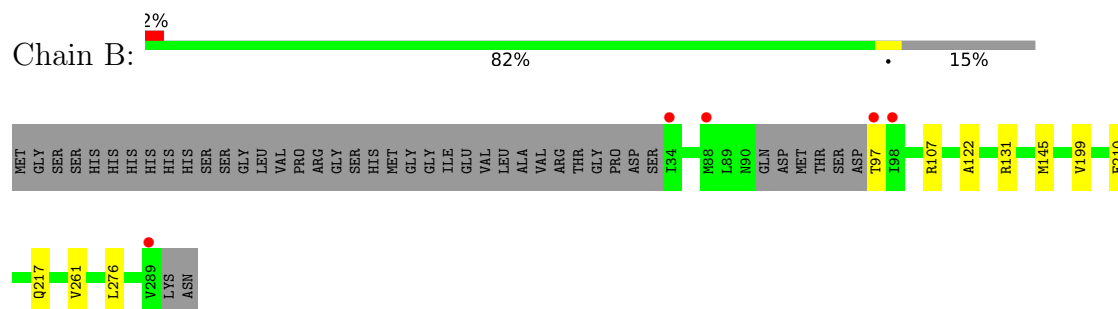
3 Residue-property plots [i](#)

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

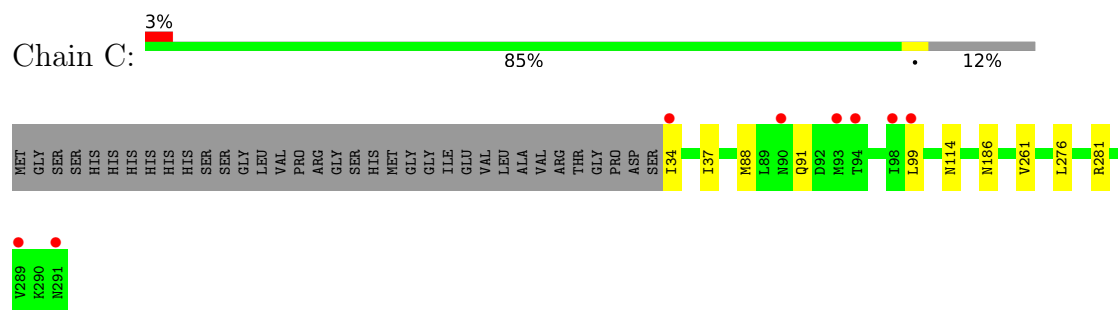
- Molecule 1: Capsid protein VP1



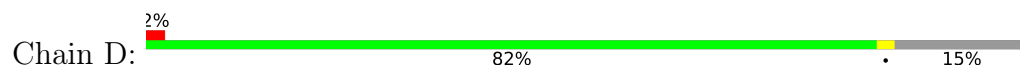
- Molecule 1: Capsid protein VP1

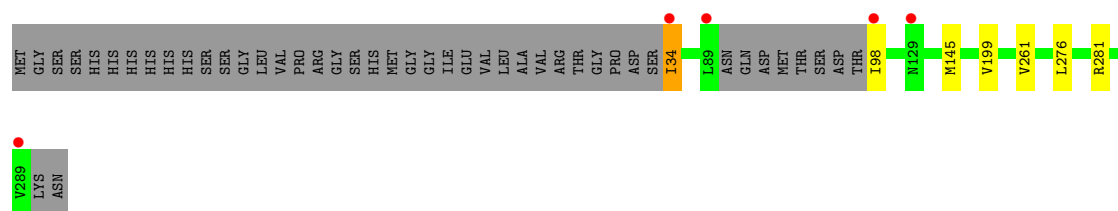


- Molecule 1: Capsid protein VP1

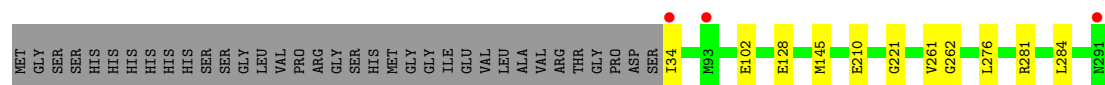
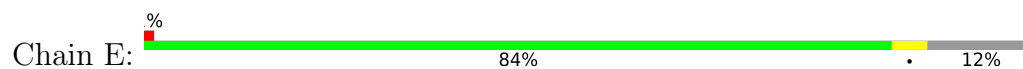


- Molecule 1: Capsid protein VP1

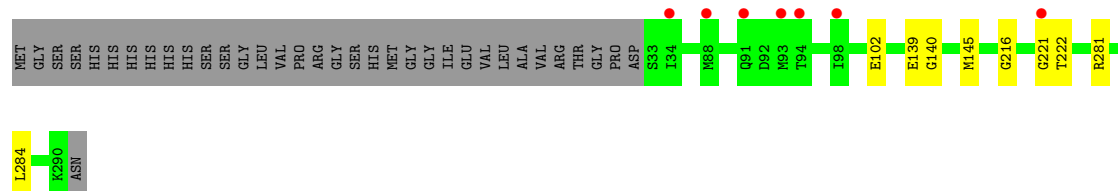
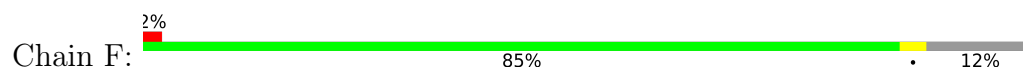




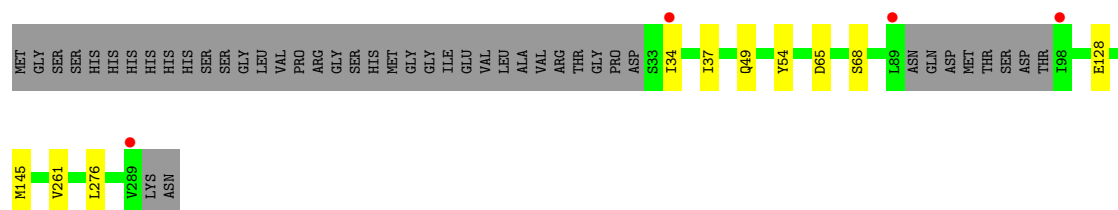
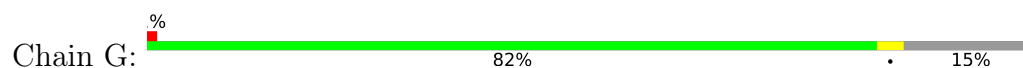
- Molecule 1: Capsid protein VP1



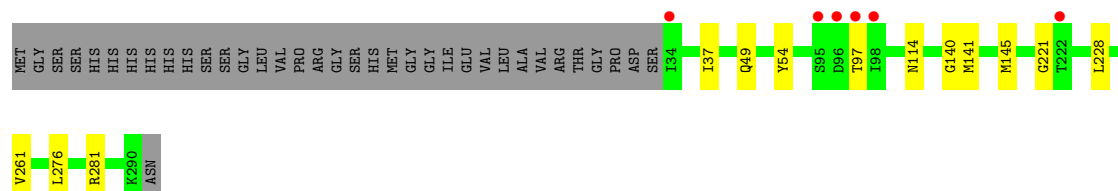
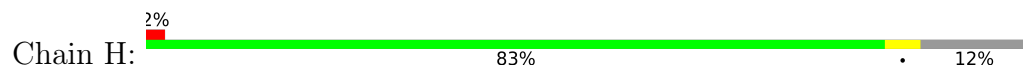
- Molecule 1: Capsid protein VP1



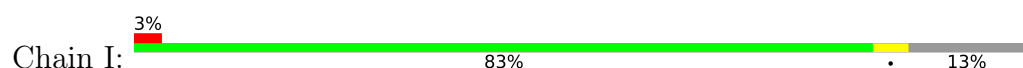
- Molecule 1: Capsid protein VP1

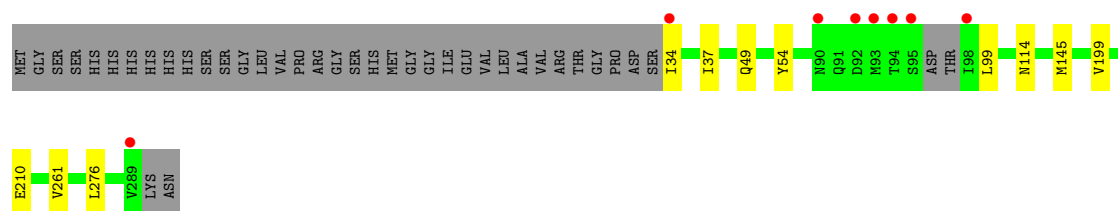


- Molecule 1: Capsid protein VP1

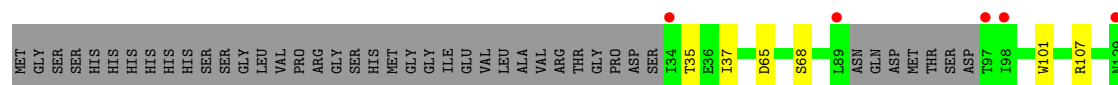
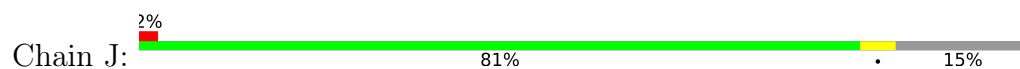


- Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1



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



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



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.93	0/2047	1.13	1/2782 (0.0%)
1	B	0.92	0/2004	1.07	0/2723
1	C	0.94	0/2057	1.10	1/2799 (0.0%)
1	D	0.92	0/1983	1.07	0/2695
1	E	0.95	1/2070 (0.0%)	1.09	2/2815 (0.1%)
1	F	0.94	0/2064	1.09	0/2807
1	G	0.94	0/1996	1.04	1/2713 (0.0%)
1	H	0.93	0/2061	1.09	0/2801
1	I	0.93	0/2039	1.08	0/2770
1	J	0.92	0/2011	1.06	0/2732
All	All	0.93	1/20332 (0.0%)	1.08	5/27637 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	221	GLY	C-O	6.12	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASN	CB-CA-C	6.32	121.39	110.01
1	A	175	ASN	CB-CA-C	6.14	116.34	111.00
1	G	128	GLU	CB-CG-CD	5.39	121.76	112.60
1	E	262	GLY	CA-C-O	-5.27	117.28	120.91
1	E	128	GLU	CB-CG-CD	5.10	121.27	112.60

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	1995	0	1889	6	0
1	B	1950	0	1877	10	0
1	C	1999	0	1903	9	0
1	D	1929	0	1846	5	0
1	E	2012	0	1915	5	0
1	F	2009	0	1908	6	0
1	G	1942	0	1850	6	0
1	H	2006	0	1917	11	0
1	I	1982	0	1898	9	0
1	J	1957	0	1875	11	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

Continued on next page...

Continued from previous page...

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	2	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	70	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 (70) 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

Continued on next page...

Continued from previous page...

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:D:145[A]:MET:C	1:D:145[A]:MET:SD	2.92	0.53
1:H:37:ILE:C	1:H:37:ILE:HD12	2.33	0.53
1:B:145[A]:MET:C	1:B:145[A]:MET:SD	2.93	0.52
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:37:ILE:HD12	1:A:37:ILE:C	2.38	0.49
1:E:145[A]:MET:SD	1:E:145[A]:MET:C	2.95	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:J:145[A]:MET:C	1:J:145[A]:MET:SD	2.96	0.48
1:D:34:ILE:N	8:D:505:HOH:O	2.47	0.48
1:G:145[A]:MET:C	1:G:145[A]:MET:SD	2.97	0.48
1:C:91:GLN:OE1	1:C:91:GLN:HA	2.13	0.48
1:G:37:ILE:C	1:G:37:ILE:HD12	2.39	0.48
1:J:35:THR:HG22	1:J:101:TRP:CZ3	2.49	0.47
1:I:145[A]:MET:SD	1:I:145[A]:MET:C	2.97	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: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:145[A]:MET:SD	1:A:145[A]:MET:C	3.00	0.44
1:J:37:ILE:C	1:J:37:ILE:HD12	2.42	0.44
1:A:141:MET:O	1:A:141:MET:HG3	2.18	0.44
1:F:145[A]:MET:C	1:F:145[A]:MET:SD	3.01	0.43
1:I:37:ILE:HD12	1:I:37:ILE:C	2.43	0.43
1:E:102:GLU:O	1:E:284:LEU:HA	2.18	0.43
1:J:145[A]:MET:HA	1:J:215:PHE:O	2.18	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:37:ILE:C	1:C:37:ILE:HD12	2.46	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:H:145[A]:MET:C	1:H:145[A]:MET:SD	3.05	0.40
1:J:107:ARG:HH11	1:J:107:ARG:HB3	1.85	0.40
1:G:145[A]:MET:HE2	1:G:145[A]:MET:HB2	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	14
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 ⓘ

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%)	207 (100%)	1 (0%)	81	70
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%)	201 (99%)	2 (1%)	68	50
1	E	215/249 (86%)	214 (100%)	1 (0%)	81	70
1	F	214/249 (86%)	213 (100%)	1 (0%)	81	70
1	G	206/249 (83%)	205 (100%)	1 (0%)	81	70
1	H	214/249 (86%)	214 (100%)	0	100	100
1	I	212/249 (85%)	211 (100%)	1 (0%)	81	70
1	J	210/249 (84%)	210 (100%)	0	100	100
All	All	2104/2490 (84%)	2097 (100%)	7 (0%)	86	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	D	34	ILE
1	D	98	ILE
1	E	34	ILE
1	F	222	THR
1	G	34	ILE
1	I	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	266	GLN
1	E	59	ASN
1	F	266	GLN
1	I	266	GLN
1	J	266	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
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(°)	Ideal(°)
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.

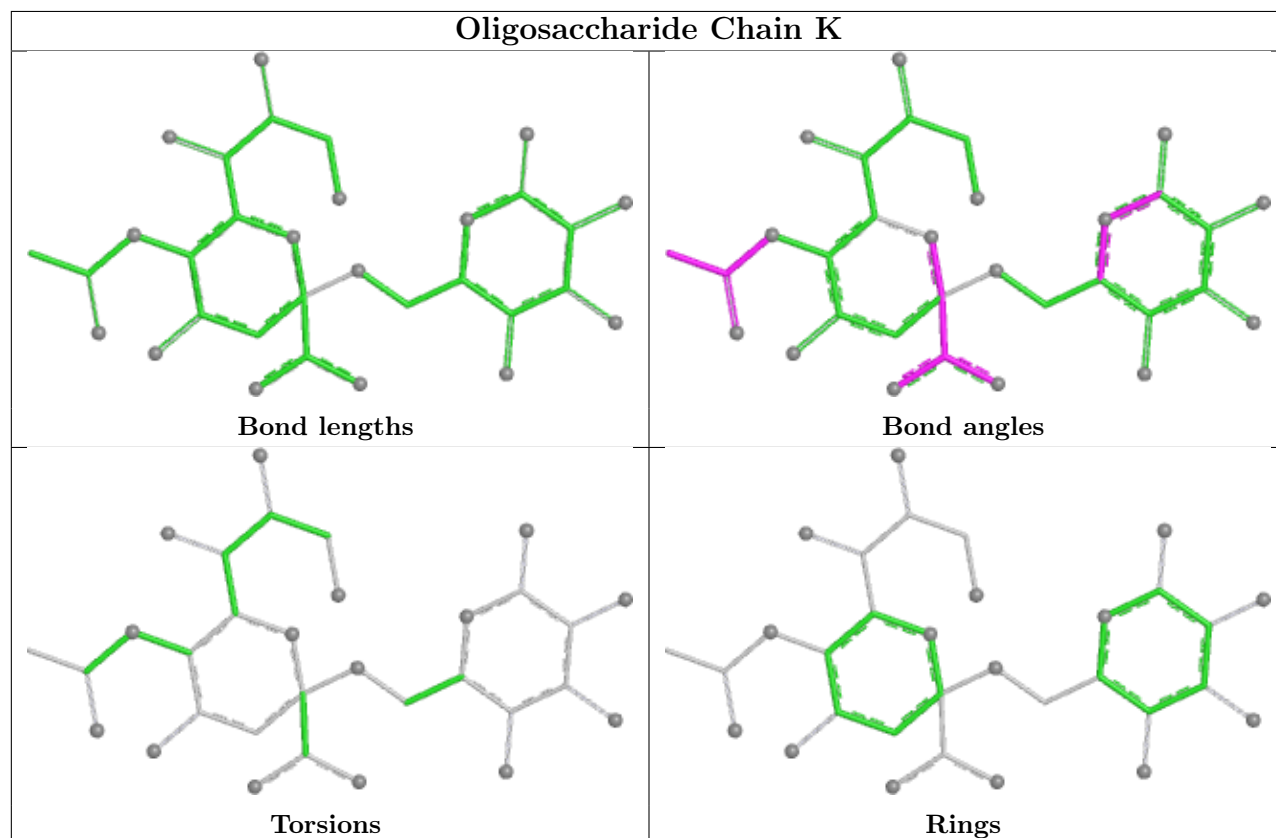
All (1) torsion outliers are listed below:

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

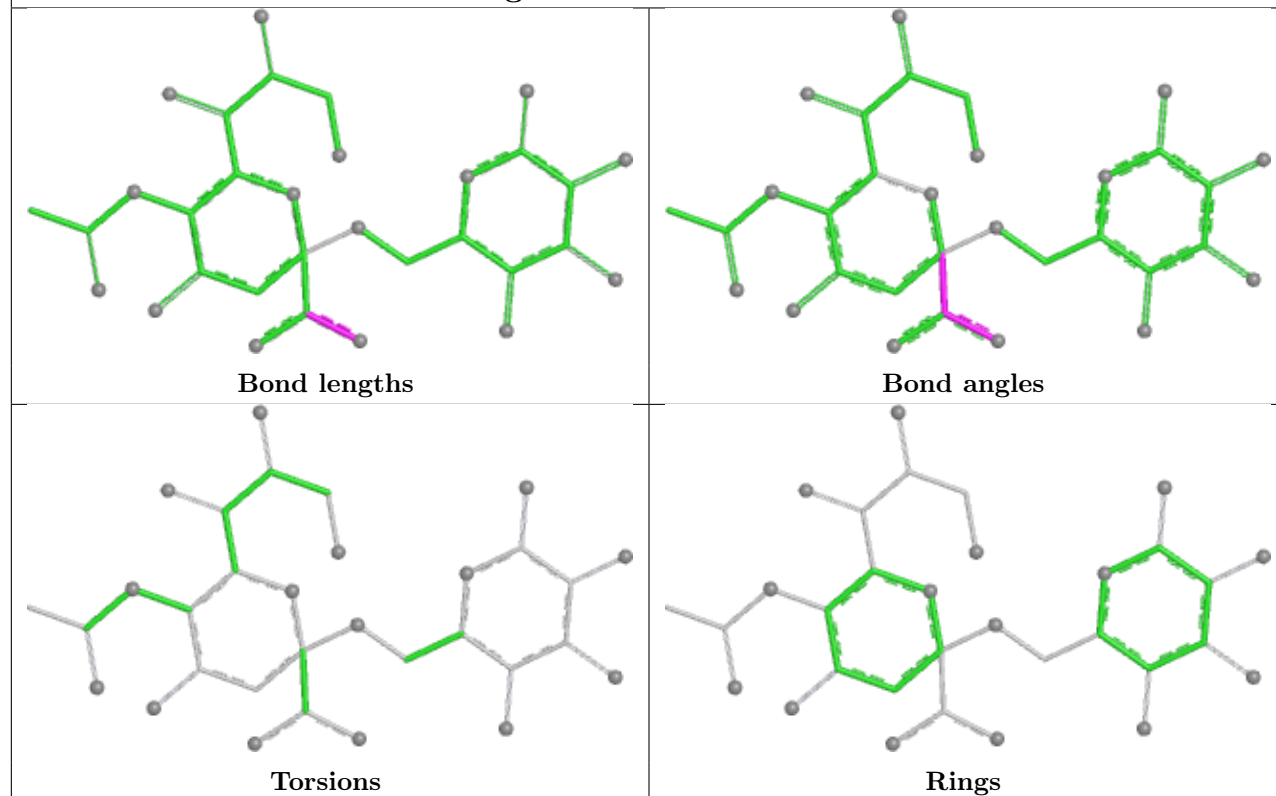
There are no ring outliers.

No monomer is involved in short contacts.

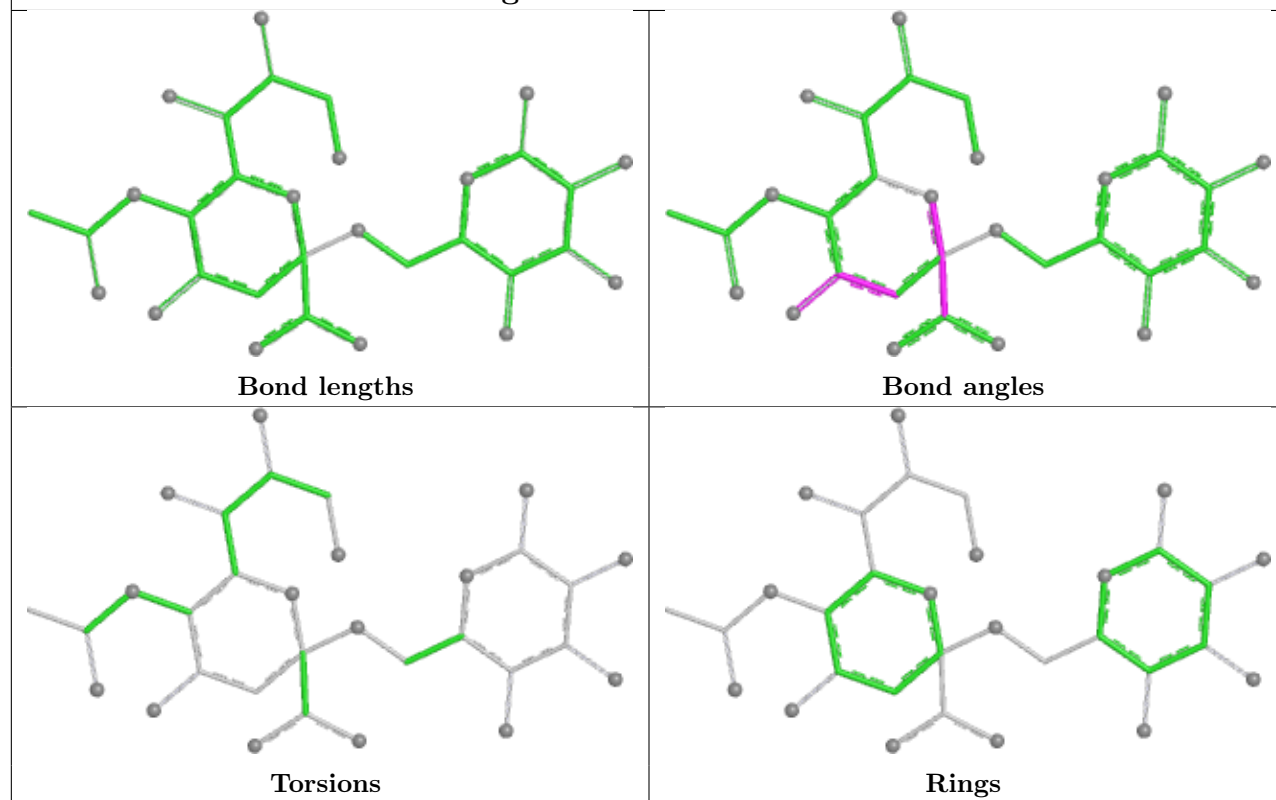
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

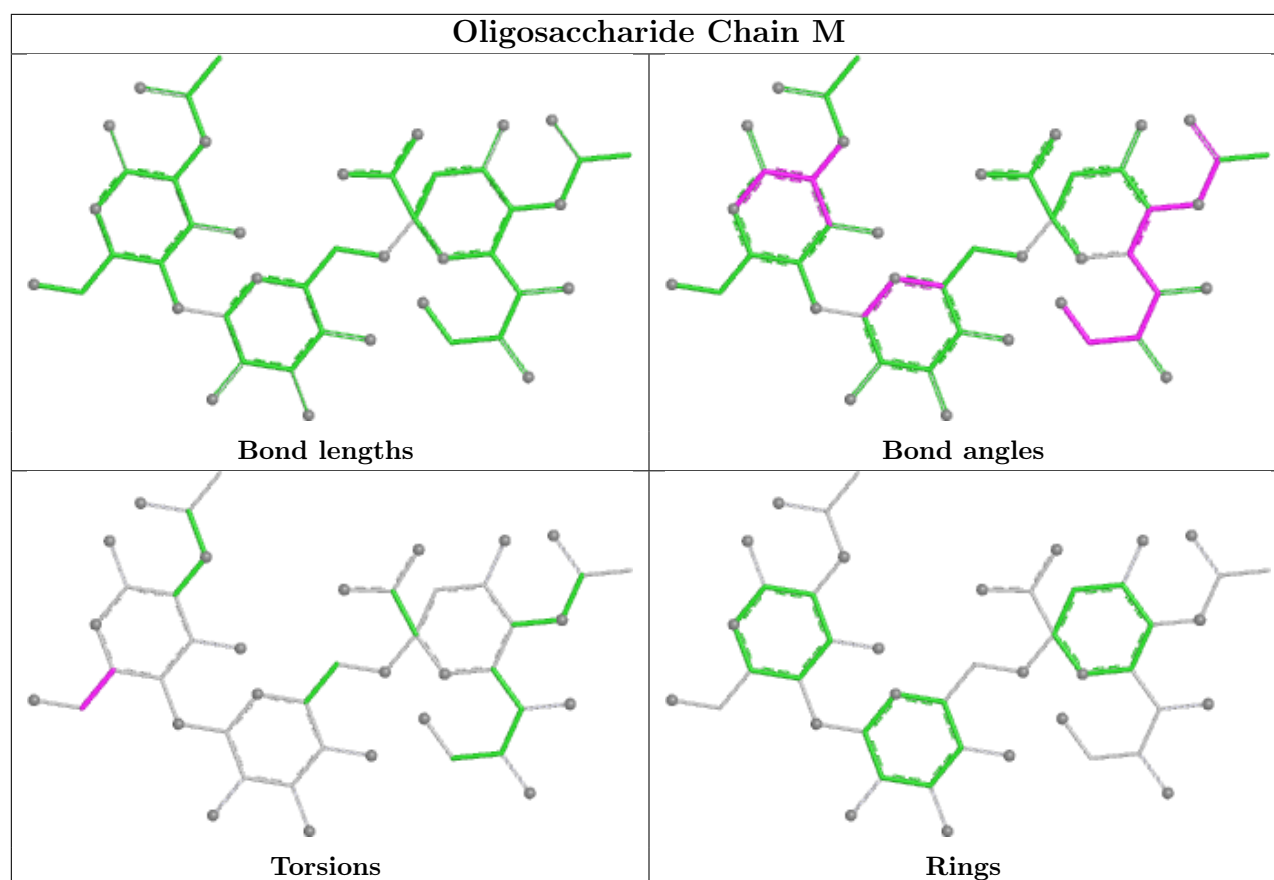


Oligosaccharide Chain L



Oligosaccharide Chain N





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	$\# Z > 2$
5	EDO	B	403	-	3,3,3	0.11	0	2,2,2	0.19	0
5	EDO	A	503	-	3,3,3	0.16	0	2,2,2	0.25	0
4	GOL	D	404	-	5,5,5	0.12	0	5,5,5	0.33	0
5	EDO	G	406	-	3,3,3	0.12	0	2,2,2	0.25	0
5	EDO	H	405	-	3,3,3	0.15	0	2,2,2	0.27	0
4	GOL	E	401	-	5,5,5	0.10	0	5,5,5	0.22	0
4	GOL	G	404	-	5,5,5	0.10	0	5,5,5	0.34	0
4	GOL	I	405	-	5,5,5	0.17	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	404[A]	-	5,5,5	0.10	0	5,5,5	0.22	0
7	SIA	C	401	-	21,21,21	1.09	1 (4%)	24,31,31	1.18	1 (4%)
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
4	GOL	B	402	-	5,5,5	0.13	0	5,5,5	0.38	0
4	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.25	0
4	GOL	H	403	-	5,5,5	0.12	0	5,5,5	0.29	0
4	GOL	I	401	-	5,5,5	0.14	0	5,5,5	0.33	0
5	EDO	D	405	-	3,3,3	0.07	0	2,2,2	0.26	0
5	EDO	I	406	-	3,3,3	0.24	0	2,2,2	0.34	0
4	GOL	E	402	-	5,5,5	0.08	0	5,5,5	0.24	0
4	GOL	J	403	-	5,5,5	0.13	0	5,5,5	0.34	0
5	EDO	C	402	-	3,3,3	0.23	0	2,2,2	0.33	0
5	EDO	E	404	-	3,3,3	0.13	0	2,2,2	0.13	0
4	GOL	G	405	-	5,5,5	0.11	0	5,5,5	0.27	0
4	GOL	H	401	-	5,5,5	0.10	0	5,5,5	0.40	0
4	GOL	H	402	-	5,5,5	0.16	0	5,5,5	0.34	0
5	EDO	C	403	-	3,3,3	0.19	0	2,2,2	0.33	0
5	EDO	F	404	-	3,3,3	0.14	0	2,2,2	0.26	0
5	EDO	E	403	-	3,3,3	0.15	0	2,2,2	0.32	0
4	GOL	I	404	-	5,5,5	0.15	0	5,5,5	0.35	0
7	SIA	B	401	-	21,21,21	1.15	1 (4%)	24,31,31	1.52	6 (25%)
4	GOL	H	404[B]	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	I	403	-	5,5,5	0.20	0	5,5,5	0.43	0
4	GOL	F	403	-	5,5,5	0.16	0	5,5,5	0.36	0
4	GOL	I	402	-	5,5,5	0.17	0	5,5,5	0.29	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
5	EDO	B	403	-	-	1/1/1/1	-
5	EDO	A	503	-	-	1/1/1/1	-
4	GOL	D	404	-	-	2/4/4/4	-
5	EDO	G	406	-	-	1/1/1/1	-
5	EDO	H	405	-	-	1/1/1/1	-
4	GOL	E	401	-	-	0/4/4/4	-
4	GOL	G	404	-	-	2/4/4/4	-
4	GOL	I	405	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	403	GOL	O2-C2-C3-O3
7	C	401	SIA	O1B-C1-C2-C3
4	B	402	GOL	O2-C2-C3-O3

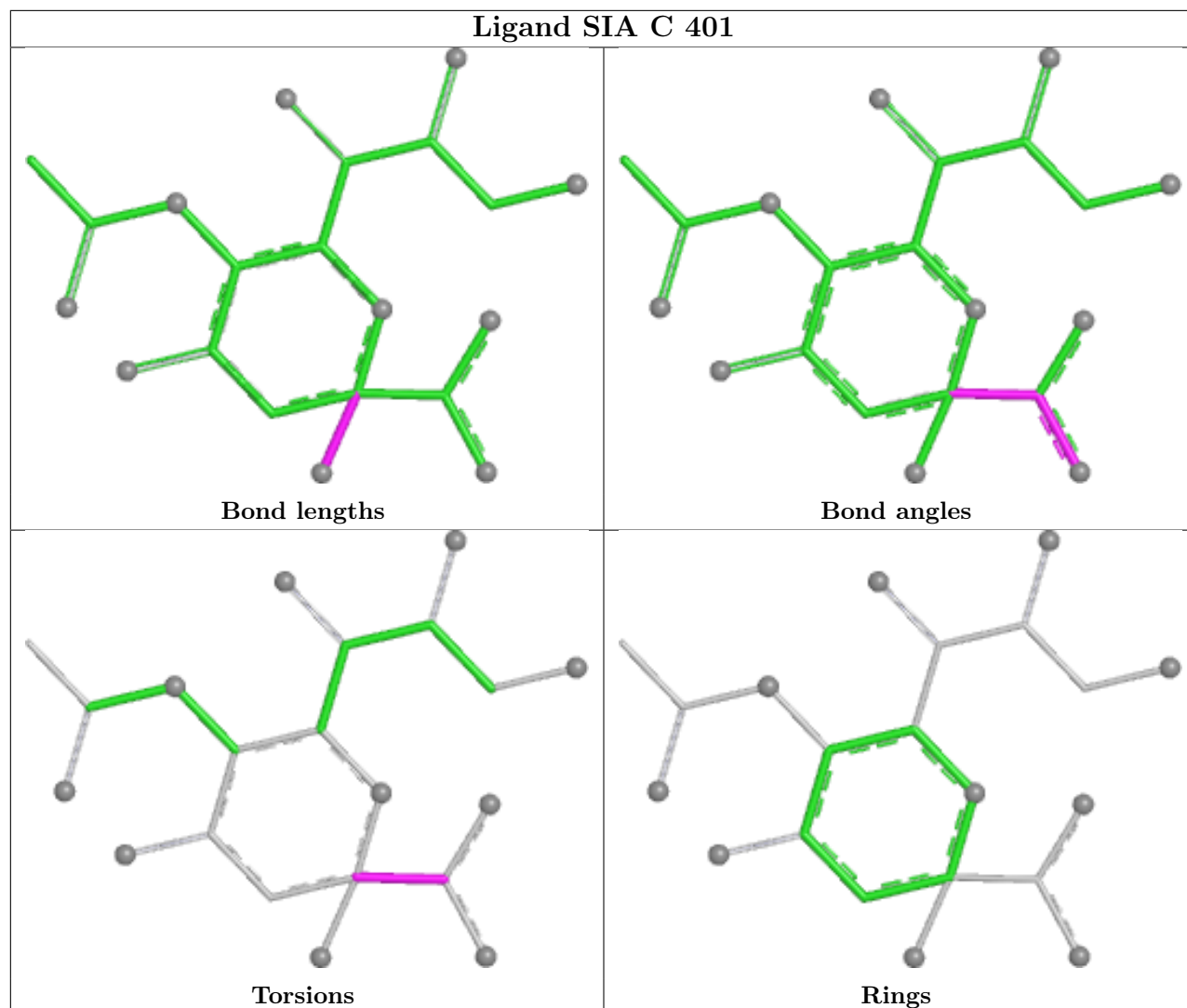
There are no ring outliers.

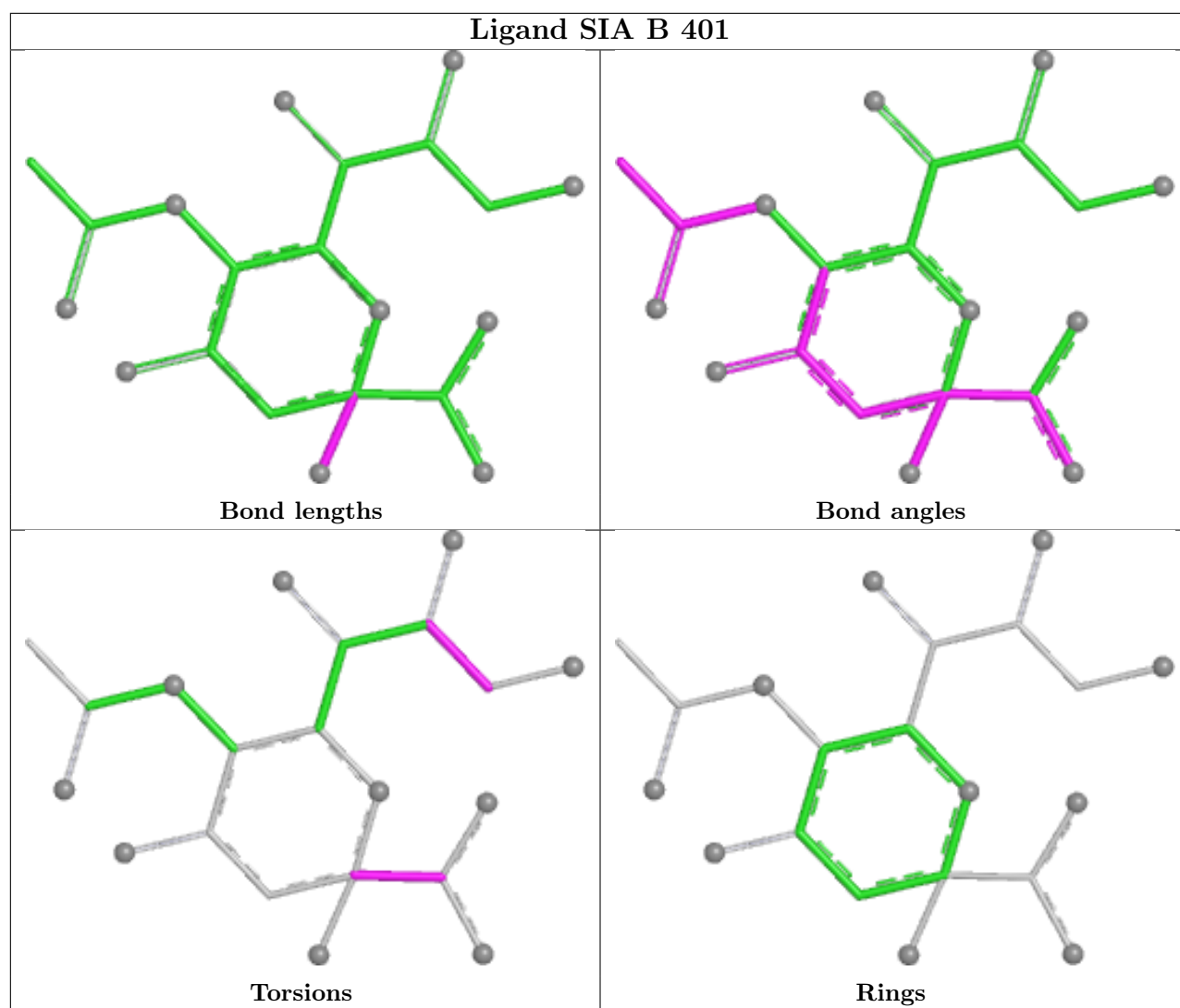
2 monomers are involved in 2 short contacts:

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

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

Ligand SIA C 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-0.18	9 (3%)	47	49	7, 17, 37, 61	3 (1%)
1	B	250/293 (85%)	-0.30	5 (2%)	65	69	7, 17, 30, 50	2 (0%)
1	C	258/293 (88%)	-0.16	8 (3%)	51	54	10, 19, 37, 58	2 (0%)
1	D	248/293 (84%)	-0.28	5 (2%)	65	69	7, 17, 31, 41	2 (0%)
1	E	258/293 (88%)	-0.23	3 (1%)	76	80	8, 18, 33, 42	4 (1%)
1	F	258/293 (88%)	-0.11	7 (2%)	56	59	8, 19, 39, 51	3 (1%)
1	G	249/293 (84%)	-0.33	4 (1%)	70	74	7, 16, 31, 44	3 (1%)
1	H	257/293 (87%)	-0.37	6 (2%)	61	64	7, 15, 30, 42	3 (1%)
1	I	254/293 (86%)	-0.35	8 (3%)	51	54	6, 15, 33, 45	3 (1%)
1	J	249/293 (84%)	-0.26	6 (2%)	59	63	7, 16, 35, 59	3 (1%)
All	All	2538/2930 (86%)	-0.26	61 (2%)	59	63	6, 17, 34, 61	28 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	98	ILE	5.0
1	I	94	THR	4.1
1	J	34	ILE	4.1
1	J	98	ILE	4.1
1	A	92	ASP	4.1
1	A	129	ASN	3.9
1	J	97	THR	3.9
1	C	34	ILE	3.7
1	G	98	ILE	3.6
1	I	95	SER	3.6
1	J	289	VAL	3.6
1	F	34	ILE	3.5
1	B	289	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	289	VAL	3.1
1	I	93	MET	3.1
1	D	34	ILE	3.1
1	A	94	THR	3.1
1	A	95	SER	3.0
1	A	97	THR	3.0
1	C	98	ILE	3.0
1	I	34	ILE	3.0
1	A	96	ASP	2.9
1	A	93	MET	2.9
1	H	34	ILE	2.9
1	I	98	ILE	2.9
1	F	94	THR	2.9
1	B	97	THR	2.8
1	G	34	ILE	2.8
1	J	89	LEU	2.8
1	C	94	THR	2.8
1	D	98	ILE	2.6
1	B	98	ILE	2.6
1	E	34	ILE	2.6
1	C	99	LEU	2.6
1	A	34	ILE	2.6
1	A	90	ASN	2.5
1	I	289	VAL	2.5
1	E	291	ASN	2.4
1	D	129	ASN	2.4
1	F	98	ILE	2.4
1	F	93	MET	2.4
1	C	90	ASN	2.3
1	D	289	VAL	2.3
1	I	90	ASN	2.3
1	H	95	SER	2.3
1	D	89	LEU	2.3
1	I	92	ASP	2.3
1	H	97	THR	2.3
1	G	89	LEU	2.3
1	H	96	ASP	2.2
1	F	221[A]	GLY	2.2
1	F	88	MET	2.1
1	F	91	GLN	2.1
1	B	34	ILE	2.1
1	C	291	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	88	MET	2.1
1	C	93	MET	2.1
1	C	289	VAL	2.0
1	H	222	THR	2.0
1	E	93	MET	2.0
1	J	129	ASN	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](#)

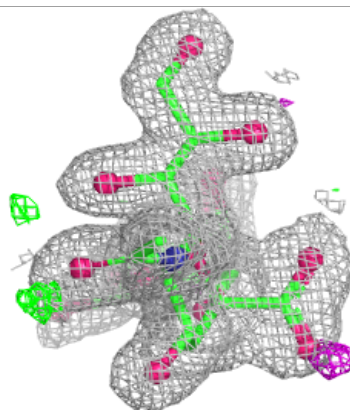
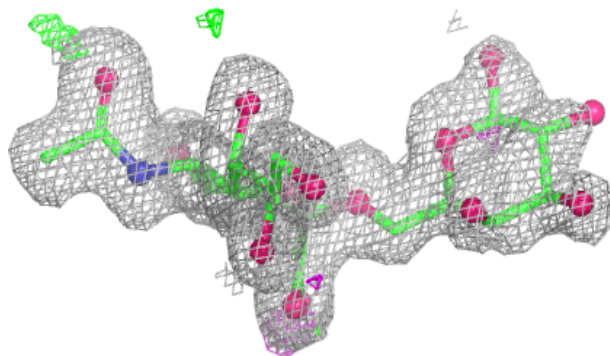
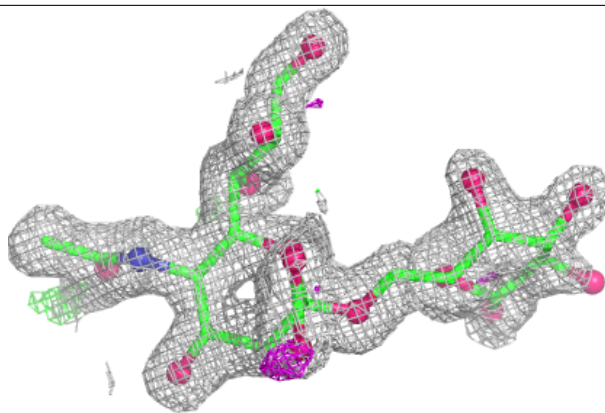
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	L	1	12/12	0.79	0.12	41,50,51,53	0
2	GAL	N	1	12/12	0.81	0.12	32,41,44,45	0
2	GAL	K	1	12/12	0.83	0.12	32,42,47,48	0
3	NAG	M	1	15/15	0.84	0.11	42,44,48,50	0
3	GAL	M	2	11/12	0.84	0.11	29,40,44,44	0
2	SIA	L	2	20/21	0.90	0.09	24,32,38,39	0
2	SIA	K	2	20/21	0.94	0.07	20,25,31,32	0
2	SIA	N	2	20/21	0.94	0.07	18,25,32,34	0
3	SIA	M	3	20/21	0.94	0.08	17,23,31,31	0

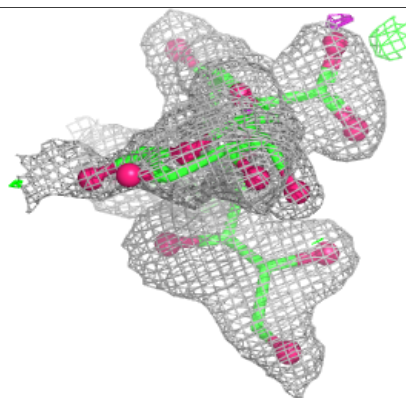
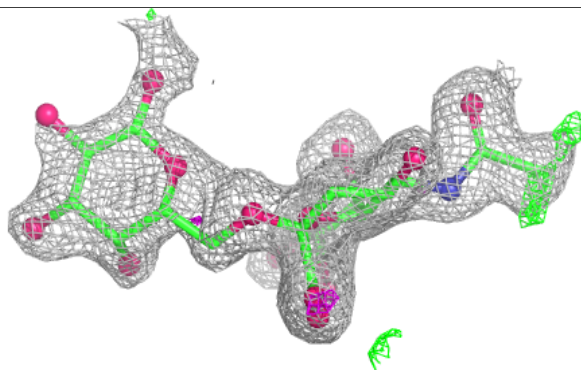
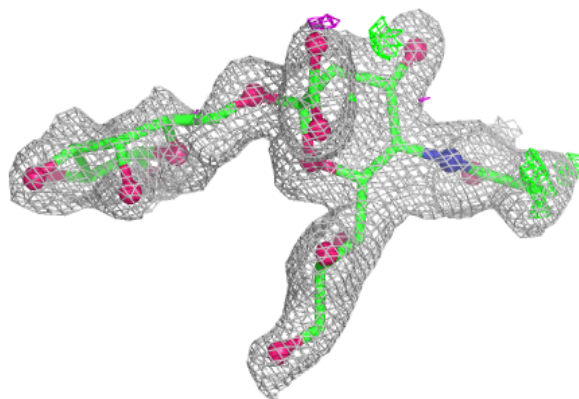
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

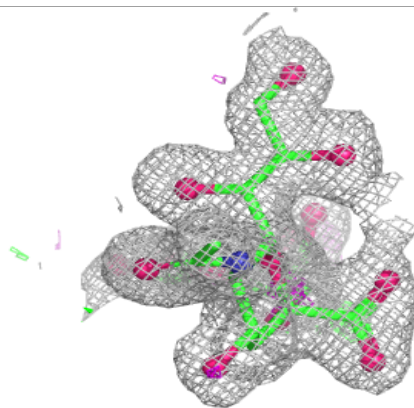
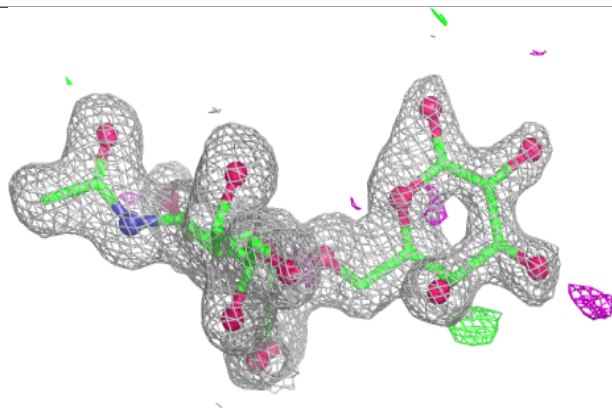
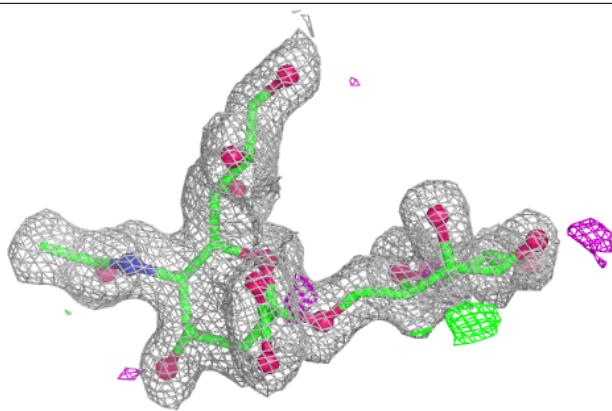
**Electron density around Chain L:**

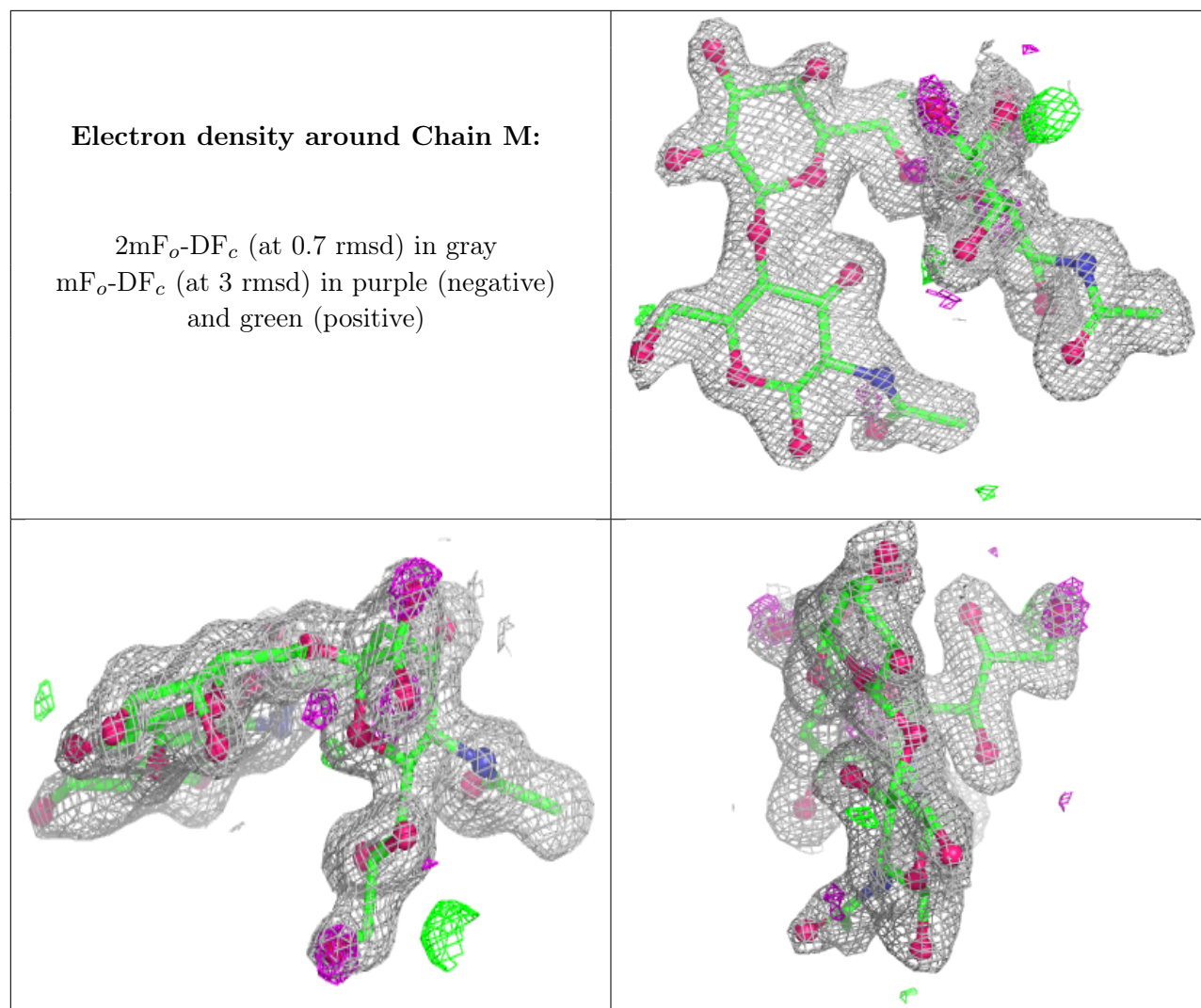
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	502	6/6	0.84	0.14	25,32,36,38	0
5	EDO	C	403	4/4	0.84	0.13	39,39,40,40	0
4	GOL	I	404	6/6	0.85	0.13	25,31,35,37	0
4	GOL	G	404	6/6	0.85	0.12	25,31,34,36	0
4	GOL	E	402	6/6	0.86	0.13	32,37,39,42	0
5	EDO	A	503	4/4	0.86	0.13	39,39,39,40	0
4	GOL	B	402	6/6	0.86	0.13	29,31,31,35	0
4	GOL	E	401	6/6	0.87	0.13	33,34,35,35	0

Continued on next page...

Continued from previous page...

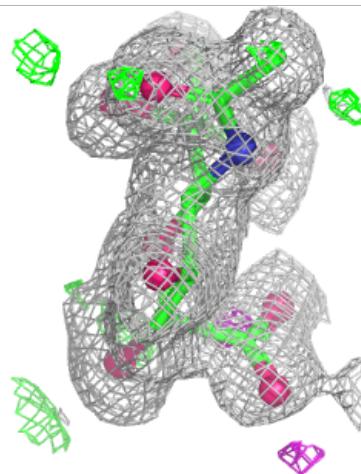
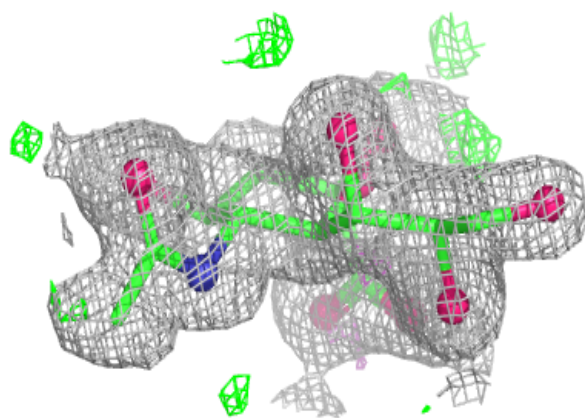
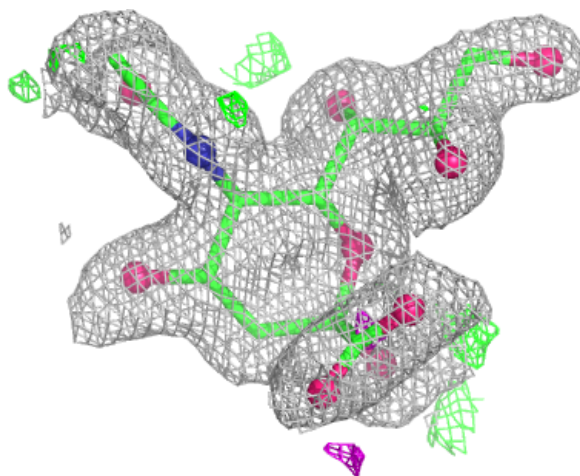
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	J	403	6/6	0.87	0.11	25,27,28,31	0
5	EDO	F	404	4/4	0.87	0.14	38,40,41,44	0
5	EDO	G	406	4/4	0.87	0.13	39,40,40,42	0
4	GOL	D	403	6/6	0.88	0.11	27,29,30,32	0
5	EDO	D	405	4/4	0.88	0.12	40,41,41,41	0
5	EDO	E	403	4/4	0.88	0.13	38,38,38,39	0
4	GOL	F	403	6/6	0.88	0.11	28,30,31,32	0
5	EDO	B	403	4/4	0.88	0.12	35,36,37,39	0
5	EDO	H	405	4/4	0.88	0.12	36,36,37,39	0
4	GOL	D	404	6/6	0.89	0.11	30,38,39,43	0
4	GOL	H	403	6/6	0.89	0.11	24,31,34,37	0
5	EDO	I	406	4/4	0.89	0.12	34,35,36,37	0
4	GOL	H	404[B]	6/6	0.90	0.10	30,32,34,36	6
4	GOL	H	404[A]	6/6	0.90	0.10	17,17,19,21	6
5	EDO	J	404	4/4	0.90	0.11	35,35,36,36	0
7	SIA	C	401	21/21	0.90	0.10	22,32,36,38	0
7	SIA	B	401	21/21	0.91	0.09	19,28,34,38	0
4	GOL	A	501	6/6	0.92	0.08	24,26,26,27	0
4	GOL	I	405	6/6	0.92	0.10	23,26,27,29	0
4	GOL	I	401	6/6	0.92	0.10	25,28,30,31	0
6	MG	F	406	1/1	0.93	0.18	37,37,37,37	0
4	GOL	H	401	6/6	0.93	0.11	21,23,24,27	0
4	GOL	G	405	6/6	0.93	0.08	24,27,28,29	0
6	MG	H	407	1/1	0.94	0.22	40,40,40,40	0
5	EDO	C	402	4/4	0.94	0.09	26,27,27,29	0
4	GOL	H	402	6/6	0.94	0.10	16,21,21,23	0
6	MG	I	408	1/1	0.95	0.17	41,41,41,41	0
6	MG	C	404	1/1	0.96	0.13	28,28,28,28	0
5	EDO	E	404	4/4	0.96	0.08	25,26,26,27	0
4	GOL	I	402	6/6	0.96	0.07	17,19,19,20	0
4	GOL	I	403	6/6	0.97	0.06	21,23,24,24	0
6	MG	F	405	1/1	0.97	0.11	23,23,23,23	0
6	MG	A	504	1/1	0.97	0.10	21,21,21,21	0
6	MG	F	407	1/1	0.97	0.06	22,22,22,22	0
6	MG	I	407	1/1	0.98	0.06	19,19,19,19	0
6	MG	C	405	1/1	0.98	0.17	28,28,28,28	0
6	MG	D	406	1/1	0.98	0.04	21,21,21,21	0
6	MG	A	505	1/1	0.98	0.04	20,20,20,20	0
6	MG	H	406	1/1	0.99	0.03	21,21,21,21	0
6	MG	B	404	1/1	0.99	0.02	13,13,13,13	0
6	MG	G	407	1/1	0.99	0.09	18,18,18,18	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.

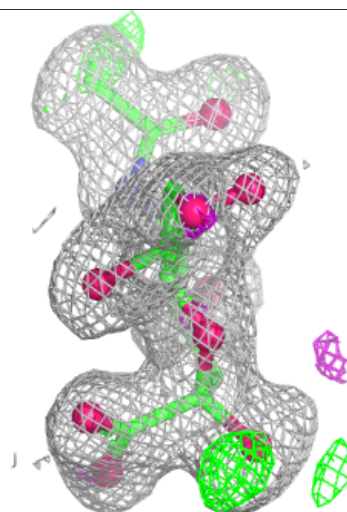
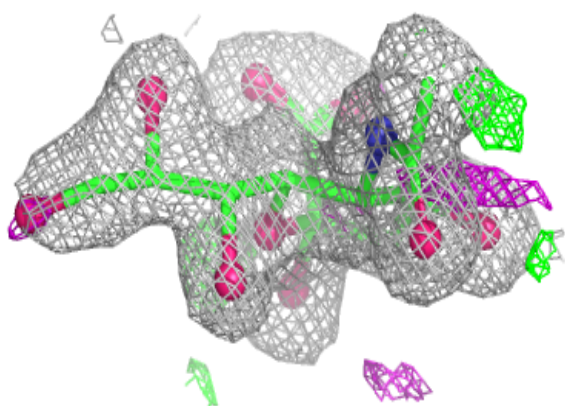
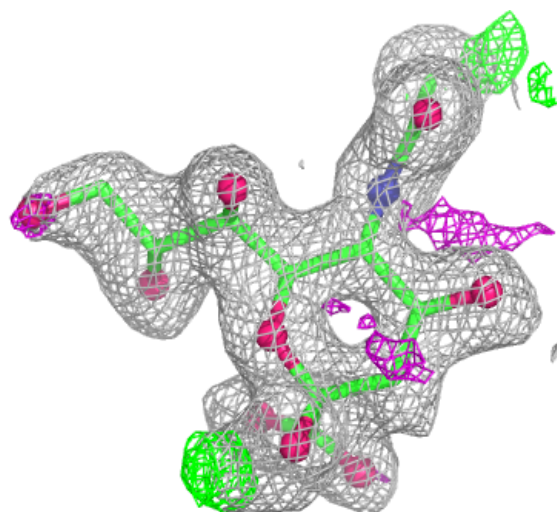
Electron density around SIA C 401:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.