wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2022 – 05:46 pm BST

PDB ID	:	7B6S
Title	:	Sheep Polyomavirus VP1 in complex with 10 mM Forssman antigen pentaose
Authors	:	Rustmeier, N.H.; Stehle, T.
Deposited on	:	2020-12-08
Resolution	:	1.92 Å(reported)

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

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

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

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

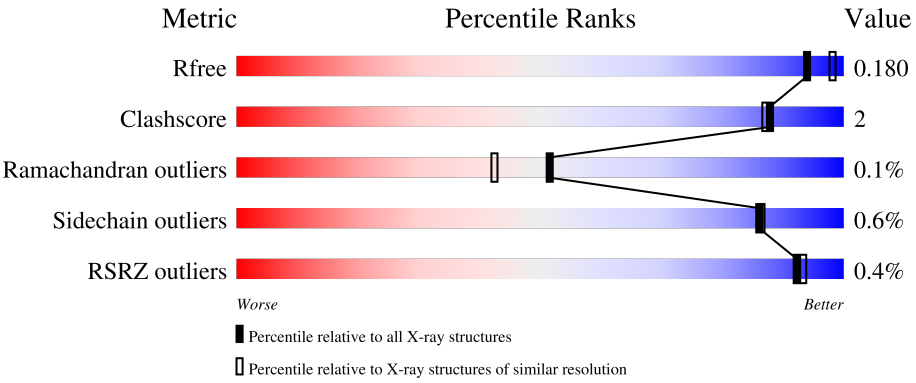
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	AAA	276	91% 6% ·
1	BBB	276	% 91% · 6%
1	CCC	276	88% 7% 5%
1	DDD	276	92% 5% ·
1	EEE	276	% 90% · 5%

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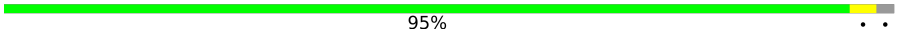
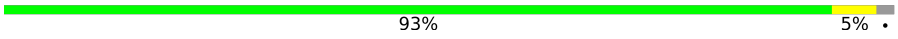
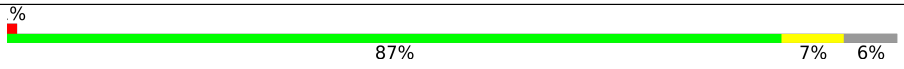
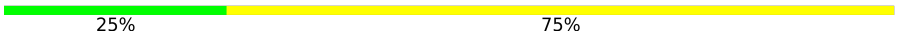
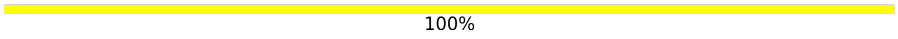
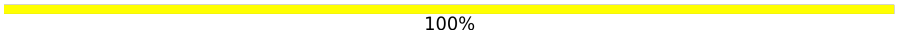
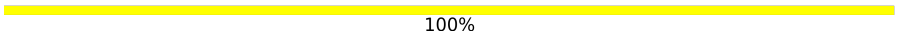
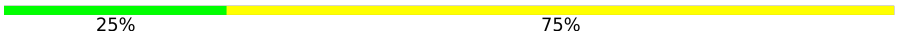
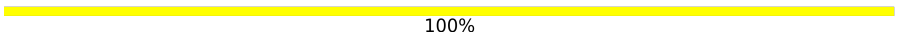
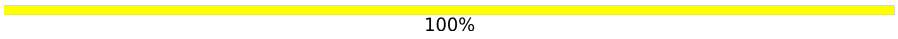
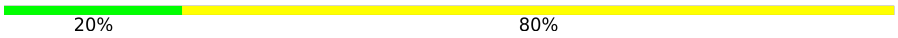
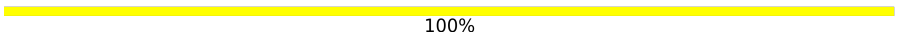
Mol	Chain	Length	Quality of chain
1	FFF	276	
1	GGG	276	
1	HHH	276	
1	III	276	
1	JJJ	276	
2	AaA	4	
2	BaB	4	
2	DaD	4	
2	FbF	4	
2	HaH	4	
2	IaI	4	
3	CaC	5	
3	EaE	5	
3	GaG	5	
3	JaJ	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23447 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	AAA	267	Total	C	N	O	S	0	1	0
			2070	1315	353	389	13			
1	BBB	260	Total	C	N	O	S	0	1	0
			2009	1281	341	375	12			
1	CCC	261	Total	C	N	O	S	0	1	0
			2017	1286	345	374	12			
1	DDD	269	Total	C	N	O	S	0	1	0
			2079	1323	347	396	13			
1	EEE	262	Total	C	N	O	S	0	1	0
			2032	1294	344	382	12			
1	FFF	271	Total	C	N	O	S	0	1	0
			2103	1334	356	399	14			
1	GGG	261	Total	C	N	O	S	0	1	0
			2022	1291	340	379	12			
1	HHH	271	Total	C	N	O	S	0	1	0
			2105	1335	356	400	14			
1	III	260	Total	C	N	O	S	0	1	0
			2004	1280	336	376	12			
1	JJJ	260	Total	C	N	O	S	0	1	0
			2027	1291	344	380	12			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	16	GLY	-	expression tag	UNP A0A0E3ZCF3
AAA	17	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	18	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	19	MET	-	expression tag	UNP A0A0E3ZCF3
AAA	95	SER	CYS	conflict	UNP A0A0E3ZCF3
BBB	16	GLY	-	expression tag	UNP A0A0E3ZCF3
BBB	17	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	18	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	19	MET	-	expression tag	UNP A0A0E3ZCF3

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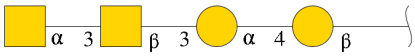
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	95	SER	CYS	conflict	UNP A0A0E3ZCF3
CCC	16	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	17	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	18	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	19	MET	-	expression tag	UNP A0A0E3ZCF3
CCC	95	SER	CYS	conflict	UNP A0A0E3ZCF3
DDD	16	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	17	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	18	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	19	MET	-	expression tag	UNP A0A0E3ZCF3
DDD	95	SER	CYS	conflict	UNP A0A0E3ZCF3
EEE	16	GLY	-	expression tag	UNP A0A0E3ZCF3
EEE	17	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	18	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	19	MET	-	expression tag	UNP A0A0E3ZCF3
EEE	95	SER	CYS	conflict	UNP A0A0E3ZCF3
FFF	16	GLY	-	expression tag	UNP A0A0E3ZCF3
FFF	17	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	18	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	19	MET	-	expression tag	UNP A0A0E3ZCF3
FFF	95	SER	CYS	conflict	UNP A0A0E3ZCF3
GGG	16	GLY	-	expression tag	UNP A0A0E3ZCF3
GGG	17	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	18	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	19	MET	-	expression tag	UNP A0A0E3ZCF3
GGG	95	SER	CYS	conflict	UNP A0A0E3ZCF3
HHH	16	GLY	-	expression tag	UNP A0A0E3ZCF3
HHH	17	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	18	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	19	MET	-	expression tag	UNP A0A0E3ZCF3
HHH	95	SER	CYS	conflict	UNP A0A0E3ZCF3
III	16	GLY	-	expression tag	UNP A0A0E3ZCF3
III	17	SER	-	expression tag	UNP A0A0E3ZCF3
III	18	HIS	-	expression tag	UNP A0A0E3ZCF3
III	19	MET	-	expression tag	UNP A0A0E3ZCF3
III	95	SER	CYS	conflict	UNP A0A0E3ZCF3
JJJ	16	GLY	-	expression tag	UNP A0A0E3ZCF3
JJJ	17	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	18	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	19	MET	-	expression tag	UNP A0A0E3ZCF3
JJJ	95	SER	CYS	conflict	UNP A0A0E3ZCF3

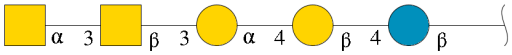
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-

2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose.



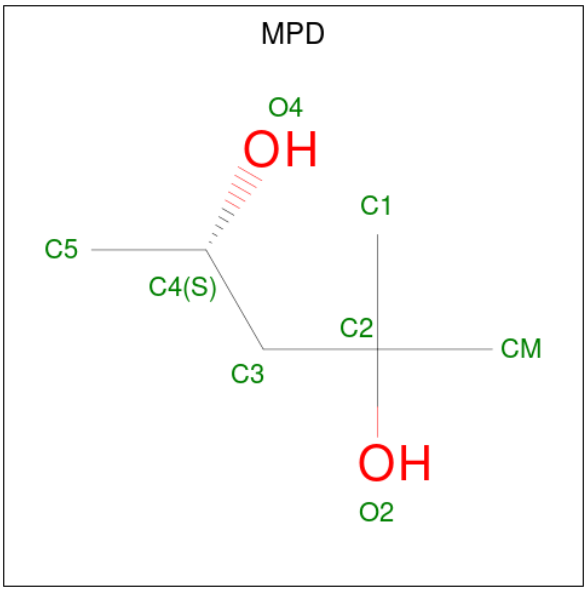
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	BaB	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	DaD	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	FbF	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	HaH	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	IaI	4	Total	C	N	O	0	0	0
			51	28	2	21			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CaC	5	Total	C	N	O	0	0	0
			62	34	2	26			
3	EaE	5	Total	C	N	O	0	0	0
			62	34	2	26			
3	GaG	5	Total	C	N	O	0	0	0
			62	34	2	26			
3	JaJ	5	Total	C	N	O	0	0	0
			62	34	2	26			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 8 6 2	0	0
4	BBB	1	Total C O 8 6 2	0	0
4	DDD	1	Total C O 8 6 2	0	0
4	FFF	1	Total C O 8 6 2	0	0
4	FFF	1	Total C O 8 6 2	0	0
4	HHH	1	Total C O 8 6 2	0	0
4	HHH	1	Total C O 8 6 2	0	0
4	III	1	Total C O 8 6 2	0	0
4	JJJ	1	Total C O 8 6 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Mg 1 1	0	0
5	BBB	1	Total Mg 1 1	0	0
5	CCC	1	Total Mg 1 1	0	0

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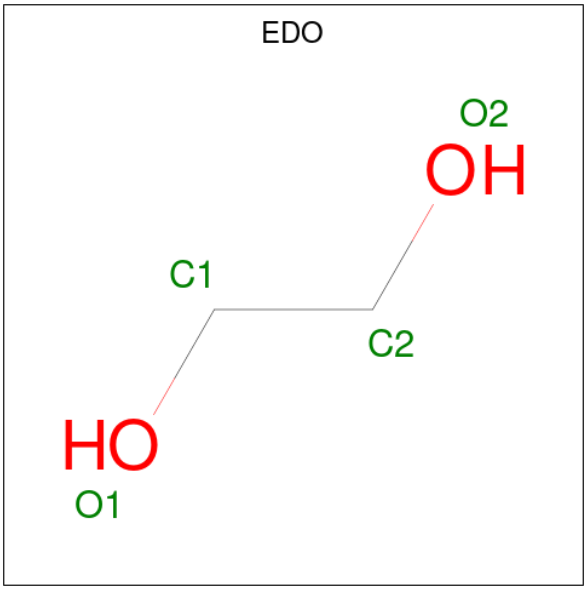
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	DDD	1	Total Mg 1 1	0	0
5	EEE	1	Total Mg 1 1	0	0
5	FFF	1	Total Mg 1 1	0	0
5	GGG	1	Total Mg 1 1	0	0
5	HHH	1	Total Mg 1 1	0	0
5	III	1	Total Mg 1 1	0	0
5	JJJ	1	Total Mg 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total C O 4 2 2	0	0
6	DDD	1	Total C O 4 2 2	0	0
6	DDD	1	Total C O 4 2 2	0	0
6	EEE	1	Total C O 4 2 2	0	0

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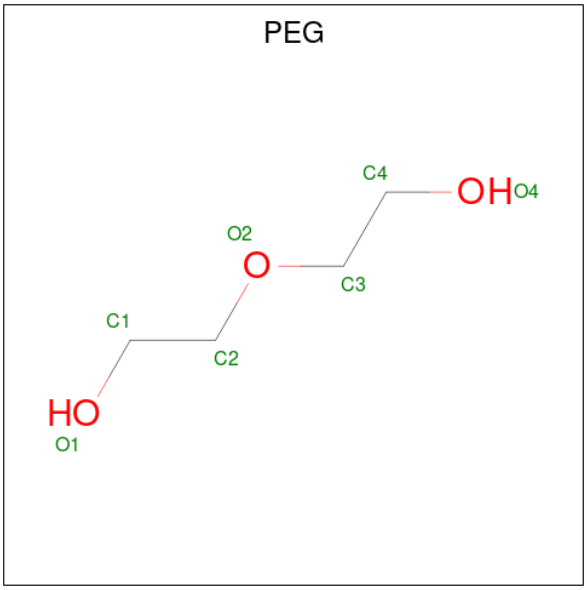
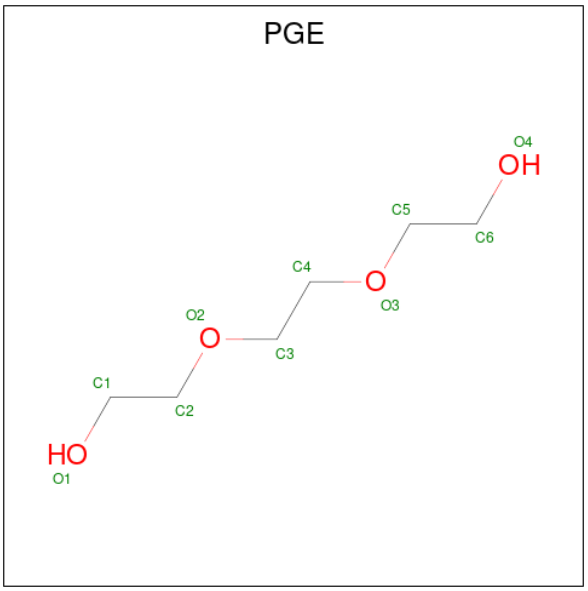
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	HHH	1	Total C O 4 2 2	0	0
6	JJJ	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	CCC	1	Total C O 7 4 3	0	0
7	EEE	1	Total C O 7 4 3	0	0
7	GGG	1	Total C O 7 4 3	0	0
7	HHH	1	Total C O 7 4 3	0	0
7	III	1	Total C O 7 4 3	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	FFF	1	Total C O 10 6 4	0	0
8	GGG	1	Total C O 10 6 4	0	0
8	III	1	Total C O 10 6 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	223	Total O 225 225	0	2
9	BBB	194	Total O 197 197	0	3
9	CCC	208	Total O 209 209	0	1
9	DDD	239	Total O 241 241	0	2
9	EEE	206	Total O 208 208	0	2
9	FFF	256	Total O 259 259	0	3
9	GGG	215	Total O 219 219	0	4
9	HHH	250	Total O 250 250	0	0
9	III	219	Total O 219 219	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	JJJ	225	Total 227	O 227	0	2

3 Residue-property plots (i)

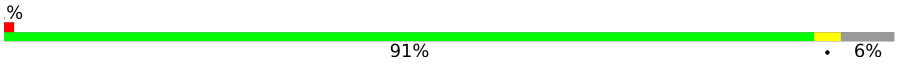
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

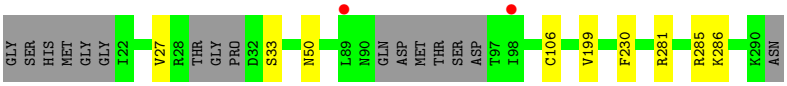
• Molecule 1: Capsid protein VP1

Chain AAA:

• Molecule 1: Capsid protein VP1

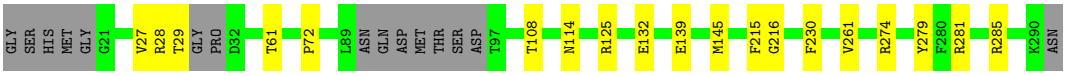
Chain BBB:





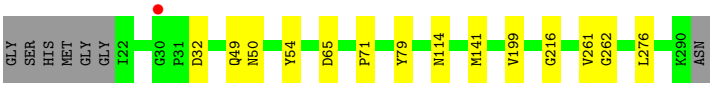
• Molecule 1: Capsid protein VP1

Chain CCC:



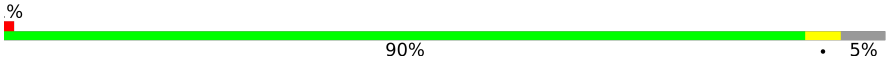
• Molecule 1: Capsid protein VP1

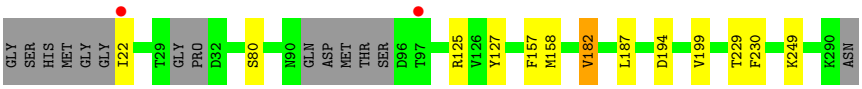
Chain DDD:



• Molecule 1: Capsid protein VP1

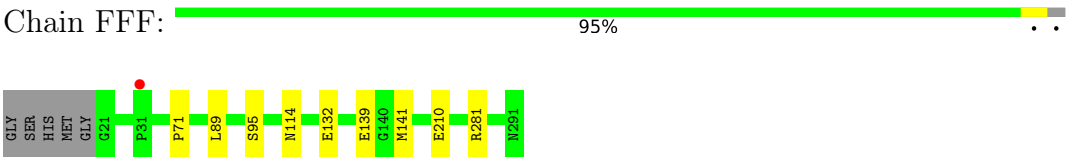
Chain EEE:





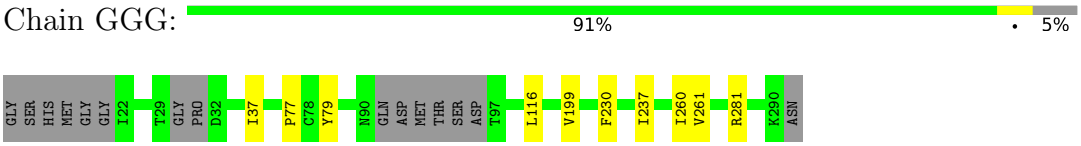
• Molecule 1: Capsid protein VP1

Chain FFF:



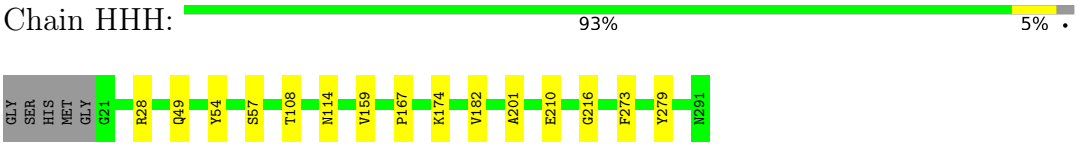
• Molecule 1: Capsid protein VP1

Chain GGG:



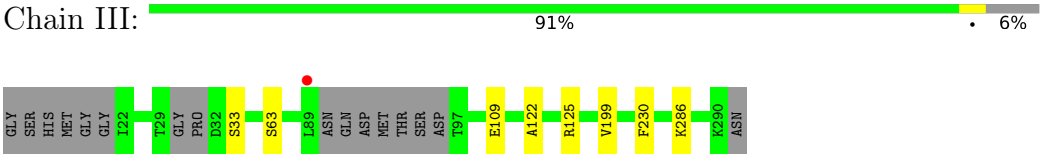
• Molecule 1: Capsid protein VP1

Chain HHH:



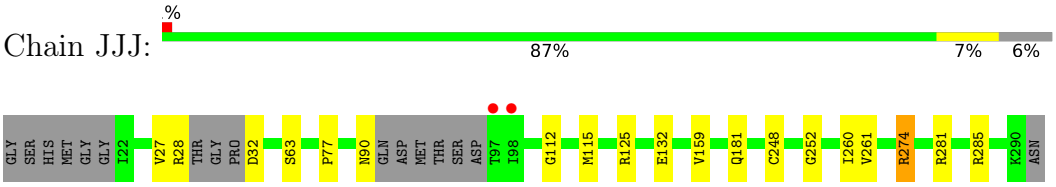
• Molecule 1: Capsid protein VP1

Chain III:



• Molecule 1: Capsid protein VP1

Chain JJJ:



• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

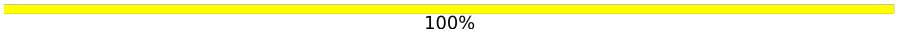
Chain AaA:

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain BaB:

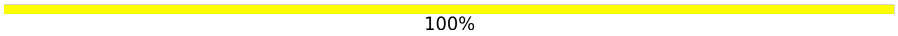
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain DaD:



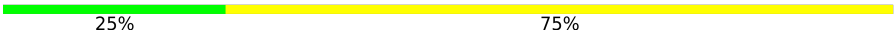
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain FbF:



• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain HaH:

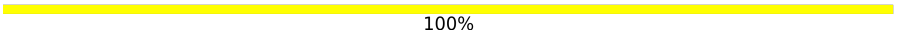


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain IaI:

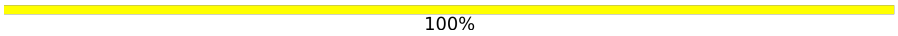
• Molecule 3: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain CaC:



• Molecule 3: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain EaE:



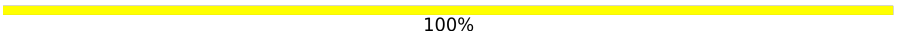
• Molecule 3: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopy

ranose

Chain GaG:

• Molecule 3: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain JaJ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	130.49Å 130.49Å 222.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.71 – 1.92 42.71 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.71-1.92) 99.8 (42.71-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.149 , 0.176 0.154 , 0.180	Depositor DCC
R_{free} test set	3211 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l 0.209 for h,-h-k,-l 0.050 for -k,-h,-l	Xtriage
Reported twinning fraction	0.784 for H, K, L 0.216 for K, H, -L	Depositor
Outliers	0 of 321066 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	23447	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, GLA, BGC, MG, GAL, NGA, A2G, EDO, PEG, PGE

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	AAA	0.75	0/2124	0.84	0/2886
1	BBB	0.72	0/2062	0.85	0/2802
1	CCC	0.72	0/2070	0.86	0/2811
1	DDD	0.72	0/2134	0.87	0/2903
1	EEE	0.72	0/2085	0.85	0/2832
1	FFF	0.75	0/2159	0.89	0/2934
1	GGG	0.73	0/2075	0.86	0/2819
1	HHH	0.74	0/2161	0.87	0/2936
1	III	0.71	0/2057	0.85	0/2797
1	JJJ	0.73	0/2080	0.85	0/2825
All	All	0.73	0/21007	0.86	0/28545

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2070	0	1988	10	0
1	BBB	2009	0	1920	8	0
1	CCC	2017	0	1940	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	2079	0	1988	9	0
1	EEE	2032	0	1946	10	0
1	FFF	2103	0	2020	8	0
1	GGG	2022	0	1939	8	0
1	HHH	2105	0	2025	12	0
1	III	2004	0	1921	6	0
1	JJJ	2027	0	1955	10	0
2	AaA	51	0	44	0	0
2	BaB	51	0	44	0	0
2	DaD	51	0	44	0	0
2	FbF	51	0	44	0	0
2	HaH	51	0	44	0	0
2	IaI	51	0	44	0	0
3	CaC	62	0	53	0	0
3	EaE	62	0	53	0	0
3	GaG	62	0	53	0	0
3	JaJ	62	0	53	0	0
4	AAA	8	0	14	1	0
4	BBB	8	0	14	0	0
4	DDD	8	0	14	1	0
4	FFF	16	0	28	1	0
4	HHH	16	0	28	0	0
4	III	8	0	14	1	0
4	JJJ	8	0	14	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
5	EEE	1	0	0	0	0
5	FFF	1	0	0	0	0
5	GGG	1	0	0	0	0
5	HHH	1	0	0	0	0
5	III	1	0	0	0	0
5	JJJ	1	0	0	0	0
6	CCC	4	0	6	0	0
6	DDD	8	0	12	0	0
6	EEE	4	0	6	0	0
6	HHH	4	0	6	0	0
6	JJJ	4	0	6	0	0
7	CCC	7	0	10	2	0
7	EEE	7	0	10	0	0
7	GGG	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	HHH	7	0	10	0	0
7	III	7	0	10	0	0
8	FFF	10	0	14	0	0
8	GGG	10	0	14	0	0
8	III	10	0	14	0	0
9	AAA	225	0	0	1	0
9	BBB	197	0	0	3	0
9	CCC	209	0	0	5	0
9	DDD	241	0	0	1	0
9	EEE	208	0	0	1	0
9	FFF	259	0	0	2	0
9	GGG	219	0	0	0	0
9	HHH	250	0	0	7	0
9	III	219	0	0	1	0
9	JJJ	227	0	0	3	0
All	All	23447	0	20372	82	0

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

The worst 5 of 82 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:JJJ:281:ARG:NH2	9:JJJ:501:HOH:O	2.22	0.70
1:HHH:174:LYS:NZ	9:HHH:504:HOH:O	2.32	0.62
1:AAA:65:ASP:HB2	9:AAA:510:HOH:O	2.00	0.61
1:HHH:210:GLU:HG3	9:HHH:532:HOH:O	2.00	0.61
1:DDD:49:GLN:HG2	1:DDD:54:TYR:CZ	2.37	0.59

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	AAA	264/276 (96%)	252 (96%)	12 (4%)	0	100 100
1	BBB	255/276 (92%)	244 (96%)	11 (4%)	0	100 100
1	CCC	256/276 (93%)	246 (96%)	10 (4%)	0	100 100
1	DDD	268/276 (97%)	257 (96%)	11 (4%)	0	100 100
1	EEE	257/276 (93%)	246 (96%)	10 (4%)	1 (0%)	34 24
1	FFF	270/276 (98%)	259 (96%)	11 (4%)	0	100 100
1	GGG	256/276 (93%)	244 (95%)	12 (5%)	0	100 100
1	HHH	270/276 (98%)	260 (96%)	9 (3%)	1 (0%)	34 24
1	III	255/276 (92%)	243 (95%)	12 (5%)	0	100 100
1	JJJ	255/276 (92%)	244 (96%)	11 (4%)	0	100 100
All	All	2606/2760 (94%)	2495 (96%)	109 (4%)	2 (0%)	51 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EEE	182	VAL
1	HHH	182	VAL

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	AAA	221/234 (94%)	217 (98%)	4 (2%)	59 53
1	BBB	212/234 (91%)	212 (100%)	0	100 100
1	CCC	213/234 (91%)	212 (100%)	1 (0%)	88 89
1	DDD	222/234 (95%)	220 (99%)	2 (1%)	78 78
1	EEE	216/234 (92%)	216 (100%)	0	100 100
1	FFF	226/234 (97%)	224 (99%)	2 (1%)	78 78
1	GGG	214/234 (92%)	214 (100%)	0	100 100
1	HHH	227/234 (97%)	227 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	III	213/234 (91%)	213 (100%)	0	100 100
1	JJJ	218/234 (93%)	214 (98%)	4 (2%)	59 53
All	All	2182/2340 (93%)	2169 (99%)	13 (1%)	86 86

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FFF	95	SER
1	FFF	132	GLU
1	JJJ	274	ARG
1	JJJ	90	ASN
1	JJJ	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

44 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	AaA	1	2	12,12,12	0.48	0	17,17,17	0.67	0
2	GLA	AaA	2	2	11,11,12	0.54	0	15,15,17	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NGA	AaA	3	2	14,14,15	0.86	0	17,19,21	1.34	1 (5%)
2	A2G	AaA	4	2	14,14,15	0.67	0	17,19,21	1.26	1 (5%)
2	GAL	BaB	1	2	12,12,12	0.71	0	17,17,17	1.44	3 (17%)
2	GLA	BaB	2	2	11,11,12	1.10	1 (9%)	15,15,17	0.77	0
2	NGA	BaB	3	2	14,14,15	0.91	0	17,19,21	1.19	2 (11%)
2	A2G	BaB	4	2	14,14,15	0.99	0	17,19,21	1.44	3 (17%)
3	BGC	CaC	1	3	12,12,12	0.49	0	17,17,17	1.15	2 (11%)
3	GAL	CaC	2	3	11,11,12	0.65	0	15,15,17	2.31	6 (40%)
3	GLA	CaC	3	3	11,11,12	0.89	0	15,15,17	1.79	3 (20%)
3	NGA	CaC	4	3	14,14,15	0.74	0	17,19,21	1.34	3 (17%)
3	A2G	CaC	5	3	14,14,15	0.50	0	17,19,21	1.28	1 (5%)
2	GAL	DaD	1	2	12,12,12	0.69	0	17,17,17	1.11	1 (5%)
2	GLA	DaD	2	2	11,11,12	0.54	0	15,15,17	1.31	1 (6%)
2	NGA	DaD	3	2	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
2	A2G	DaD	4	2	14,14,15	0.81	0	17,19,21	1.60	1 (5%)
3	BGC	EaE	1	3	12,12,12	0.55	0	17,17,17	1.72	5 (29%)
3	GAL	EaE	2	3	11,11,12	0.55	0	15,15,17	1.82	3 (20%)
3	GLA	EaE	3	3	11,11,12	0.80	0	15,15,17	1.65	3 (20%)
3	NGA	EaE	4	3	14,14,15	0.75	0	17,19,21	1.08	1 (5%)
3	A2G	EaE	5	3	14,14,15	0.73	0	17,19,21	1.89	4 (23%)
2	GAL	FbF	1	2	12,12,12	0.65	0	17,17,17	1.18	1 (5%)
2	GLA	FbF	2	2	11,11,12	0.63	0	15,15,17	1.83	5 (33%)
2	NGA	FbF	3	2	14,14,15	0.90	0	17,19,21	1.30	3 (17%)
2	A2G	FbF	4	2	14,14,15	0.42	0	17,19,21	1.70	3 (17%)
3	BGC	GaG	1	3	12,12,12	0.56	0	17,17,17	1.04	0
3	GAL	GaG	2	3	11,11,12	0.80	0	15,15,17	2.19	7 (46%)
3	GLA	GaG	3	3	11,11,12	0.86	0	15,15,17	1.43	3 (20%)
3	NGA	GaG	4	3	14,14,15	0.77	0	17,19,21	1.87	6 (35%)
3	A2G	GaG	5	3	14,14,15	0.84	0	17,19,21	1.44	2 (11%)
2	GAL	HaH	1	2	12,12,12	0.59	0	17,17,17	0.95	0
2	GLA	HaH	2	2	11,11,12	0.75	0	15,15,17	1.38	3 (20%)
2	NGA	HaH	3	2	14,14,15	0.87	0	17,19,21	1.06	2 (11%)
2	A2G	HaH	4	2	14,14,15	0.54	0	17,19,21	1.12	2 (11%)
2	GAL	IaI	1	2	12,12,12	0.47	0	17,17,17	0.99	0
2	GLA	IaI	2	2	11,11,12	0.93	1 (9%)	15,15,17	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NGA	IaI	3	2	14,14,15	1.01	0	17,19,21	1.47	3 (17%)
2	A2G	IaI	4	2	14,14,15	0.91	1 (7%)	17,19,21	1.56	4 (23%)
3	BGC	JaJ	1	3	12,12,12	0.57	0	17,17,17	1.90	4 (23%)
3	GAL	JaJ	2	3	11,11,12	0.82	0	15,15,17	1.47	2 (13%)
3	GLA	JaJ	3	3	11,11,12	1.24	1 (9%)	15,15,17	2.34	5 (33%)
3	NGA	JaJ	4	3	14,14,15	0.81	0	17,19,21	1.08	1 (5%)
3	A2G	JaJ	5	3	14,14,15	0.82	0	17,19,21	1.19	2 (11%)

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	AaA	1	2	-	0/2/22/22	0/1/1/1
2	GLA	AaA	2	2	-	1/2/19/22	0/1/1/1
2	NGA	AaA	3	2	-	0/6/23/26	0/1/1/1
2	A2G	AaA	4	2	-	0/6/23/26	0/1/1/1
2	GAL	BaB	1	2	-	2/2/22/22	0/1/1/1
2	GLA	BaB	2	2	-	1/2/19/22	0/1/1/1
2	NGA	BaB	3	2	-	0/6/23/26	0/1/1/1
2	A2G	BaB	4	2	-	1/6/23/26	0/1/1/1
3	BGC	CaC	1	3	-	2/2/22/22	0/1/1/1
3	GAL	CaC	2	3	-	1/2/19/22	0/1/1/1
3	GLA	CaC	3	3	-	2/2/19/22	0/1/1/1
3	NGA	CaC	4	3	-	0/6/23/26	0/1/1/1
3	A2G	CaC	5	3	-	0/6/23/26	0/1/1/1
2	GAL	DaD	1	2	-	1/2/22/22	0/1/1/1
2	GLA	DaD	2	2	-	1/2/19/22	0/1/1/1
2	NGA	DaD	3	2	-	0/6/23/26	0/1/1/1
2	A2G	DaD	4	2	-	0/6/23/26	0/1/1/1
3	BGC	EaE	1	3	-	2/2/22/22	0/1/1/1
3	GAL	EaE	2	3	-	0/2/19/22	0/1/1/1
3	GLA	EaE	3	3	-	1/2/19/22	0/1/1/1
3	NGA	EaE	4	3	-	0/6/23/26	0/1/1/1
3	A2G	EaE	5	3	-	0/6/23/26	0/1/1/1
2	GAL	FbF	1	2	-	0/2/22/22	0/1/1/1
2	GLA	FbF	2	2	-	1/2/19/22	0/1/1/1
2	NGA	FbF	3	2	-	0/6/23/26	0/1/1/1
2	A2G	FbF	4	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	GaG	1	3	-	0/2/22/22	0/1/1/1
3	GAL	GaG	2	3	-	1/2/19/22	0/1/1/1
3	GLA	GaG	3	3	-	1/2/19/22	0/1/1/1
3	NGA	GaG	4	3	-	0/6/23/26	0/1/1/1
3	A2G	GaG	5	3	-	0/6/23/26	0/1/1/1
2	GAL	HaH	1	2	-	2/2/22/22	0/1/1/1
2	GLA	HaH	2	2	-	2/2/19/22	0/1/1/1
2	NGA	HaH	3	2	-	0/6/23/26	0/1/1/1
2	A2G	HaH	4	2	-	0/6/23/26	0/1/1/1
2	GAL	IaI	1	2	-	2/2/22/22	0/1/1/1
2	GLA	IaI	2	2	-	1/2/19/22	0/1/1/1
2	NGA	IaI	3	2	-	1/6/23/26	0/1/1/1
2	A2G	IaI	4	2	-	0/6/23/26	0/1/1/1
3	BGC	JaJ	1	3	-	0/2/22/22	0/1/1/1
3	GAL	JaJ	2	3	-	1/2/19/22	0/1/1/1
3	GLA	JaJ	3	3	-	1/2/19/22	0/1/1/1
3	NGA	JaJ	4	3	-	0/6/23/26	0/1/1/1
3	A2G	JaJ	5	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	2	GLA	C2-C3	-2.86	1.48	1.52
3	JaJ	3	GLA	C4-C5	2.30	1.57	1.53
2	IaI	2	GLA	C2-C3	-2.24	1.49	1.52
2	IaI	4	A2G	C1-C2	2.05	1.55	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CaC	2	GAL	C1-O5-C5	5.49	119.64	112.19
3	JaJ	3	GLA	C1-C2-C3	5.24	116.11	109.67
3	JaJ	1	BGC	C4-C3-C2	-5.11	101.90	110.82
3	GaG	2	GAL	C1-O5-C5	4.98	118.94	112.19
3	CaC	3	GLA	C1-C2-C3	4.88	115.66	109.67

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BaB	1	GAL	O5-C5-C6-O6

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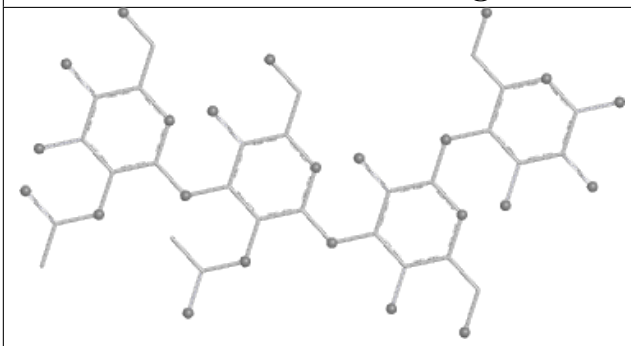
Mol	Chain	Res	Type	Atoms
2	HaH	2	GLA	O5-C5-C6-O6
3	EaE	1	BGC	C4-C5-C6-O6
2	HaH	1	GAL	O5-C5-C6-O6
3	CaC	3	GLA	O5-C5-C6-O6

There are no ring outliers.

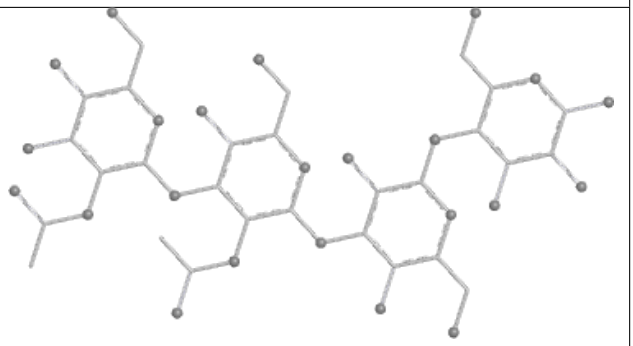
No monomer is involved in short contacts.

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

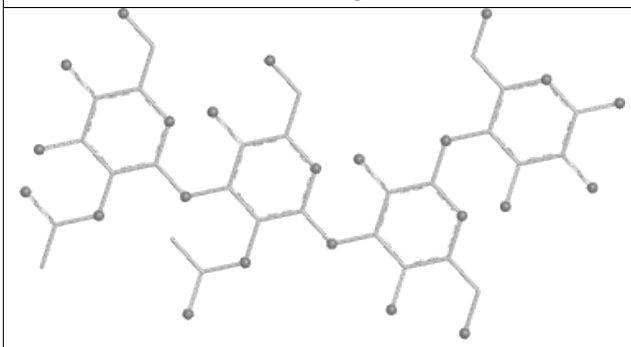
Oligosaccharide Chain AaA



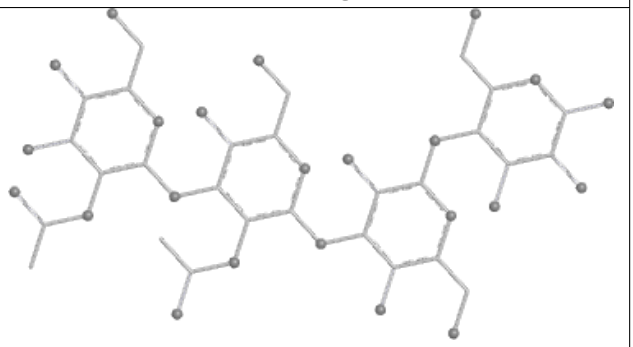
Bond lengths



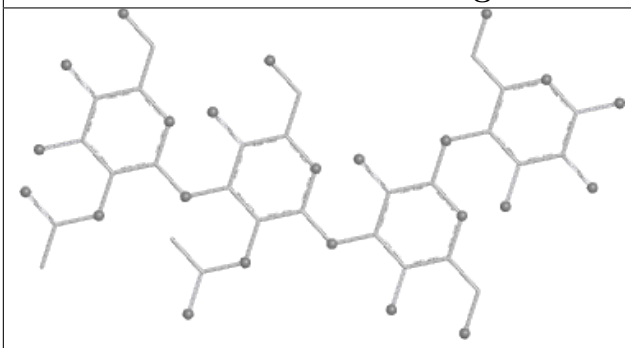
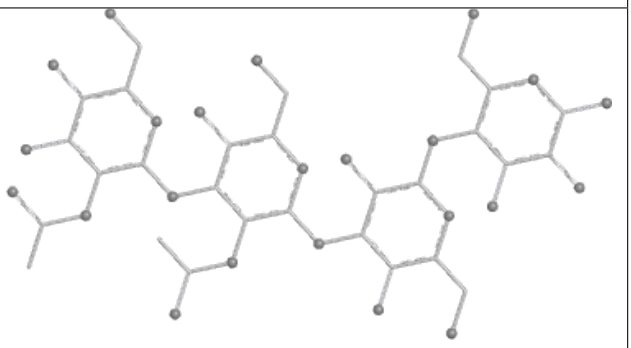
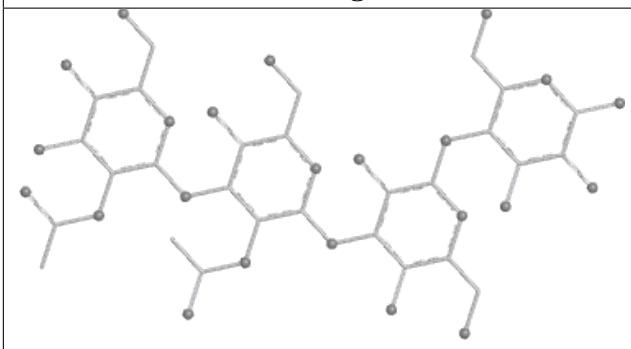
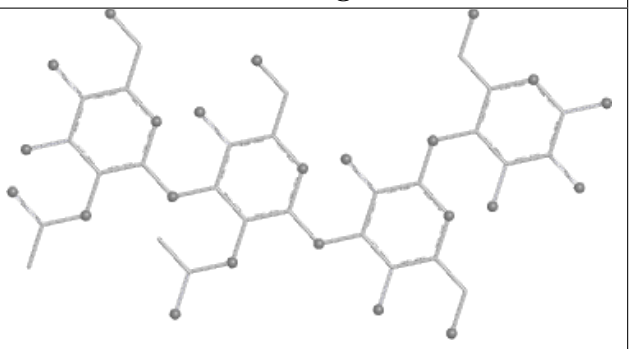
Bond angles

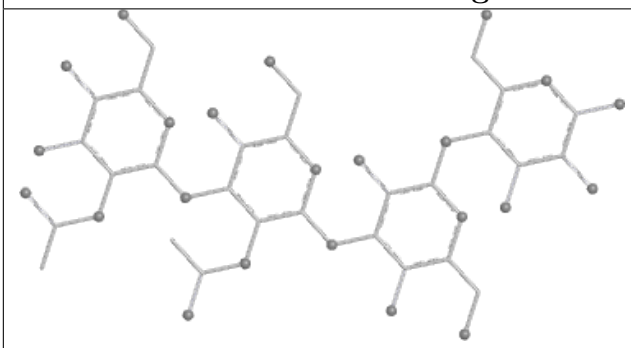
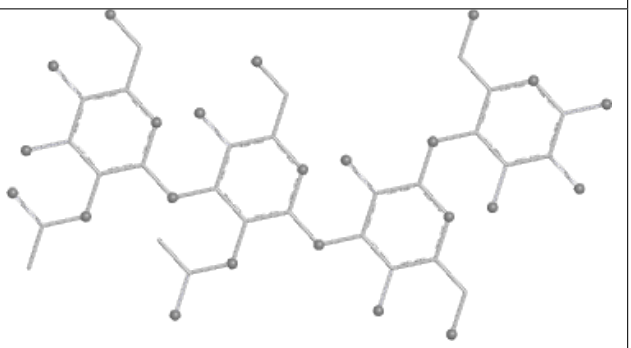
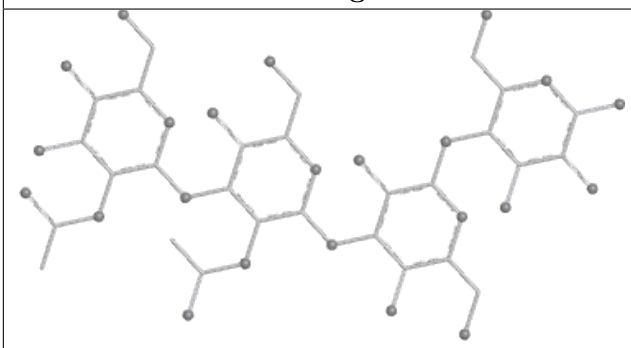
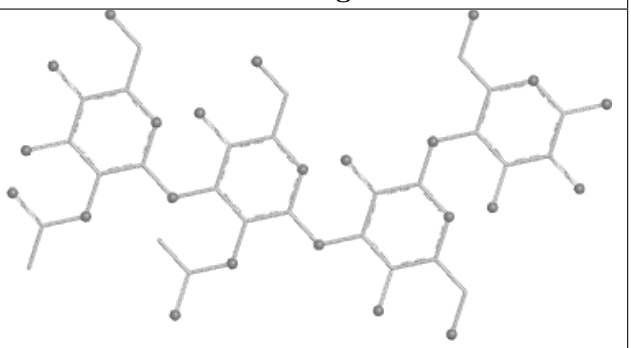


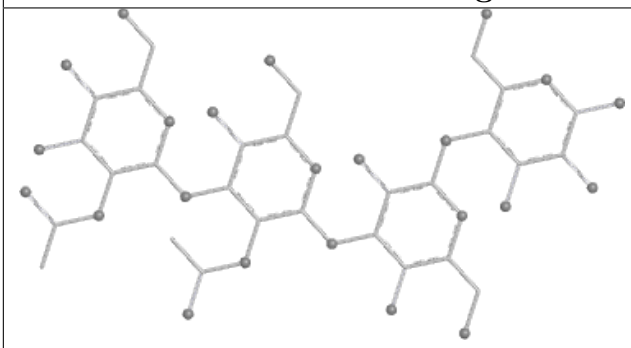
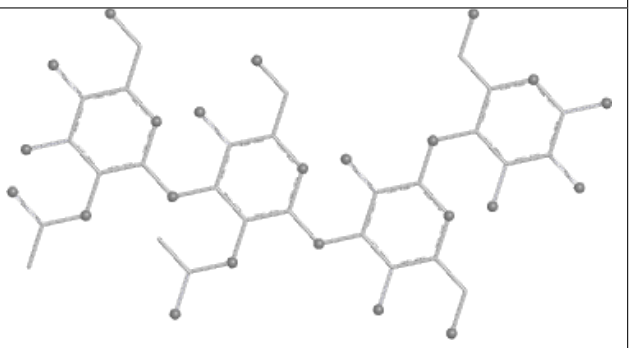
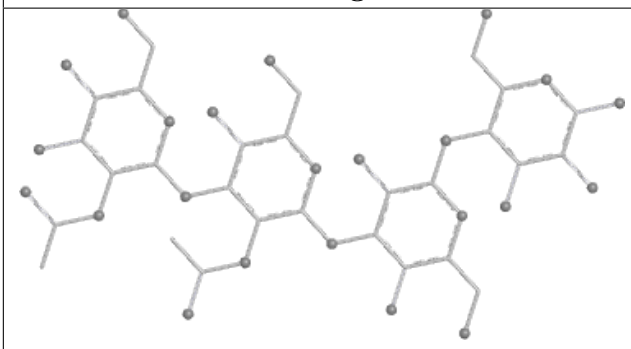
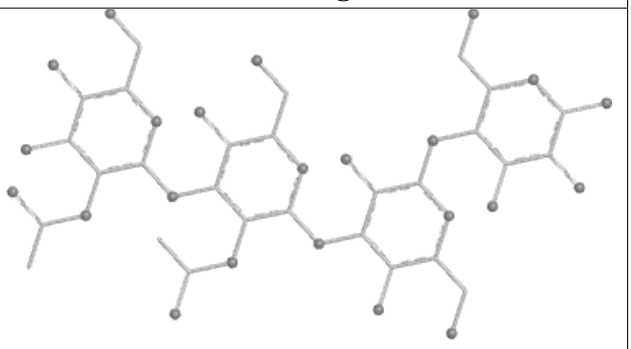
Torsions

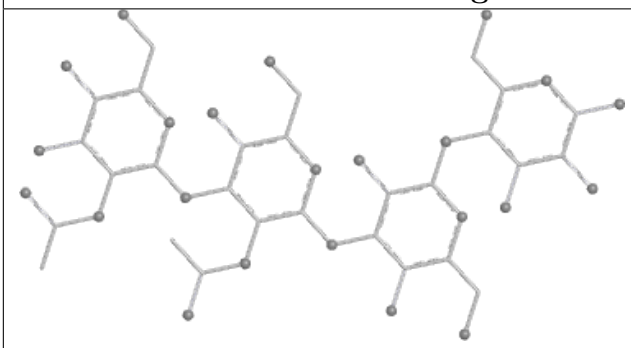
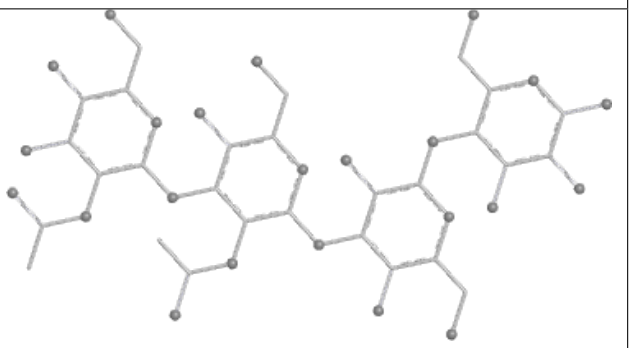
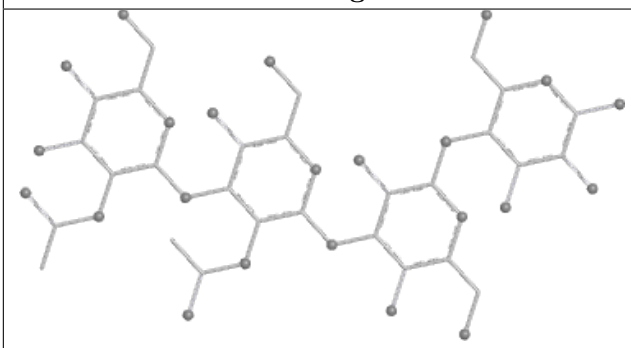
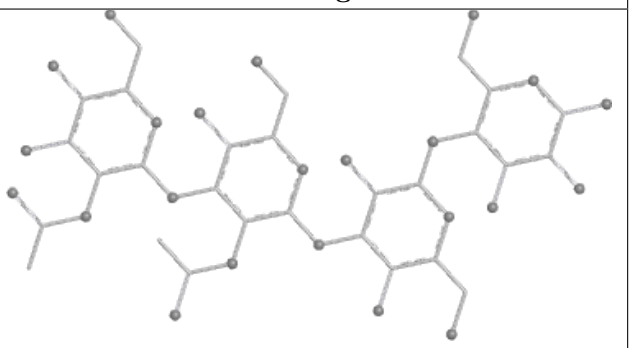


Rings

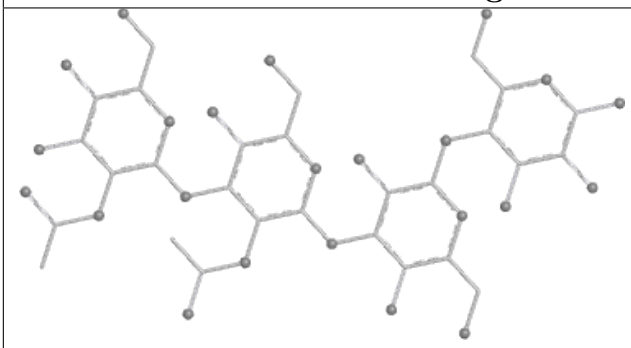
Oligosaccharide Chain BaB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain DaD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

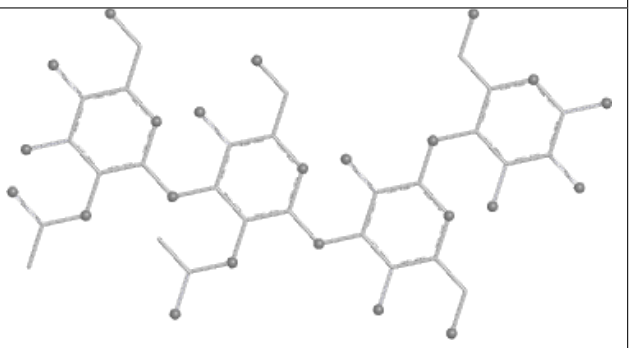
Oligosaccharide Chain FbF	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain HaH	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

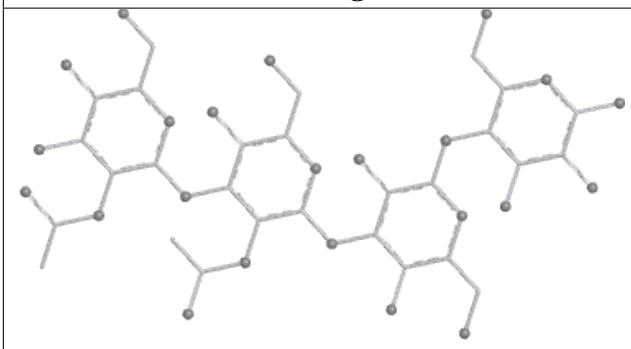
Oligosaccharide Chain IaI



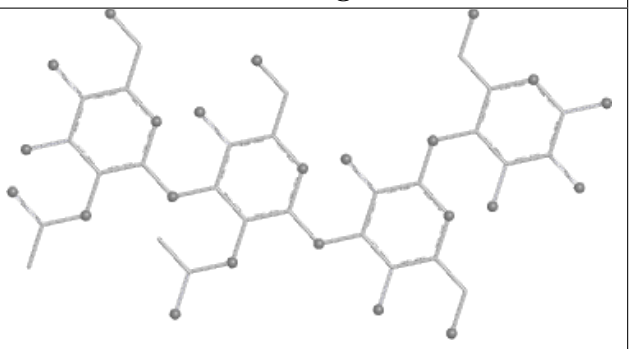
Bond lengths



Bond angles

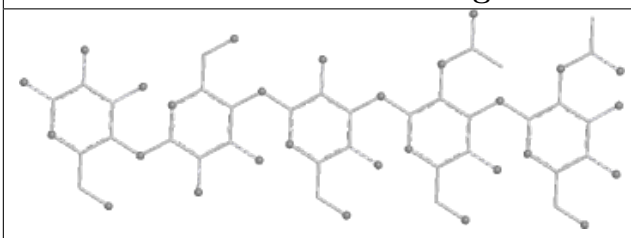


Torsions

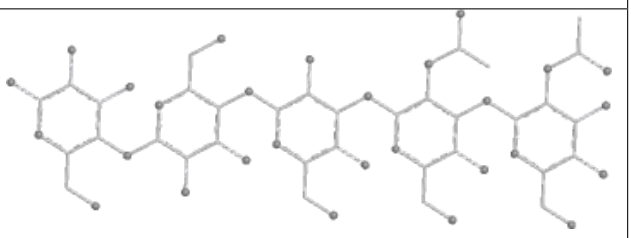


Rings

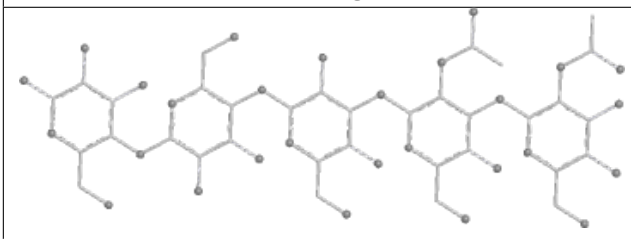
Oligosaccharide Chain CaC



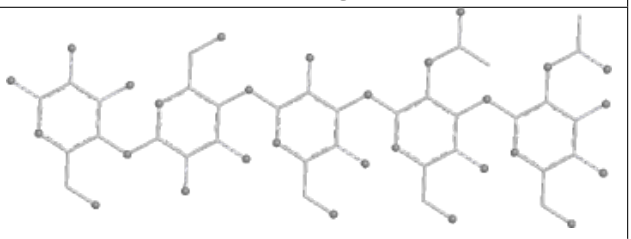
Bond lengths



Bond angles

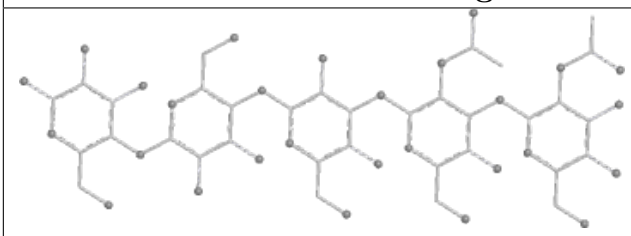


Torsions

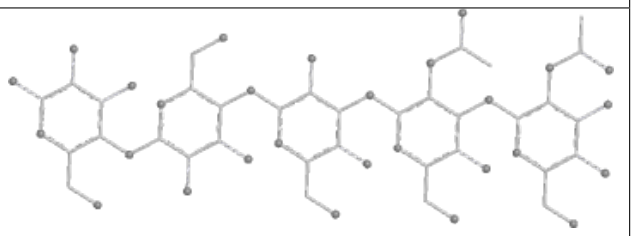


Rings

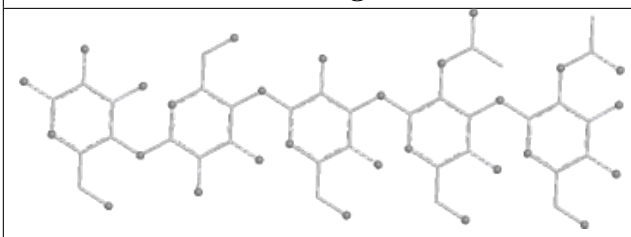
Oligosaccharide Chain EaE



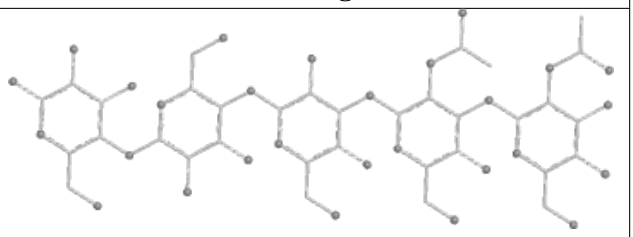
Bond lengths



Bond angles

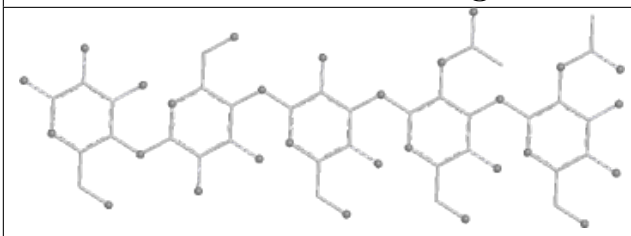


Torsions

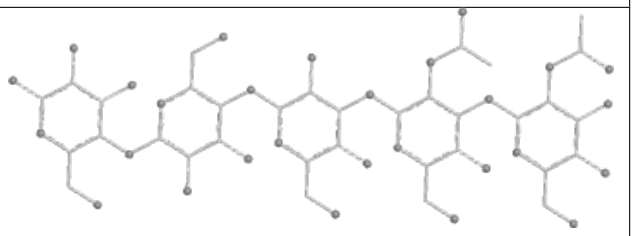


Rings

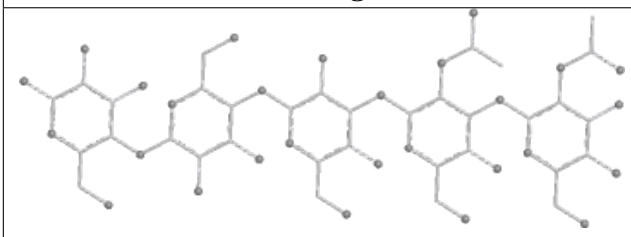
Oligosaccharide Chain GaG



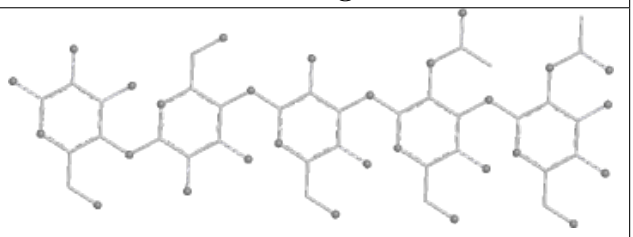
Bond lengths



Bond angles

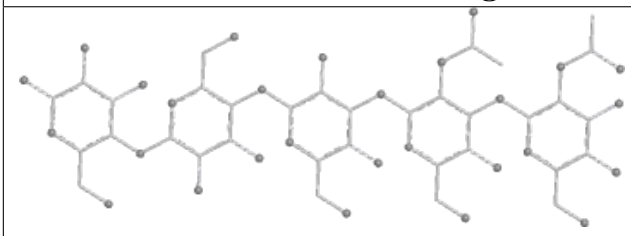


Torsions

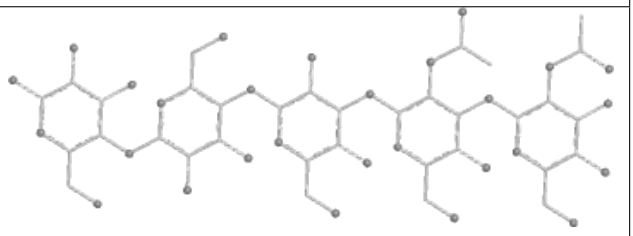


Rings

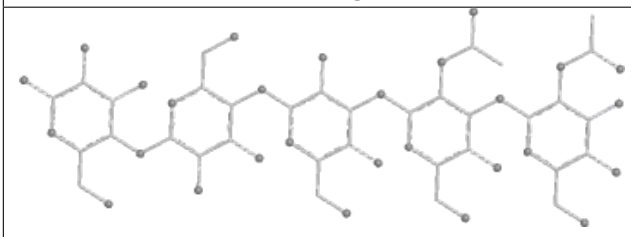
Oligosaccharide Chain JaJ



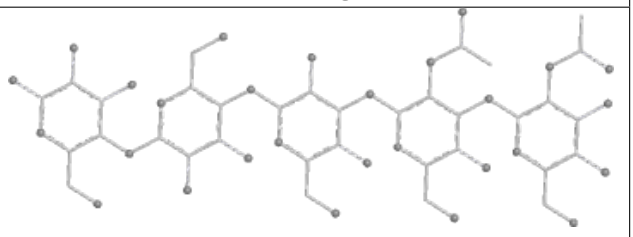
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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	MPD	HHH	401	-	7,7,7	0.21	0	9,10,10	0.66	0
4	MPD	HHH	402	-	7,7,7	0.28	0	9,10,10	0.65	0
7	PEG	CCC	502	-	6,6,6	0.43	0	5,5,5	0.38	0
6	EDO	DDD	403	-	3,3,3	0.20	0	2,2,2	0.30	0
4	MPD	DDD	401	-	7,7,7	0.14	0	9,10,10	0.69	0
4	MPD	JJJ	401	-	7,7,7	0.32	0	9,10,10	0.38	0
8	PGE	GGG	2302	-	9,9,9	0.25	0	8,8,8	0.22	0
6	EDO	EEE	401	-	3,3,3	0.12	0	2,2,2	0.42	0
7	PEG	GGG	2301	-	6,6,6	0.24	0	5,5,5	0.17	0
7	PEG	EEE	402	-	6,6,6	0.20	0	5,5,5	0.13	0
4	MPD	III	401	-	7,7,7	0.20	0	9,10,10	0.59	0
4	MPD	FFF	303	-	7,7,7	0.20	0	9,10,10	0.59	0
7	PEG	HHH	403	-	6,6,6	0.16	0	5,5,5	0.17	0
7	PEG	III	402	-	6,6,6	0.14	0	5,5,5	0.15	0
6	EDO	DDD	402	-	3,3,3	0.12	0	2,2,2	0.26	0
6	EDO	CCC	501	-	3,3,3	0.10	0	2,2,2	0.21	0
4	MPD	FFF	302	-	7,7,7	0.16	0	9,10,10	0.53	0
8	PGE	FFF	301	-	9,9,9	0.27	0	8,8,8	0.20	0
6	EDO	HHH	404	-	3,3,3	0.24	0	2,2,2	0.47	0
6	EDO	JJJ	402	-	3,3,3	0.13	0	2,2,2	0.27	0
8	PGE	III	403	-	9,9,9	0.23	0	8,8,8	0.17	0
4	MPD	BBB	401	-	7,7,7	0.22	0	9,10,10	0.27	0
4	MPD	AAA	401	-	7,7,7	0.26	0	9,10,10	0.39	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	MPD	HHH	401	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	HHH	402	-	-	1/5/5/5	-
7	PEG	CCC	502	-	-	3/4/4/4	-
6	EDO	DDD	403	-	-	0/1/1/1	-
4	MPD	DDD	401	-	-	1/5/5/5	-
4	MPD	JJJ	401	-	-	3/5/5/5	-
8	PGE	GGG	2302	-	-	4/7/7/7	-
6	EDO	EEE	401	-	-	1/1/1/1	-
7	PEG	GGG	2301	-	-	3/4/4/4	-
7	PEG	EEE	402	-	-	2/4/4/4	-
4	MPD	III	401	-	-	2/5/5/5	-
4	MPD	FFF	303	-	-	1/5/5/5	-
7	PEG	HHH	403	-	-	2/4/4/4	-
7	PEG	III	402	-	-	3/4/4/4	-
6	EDO	DDD	402	-	-	1/1/1/1	-
6	EDO	CCC	501	-	-	1/1/1/1	-
4	MPD	FFF	302	-	-	3/5/5/5	-
8	PGE	FFF	301	-	-	5/7/7/7	-
6	EDO	HHH	404	-	-	1/1/1/1	-
6	EDO	JJJ	402	-	-	0/1/1/1	-
8	PGE	III	403	-	-	4/7/7/7	-
4	MPD	BBB	401	-	-	0/5/5/5	-
4	MPD	AAA	401	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	HHH	401	MPD	O2-C2-C3-C4
4	HHH	401	MPD	CM-C2-C3-C4
7	CCC	502	PEG	O2-C3-C4-O4
7	III	402	PEG	O1-C1-C2-O2
8	FFF	301	PGE	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	CCC	502	PEG	2	0
4	DDD	401	MPD	1	0
4	III	401	MPD	1	0
4	FFF	302	MPD	1	0
4	AAA	401	MPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	267/276 (96%)	-0.47	1 (0%) 92 93	24, 29, 43, 52	0
1	BBB	260/276 (94%)	-0.39	2 (0%) 86 87	19, 31, 50, 72	0
1	CCC	261/276 (94%)	-0.44	0 100 100	20, 28, 52, 76	0
1	DDD	269/276 (97%)	-0.47	1 (0%) 92 93	19, 27, 43, 59	0
1	EEE	262/276 (94%)	-0.46	2 (0%) 86 87	21, 28, 50, 71	0
1	FFF	271/276 (98%)	-0.50	1 (0%) 92 93	18, 24, 42, 58	0
1	GGG	261/276 (94%)	-0.47	0 100 100	20, 25, 49, 70	0
1	HHH	271/276 (98%)	-0.50	0 100 100	20, 27, 42, 62	0
1	III	260/276 (94%)	-0.40	1 (0%) 92 93	21, 29, 48, 75	0
1	JJJ	260/276 (94%)	-0.42	2 (0%) 86 87	18, 27, 50, 68	0
All	All	2642/2760 (95%)	-0.45	10 (0%) 92 93	18, 28, 48, 76	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	22	ILE	5.2
1	AAA	29	THR	2.9
1	III	89	LEU	2.6
1	FFF	31	PRO	2.5
1	BBB	89	LEU	2.5

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	CaC	1	12/12	0.85	0.23	38,47,54,62	0
3	BGC	GaG	1	12/12	0.86	0.18	39,52,68,69	0
3	BGC	JaJ	1	12/12	0.89	0.18	40,47,64,68	0
3	BGC	EaE	1	12/12	0.90	0.17	41,49,58,64	0
2	GAL	HaH	1	12/12	0.91	0.08	41,47,52,55	0
2	GLA	BaB	2	11/12	0.93	0.10	29,31,34,35	0
2	GAL	BaB	1	12/12	0.93	0.09	42,48,56,57	0
3	GAL	CaC	2	11/12	0.94	0.11	25,30,35,42	0
2	GAL	IaI	1	12/12	0.94	0.08	40,45,53,61	0
3	GAL	JaJ	2	11/12	0.94	0.09	30,32,37,38	0
3	A2G	EaE	5	14/15	0.95	0.09	27,30,35,36	0
2	GLA	IaI	2	11/12	0.95	0.09	29,32,35,35	0
2	A2G	AaA	4	14/15	0.96	0.07	30,32,36,36	0
2	NGA	HaH	3	14/15	0.96	0.10	29,31,34,35	0
3	GAL	EaE	2	11/12	0.96	0.09	34,37,44,50	0
3	NGA	EaE	4	14/15	0.96	0.07	27,30,31,33	0
2	GAL	AaA	1	12/12	0.96	0.06	36,43,50,51	0
2	GLA	AaA	2	11/12	0.96	0.07	29,32,34,38	0
3	NGA	GaG	4	14/15	0.96	0.08	22,25,27,29	0
3	A2G	GaG	5	14/15	0.96	0.08	26,27,31,35	0
2	NGA	IaI	3	14/15	0.96	0.09	25,28,31,33	0
2	GAL	DaD	1	12/12	0.96	0.08	32,40,43,54	0
3	GLA	JaJ	3	11/12	0.96	0.08	22,24,26,27	0
3	NGA	JaJ	4	14/15	0.96	0.08	21,25,26,26	0
3	GLA	EaE	3	11/12	0.97	0.08	26,28,30,31	0
2	NGA	AaA	3	14/15	0.97	0.09	26,28,33,34	0
2	GAL	FbF	1	12/12	0.97	0.07	27,38,47,48	0
2	A2G	FbF	4	14/15	0.97	0.08	22,25,30,31	0
3	GAL	GaG	2	11/12	0.97	0.08	30,33,38,43	0
3	GLA	GaG	3	11/12	0.97	0.08	23,25,27,27	0
2	A2G	IaI	4	14/15	0.97	0.07	26,31,37,39	0
2	NGA	BaB	3	14/15	0.97	0.07	25,30,32,33	0
2	GLA	HaH	2	11/12	0.97	0.08	28,30,32,33	0
3	A2G	CaC	5	14/15	0.97	0.09	22,23,28,32	0
2	A2G	BaB	4	14/15	0.97	0.07	25,27,39,43	0
2	A2G	HaH	4	14/15	0.97	0.09	29,32,35,38	0
3	A2G	JaJ	5	14/15	0.97	0.07	23,24,29,33	0

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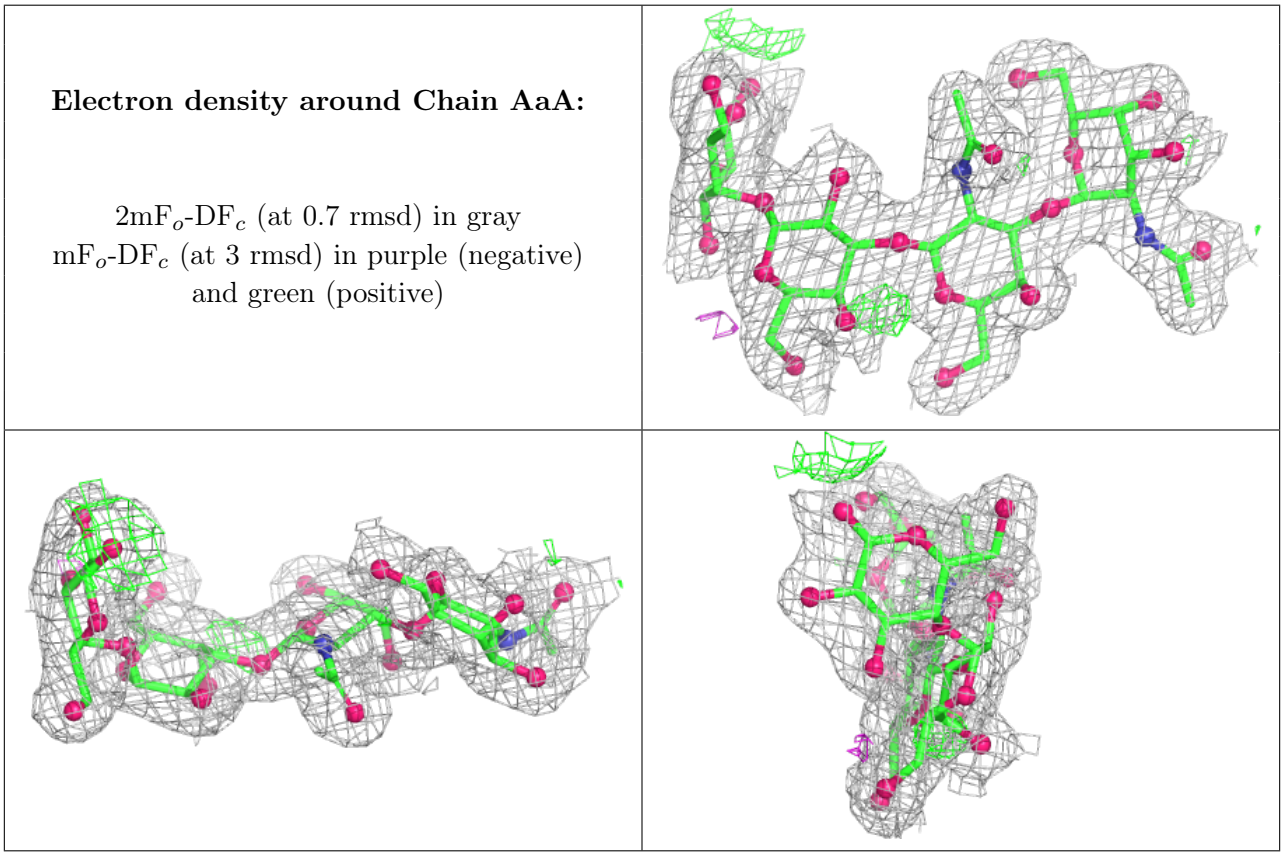
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NGA	DaD	3	14/15	0.98	0.08	20,22,25,27	0
2	A2G	DaD	4	14/15	0.98	0.07	21,25,32,34	0
2	GLA	DaD	2	11/12	0.98	0.08	25,26,26,27	0
3	GLA	CaC	3	11/12	0.98	0.09	22,24,26,26	0
2	GLA	FbF	2	11/12	0.98	0.09	23,25,26,27	0
2	NGA	FbF	3	14/15	0.99	0.08	20,23,28,29	0
3	NGA	CaC	4	14/15	0.99	0.08	21,23,26,28	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.

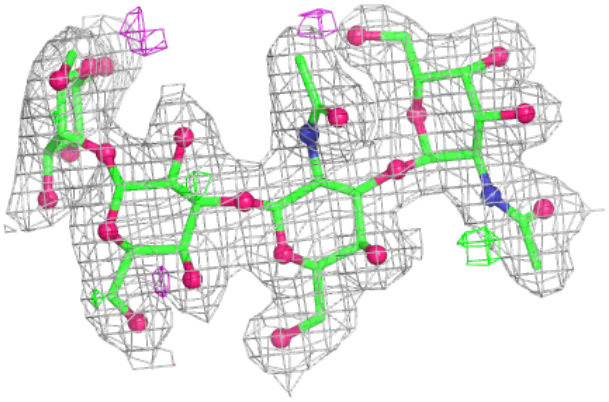
Electron density around Chain AaA:

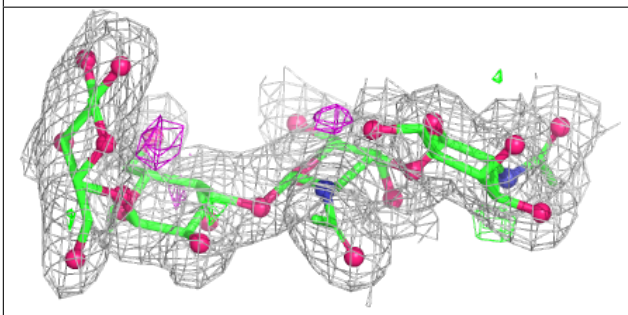
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

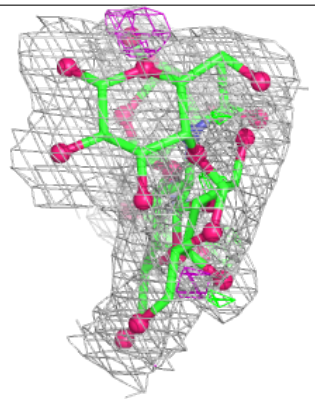


Electron density around Chain BaB:

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

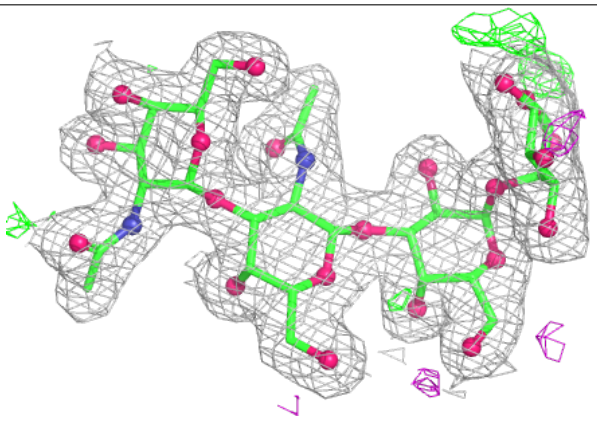


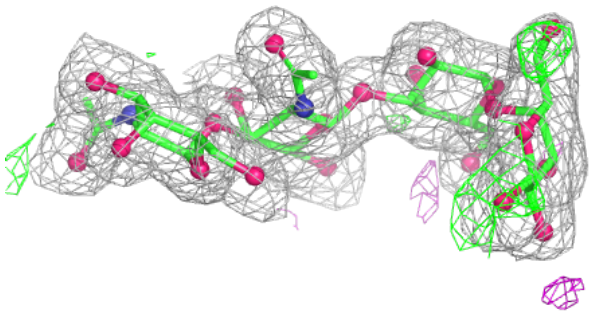


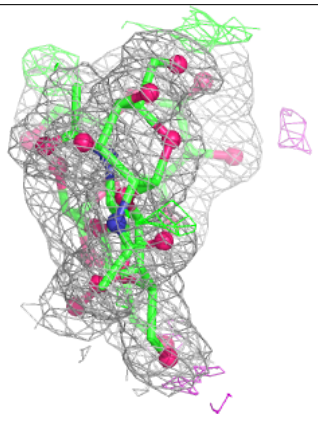


Electron density around Chain DaD:

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

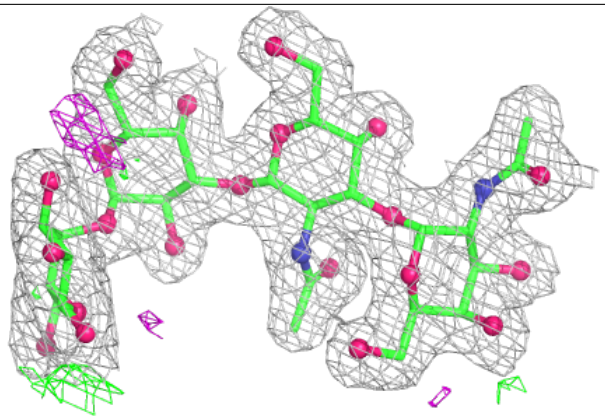


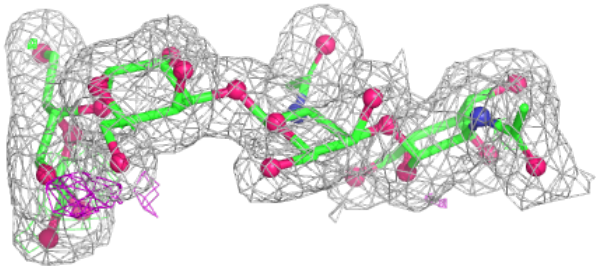


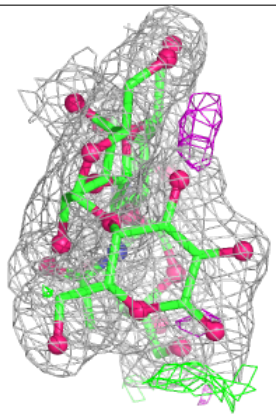


Electron density around Chain FbF:

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

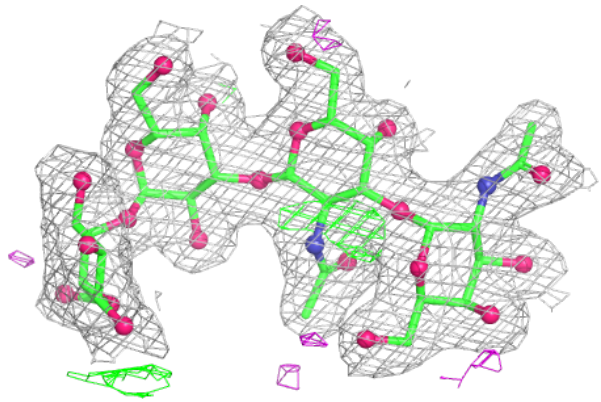


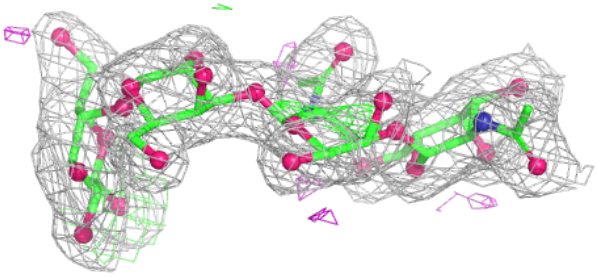


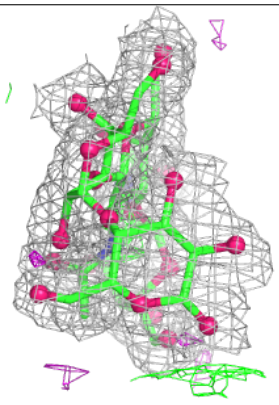


Electron density around Chain HaH:

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

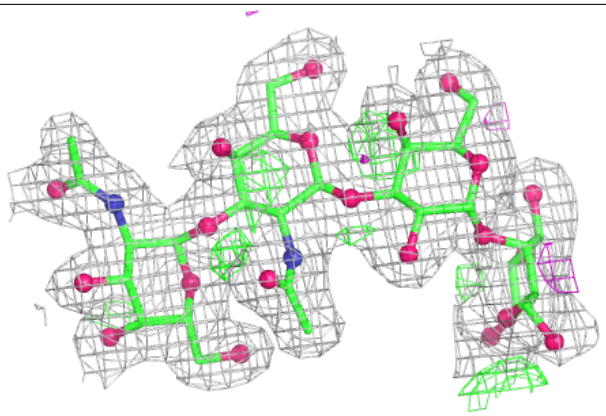


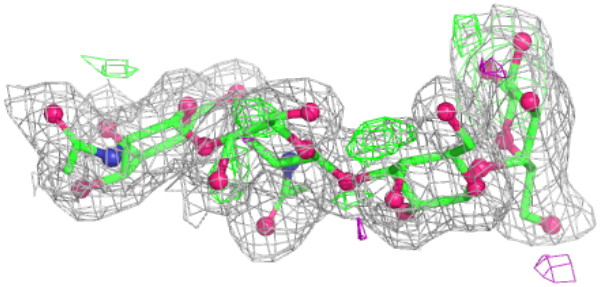


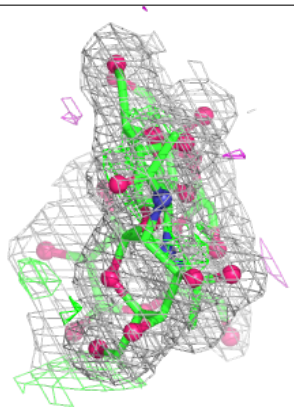


Electron density around Chain IaI:

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

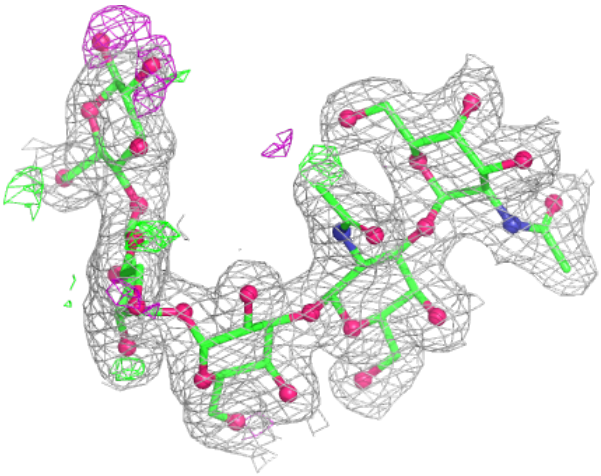


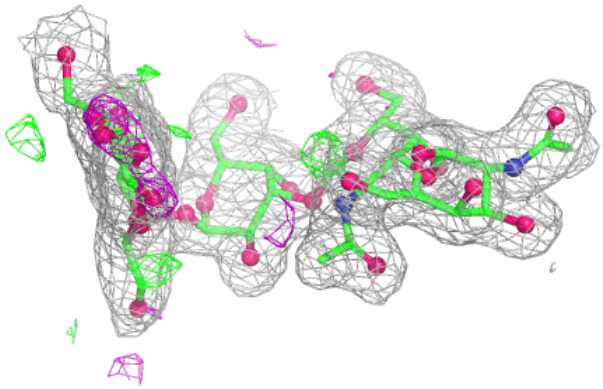


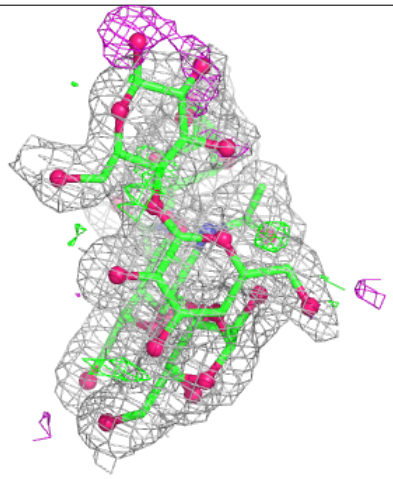


Electron density around Chain CaC:

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

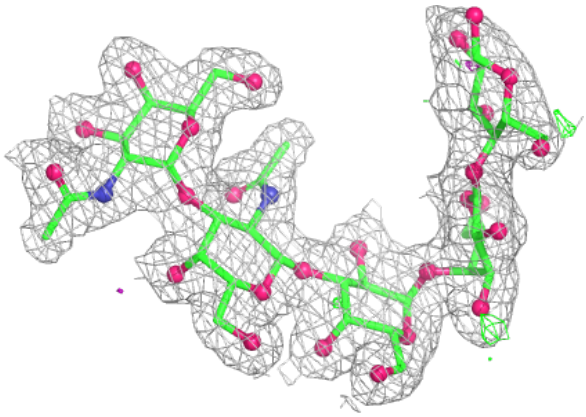


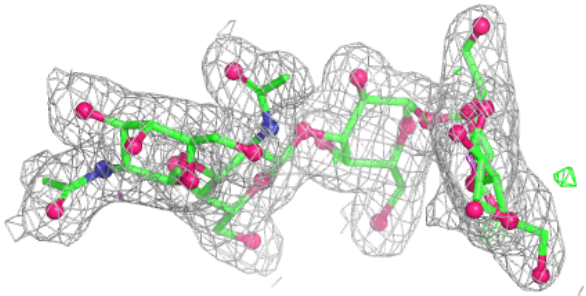


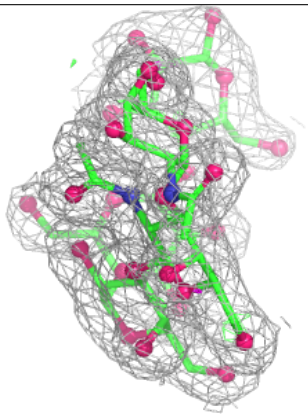


Electron density around Chain EaE:

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

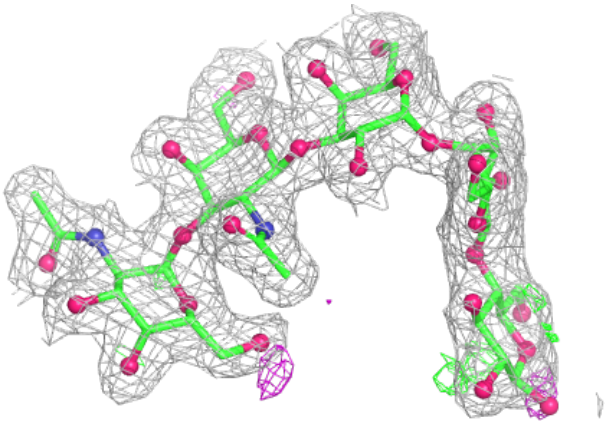


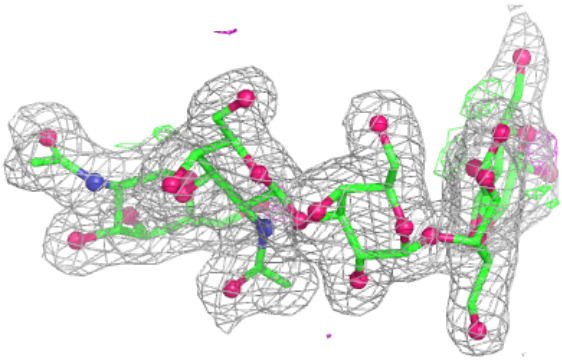


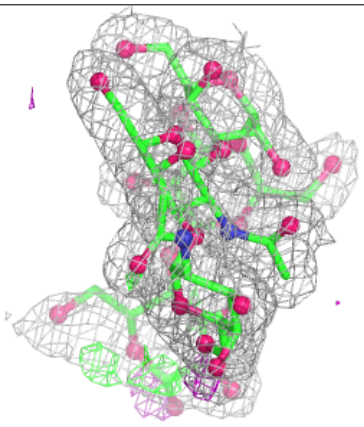


Electron density around Chain GaG:

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

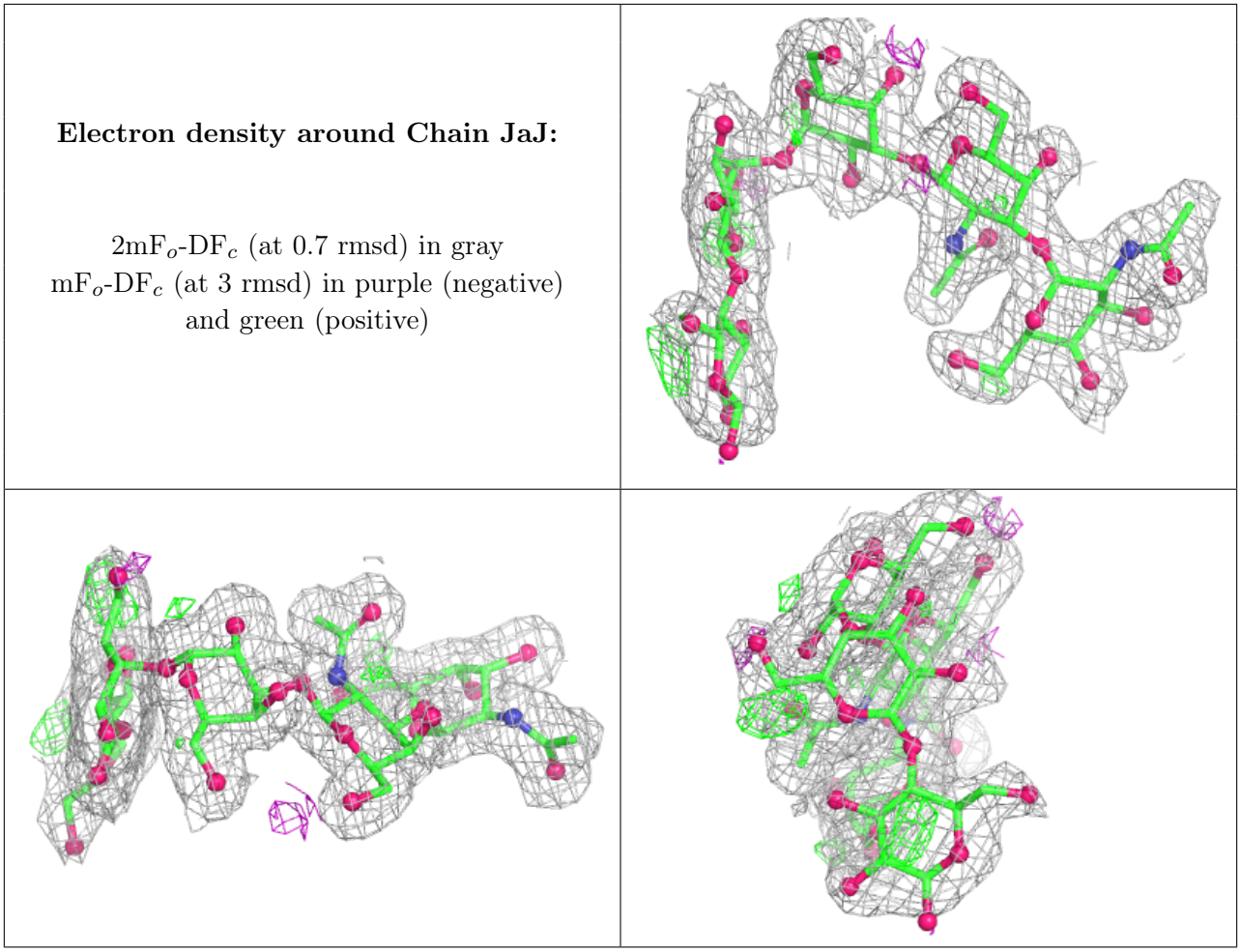






Electron density around Chain JaJ:

$2mF_o$-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
6	EDO	HHH	404	4/4	0.69	0.13	61,62,64,65	0
6	EDO	DDD	402	4/4	0.80	0.11	66,67,67,67	0
4	MPD	JJJ	401	8/8	0.82	0.18	38,43,46,49	0
7	PEG	EEE	402	7/7	0.82	0.15	51,58,64,64	0
8	PGE	III	403	10/10	0.84	0.20	41,55,60,61	0
8	PGE	GGG	2302	10/10	0.85	0.18	39,56,62,63	0
8	PGE	FFF	301	10/10	0.85	0.15	33,51,55,57	0
4	MPD	HHH	401	8/8	0.86	0.20	40,55,62,67	0
4	MPD	FFF	303	8/8	0.87	0.18	37,47,51,53	0
7	PEG	GGG	2301	7/7	0.87	0.17	56,59,62,63	0
7	PEG	III	402	7/7	0.87	0.10	63,68,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	EEE	401	4/4	0.88	0.12	52,54,54,55	0
7	PEG	HHH	403	7/7	0.88	0.12	57,59,60,62	0
6	EDO	DDD	403	4/4	0.89	0.10	50,51,53,53	0
4	MPD	III	401	8/8	0.89	0.13	31,39,43,45	0
5	MG	III	404	1/1	0.91	0.10	42,42,42,42	0
6	EDO	CCC	501	4/4	0.92	0.12	59,59,60,62	0
4	MPD	BBB	401	8/8	0.92	0.15	36,46,55,56	0
7	PEG	CCC	502	7/7	0.93	0.25	36,39,43,48	0
6	EDO	JJJ	402	4/4	0.93	0.08	48,51,53,57	0
4	MPD	AAA	401	8/8	0.94	0.14	35,42,54,54	0
4	MPD	DDD	401	8/8	0.94	0.14	32,45,47,48	0
5	MG	GGG	2303	1/1	0.94	0.10	38,38,38,38	0
5	MG	HHH	405	1/1	0.96	0.06	45,45,45,45	0
5	MG	AAA	402	1/1	0.96	0.06	49,49,49,49	0
5	MG	CCC	503	1/1	0.96	0.06	42,42,42,42	0
4	MPD	FFF	302	8/8	0.96	0.10	27,40,50,51	0
4	MPD	HHH	402	8/8	0.97	0.11	33,48,53,57	0
5	MG	EEE	403	1/1	0.98	0.07	49,49,49,49	0
5	MG	BBB	402	1/1	0.98	0.06	47,47,47,47	0
5	MG	DDD	404	1/1	0.98	0.11	39,39,39,39	0
5	MG	FFF	304	1/1	0.99	0.07	39,39,39,39	0
5	MG	JJJ	403	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.