Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2022 – 04:39 pm BST

PDB ID	:	7B6V
Title	:	Sheep Polyomavirus VP1 in complex with 5 mM Forssman antigen pentaose and 20 mM 3'-sialyllactosamine
Authors	:	Rustmeier, N.H.; Stehle, T.
Deposited on	:	2020-12-08
Resolution	:	1.80 Å(reported)

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

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

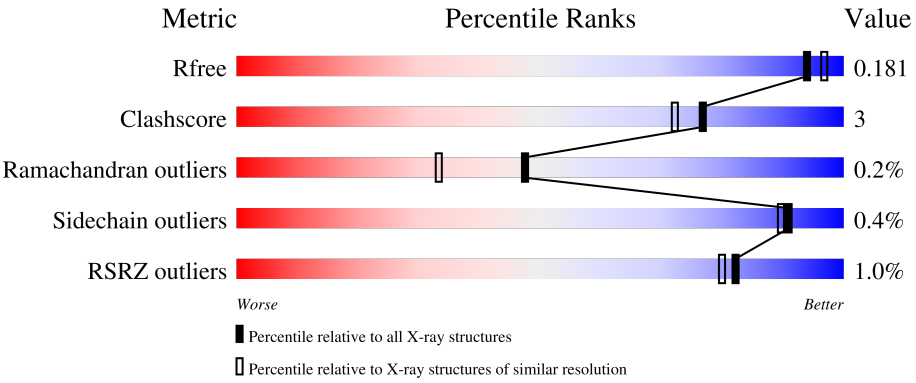
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	AAA	276	91% 6% .
1	BBB	276	% 87% 6% 7%
1	CCC	276	% 88% 6% 6%
1	DDD	276	% 90% 7% .
1	EEE	276	% 84% 9% 6%

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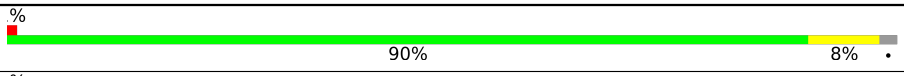
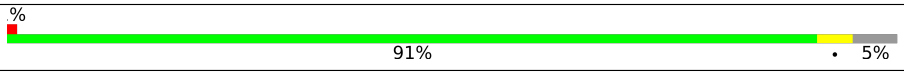
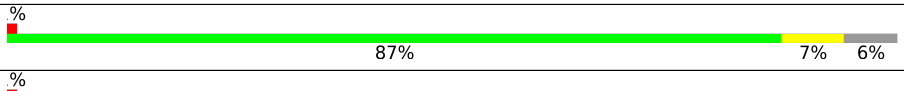
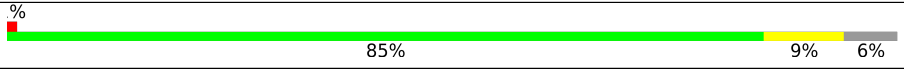
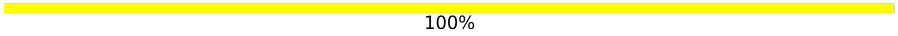
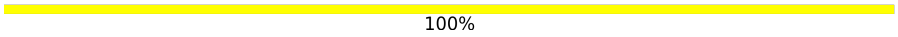
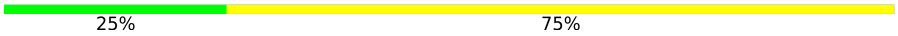
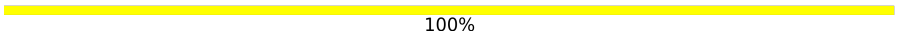
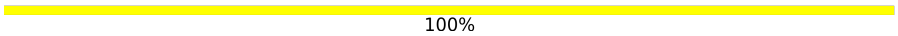
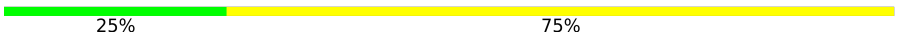
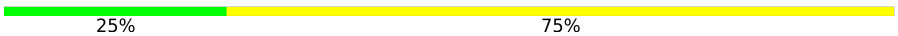
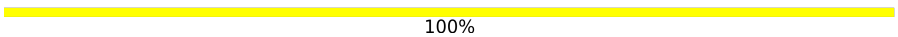
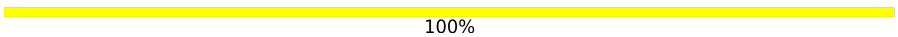
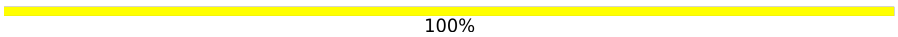
Mol	Chain	Length	Quality of chain
1	FFF	276	
1	GGG	276	
1	HHH	276	
1	III	276	
1	JJJ	276	
2	AaA	4	
2	BaB	4	
2	DaD	4	
2	EaE	4	
2	FaF	4	
2	GaG	4	
2	HaH	4	
2	IaI	4	
2	JaJ	4	
3	CaC	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23360 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	268	Total	C	N	O	S	0	0	0
			2073	1316	351	392	14			
1	BBB	257	Total	C	N	O	S	0	1	0
			1986	1267	335	372	12			
1	CCC	259	Total	C	N	O	S	0	1	0
			1996	1273	338	373	12			
1	DDD	268	Total	C	N	O	S	0	1	0
			2078	1322	349	394	13			
1	EEE	259	Total	C	N	O	S	0	0	0
			1998	1272	336	378	12			
1	FFF	271	Total	C	N	O	S	0	0	0
			2094	1329	353	398	14			
1	GGG	261	Total	C	N	O	S	0	0	0
			2013	1284	339	378	12			
1	HHH	271	Total	C	N	O	S	0	0	0
			2094	1330	351	399	14			
1	III	260	Total	C	N	O	S	0	0	0
			1988	1268	335	373	12			
1	JJJ	259	Total	C	N	O	S	0	0	0
			2002	1278	335	377	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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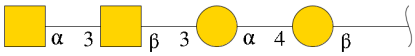
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	95	SER	CYS	conflict	UNP A0A0E3ZCF3
CCC	16	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	17	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	18	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	19	MET	-	expression tag	UNP A0A0E3ZCF3
CCC	95	SER	CYS	conflict	UNP A0A0E3ZCF3
DDD	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

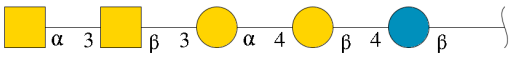
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-

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



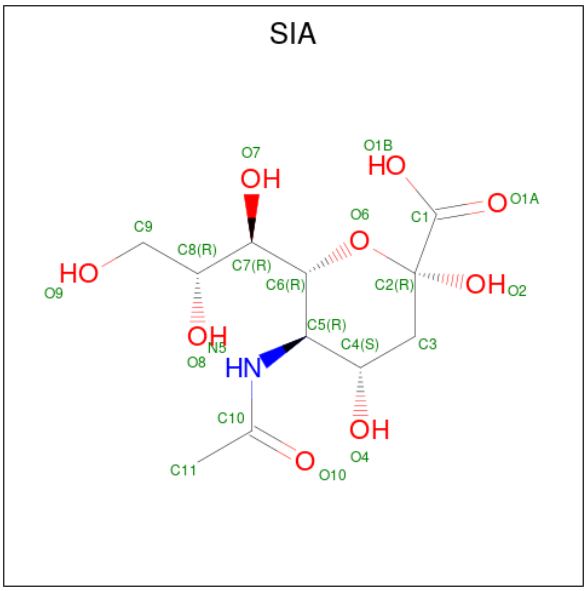
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	BaB	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	DaD	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	EaE	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	FaF	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	GaG	4	Total	C	N	O	0	0	0
			51	28	2	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			
2	JaJ	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			

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C N O 21 11 1 9	0	0
4	DDD	1	Total C N O 21 11 1 9	0	0
4	FFF	1	Total C N O 21 11 1 9	0	0
4	HHH	1	Total C N O 21 11 1 9	0	0
4	III	1	Total C N O 21 11 1 9	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
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

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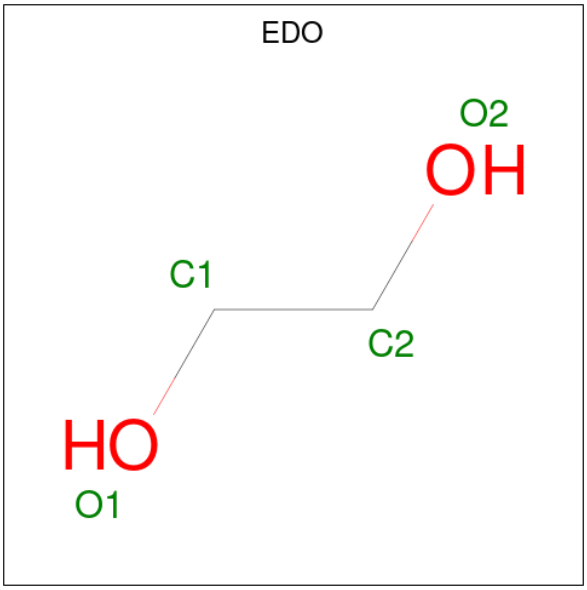
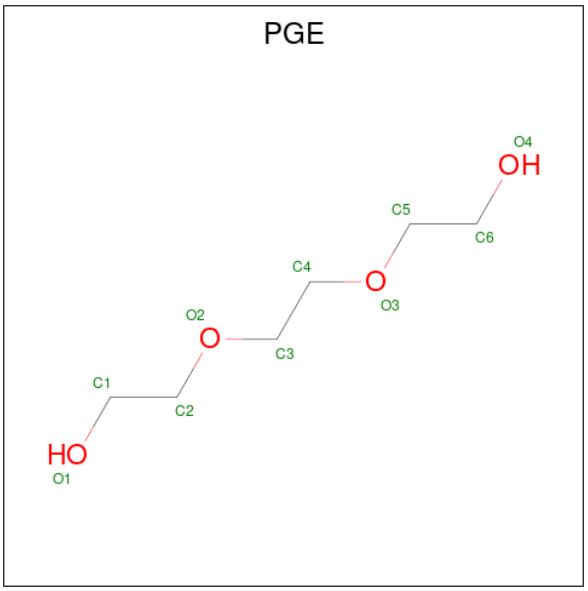
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	HHH	1	Total Mg 1 1	0	0
5	III	1	Total Mg 1 1	0	0
5	JJJ	1	Total Mg 1 1	0	0

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



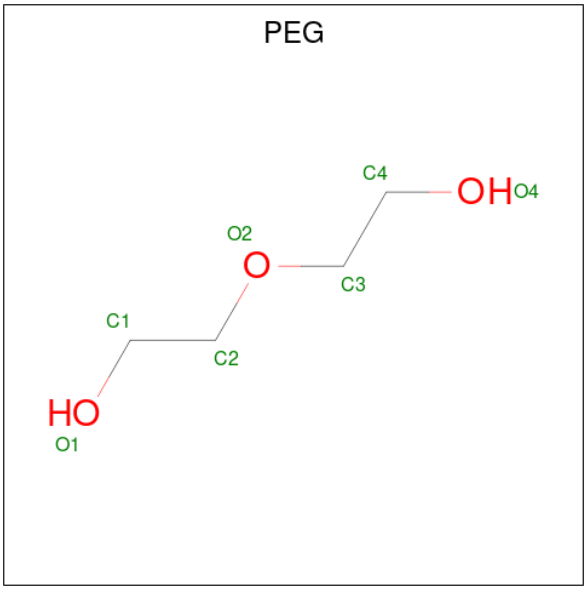
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	EEE	1	Total C O 4 2 2	0	0
6	EEE	1	Total C O 4 2 2	0	0
6	HHH	1	Total C O 4 2 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	JJJ	1	Total C O 10 6 4	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	JJJ	1	Total C O 7 4 3	0	0

- Molecule 9 is water.

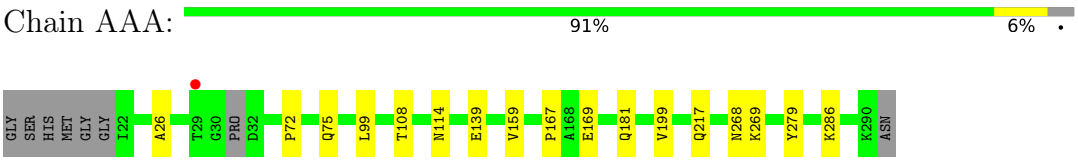
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	246	Total O 249 249	0	3
9	BBB	213	Total O 215 215	0	2
9	CCC	215	Total O 216 216	0	1
9	DDD	255	Total O 258 258	0	3
9	EEE	217	Total O 218 218	0	1
9	FFF	266	Total O 270 270	0	4
9	GGG	242	Total O 244 244	0	2
9	HHH	252	Total O 254 254	0	2
9	III	214	Total O 215 215	0	1
9	JJJ	232	Total O 234 234	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.

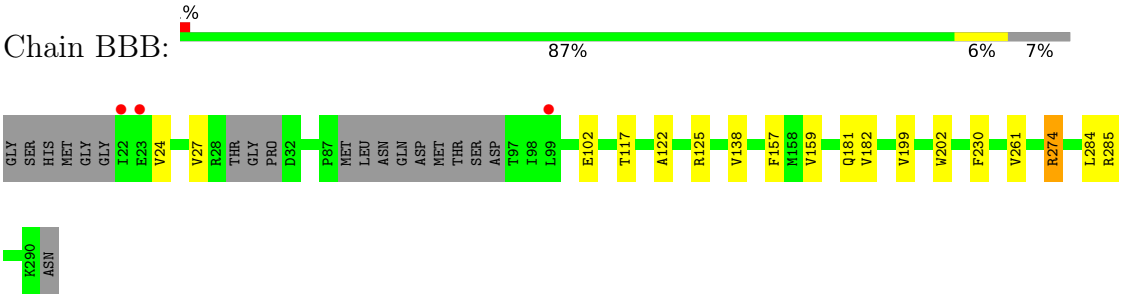
• Molecule 1: Capsid protein VP1

Chain AAA:



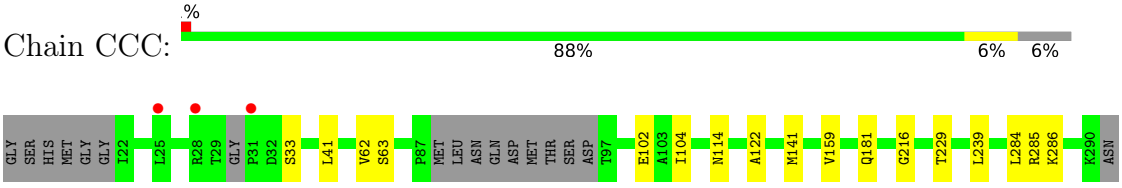
• Molecule 1: Capsid protein VP1

Chain BBB:



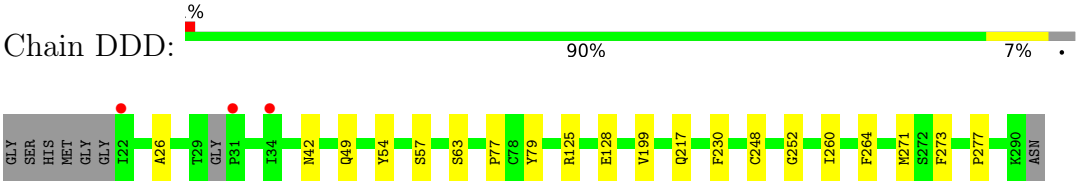
• Molecule 1: Capsid protein VP1

Chain CCC:



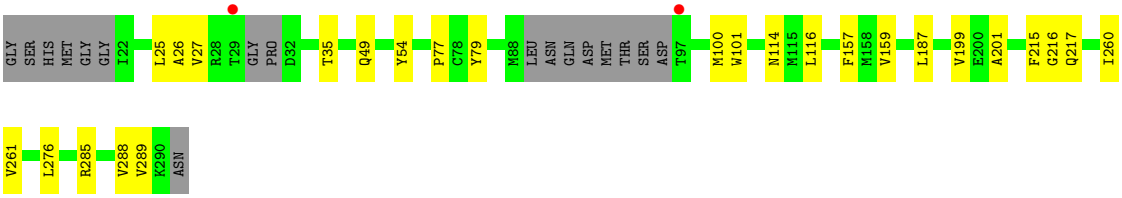
• Molecule 1: Capsid protein VP1

Chain DDD:



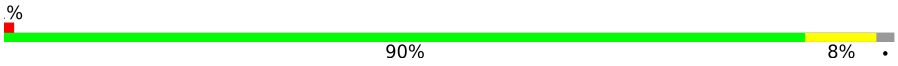
• Molecule 1: Capsid protein VP1

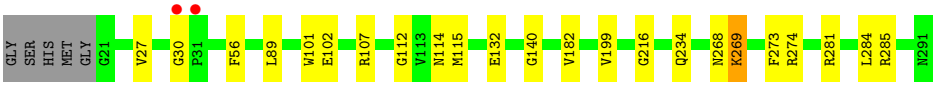
Chain EEE:



• Molecule 1: Capsid protein VP1

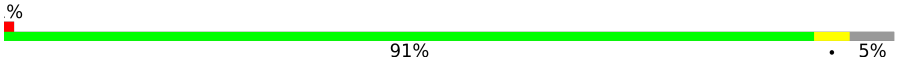
Chain FFF:

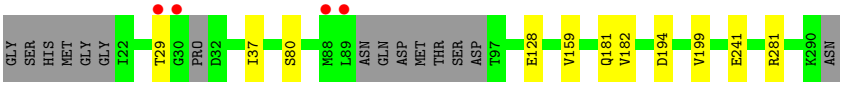




• Molecule 1: Capsid protein VP1

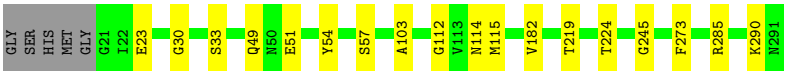
Chain GGG:





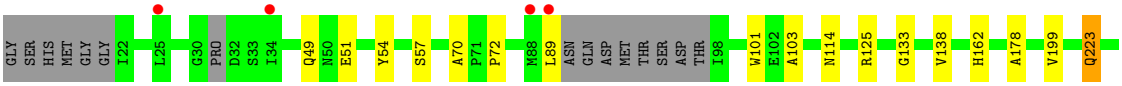
• Molecule 1: Capsid protein VP1

Chain HHH:



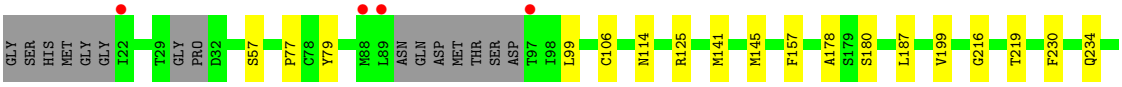
• Molecule 1: Capsid protein VP1

Chain III:



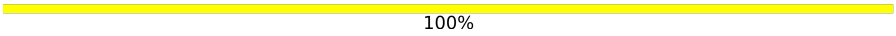
• Molecule 1: Capsid protein VP1

Chain JJJ:



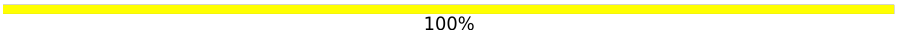
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain AaA:



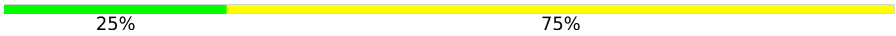
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain BaB:



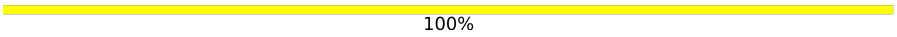
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain DaD:



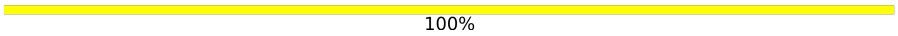
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain EaE:



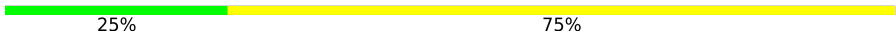
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain FaF:



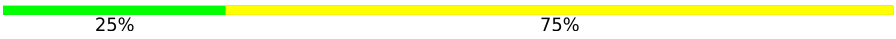
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain GaG:



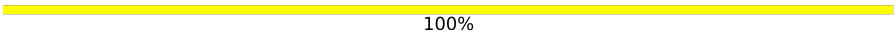
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain HaH:



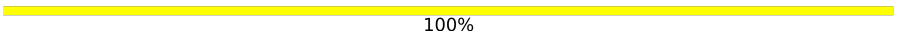
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain IaI:



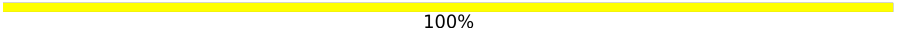
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain JaJ:



• 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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	130.40Å 130.40Å 221.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 1.80 48.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.85-1.80) 99.8 (48.85-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.152 , 0.177 0.156 , 0.181	Depositor DCC
R_{free} test set	6482 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.084 for -h,-k,l 0.357 for h,-h-k,-l 0.084 for -k,-h,-l	Xtriage
Reported twinning fraction	0.641 for H, K, L 0.359 for K, H, -L	Depositor
Outliers	0 of 390440 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	23360	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: SIA, PEG, MG, PGE, GAL, NGA, GLA, BGC, A2G, EDO

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	0.88	0/2886
1	BBB	0.71	0/2036	0.88	0/2767
1	CCC	0.72	0/2049	0.90	0/2783
1	DDD	0.73	0/2133	0.90	0/2900
1	EEE	0.74	0/2048	0.88	0/2783
1	FFF	0.75	0/2147	0.90	0/2920
1	GGG	0.77	0/2063	0.89	0/2803
1	HHH	0.73	0/2147	0.89	0/2920
1	III	0.72	0/2038	0.89	0/2771
1	JJJ	0.74	0/2052	0.88	0/2788
All	All	0.74	0/20837	0.89	0/28321

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	2073	0	1986	9	0
1	BBB	1986	0	1891	11	0
1	CCC	1996	0	1905	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	2078	0	1998	15	0
1	EEE	1998	0	1898	16	0
1	FFF	2094	0	2007	17	0
1	GGG	2013	0	1928	7	0
1	HHH	2094	0	2002	10	0
1	III	1988	0	1882	14	0
1	JJJ	2002	0	1918	20	0
2	AaA	51	0	44	0	0
2	BaB	51	0	44	0	0
2	DaD	51	0	44	0	0
2	EaE	51	0	44	0	0
2	FaF	51	0	44	0	0
2	GaG	51	0	44	0	0
2	HaH	51	0	44	0	0
2	IaI	51	0	44	0	0
2	JaJ	51	0	44	0	0
3	CaC	62	0	53	0	0
4	AAA	21	0	18	1	0
4	DDD	21	0	18	0	0
4	FFF	21	0	18	0	0
4	HHH	21	0	18	0	0
4	III	21	0	18	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	EEE	8	0	12	1	0
6	HHH	4	0	6	0	0
7	JJJ	10	0	14	0	0
8	JJJ	7	0	10	2	0
9	AAA	249	0	0	0	0
9	BBB	215	0	0	0	0
9	CCC	216	0	0	0	0
9	DDD	258	0	0	2	0
9	EEE	218	0	0	2	0
9	FFF	270	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	GGG	244	0	0	2	0
9	HHH	254	0	0	0	0
9	III	215	0	0	1	0
9	JJJ	234	0	0	3	0
All	All	23360	0	19996	113	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 3.

All (113) 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:FFF:89:LEU:HD21	1:FFF:101:TRP:CZ2	2.25	0.72
1:FFF:281:ARG:NH2	9:FFF:502:HOH:O	2.25	0.70
1:JJJ:281:ARG:NH2	9:JJJ:502:HOH:O	2.26	0.68
1:FFF:89:LEU:HG	9:FFF:609:HOH:O	1.94	0.68
1:CCC:229:THR:HG22	1:DDD:217:GLN:HG2	1.76	0.67
1:GGG:281:ARG:NH1	9:GGG:406:HOH:O	2.29	0.62
1:BBB:125[B]:ARG:HD3	1:CCC:62:VAL:HB	1.83	0.61
1:DDD:49:GLN:HG2	1:DDD:54:TYR:CZ	2.37	0.59
1:FFF:268:ASN:O	1:FFF:269:LYS:HB2	2.03	0.58
1:JJJ:234:GLN:NE2	8:JJJ:402:PEG:H12	2.19	0.57
1:III:114:ASN:HB2	1:JJJ:199:VAL:O	2.05	0.57
1:III:103:ALA:O	1:III:245:GLY:HA3	2.07	0.54
1:EEE:116:LEU:HD11	1:EEE:261:VAL:HG11	1.91	0.53
1:III:51:GLU:O	1:JJJ:178:ALA:HB1	2.09	0.53
1:JJJ:79:TYR:CE2	1:JJJ:199:VAL:HA	2.45	0.52
1:HHH:219:THR:HG22	1:HHH:224:THR:HG21	1.92	0.52
1:DDD:77:PRO:HG3	1:DDD:260:ILE:HD11	1.92	0.52
1:EEE:25:LEU:HB2	1:EEE:288:VAL:HG13	1.92	0.51
1:AAA:99:LEU:HD13	1:AAA:286:LYS:HD3	1.94	0.50
1:III:138:VAL:HG11	1:III:261:VAL:HG23	1.94	0.50
1:EEE:217:GLN:HG2	9:EEE:653:HOH:O	2.12	0.49
1:III:162:HIS:CD2	1:III:178:ALA:HA	2.47	0.49
1:DDD:125:ARG:HD2	9:DDD:619:HOH:O	2.10	0.49
1:EEE:215:PHE:HB3	6:EEE:401:EDO:H12	1.94	0.49
1:III:125:ARG:HD3	1:III:133:GLY:O	2.12	0.49
1:JJJ:125:ARG:HD2	9:JJJ:620:HOH:O	2.12	0.49
1:EEE:27:VAL:HG13	1:EEE:285:ARG:HD2	1.95	0.49
1:GGG:37:ILE:C	1:GGG:37:ILE:HD12	2.34	0.48
1:AAA:199:VAL:O	1:EEE:114:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:26:ALA:O	1:EEE:288:VAL:HG12	2.13	0.48
1:BBB:138:VAL:HG11	1:BBB:261:VAL:HG23	1.96	0.48
1:III:57:SER:HB3	1:III:273:PHE:HB2	1.96	0.48
1:FFF:114:ASN:HB2	1:GGG:199:VAL:O	2.14	0.47
1:JJJ:234:GLN:NE2	8:JJJ:402:PEG:C1	2.77	0.47
1:AAA:114:ASN:HB2	1:BBB:199:VAL:O	2.14	0.47
1:AAA:72:PRO:HG2	1:AAA:75:GLN:NE2	2.29	0.47
1:HHH:23:GLU:HB2	1:HHH:290:LYS:CG	2.44	0.47
1:HHH:112:GLY:O	1:HHH:115:MET:HG2	2.13	0.47
1:CCC:114:ASN:HB2	1:DDD:199:VAL:O	2.15	0.47
1:FFF:140:GLY:O	9:FFF:501:HOH:O	2.20	0.46
1:JJJ:261:VAL:HG22	1:JJJ:274:ARG:O	2.15	0.46
1:DDD:57:SER:HB3	1:DDD:273:PHE:HB2	1.97	0.46
1:EEE:77:PRO:HG3	1:EEE:260:ILE:HD11	1.96	0.46
1:EEE:157:PHE:HB3	1:EEE:187:LEU:HB3	1.97	0.46
1:FFF:89:LEU:HD21	1:FFF:101:TRP:HZ2	1.77	0.46
1:FFF:107:ARG:HG2	1:FFF:234:GLN:O	2.15	0.46
1:AAA:159:VAL:O	1:AAA:181:GLN:HA	2.15	0.46
1:AAA:167:PRO:HB2	1:AAA:169:GLU:OE1	2.15	0.46
1:EEE:79:TYR:CE2	1:EEE:199:VAL:HA	2.52	0.45
1:BBB:122:ALA:HA	1:CCC:63:SER:O	2.16	0.45
1:EEE:35:THR:HG22	1:EEE:101:TRP:CZ3	2.52	0.45
1:JJJ:57:SER:HB3	1:JJJ:273:PHE:HB2	1.98	0.45
1:JJJ:77:PRO:HG3	1:JJJ:260:ILE:HD11	1.98	0.45
9:FFF:733:HOH:O	1:GGG:241:GLU:HG2	2.16	0.45
1:BBB:230:PHE:CE2	1:CCC:216:GLY:HA3	2.52	0.45
1:DDD:79:TYR:CE2	1:DDD:199:VAL:HA	2.52	0.45
1:DDD:230:PHE:CE2	1:EEE:216:GLY:HA3	2.52	0.45
1:HHH:51:GLU:O	1:III:178:ALA:HB1	2.17	0.44
1:III:70:ALA:O	1:III:72:PRO:HD3	2.17	0.44
1:AAA:26:ALA:HB2	1:FFF:30:GLY:HA2	1.99	0.44
1:JJJ:180:SER:HB3	1:JJJ:187:LEU:CD1	2.47	0.44
1:CCC:159:VAL:O	1:CCC:181:GLN:HA	2.17	0.44
1:JJJ:99:LEU:HB2	9:JJJ:629:HOH:O	2.17	0.44
1:FFF:27:VAL:HG13	1:FFF:285:ARG:HD2	2.00	0.43
1:HHH:49:GLN:HG2	1:HHH:54:TYR:CZ	2.54	0.43
1:HHH:103:ALA:O	1:HHH:245:GLY:HA3	2.18	0.43
1:FFF:89:LEU:HB2	9:FFF:609:HOH:O	2.19	0.43
1:GGG:159:VAL:O	1:GGG:181:GLN:HA	2.18	0.43
1:HHH:33:SER:O	1:HHH:285:ARG:HA	2.18	0.43
1:CCC:41:LEU:HD23	1:CCC:41:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:159:VAL:HG12	1:EEE:201:ALA:HA	1.99	0.43
1:JJJ:145:MET:C	1:JJJ:145:MET:SD	2.97	0.43
1:BBB:159:VAL:O	1:BBB:181:GLN:HA	2.19	0.43
1:JJJ:157:PHE:HB3	1:JJJ:187:LEU:HB3	2.01	0.43
1:CCC:122:ALA:HA	1:DDD:63:SER:O	2.19	0.42
1:III:89:LEU:HD11	1:III:101:TRP:CD1	2.54	0.42
1:CCC:33:SER:HA	1:CCC:286:LYS:HD2	2.01	0.42
1:JJJ:263:PHE:HA	1:JJJ:272:SER:O	2.19	0.42
1:EEE:261:VAL:HG21	1:EEE:276:LEU:HG	2.00	0.42
1:HHH:57:SER:HB3	1:HHH:273:PHE:HB2	2.00	0.42
1:DDD:42:ASN:OD1	1:DDD:277:PRO:HB3	2.20	0.42
1:FFF:56:PHE:HA	1:FFF:273:PHE:O	2.19	0.42
1:BBB:117:THR:HA	1:CCC:141:MET:SD	2.60	0.42
1:III:223:GLN:OE1	9:III:501:HOH:O	2.22	0.42
1:III:230:PHE:CZ	1:JJJ:216:GLY:HA3	2.55	0.41
1:FFF:112:GLY:O	1:FFF:115:MET:HG2	2.21	0.41
1:III:49:GLN:HG2	1:III:54:TYR:CZ	2.55	0.41
1:BBB:27:VAL:CG1	1:BBB:285:ARG:HD2	2.50	0.41
1:DDD:128:GLU:OE1	9:DDD:501:HOH:O	2.21	0.41
1:JJJ:106:CYS:HA	1:JJJ:281:ARG:O	2.21	0.41
1:EEE:100:MET:HE2	1:EEE:289:VAL:HG21	2.03	0.41
1:AAA:268:ASN:O	1:AAA:269:LYS:HB2	2.20	0.41
1:BBB:102:GLU:O	1:BBB:284:LEU:HA	2.20	0.41
1:FFF:102:GLU:O	1:FFF:284:LEU:HA	2.21	0.41
1:GGG:128:GLU:HG2	9:GGG:486:HOH:O	2.19	0.41
1:HHH:114:ASN:HB2	1:III:199:VAL:O	2.21	0.41
1:CCC:104:ILE:HG22	1:CCC:239:LEU:HD21	2.03	0.41
1:FFF:199:VAL:O	1:JJJ:114:ASN:HB2	2.20	0.41
1:CCC:33:SER:O	1:CCC:285:ARG:HA	2.21	0.41
1:JJJ:141:MET:HA	1:JJJ:219:THR:O	2.21	0.41
1:BBB:157:PHE:HB2	1:BBB:202:TRP:CZ3	2.56	0.41
1:GGG:80:SER:HA	1:GGG:194:ASP:OD1	2.20	0.41
1:BBB:261:VAL:HG22	1:BBB:274:ARG:O	2.20	0.40
1:FFF:107:ARG:HD3	9:FFF:715:HOH:O	2.20	0.40
1:AAA:108:THR:HA	1:AAA:279:TYR:O	2.20	0.40
4:AAA:401:SIA:H91	9:EEE:553:HOH:O	2.20	0.40
1:DDD:264:PHE:O	1:DDD:271:MET:HA	2.21	0.40
1:CCC:102:GLU:O	1:CCC:284:LEU:HA	2.21	0.40
1:DDD:26:ALA:HB2	1:HHH:30:GLY:HA2	2.03	0.40
1:DDD:248:CYS:HB3	1:DDD:252:GLY:O	2.22	0.40
1:EEE:49:GLN:HA	1:EEE:54:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:216:GLY:HA3	1:JJJ:230:PHE:CZ	2.57	0.40
1:DDD:77:PRO:CG	1:DDD:260:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	264/276 (96%)	250 (95%)	14 (5%)	0	100	100
1	BBB	252/276 (91%)	241 (96%)	10 (4%)	1 (0%)	34	21
1	CCC	254/276 (92%)	240 (94%)	14 (6%)	0	100	100
1	DDD	265/276 (96%)	252 (95%)	13 (5%)	0	100	100
1	EEE	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	FFF	269/276 (98%)	256 (95%)	12 (4%)	1 (0%)	34	21
1	GGG	255/276 (92%)	242 (95%)	12 (5%)	1 (0%)	34	21
1	HHH	269/276 (98%)	258 (96%)	10 (4%)	1 (0%)	34	21
1	III	254/276 (92%)	241 (95%)	13 (5%)	0	100	100
1	JJJ	253/276 (92%)	240 (95%)	13 (5%)	0	100	100
All	All	2588/2760 (94%)	2463 (95%)	121 (5%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	182	VAL
1	FFF	182	VAL
1	HHH	182	VAL
1	GGG	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	222/234 (95%)	220 (99%)	2 (1%)	78 75
1	BBB	209/234 (89%)	207 (99%)	2 (1%)	76 71
1	CCC	210/234 (90%)	210 (100%)	0	100 100
1	DDD	224/234 (96%)	224 (100%)	0	100 100
1	EEE	211/234 (90%)	211 (100%)	0	100 100
1	FFF	225/234 (96%)	222 (99%)	3 (1%)	69 62
1	GGG	213/234 (91%)	212 (100%)	1 (0%)	88 87
1	HHH	224/234 (96%)	224 (100%)	0	100 100
1	III	207/234 (88%)	206 (100%)	1 (0%)	88 87
1	JJJ	213/234 (91%)	213 (100%)	0	100 100
All	All	2158/2340 (92%)	2149 (100%)	9 (0%)	91 89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	139	GLU
1	AAA	217	GLN
1	BBB	24	VAL
1	BBB	274	ARG
1	FFF	132	GLU
1	FFF	269	LYS
1	FFF	274	ARG
1	GGG	29	THR
1	III	223	GLN

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)

41 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	0.33	0	17,17,17	1.10	1 (5%)
2	GLA	AaA	2	2	11,11,12	0.63	0	15,15,17	1.09	1 (6%)
2	NGA	AaA	3	2	14,14,15	0.98	0	17,19,21	1.80	4 (23%)
2	A2G	AaA	4	2	14,14,15	0.59	0	17,19,21	1.42	3 (17%)
2	GAL	BaB	1	2	12,12,12	0.64	0	17,17,17	1.41	2 (11%)
2	GLA	BaB	2	2	11,11,12	0.64	0	15,15,17	1.15	1 (6%)
2	NGA	BaB	3	2	14,14,15	0.95	0	17,19,21	1.75	4 (23%)
2	A2G	BaB	4	2	14,14,15	0.70	0	17,19,21	1.22	3 (17%)
3	BGC	CaC	1	3	12,12,12	0.55	0	17,17,17	1.22	2 (11%)
3	GAL	CaC	2	3	11,11,12	0.61	0	15,15,17	1.28	3 (20%)
3	GLA	CaC	3	3	11,11,12	0.70	0	15,15,17	1.85	4 (26%)
3	NGA	CaC	4	3	14,14,15	0.85	1 (7%)	17,19,21	1.11	1 (5%)
3	A2G	CaC	5	3	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	GAL	DaD	1	2	12,12,12	0.63	0	17,17,17	1.16	1 (5%)
2	GLA	DaD	2	2	11,11,12	0.69	0	15,15,17	1.10	1 (6%)
2	NGA	DaD	3	2	14,14,15	0.74	0	17,19,21	0.85	0
2	A2G	DaD	4	2	14,14,15	0.67	0	17,19,21	1.60	6 (35%)
2	GAL	EaE	1	2	12,12,12	0.55	0	17,17,17	1.21	2 (11%)
2	GLA	EaE	2	2	11,11,12	0.73	0	15,15,17	1.58	4 (26%)
2	NGA	EaE	3	2	14,14,15	0.78	0	17,19,21	1.26	3 (17%)
2	A2G	EaE	4	2	14,14,15	0.82	1 (7%)	17,19,21	1.77	4 (23%)
2	GAL	FaF	1	2	12,12,12	0.77	0	17,17,17	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLA	FaF	2	2	11,11,12	0.57	0	15,15,17	1.60	4 (26%)
2	NGA	FaF	3	2	14,14,15	0.75	1 (7%)	17,19,21	1.38	2 (11%)
2	A2G	FaF	4	2	14,14,15	0.82	0	17,19,21	1.61	3 (17%)
2	GAL	GaG	1	2	12,12,12	0.59	0	17,17,17	1.30	1 (5%)
2	GLA	GaG	2	2	11,11,12	0.90	0	15,15,17	0.91	0
2	NGA	GaG	3	2	14,14,15	0.68	0	17,19,21	1.73	4 (23%)
2	A2G	GaG	4	2	14,14,15	1.02	0	17,19,21	1.18	1 (5%)
2	GAL	HaH	1	2	12,12,12	0.52	0	17,17,17	0.93	0
2	GLA	HaH	2	2	11,11,12	0.56	0	15,15,17	1.07	1 (6%)
2	NGA	HaH	3	2	14,14,15	0.38	0	17,19,21	1.33	2 (11%)
2	A2G	HaH	4	2	14,14,15	0.49	0	17,19,21	1.34	1 (5%)
2	GAL	IaI	1	2	12,12,12	0.52	0	17,17,17	1.22	2 (11%)
2	GLA	IaI	2	2	11,11,12	0.56	0	15,15,17	1.15	2 (13%)
2	NGA	IaI	3	2	14,14,15	0.68	0	17,19,21	1.21	3 (17%)
2	A2G	IaI	4	2	14,14,15	0.72	0	17,19,21	1.26	2 (11%)
2	GAL	JaJ	1	2	12,12,12	0.75	0	17,17,17	1.51	3 (17%)
2	GLA	JaJ	2	2	11,11,12	1.40	2 (18%)	15,15,17	2.42	5 (33%)
2	NGA	JaJ	3	2	14,14,15	0.73	0	17,19,21	1.46	2 (11%)
2	A2G	JaJ	4	2	14,14,15	0.93	0	17,19,21	1.18	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	-	0/2/22/22	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	-	0/2/19/22	0/1/1/1
3	GLA	CaC	3	3	-	1/2/19/22	0/1/1/1
3	NGA	CaC	4	3	-	0/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	JaJ	2	GLA	C4-C5	2.88	1.59	1.53
2	JaJ	2	GLA	O3-C3	2.85	1.49	1.43
2	EaE	4	A2G	O5-C1	2.34	1.47	1.43
2	FaF	3	NGA	O5-C1	-2.32	1.40	1.43
3	CaC	4	NGA	O5-C5	-2.09	1.39	1.43

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JaJ	2	GLA	O3-C3-C4	5.50	123.06	110.35
2	AaA	3	NGA	C1-O5-C5	5.13	119.14	112.19
2	EaE	4	A2G	O5-C5-C6	4.59	114.40	107.20
2	FaF	4	A2G	O5-C5-C6	4.34	114.01	107.20
2	JaJ	2	GLA	C1-C2-C3	4.30	114.95	109.67
2	EaE	4	A2G	C6-C5-C4	-4.12	103.36	113.00
3	CaC	3	GLA	O3-C3-C2	-3.81	102.69	109.99
2	BaB	3	NGA	O4-C4-C3	-3.78	101.62	110.35
2	BaB	1	GAL	O5-C5-C6	3.62	115.44	106.44
2	GaG	3	NGA	O3-C3-C2	-3.59	102.04	109.47
2	AaA	4	A2G	C1-O5-C5	3.53	116.98	112.19
2	JaJ	2	GLA	O3-C3-C2	-3.51	103.27	109.99
2	GaG	1	GAL	O3-C3-C4	3.40	118.20	110.35
2	HaH	4	A2G	C1-O5-C5	3.39	116.78	112.19
2	GaG	3	NGA	O3-C3-C4	3.38	118.16	110.35
3	CaC	3	GLA	O4-C4-C3	-3.31	102.71	110.35
2	DaD	4	A2G	O4-C4-C5	3.15	117.11	109.30
2	JaJ	1	GAL	O2-C2-C1	3.14	116.44	109.16
3	CaC	1	BGC	C1-O5-C5	3.10	119.50	113.66
2	IaI	2	GLA	C2-C3-C4	-3.05	105.61	110.89
2	JaJ	2	GLA	O2-C2-C3	-3.00	104.13	110.14
2	GaG	3	NGA	O5-C1-C2	2.96	115.96	111.29
2	FaF	2	GLA	C1-O5-C5	2.91	116.14	112.19
2	EaE	2	GLA	O3-C3-C2	-2.90	104.43	109.99
3	CaC	4	NGA	O3-C3-C2	-2.89	103.48	109.47
2	EaE	2	GLA	O3-C3-C4	2.86	116.96	110.35
2	JaJ	2	GLA	O5-C1-C2	-2.86	106.36	110.77
2	FaF	3	NGA	O7-C7-C8	-2.83	116.81	122.06
2	JaJ	1	GAL	O3-C3-C2	-2.82	103.83	110.35
2	DaD	2	GLA	O3-C3-C4	2.80	116.83	110.35
2	HaH	2	GLA	C1-O5-C5	2.73	115.90	112.19
2	FaF	2	GLA	O3-C3-C2	-2.73	104.77	109.99
2	AaA	4	A2G	O5-C1-C2	2.73	115.59	111.29
2	EaE	4	A2G	O3-C3-C2	2.72	115.09	109.47
2	EaE	2	GLA	O5-C5-C6	-2.70	102.97	107.20
2	FaF	4	A2G	O4-C4-C3	-2.69	104.12	110.35
2	HaH	3	NGA	C4-C3-C2	-2.69	107.08	111.02
2	DaD	4	A2G	O5-C5-C6	2.67	111.39	107.20
2	JaJ	3	NGA	C2-N2-C7	-2.64	119.15	122.90
2	BaB	3	NGA	O5-C1-C2	2.62	115.43	111.29
2	BaB	1	GAL	C4-C3-C2	-2.62	106.25	110.82
3	CaC	3	GLA	O2-C2-C3	2.61	115.37	110.14
2	DaD	4	A2G	C4-C3-C2	-2.61	107.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BaB	4	A2G	O3-C3-C2	2.61	114.87	109.47
2	AaA	1	GAL	O3-C3-C2	-2.60	104.33	110.35
3	CaC	2	GAL	O6-C6-C5	-2.60	102.36	111.29
2	BaB	3	NGA	C6-C5-C4	2.59	119.08	113.00
3	CaC	5	A2G	O6-C6-C5	-2.55	102.55	111.29
2	EaE	1	GAL	C4-C3-C2	-2.52	106.43	110.82
2	JaJ	1	GAL	O3-C3-C4	2.48	116.09	110.35
2	EaE	1	GAL	O4-C4-C3	-2.47	104.64	110.35
2	EaE	2	GLA	C6-C5-C4	2.46	118.77	113.00
2	BaB	4	A2G	O7-C7-N2	2.38	126.33	121.95
2	DaD	4	A2G	O5-C5-C4	2.37	116.61	110.83
3	CaC	1	BGC	O5-C5-C4	2.36	113.99	109.69
3	CaC	2	GAL	C3-C4-C5	-2.36	106.03	110.24
2	GaG	3	NGA	C1-C2-N2	-2.34	106.50	110.49
2	BaB	4	A2G	O7-C7-C8	-2.33	117.72	122.06
3	CaC	2	GAL	C2-C3-C4	-2.31	106.90	110.89
2	AaA	3	NGA	C4-C3-C2	-2.29	107.66	111.02
2	JaJ	4	A2G	C1-O5-C5	2.28	115.28	112.19
2	GaG	4	A2G	O5-C5-C6	2.28	110.78	107.20
2	IaI	4	A2G	O3-C3-C4	-2.28	105.08	110.35
2	EaE	3	NGA	O4-C4-C3	-2.25	105.14	110.35
3	CaC	3	GLA	C1-O5-C5	2.23	115.22	112.19
2	FaF	4	A2G	C3-C4-C5	2.22	114.20	110.24
2	IaI	3	NGA	C2-N2-C7	2.21	126.05	122.90
2	FaF	1	GAL	O5-C1-C2	-2.20	106.35	110.28
2	JaJ	4	A2G	C8-C7-N2	-2.20	112.37	116.10
2	AaA	4	A2G	C2-N2-C7	-2.20	119.77	122.90
2	IaI	2	GLA	O5-C5-C6	2.20	110.65	107.20
2	HaH	3	NGA	O5-C1-C2	2.19	114.74	111.29
2	IaI	1	GAL	C6-C5-C4	2.19	118.12	113.00
2	AaA	3	NGA	O4-C4-C5	-2.17	103.91	109.30
2	EaE	3	NGA	O5-C5-C6	-2.16	103.81	107.20
2	BaB	3	NGA	O7-C7-C8	-2.16	118.04	122.06
2	DaD	1	GAL	O5-C5-C6	2.09	111.64	106.44
2	EaE	3	NGA	O4-C4-C5	2.09	114.49	109.30
2	BaB	2	GLA	O2-C2-C3	2.09	114.32	110.14
2	JaJ	3	NGA	O7-C7-C8	-2.09	118.18	122.06
2	IaI	4	A2G	O4-C4-C3	-2.09	105.53	110.35
2	FaF	2	GLA	O3-C3-C4	2.08	115.16	110.35
2	IaI	3	NGA	O3-C3-C2	-2.08	105.17	109.47
2	AaA	2	GLA	O3-C3-C2	-2.07	106.02	109.99
2	DaD	4	A2G	O5-C1-C2	2.07	114.55	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DaD	4	A2G	O4-C4-C3	-2.07	105.57	110.35
2	IaI	1	GAL	O4-C4-C3	-2.03	105.66	110.35
2	FaF	3	NGA	C1-O5-C5	2.02	114.93	112.19
2	FaF	2	GLA	O5-C5-C6	-2.02	104.04	107.20
2	IaI	3	NGA	O7-C7-N2	2.01	125.65	121.95
2	EaE	4	A2G	O3-C3-C4	-2.01	105.69	110.35
2	AaA	3	NGA	O5-C5-C6	-2.00	104.06	107.20

There are no chirality outliers.

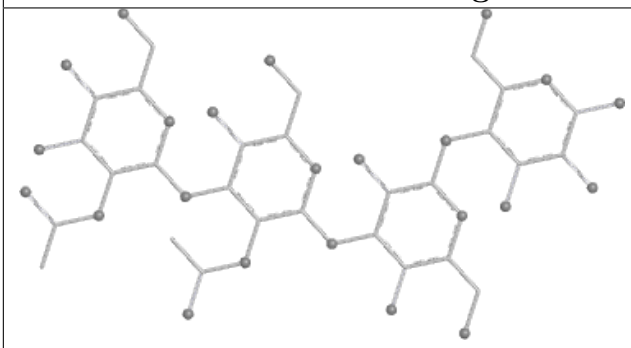
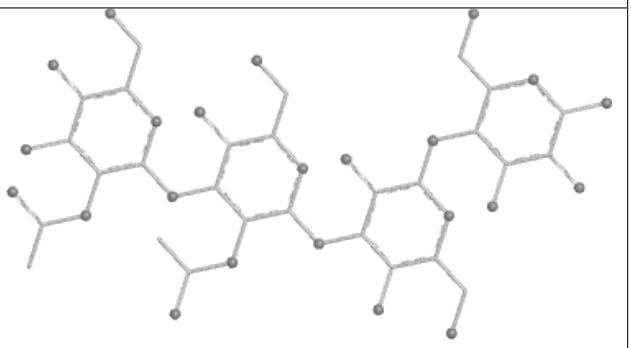
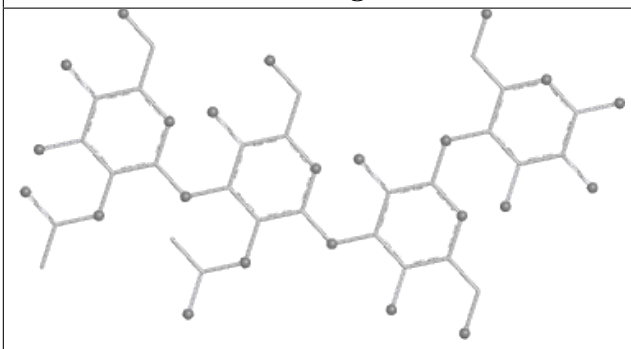
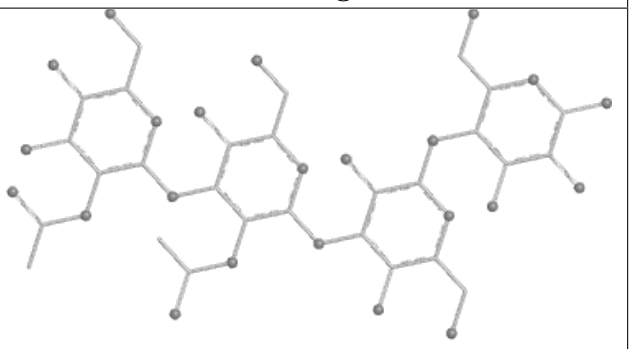
All (21) torsion outliers are listed below:

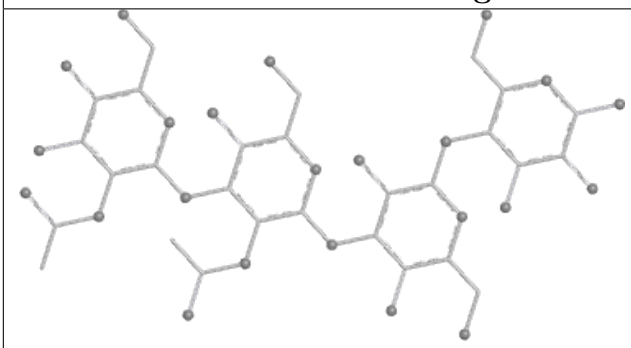
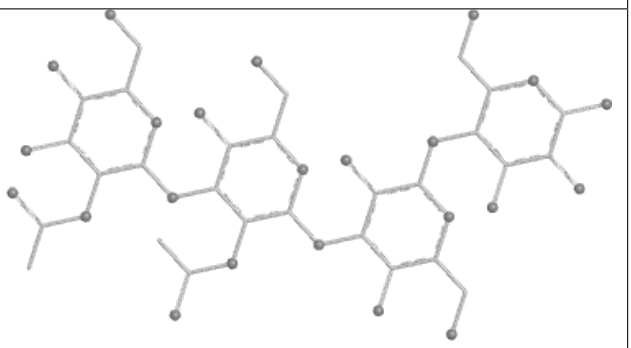
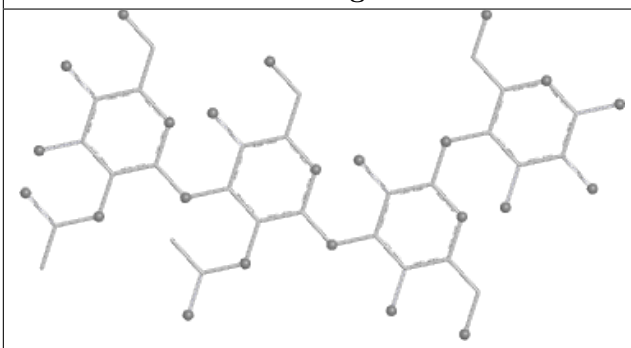
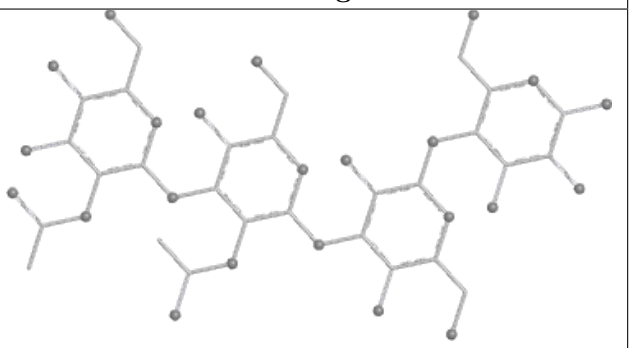
Mol	Chain	Res	Type	Atoms
2	HaH	1	GAL	O5-C5-C6-O6
2	IaI	1	GAL	O5-C5-C6-O6
3	CaC	1	BGC	C4-C5-C6-O6
2	JaJ	1	GAL	O5-C5-C6-O6
2	EaE	2	GLA	O5-C5-C6-O6
2	HaH	1	GAL	C4-C5-C6-O6
3	CaC	1	BGC	O5-C5-C6-O6
2	DaD	2	GLA	O5-C5-C6-O6
2	HaH	2	GLA	O5-C5-C6-O6
2	FaF	1	GAL	O5-C5-C6-O6
2	FaF	2	GLA	O5-C5-C6-O6
2	BaB	2	GLA	O5-C5-C6-O6
2	GaG	1	GAL	O5-C5-C6-O6
2	IaI	2	GLA	O5-C5-C6-O6
2	EaE	1	GAL	O5-C5-C6-O6
2	AaA	2	GLA	O5-C5-C6-O6
2	JaJ	2	GLA	O5-C5-C6-O6
3	CaC	3	GLA	O5-C5-C6-O6
2	GaG	2	GLA	O5-C5-C6-O6
2	IaI	1	GAL	C4-C5-C6-O6
2	BaB	4	A2G	O5-C5-C6-O6

There are no ring outliers.

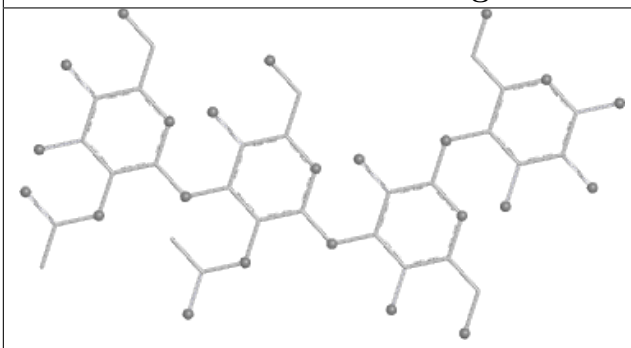
No monomer is involved in short contacts.

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

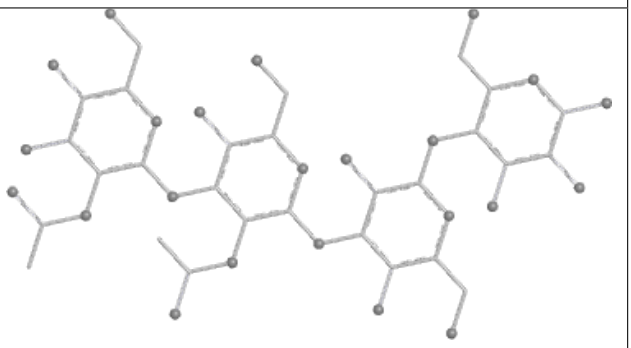
Oligosaccharide Chain AaA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

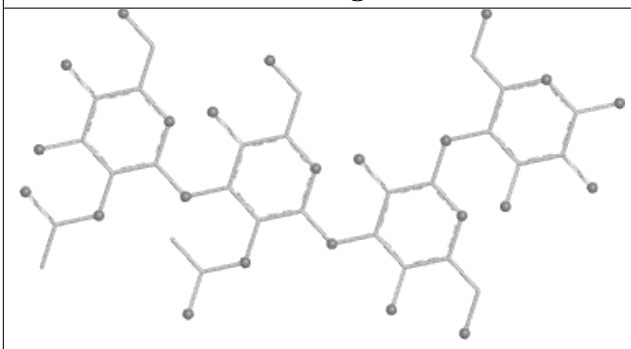
Oligosaccharide Chain DaD



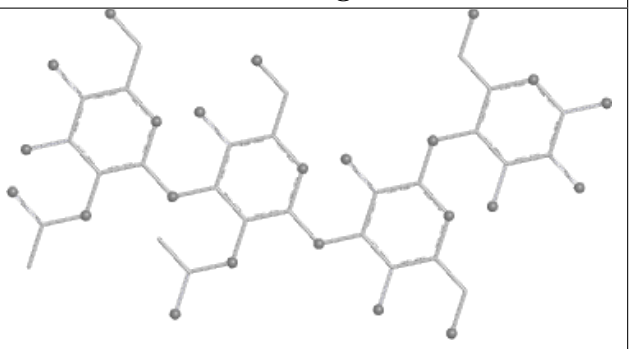
Bond lengths



Bond angles

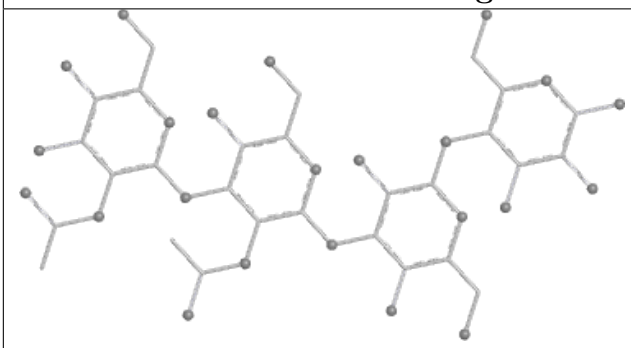


Torsions

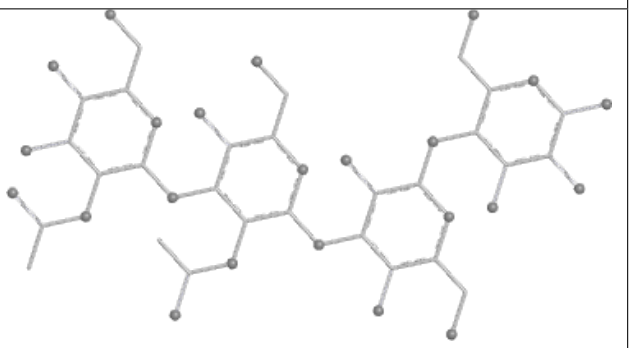


Rings

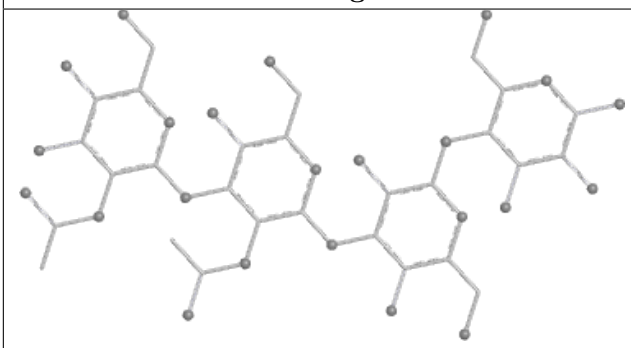
Oligosaccharide Chain EaE



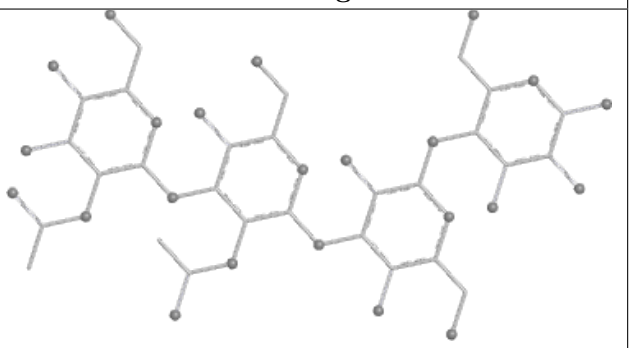
Bond lengths



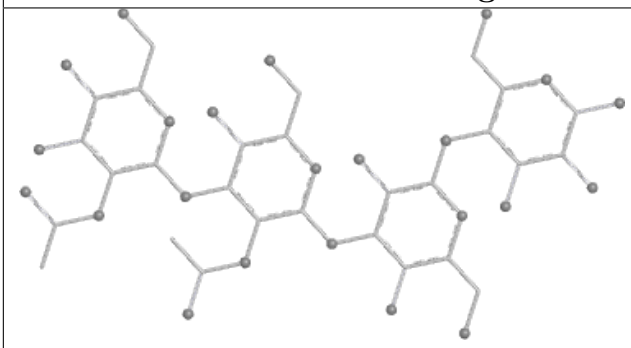
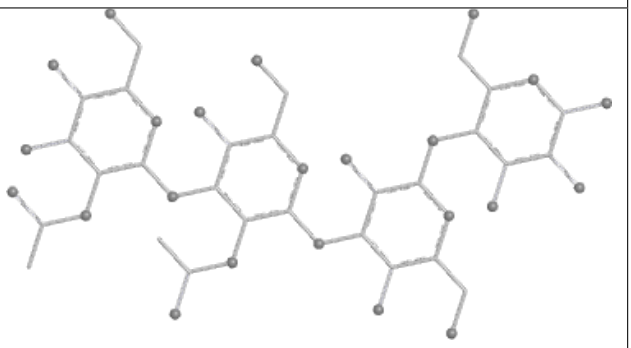
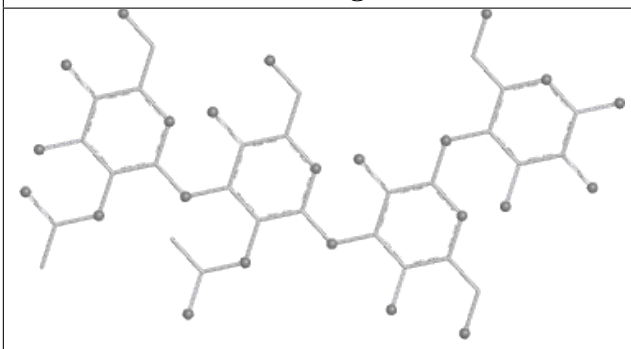
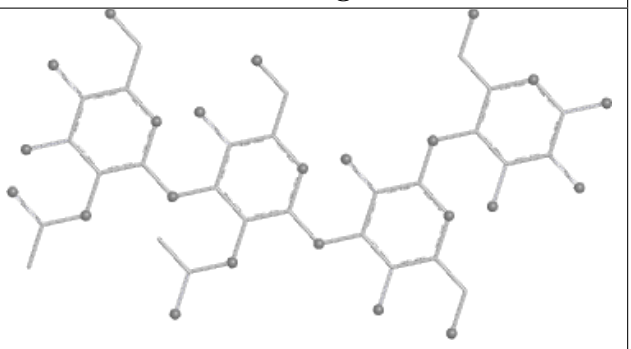
Bond angles

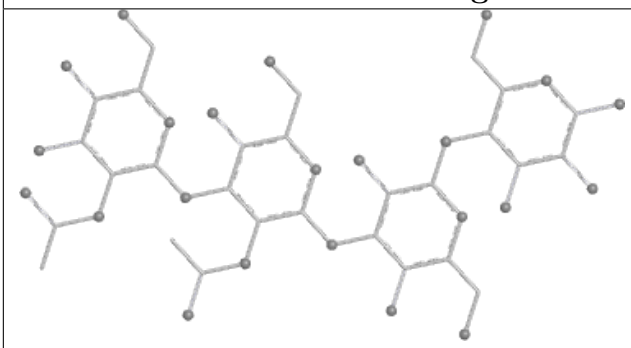
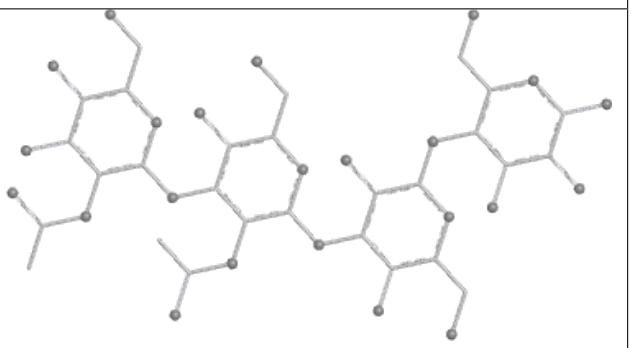
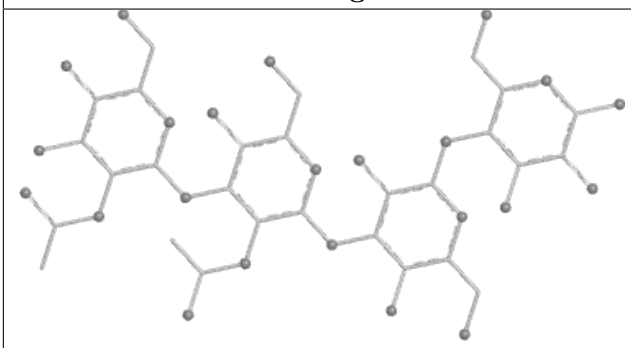
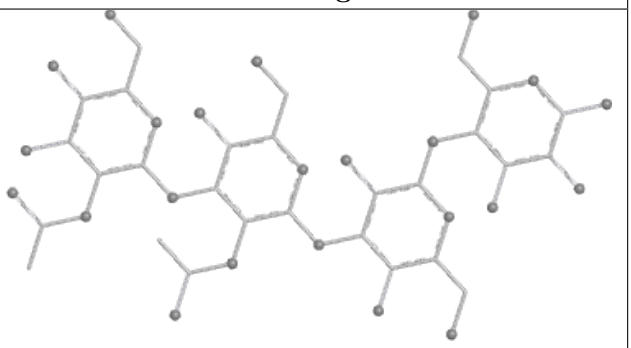


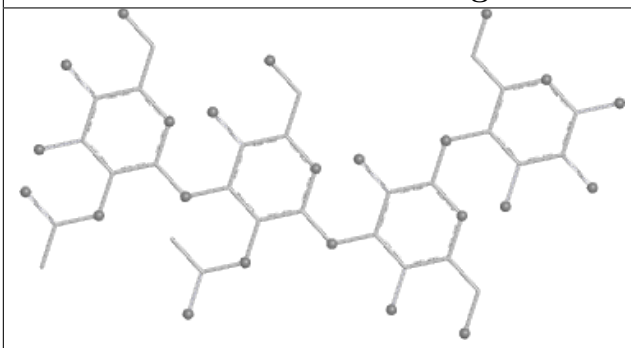
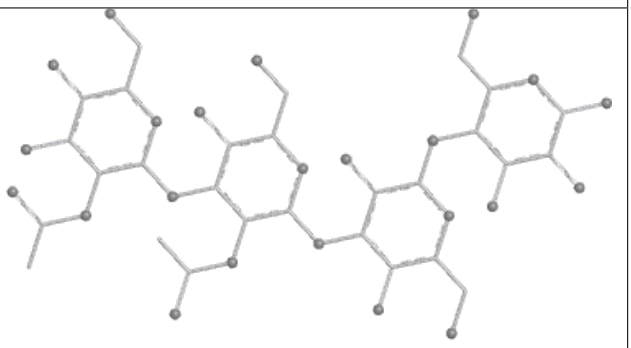
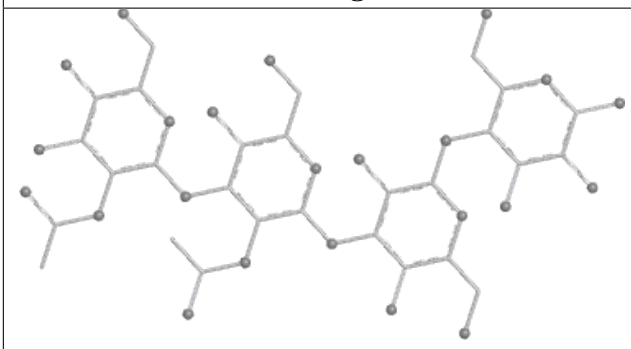
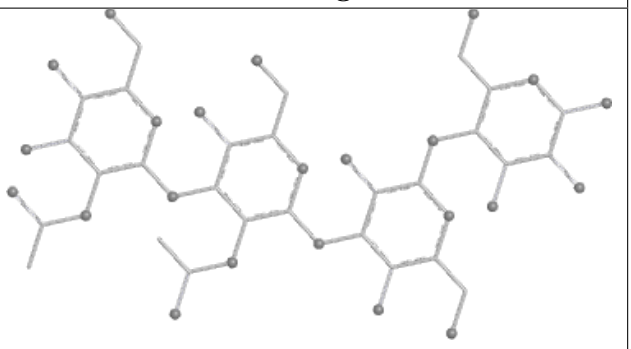
Torsions

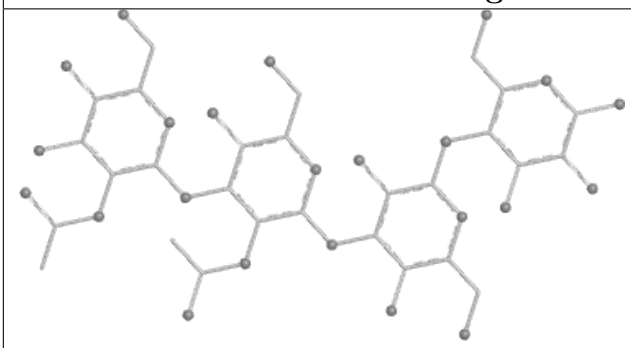
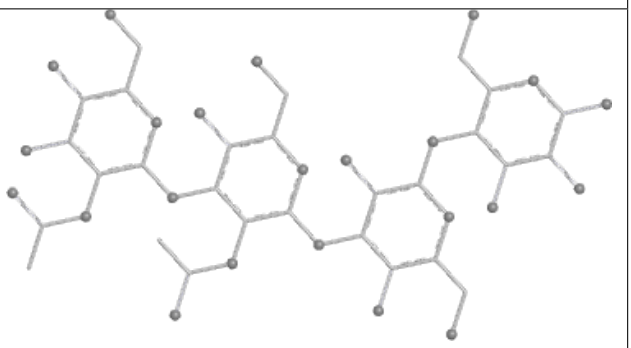
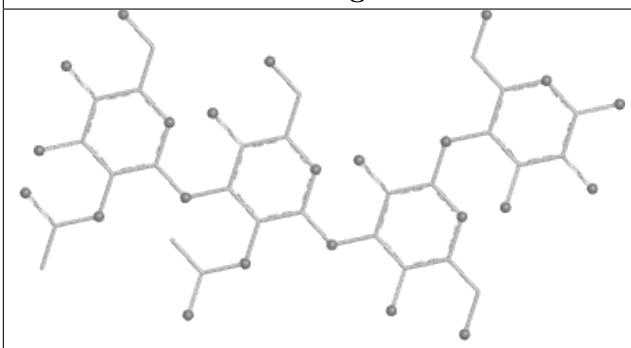
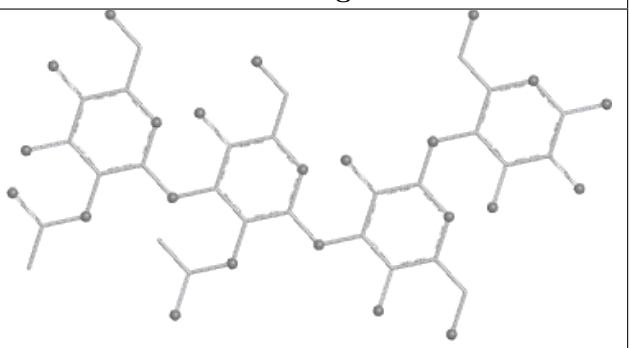


Rings

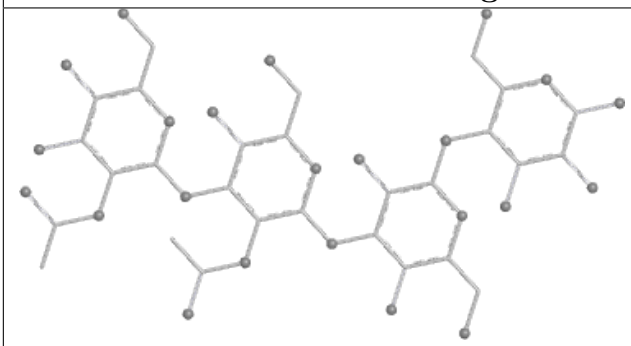
Oligosaccharide Chain FaF	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

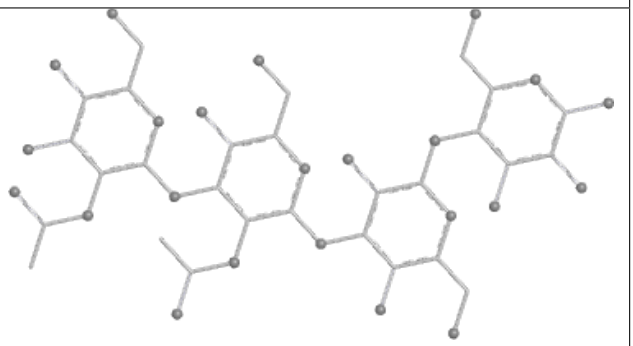
Oligosaccharide Chain HaH	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

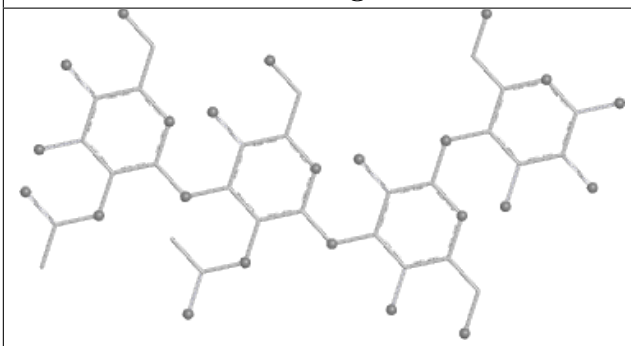
Oligosaccharide Chain JaJ



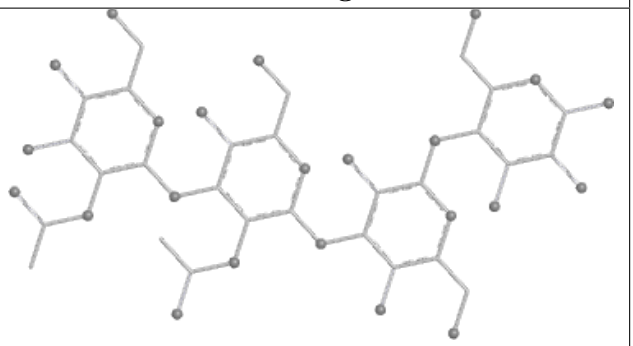
Bond lengths



Bond angles

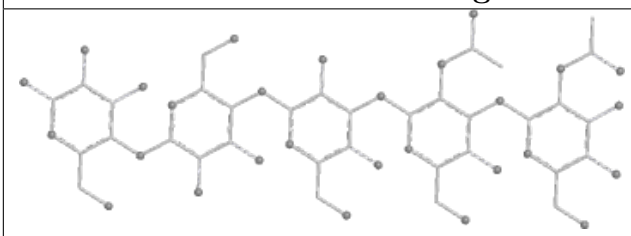


Torsions

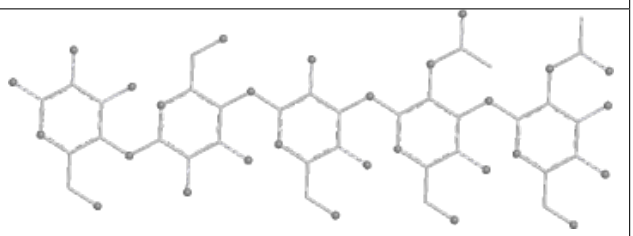


Rings

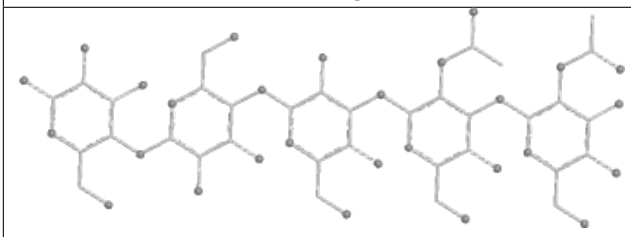
Oligosaccharide Chain CaC



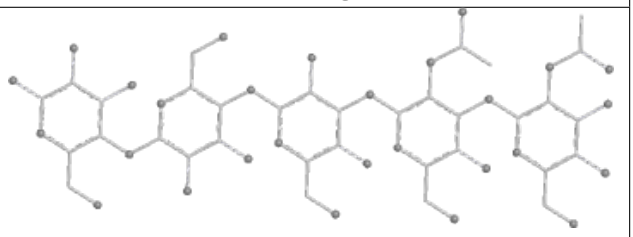
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
7	PGE	JJJ	401	-	9,9,9	0.25	0	8,8,8	0.12	0
4	SIA	HHH	401	-	21,21,21	1.38	2 (9%)	25,31,31	1.85	3 (12%)
8	PEG	JJJ	402	-	6,6,6	0.14	0	5,5,5	0.11	0
4	SIA	AAA	401	-	21,21,21	1.35	4 (19%)	25,31,31	1.35	3 (12%)
6	EDO	EEE	402	-	3,3,3	0.09	0	2,2,2	0.14	0
4	SIA	III	401	-	21,21,21	1.21	2 (9%)	25,31,31	1.33	3 (12%)
4	SIA	FFF	401	-	21,21,21	1.34	1 (4%)	25,31,31	0.99	2 (8%)
6	EDO	EEE	401	-	3,3,3	0.20	0	2,2,2	0.29	0
4	SIA	DDD	401	-	21,21,21	1.71	3 (14%)	25,31,31	1.29	2 (8%)
6	EDO	HHH	402	-	3,3,3	0.10	0	2,2,2	0.26	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
7	PGE	JJJ	401	-	-	4/7/7/7	-
4	SIA	HHH	401	-	-	3/20/38/38	0/1/1/1
8	PEG	JJJ	402	-	-	0/4/4/4	-
4	SIA	AAA	401	-	-	2/20/38/38	0/1/1/1
6	EDO	EEE	402	-	-	1/1/1/1	-
4	SIA	III	401	-	-	4/20/38/38	0/1/1/1
4	SIA	FFF	401	-	-	2/20/38/38	0/1/1/1
6	EDO	EEE	401	-	-	1/1/1/1	-
4	SIA	DDD	401	-	-	3/20/38/38	0/1/1/1
6	EDO	HHH	402	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	401	SIA	O2-C2	5.22	1.46	1.39
4	HHH	401	SIA	O2-C2	5.00	1.46	1.39
4	FFF	401	SIA	O2-C2	4.54	1.45	1.39
4	AAA	401	SIA	O2-C2	3.76	1.44	1.39
4	III	401	SIA	O2-C2	3.74	1.44	1.39
4	DDD	401	SIA	C4-C5	3.02	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	401	SIA	C3-C2	2.65	1.55	1.51
4	AAA	401	SIA	C3-C2	2.55	1.54	1.51
4	AAA	401	SIA	C2-C1	-2.36	1.50	1.53
4	III	401	SIA	O6-C2	2.31	1.45	1.43
4	HHH	401	SIA	C2-C1	-2.08	1.50	1.53
4	AAA	401	SIA	C4-C5	2.03	1.54	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	HHH	401	SIA	O2-C2-C3	5.76	117.72	109.40
4	HHH	401	SIA	O1A-C1-C2	-4.46	116.83	123.59
4	AAA	401	SIA	O2-C2-C3	4.31	115.63	109.40
4	HHH	401	SIA	O2-C2-C1	-4.13	102.36	110.76
4	III	401	SIA	C3-C4-C5	3.38	115.17	109.98
4	III	401	SIA	O6-C6-C5	-3.26	106.59	109.78
4	III	401	SIA	O2-C2-C1	-3.02	104.61	110.76
4	AAA	401	SIA	O1A-C1-C2	-2.89	119.20	123.59
4	DDD	401	SIA	C3-C4-C5	2.63	114.02	109.98
4	DDD	401	SIA	O6-C6-C5	-2.52	107.31	109.78
4	FFF	401	SIA	O1A-C1-C2	-2.38	119.99	123.59
4	AAA	401	SIA	O2-C2-C1	-2.28	106.11	110.76
4	FFF	401	SIA	O6-C6-C7	-2.07	104.10	107.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	HHH	401	SIA	O8-C8-C9-O9
4	III	401	SIA	O1B-C1-C2-O6
4	III	401	SIA	C7-C8-C9-O9
4	III	401	SIA	O8-C8-C9-O9
4	HHH	401	SIA	C7-C8-C9-O9
7	JJJ	401	PGE	O1-C1-C2-O2
6	EEE	401	EDO	O1-C1-C2-O2
4	DDD	401	SIA	C7-C8-C9-O9
4	AAA	401	SIA	O1A-C1-C2-C3
4	FFF	401	SIA	O1A-C1-C2-C3
7	JJJ	401	PGE	O3-C5-C6-O4
4	AAA	401	SIA	O1A-C1-C2-O6
4	FFF	401	SIA	O1A-C1-C2-O6
4	DDD	401	SIA	O1B-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	III	401	SIA	O1B-C1-C2-C3
7	JJJ	401	PGE	C4-C3-O2-C2
7	JJJ	401	PGE	C6-C5-O3-C4
4	DDD	401	SIA	O1A-C1-C2-O2
4	HHH	401	SIA	O1A-C1-C2-O2
6	EEE	402	EDO	O1-C1-C2-O2

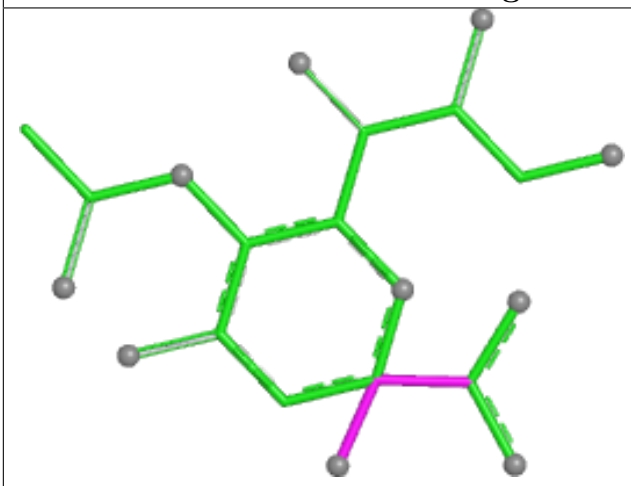
There are no ring outliers.

3 monomers are involved in 4 short contacts:

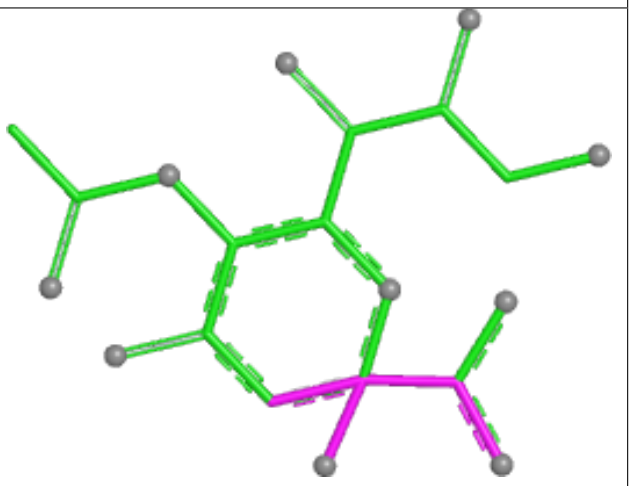
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	JJJ	402	PEG	2	0
4	AAA	401	SIA	1	0
6	EEE	401	EDO	1	0

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

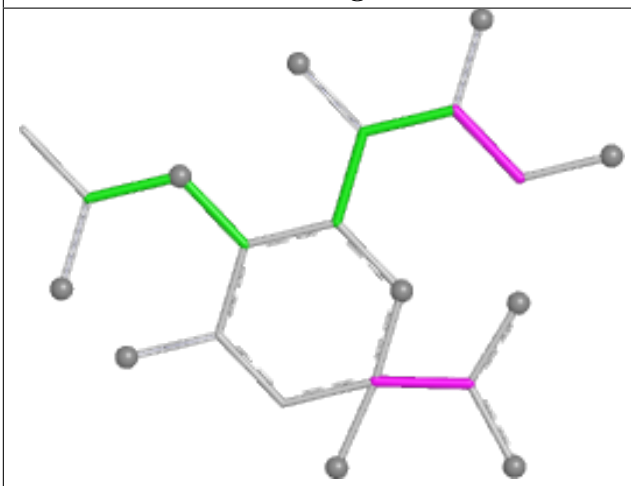
Ligand SIA HHH 401



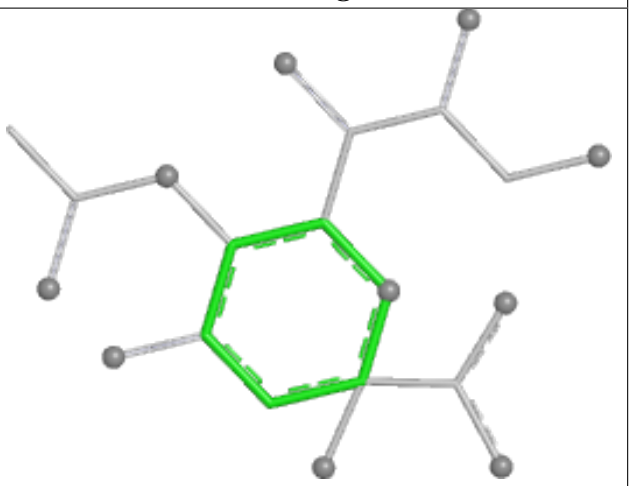
Bond lengths



Bond angles

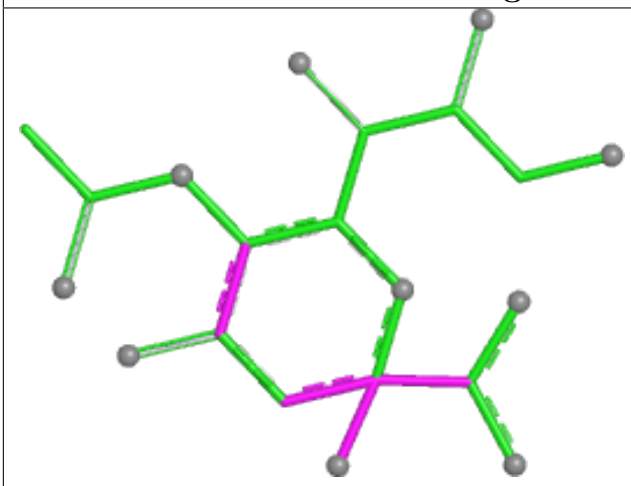


Torsions

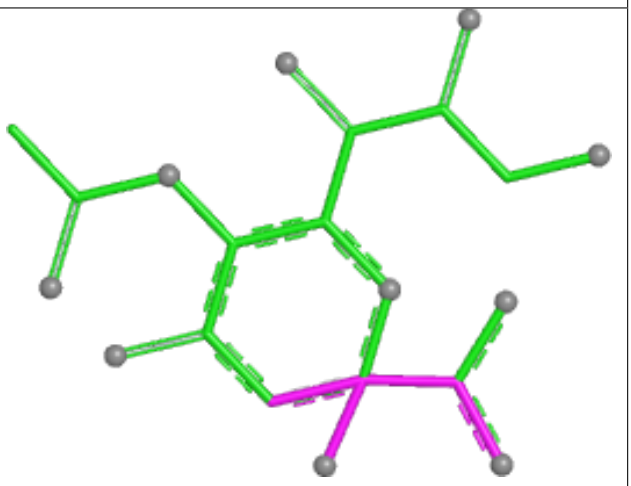


Rings

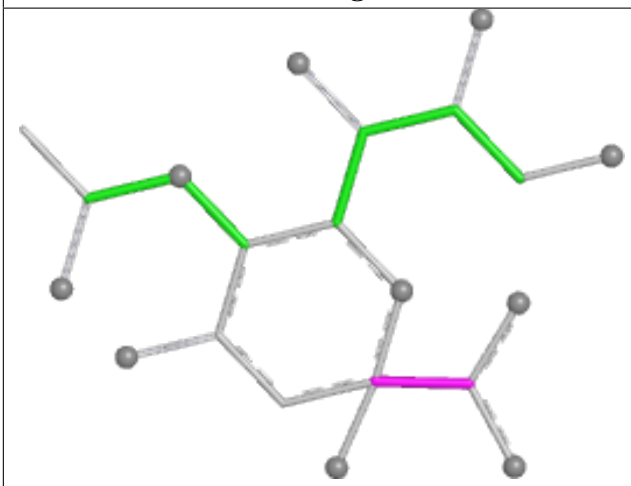
Ligand SIA AAA 401



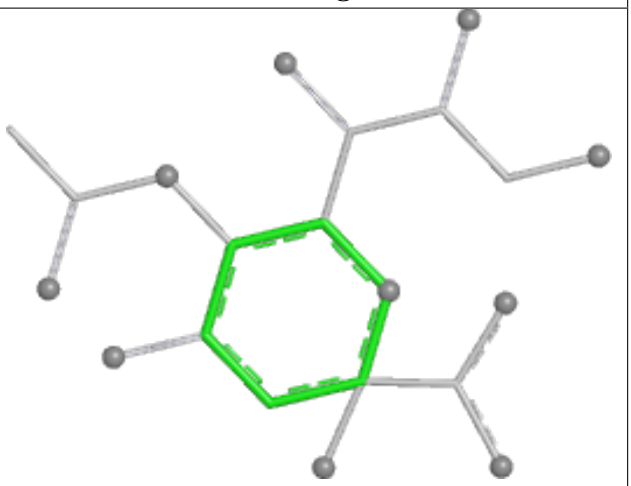
Bond lengths



Bond angles

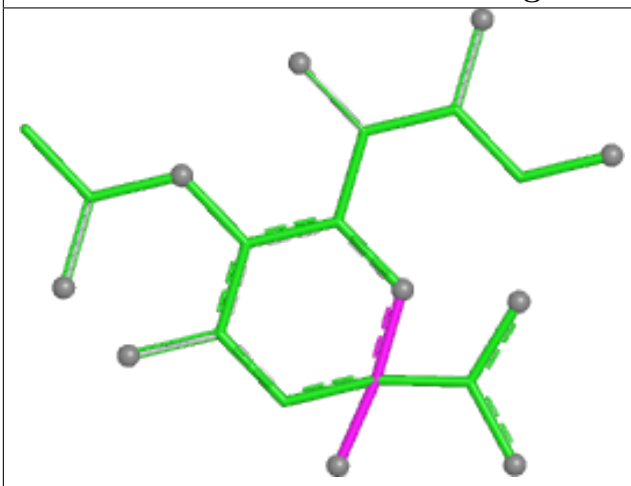


Torsions

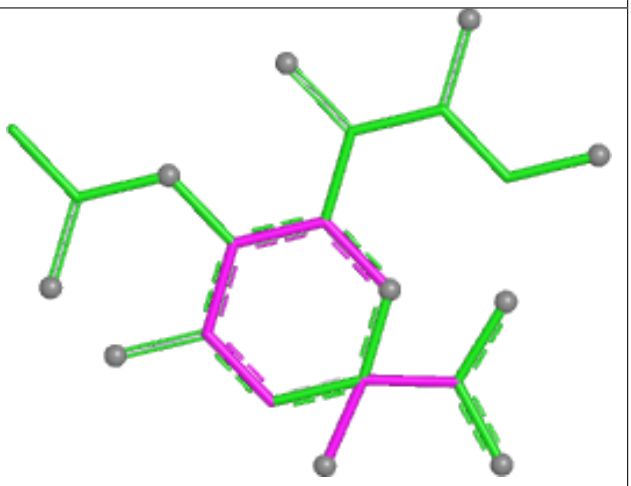


Rings

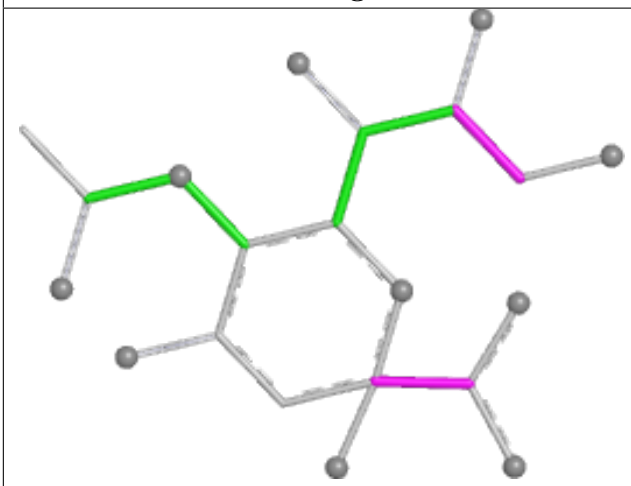
Ligand SIA III 401



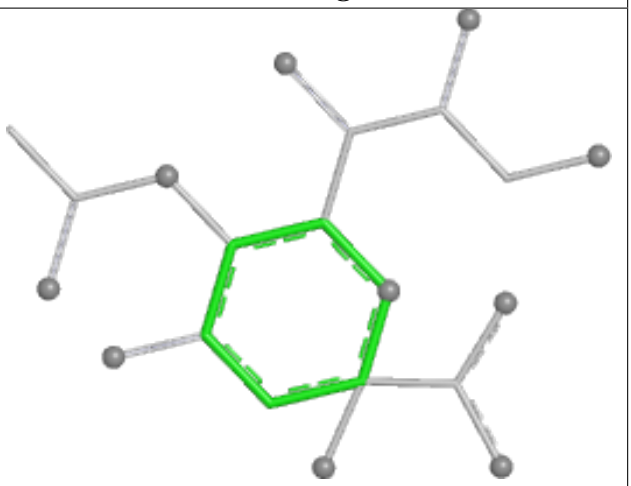
Bond lengths



Bond angles

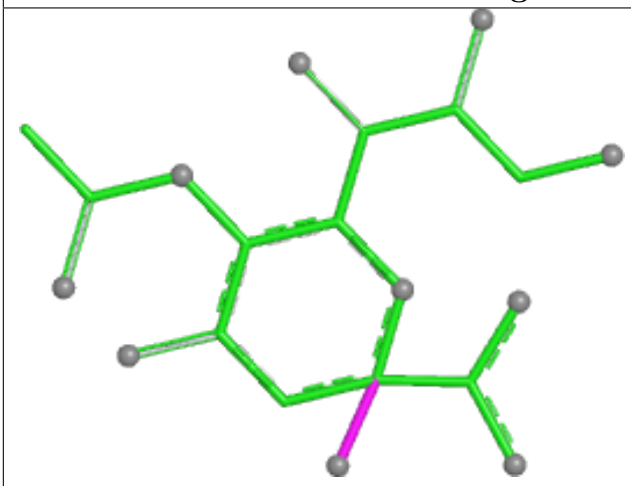


Torsions

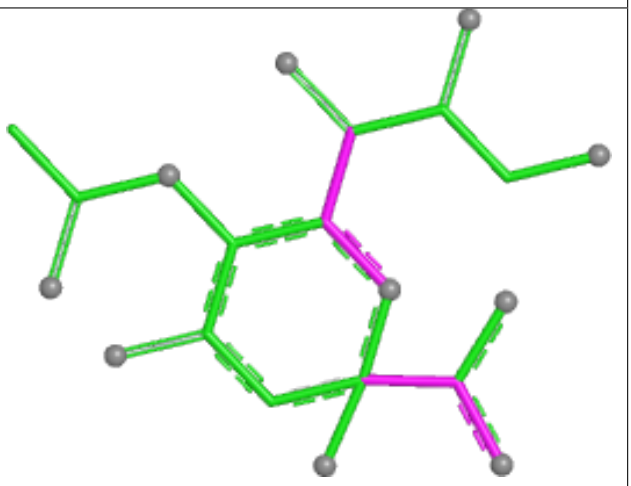


Rings

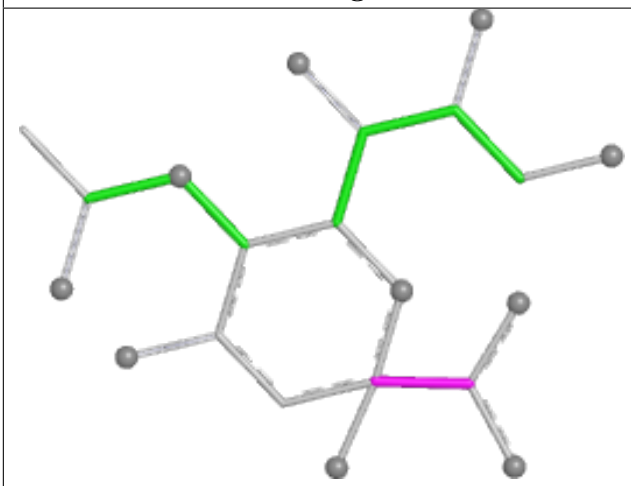
Ligand SIA FFF 401



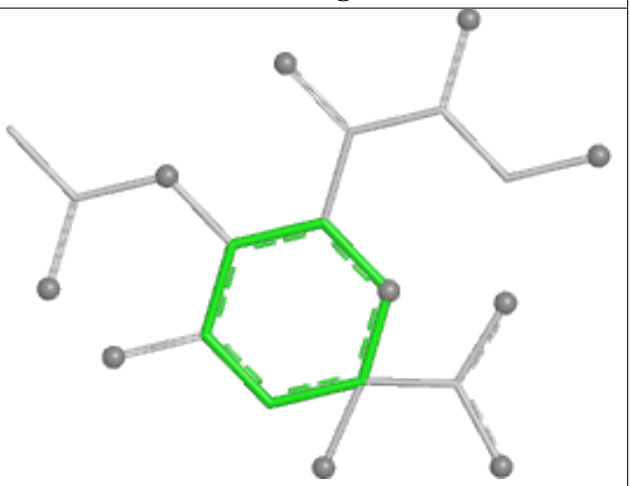
Bond lengths



Bond angles

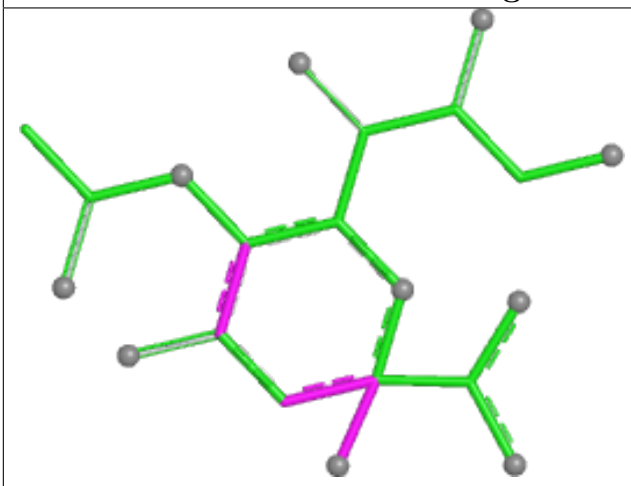


Torsions

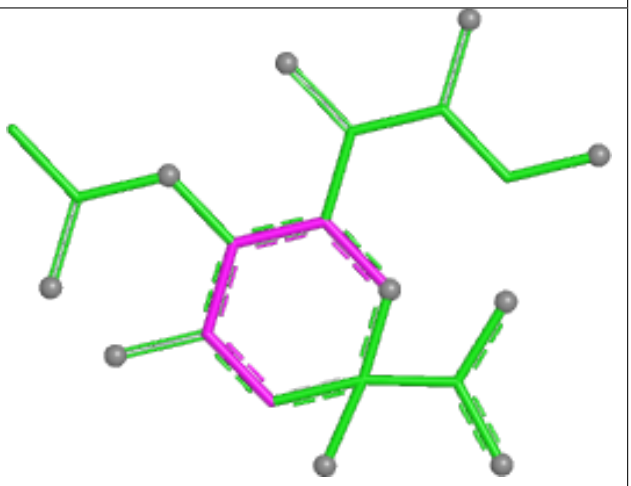


Rings

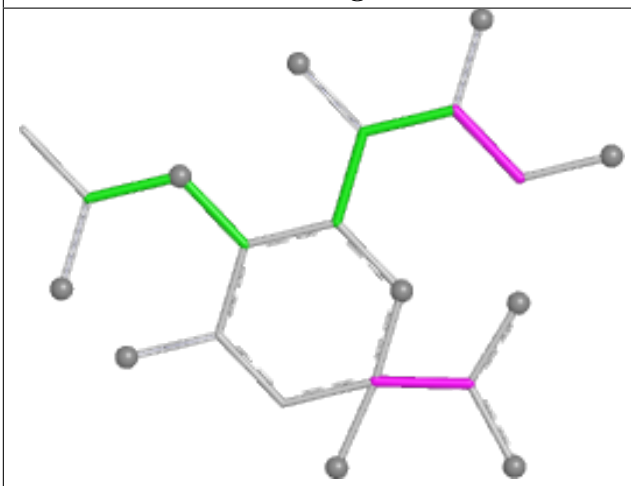
Ligand SIA DDD 401



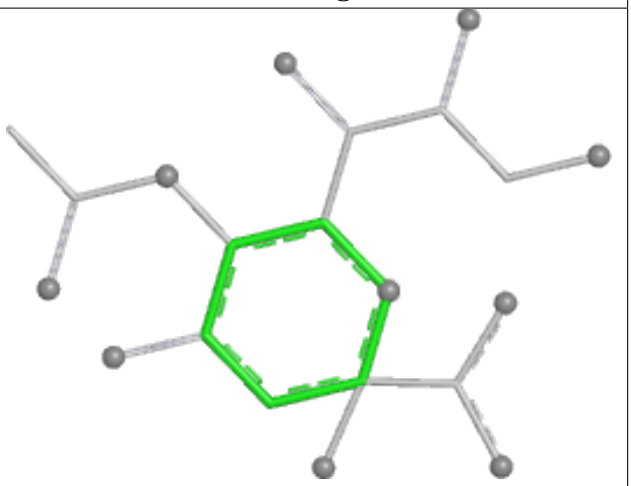
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	268/276 (97%)	-0.40	1 (0%)	92	90	17, 24, 39, 55	0
1	BBB	257/276 (93%)	-0.31	3 (1%)	79	76	18, 26, 46, 56	0
1	CCC	259/276 (93%)	-0.34	3 (1%)	79	76	16, 25, 49, 64	0
1	DDD	268/276 (97%)	-0.38	3 (1%)	80	78	16, 24, 40, 50	0
1	EEE	259/276 (93%)	-0.37	2 (0%)	86	84	17, 24, 47, 69	0
1	FFF	271/276 (98%)	-0.39	2 (0%)	87	86	17, 22, 38, 55	0
1	GGG	261/276 (94%)	-0.31	4 (1%)	73	70	17, 23, 45, 61	0
1	HHH	271/276 (98%)	-0.43	0	100	100	18, 24, 39, 51	0
1	III	260/276 (94%)	-0.23	4 (1%)	73	70	18, 26, 47, 65	0
1	JJJ	259/276 (93%)	-0.34	4 (1%)	73	70	16, 24, 47, 62	0
All	All	2633/2760 (95%)	-0.35	26 (0%)	82	80	16, 24, 44, 69	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	88	MET	4.4
1	BBB	22	ILE	3.2
1	GGG	29	THR	3.0
1	CCC	25	LEU	2.9
1	III	89	LEU	2.8
1	AAA	29	THR	2.7
1	JJJ	89	LEU	2.6
1	EEE	29	THR	2.6
1	DDD	22	ILE	2.5
1	DDD	34	ILE	2.5
1	DDD	31	PRO	2.5
1	GGG	89	LEU	2.5
1	JJJ	97	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	23	GLU	2.4
1	CCC	28	ARG	2.3
1	CCC	31	PRO	2.3
1	FFF	30	GLY	2.3
1	BBB	99	LEU	2.2
1	III	34	ILE	2.2
1	GGG	88	MET	2.2
1	FFF	31	PRO	2.2
1	III	25	LEU	2.1
1	JJJ	22	ILE	2.1
1	JJJ	88	MET	2.1
1	GGG	30	GLY	2.0
1	EEE	97	THR	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	HaH	1	12/12	0.91	0.09	32,40,45,47	0
3	BGC	CaC	1	12/12	0.91	0.17	37,46,49,57	0
2	GAL	IaI	1	12/12	0.92	0.10	36,40,44,45	0
2	GAL	BaB	1	12/12	0.93	0.08	29,34,41,42	0
2	GAL	GaG	1	12/12	0.94	0.08	22,26,32,34	0
2	GLA	IaI	2	11/12	0.94	0.09	20,26,28,30	0
2	GAL	JaJ	1	12/12	0.94	0.08	19,25,29,32	0
2	GAL	EaE	1	12/12	0.94	0.09	26,31,36,38	0
3	GAL	CaC	2	11/12	0.94	0.10	22,27,33,38	0
2	GAL	FaF	1	12/12	0.95	0.08	25,38,44,48	0
2	NGA	HaH	3	14/15	0.95	0.09	24,26,27,27	0
2	A2G	JaJ	4	14/15	0.95	0.07	20,23,26,28	0
2	A2G	HaH	4	14/15	0.95	0.08	21,27,29,31	0
2	GLA	BaB	2	11/12	0.95	0.09	23,25,29,29	0
2	A2G	BaB	4	14/15	0.96	0.08	21,23,31,32	0

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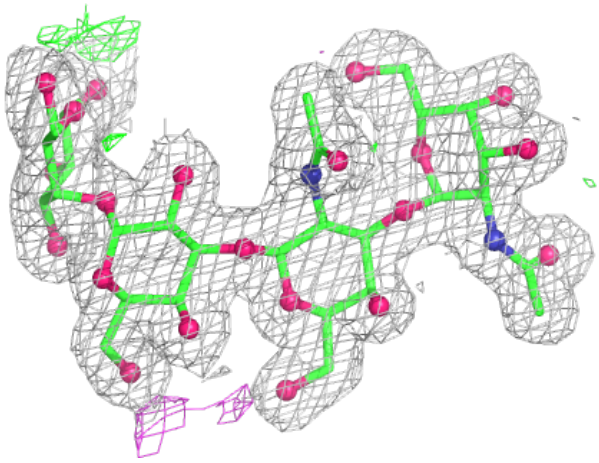
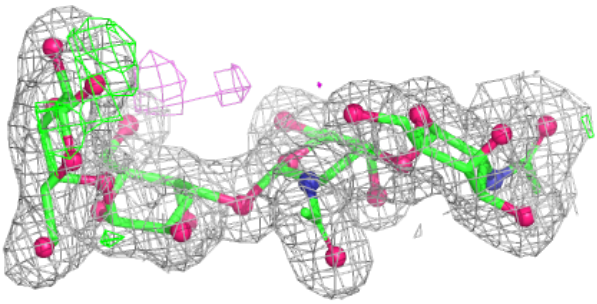
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A2G	IaI	4	14/15	0.96	0.07	22,28,31,32	0
2	NGA	AaA	3	14/15	0.96	0.08	19,23,24,24	0
3	A2G	CaC	5	14/15	0.96	0.10	20,20,23,24	0
2	A2G	GaG	4	14/15	0.97	0.08	23,25,29,29	0
2	GAL	DaD	1	12/12	0.97	0.07	25,33,39,39	0
2	A2G	DaD	4	14/15	0.97	0.07	18,24,28,28	0
2	A2G	AaA	4	14/15	0.97	0.07	22,25,29,33	0
2	GLA	EaE	2	11/12	0.97	0.08	19,21,22,22	0
2	NGA	EaE	3	14/15	0.97	0.07	20,21,23,23	0
2	A2G	EaE	4	14/15	0.97	0.07	20,23,26,26	0
2	NGA	BaB	3	14/15	0.97	0.07	21,22,25,26	0
2	GLA	JaJ	2	11/12	0.97	0.07	18,20,21,22	0
2	NGA	JaJ	3	14/15	0.97	0.07	18,19,22,24	0
2	GLA	FaF	2	11/12	0.97	0.07	16,19,22,23	0
2	A2G	FaF	4	14/15	0.97	0.09	18,21,25,29	0
2	GAL	AaA	1	12/12	0.97	0.06	30,37,41,43	0
2	NGA	GaG	3	14/15	0.97	0.07	18,20,23,24	0
2	GLA	HaH	2	11/12	0.98	0.07	23,27,30,30	0
2	NGA	DaD	3	14/15	0.98	0.08	20,22,25,27	0
2	GLA	GaG	2	11/12	0.98	0.07	20,21,24,24	0
2	GLA	AaA	2	11/12	0.98	0.06	22,24,25,27	0
2	NGA	FaF	3	14/15	0.98	0.09	18,19,22,22	0
2	NGA	IaI	3	14/15	0.98	0.07	23,25,29,30	0
3	GLA	CaC	3	11/12	0.98	0.08	19,19,21,22	0
3	NGA	CaC	4	14/15	0.98	0.07	17,19,22,23	0
2	GLA	DaD	2	11/12	0.98	0.06	20,24,25,25	0

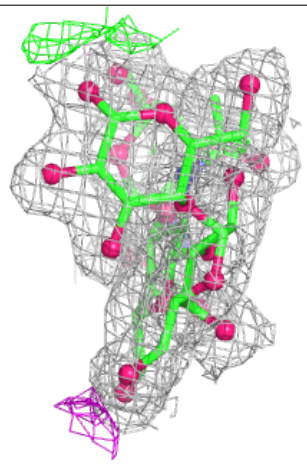
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain AaA:

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

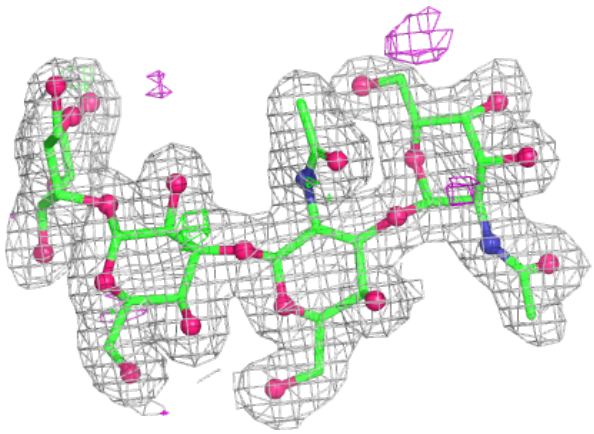


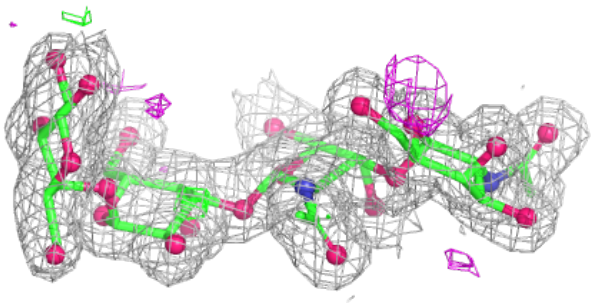


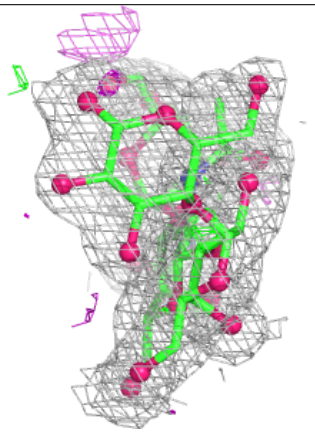


Electron density around Chain BaB:

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

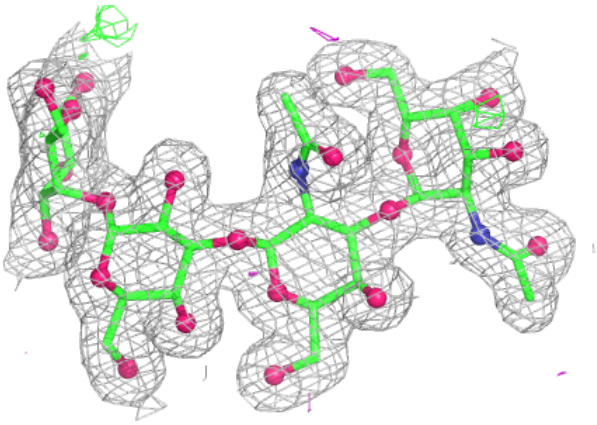


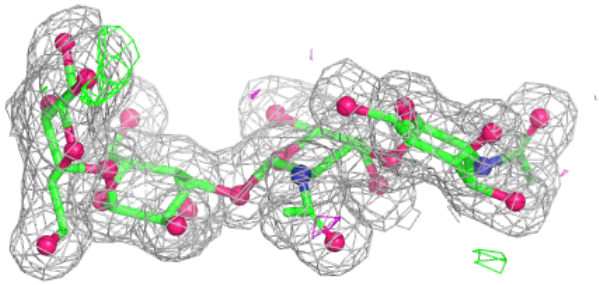


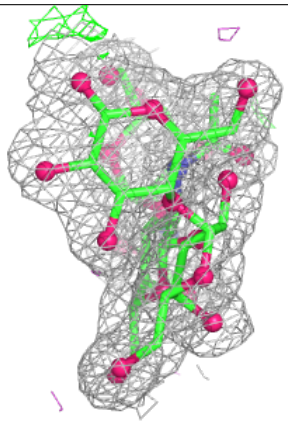


Electron density around Chain DaD:

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

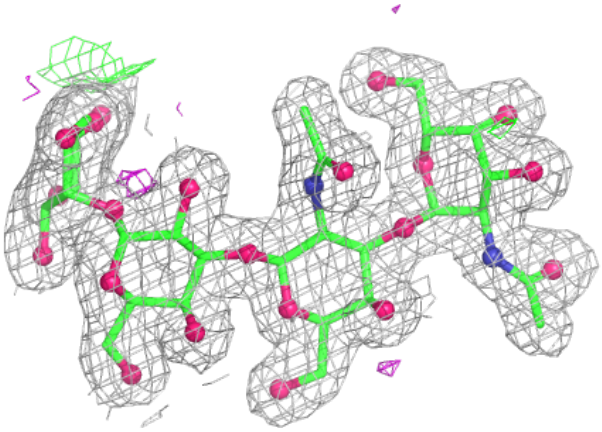


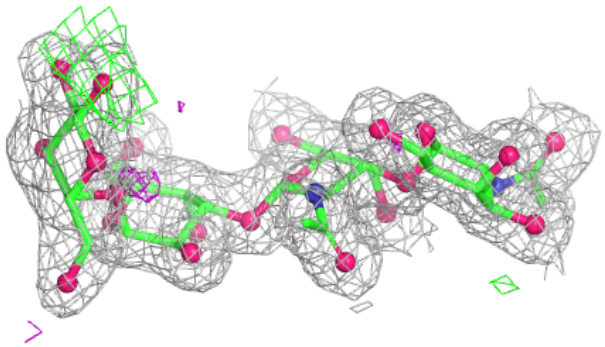


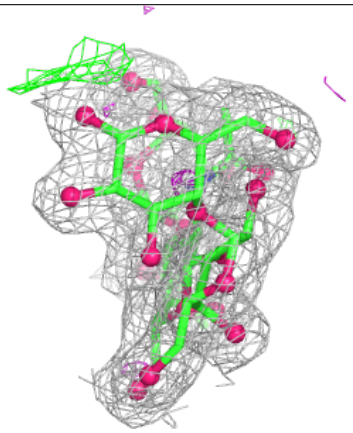


Electron density around Chain EaE:

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

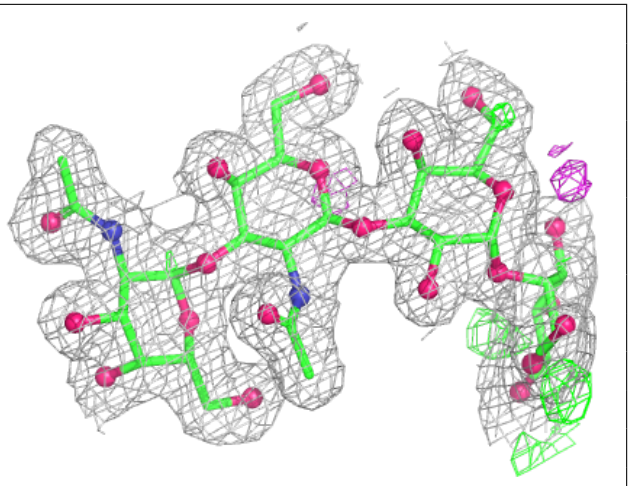


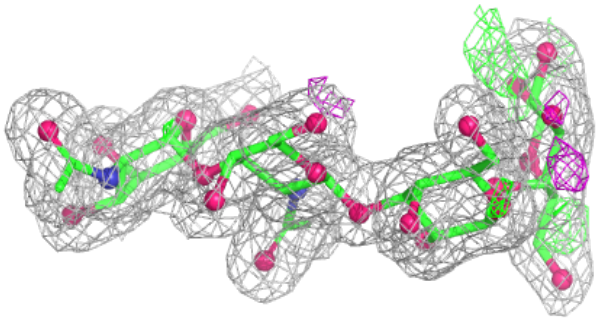


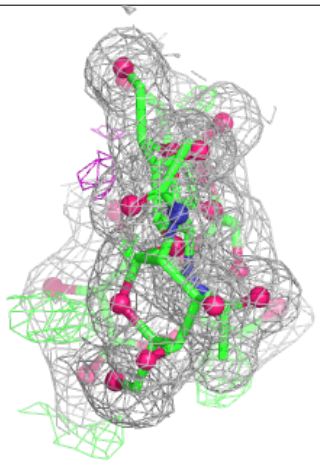


Electron density around Chain FaF:

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

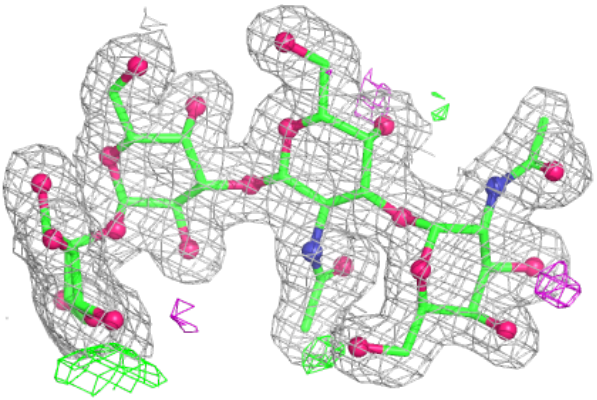


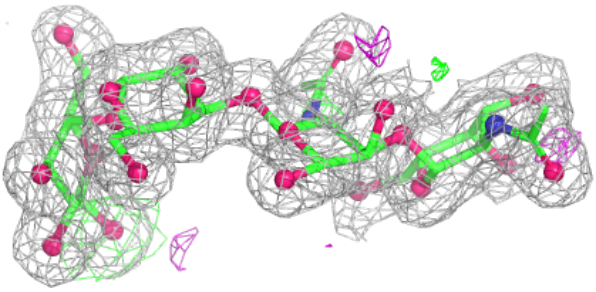


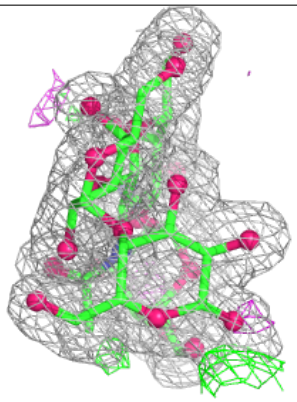


Electron density around Chain GaG:

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

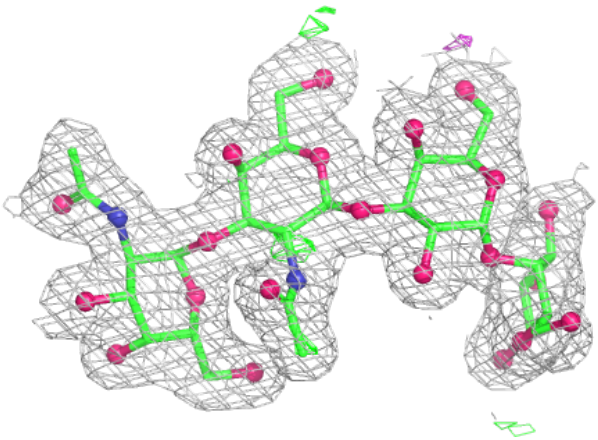


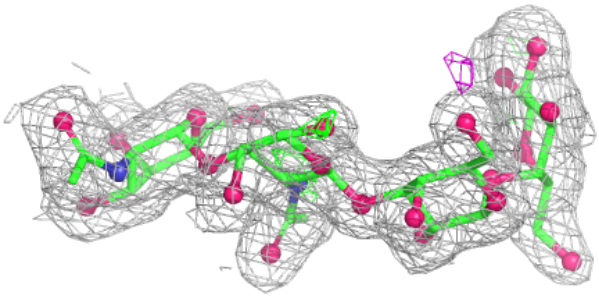


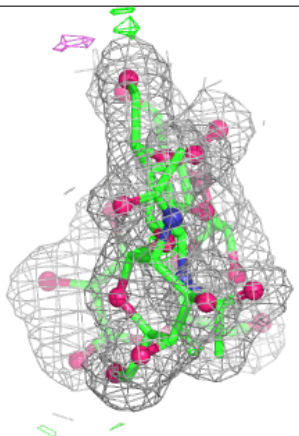


Electron density around Chain HaH:

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

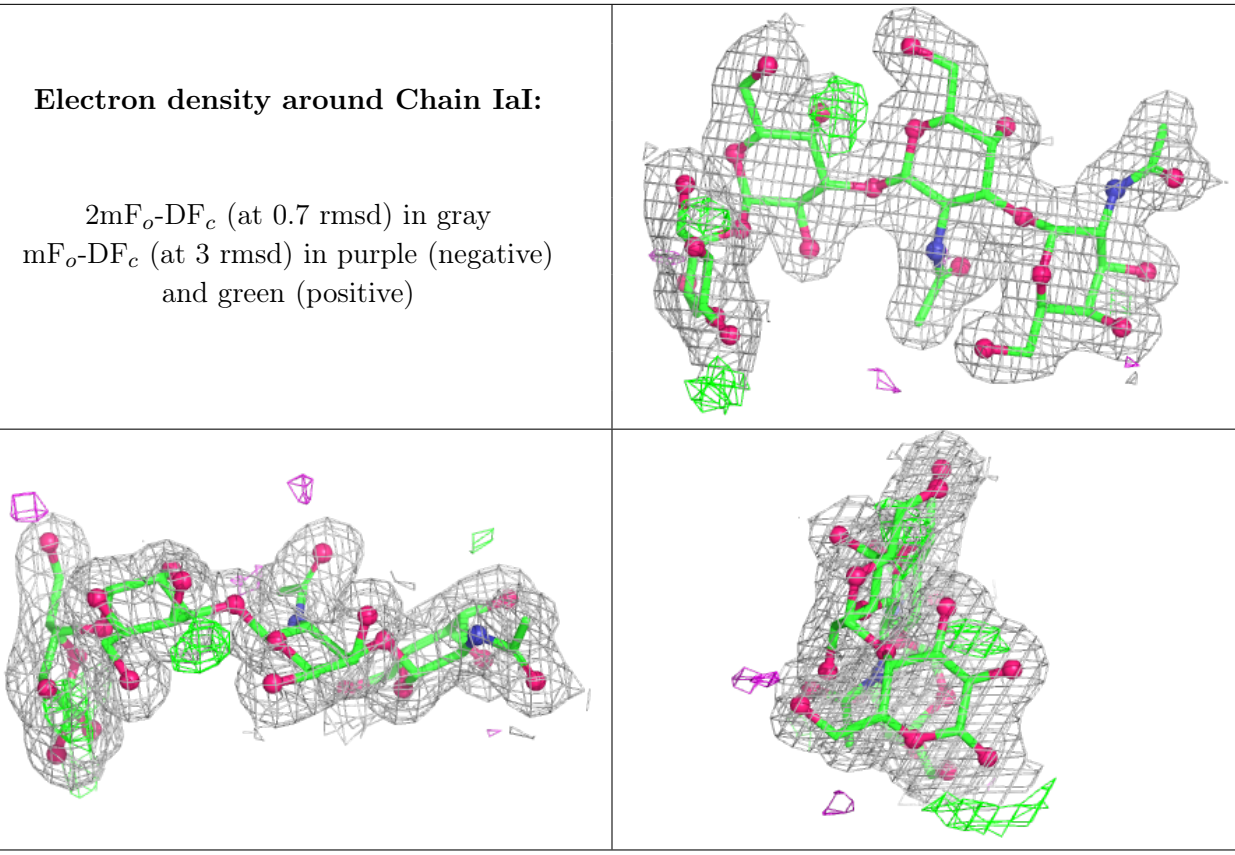






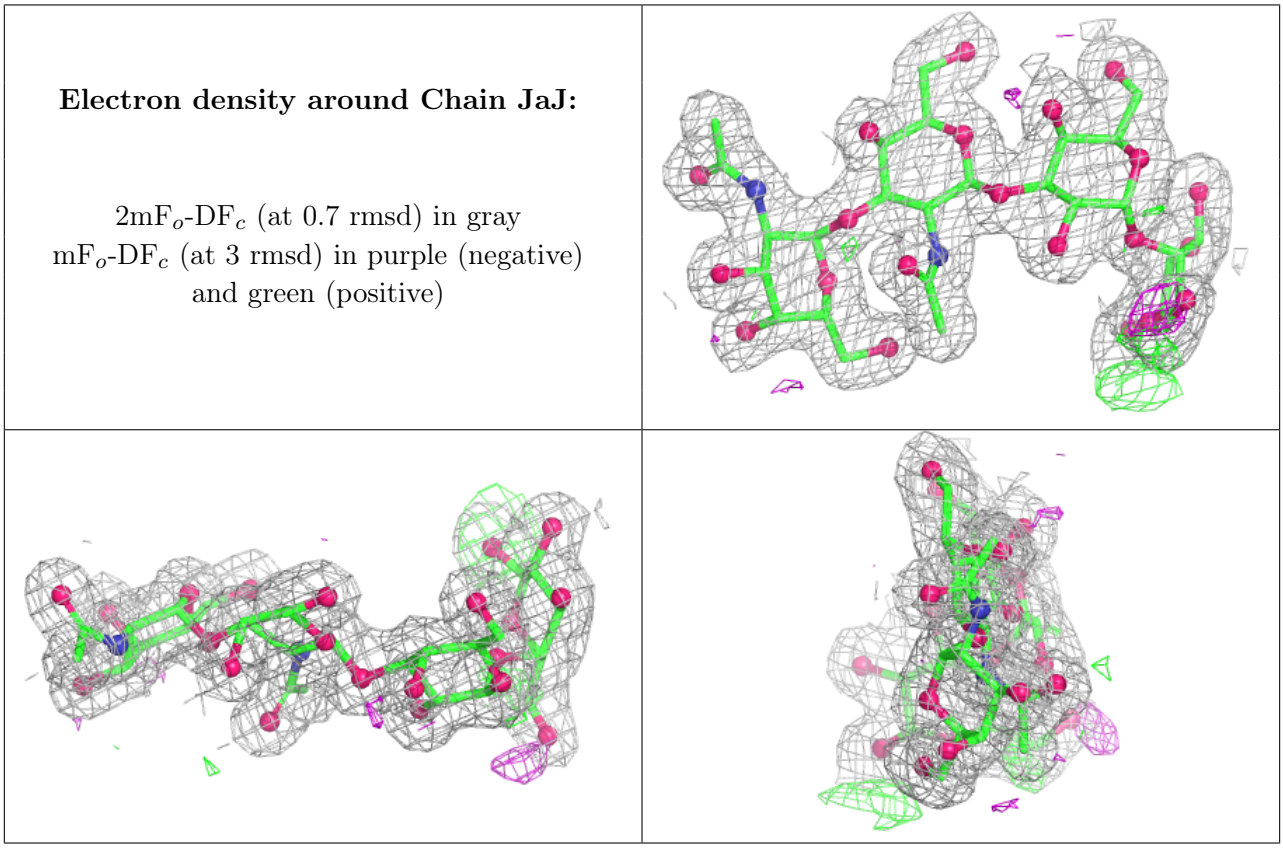
Electron density around Chain IaI:

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



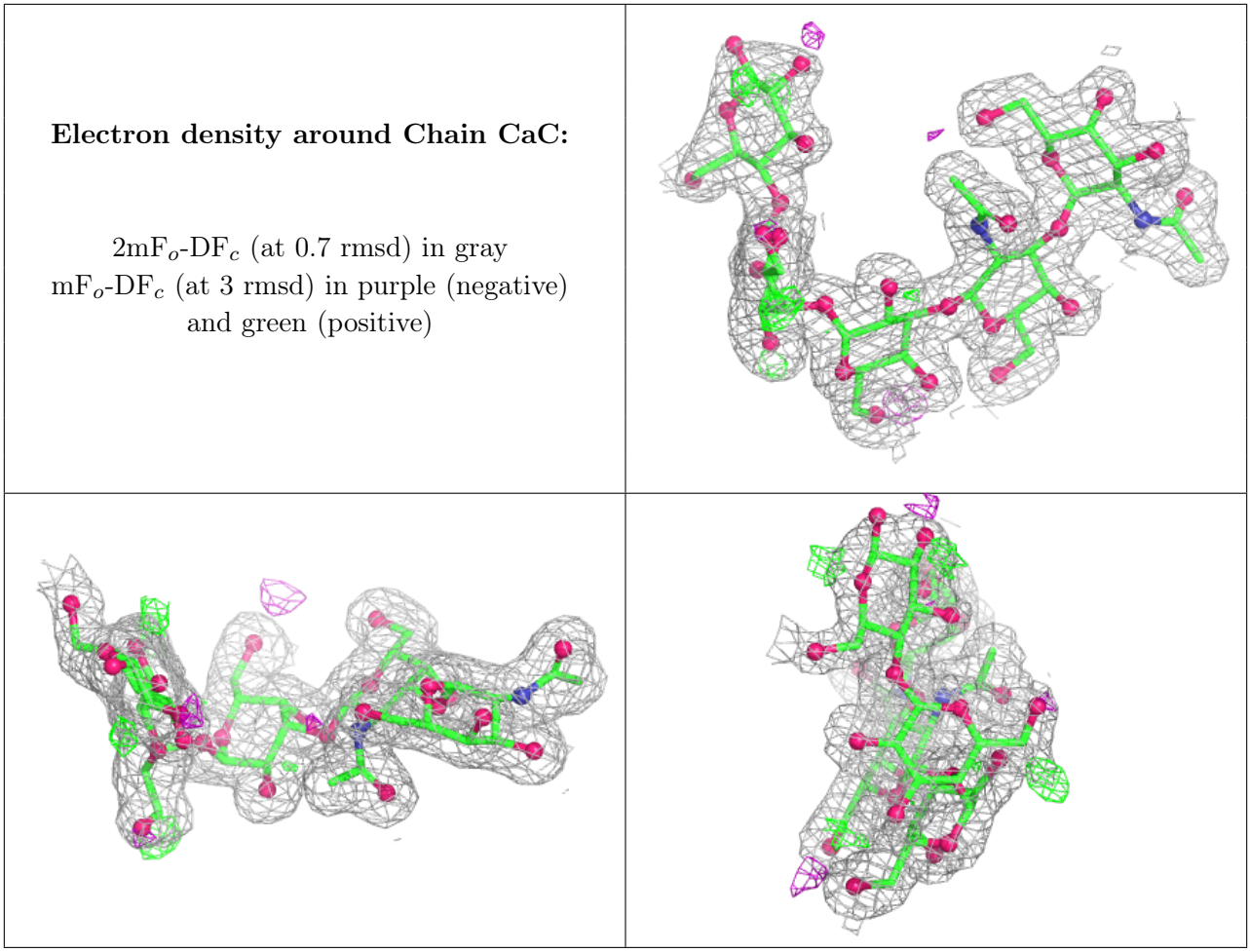
Electron density around Chain JaJ:

$2mF_o$-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)



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
7	PGE	JJJ	401	10/10	0.80	0.17	42,56,59,60	0
4	SIA	III	401	21/21	0.85	0.14	25,39,50,54	0
6	EDO	EEE	401	4/4	0.89	0.09	39,39,40,42	0
8	PEG	JJJ	402	7/7	0.89	0.15	45,49,53,61	0
4	SIA	HHH	401	21/21	0.90	0.13	27,37,45,49	0
4	SIA	AAA	401	21/21	0.91	0.11	26,35,40,47	0
4	SIA	DDD	401	21/21	0.92	0.11	21,32,38,41	0
6	EDO	HHH	402	4/4	0.92	0.09	51,52,52,53	0
4	SIA	FFF	401	21/21	0.93	0.11	20,32,39,42	0
5	MG	HHH	403	1/1	0.93	0.09	39,39,39,39	0
6	EDO	EEE	402	4/4	0.94	0.12	46,50,51,53	0

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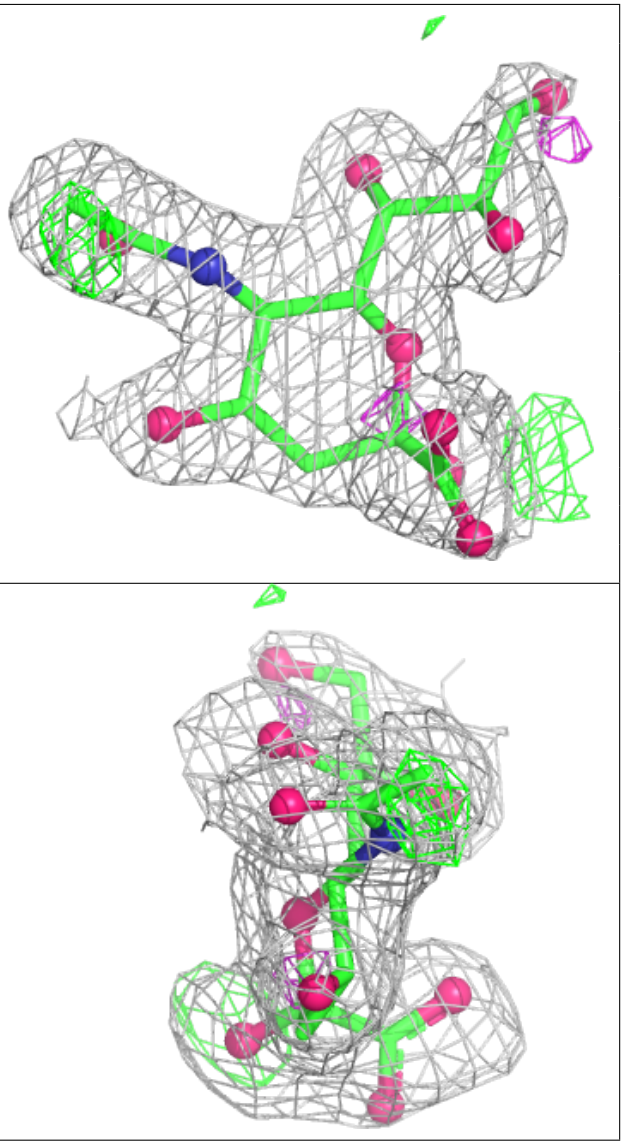
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	BBB	301	1/1	0.96	0.11	43,43,43,43	0
5	MG	DDD	402	1/1	0.96	0.13	36,36,36,36	0
5	MG	GGG	301	1/1	0.96	0.14	39,39,39,39	0
5	MG	III	402	1/1	0.97	0.07	36,36,36,36	0
5	MG	CCC	301	1/1	0.98	0.04	43,43,43,43	0
5	MG	EEE	403	1/1	0.98	0.06	45,45,45,45	0
5	MG	JJJ	403	1/1	0.99	0.06	39,39,39,39	0
5	MG	FFF	402	1/1	0.99	0.11	39,39,39,39	0
5	MG	AAA	402	1/1	0.99	0.04	36,36,36,36	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.

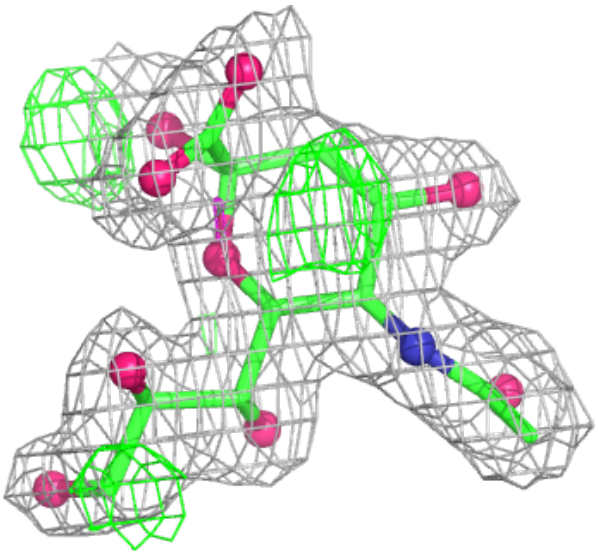
Electron density around SIA III 401:

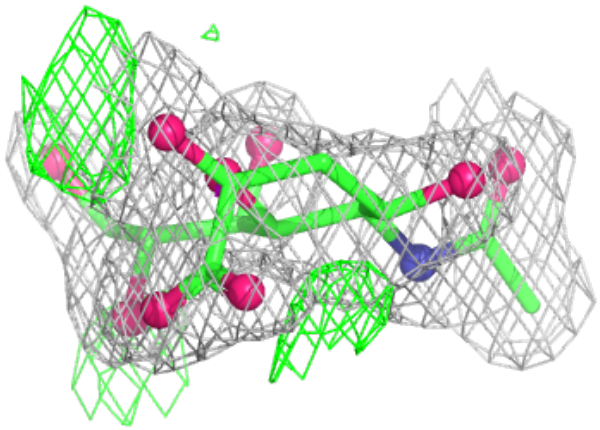
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SIA HHH 401:

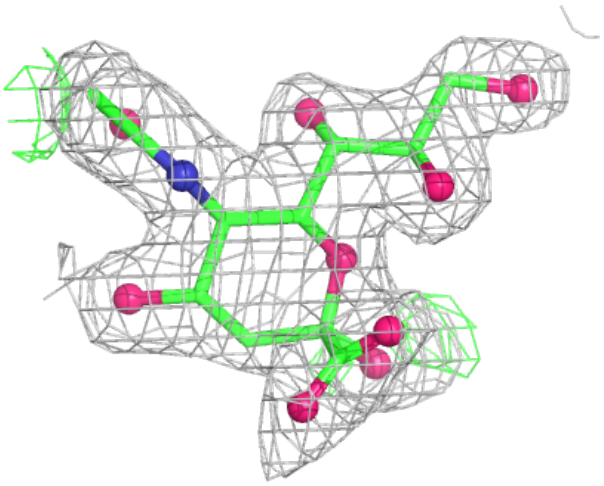
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

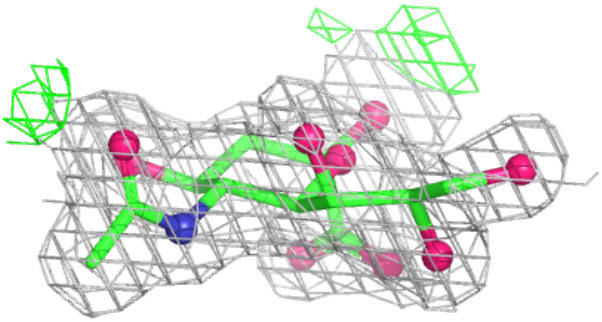


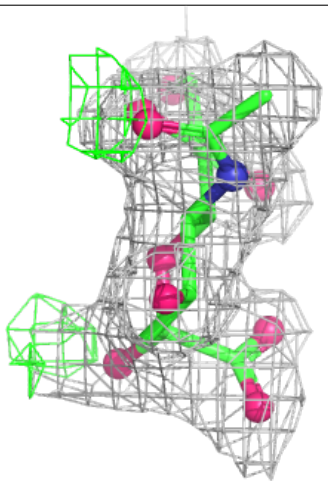


Electron density around SIA AAA 401:

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

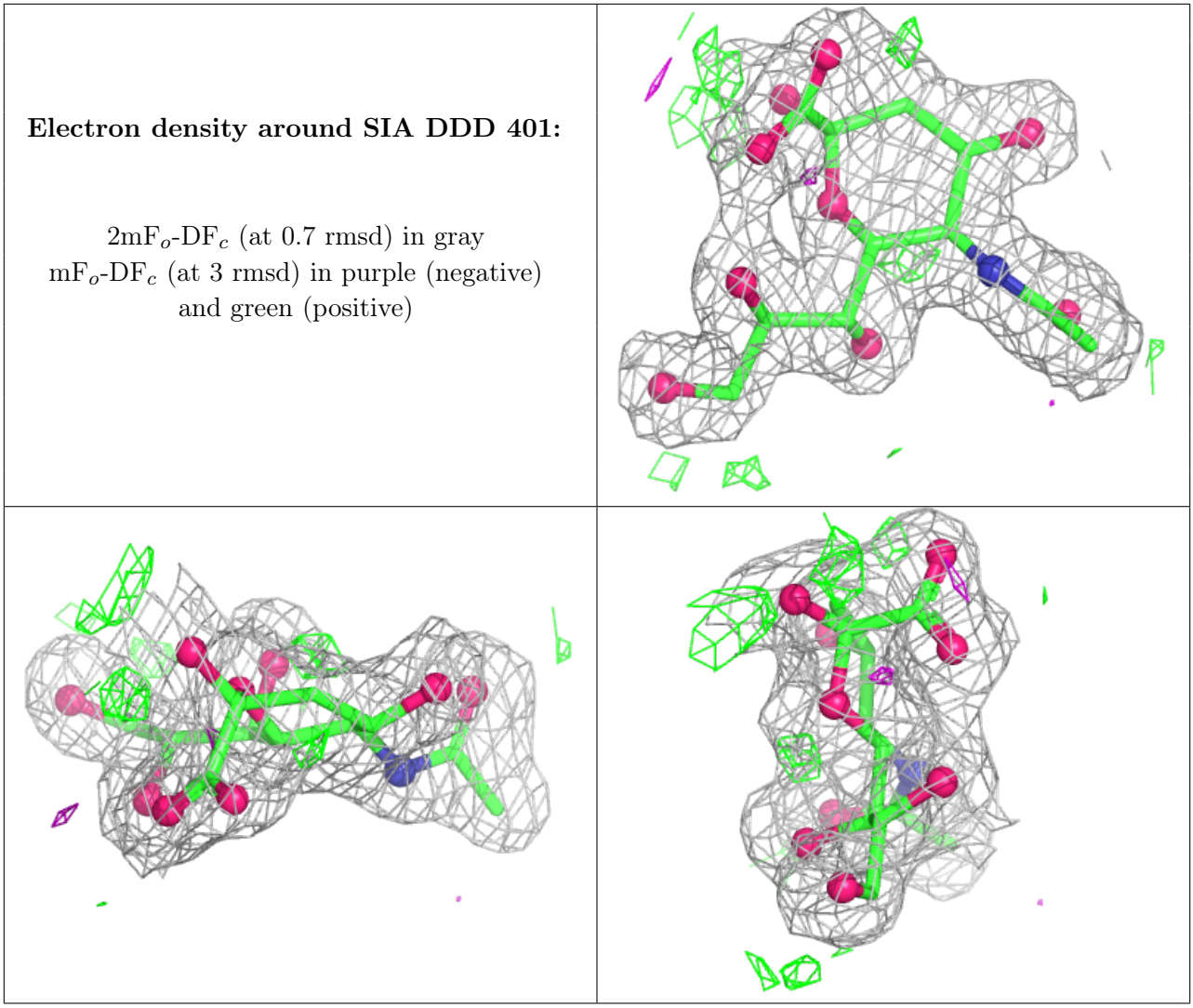






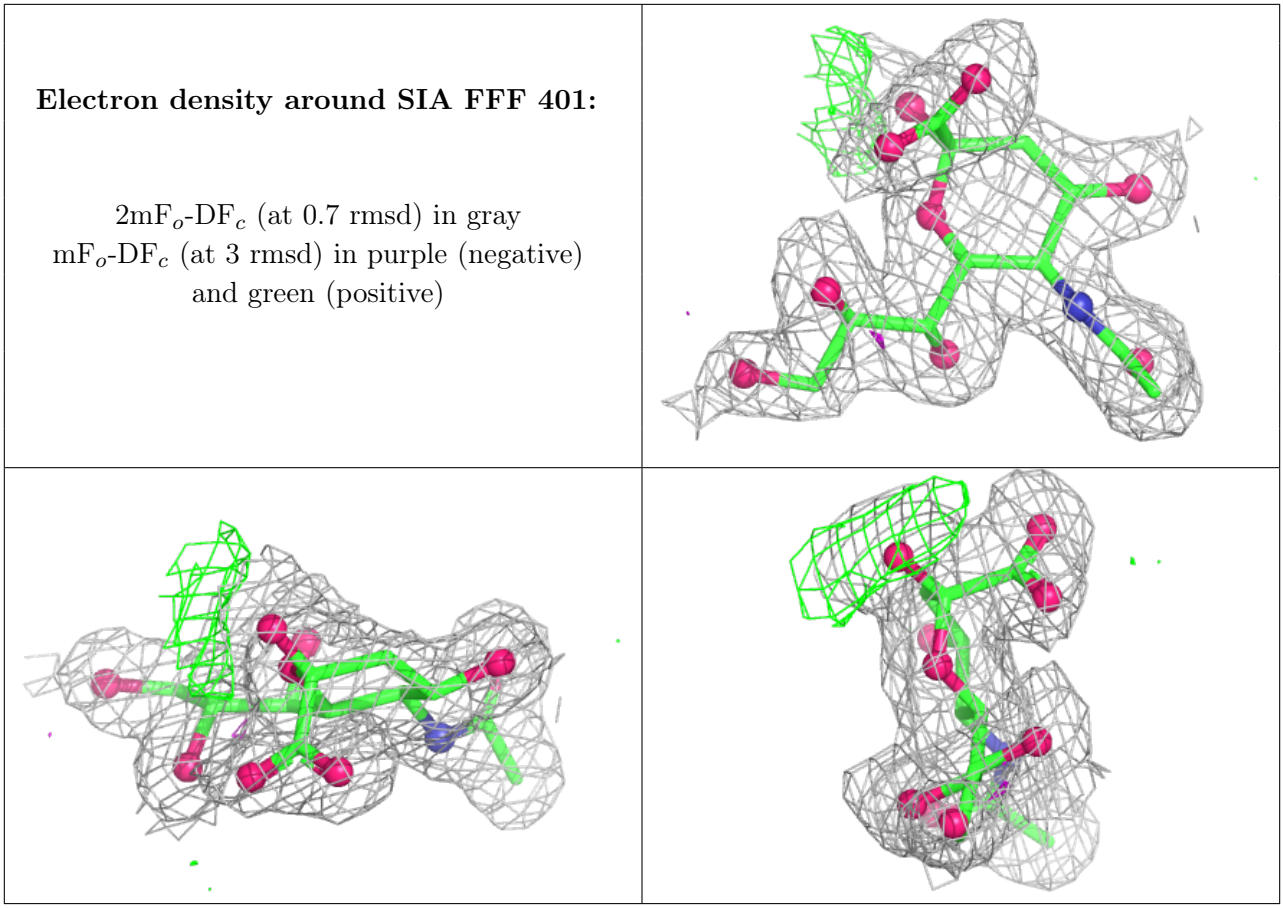
Electron density around SIA DDD 401:

$2mF_o$-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 FFF 401:

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



6.5 Other polymers

There are no such residues in this entry.