



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:21 AM UTC

PDB ID : 7B6T / pdb_00007b6t
Title : Sheep Polyomavirus VP1 in complex with 10 mM globo-N-tetraose
Authors : Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-12-08
Resolution : 1.70 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

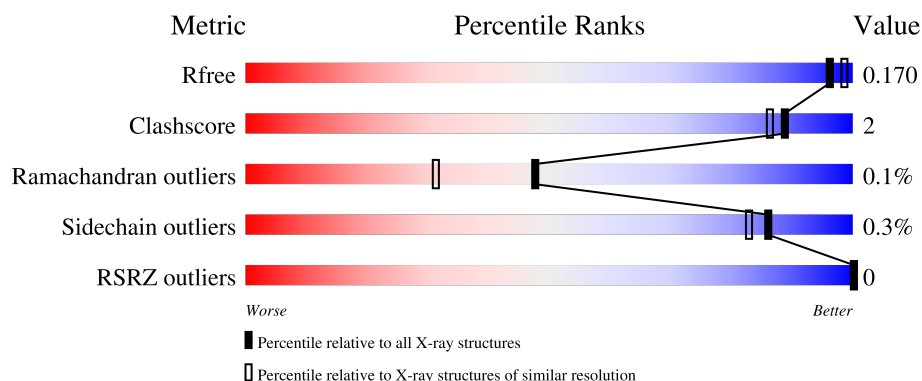
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



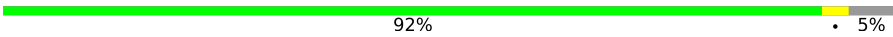
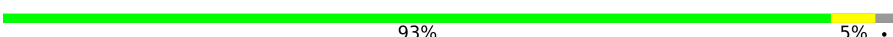
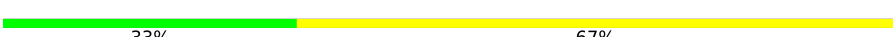
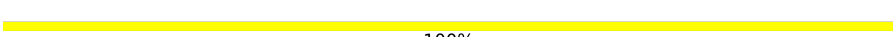
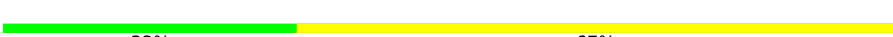
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	AAA	276	89% 6% 5%
1	BBB	276	92% 6% .
1	CCC	276	91% . 6%
1	DDD	276	94% . .
1	EEE	276	90% . 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	276	 92% • 5%
1	GGG	276	 92% 5% •
1	HHH	276	 91% • 5%
1	III	276	 93% 5% •
1	JJJ	276	 91% • 6%
2	AaA	3	 33% 67%
2	CaC	3	 100%
2	FaF	3	 33% 67%
2	HaH	3	 67% 33%
3	BaB	2	 100%
3	DaD	2	 50% 50%
3	JaJ	2	 50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24010 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	262	Total	C	N	O	S	0	0	0
			2011	1286	337	376	12			
1	BBB	271	Total	C	N	O	S	0	0	0
			2087	1325	351	397	14			
1	CCC	260	Total	C	N	O	S	0	0	0
			2006	1280	338	376	12			
1	DDD	271	Total	C	N	O	S	0	0	0
			2088	1326	351	397	14			
1	EEE	259	Total	C	N	O	S	0	0	0
			1989	1269	335	373	12			
1	FFF	261	Total	C	N	O	S	0	1	0
			2005	1281	337	375	12			
1	GGG	270	Total	C	N	O	S	0	0	0
			2075	1321	348	393	13			
1	HHH	261	Total	C	N	O	S	0	2	0
			2015	1285	338	380	12			
1	III	270	Total	C	N	O	S	0	0	0
			2070	1320	347	390	13			
1	JJJ	260	Total	C	N	O	S	0	0	0
			1997	1275	335	375	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

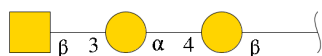
Continued on next page...

Continued from previous page...

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	19	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	20	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	21	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	22	MET	-	expression tag	UNP A0A0E3ZCF3
DDD	98	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

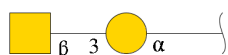
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-a

lpha-D-galactopyranose-(1-4)-beta-D-galactopyranose.



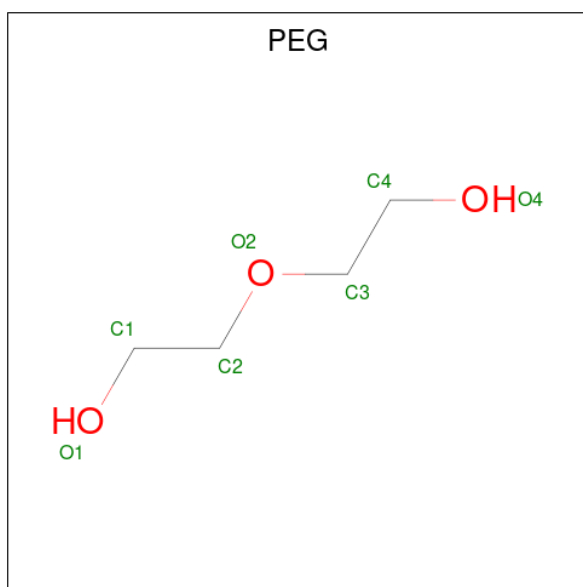
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	CaC	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	FaF	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	HaH	3	Total	C	N	O	0	0	0
			37	20	1	16			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	BaB	2	Total	C	N	O	0	0	0
			26	14	1	11			
3	DaD	2	Total	C	N	O	0	0	0
			26	14	1	11			
3	JaJ	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		
4	CCC	1	Total	C	O	0	0
			7	4	3		
4	CCC	1	Total	C	O	0	0
			7	4	3		
4	DDD	1	Total	C	O	0	0
			7	4	3		
4	EEE	1	Total	C	O	0	0
			7	4	3		
4	FFF	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

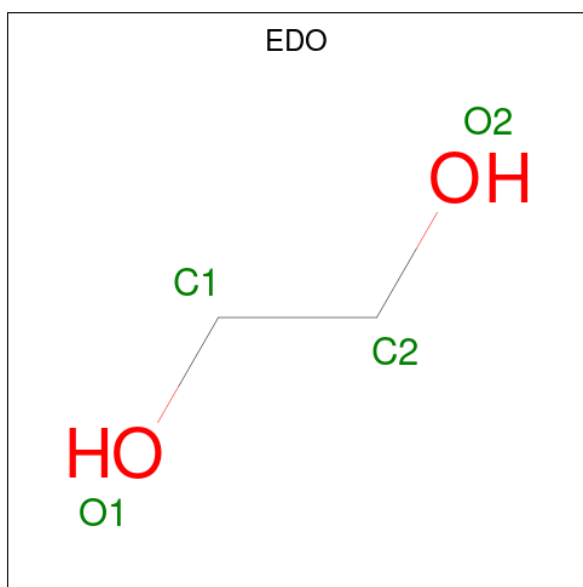
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	GGG	2	Total 2	Mg 2	0	0
5	HHH	1	Total 1	Mg 1	0	0
5	III	2	Total 2	Mg 2	0	0
5	JJJ	1	Total 1	Mg 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	1	Total 1	K 1	0	0
6	BBB	1	Total 1	K 1	0	0
6	CCC	1	Total 1	K 1	0	0
6	DDD	1	Total 1	K 1	0	0
6	EEE	1	Total 1	K 1	0	0
6	FFF	1	Total 1	K 1	0	0
6	HHH	1	Total 1	K 1	0	0
6	III	1	Total 1	K 1	0	0
6	JJJ	1	Total 1	K 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



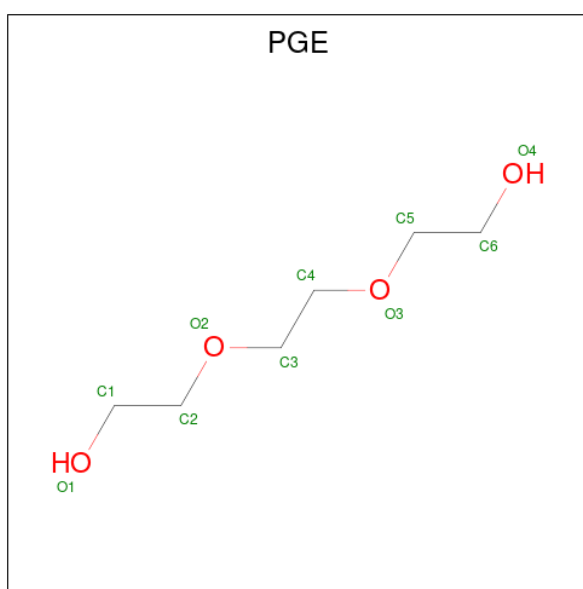
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	EEE	1	Total	C	O	0	0
			4	2	2		
7	FFF	1	Total	C	O	0	0
			4	2	2		
7	FFF	1	Total	C	O	0	0
			4	2	2		
7	FFF	1	Total	C	O	0	0
			4	2	2		
7	HHH	1	Total	C	O	0	0
			4	2	2		
7	HHH	1	Total	C	O	0	0
			4	2	2		
7	HHH	1	Total	C	O	0	0
			4	2	2		
7	HHH	1	Total	C	O	0	0
			4	2	2		
7	III	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

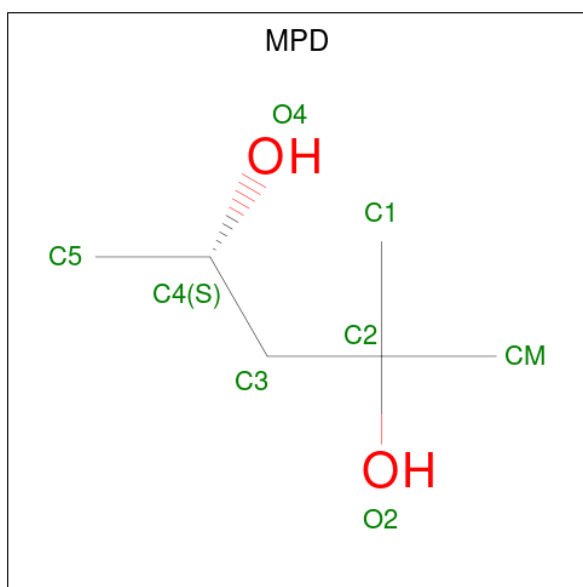
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	III	1	Total	C	O	0	0
			4	2	2		
7	III	1	Total	C	O	0	0
			4	2	2		
7	JJJ	1	Total	C	O	0	0
			4	2	2		
7	JJJ	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	BBB	1	Total	C	O	0	0
			8	5	3		
8	BBB	1	Total	C	O	0	0
			8	5	3		
8	BBB	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	EEE	1	Total	C	O	0	0
			8	6	2		
9	GGG	1	Total	C	O	0	0
			8	6	2		
9	III	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	320	Total	O	0	6
			326	326		
10	BBB	327	Total	O	0	3
			330	330		
10	CCC	318	Total	O	0	1
			319	319		
10	DDD	333	Total	O	0	6
			339	339		
10	EEE	318	Total	O	0	3
			321	321		
10	FFF	317	Total	O	0	8
			325	325		
10	GGG	341	Total	O	0	6
			347	347		
10	HHH	315	Total	O	0	8
			323	323		
10	III	338	Total	O	0	8
			346	346		

Continued on next page...

Continued from previous page...

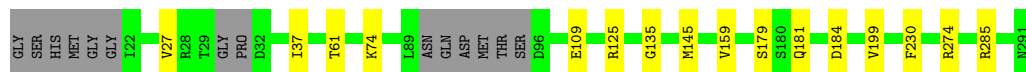
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	JJJ	276	Total 280	O 280	0	5

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:  89% 6% 5%



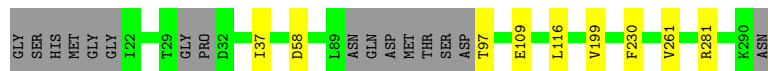
- Molecule 1: Capsid protein VP1

Chain BBB:  92% 6% .

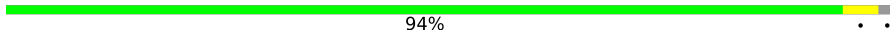


- Molecule 1: Capsid protein VP1

Chain CCC:  91% . 6%



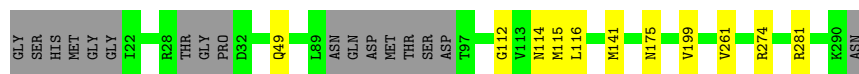
- Molecule 1: Capsid protein VP1

Chain DDD:  94% . .



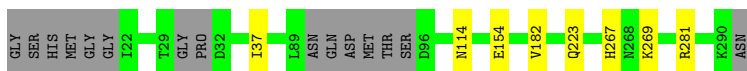
- Molecule 1: Capsid protein VP1

Chain EEE:  90% . 6%



- Molecule 1: Capsid protein VP1

Chain FFF:  92% . 5%



- Molecule 1: Capsid protein VP1

Chain GGG: 92% 5%



- Molecule 1: Capsid protein VP1

Chain HHH: 91% 5%



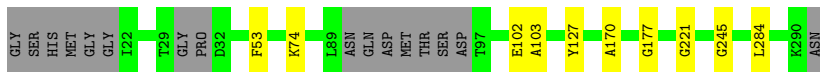
- Molecule 1: Capsid protein VP1

Chain III: 93% 5%



- Molecule 1: Capsid protein VP1

Chain JJJ: 91% 6%



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

Chain AaA: 33% 67%

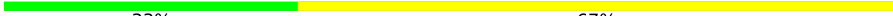


- Molecule 2: 2-acetamido-2-deoxy-beta-D-galactopyranose-(1-3)-alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain CaC: 100%



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

Chain FaF:  33% 67%

GLA1
GLA2
NGA3

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

Chain HaH:  67% 33%

GLA1
GLA2
NGA3

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

Chain BaB:  100%

GLA1
NGA2

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

Chain DaD:  50% 50%

GLA3
NGA2

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

Chain JaJ:  50% 50%

GLA3
NGA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	130.27Å 130.27Å 222.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.91 – 1.70 48.91 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-1.70) 100.0 (48.91-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.143 , 0.165 0.149 , 0.170	Depositor DCC
R_{free} test set	4628 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l 0.219 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
Reported twinning fraction	0.792 for H, K, L 0.208 for K, H, -L	Depositor
Outliers	0 of 462791 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24010	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.05	0/2061	1.17	1/2801 (0.0%)
1	BBB	1.06	2/2140 (0.1%)	1.18	1/2910 (0.0%)
1	CCC	1.01	0/2056	1.16	1/2794 (0.0%)
1	DDD	1.03	1/2141 (0.0%)	1.20	0/2911
1	EEE	1.01	0/2039	1.22	1/2772 (0.0%)
1	FFF	1.03	1/2058 (0.0%)	1.18	0/2797
1	GGG	1.04	1/2128 (0.0%)	1.20	0/2894
1	HHH	1.02	0/2069	1.17	2/2813 (0.1%)
1	III	1.07	0/2123	1.19	1/2889 (0.0%)
1	JJJ	1.04	1/2047 (0.0%)	1.19	3/2782 (0.1%)
All	All	1.04	6/20862 (0.0%)	1.19	10/28363 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	154	GLU	C-O	5.61	1.30	1.24
1	DDD	192	GLY	C-O	5.49	1.29	1.23
1	GGG	221	GLY	C-O	5.44	1.29	1.23
1	JJJ	221	GLY	C-O	5.25	1.30	1.23
1	BBB	221	GLY	C-O	5.24	1.29	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	175	ASN	O-C-N	-6.09	118.73	121.53
1	HHH	178	ALA	CA-C-N	5.69	128.69	120.38
1	HHH	178	ALA	C-N-CA	5.69	128.69	120.38
1	JJJ	53	PHE	CA-CB-CG	-5.58	108.22	113.80
1	CCC	58	ASP	N-CA-C	-5.43	103.36	110.53

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	2011	0	1922	10	0
1	BBB	2087	0	1995	12	0
1	CCC	2006	0	1923	6	0
1	DDD	2088	0	1996	9	0
1	EEE	1989	0	1892	7	0
1	FFF	2005	0	1909	6	0
1	GGG	2075	0	1984	11	0
1	HHH	2015	0	1918	8	0
1	III	2070	0	1976	10	0
1	JJJ	1997	0	1900	4	0
2	AaA	37	0	33	0	0
2	CaC	37	0	33	0	0
2	FaF	37	0	33	0	0
2	HaH	37	0	33	1	0
3	BaB	26	0	24	0	0
3	DaD	26	0	24	0	0
3	JaJ	26	0	24	0	0
4	AAA	7	0	10	0	0
4	CCC	14	0	20	0	0
4	DDD	7	0	10	1	0
4	EEE	7	0	10	0	0
4	FFF	7	0	10	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	2	0	0	0	0
5	HHH	1	0	0	0	0
5	III	2	0	0	0	0
5	JJJ	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
6	EEE	1	0	0	0	0
6	FFF	1	0	0	0	0
6	HHH	1	0	0	0	0
6	III	1	0	0	0	0
6	JJJ	1	0	0	0	0
7	BBB	8	0	12	1	0
7	CCC	12	0	18	1	0
7	EEE	4	0	6	0	0
7	FFF	12	0	18	1	0
7	HHH	16	0	24	1	0
7	III	12	0	18	3	0
7	JJJ	8	0	12	1	0
8	BBB	26	0	32	1	0
9	EEE	8	0	14	0	0
9	GGG	8	0	14	1	0
9	III	8	0	14	0	0
10	AAA	326	0	0	3	0
10	BBB	330	0	0	4	0
10	CCC	319	0	0	2	0
10	DDD	339	0	0	4	0
10	EEE	321	0	0	2	0
10	FFF	325	0	0	2	0
10	GGG	347	0	0	5	0
10	HHH	323	0	0	3	0
10	III	346	0	0	0	0
10	JJJ	280	0	0	0	0
All	All	24010	0	19861	77	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 77 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:EEE:281:ARG:NH2	10:EEE:601:HOH:O	2.20	0.74
1:CCC:281:ARG:NH1	10:CCC:401:HOH:O	2.20	0.73
1:FFF:281:ARG:NH2	10:FFF:501:HOH:O	2.22	0.72
1:BBB:89:LEU:H	1:BBB:89:LEU:HD23	1.53	0.71
1:JJJ:170:ALA:O	7:JJJ:401:EDO:H12	1.91	0.70

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	256/276 (93%)	244 (95%)	12 (5%)	0	100	100
1	BBB	269/276 (98%)	258 (96%)	11 (4%)	0	100	100
1	CCC	254/276 (92%)	243 (96%)	11 (4%)	0	100	100
1	DDD	269/276 (98%)	259 (96%)	10 (4%)	0	100	100
1	EEE	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	FFF	256/276 (93%)	245 (96%)	10 (4%)	1 (0%)	30	16
1	GGG	268/276 (97%)	256 (96%)	11 (4%)	1 (0%)	30	16
1	HHH	259/276 (94%)	247 (95%)	12 (5%)	0	100	100
1	III	268/276 (97%)	258 (96%)	10 (4%)	0	100	100
1	JJJ	254/276 (92%)	243 (96%)	11 (4%)	0	100	100
All	All	2606/2760 (94%)	2496 (96%)	108 (4%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	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	211/234 (90%)	209 (99%)	2 (1%)	70	62
1	BBB	223/234 (95%)	221 (99%)	2 (1%)	70	62
1	CCC	213/234 (91%)	212 (100%)	1 (0%)	81	76
1	DDD	223/234 (95%)	223 (100%)	0	100	100
1	EEE	209/234 (89%)	208 (100%)	1 (0%)	81	76
1	FFF	210/234 (90%)	210 (100%)	0	100	100
1	GGG	220/234 (94%)	220 (100%)	0	100	100
1	HHH	212/234 (91%)	212 (100%)	0	100	100
1	III	218/234 (93%)	218 (100%)	0	100	100
1	JJJ	209/234 (89%)	209 (100%)	0	100	100
All	All	2148/2340 (92%)	2142 (100%)	6 (0%)	86	83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	274	ARG
1	CCC	97	THR
1	EEE	274	ARG
1	AAA	274	ARG
1	AAA	109	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	0.41	0	17,17,17	1.07	0
2	GLA	AaA	2	2	11,11,12	0.71	0	15,15,17	1.40	3 (20%)
2	NGA	AaA	3	2	14,14,15	0.49	0	17,19,21	1.35	1 (5%)
3	GLA	BaB	1	3	12,12,12	0.60	0	17,17,17	1.22	1 (5%)
3	NGA	BaB	2	3	14,14,15	0.47	0	17,19,21	1.00	1 (5%)
2	GAL	CaC	1	2	12,12,12	0.64	0	17,17,17	1.15	2 (11%)
2	GLA	CaC	2	2	11,11,12	0.48	0	15,15,17	1.34	2 (13%)
2	NGA	CaC	3	2	14,14,15	0.56	0	17,19,21	1.33	1 (5%)
3	GLA	DaD	1	3	12,12,12	0.57	0	17,17,17	0.93	0
3	NGA	DaD	2	3	14,14,15	0.43	0	17,19,21	1.21	1 (5%)
2	GAL	FaF	1	2	12,12,12	0.47	0	17,17,17	0.70	0
2	GLA	FaF	2	2	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
2	NGA	FaF	3	2	14,14,15	0.54	0	17,19,21	1.16	2 (11%)
2	GAL	HaH	1	2	12,12,12	0.53	0	17,17,17	1.27	3 (17%)
2	GLA	HaH	2	2	11,11,12	0.46	0	15,15,17	1.09	1 (6%)
2	NGA	HaH	3	2	14,14,15	0.66	0	17,19,21	1.09	1 (5%)
3	GLA	JaJ	1	3	12,12,12	0.50	0	17,17,17	0.56	0
3	NGA	JaJ	2	3	14,14,15	0.45	0	17,19,21	1.71	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
3	GLA	BaB	1	3	-	1/2/22/22	0/1/1/1
3	NGA	BaB	2	3	-	0/6/23/26	0/1/1/1
2	GAL	CaC	1	2	-	2/2/22/22	0/1/1/1
2	GLA	CaC	2	2	-	1/2/19/22	0/1/1/1
2	NGA	CaC	3	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLA	DaD	1	3	-	1/2/22/22	0/1/1/1
3	NGA	DaD	2	3	-	1/6/23/26	0/1/1/1
2	GAL	FaF	1	2	-	0/2/22/22	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	GAL	HaH	1	2	-	1/2/22/22	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
3	GLA	JaJ	1	3	-	1/2/22/22	0/1/1/1
3	NGA	JaJ	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	JaJ	2	NGA	C1-O5-C5	5.57	119.65	112.19
2	AaA	3	NGA	C1-O5-C5	4.50	118.22	112.19
2	CaC	3	NGA	C1-O5-C5	4.23	117.86	112.19
3	BaB	1	GLA	C1-O5-C5	3.61	120.64	113.65
2	AaA	2	GLA	O3-C3-C2	-3.58	102.76	110.05

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

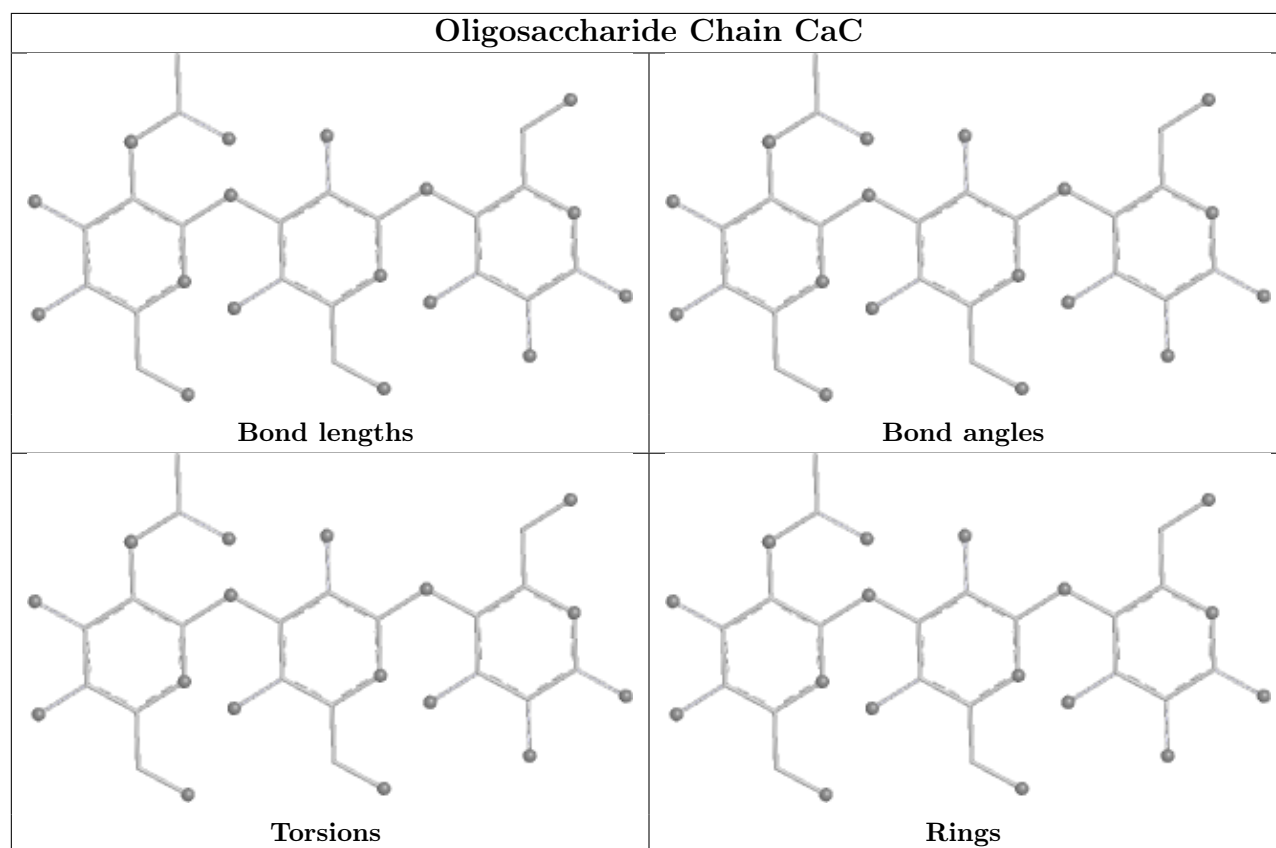
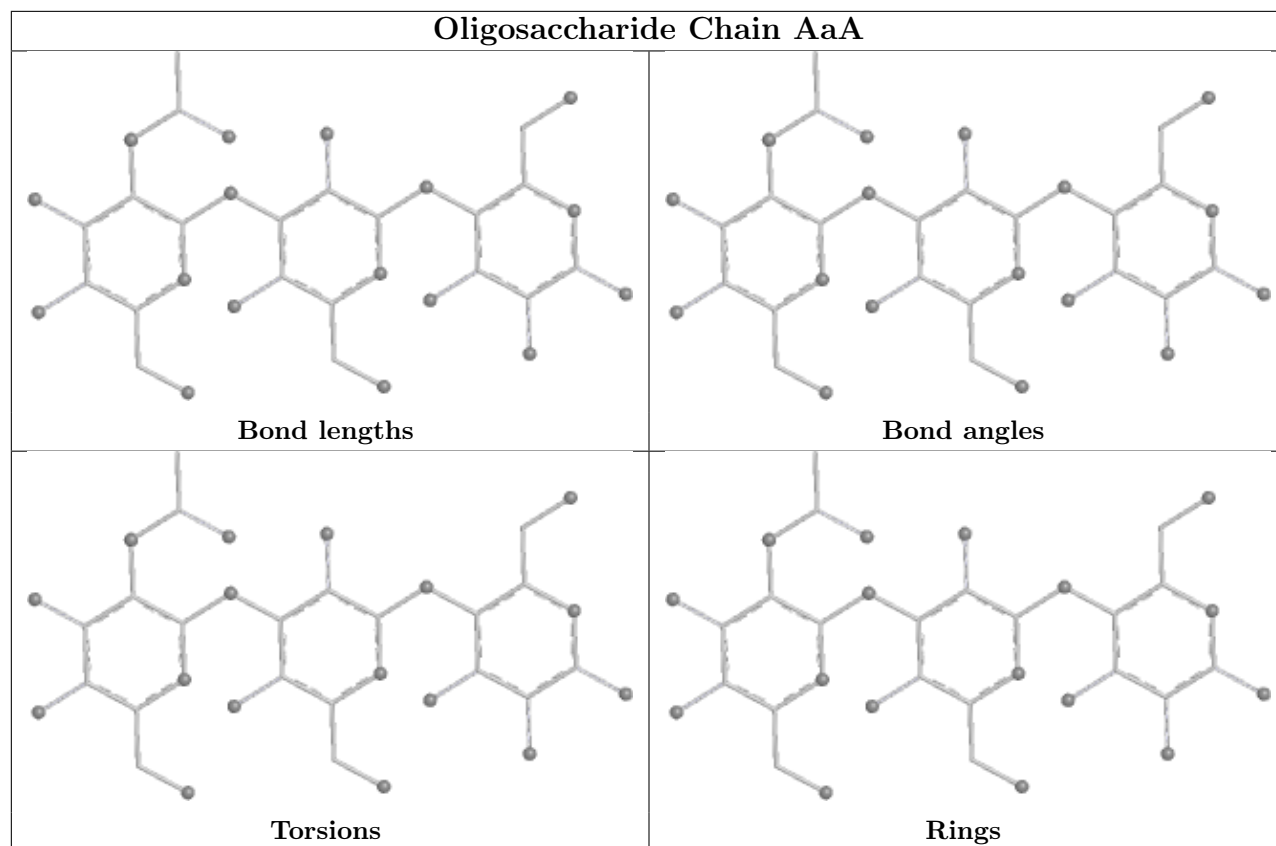
Mol	Chain	Res	Type	Atoms
2	HaH	1	GAL	O5-C5-C6-O6
3	BaB	1	GLA	O5-C5-C6-O6
2	CaC	1	GAL	C4-C5-C6-O6
2	AaA	2	GLA	O5-C5-C6-O6
2	CaC	2	GLA	O5-C5-C6-O6

There are no ring outliers.

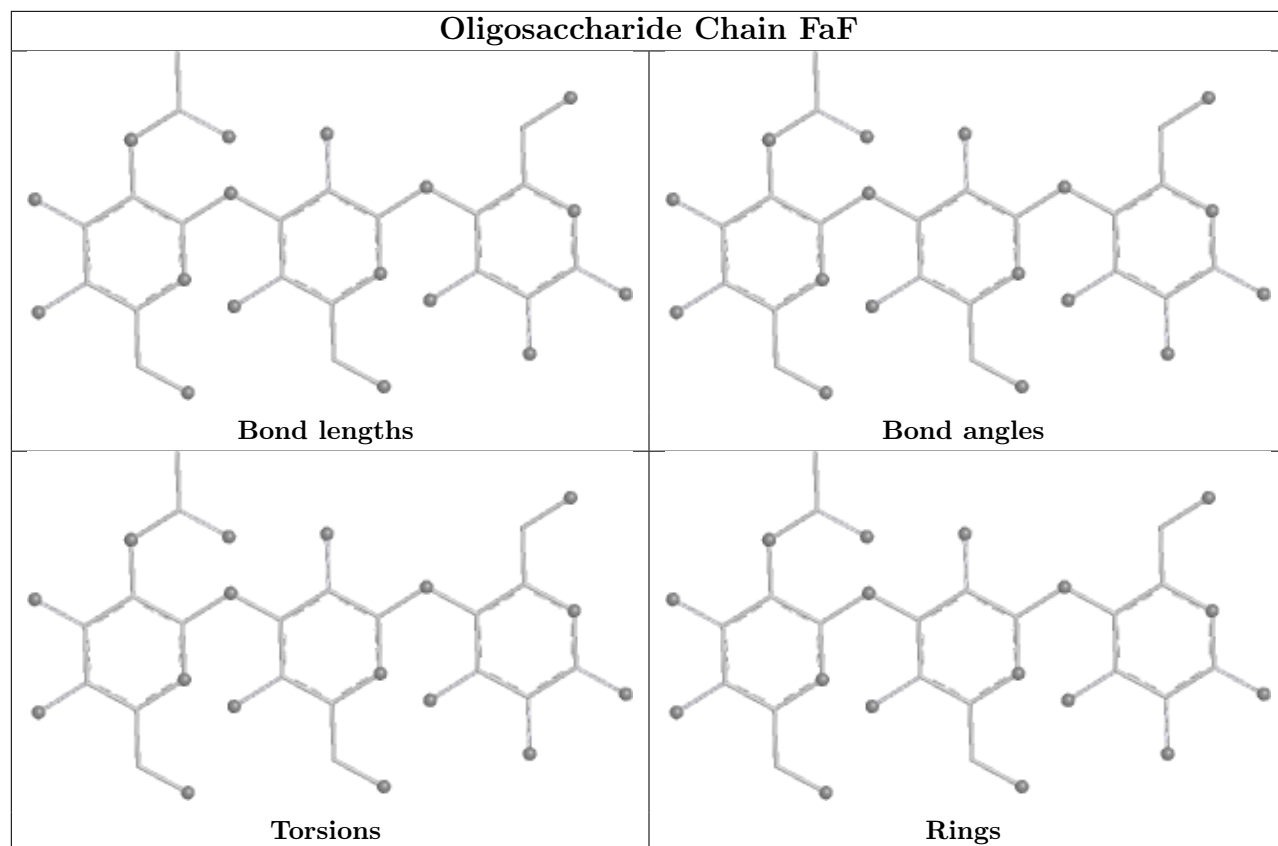
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	HaH	3	NGA	1	0

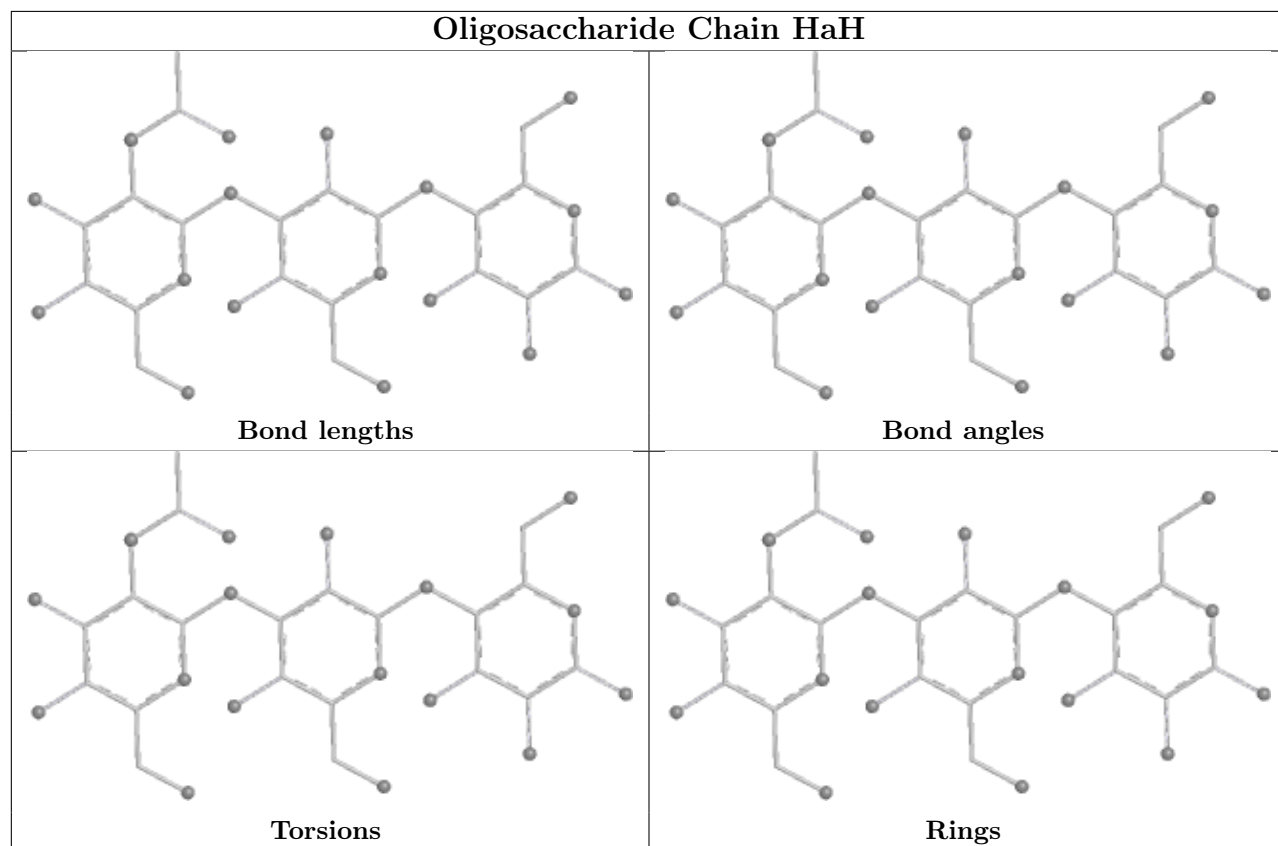
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

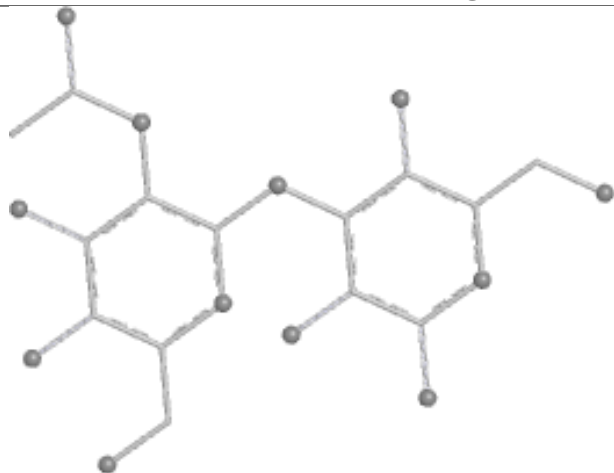
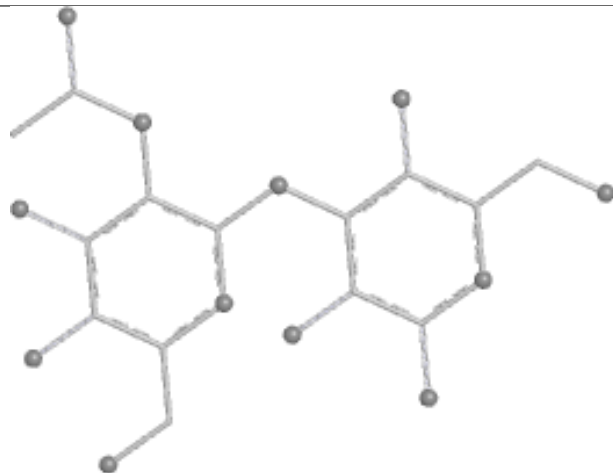
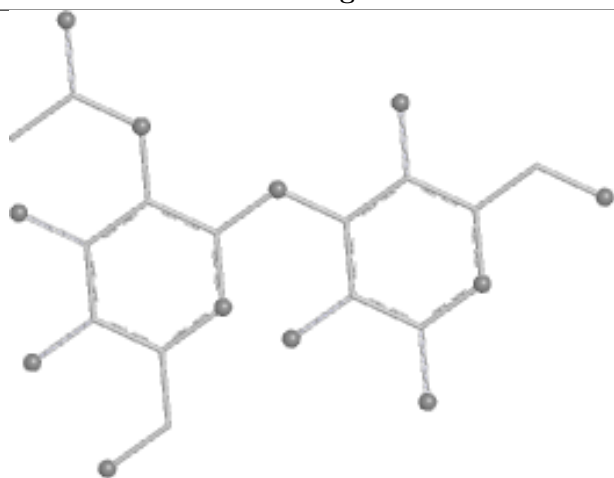
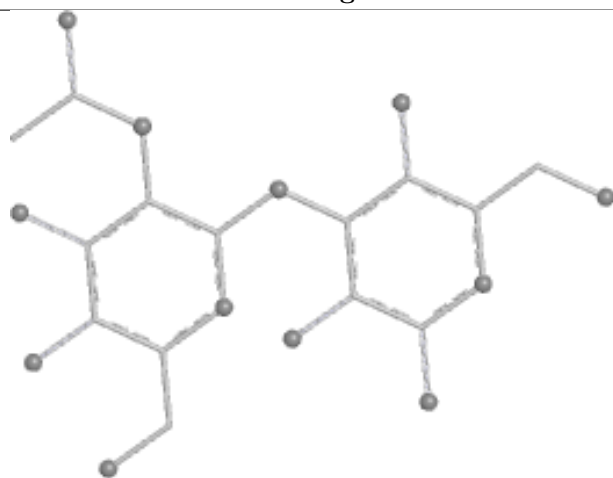


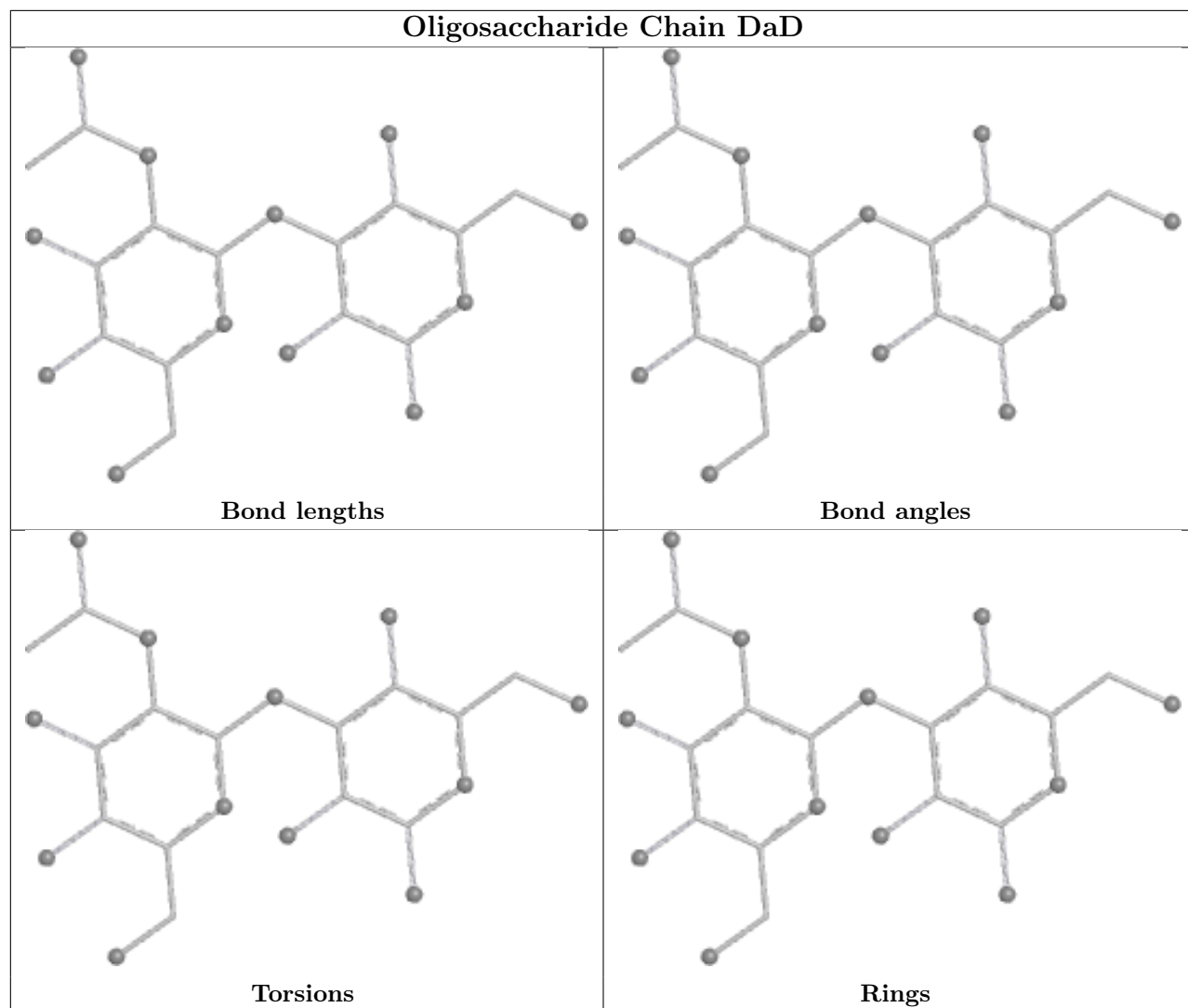
Oligosaccharide Chain FaF

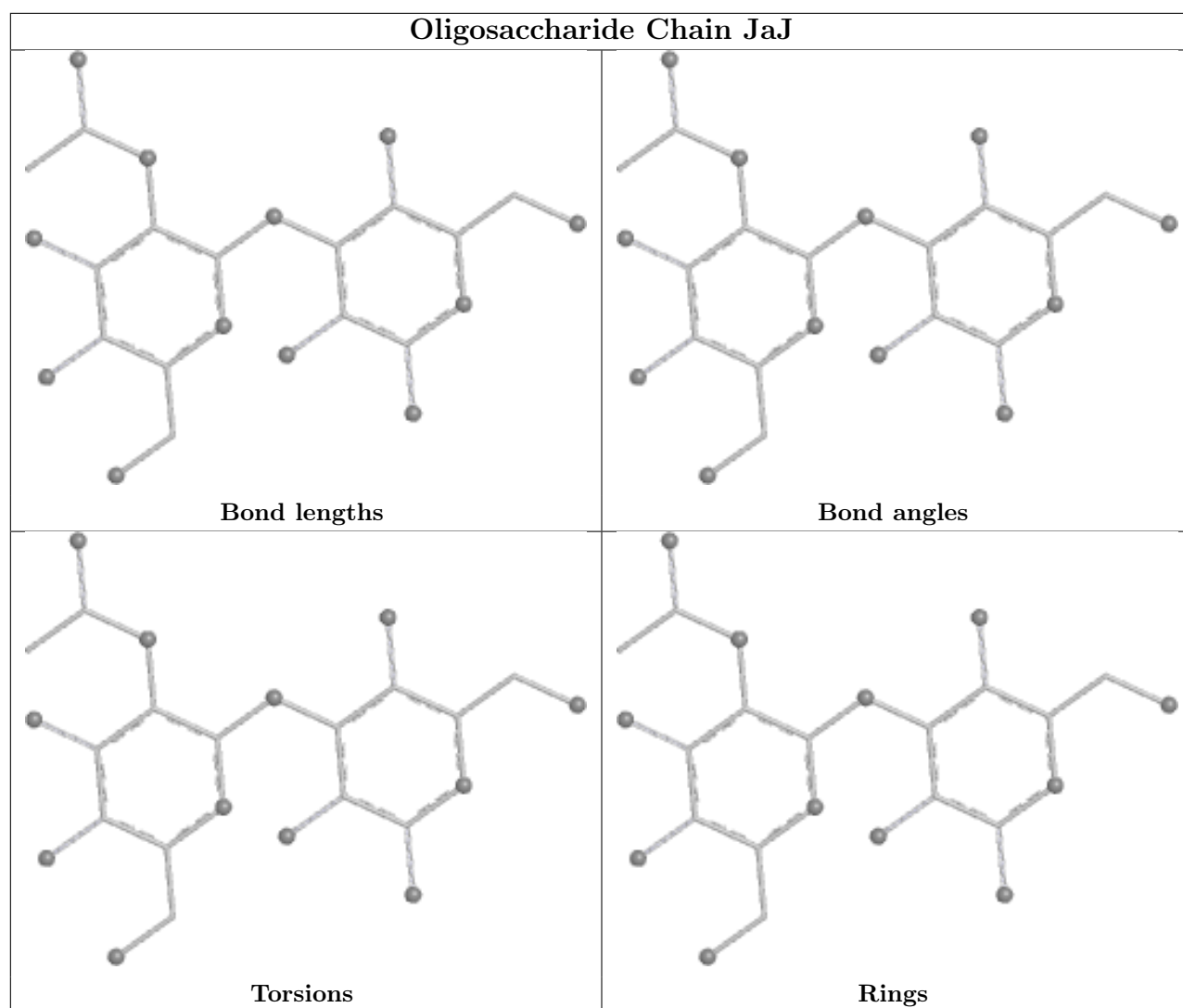


Oligosaccharide Chain HaH



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





5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 21 are monoatomic - leaving 30 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	PEG	DDD	401	-	6,6,6	0.17	0	5,5,5	0.12	0
7	EDO	FFF	401	-	3,3,3	0.24	0	2,2,2	0.11	0
8	PGE	BBB	403	-	7,7,9	0.23	0	6,6,8	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	AAA	401	-	6,6,6	0.26	0	5,5,5	0.11	0
7	EDO	FFF	402	-	3,3,3	0.41	0	2,2,2	0.50	0
7	EDO	BBB	401	-	3,3,3	0.26	0	2,2,2	0.28	0
7	EDO	HHH	402	-	3,3,3	0.10	0	2,2,2	0.22	0
7	EDO	III	303	-	3,3,3	0.09	0	2,2,2	0.28	0
7	EDO	HHH	401	-	3,3,3	0.14	0	2,2,2	0.29	0
4	PEG	CCC	304	-	6,6,6	0.11	0	5,5,5	0.14	0
4	PEG	CCC	301	-	6,6,6	0.24	0	5,5,5	0.50	0
7	EDO	BBB	405	-	3,3,3	0.11	0	2,2,2	0.28	0
4	PEG	EEE	501	-	6,6,6	0.16	0	5,5,5	0.08	0
7	EDO	EEE	502	-	3,3,3	0.13	0	2,2,2	0.30	0
7	EDO	HHH	403	-	3,3,3	0.09	0	2,2,2	0.28	0
7	EDO	FFF	404	-	3,3,3	0.19	0	2,2,2	0.08	0
9	MPD	GGG	301	-	7,7,7	0.19	0	9,10,10	0.69	0
7	EDO	CCC	305	-	3,3,3	0.22	0	2,2,2	0.80	0
9	MPD	EEE	503	-	7,7,7	0.27	0	9,10,10	0.39	0
7	EDO	JJJ	401	-	3,3,3	0.18	0	2,2,2	0.29	0
8	PGE	BBB	402	-	7,7,9	0.30	0	6,6,8	0.17	0
8	PGE	BBB	404	-	9,9,9	0.21	0	8,8,8	0.18	0
7	EDO	HHH	404	-	3,3,3	0.13	0	2,2,2	0.17	0
7	EDO	CCC	302	-	3,3,3	0.05	0	2,2,2	0.25	0
9	MPD	III	302	-	7,7,7	0.27	0	9,10,10	0.59	0
7	EDO	JJJ	402	-	3,3,3	0.21	0	2,2,2	0.15	0
7	EDO	CCC	303	-	3,3,3	0.09	0	2,2,2	0.23	0
4	PEG	FFF	403	-	6,6,6	0.14	0	5,5,5	0.13	0
7	EDO	III	304	-	3,3,3	0.08	0	2,2,2	0.20	0
7	EDO	III	301	-	3,3,3	0.07	0	2,2,2	0.08	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	PEG	DDD	401	-	-	4/4/4/4	-
7	EDO	FFF	401	-	-	1/1/1/1	-
8	PGE	BBB	403	-	-	2/5/5/7	-
4	PEG	AAA	401	-	-	1/4/4/4	-
7	EDO	FFF	402	-	-	1/1/1/1	-
7	EDO	BBB	401	-	-	1/1/1/1	-
7	EDO	HHH	402	-	-	1/1/1/1	-
7	EDO	III	303	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	HHH	401	-	-	0/1/1/1	-
4	PEG	CCC	304	-	-	0/4/4/4	-
4	PEG	CCC	301	-	-	2/4/4/4	-
7	EDO	BBB	405	-	-	1/1/1/1	-
4	PEG	EEE	501	-	-	3/4/4/4	-
7	EDO	EEE	502	-	-	1/1/1/1	-
7	EDO	HHH	403	-	-	1/1/1/1	-
7	EDO	FFF	404	-	-	1/1/1/1	-
9	MPD	GGG	301	-	-	0/5/5/5	-
7	EDO	CCC	305	-	-	1/1/1/1	-
9	MPD	EEE	503	-	-	2/5/5/5	-
7	EDO	JJJ	401	-	-	0/1/1/1	-
8	PGE	BBB	402	-	-	5/5/5/7	-
8	PGE	BBB	404	-	-	3/7/7/7	-
7	EDO	HHH	404	-	-	1/1/1/1	-
7	EDO	CCC	302	-	-	1/1/1/1	-
9	MPD	III	302	-	-	1/5/5/5	-
7	EDO	JJJ	402	-	-	1/1/1/1	-
7	EDO	CCC	303	-	-	1/1/1/1	-
4	PEG	FFF	403	-	-	3/4/4/4	-
7	EDO	III	304	-	-	1/1/1/1	-
7	EDO	III	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	EEE	503	MPD	C2-C3-C4-O4
4	CCC	301	PEG	C1-C2-O2-C3
8	BBB	404	PGE	O1-C1-C2-O2
8	BBB	404	PGE	O3-C5-C6-O4
4	DDD	401	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	401	PEG	1	0
7	FFF	402	EDO	1	0
7	BBB	401	EDO	1	0
7	III	303	EDO	3	0
7	HHH	403	EDO	1	0
9	GGG	301	MPD	1	0
7	CCC	305	EDO	1	0
7	JJJ	401	EDO	1	0
8	BBB	404	PGE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	262/276 (94%)	-1.21	0 100 100	15, 20, 40, 65	0
1	BBB	271/276 (98%)	-1.23	0 100 100	14, 19, 35, 51	0
1	CCC	260/276 (94%)	-1.20	0 100 100	15, 20, 40, 66	0
1	DDD	271/276 (98%)	-1.25	0 100 100	16, 21, 34, 50	0
1	EEE	259/276 (93%)	-1.15	0 100 100	15, 22, 42, 64	0
1	FFF	261/276 (94%)	-1.19	0 100 100	13, 21, 41, 64	1 (0%)
1	GGG	270/276 (97%)	-1.21	0 100 100	14, 21, 35, 58	0
1	HHH	261/276 (94%)	-1.17	0 100 100	14, 20, 40, 63	2 (0%)
1	III	270/276 (97%)	-1.17	0 100 100	16, 22, 37, 59	0
1	JJJ	260/276 (94%)	-1.11	0 100 100	15, 22, 43, 66	0
All	All	2645/2760 (95%)	-1.19	0 100 100	13, 21, 39, 66	3 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	AaA	1	12/12	-	-	24,34,38,40	12

Continued on next page...

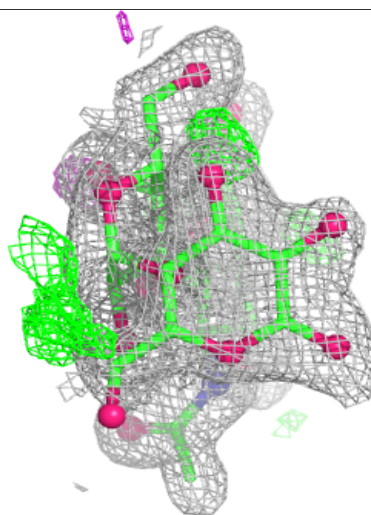
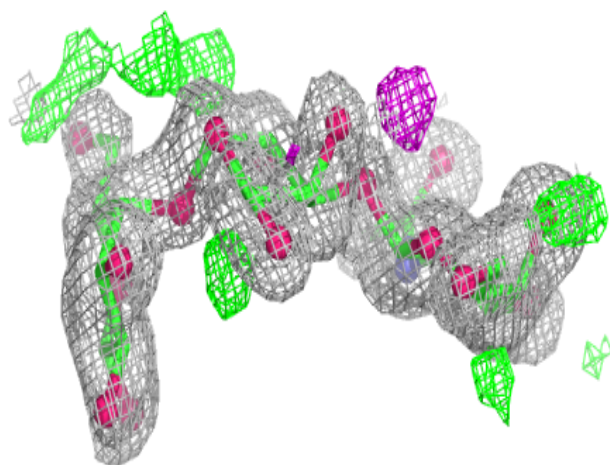
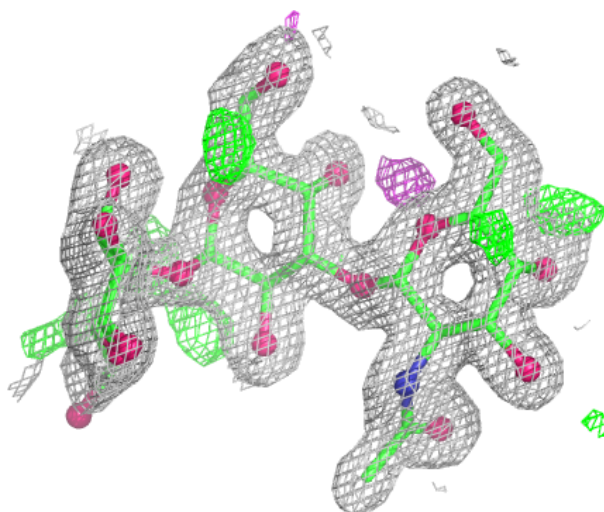
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLA	AaA	2	11/12	-	-	22,25,28,30	11
2	NGA	AaA	3	14/15	-	-	22,24,26,27	14
2	GAL	CaC	1	12/12	-	-	30,37,39,43	12
2	GLA	CaC	2	11/12	-	-	24,29,32,35	11
2	NGA	CaC	3	14/15	-	-	22,26,28,30	14
2	GAL	FaF	1	12/12	-	-	23,32,37,40	12
2	GLA	FaF	2	11/12	-	-	22,27,28,28	11
2	NGA	FaF	3	14/15	-	-	23,25,26,29	14
2	GAL	HaH	1	12/12	-	-	28,32,36,38	12
2	GLA	HaH	2	11/12	-	-	21,23,25,25	11
2	NGA	HaH	3	14/15	-	-	22,24,25,26	14
3	GLA	BaB	1	12/12	-	-	28,32,34,34	12
3	NGA	BaB	2	14/15	-	-	29,30,31,32	14
3	GLA	DaD	1	12/12	-	-	31,35,36,37	12
3	NGA	DaD	2	14/15	-	-	27,28,31,31	14
3	GLA	JaJ	1	12/12	-	-	29,33,35,36	12
3	NGA	JaJ	2	14/15	-	-	24,27,31,33	14

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.

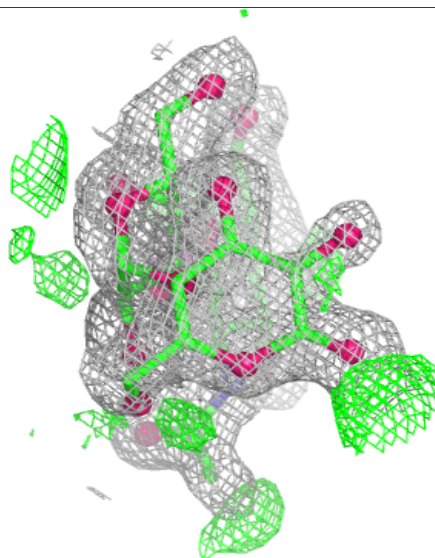
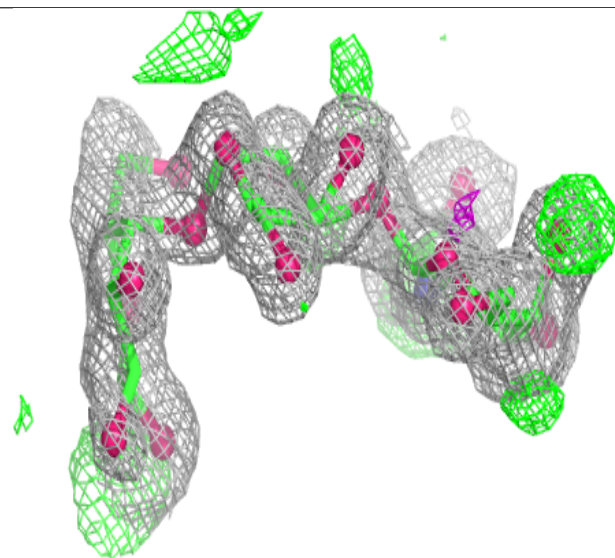
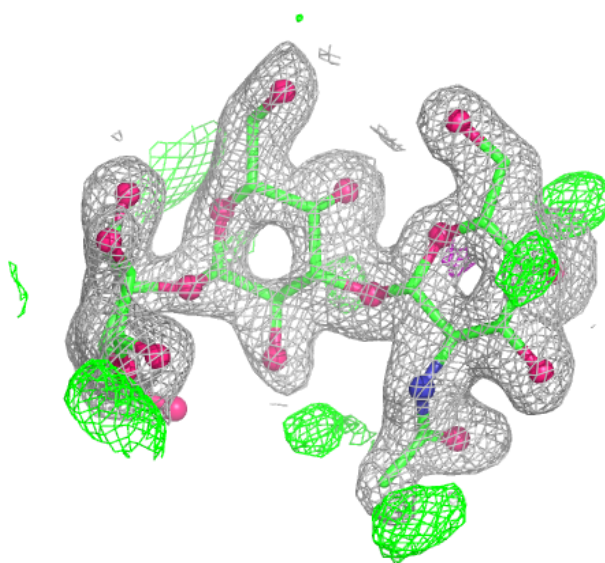
Electron density around Chain AaA:

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



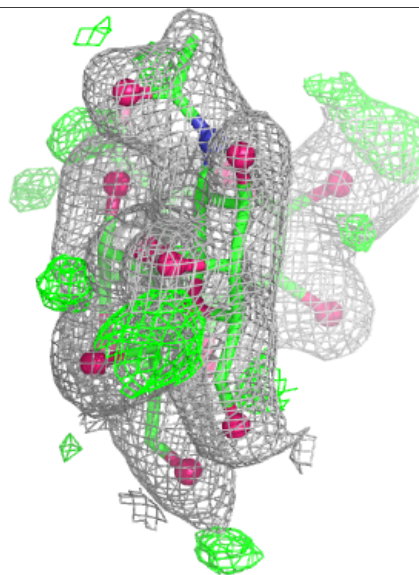
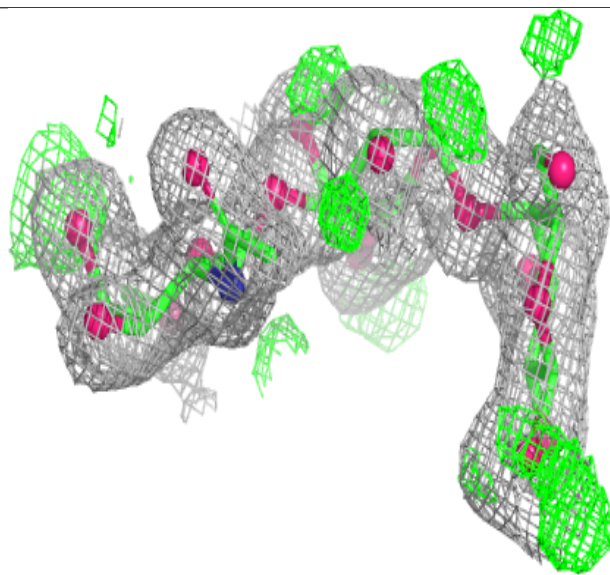
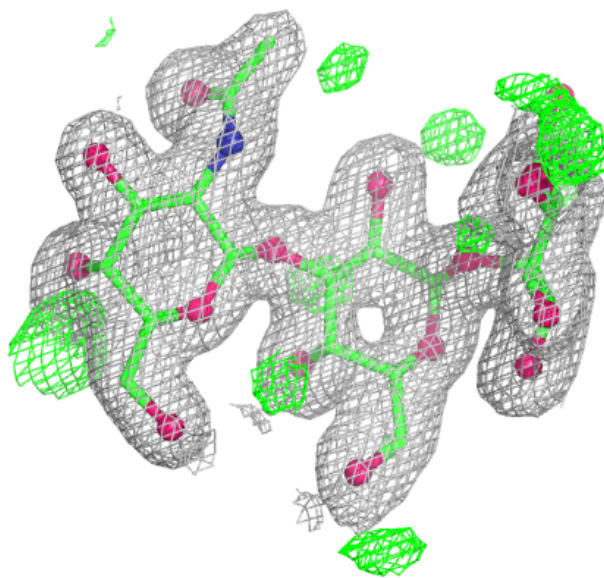
Electron density around Chain CaC:

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



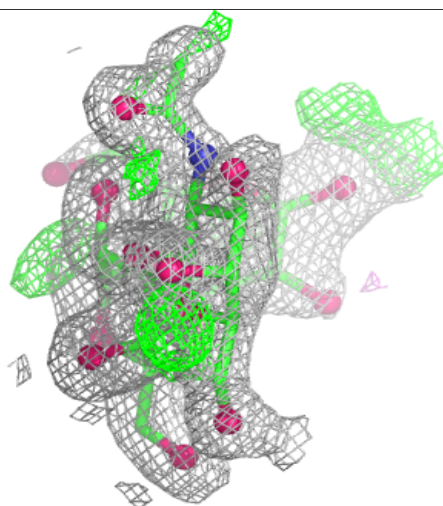
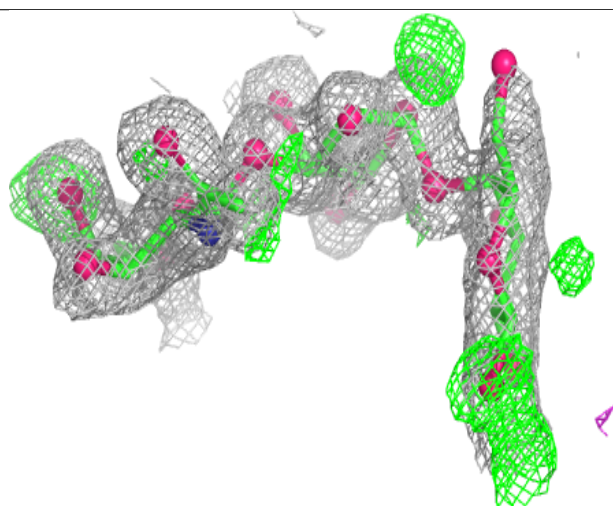
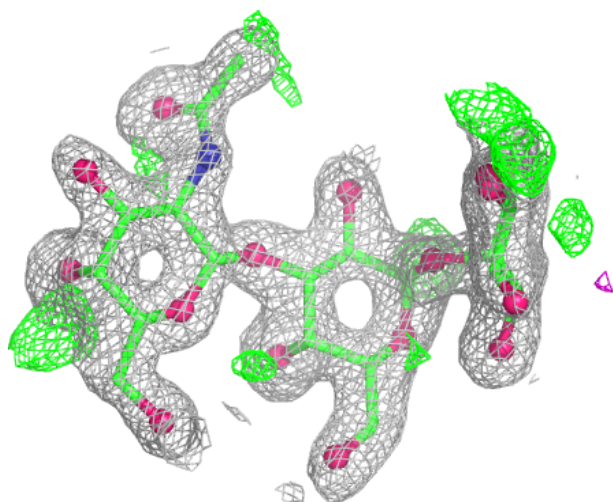
Electron density around Chain FaF:

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



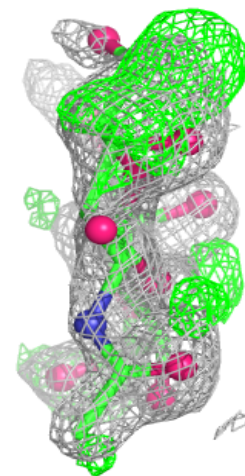
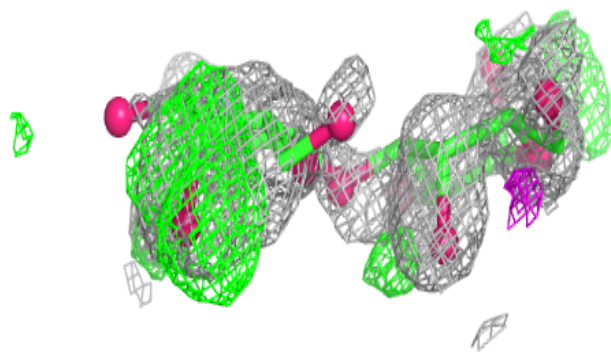
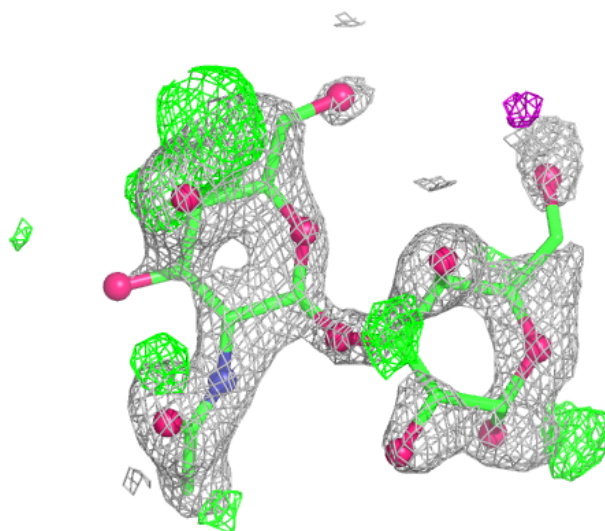
Electron density around Chain HaH:

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



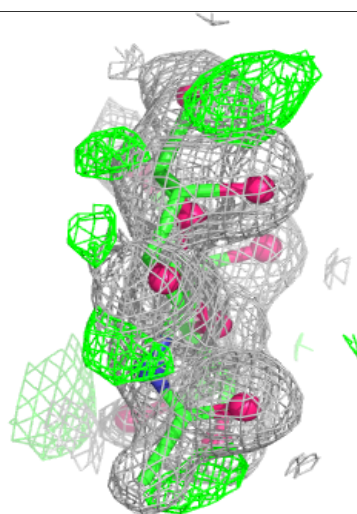
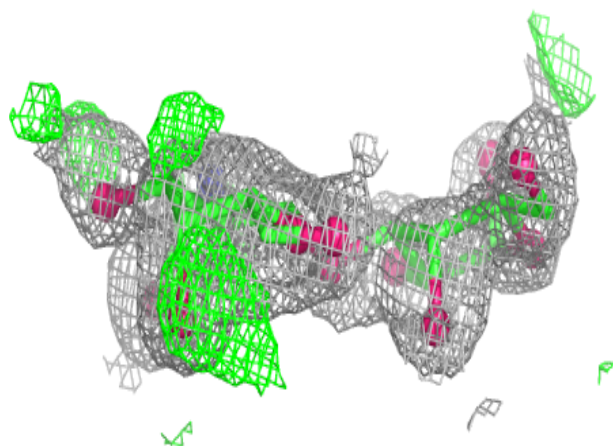
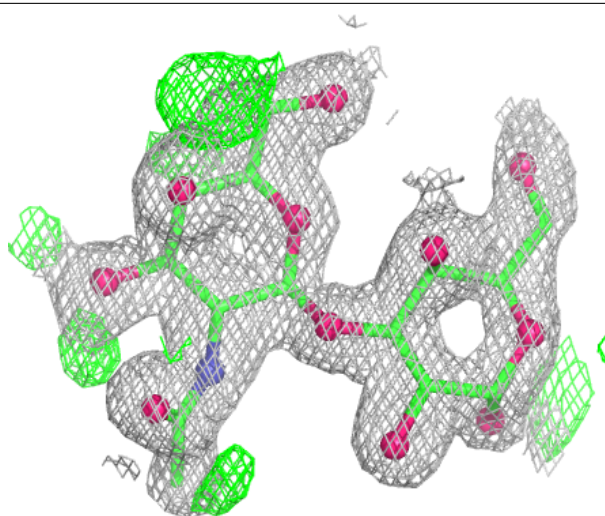
Electron density around Chain BaB:

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



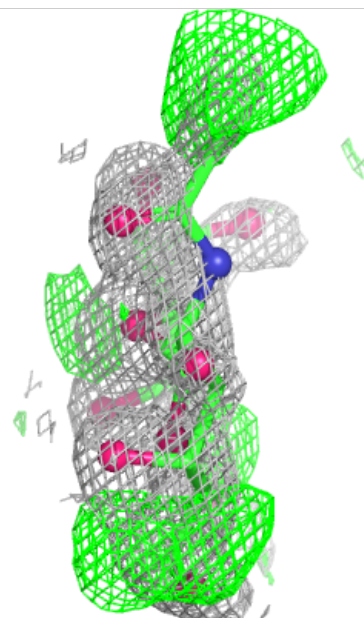
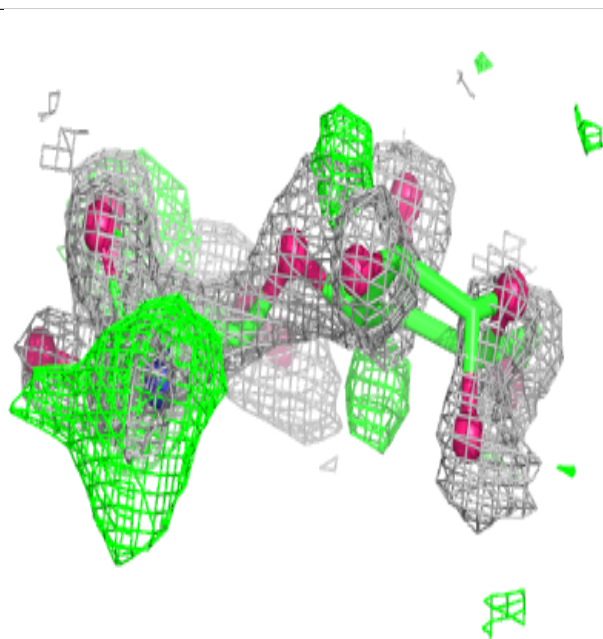
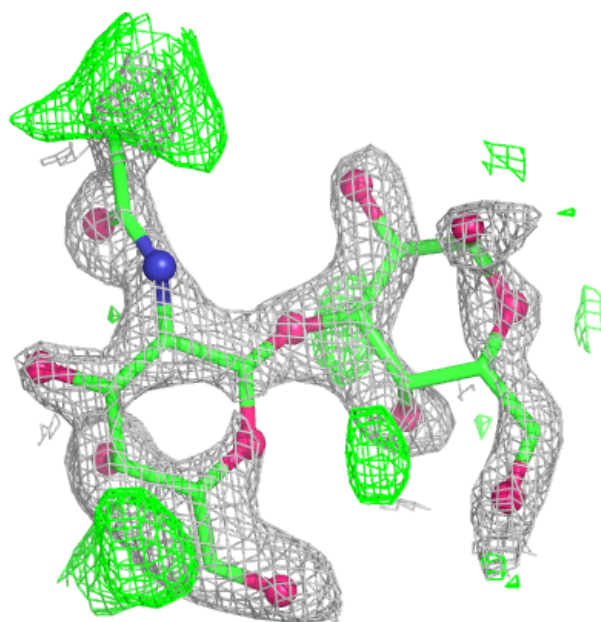
Electron density around Chain DaD:

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



Electron density around Chain 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	FFF	402	4/4	0.95	0.09	36,36,38,39	0
4	PEG	FFF	403	7/7	0.97	0.08	69,69,72,73	0
7	EDO	BBB	401	4/4	0.97	0.10	32,34,37,38	0
4	PEG	CCC	301	7/7	0.97	0.07	39,42,43,45	0
7	EDO	JJJ	402	4/4	0.97	0.07	35,38,38,42	0
8	PGE	BBB	404	10/10	0.97	0.07	53,56,57,58	0
5	MG	EEE	504	1/1	0.98	0.04	34,34,34,34	0
6	K	DDD	403	1/1	0.98	0.10	51,51,51,51	0
4	PEG	CCC	304	7/7	0.98	0.06	48,53,57,58	0
7	EDO	BBB	405	4/4	0.98	0.06	44,44,44,51	0
7	EDO	CCC	302	4/4	0.98	0.06	52,53,54,58	0
7	EDO	CCC	303	4/4	0.98	0.08	51,51,55,60	0
7	EDO	CCC	305	4/4	0.98	0.06	25,30,30,35	0
7	EDO	EEE	502	4/4	0.98	0.07	53,55,55,57	0
7	EDO	FFF	401	4/4	0.98	0.10	35,38,39,42	0
4	PEG	DDD	401	7/7	0.98	0.06	54,56,60,60	0
7	EDO	FFF	404	4/4	0.98	0.05	39,40,42,48	0
7	EDO	HHH	401	4/4	0.98	0.07	50,50,51,52	0
7	EDO	HHH	404	4/4	0.98	0.06	45,45,45,46	0
7	EDO	III	301	4/4	0.98	0.06	56,56,58,62	0
7	EDO	III	303	4/4	0.98	0.06	38,39,43,46	0
7	EDO	III	304	4/4	0.98	0.07	42,46,49,53	0
7	EDO	JJJ	401	4/4	0.98	0.08	35,37,38,44	0
4	PEG	EEE	501	7/7	0.98	0.07	61,61,66,67	0
8	PGE	BBB	402	8/10	0.98	0.07	30,42,49,49	0
8	PGE	BBB	403	8/10	0.98	0.07	47,53,55,57	0
4	PEG	AAA	401	7/7	0.98	0.07	41,51,56,58	0
9	MPD	EEE	503	8/8	0.98	0.06	27,38,41,43	0
9	MPD	III	302	8/8	0.98	0.07	30,40,44,45	0
6	K	CCC	307	1/1	0.99	0.04	36,36,36,36	0
5	MG	DDD	402	1/1	0.99	0.03	32,32,32,32	0
6	K	EEE	505	1/1	0.99	0.07	39,39,39,39	0
7	EDO	HHH	402	4/4	0.99	0.04	49,51,51,52	0
7	EDO	HHH	403	4/4	0.99	0.05	46,48,51,51	0
6	K	FFF	406	1/1	0.99	0.08	44,44,44,44	0
6	K	HHH	406	1/1	0.99	0.08	44,44,44,44	0
6	K	III	307	1/1	0.99	0.07	42,42,42,42	0
6	K	JJJ	404	1/1	0.99	0.08	44,44,44,44	0
5	MG	FFF	405	1/1	0.99	0.04	34,34,34,34	0
5	MG	GGG	302	1/1	0.99	0.04	35,35,35,35	0
5	MG	GGG	303	1/1	0.99	0.03	31,31,31,31	0
5	MG	III	305	1/1	0.99	0.04	39,39,39,39	0
5	MG	JJJ	403	1/1	0.99	0.03	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	AAA	403	1/1	0.99	0.06	38,38,38,38	0
9	MPD	GGG	301	8/8	0.99	0.06	26,40,46,46	0
6	K	BBB	407	1/1	0.99	0.10	40,40,40,40	0
5	MG	III	306	1/1	1.00	0.03	29,29,29,29	0
5	MG	AAA	402	1/1	1.00	0.03	28,28,28,28	0
5	MG	BBB	406	1/1	1.00	0.02	34,34,34,34	0
5	MG	HHH	405	1/1	1.00	0.01	34,34,34,34	0
5	MG	CCC	306	1/1	1.00	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.