



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:33 AM BST

PDB ID : 5CPX
Title : Crystal structure of murine polyomavirus PTA strain VP1 in complex with the DSLNT glycan
Authors : Buch, M.H.C.; Liaci, A.M.; Neu, U.; Stehle, T.
Deposited on : 2015-07-21
Resolution : 1.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

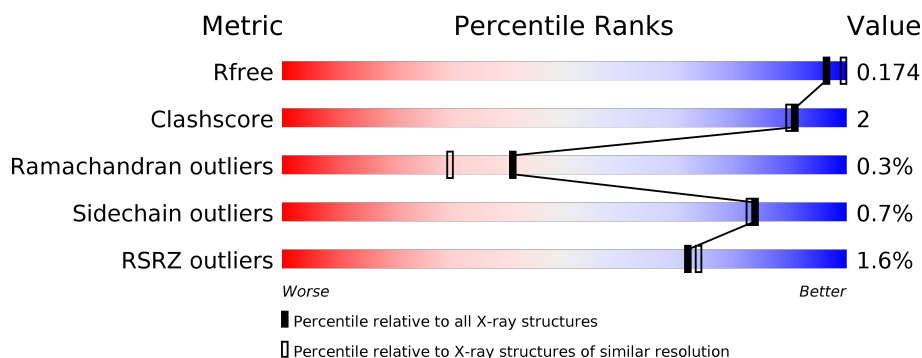
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	284	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	B	284	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div></div> </div> </div>
1	C	284	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	D	284	<div> <div></div> <div> <div></div> <div>96%</div> <div></div> </div> </div>
1	E	284	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
2	F	3	<div> <div></div> <div> <div></div> <div>100%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	3	 33% 67%
2	J	3	 33% 67%
3	G	2	 50% 50%
3	H	2	 50% 50%

2 Entry composition [i](#)

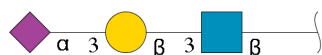
There are 5 unique types of molecules in this entry. The entry contains 12830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VP1.

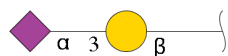
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	10	0
			2208	1412	370	417	9			
1	B	277	Total	C	N	O	S	0	5	0
			2183	1395	369	411	8			
1	C	278	Total	C	N	O	S	0	5	0
			2190	1401	368	413	8			
1	D	283	Total	C	N	O	S	0	2	0
			2216	1408	371	425	12			
1	E	278	Total	C	N	O	S	0	8	0
			2199	1404	372	415	8			

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



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

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	H	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	324	Total	O	0	0
			324	324		
5	B	279	Total	O	0	0
			279	279		
5	C	306	Total	O	0	0
			306	306		
5	D	361	Total	O	0	0
			361	361		

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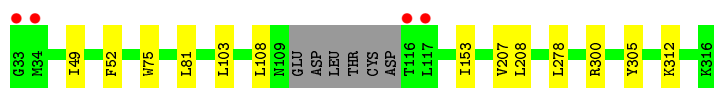
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	346	Total	O	0	0
			346	346		

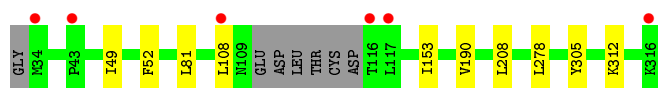
3 Residue-property plots [i](#)

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.

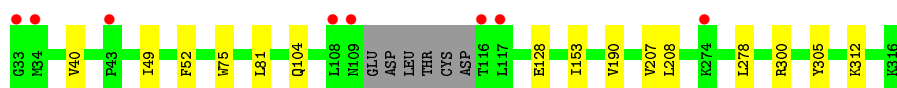
- Molecule 1: VP1



- Molecule 1: VP1



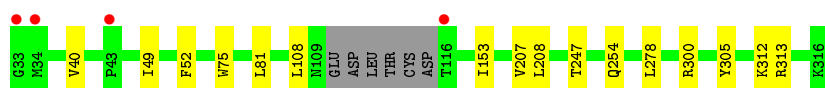
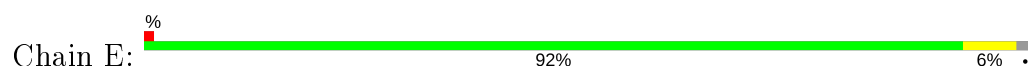
- Molecule 1: VP1




- Molecule 1: VP1



- Molecule 1: VP1




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

Chain F:  100%


HA01
GAL2
SIA3

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

Chain I:  33% 67%

HA01
GAL2
SIA3

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

Chain J:  33% 67%

HA01
GAL2
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain G:  50% 50%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain H:  50% 50%

GAL1
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.73Å 219.73Å 100.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.36 – 1.87 48.36 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.36-1.87) 99.8 (48.36-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.176 0.153 , 0.174	Depositor DCC
R_{free} test set	6850 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/2286	0.58	0/3115
1	B	0.40	0/2245	0.57	0/3057
1	C	0.40	0/2264	0.56	0/3088
1	D	0.42	0/2276	0.58	0/3102
1	E	0.42	0/2271	0.59	0/3095
All	All	0.42	0/11342	0.58	0/15457

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2195	10	0
1	B	2183	0	2168	6	0
1	C	2190	0	2183	9	0
1	D	2216	0	2188	8	0
1	E	2199	0	2177	10	0
2	F	46	0	40	0	0
2	I	46	0	40	0	0
2	J	46	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	32	0	28	0	0
3	H	32	0	28	0	0
4	A	4	0	4	0	0
4	B	4	0	4	0	0
4	D	4	0	4	0	0
4	E	4	0	4	0	0
5	A	324	0	0	0	0
5	B	279	0	0	0	0
5	C	306	0	0	2	0
5	D	361	0	0	0	0
5	E	346	0	0	1	0
All	All	12830	0	11103	37	0

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

All (37) 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:B:49:ILE:HD11	1:B:278:LEU:HD23	1.51	0.92
1:E:49:ILE:HD11	1:E:278:LEU:HD23	1.56	0.86
1:D:49:ILE:HD11	1:D:278:LEU:CD2	2.19	0.72
1:B:49:ILE:HD11	1:B:278:LEU:CD2	2.21	0.71
1:E:49:ILE:HD11	1:E:278:LEU:CD2	2.21	0.70
1:D:49:ILE:HD11	1:D:278:LEU:HD23	1.75	0.66
1:E:254:GLN:HG3	5:E:771:HOH:O	2.00	0.61
1:C:49:ILE:HD11	1:C:278:LEU:CD2	2.34	0.58
1:C:49:ILE:HD11	1:C:278:LEU:HD23	1.85	0.57
1:D:153:ILE:HA	1:E:81:LEU:HD21	1.89	0.53
1:A:49:ILE:HD13	1:A:103:LEU:HD13	1.91	0.52
1:A:49:ILE:HD11	1:A:278:LEU:HD23	1.92	0.52
1:A:52[B]:PHE:CE1	1:A:305:TYR:HB2	2.46	0.51
1:B:52[B]:PHE:CE1	1:B:305:TYR:HB2	2.46	0.51
1:D:40:VAL:HB	1:D:312:LYS:HB2	1.95	0.49
1:A:49:ILE:HD13	1:A:103:LEU:CD1	2.42	0.48
1:D:52[A]:PHE:CE1	1:D:305:TYR:HB2	2.48	0.48
1:C:52[A]:PHE:CE1	1:C:305:TYR:HB2	2.49	0.48
1:A:49:ILE:CD1	1:A:103:LEU:HD12	2.46	0.46
1:A:49:ILE:CD1	1:A:103:LEU:CD1	2.95	0.44
1:C:104:GLN:HG2	5:C:722:HOH:O	2.18	0.44
1:A:81:LEU:HD21	1:E:153:ILE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108[B]:LEU:HD21	1:B:312:LYS:HE2	2.00	0.43
1:E:40:VAL:HB	1:E:312:LYS:HB2	1.99	0.43
1:C:153:ILE:HA	1:D:81:LEU:HD21	2.00	0.43
1:A:153:ILE:HA	1:B:81:LEU:HD21	2.01	0.42
1:E:52[A]:PHE:CE1	1:E:305:TYR:HB2	2.55	0.42
1:C:75:TRP:CZ3	1:C:300:ARG:HB2	2.55	0.41
1:C:40:VAL:HB	1:C:312:LYS:HB2	2.02	0.41
1:E:108[B]:LEU:HD21	1:E:312:LYS:HE2	2.02	0.41
1:E:75:TRP:CZ3	1:E:300:ARG:HB2	2.56	0.41
1:D:49:ILE:HD11	1:D:278:LEU:HD22	1.99	0.41
1:A:75:TRP:CZ3	1:A:300:ARG:HB2	2.55	0.41
1:D:156:PRO:HD2	1:E:247:THR:HG22	2.03	0.41
1:A:108[A]:LEU:HD21	1:A:312:LYS:HE2	2.03	0.40
1:B:153:ILE:HA	1:C:81:LEU:HD21	2.03	0.40
1:C:128:GLU:OE1	5:C:501:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/284 (100%)	274 (97%)	8 (3%)	1 (0%)	34	22
1	B	277/284 (98%)	272 (98%)	5 (2%)	0	100	100
1	C	281/284 (99%)	274 (98%)	6 (2%)	1 (0%)	34	22
1	D	283/284 (100%)	274 (97%)	8 (3%)	1 (0%)	34	22
1	E	281/284 (99%)	273 (97%)	7 (2%)	1 (0%)	34	22
All	All	1405/1420 (99%)	1367 (97%)	34 (2%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	VAL
1	C	207	VAL
1	D	207	VAL
1	E	207	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	A	246/250 (98%)	245 (100%)	1 (0%)	91	90
1	B	241/250 (96%)	239 (99%)	2 (1%)	81	80
1	C	244/250 (98%)	242 (99%)	2 (1%)	81	80
1	D	248/250 (99%)	247 (100%)	1 (0%)	91	90
1	E	243/250 (97%)	240 (99%)	3 (1%)	71	67
All	All	1222/1250 (98%)	1213 (99%)	9 (1%)	84	83

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

Mol	Chain	Res	Type
1	A	208	LEU
1	B	190	VAL
1	B	208	LEU
1	C	190	VAL
1	C	208	LEU
1	D	208	LEU
1	E	208	LEU
1	E	313[A]	ARG
1	E	313[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	NAG	F	1	2	15,15,15	0.48	0	21,21,21	0.96	1 (4%)
2	GAL	F	2	2	11,11,12	0.60	0	15,15,17	1.13	1 (6%)
2	SIA	F	3	2	17,20,21	0.41	0	21,28,31	0.86	2 (9%)
3	GAL	G	1	3	12,12,12	0.53	0	17,17,17	0.65	0
3	SIA	G	2	3	17,20,21	0.40	0	21,28,31	0.96	1 (4%)
3	GAL	H	1	3	12,12,12	0.60	0	17,17,17	0.67	0
3	SIA	H	2	3	17,20,21	0.48	0	21,28,31	0.90	1 (4%)
2	NAG	I	1	2	15,15,15	0.50	0	21,21,21	0.88	1 (4%)
2	GAL	I	2	2	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
2	SIA	I	3	2	17,20,21	0.50	0	21,28,31	0.80	0
2	NAG	J	1	2	15,15,15	0.48	0	21,21,21	0.78	0
2	GAL	J	2	2	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
2	SIA	J	3	2	17,20,21	0.49	0	21,28,31	0.97	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	SIA	F	3	2	-	4/14/34/38	0/1/1/1
3	GAL	G	1	3	-	0/2/22/22	0/1/1/1
3	SIA	G	2	3	-	6/14/34/38	0/1/1/1
3	GAL	H	1	3	-	0/2/22/22	0/1/1/1
3	SIA	H	2	3	-	4/14/34/38	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	2/14/34/38	0/1/1/1
2	NAG	J	1	2	-	2/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/14/34/38	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GAL	C1-O5-C5	2.79	115.98	112.19
2	F	1	NAG	C3-C4-C5	2.56	114.81	110.24
2	J	3	SIA	C6-O6-C2	2.56	116.82	111.34
2	J	3	SIA	O9-C9-C8	-2.48	105.67	111.07
2	I	2	GAL	C1-O5-C5	2.42	115.47	112.19
2	I	1	NAG	C1-C2-C3	2.39	113.81	110.54
2	I	2	GAL	O3-C3-C2	2.37	114.54	109.99
3	G	2	SIA	C6-O6-C2	2.32	116.31	111.34
2	J	2	GAL	C1-C2-C3	2.27	112.46	109.67
3	H	2	SIA	C6-O6-C2	2.24	116.13	111.34
2	F	3	SIA	C6-O6-C2	2.20	116.04	111.34
2	J	2	GAL	O3-C3-C2	2.14	114.10	109.99
2	F	3	SIA	O9-C9-C8	-2.01	106.70	111.07

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	SIA	C7-C8-C9-O9
3	G	2	SIA	O8-C8-C9-O9
2	J	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6

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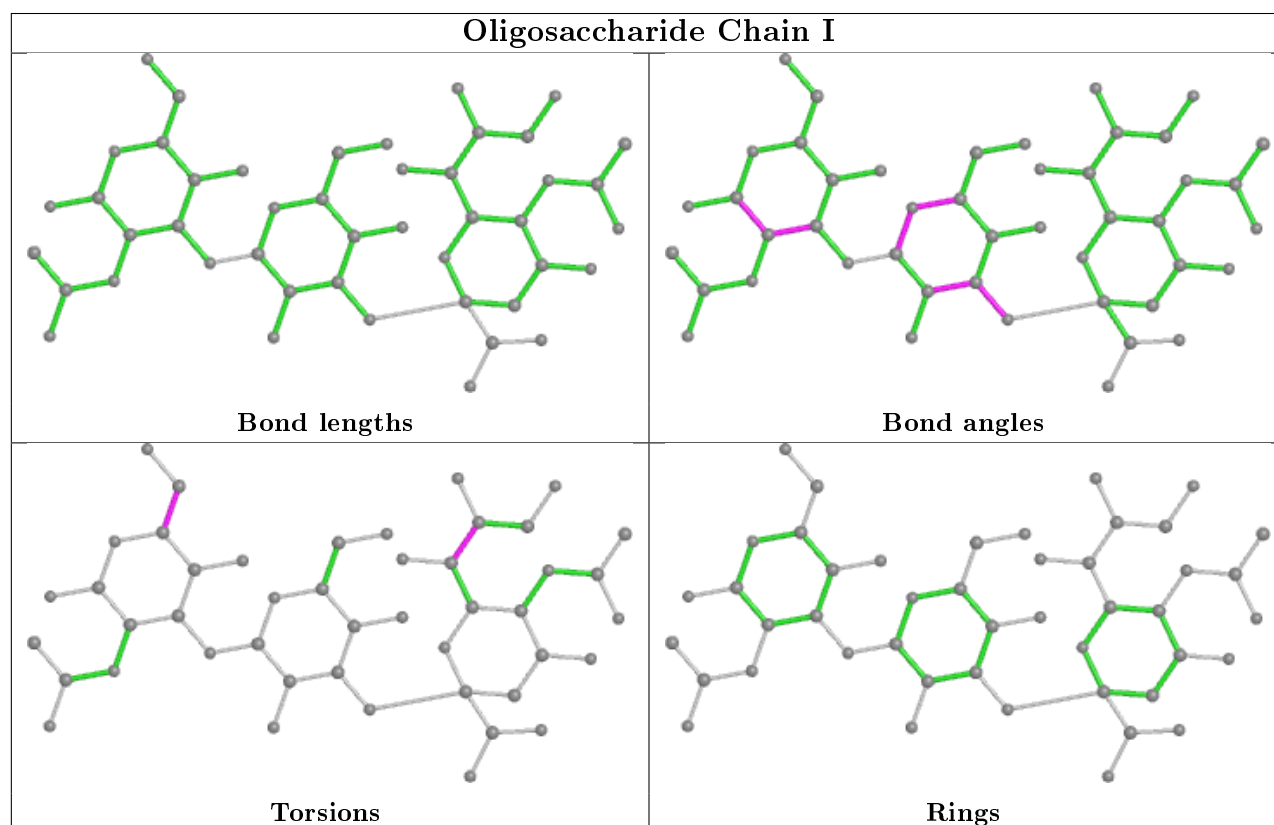
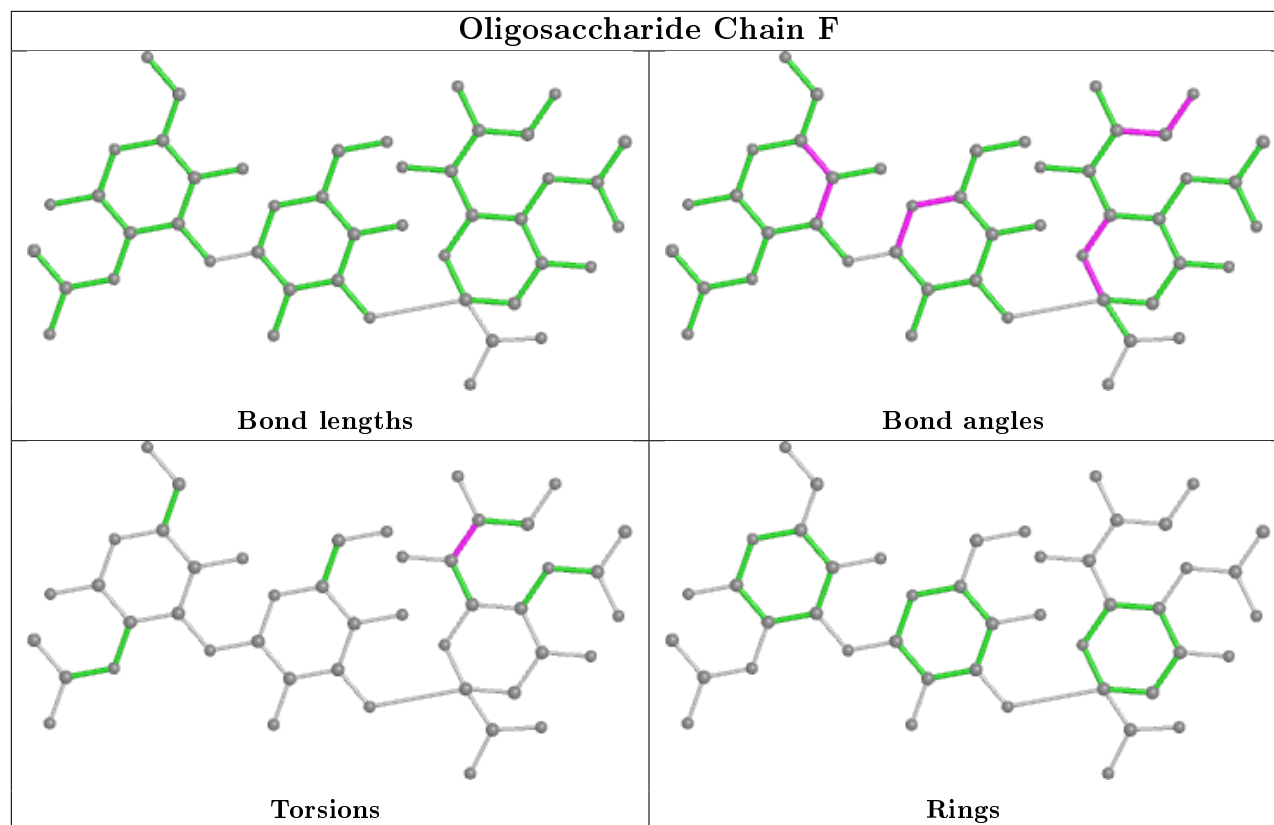
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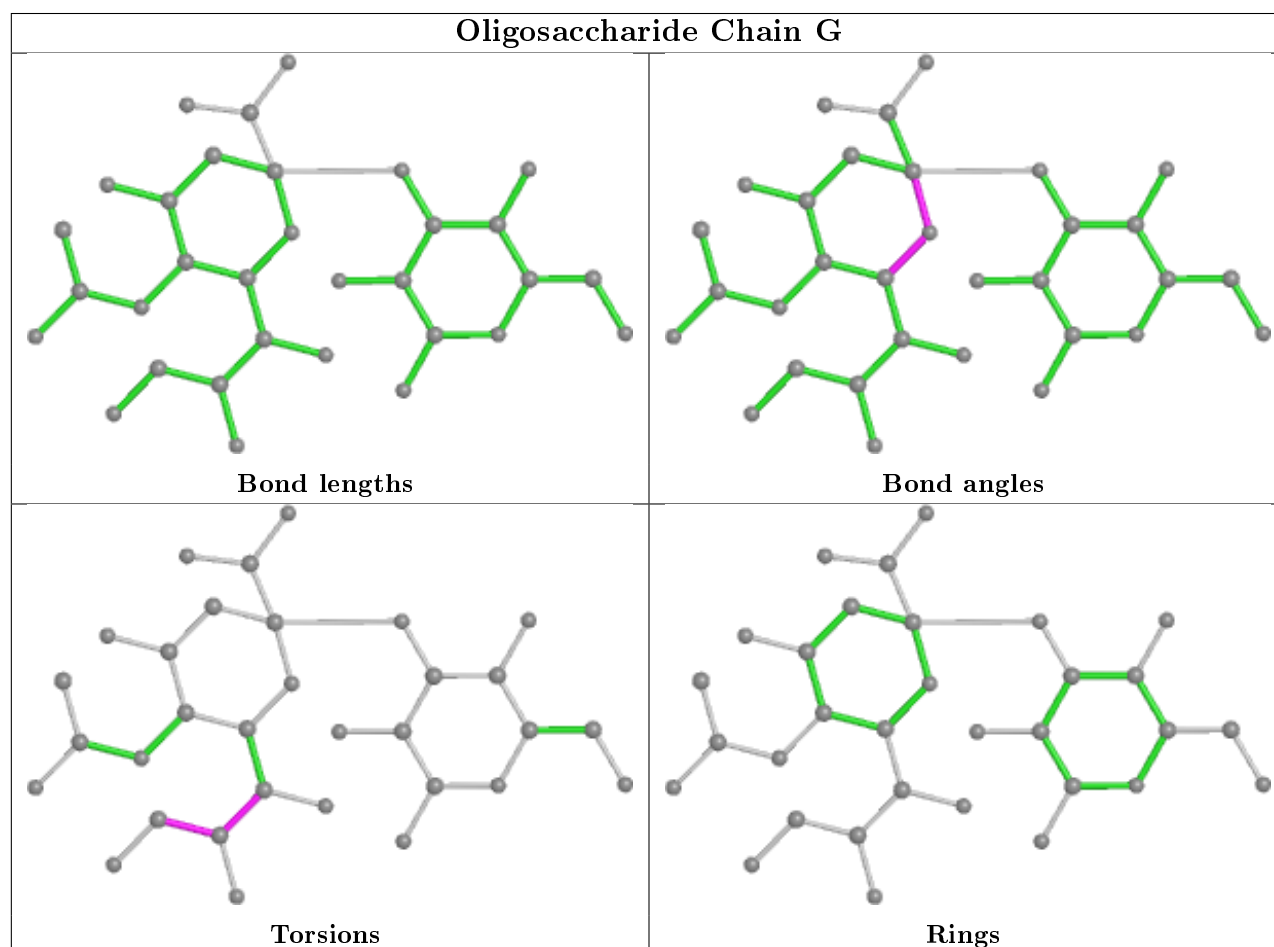
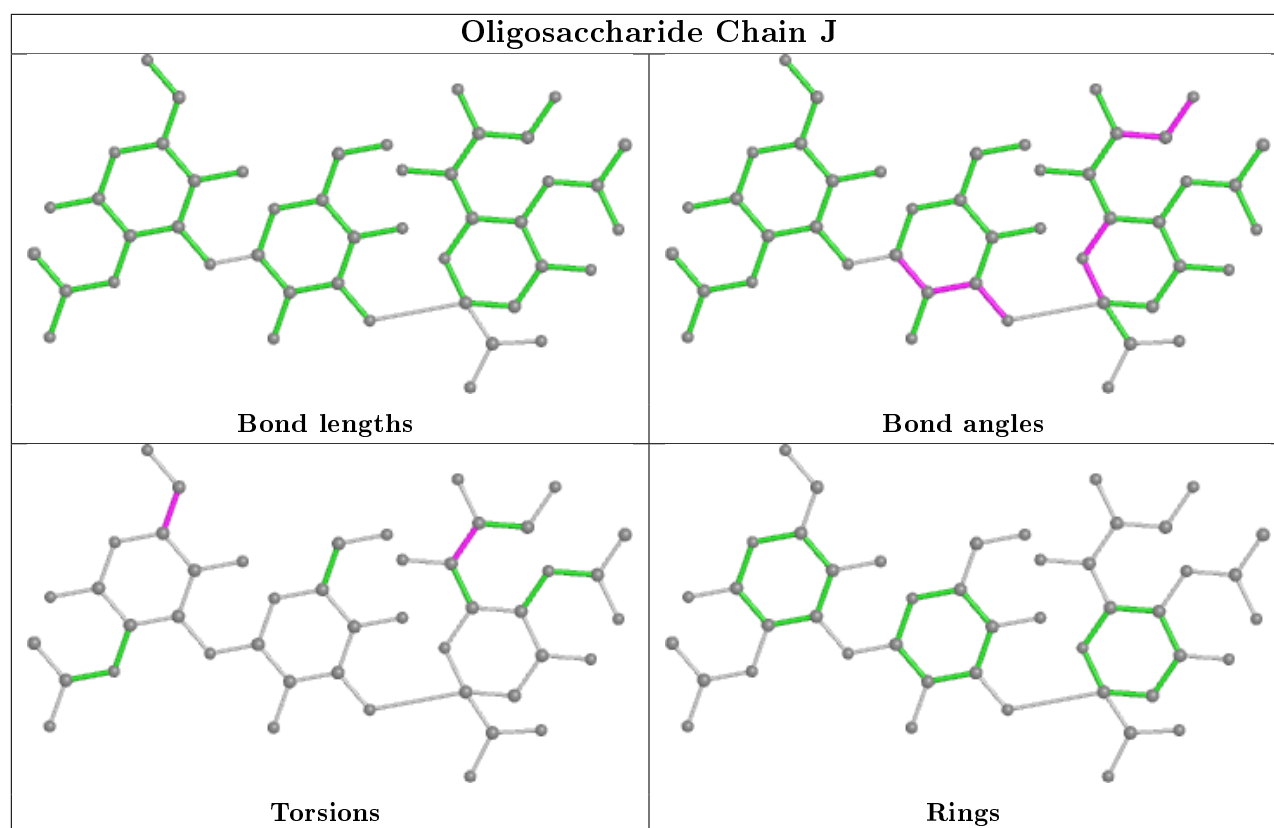
Mol	Chain	Res	Type	Atoms
3	G	2	SIA	O7-C7-C8-O8
3	H	2	SIA	O7-C7-C8-C9
2	J	3	SIA	O7-C7-C8-C9
3	G	2	SIA	O7-C7-C8-C9
3	G	2	SIA	C6-C7-C8-C9
3	G	2	SIA	C6-C7-C8-O8
2	J	3	SIA	C6-C7-C8-C9
2	I	1	NAG	C4-C5-C6-O6
2	J	3	SIA	C6-C7-C8-O8
2	J	3	SIA	O7-C7-C8-O8
3	H	2	SIA	C6-C7-C8-O8
2	I	1	NAG	O5-C5-C6-O6
3	H	2	SIA	C6-C7-C8-C9
2	F	3	SIA	C6-C7-C8-O8
3	H	2	SIA	O7-C7-C8-O8
2	F	3	SIA	O7-C7-C8-C9
2	F	3	SIA	O7-C7-C8-O8
2	I	3	SIA	C6-C7-C8-O8
2	F	3	SIA	C6-C7-C8-C9
2	I	3	SIA	O7-C7-C8-C9

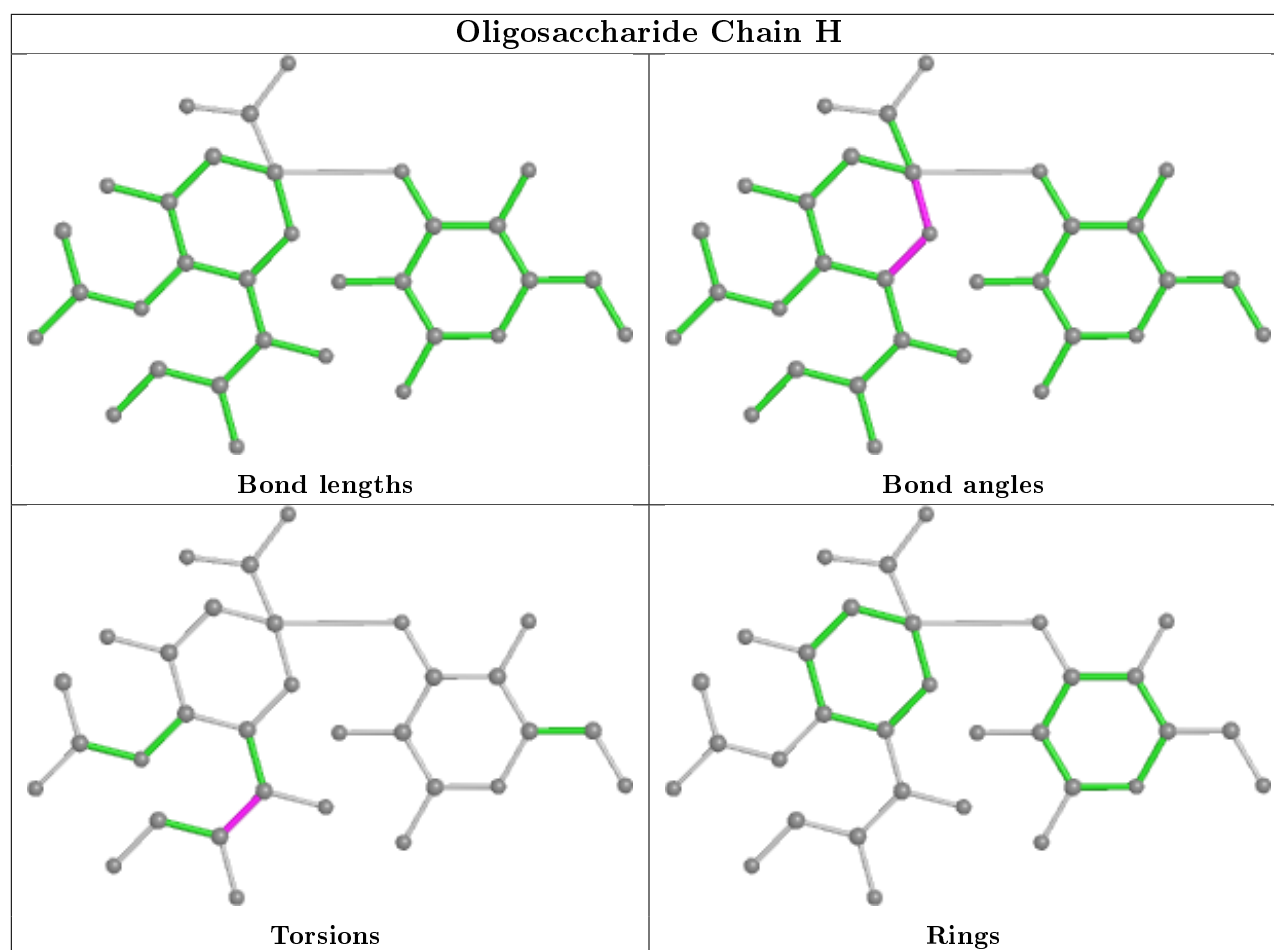
There are no ring outliers.

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.







5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
4	GOL	D	401	-	3,3,5	0.47	0	2,2,5	0.36	0
4	GOL	B	401	-	3,3,5	0.48	0	2,2,5	0.27	0
4	GOL	E	401	-	3,3,5	0.41	0	2,2,5	0.52	0
4	GOL	A	401	-	3,3,5	0.41	0	2,2,5	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	401	-	-	1/1/1/4	-
4	GOL	B	401	-	-	0/1/1/4	-
4	GOL	E	401	-	-	1/1/1/4	-
4	GOL	A	401	-	-	0/1/1/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	GOL	O1-C1-C2-O2
4	E	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	278/284 (97%)	-0.48	4 (1%) 75 77	8, 15, 39, 62	4 (1%)
1	B	277/284 (97%)	-0.41	6 (2%) 62 63	11, 19, 40, 67	3 (1%)
1	C	278/284 (97%)	-0.36	8 (2%) 51 53	11, 19, 43, 70	2 (0%)
1	D	283/284 (99%)	-0.50	1 (0%) 92 93	9, 16, 34, 67	1 (0%)
1	E	278/284 (97%)	-0.50	4 (1%) 75 77	8, 15, 41, 70	1 (0%)
All	All	1394/1420 (98%)	-0.45	23 (1%) 72 74	8, 17, 40, 70	11 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	GLY	4.2
1	B	316	LYS	4.0
1	D	43	PRO	3.9
1	E	116	THR	3.9
1	C	116	THR	3.7
1	C	117	LEU	3.2
1	E	33	GLY	3.1
1	A	116	THR	3.0
1	A	34	MET	2.9
1	B	34	MET	2.8
1	B	116	THR	2.8
1	B	108[A]	LEU	2.7
1	E	34	MET	2.7
1	A	33	GLY	2.5
1	E	43	PRO	2.5
1	B	117	LEU	2.3
1	C	43	PRO	2.3
1	B	43	PRO	2.2
1	C	108	LEU	2.2
1	C	109	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	274	LYS	2.1
1	A	117	LEU	2.1
1	C	34	MET	2.0

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

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

6.3 Carbohydrates [i](#)

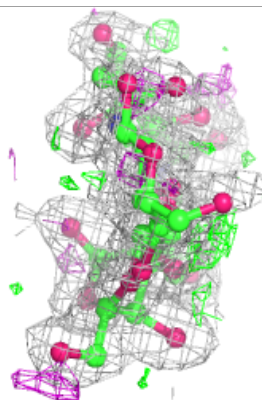
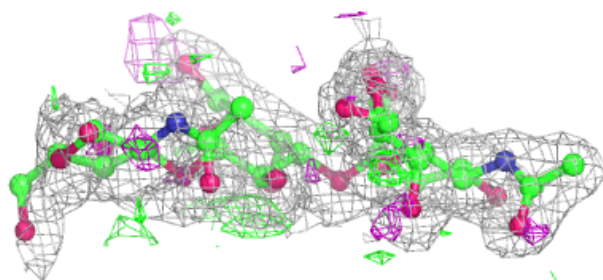
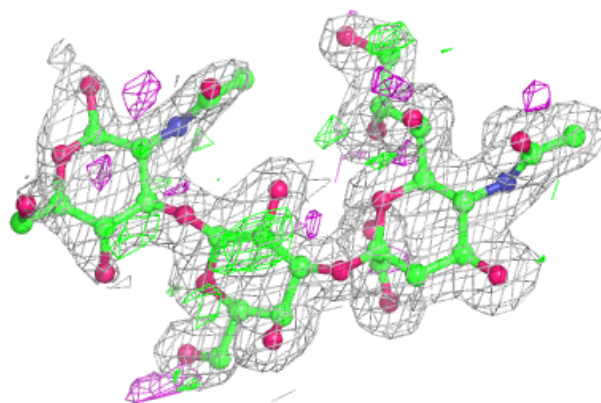
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	1	15/15	0.82	0.24	47,68,85,92	0
2	NAG	I	1	15/15	0.89	0.26	34,61,74,76	0
2	NAG	J	1	15/15	0.90	0.20	31,49,76,85	0
3	GAL	H	1	12/12	0.91	0.18	26,31,37,37	0
2	GAL	I	2	11/12	0.93	0.11	25,27,32,40	0
3	GAL	G	1	12/12	0.94	0.17	26,33,41,44	0
3	SIA	G	2	20/21	0.95	0.11	18,26,38,50	0
2	GAL	F	2	11/12	0.95	0.14	22,29,36,41	0
2	GAL	J	2	11/12	0.96	0.11	20,25,28,31	0
2	SIA	F	3	20/21	0.96	0.09	17,21,30,37	0
3	SIA	H	2	20/21	0.96	0.13	17,24,34,46	0
2	SIA	I	3	20/21	0.97	0.09	14,21,32,47	0
2	SIA	J	3	20/21	0.97	0.09	13,19,28,39	0

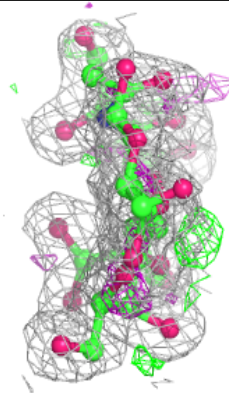
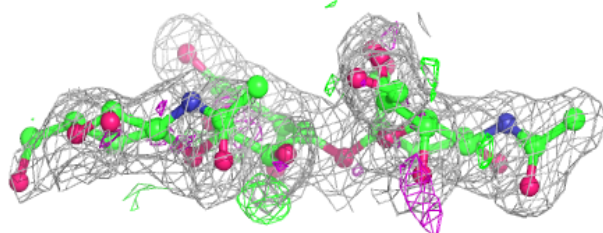
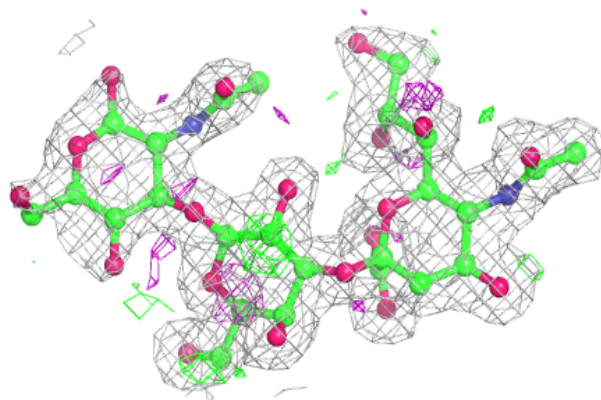
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

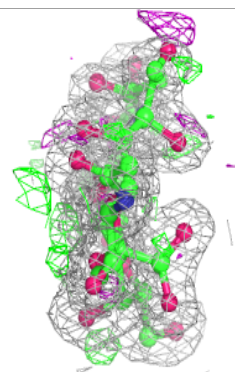
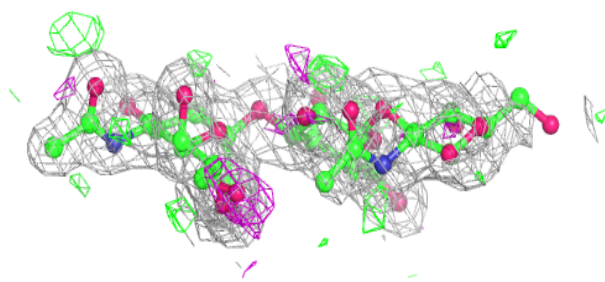
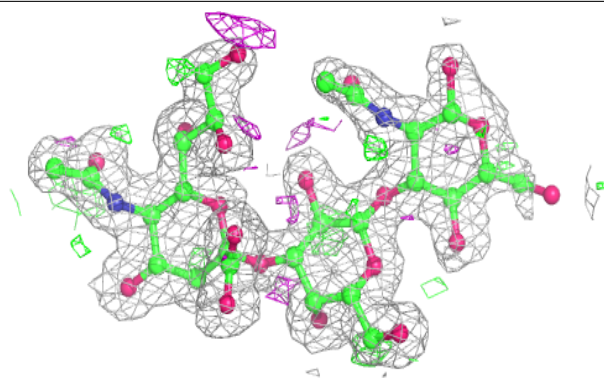
**Electron density around Chain I:**

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



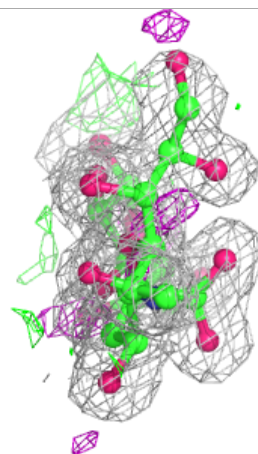
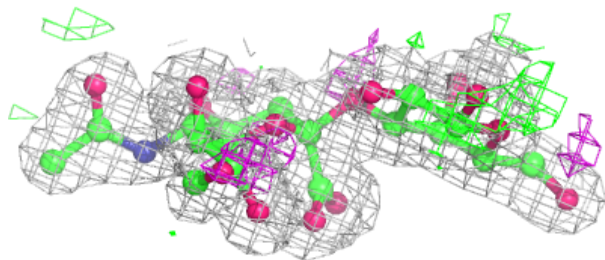
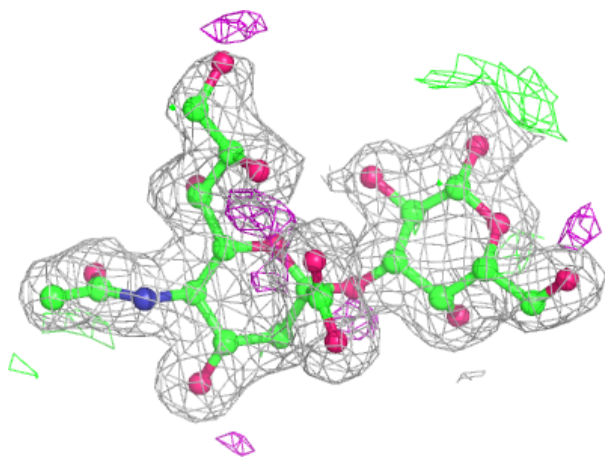
Electron density around Chain J:

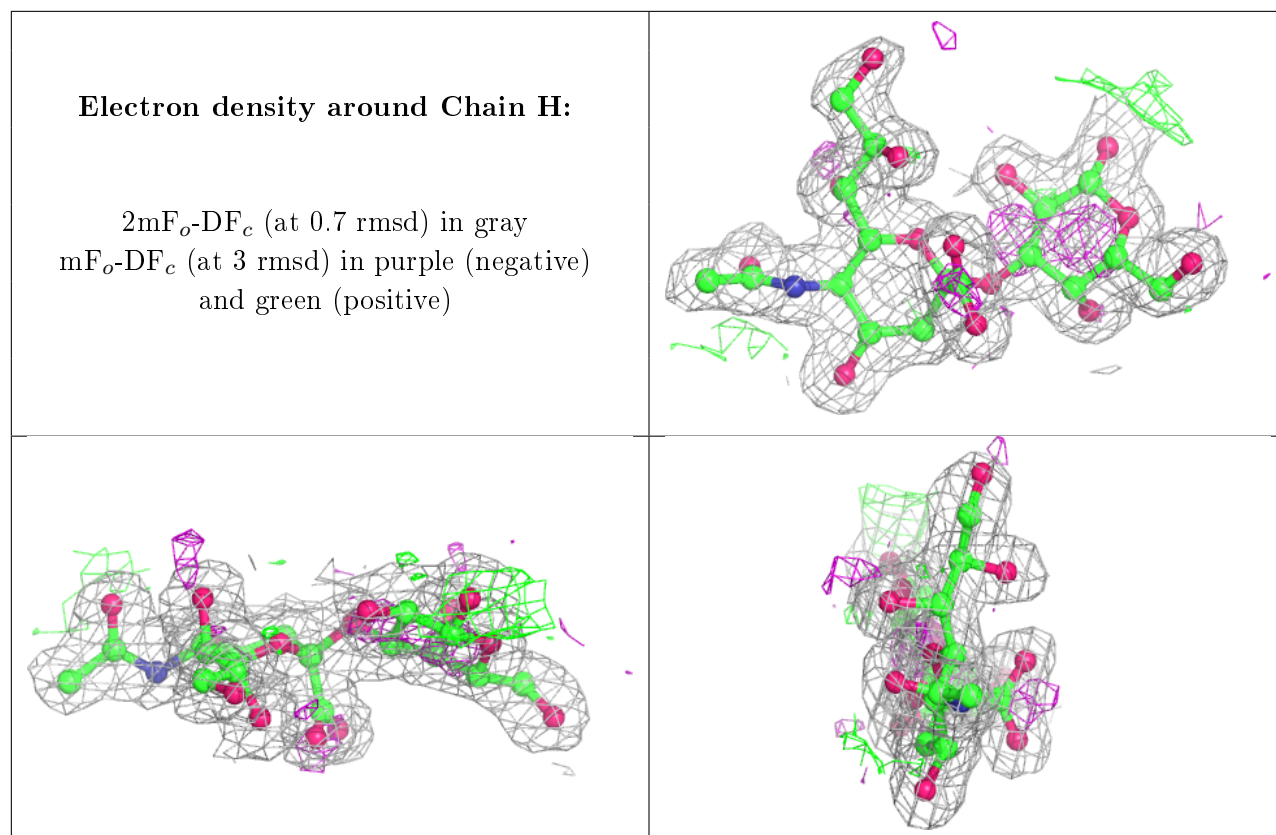
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	E	401	4/6	0.86	0.33	40,46,51,54	0
4	GOL	D	401	4/6	0.91	0.28	31,33,42,56	0
4	GOL	B	401	4/6	0.92	0.32	36,45,61,64	0
4	GOL	A	401	4/6	0.92	0.28	46,49,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.