wwPDB X-ray Structure Validation Summary Report (i)

Sep 19, 2023 – 10:57 AM EDT

PDB ID	:	5ESV
Title	:	Crystal Structure of Broadly Neutralizing Antibody CH03, Isolated from Donor CH0219, in Complex with Scaffolded Trimeric HIV-1 Env V1V2 Domain from the Clade C Superinfecting Strain of Donor CAP256.
Authors	:	Gorman, J.; Yang, M.; Kwong, P.D.
Deposited on	:	2015-11-17
Resolution	:	3.10 Å(reported)

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

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

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

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

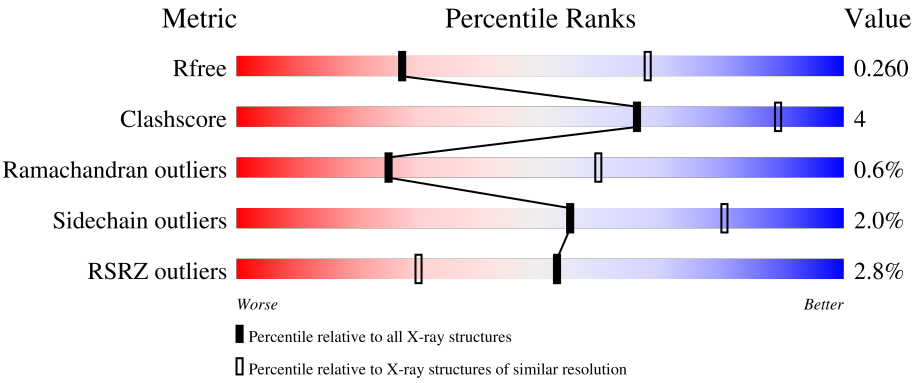
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	244	89% 5% 6%
1	C	244	4% 86% 9% 6%
1	H	244	89% 5% 6%
2	B	215	92% 7%
2	D	215	92% 7%

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Mol	Chain	Length	Quality of chain
2	L	215	3% 93% 7%
3	E	211	3% 78% 5% 17%
3	F	211	3% 73% 9% 15%
3	G	211	9% 69% 16% 11%
4	I	2	100%
5	J	5	20% 40% 40%
6	K	7	14% 43% 43%
6	M	7	14% 43% 43%
6	P	7	14% 43% 43%
6	Q	7	29% 43% 29%
6	T	7	14% 71% 14%
7	N	3	67% 33%
7	O	3	33% 33% 33%
8	R	6	17% 83%
8	S	6	33% 33% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	I	2	-	-	-	X
5	MAN	J	4	-	-	-	X
6	MAN	K	6	-	-	-	X
6	NAG	P	1	X	-	-	-
7	NAG	N	1	-	-	-	X
7	BMA	N	3	-	-	-	X
8	MAN	R	6	-	-	-	X
9	ZN	E	422	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29608 atoms, of which 14564 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 CH03 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	0	0
			3429	1102	1684	300	336	7			
1	C	230	Total	C	H	N	O	S	0	0	0
			3412	1099	1673	297	336	7			
1	H	229	Total	C	H	N	O	S	0	0	0
			3415	1098	1677	299	334	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP S6BGE0
A	220	LEU	-	expression tag	UNP S6BGE0
A	221	GLU	-	expression tag	UNP S6BGE0
A	222	VAL	-	expression tag	UNP S6BGE0
A	223	LEU	-	expression tag	UNP S6BGE0
A	224	PHE	-	expression tag	UNP S6BGE0
C	219	GLY	-	expression tag	UNP S6BGE0
C	220	LEU	-	expression tag	UNP S6BGE0
C	221	GLU	-	expression tag	UNP S6BGE0
C	222	VAL	-	expression tag	UNP S6BGE0
C	223	LEU	-	expression tag	UNP S6BGE0
C	224	PHE	-	expression tag	UNP S6BGE0
H	219	GLY	-	expression tag	UNP S6BGE0
H	220	LEU	-	expression tag	UNP S6BGE0
H	221	GLU	-	expression tag	UNP S6BGE0
H	222	VAL	-	expression tag	UNP S6BGE0
H	223	LEU	-	expression tag	UNP S6BGE0
H	224	PHE	-	expression tag	UNP S6BGE0

- Molecule 2 is a protein called CH03 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	213	Total	C	H	N	O	S	0	0	0
			3241	1033	1598	283	323	4			
2	D	214	Total	C	H	N	O	S	0	0	0
			3256	1038	1604	284	326	4			
2	L	214	Total	C	H	N	O	S	0	0	0
			3256	1038	1604	284	326	4			

- Molecule 3 is a protein called 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	176	Total	C	H	N	O	S	0	0	0
			2673	833	1335	239	259	7			
3	F	179	Total	C	H	N	O	S	0	0	0
			2726	861	1356	242	260	7			
3	G	187	Total	C	H	N	O	S	0	0	0
			2831	887	1411	251	275	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	111	SER	-	expression tag	UNP P44815
E	112	LEU	-	expression tag	UNP P44815
E	125	GLY	-	linker	UNP P44815
E	198	GLY	-	linker	UNP W6ICC0
E	199	GLY	-	linker	UNP W6ICC0
E	200	SER	-	linker	UNP W6ICC0
E	201	GLY	-	linker	UNP W6ICC0
E	?	-	ASP	deletion	UNP P44815
E	?	-	THR	deletion	UNP P44815
E	?	-	ASP	deletion	UNP P44815
E	?	-	MET	deletion	UNP P44815
E	?	-	GLN	deletion	UNP P44815
E	?	-	TYR	deletion	UNP P44815
E	323	GLY	-	expression tag	UNP P44815
E	324	LEU	-	expression tag	UNP P44815
E	325	GLU	-	expression tag	UNP P44815
E	326	VAL	-	expression tag	UNP P44815
E	327	LEU	-	expression tag	UNP P44815
E	328	PHE	-	expression tag	UNP P44815
E	329	GLN	-	expression tag	UNP P44815
F	111	SER	-	expression tag	UNP P44815
F	112	LEU	-	expression tag	UNP P44815

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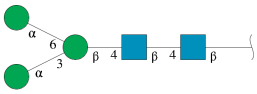
Chain	Residue	Modelled	Actual	Comment	Reference
F	125	GLY	-	linker	UNP P44815
F	198	GLY	-	linker	UNP W6ICC0
F	199	GLY	-	linker	UNP W6ICC0
F	200	SER	-	linker	UNP W6ICC0
F	201	GLY	-	linker	UNP W6ICC0
F	?	-	ASP	deletion	UNP P44815
F	?	-	THR	deletion	UNP P44815
F	?	-	ASP	deletion	UNP P44815
F	?	-	MET	deletion	UNP P44815
F	?	-	GLN	deletion	UNP P44815
F	?	-	TYR	deletion	UNP P44815
F	323	GLY	-	expression tag	UNP P44815
F	324	LEU	-	expression tag	UNP P44815
F	325	GLU	-	expression tag	UNP P44815
F	326	VAL	-	expression tag	UNP P44815
F	327	LEU	-	expression tag	UNP P44815
F	328	PHE	-	expression tag	UNP P44815
F	329	GLN	-	expression tag	UNP P44815
G	111	SER	-	expression tag	UNP P44815
G	112	LEU	-	expression tag	UNP P44815
G	125	GLY	-	linker	UNP P44815
G	198	GLY	-	linker	UNP W6ICC0
G	199	GLY	-	linker	UNP W6ICC0
G	200	SER	-	linker	UNP W6ICC0
G	201	GLY	-	linker	UNP W6ICC0
G	?	-	ASP	deletion	UNP P44815
G	?	-	THR	deletion	UNP P44815
G	?	-	ASP	deletion	UNP P44815
G	?	-	MET	deletion	UNP P44815
G	?	-	GLN	deletion	UNP P44815
G	?	-	TYR	deletion	UNP P44815
G	323	GLY	-	expression tag	UNP P44815
G	324	LEU	-	expression tag	UNP P44815
G	325	GLU	-	expression tag	UNP P44815
G	326	VAL	-	expression tag	UNP P44815
G	327	LEU	-	expression tag	UNP P44815
G	328	PHE	-	expression tag	UNP P44815
G	329	GLN	-	expression tag	UNP P44815

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

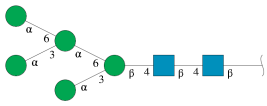
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



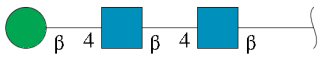
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



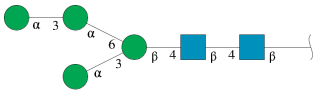
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	7	Total	C	H	N	O	0	0	0
			151	46	68	2	35			
6	M	7	Total	C	H	N	O	0	0	0
			152	46	69	2	35			
6	P	7	Total	C	H	N	O	0	0	0
			152	46	69	2	35			
6	Q	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			
6	T	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
7	O	3	Total	C	H	N	O	0	0	0
			71	22	32	2	15			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

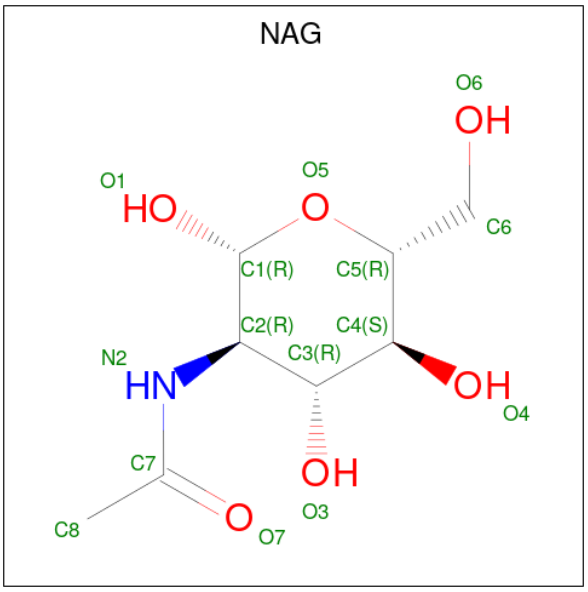


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	R	6	Total	C	H	N	O	0	0	0
			133	40	61	2	30			
8	S	6	Total	C	H	N	O	0	0	0
			132	40	60	2	30			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Zn	0	0
			1	1		
9	F	1	Total	Zn	0	0
			1	1		
9	G	1	Total	Zn	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total C H N O 26 8 12 1 5	0	0

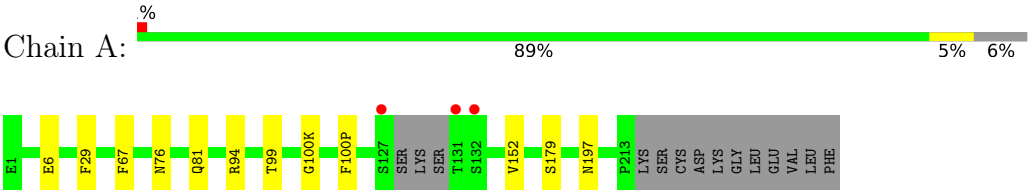
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total O 2 2	0	0
11	H	2	Total O 2 2	0	0

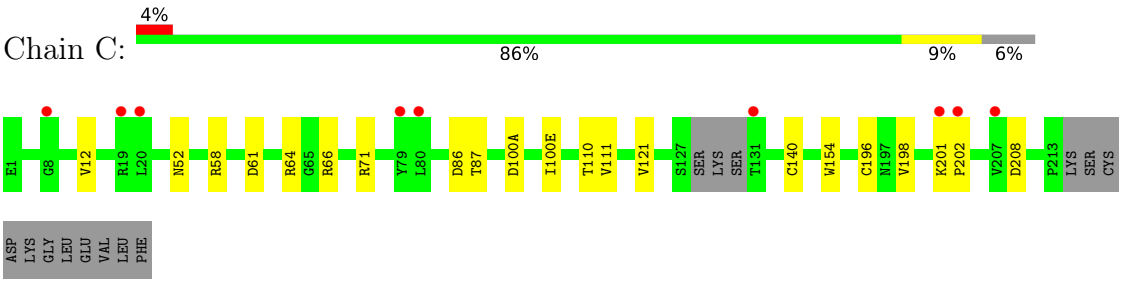
3 Residue-property plots (i)

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.

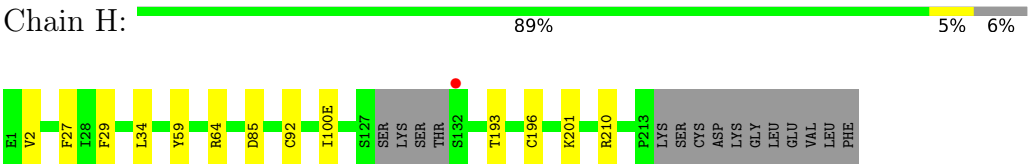
• Molecule 1: CH03 Heavy Chain



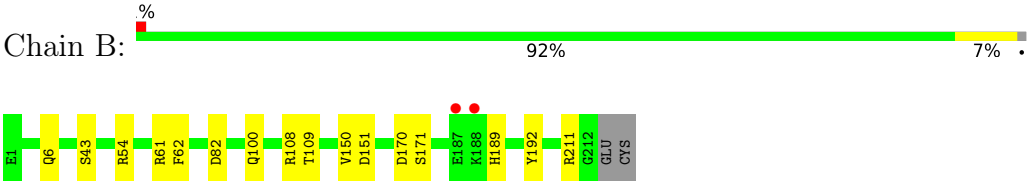
• Molecule 1: CH03 Heavy Chain



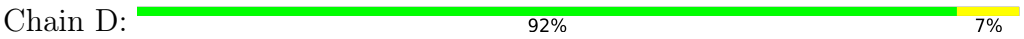
• Molecule 1: CH03 Heavy Chain

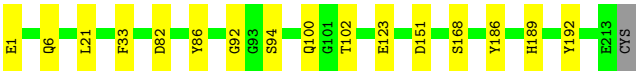


• Molecule 2: CH03 Light Chain



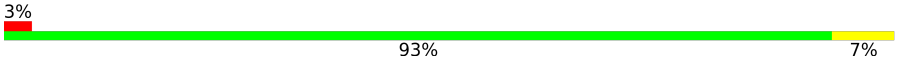
• Molecule 2: CH03 Light Chain





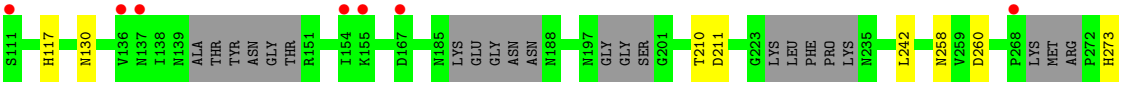
• Molecule 2: CH03 Light Chain

Chain L:



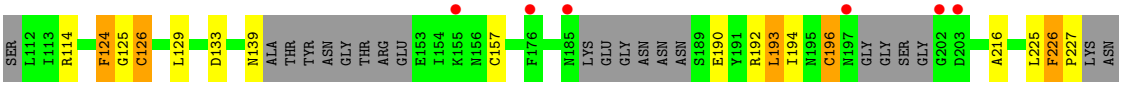
• Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160

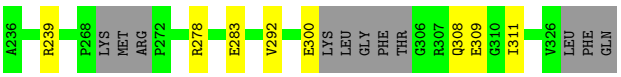
Chain E:



• Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160

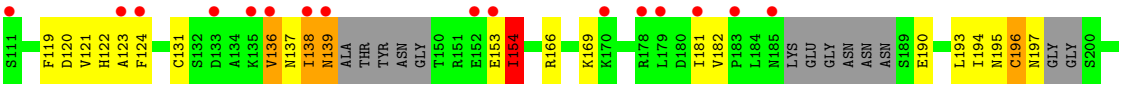
Chain F:

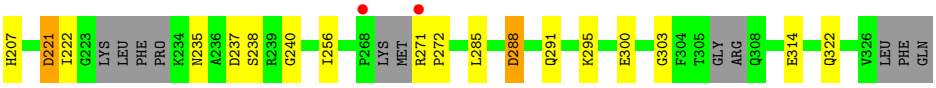




• Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160

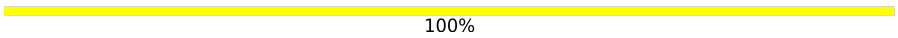
Chain G:





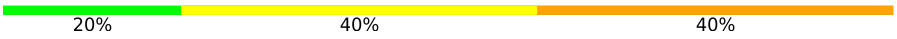
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



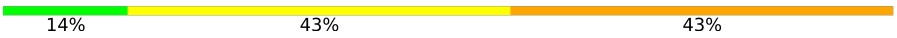
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

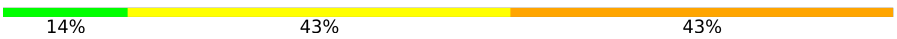


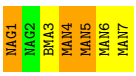
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

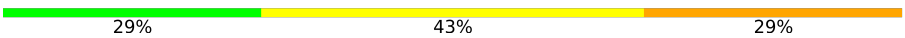
Chain P:

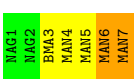




• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

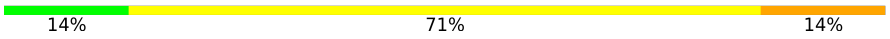
Chain Q:





• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

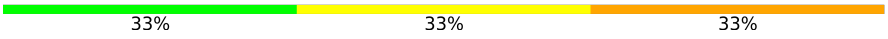


• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

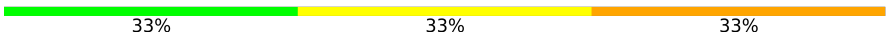


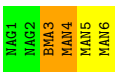
• Molecule 8: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 8: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.69Å 98.21Å 170.63Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	41.99 – 3.10 41.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.99-3.10) 99.1 (41.99-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX (dev_2247: ???)	Depositor
R, R_{free}	0.208 , 0.259 0.209 , 0.260	Depositor DCC
R_{free} test set	2004 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	29608	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: MAN, ZN, BMA, 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	0.28	0/1789	0.48	0/2435
1	C	0.27	0/1783	0.46	0/2428
1	H	0.29	0/1782	0.48	0/2425
2	B	0.29	0/1682	0.47	0/2283
2	D	0.26	0/1691	0.46	0/2295
2	L	0.28	0/1691	0.46	0/2295
3	E	0.26	0/1346	0.47	0/1809
3	F	0.27	0/1381	0.48	0/1855
3	G	0.30	0/1430	0.53	0/1922
All	All	0.28	0/14575	0.48	0/19747

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	195	ASN	Peptide

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	1745	1684	1684	6	0
1	C	1739	1673	1673	11	0
1	H	1738	1677	1677	5	0
2	B	1643	1598	1598	8	0
2	D	1652	1604	1604	10	0
2	L	1652	1604	1604	7	0
3	E	1338	1335	1332	7	0
3	F	1370	1356	1373	21	0
3	G	1420	1411	1408	25	0
4	I	28	25	25	1	0
5	J	61	52	52	1	0
6	K	83	68	70	5	0
6	M	83	69	70	2	0
6	P	83	69	70	4	0
6	Q	83	70	70	2	0
6	T	83	70	70	1	0
7	N	39	34	34	2	0
7	O	39	32	34	2	0
8	R	72	61	61	6	0
8	S	72	60	61	2	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	G	14	12	13	0	0
11	A	2	0	0	0	0
11	H	2	0	0	0	0
All	All	15044	14564	14583	118	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 4.

The worst 5 of 118 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)
6:P:4:MAN:O2	6:P:5:MAN:H2	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ARG:NH1	2:B:109:THR:O	2.08	0.86
1:C:52:ASN:O	1:C:71:ARG:NH2	2.21	0.72
3:G:288:ASP:N	3:G:288:ASP:OD1	2.25	0.70
3:E:117:HIS:O	3:G:295:LYS:NZ	2.27	0.68

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	A	226/244 (93%)	212 (94%)	13 (6%)	1 (0%)	34 69
1	C	226/244 (93%)	209 (92%)	17 (8%)	0	100 100
1	H	225/244 (92%)	212 (94%)	13 (6%)	0	100 100
2	B	211/215 (98%)	200 (95%)	11 (5%)	0	100 100
2	D	212/215 (99%)	201 (95%)	11 (5%)	0	100 100
2	L	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	29 64
3	E	162/211 (77%)	151 (93%)	9 (6%)	2 (1%)	13 44
3	F	165/211 (78%)	149 (90%)	14 (8%)	2 (1%)	13 44
3	G	173/211 (82%)	153 (88%)	16 (9%)	4 (2%)	6 28
All	All	1812/2010 (90%)	1690 (93%)	112 (6%)	10 (1%)	25 59

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	124	PHE
3	F	226	PHE
3	E	274	ILE
3	E	258	ASN
3	G	154	ILE

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	191/204 (94%)	190 (100%)	1 (0%)	88 94
1	C	190/204 (93%)	189 (100%)	1 (0%)	88 94
1	H	190/204 (93%)	186 (98%)	4 (2%)	53 79
2	B	182/184 (99%)	181 (100%)	1 (0%)	88 94
2	D	183/184 (100%)	182 (100%)	1 (0%)	88 94
2	L	183/184 (100%)	182 (100%)	1 (0%)	88 94
3	E	141/170 (83%)	139 (99%)	2 (1%)	67 86
3	F	144/170 (85%)	138 (96%)	6 (4%)	30 62
3	G	149/170 (88%)	135 (91%)	14 (9%)	8 32
All	All	1553/1674 (93%)	1522 (98%)	31 (2%)	55 80

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	136	VAL
1	H	92	CYS
3	G	154	ILE
1	H	196	CYS
3	G	288	ASP

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

Mol	Chain	Res	Type
3	G	122	HIS

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)

60 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	$\#\|Z\| > 2$
4	NAG	I	1	4,3	14,14,15	0.56	0	17,19,21	0.61	0
4	NAG	I	2	4	14,14,15	0.48	0	17,19,21	1.00	1 (5%)
5	NAG	J	1	5,3	14,14,15	0.56	0	17,19,21	0.63	0
5	NAG	J	2	5	14,14,15	0.32	0	17,19,21	1.04	1 (5%)
5	BMA	J	3	5	11,11,12	1.45	2 (18%)	15,15,17	1.93	4 (26%)
5	MAN	J	4	5	11,11,12	0.91	1 (9%)	15,15,17	1.68	3 (20%)
5	MAN	J	5	5	11,11,12	0.92	0	15,15,17	0.93	2 (13%)
6	NAG	K	1	6,3	14,14,15	0.43	0	17,19,21	0.35	0
6	NAG	K	2	6	14,14,15	0.70	1 (7%)	17,19,21	0.71	0
6	BMA	K	3	6	11,11,12	1.59	1 (9%)	15,15,17	1.13	1 (6%)
6	MAN	K	4	6	11,11,12	2.24	3 (27%)	15,15,17	2.26	6 (40%)
6	MAN	K	5	6	11,11,12	1.15	1 (9%)	15,15,17	2.05	4 (26%)
6	MAN	K	6	6	11,11,12	1.58	2 (18%)	15,15,17	1.70	3 (20%)
6	MAN	K	7	6	11,11,12	0.86	1 (9%)	15,15,17	1.09	1 (6%)
6	NAG	M	1	6,3	14,14,15	0.44	0	17,19,21	0.43	0
6	NAG	M	2	6	14,14,15	0.66	1 (7%)	17,19,21	0.57	0
6	BMA	M	3	6	11,11,12	0.78	1 (9%)	15,15,17	1.07	0
6	MAN	M	4	6	11,11,12	1.67	2 (18%)	15,15,17	1.49	4 (26%)
6	MAN	M	5	6	11,11,12	1.26	2 (18%)	15,15,17	1.42	1 (6%)
6	MAN	M	6	6	11,11,12	1.00	1 (9%)	15,15,17	1.01	2 (13%)
6	MAN	M	7	6	11,11,12	1.13	1 (9%)	15,15,17	0.79	0
7	NAG	N	1	7,3	14,14,15	0.98	1 (7%)	17,19,21	0.81	0
7	NAG	N	2	7	14,14,15	0.82	1 (7%)	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	N	3	7	11,11,12	1.02	0	15,15,17	1.01	1 (6%)
7	NAG	O	1	7,3	14,14,15	0.36	0	17,19,21	0.42	0
7	NAG	O	2	7	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
7	BMA	O	3	7	11,11,12	1.58	2 (18%)	15,15,17	1.79	4 (26%)
6	NAG	P	1	6,3	14,14,15	1.78	2 (14%)	17,19,21	1.23	2 (11%)
6	NAG	P	2	6	14,14,15	0.41	0	17,19,21	0.59	0
6	BMA	P	3	6	11,11,12	0.92	1 (9%)	15,15,17	0.80	1 (6%)
6	MAN	P	4	6	11,11,12	1.25	1 (9%)	15,15,17	2.02	4 (26%)
6	MAN	P	5	6	11,11,12	1.21	2 (18%)	15,15,17	1.98	1 (6%)
6	MAN	P	6	6	11,11,12	1.22	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	P	7	6	11,11,12	0.77	1 (9%)	15,15,17	1.11	1 (6%)
6	NAG	Q	1	6,3	14,14,15	0.26	0	17,19,21	0.65	0
6	NAG	Q	2	6	14,14,15	0.25	0	17,19,21	0.61	0
6	BMA	Q	3	6	11,11,12	1.14	2 (18%)	15,15,17	1.53	3 (20%)
6	MAN	Q	4	6	11,11,12	1.05	1 (9%)	15,15,17	1.59	3 (20%)
6	MAN	Q	5	6	11,11,12	1.14	1 (9%)	15,15,17	1.06	1 (6%)
6	MAN	Q	6	6	11,11,12	0.94	1 (9%)	15,15,17	1.22	2 (13%)
6	MAN	Q	7	6	11,11,12	0.89	0	15,15,17	2.29	3 (20%)
8	NAG	R	1	8,3	14,14,15	0.59	0	17,19,21	1.33	2 (11%)
8	NAG	R	2	8	14,14,15	0.43	0	17,19,21	1.00	2 (11%)
8	BMA	R	3	8	11,11,12	1.26	2 (18%)	15,15,17	1.40	3 (20%)
8	MAN	R	4	8	11,11,12	0.99	1 (9%)	15,15,17	1.27	2 (13%)
8	MAN	R	5	8	11,11,12	1.50	3 (27%)	15,15,17	1.47	4 (26%)
8	MAN	R	6	8	11,11,12	1.29	2 (18%)	15,15,17	1.55	3 (20%)
8	NAG	S	1	8,3	14,14,15	0.30	0	17,19,21	0.48	0
8	NAG	S	2	8	14,14,15	0.37	0	17,19,21	0.47	0
8	BMA	S	3	8	11,11,12	0.74	0	15,15,17	1.20	1 (6%)
8	MAN	S	4	8	11,11,12	0.95	1 (9%)	15,15,17	1.66	1 (6%)
8	MAN	S	5	8	11,11,12	1.29	3 (27%)	15,15,17	2.09	5 (33%)
8	MAN	S	6	8	11,11,12	1.22	1 (9%)	15,15,17	1.25	3 (20%)
6	NAG	T	1	6,3	14,14,15	0.29	0	17,19,21	0.41	0
6	NAG	T	2	6	14,14,15	0.49	0	17,19,21	0.38	0
6	BMA	T	3	6	11,11,12	0.85	1 (9%)	15,15,17	1.25	2 (13%)
6	MAN	T	4	6	11,11,12	1.27	2 (18%)	15,15,17	0.96	1 (6%)
6	MAN	T	5	6	11,11,12	0.98	1 (9%)	15,15,17	1.53	2 (13%)
6	MAN	T	6	6	11,11,12	0.88	0	15,15,17	1.42	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	T	7	6	11,11,12	0.91	1 (9%)	15,15,17	2.47	2 (13%)

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	NAG	I	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	1/1/1/1
5	MAN	J	5	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
6	MAN	K	6	6	-	2/2/19/22	0/1/1/1
6	MAN	K	7	6	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	2/2/19/22	1/1/1/1
6	MAN	M	6	6	-	2/2/19/22	0/1/1/1
6	MAN	M	7	6	-	0/2/19/22	0/1/1/1
7	NAG	N	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	2/2/19/22	0/1/1/1
7	NAG	O	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
6	NAG	P	1	6,3	1/1/6/7	3/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	MAN	P	5	6	-	2/2/19/22	0/1/1/1
6	MAN	P	6	6	-	0/2/19/22	0/1/1/1
6	MAN	P	7	6	-	2/2/19/22	0/1/1/1
6	NAG	Q	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	6	6	-	1/2/19/22	1/1/1/1
6	MAN	Q	7	6	-	1/2/19/22	0/1/1/1
8	NAG	R	1	8,3	-	3/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	2/2/19/22	0/1/1/1
8	MAN	R	4	8	-	1/2/19/22	1/1/1/1
8	MAN	R	5	8	-	2/2/19/22	0/1/1/1
8	MAN	R	6	8	-	1/2/19/22	0/1/1/1
8	NAG	S	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	1/2/19/22	1/1/1/1
8	MAN	S	5	8	-	2/2/19/22	0/1/1/1
8	MAN	S	6	8	-	2/2/19/22	0/1/1/1
6	NAG	T	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	1/2/19/22	0/1/1/1
6	MAN	T	4	6	-	0/2/19/22	0/1/1/1
6	MAN	T	5	6	-	2/2/19/22	0/1/1/1
6	MAN	T	6	6	-	2/2/19/22	0/1/1/1
6	MAN	T	7	6	-	0/2/19/22	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	O5-C1	-5.67	1.34	1.43
6	K	4	MAN	C4-C5	4.90	1.63	1.53
6	K	3	BMA	O5-C1	-4.54	1.36	1.43
6	M	4	MAN	O5-C1	-3.64	1.37	1.43
7	O	3	BMA	C2-C3	3.59	1.57	1.52

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	7	MAN	C1-O5-C5	7.79	122.74	112.19
6	Q	7	MAN	C1-O5-C5	7.17	121.90	112.19
6	P	5	MAN	C1-O5-C5	6.64	121.19	112.19
6	P	4	MAN	O3-C3-C2	5.27	120.09	109.99
8	S	5	MAN	C1-C2-C3	5.09	115.92	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	P	1	NAG	C1

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	C3-C2-N2-C7
7	N	1	NAG	C3-C2-N2-C7
8	R	2	NAG	C3-C2-N2-C7
6	M	6	MAN	C4-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	4	MAN	C1-C2-C3-C4-C5-O5
6	Q	6	MAN	C1-C2-C3-C4-C5-O5
8	R	4	MAN	C1-C2-C3-C4-C5-O5
6	M	5	MAN	C1-C2-C3-C4-C5-O5
8	S	4	MAN	C1-C2-C3-C4-C5-O5

25 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	3	BMA	1	0
8	R	4	MAN	1	0
7	O	2	NAG	2	0
6	Q	6	MAN	1	0
7	N	1	NAG	2	0
6	K	3	BMA	3	0
8	S	3	BMA	1	0
6	K	6	MAN	2	0
8	R	1	NAG	2	0

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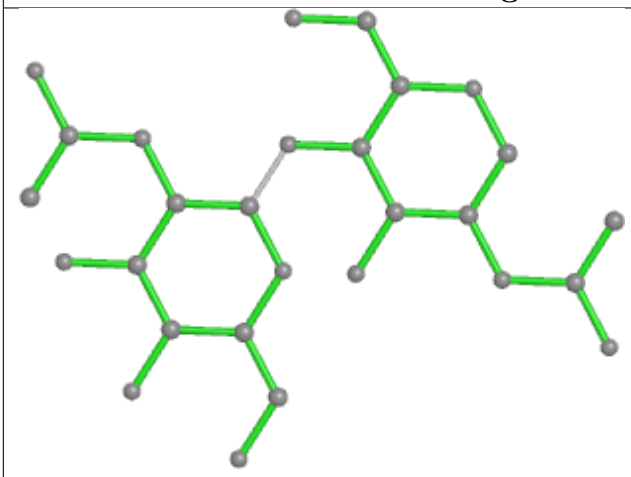
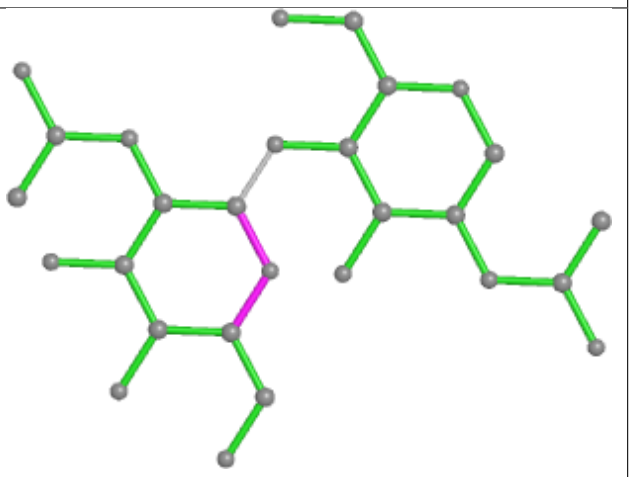
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	5	MAN	1	0
6	M	4	MAN	1	0
4	I	1	NAG	1	0
6	K	4	MAN	5	0
8	S	4	MAN	1	0
8	R	5	MAN	1	0
6	P	1	NAG	1	0
8	R	3	BMA	1	0
5	J	3	BMA	1	0
6	Q	7	MAN	1	0
8	R	2	NAG	3	0
5	J	2	NAG	1	0
6	T	2	NAG	1	0
6	P	5	MAN	3	0
6	M	2	NAG	1	0
6	P	4	MAN	3	0

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

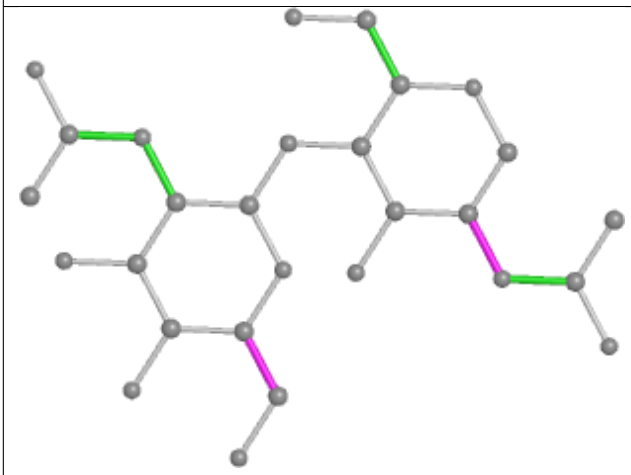
Oligosaccharide Chain I



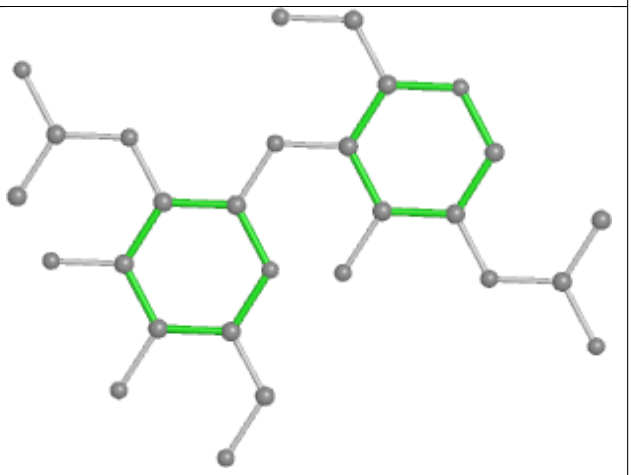
Bond lengths



Bond angles

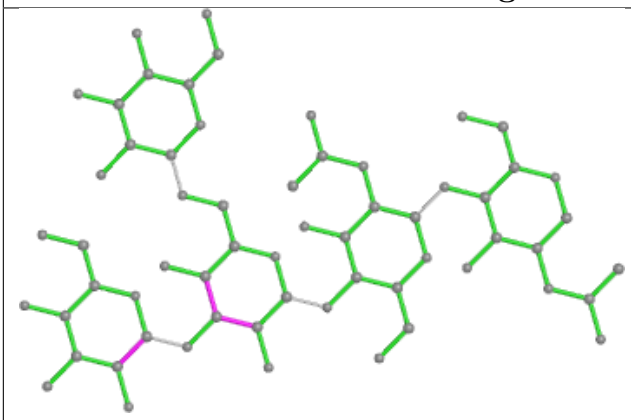


Torsions

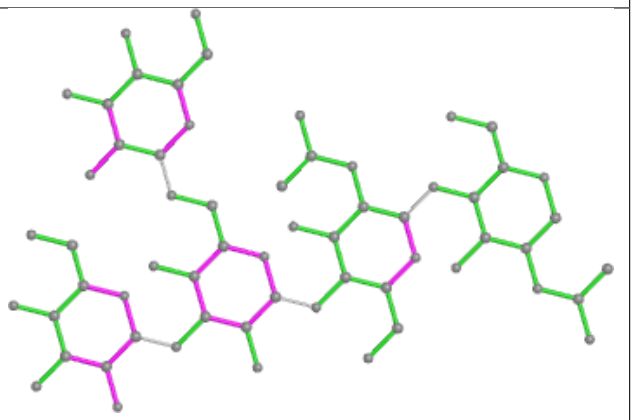


Rings

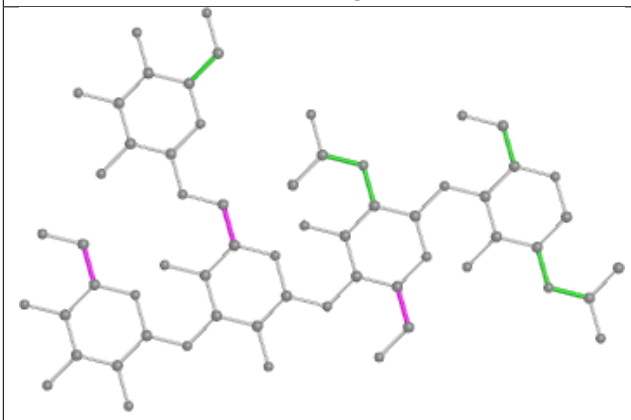
Oligosaccharide Chain J



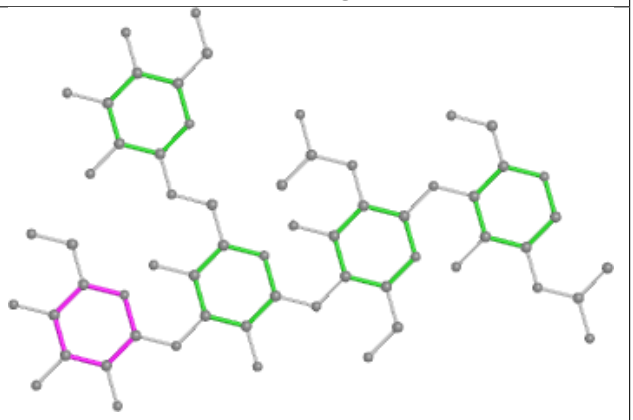
Bond lengths



Bond angles

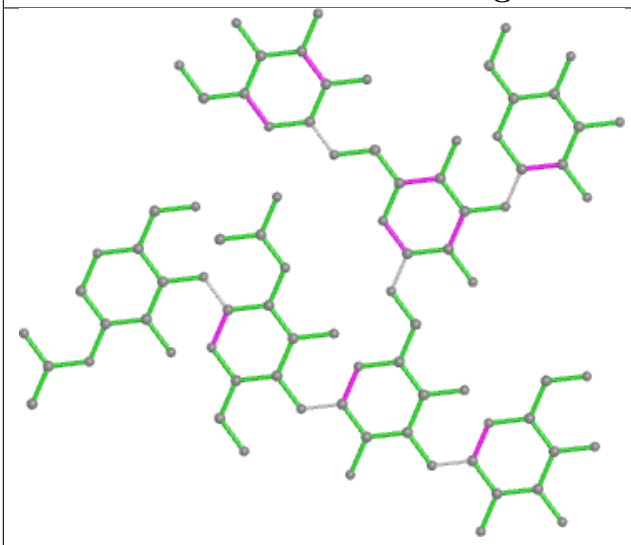


Torsions

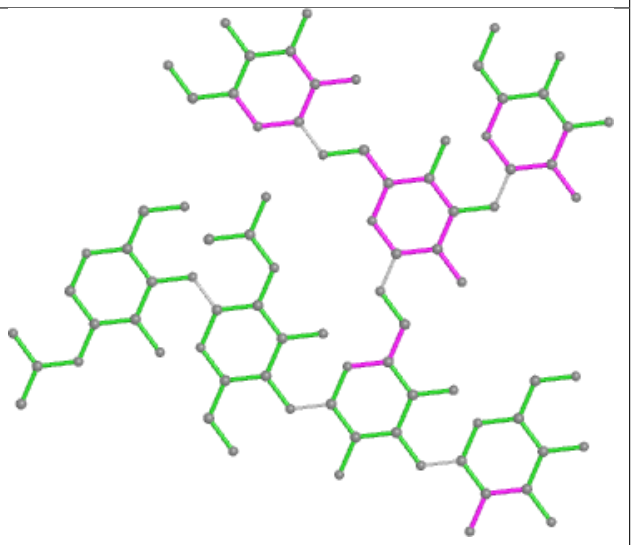


Rings

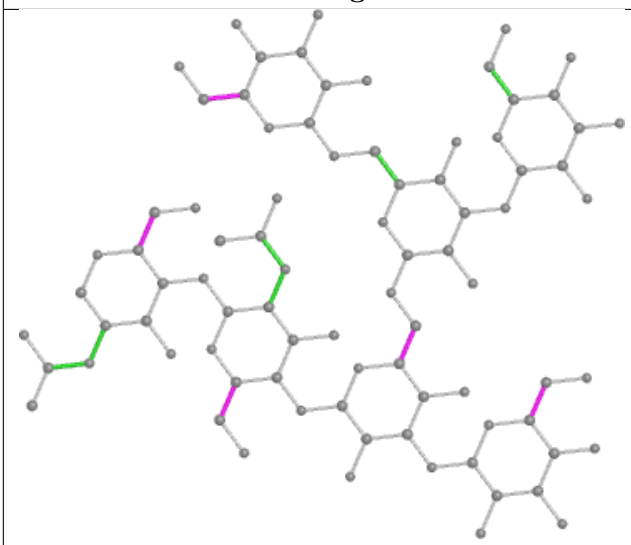
Oligosaccharide Chain K



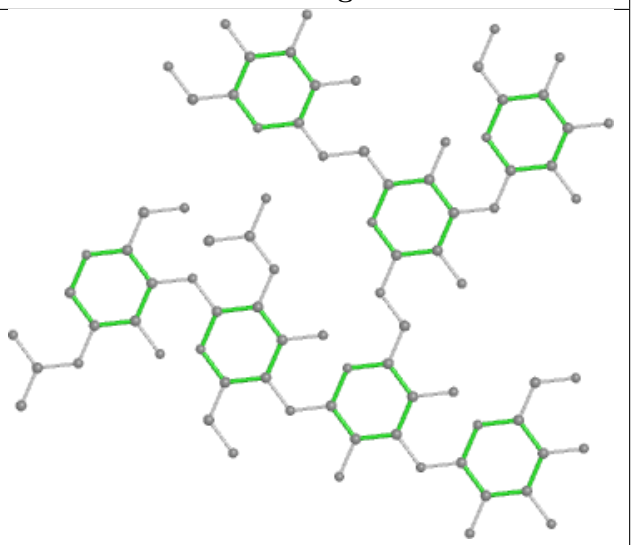
Bond lengths



Bond angles

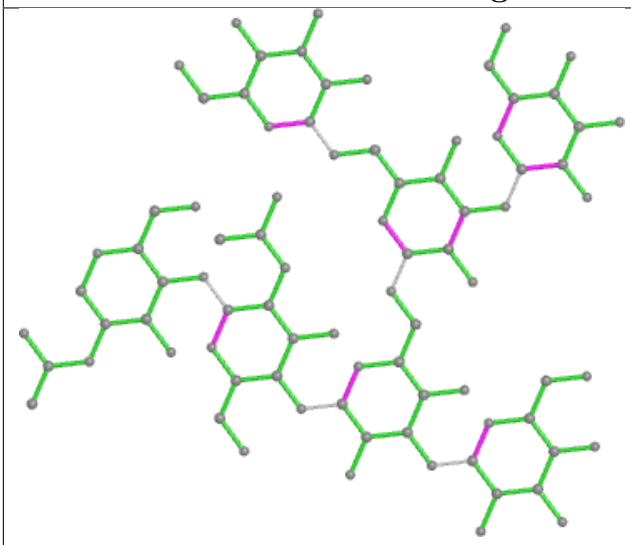


Torsions

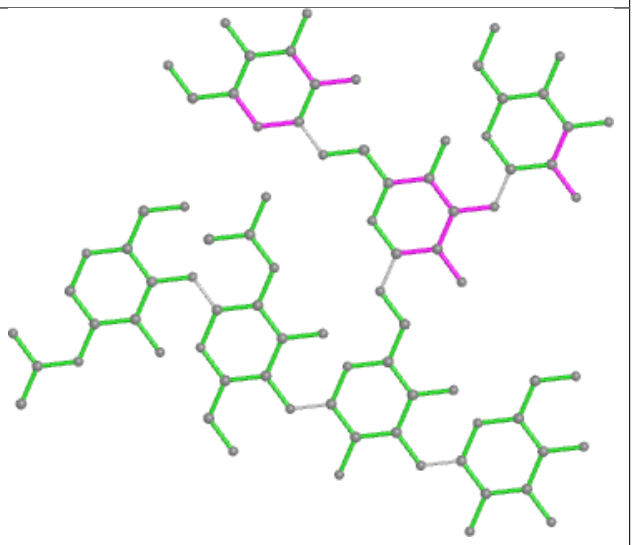


Rings

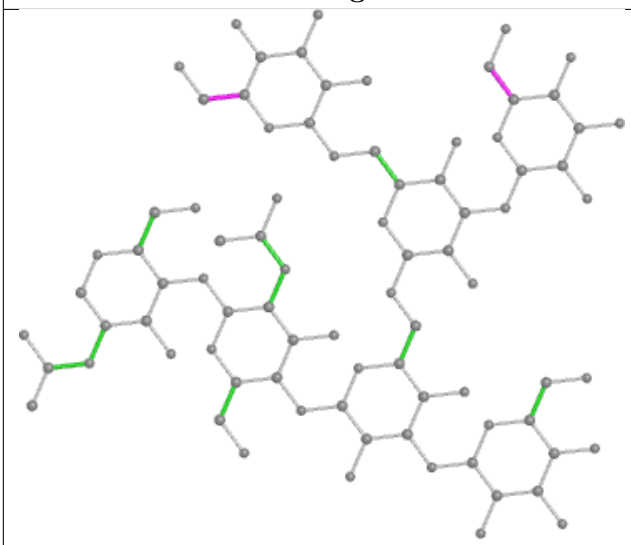
Oligosaccharide Chain M



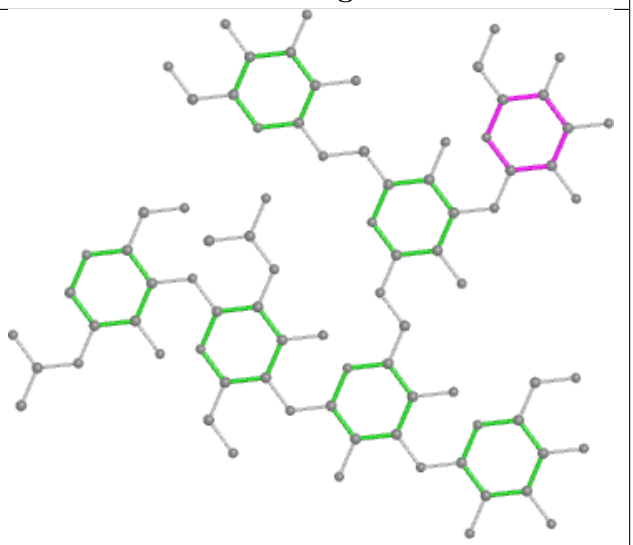
Bond lengths



Bond angles

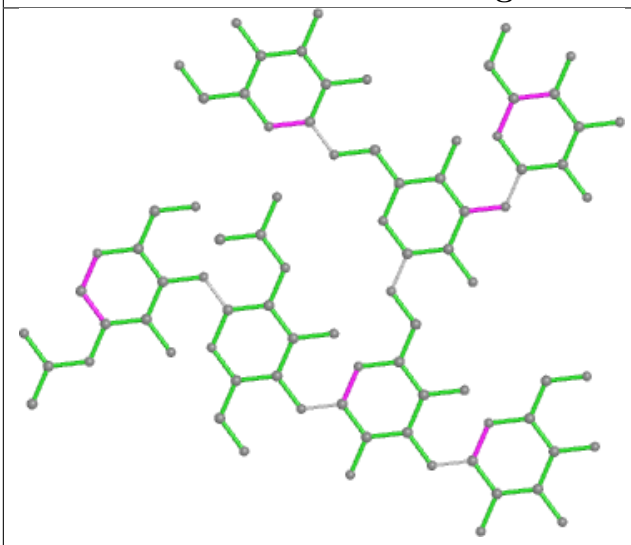


Torsions

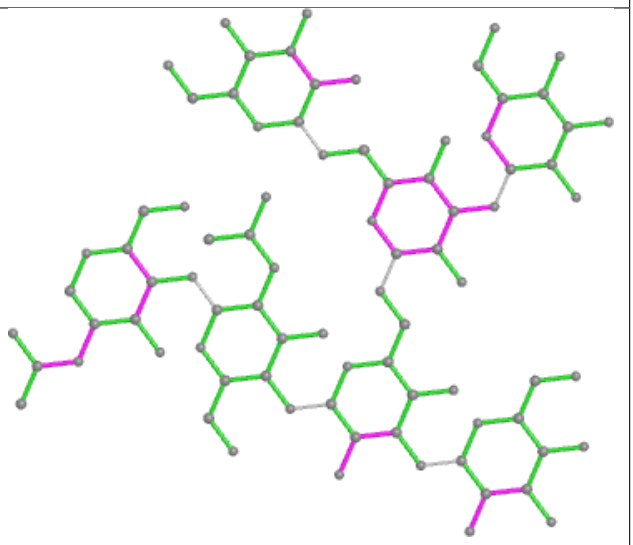


Rings

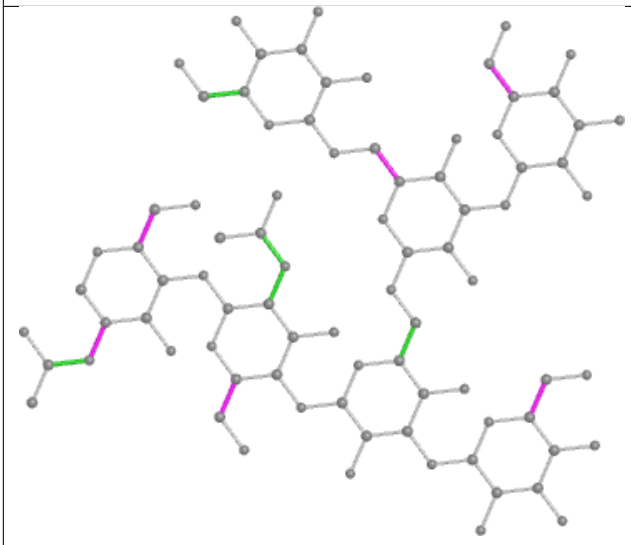
Oligosaccharide Chain P



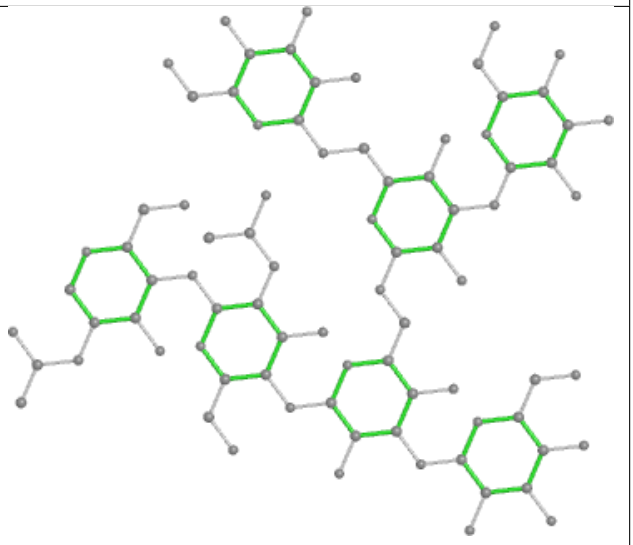
Bond lengths



Bond angles

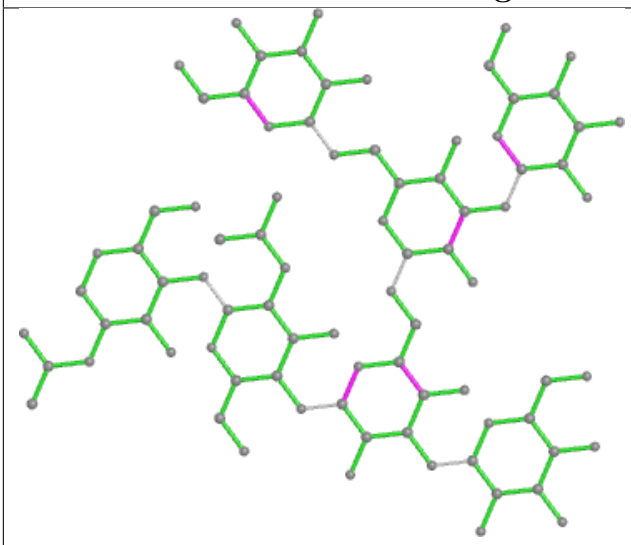


Torsions

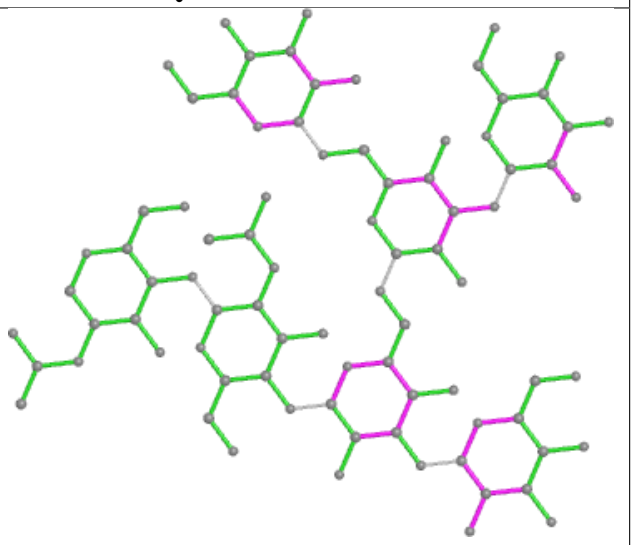


Rings

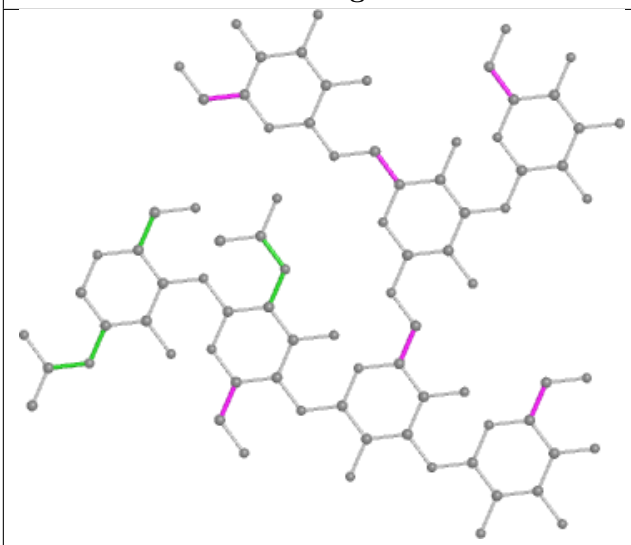
Oligosaccharide Chain Q



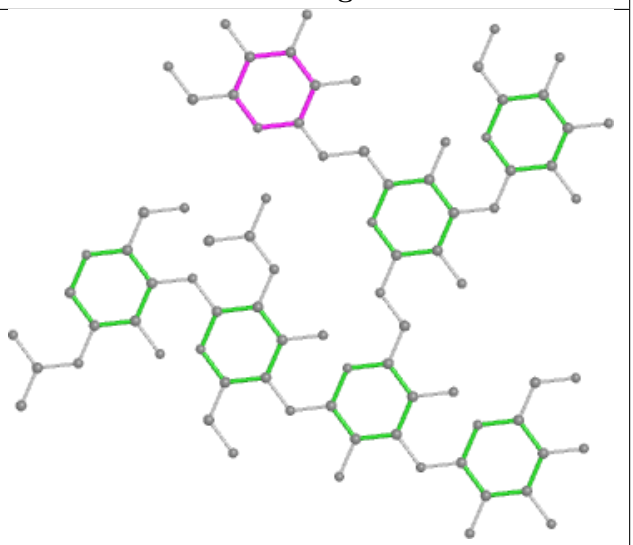
Bond lengths



Bond angles

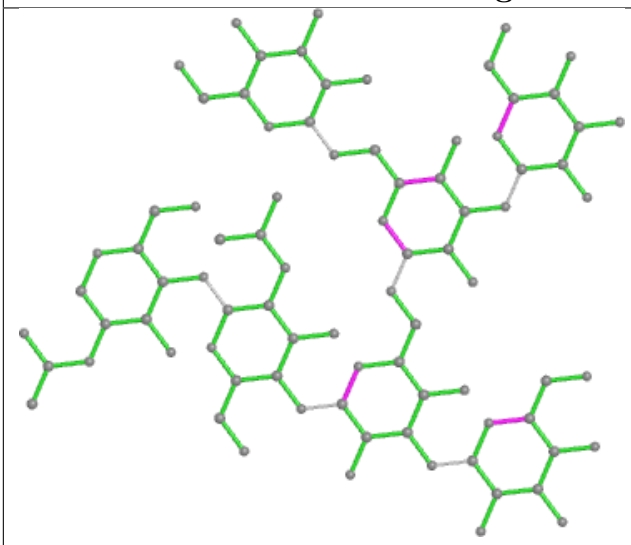


Torsions

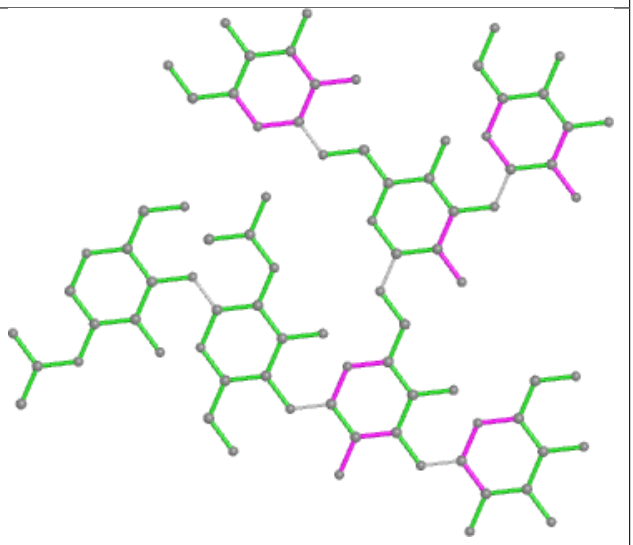


Rings

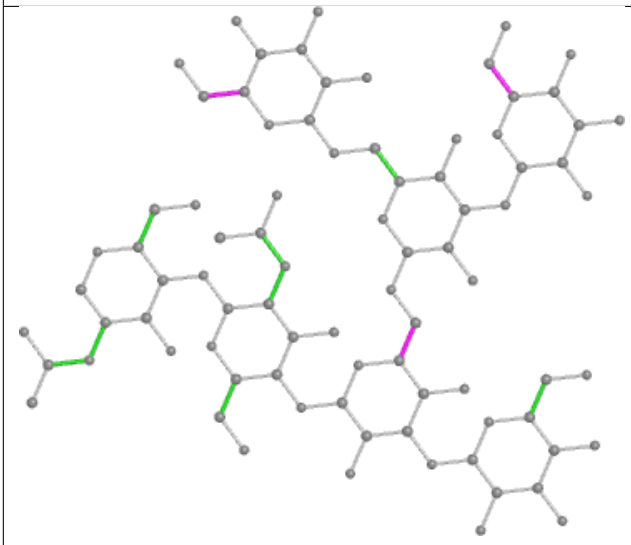
Oligosaccharide Chain T



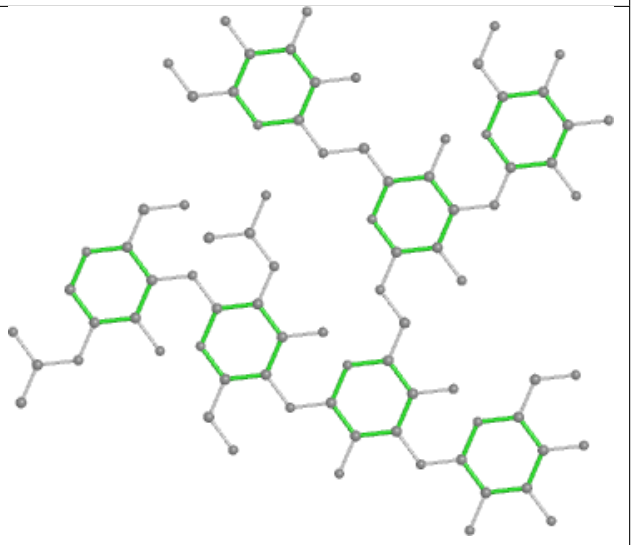
Bond lengths



Bond angles

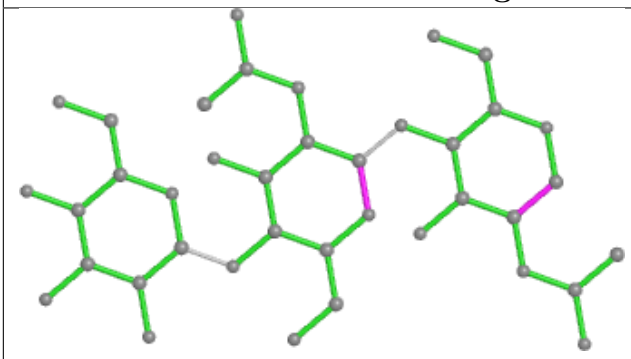


Torsions

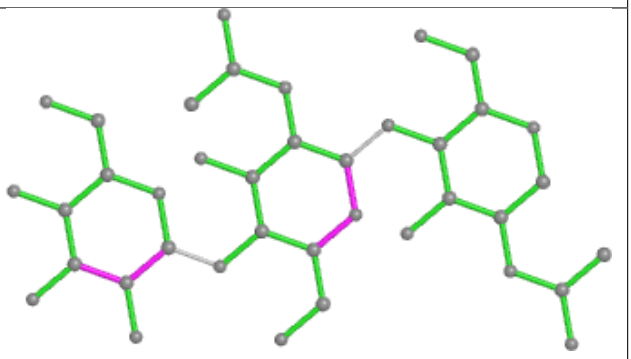


Rings

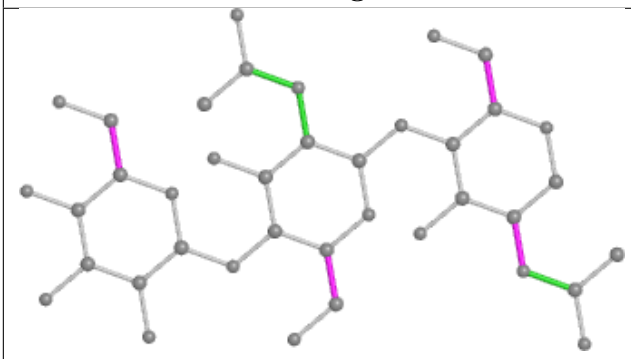
Oligosaccharide Chain N



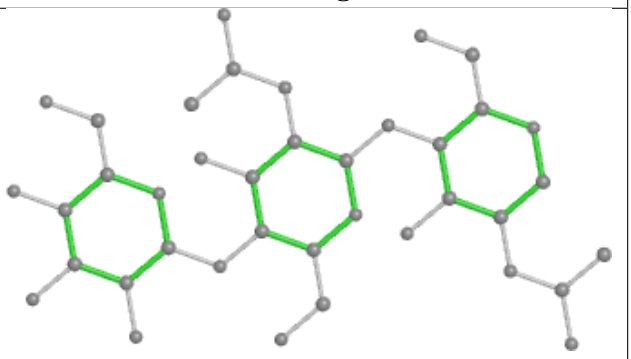
Bond lengths



Bond angles

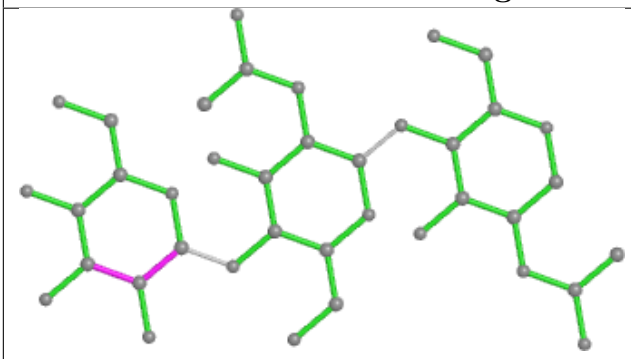


Torsions

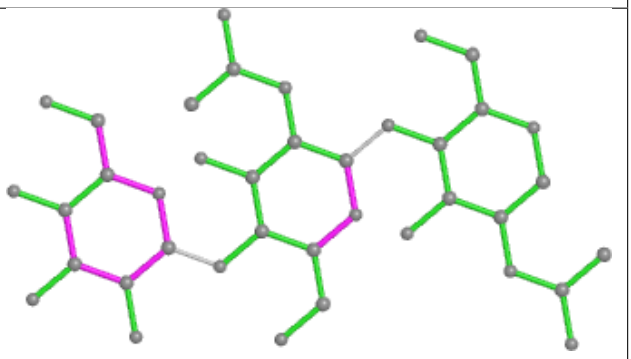


Rings

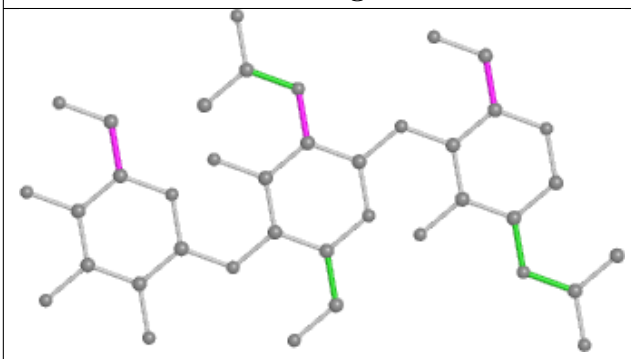
Oligosaccharide Chain O



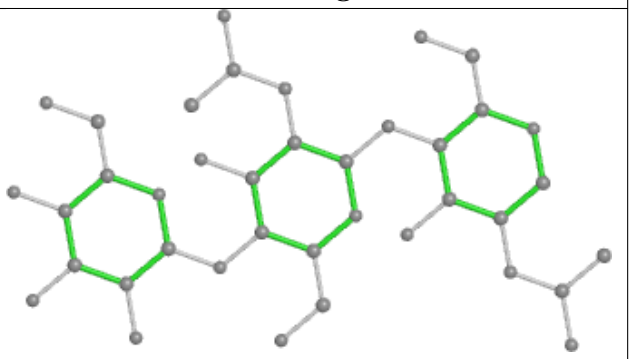
Bond lengths



Bond angles

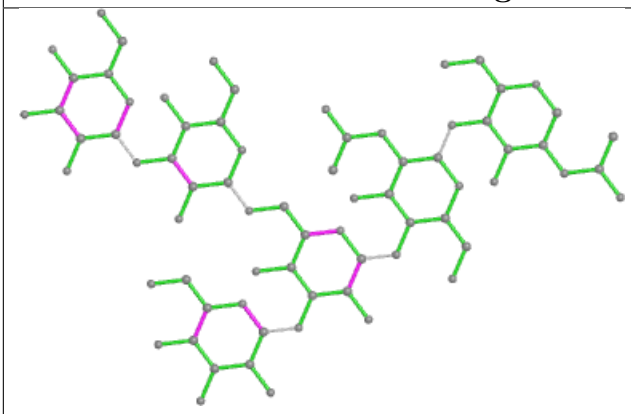


Torsions

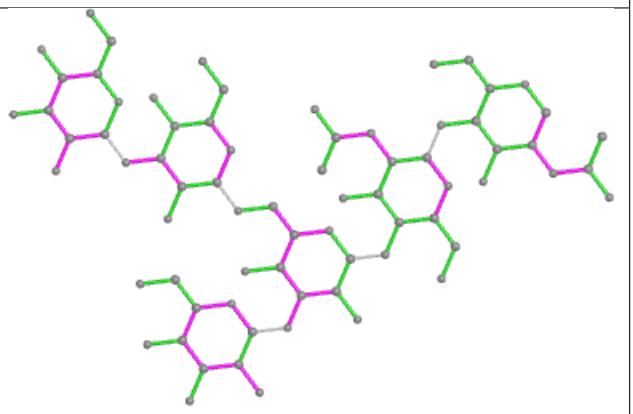


Rings

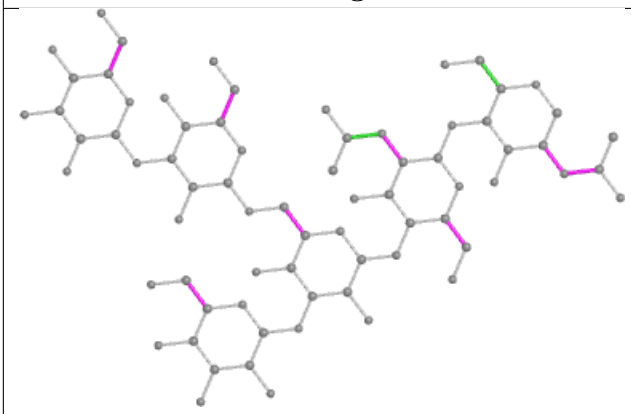
Oligosaccharide Chain R



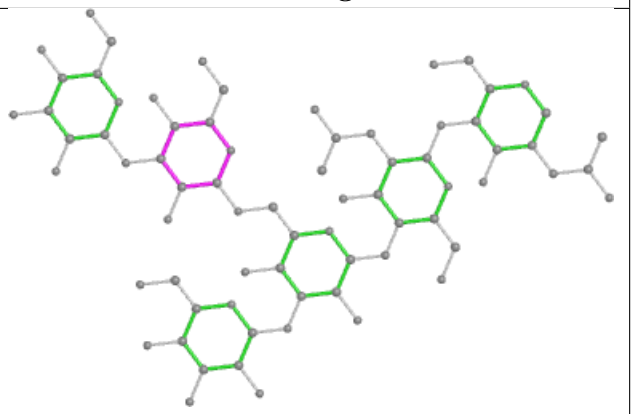
Bond lengths



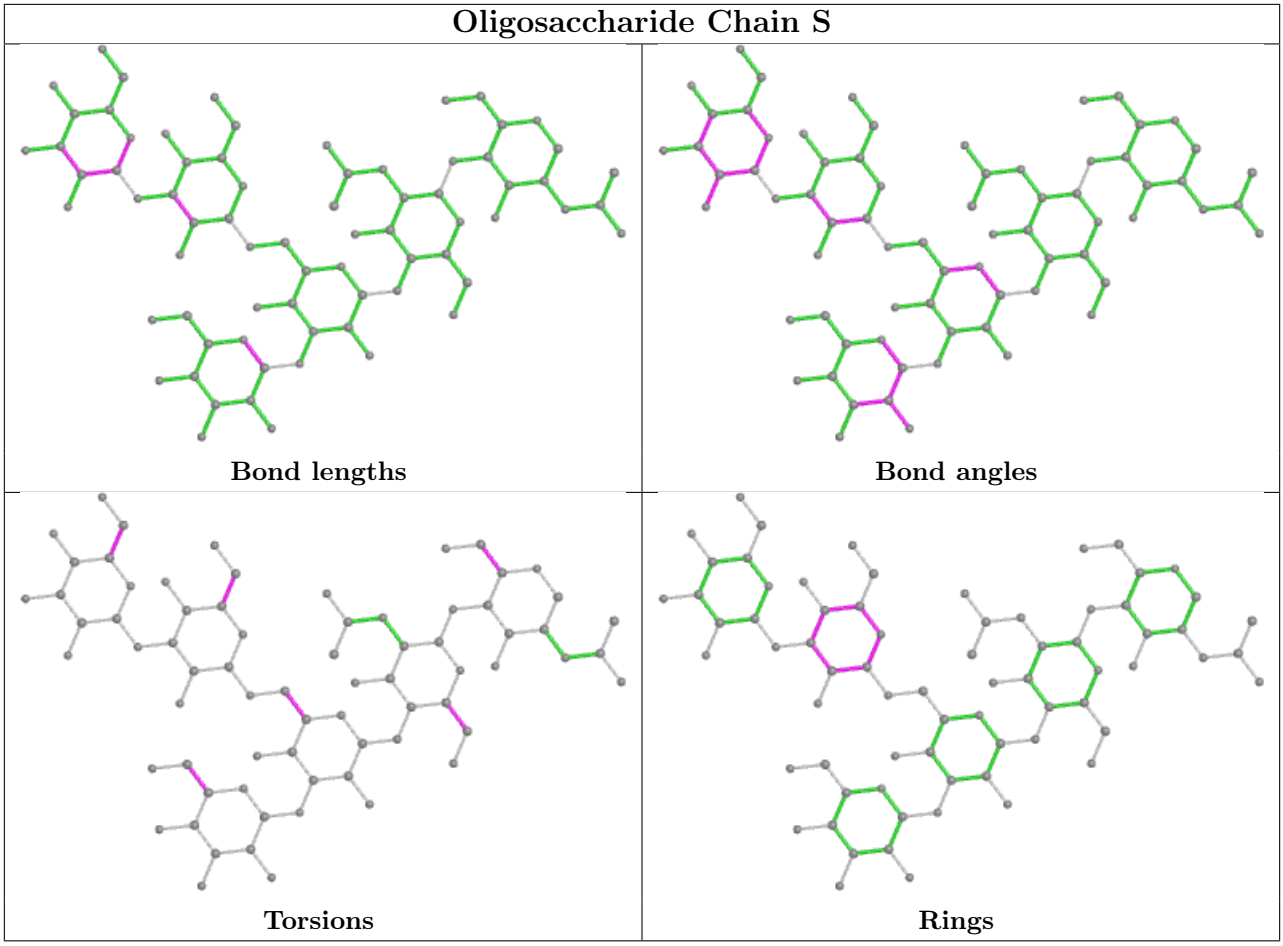
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
10	NAG	G	401	3	14,14,15	0.67	1 (7%)	17,19,21	0.49	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
10	NAG	G	401	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	401	NAG	O5-C1	-2.19	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	G	401	NAG	O5-C5-C6-O6

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, 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	A	230/244 (94%)	-0.01	3 (1%) 77 59	31, 54, 92, 138	0
1	C	230/244 (94%)	0.38	9 (3%) 39 20	61, 97, 137, 157	0
1	H	229/244 (93%)	-0.04	1 (0%) 92 84	38, 61, 98, 117	0
2	B	213/215 (99%)	-0.02	2 (0%) 84 69	33, 59, 92, 123	0
2	D	214/215 (99%)	0.04	0 100 100	54, 78, 109, 140	0
2	L	214/215 (99%)	0.08	6 (2%) 53 30	32, 61, 122, 158	0
3	E	176/211 (83%)	0.35	7 (3%) 38 19	38, 78, 134, 177	0
3	F	179/211 (84%)	0.27	6 (3%) 45 24	36, 86, 148, 171	0
3	G	187/211 (88%)	0.52	18 (9%) 8 2	39, 80, 150, 168	0
All	All	1872/2010 (93%)	0.16	52 (2%) 53 30	31, 71, 131, 177	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	111	SER	6.6
3	G	268	PRO	6.2
3	E	111	SER	6.1
3	F	202	GLY	6.1
1	A	131	THR	4.5

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

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

6.3 Carbohydrates

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
5	MAN	J	4	11/12	0.44	0.67	127,132,158,162	0
5	BMA	J	3	11/12	0.51	0.36	113,122,147,148	0
8	MAN	R	6	11/12	0.54	0.52	132,135,162,165	0
7	BMA	N	3	11/12	0.55	0.48	134,137,163,164	0
8	MAN	S	5	11/12	0.60	0.36	121,125,149,152	0
6	MAN	K	6	11/12	0.62	0.50	112,119,142,144	0
7	BMA	O	3	11/12	0.64	0.31	113,121,145,146	0
6	MAN	K	4	11/12	0.67	0.23	95,104,125,125	0
6	MAN	Q	6	11/12	0.68	0.24	124,127,151,153	0
7	NAG	N	2	14/15	0.69	0.37	120,138,162,166	0
7	NAG	O	2	14/15	0.71	0.39	128,133,160,160	0
6	MAN	K	5	11/12	0.72	0.29	103,108,128,129	0
6	MAN	P	5	11/12	0.73	0.24	92,103,124,125	0
6	MAN	Q	7	11/12	0.75	0.28	121,130,156,157	0
7	NAG	N	1	14/15	0.75	0.50	127,136,159,163	0
6	MAN	T	6	11/12	0.76	0.26	86,93,110,113	0
8	MAN	S	4	11/12	0.76	0.23	107,114,137,137	0
6	MAN	P	6	11/12	0.76	0.31	101,107,128,130	0
6	MAN	Q	5	11/12	0.77	0.30	130,136,163,167	0
6	MAN	M	5	11/12	0.77	0.34	68,80,96,98	0
5	MAN	J	5	11/12	0.77	0.34	107,112,133,134	0
4	NAG	I	2	14/15	0.77	0.47	101,109,130,133	0
5	NAG	J	2	14/15	0.78	0.28	94,108,126,130	0
8	BMA	R	3	11/12	0.80	0.24	121,126,152,154	0
8	NAG	S	1	14/15	0.81	0.33	109,129,156,156	0
8	MAN	R	4	11/12	0.81	0.28	121,126,150,151	0
8	NAG	R	2	14/15	0.81	0.34	107,115,136,138	0
8	NAG	R	1	14/15	0.83	0.25	87,94,111,113	0
8	MAN	R	5	11/12	0.83	0.37	121,127,151,152	0
4	NAG	I	1	14/15	0.84	0.34	94,110,133,133	0
6	MAN	T	7	11/12	0.84	0.18	87,97,115,118	0
7	NAG	O	1	14/15	0.87	0.23	109,119,139,143	0
6	MAN	T	5	11/12	0.87	0.24	93,101,122,123	0
6	MAN	M	7	11/12	0.87	0.22	56,67,80,82	0
6	NAG	Q	2	14/15	0.89	0.20	79,88,101,105	0
6	BMA	Q	3	11/12	0.89	0.21	96,104,122,126	0
6	MAN	Q	4	11/12	0.89	0.19	108,121,146,146	0
6	BMA	P	3	11/12	0.90	0.24	48,55,68,68	0
8	NAG	S	2	14/15	0.90	0.20	95,107,129,129	0
6	MAN	P	4	11/12	0.91	0.18	70,87,107,107	0

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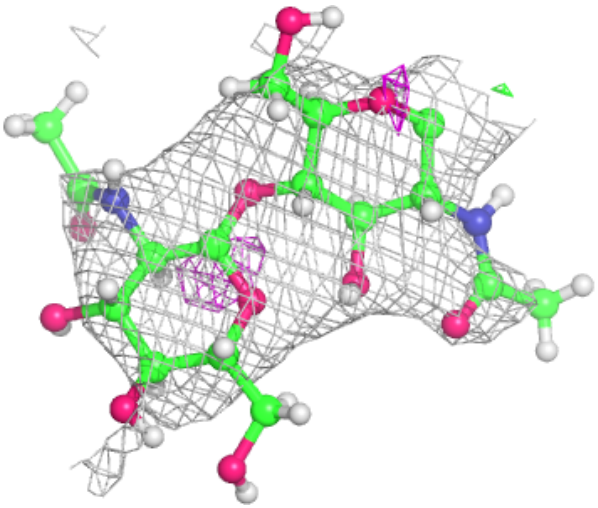
Continued from previous page...

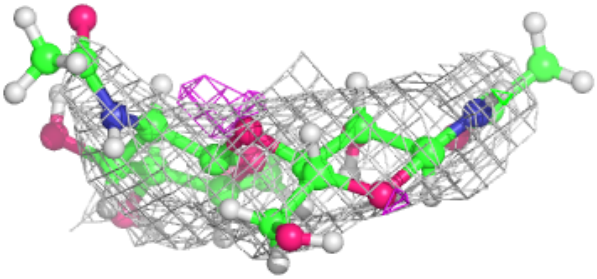
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	J	1	14/15	0.91	0.27	76,83,98,100	0
6	NAG	Q	1	14/15	0.92	0.22	82,87,102,105	0
6	NAG	M	1	14/15	0.92	0.20	45,56,66,66	0
6	NAG	P	2	14/15	0.92	0.20	55,67,80,80	0
6	NAG	T	1	14/15	0.92	0.22	50,60,72,72	0
6	MAN	T	4	11/12	0.92	0.18	77,82,98,99	0
6	NAG	K	2	14/15	0.92	0.24	79,98,116,116	0
6	NAG	K	1	14/15	0.93	0.16	88,96,115,117	0
6	BMA	K	3	11/12	0.93	0.23	60,75,89,91	0
6	NAG	P	1	14/15	0.93	0.22	68,84,95,101	0
8	BMA	S	3	11/12	0.93	0.20	88,95,118,118	0
6	MAN	M	4	11/12	0.93	0.23	62,67,78,81	0
6	BMA	T	3	11/12	0.93	0.20	61,71,82,86	0
8	MAN	S	6	11/12	0.93	0.18	79,87,105,106	0
6	NAG	M	2	14/15	0.94	0.19	40,48,58,64	0
6	MAN	K	7	11/12	0.95	0.22	41,50,58,65	0
6	MAN	M	6	11/12	0.95	0.28	70,79,91,96	0
6	NAG	T	2	14/15	0.96	0.17	49,59,69,71	0
6	MAN	P	7	11/12	0.96	0.19	34,42,51,54	0
6	BMA	M	3	11/12	0.97	0.20	43,49,63,63	0

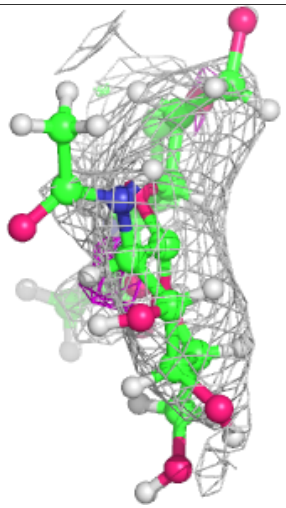
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

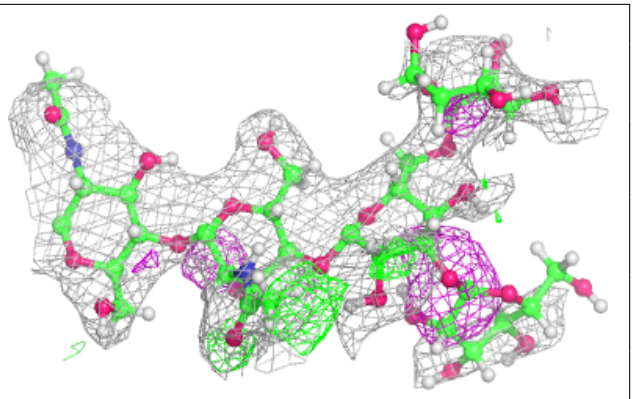


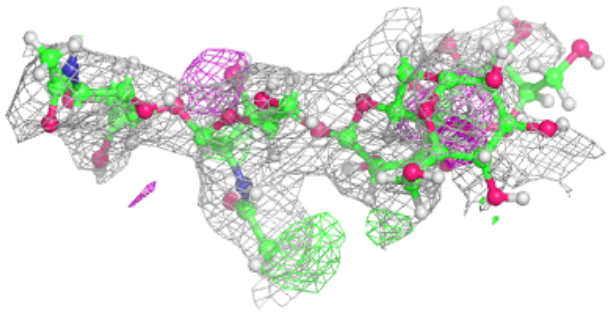


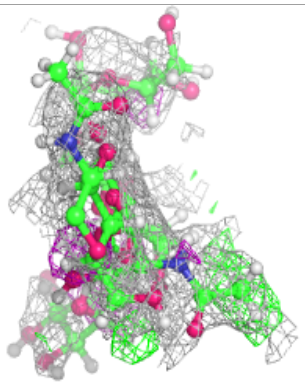


Electron density around Chain J:

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

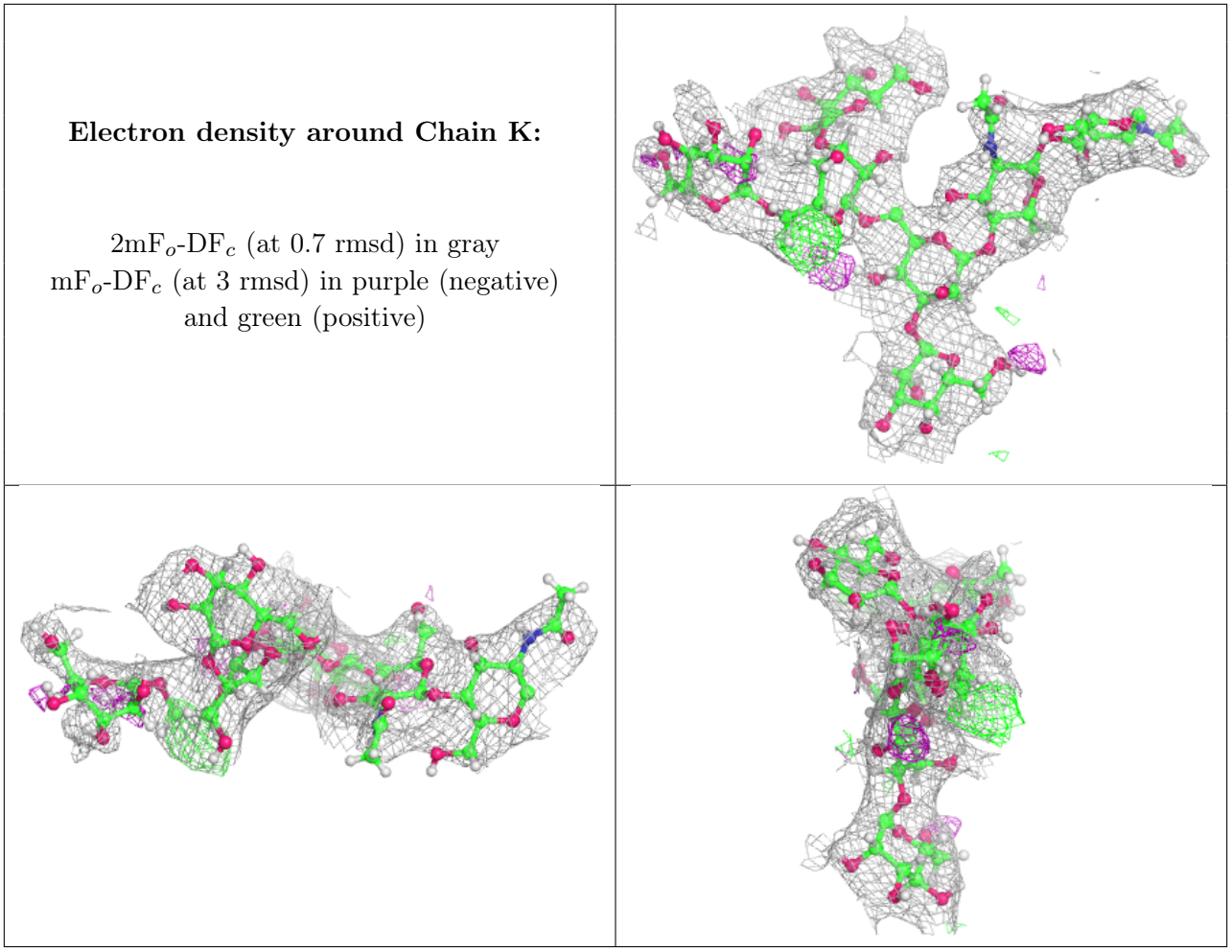






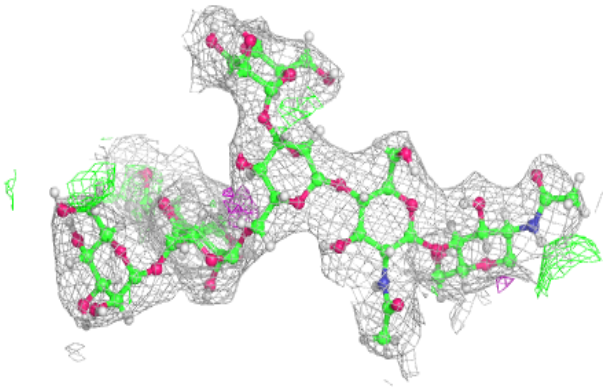
Electron density around Chain K:

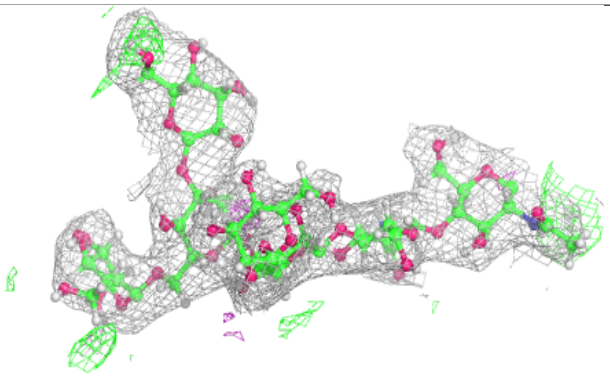
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

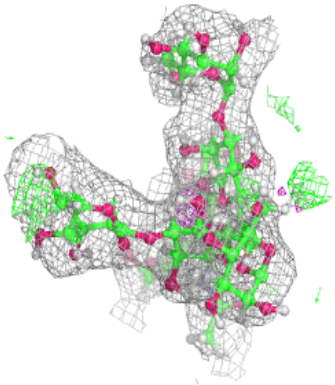


Electron density around Chain M:

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

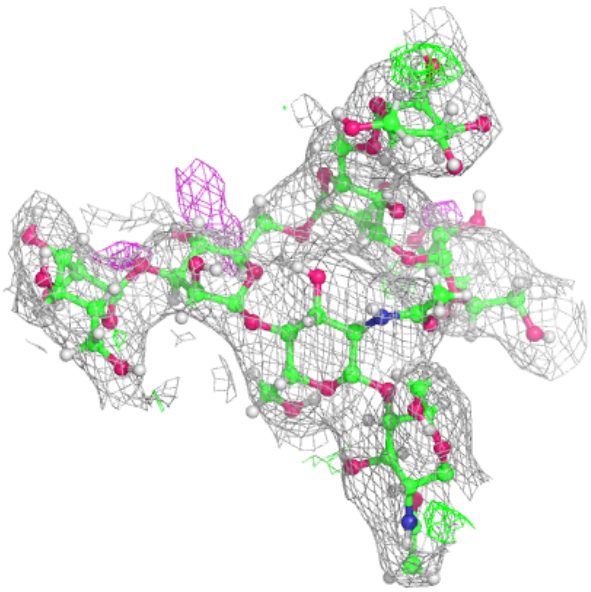


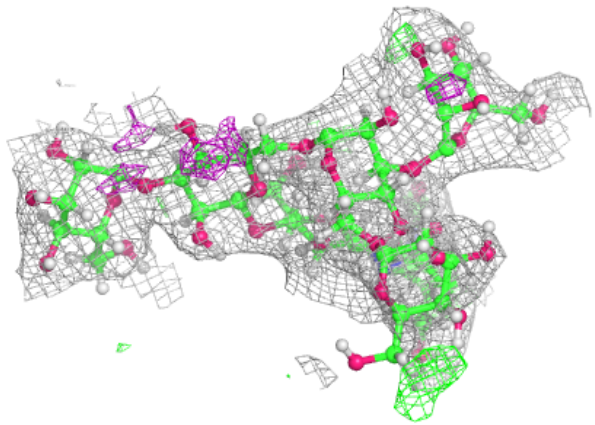


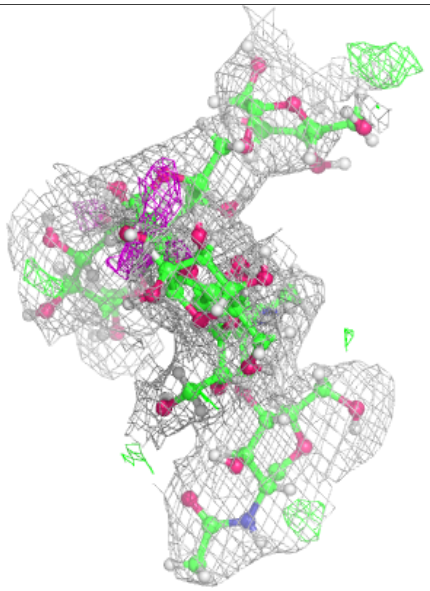


Electron density around Chain P:

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

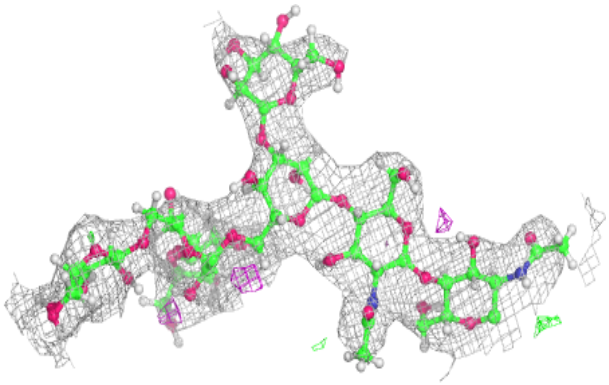


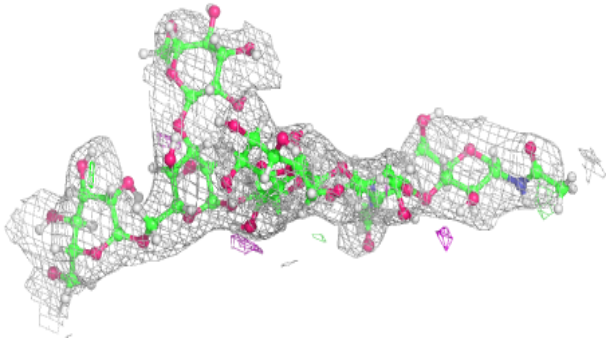


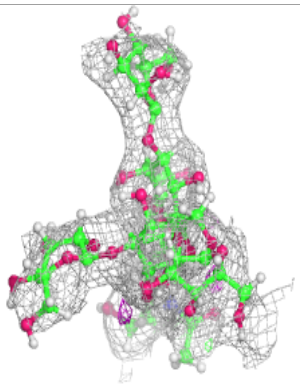


Electron density around Chain Q:

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

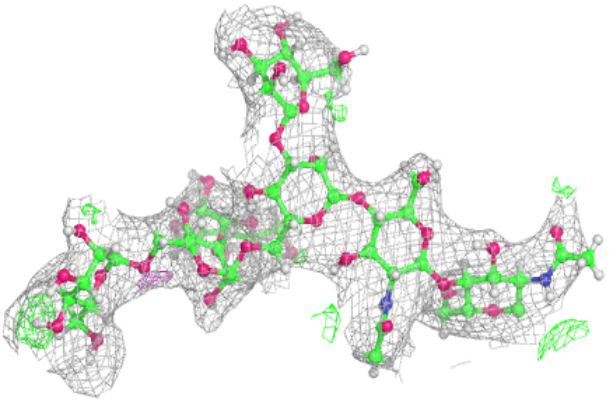


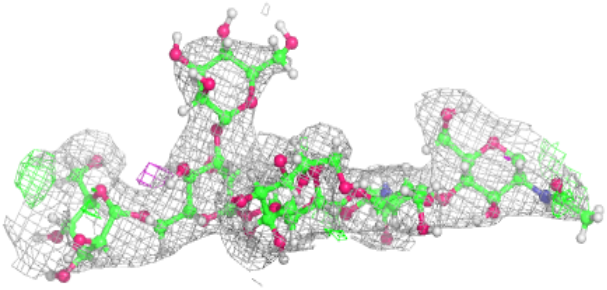


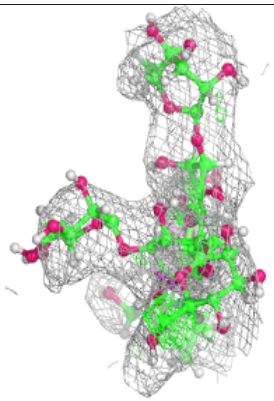


Electron density around Chain T:

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

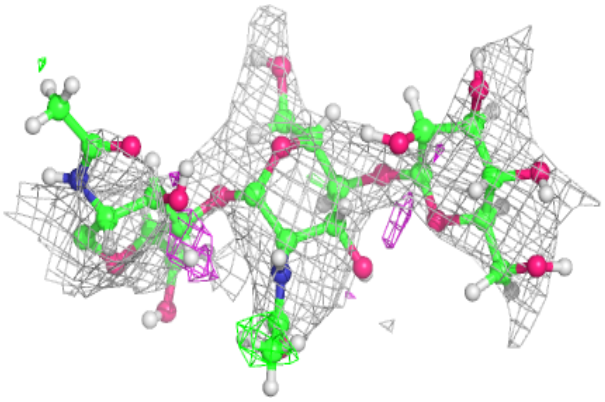


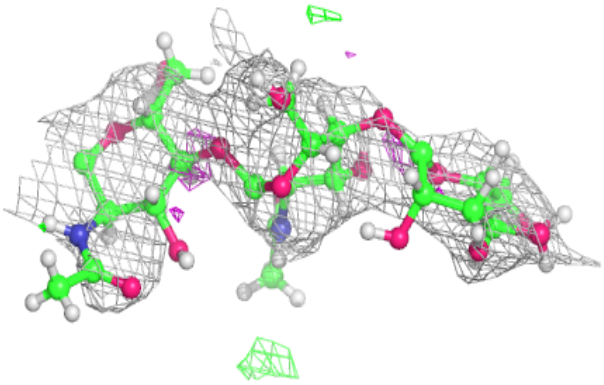


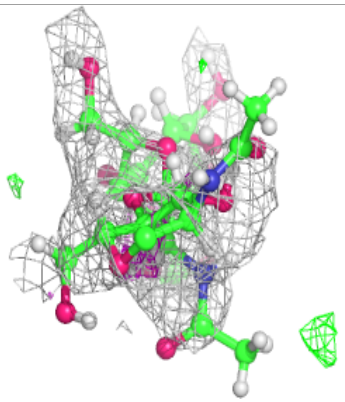


Electron density around Chain N:

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

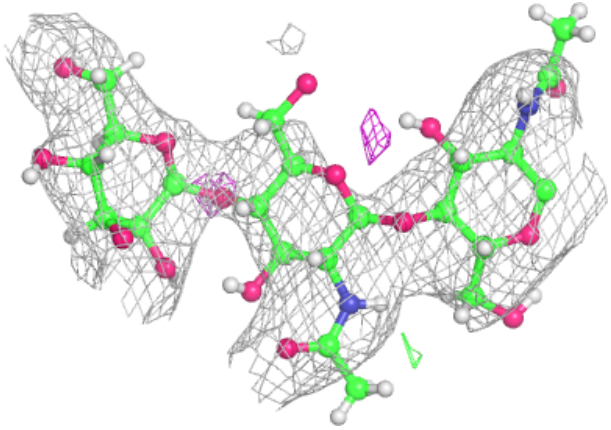


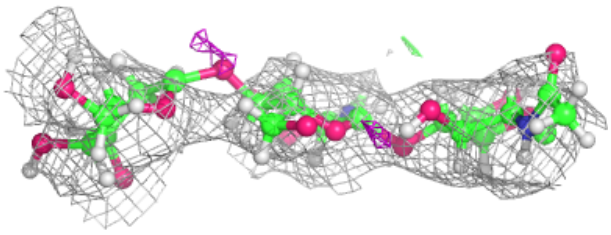


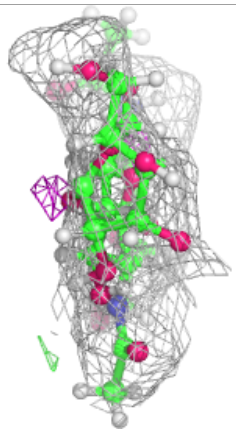


Electron density around Chain O:

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

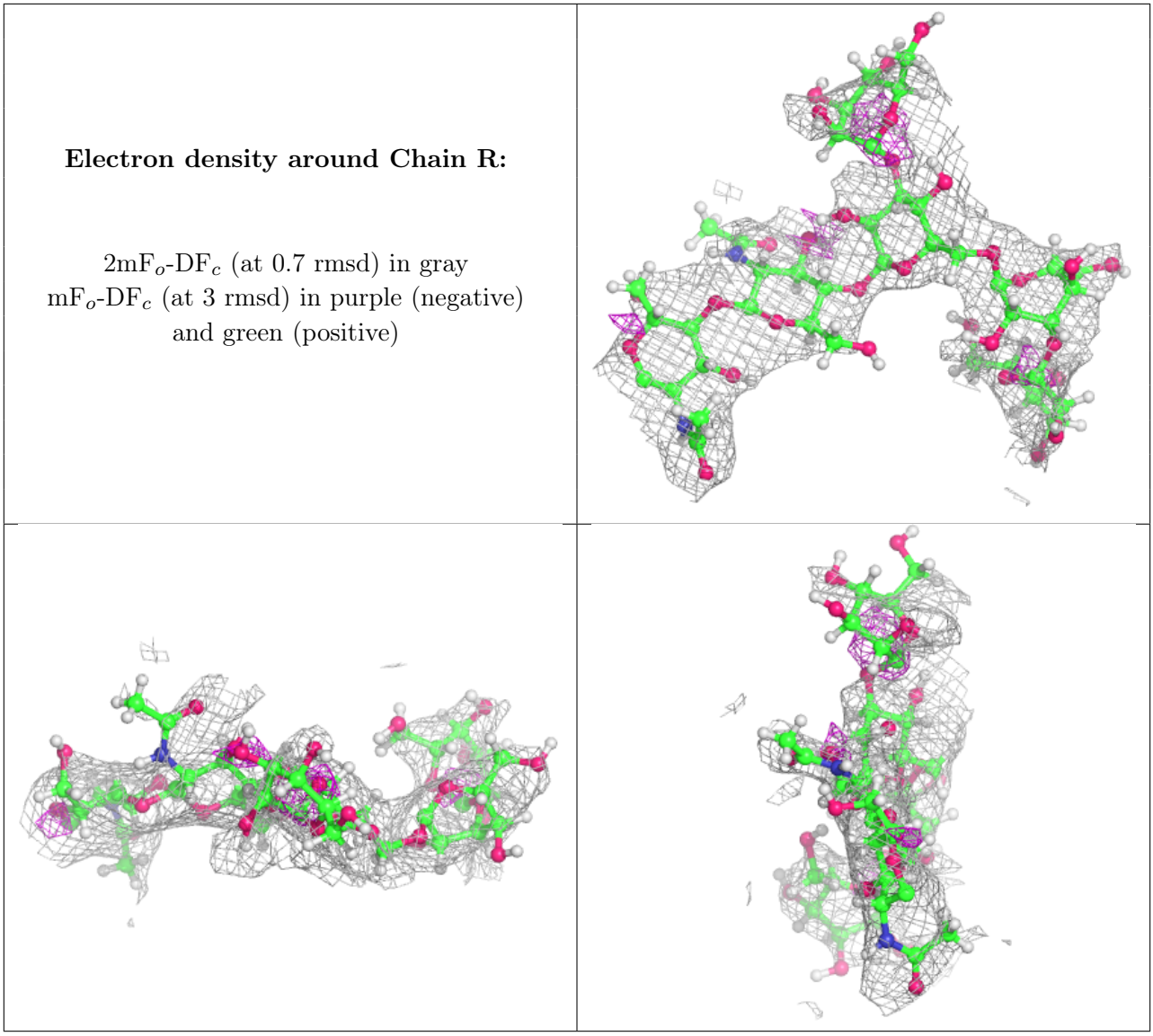






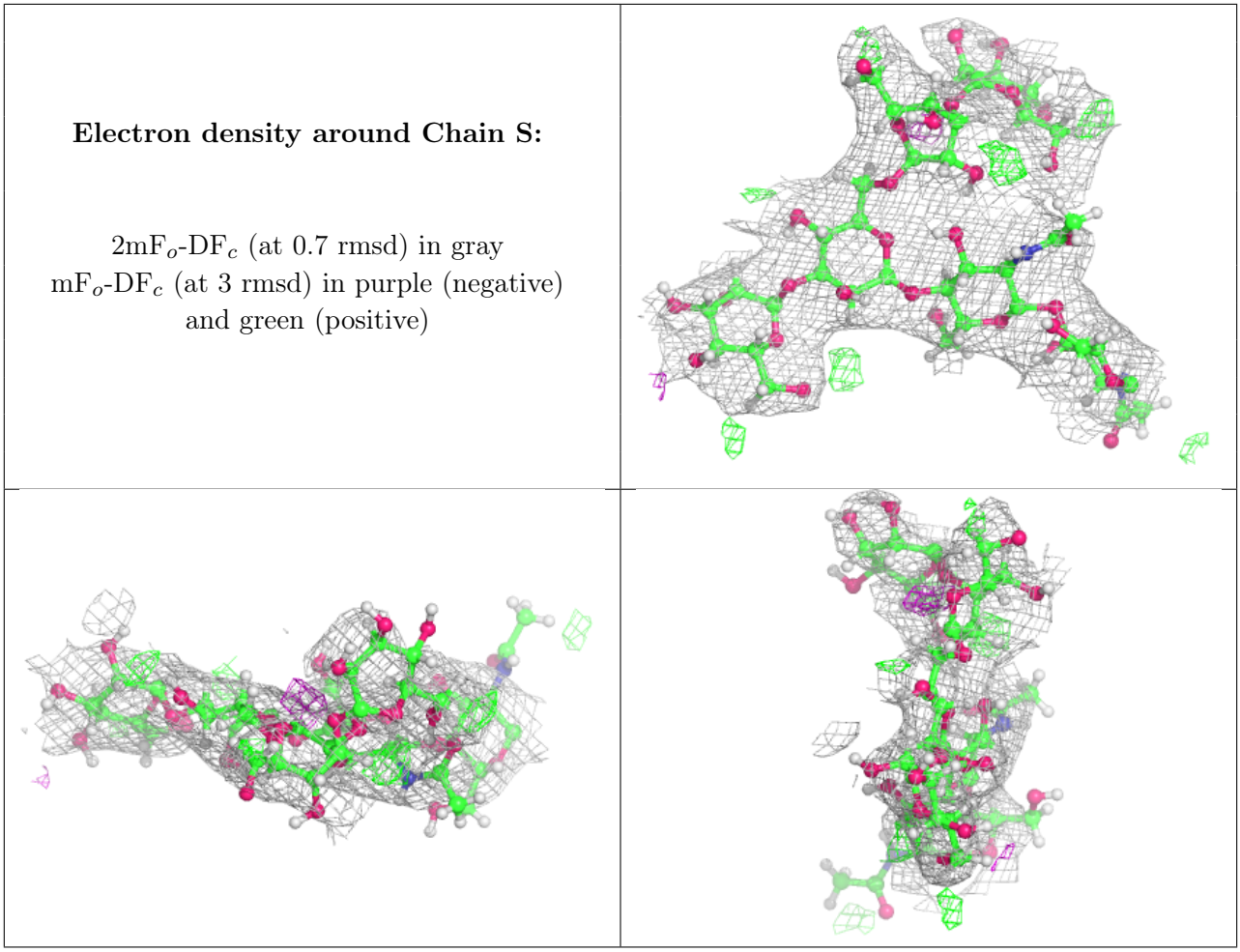
Electron density around Chain R:

$2mF_o$-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 S:

$2mF_o$-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
10	NAG	G	401	14/15	0.70	0.35	104,114,137,137	0
9	ZN	E	422	1/1	0.75	0.46	216,216,216,216	1
9	ZN	F	421	1/1	0.89	0.23	67,67,67,67	1
9	ZN	G	421	1/1	0.92	0.33	109,109,109,109	1

6.5 Other polymers

There are no such residues in this entry.