Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 02:34 PM EDT

PDB ID	:	4HG4
Title	:	Crystal structure of Fab 2G1 in complex with a H2N2 influenza virus hemagglutinin
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2012-10-06
Resolution	:	3.20 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 (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 (i)) were used in the production of this report:

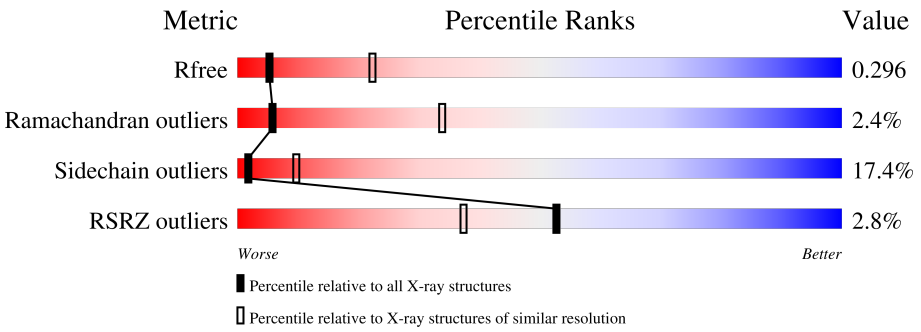
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	327	83% 15% •
1	B	327	% 81% 16% • •
1	C	327	% 83% 16% •
1	D	327	% 83% 16% •
1	E	327	83% 16% •
1	F	327	% 82% 17% • •
1	G	327	2% 83% 16% •

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Mol	Chain	Length	Quality of chain
1	H	327	83% 16%
1	I	327	83% 16%
2	a	174	2% 83% 15%
2	b	174	3% 81% 14%
2	c	174	2% 90% 8%
2	d	174	5% 91% 8%
2	e	174	3% 90% 9%
2	f	174	2% 89% 9%
2	g	174	3% 91% 7%
2	h	174	84% 11%
2	i	174	% 88% 10%
3	J	223	5% 39% 12% 48%
3	L	223	76% 18% 5%
3	N	223	77% 22%
3	P	223	7% 58% 13% 28%
3	R	223	3% 75% 20%
3	T	223	12% 76% 19%
3	V	223	10% 43% 9% 48%
3	X	223	6% 57% 15% 26%
3	Z	223	4% 57% 17% 25%
4	K	214	4% 32% 16% 50%
4	M	214	84% 15%
4	O	214	80% 20%
4	Q	214	9% 57% 16% 27%
4	S	214	2% 78% 20%

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Mol	Chain	Length	Quality of chain
4	U	214	5% 74% 24%
4	W	214	38% 10% 51%
4	Y	214	40% 10% 49%
4	z	214	3% 42% 13% 44%
5	j	2	50% 50%
5	k	2	100%
5	m	2	50% 50%
5	n	2	50% 50%
5	o	2	100%
5	q	2	50% 50%
5	r	2	100%
5	s	2	50% 50%
5	t	2	100%
6	l	3	33% 67%
6	p	3	100%

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
5	NAG	s	2	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 58742 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2531	1593	438	485	15	0	0	0
1	B	319	2503	1577	433	478	15	0	0	0
1	C	324	2539	1599	439	486	15	0	0	0
1	D	324	2539	1599	439	486	15	0	0	0
1	E	323	2531	1593	438	485	15	0	0	0
1	F	324	2539	1599	439	486	15	0	0	0
1	G	324	2539	1599	439	486	15	0	0	0
1	H	325	2548	1604	440	489	15	0	0	0
1	I	324	2539	1599	439	486	15	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP Q67085
B	9	PRO	-	expression tag	UNP Q67085
C	9	PRO	-	expression tag	UNP Q67085
D	9	PRO	-	expression tag	UNP Q67085
E	9	PRO	-	expression tag	UNP Q67085
F	9	PRO	-	expression tag	UNP Q67085
G	9	PRO	-	expression tag	UNP Q67085
H	9	PRO	-	expression tag	UNP Q67085
I	9	PRO	-	expression tag	UNP Q67085

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	a	171	1387	866	236	276	9	0	0	0
2	b	167	1345	836	229	271	9	0	0	0
2	c	172	1396	871	237	279	9	0	0	0
2	d	172	1396	871	237	279	9	0	0	0
2	e	172	1396	871	237	279	9	0	0	0
2	f	172	1396	871	237	279	9	0	0	0
2	g	172	1396	871	237	279	9	0	0	0
2	h	167	1355	845	231	270	9	0	0	0
2	i	172	1396	871	237	279	9	0	0	0

- Molecule 3 is a protein called Fab 2G1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	115	871	555	142	171	3	0	0	0
3	L	212	1578	1004	258	311	5	0	0	0
3	N	223	1648	1043	271	328	6	0	0	0
3	P	161	1207	770	195	239	3	0	0	0
3	R	214	1589	1010	260	314	5	0	0	0
3	T	213	1580	1005	259	311	5	0	0	0
3	V	117	883	564	144	172	3	0	0	0
3	X	164	1232	785	201	242	4	0	0	0
3	Z	167	1262	807	205	246	4	0	0	0

- Molecule 4 is a protein called Fab 2G1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	106	826	518	140	166	2	0	0	0
			Total	C	N	O	S			
4	M	214	1661	1037	282	337	5	0	0	0
			Total	C	N	O	S			
4	O	214	1661	1037	282	337	5	0	0	0
			Total	C	N	O	S			
4	Q	157	1217	760	206	248	3	0	0	0
			Total	C	N	O	S			
4	S	211	1642	1027	279	332	4	0	0	0
			Total	C	N	O	S			
4	U	211	1642	1027	279	332	4	0	0	0
			Total	C	N	O	S			
4	W	105	818	512	139	165	2	0	0	0
			Total	C	N	O	S			
4	Y	109	853	534	147	170	2	0	0	0
			Total	C	N	O	S			
4	z	119	915	568	155	190	2	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	j	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	k	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	m	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	n	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	o	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	q	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	r	2	28	16	2	10	0	0	0
			Total	C	N	O			
5	s	2	28	16	2	10	0	0	0

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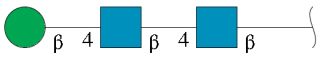
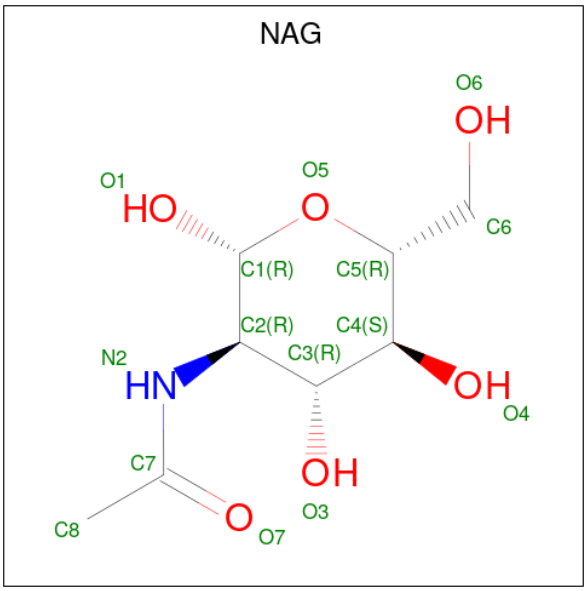
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	t	2	28	16	2	10	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	l	3	39	22	2	15	0	0	0
			Total	C	N	O			
6	p	3	39	22	2	15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	E	1	14	8	1	5	0	0

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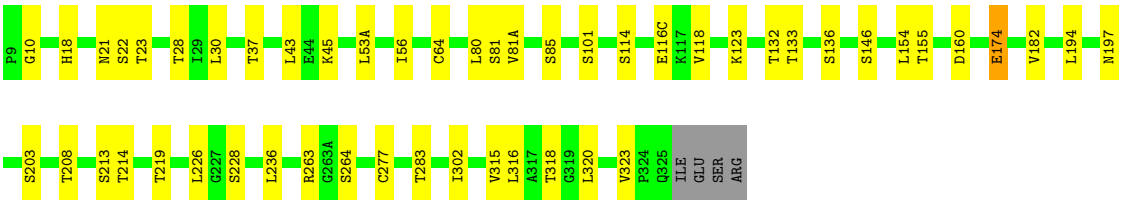
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	F	1	14	8	1	5	0	0

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.

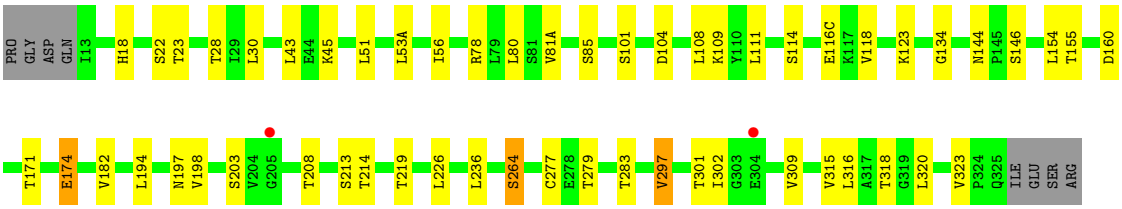
• Molecule 1: Hemagglutinin HA1

Chain A:



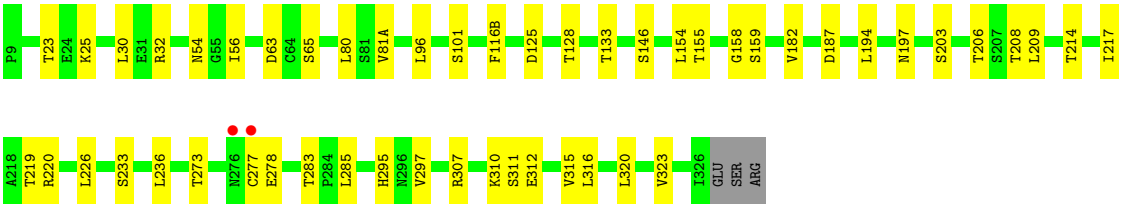
• Molecule 1: Hemagglutinin HA1

Chain B:



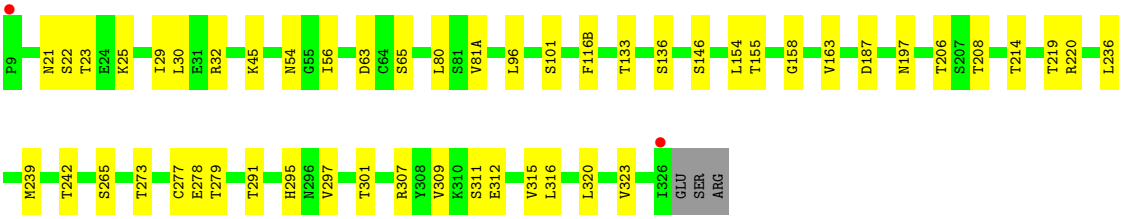
• Molecule 1: Hemagglutinin HA1

Chain C:



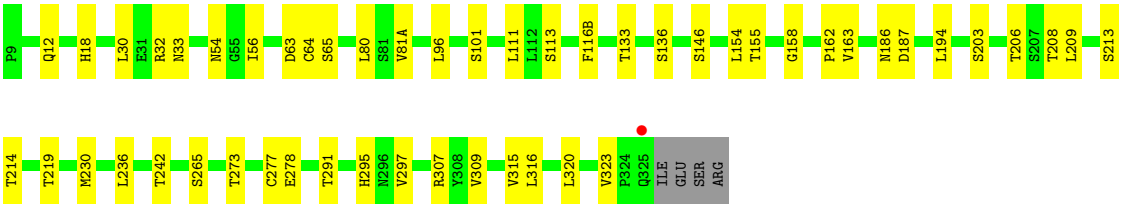
• Molecule 1: Hemagglutinin HA1

Chain D:



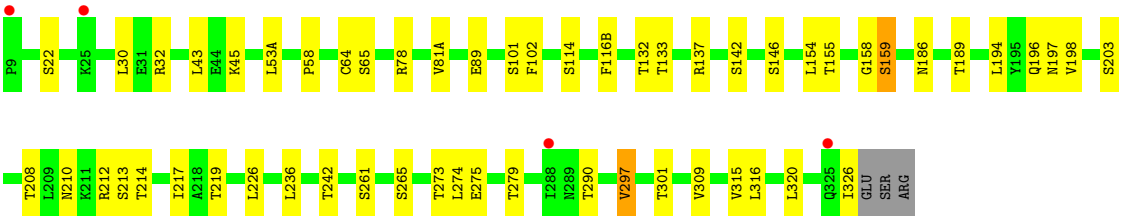
• Molecule 1: Hemagglutinin HA1

Chain E:



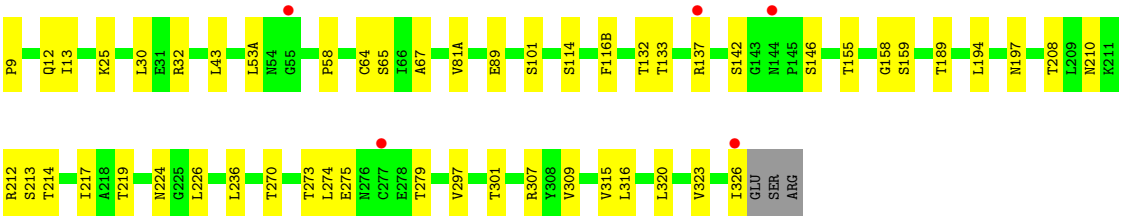
• Molecule 1: Hemagglutinin HA1

Chain F:



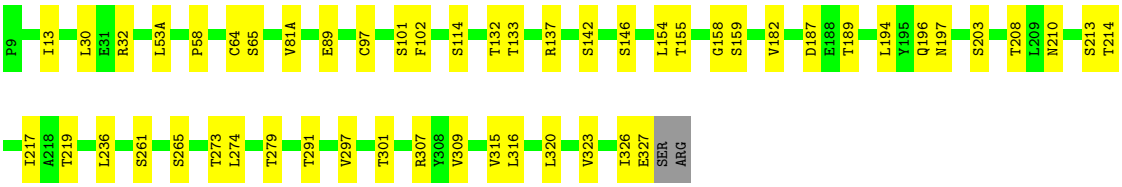
• Molecule 1: Hemagglutinin HA1

Chain G:



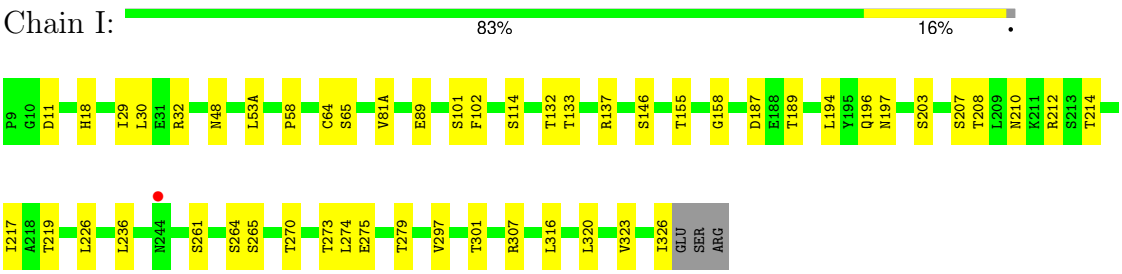
• Molecule 1: Hemagglutinin HA1

Chain H:



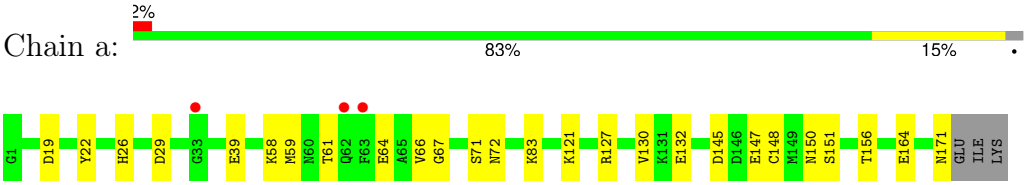
• Molecule 1: Hemagglutinin HA1

Chain I:



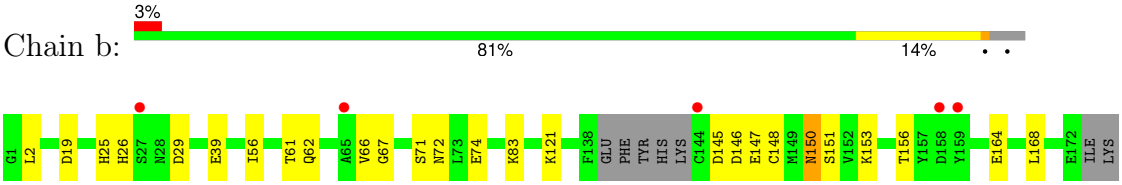
• Molecule 2: Hemagglutinin HA2

Chain a:



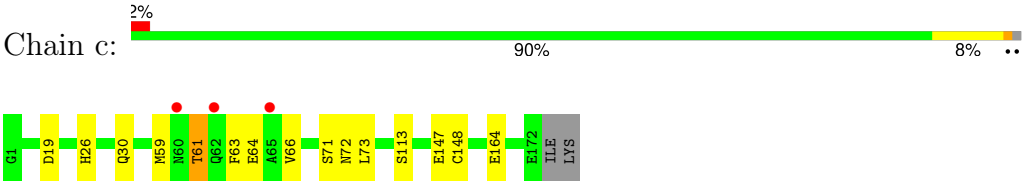
• Molecule 2: Hemagglutinin HA2

Chain b:



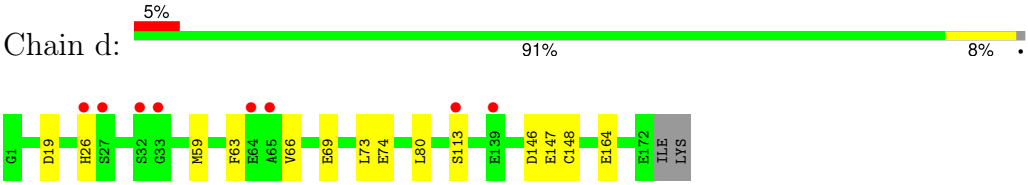
• Molecule 2: Hemagglutinin HA2

Chain c:



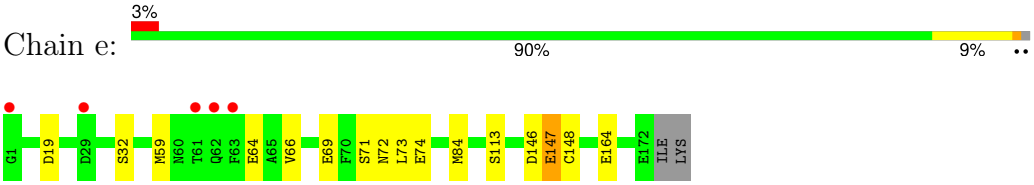
• Molecule 2: Hemagglutinin HA2

Chain d:



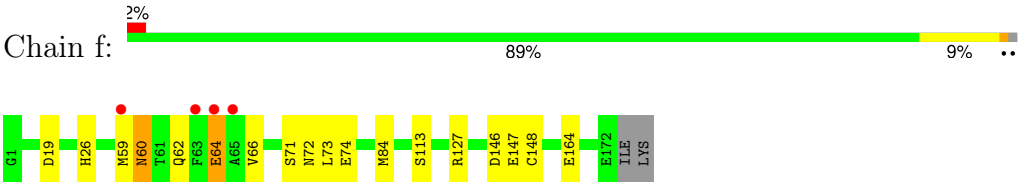
• Molecule 2: Hemagglutinin HA2

Chain e:



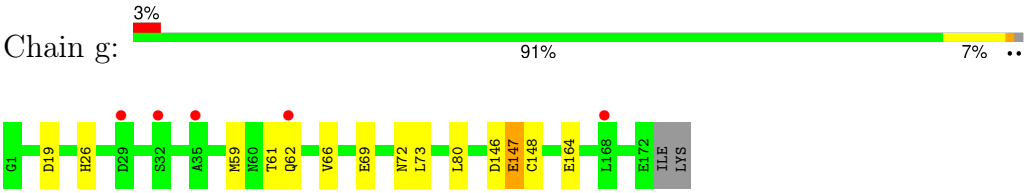
• Molecule 2: Hemagglutinin HA2

Chain f:



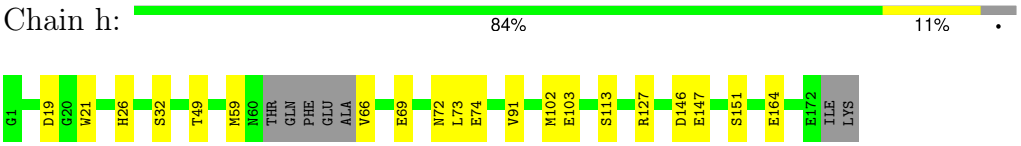
• Molecule 2: Hemagglutinin HA2

Chain g:



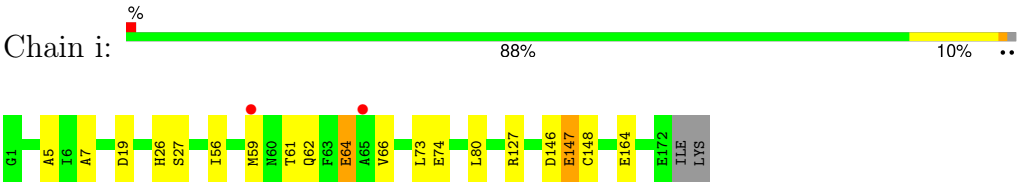
• Molecule 2: Hemagglutinin HA2

Chain h:



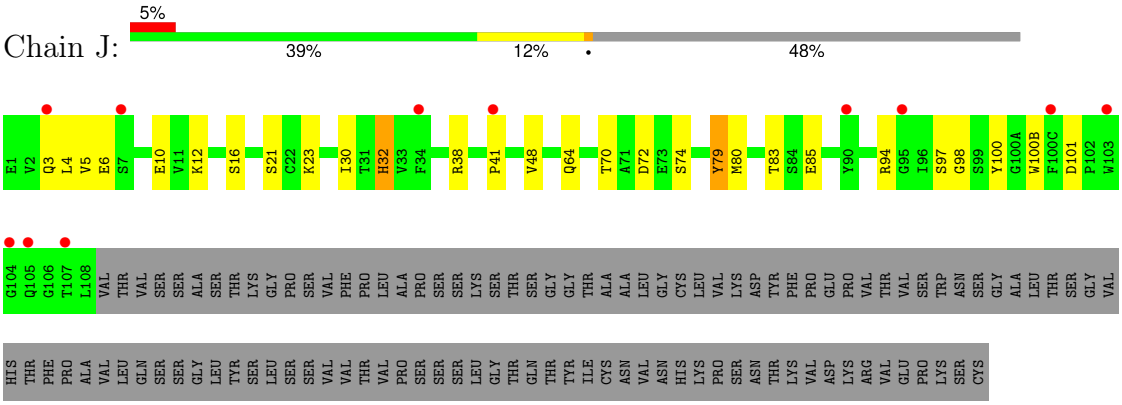
• Molecule 2: Hemagglutinin HA2

Chain i:



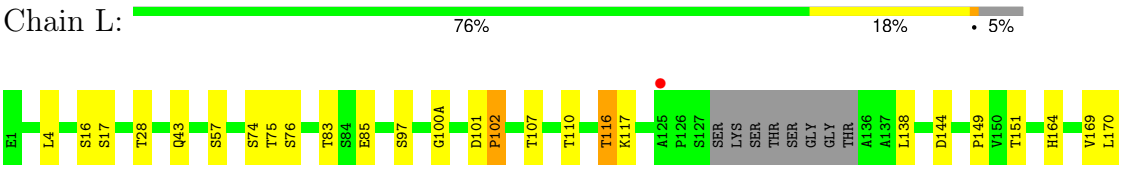
• Molecule 3: Fab 2G1 heavy chain

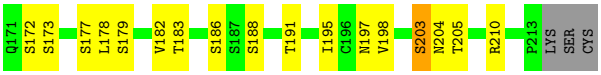
Chain J:



• Molecule 3: Fab 2G1 heavy chain

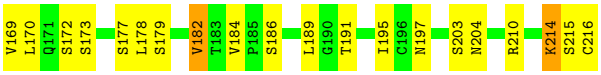
Chain L:





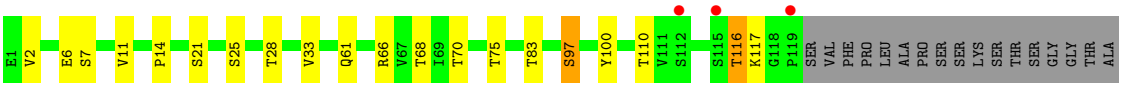
• Molecule 3: Fab 2G1 heavy chain

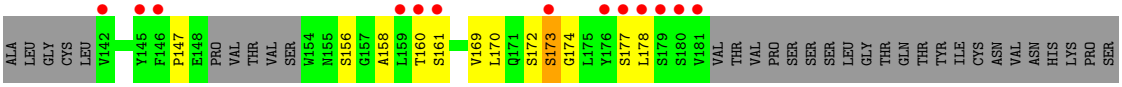
Chain N:



• Molecule 3: Fab 2G1 heavy chain

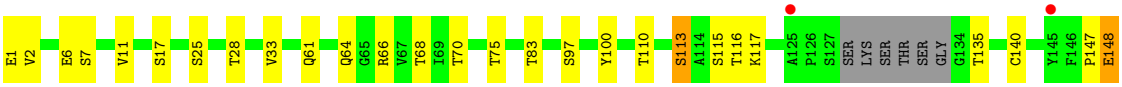
Chain P:

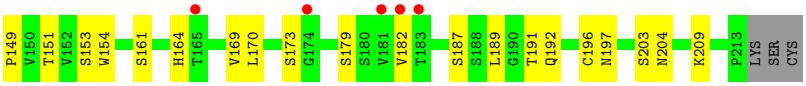




• Molecule 3: Fab 2G1 heavy chain

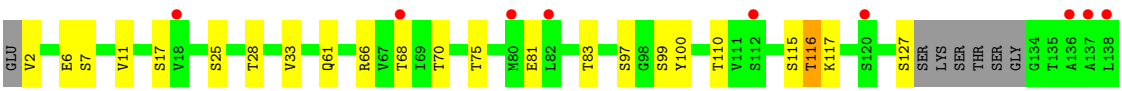
Chain R:

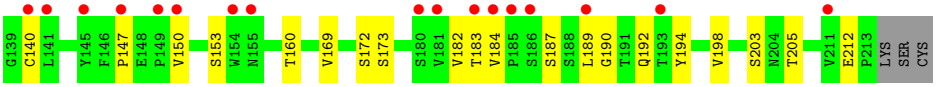




• Molecule 3: Fab 2G1 heavy chain

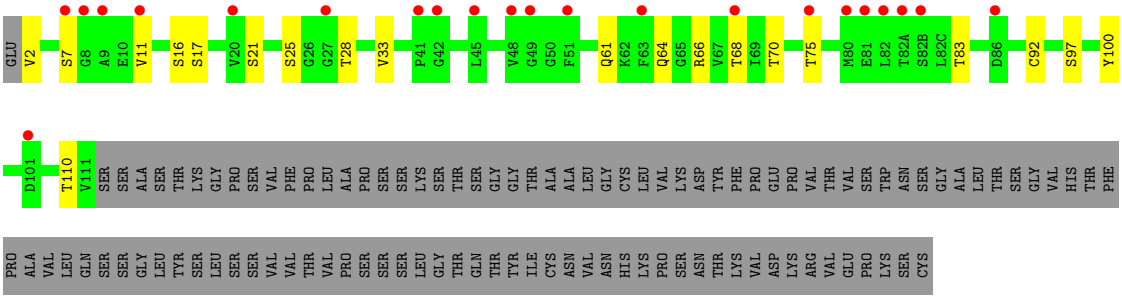
Chain T:





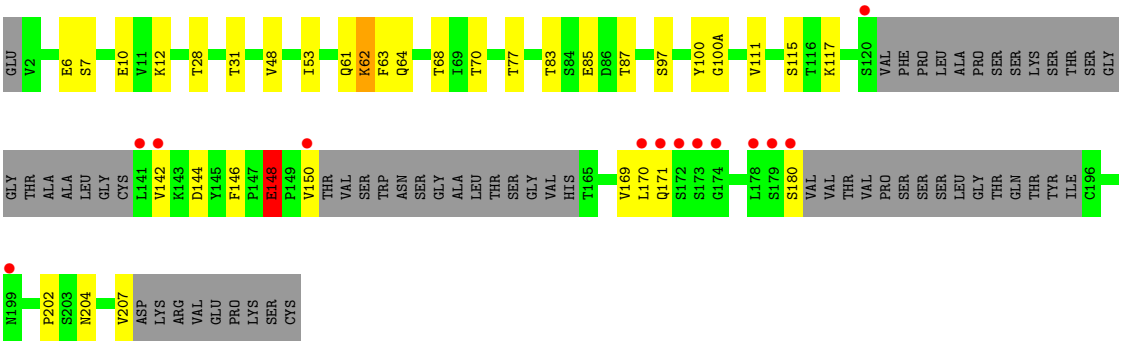
• Molecule 3: Fab 2G1 heavy chain

Chain V: 10% 43% 9% 48%



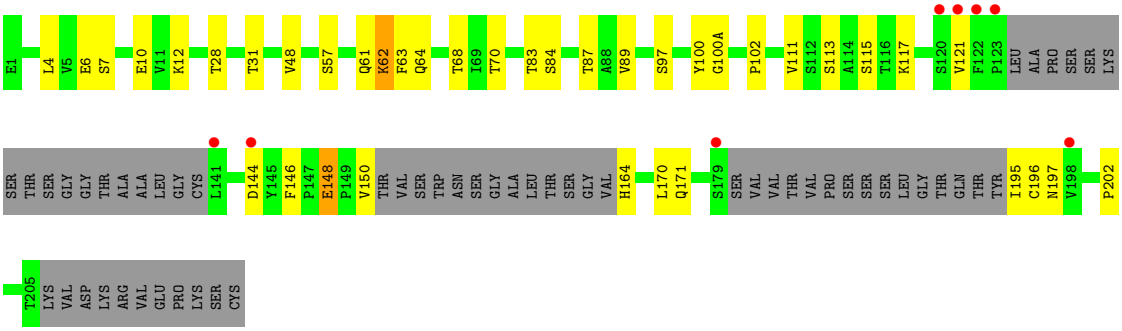
- Molecule 3: Fab 2G1 heavy chain

Chain X: 6% 57% 15% 26%



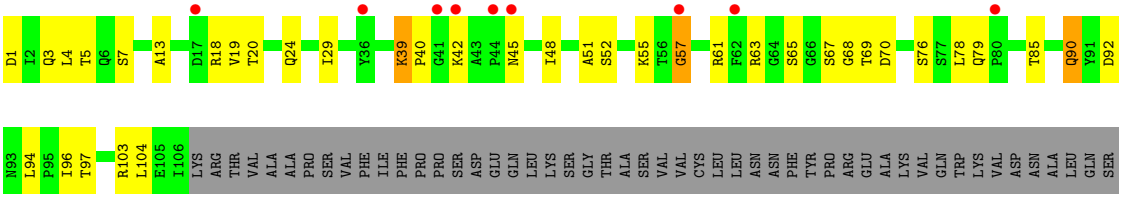
- Molecule 3: Fab 2G1 heavy chain

Chain Z: 4% 57% 17% • 25%



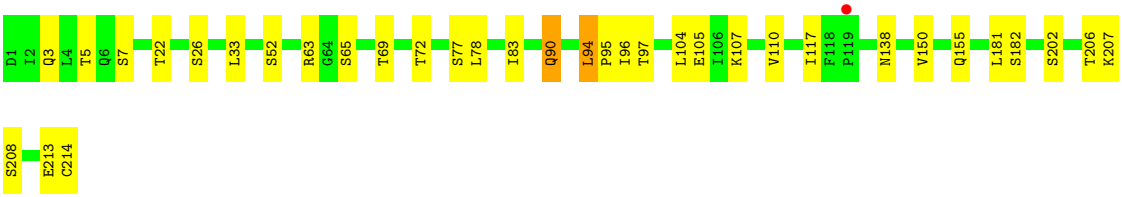
- Molecule 4: Fab 2G1 light chain

Chain K: 4% 32% 16% • 50%



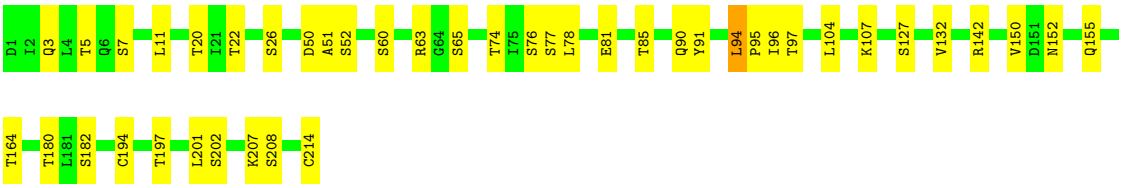
• Molecule 4: Fab 2G1 light chain

Chain M:



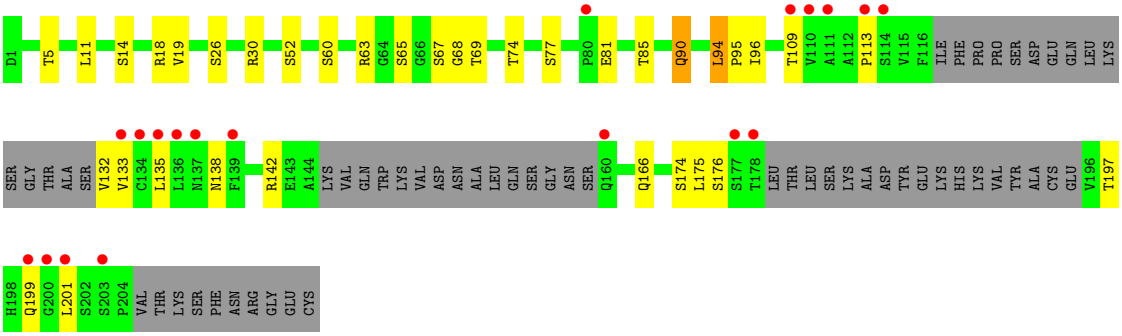
• Molecule 4: Fab 2G1 light chain

Chain O:



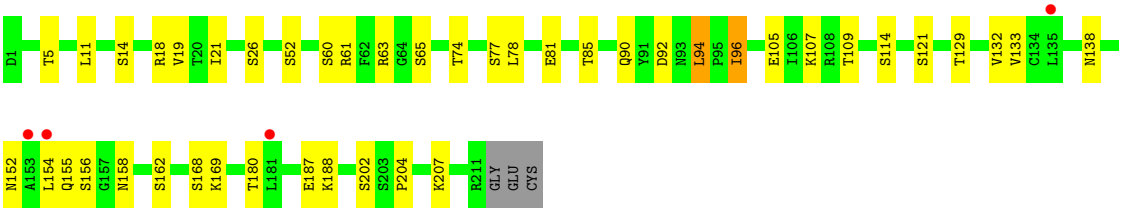
• Molecule 4: Fab 2G1 light chain

Chain Q:



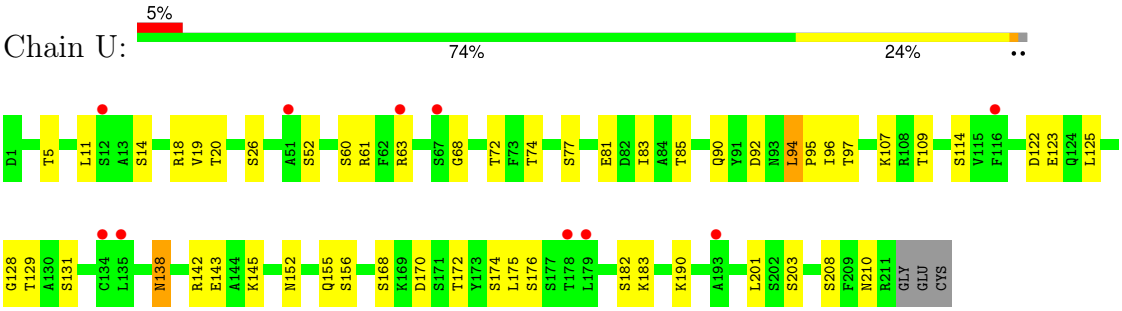
• Molecule 4: Fab 2G1 light chain

Chain S:



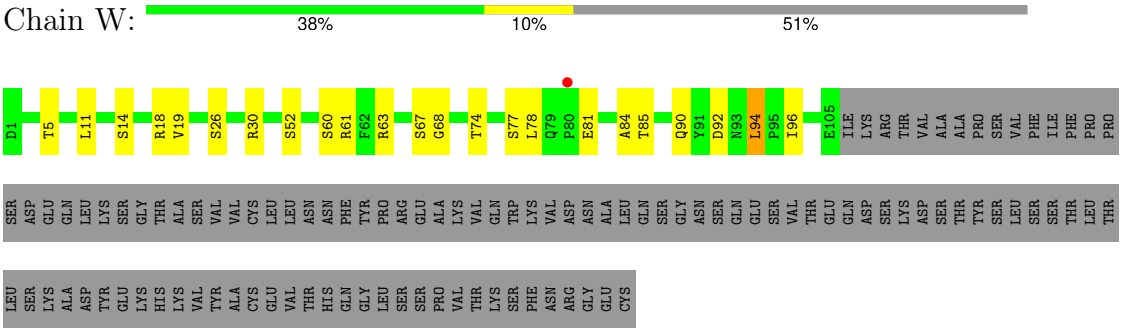
• Molecule 4: Fab 2G1 light chain

Chain U:



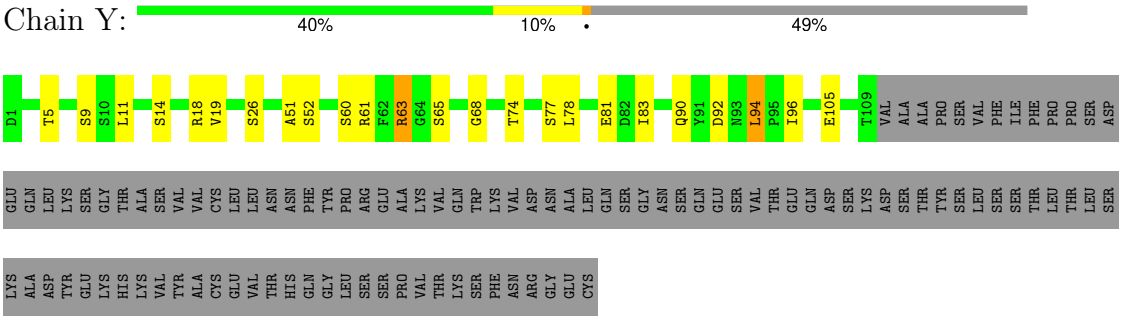
• Molecule 4: Fab 2G1 light chain

Chain W:



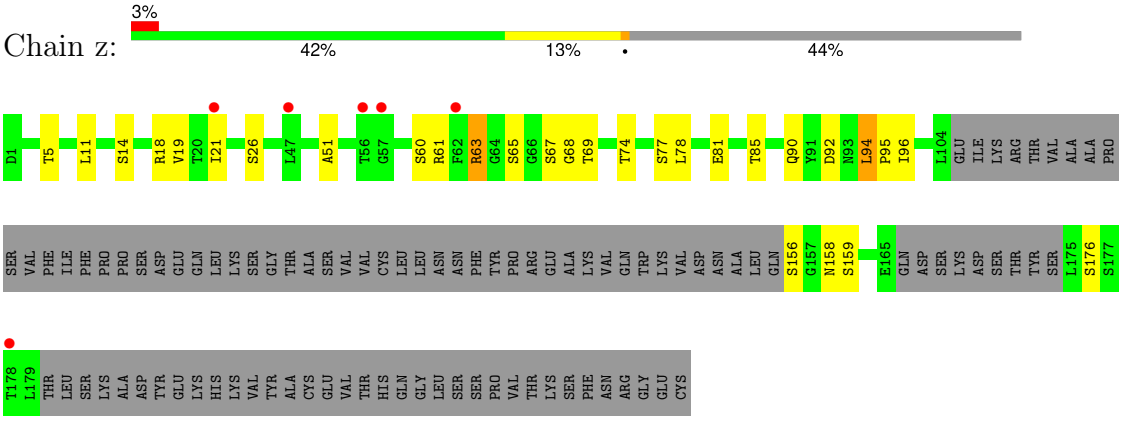
• Molecule 4: Fab 2G1 light chain

Chain Y:



• Molecule 4: Fab 2G1 light chain

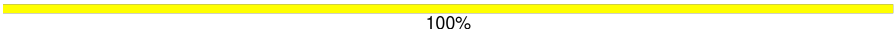
Chain z:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 

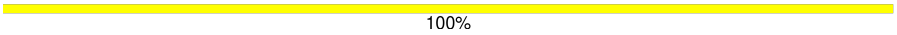
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

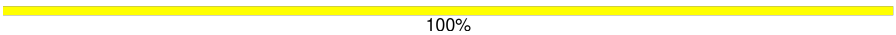
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r: 

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 50% 50%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 100%

NAG1 NAG2

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

Chain l: 33% 67%

NAG1 NAG2 BMA3

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

Chain p: 100%

NAG1 NAG2 BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.84Å 133.14Å 812.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.20 50.01 – 3.16	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.13-3.20) 87.4 (50.01-3.16)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.249 , 0.302 0.243 , 0.296	Depositor DCC
R_{free} test set	10355 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	58742	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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 (i)

5.1 Standard geometry (i)

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

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	0.51	1/2591 (0.0%)	0.68	0/3517
1	B	0.49	0/2562	0.69	0/3478
1	C	0.53	0/2599	0.74	1/3528 (0.0%)
1	D	0.44	0/2599	0.64	1/3528 (0.0%)
1	E	0.48	1/2591 (0.0%)	0.65	0/3517
1	F	0.44	1/2599 (0.0%)	0.62	0/3528
1	G	0.42	1/2599 (0.0%)	0.63	0/3528
1	H	0.50	1/2608 (0.0%)	0.69	0/3540
1	I	0.45	1/2599 (0.0%)	0.65	0/3528
2	a	0.44	0/1415	0.63	0/1900
2	b	0.45	0/1369	0.64	0/1837
2	c	0.44	0/1424	0.60	0/1912
2	d	0.43	0/1424	0.58	0/1912
2	e	0.48	0/1424	0.62	0/1912
2	f	0.47	0/1424	0.62	0/1912
2	g	0.45	0/1424	0.62	0/1912
2	h	0.55	0/1381	0.65	0/1852
2	i	0.56	0/1424	0.67	0/1912
3	J	0.49	0/893	0.69	0/1213
3	L	0.60	0/1618	0.78	1/2209 (0.0%)
3	N	0.63	0/1689	0.83	1/2304 (0.0%)
3	P	0.42	0/1237	0.59	0/1682
3	R	0.45	0/1629	0.66	0/2224
3	T	0.39	0/1620	0.61	0/2212
3	V	0.44	0/905	0.60	0/1231
3	X	0.51	0/1261	0.70	0/1713
3	Z	0.42	0/1294	0.64	0/1760
4	K	0.43	0/843	0.72	1/1146 (0.1%)
4	M	0.57	0/1695	0.75	0/2302
4	O	0.67	0/1695	0.85	1/2302 (0.0%)
4	Q	0.44	0/1239	0.65	0/1682
4	S	0.45	0/1676	0.66	1/2277 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	U	0.40	0/1676	0.60	0/2277
4	W	0.45	0/835	0.62	0/1135
4	Y	0.51	0/870	0.75	1/1181 (0.1%)
4	z	0.40	0/930	0.62	1/1261 (0.1%)
All	All	0.48	6/59661 (0.0%)	0.67	9/80864 (0.0%)

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
1	A	0	1
1	G	0	1
2	b	0	2
2	f	0	1
2	i	0	2
3	J	0	2
3	L	0	2
3	N	0	3
3	R	0	1
3	X	0	1
3	Z	0	1
4	K	0	4
4	M	0	2
4	O	0	1
4	Q	0	2
4	S	0	1
4	U	0	1
4	W	0	1
4	Y	0	1
4	z	0	1
All	All	0	31

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CYS	CB-SG	-7.01	1.70	1.82
1	E	64	CYS	CB-SG	-5.99	1.72	1.81
1	G	64	CYS	CB-SG	-5.53	1.72	1.81
1	F	64	CYS	CB-SG	-5.51	1.72	1.81
1	I	64	CYS	CB-SG	-5.20	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CYS	CB-SG	-5.06	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	220	ARG	NE-CZ-NH2	6.90	123.75	120.30
4	K	57	GLY	N-CA-C	-6.43	97.01	113.10
4	z	63	ARG	NE-CZ-NH1	-6.29	117.16	120.30
4	Y	63	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	L	102	PRO	N-CA-C	-5.32	98.28	112.10
4	S	96	ILE	CG1-CB-CG2	-5.22	99.92	111.40
3	N	182	VAL	CB-CA-C	-5.20	101.52	111.40
1	D	220	ARG	NE-CZ-NH1	5.07	122.84	120.30
4	O	50	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLY	Peptide
1	G	9	PRO	Peptide
3	J	30	ILE	Peptide
3	J	64	GLN	Peptide
4	K	39	LYS	Peptide
4	K	52	SER	Peptide
4	K	57	GLY	Peptide
4	K	90	GLN	Peptide
3	L	101	ASP	Peptide
3	L	203	SER	Peptide
4	M	90	GLN	Peptide
4	M	94	LEU	Peptide
3	N	114	ALA	Peptide
3	N	126	PRO	Peptide
3	N	203	SER	Peptide
4	O	94	LEU	Peptide
4	Q	90	GLN	Peptide
4	Q	94	LEU	Peptide
3	R	148	GLU	Peptide
4	S	94	LEU	Peptide
4	U	94	LEU	Peptide
4	W	94	LEU	Peptide
3	X	148	GLU	Peptide

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Mol	Chain	Res	Type	Group
4	Y	94	LEU	Peptide
3	Z	148	GLU	Peptide
2	b	61	THR	Peptide
2	b	62	GLN	Peptide
2	f	60	ASN	Peptide
2	i	61	THR	Peptide
2	i	62	GLN	Peptide
4	z	94	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	321/327 (98%)	292 (91%)	28 (9%)	1 (0%)	41	74
1	B	317/327 (97%)	283 (89%)	30 (10%)	4 (1%)	12	47
1	C	322/327 (98%)	288 (89%)	29 (9%)	5 (2%)	9	43
1	D	322/327 (98%)	293 (91%)	26 (8%)	3 (1%)	17	56
1	E	321/327 (98%)	291 (91%)	26 (8%)	4 (1%)	13	49
1	F	322/327 (98%)	288 (89%)	28 (9%)	6 (2%)	8	39
1	G	322/327 (98%)	285 (88%)	32 (10%)	5 (2%)	9	43
1	H	323/327 (99%)	286 (88%)	34 (10%)	3 (1%)	17	56
1	I	322/327 (98%)	287 (89%)	32 (10%)	3 (1%)	17	56
2	a	169/174 (97%)	143 (85%)	20 (12%)	6 (4%)	3	23
2	b	163/174 (94%)	135 (83%)	24 (15%)	4 (2%)	5	32
2	c	170/174 (98%)	147 (86%)	19 (11%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	170/174 (98%)	147 (86%)	21 (12%)	2 (1%)	13	49
2	e	170/174 (98%)	154 (91%)	14 (8%)	2 (1%)	13	49
2	f	170/174 (98%)	144 (85%)	22 (13%)	4 (2%)	6	34
2	g	170/174 (98%)	148 (87%)	20 (12%)	2 (1%)	13	49
2	h	163/174 (94%)	143 (88%)	15 (9%)	5 (3%)	4	26
2	i	170/174 (98%)	144 (85%)	21 (12%)	5 (3%)	4	28
3	J	113/223 (51%)	80 (71%)	26 (23%)	7 (6%)	1	11
3	L	208/223 (93%)	186 (89%)	13 (6%)	9 (4%)	2	20
3	N	221/223 (99%)	200 (90%)	14 (6%)	7 (3%)	4	26
3	P	155/223 (70%)	134 (86%)	12 (8%)	9 (6%)	1	13
3	R	210/223 (94%)	185 (88%)	18 (9%)	7 (3%)	4	25
3	T	209/223 (94%)	184 (88%)	19 (9%)	6 (3%)	4	28
3	V	115/223 (52%)	106 (92%)	8 (7%)	1 (1%)	17	56
3	X	156/223 (70%)	129 (83%)	19 (12%)	8 (5%)	2	15
3	Z	159/223 (71%)	133 (84%)	16 (10%)	10 (6%)	1	10
4	K	104/214 (49%)	77 (74%)	17 (16%)	10 (10%)	0	3
4	M	212/214 (99%)	191 (90%)	18 (8%)	3 (1%)	11	46
4	O	212/214 (99%)	190 (90%)	18 (8%)	4 (2%)	8	39
4	Q	149/214 (70%)	125 (84%)	20 (13%)	4 (3%)	5	30
4	S	209/214 (98%)	182 (87%)	20 (10%)	7 (3%)	4	25
4	U	209/214 (98%)	177 (85%)	25 (12%)	7 (3%)	4	25
4	W	103/214 (48%)	89 (86%)	10 (10%)	4 (4%)	3	22
4	Y	107/214 (50%)	94 (88%)	9 (8%)	4 (4%)	3	22
4	z	113/214 (53%)	97 (86%)	11 (10%)	5 (4%)	2	19
All	All	7371/8442 (87%)	6457 (88%)	734 (10%)	180 (2%)	6	34

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	66	VAL
1	B	264	SER
2	c	61	THR
2	e	146	ASP
2	f	62	GLN

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Mol	Chain	Res	Type
2	f	64	GLU
2	f	146	ASP
2	g	146	ASP
2	h	147	GLU
2	i	146	ASP
3	J	98	GLY
4	K	13	ALA
4	K	51	ALA
3	L	102	PRO
3	L	204	ASN
4	M	96	ILE
3	N	204	ASN
4	O	51	ALA
3	P	147	PRO
3	R	148	GLU
3	R	203	SER
3	R	204	ASN
3	T	116	THR
3	T	189	LEU
3	T	203	SER
3	X	148	GLU
3	Z	62	LYS
2	a	67	GLY
2	a	147	GLU
2	a	150	ASN
1	B	134	GLY
1	B	174	GLU
2	b	67	GLY
2	b	146	ASP
2	b	147	GLU
2	c	147	GLU
1	D	297	VAL
2	d	146	ASP
2	d	147	GLU
2	e	147	GLU
1	F	58	PRO
1	F	158	GLY
1	G	159	SER
2	g	147	GLU
1	H	58	PRO
2	h	146	ASP
1	I	58	PRO

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Mol	Chain	Res	Type
2	i	64	GLU
4	K	3	GLN
4	K	68	GLY
3	L	16	SER
3	L	116	THR
3	L	188	SER
4	M	95	PRO
4	O	96	ILE
4	O	152	ASN
3	P	100	TYR
3	P	116	THR
3	P	173	SER
3	R	100	TYR
4	S	138	ASN
4	S	187	GLU
3	T	100	TYR
3	T	190	GLY
4	U	96	ILE
4	U	128	GLY
4	U	143	GLU
3	X	61	GLN
3	X	62	LYS
3	X	63	PHE
4	Y	51	ALA
3	Z	61	GLN
1	A	174	GLU
2	b	150	ASN
1	C	297	VAL
1	E	186	ASN
1	F	159	SER
1	F	196	GLN
2	f	147	GLU
1	G	58	PRO
1	G	67	ALA
2	h	103	GLU
1	I	196	GLN
2	i	7	ALA
2	i	147	GLU
3	J	79	TYR
3	L	144	ASP
3	L	203	SER
4	M	138	ASN

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Mol	Chain	Res	Type
3	N	100	TYR
4	O	95	PRO
3	P	97	SER
3	R	113	SER
4	S	92	ASP
4	S	204	PRO
4	U	92	ASP
4	U	138	ASN
4	W	92	ASP
3	X	100	TYR
3	X	144	ASP
3	Z	63	PHE
4	z	92	ASP
2	a	127	ARG
1	C	128	THR
2	c	63	PHE
1	E	297	VAL
1	F	186	ASN
3	J	16	SER
3	J	32	HIS
3	J	83	THR
3	J	100	TYR
4	K	76	SER
4	K	92	ASP
3	N	172	SER
3	P	158	ALA
4	S	121	SER
3	V	100	TYR
4	W	84	ALA
4	Y	92	ASP
3	Z	100	TYR
3	Z	144	ASP
3	Z	196	CYS
4	z	96	ILE
2	c	30	GLN
1	D	96	LEU
1	H	196	GLN
2	h	102	MET
2	i	5	ALA
4	K	67	SER
3	L	149	PRO
3	N	132	SER

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Mol	Chain	Res	Type
3	N	214	LYS
4	Q	68	GLY
4	Q	96	ILE
4	S	114	SER
3	T	147	PRO
4	W	96	ILE
3	Z	148	GLU
4	z	51	ALA
2	a	132	GLU
1	C	310	LYS
1	E	162	PRO
1	G	224	ASN
1	I	158	GLY
4	K	40	PRO
3	L	100(A)	GLY
3	P	172	SER
3	R	149	PRO
4	S	96	ILE
4	Y	96	ILE
3	Z	100(A)	GLY
3	Z	202	PRO
1	D	158	GLY
1	F	297	VAL
1	H	158	GLY
2	h	91	VAL
3	J	41	PRO
3	P	174	GLY
3	X	202	PRO
1	B	297	VAL
1	C	158	GLY
1	G	158	GLY
4	K	94	LEU
4	Q	95	PRO
1	E	158	GLY
4	K	96	ILE
3	N	149	PRO
3	P	14	PRO
4	U	95	PRO
4	W	68	GLY
3	X	100(A)	GLY
4	Y	68	GLY
4	z	68	GLY

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Mol	Chain	Res	Type
4	z	95	PRO
4	Q	113	PRO
4	U	68	GLY
1	C	217	ILE
3	Z	102	PRO
3	R	147	PRO
3	N	147	PRO

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	285/289 (99%)	236 (83%)	49 (17%)	2 10
1	B	282/289 (98%)	228 (81%)	54 (19%)	1 8
1	C	286/289 (99%)	241 (84%)	45 (16%)	2 12
1	D	286/289 (99%)	239 (84%)	47 (16%)	2 11
1	E	285/289 (99%)	239 (84%)	46 (16%)	2 11
1	F	286/289 (99%)	235 (82%)	51 (18%)	2 9
1	G	286/289 (99%)	241 (84%)	45 (16%)	2 12
1	H	287/289 (99%)	239 (83%)	48 (17%)	2 10
1	I	286/289 (99%)	239 (84%)	47 (16%)	2 11
2	a	148/151 (98%)	128 (86%)	20 (14%)	4 18
2	b	144/151 (95%)	123 (85%)	21 (15%)	3 15
2	c	149/151 (99%)	137 (92%)	12 (8%)	11 42
2	d	149/151 (99%)	137 (92%)	12 (8%)	11 42
2	e	149/151 (99%)	134 (90%)	15 (10%)	7 29
2	f	149/151 (99%)	134 (90%)	15 (10%)	7 29
2	g	149/151 (99%)	136 (91%)	13 (9%)	10 37
2	h	145/151 (96%)	130 (90%)	15 (10%)	7 29
2	i	149/151 (99%)	135 (91%)	14 (9%)	8 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	91/185 (49%)	70 (77%)	21 (23%)	1	3
3	L	176/185 (95%)	142 (81%)	34 (19%)	1	8
3	N	185/185 (100%)	142 (77%)	43 (23%)	1	3
3	P	130/185 (70%)	104 (80%)	26 (20%)	1	6
3	R	177/185 (96%)	136 (77%)	41 (23%)	1	3
3	T	176/185 (95%)	138 (78%)	38 (22%)	1	5
3	V	93/185 (50%)	74 (80%)	19 (20%)	1	6
3	X	136/185 (74%)	106 (78%)	30 (22%)	1	4
3	Z	139/185 (75%)	109 (78%)	30 (22%)	1	5
4	K	93/190 (49%)	67 (72%)	26 (28%)	0	1
4	M	190/190 (100%)	158 (83%)	32 (17%)	2	10
4	O	190/190 (100%)	152 (80%)	38 (20%)	1	6
4	Q	140/190 (74%)	108 (77%)	32 (23%)	1	4
4	S	188/190 (99%)	151 (80%)	37 (20%)	1	7
4	U	188/190 (99%)	141 (75%)	47 (25%)	0	2
4	W	92/190 (48%)	73 (79%)	19 (21%)	1	6
4	Y	96/190 (50%)	76 (79%)	20 (21%)	1	6
4	z	105/190 (55%)	81 (77%)	24 (23%)	1	4
All	All	6485/7335 (88%)	5359 (83%)	1126 (17%)	2	10

All (1126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	21	ASN
1	A	22	SER
1	A	23	THR
1	A	28	THR
1	A	30	LEU
1	A	37	THR
1	A	43	LEU
1	A	45	LYS
1	A	53(A)	LEU
1	A	56	ILE
1	A	80	LEU
1	A	81	SER

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Mol	Chain	Res	Type
1	A	81(A)	VAL
1	A	85	SER
1	A	101	SER
1	A	114	SER
1	A	116(C)	GLU
1	A	118	VAL
1	A	123	LYS
1	A	132	THR
1	A	133	THR
1	A	136	SER
1	A	146	SER
1	A	154	LEU
1	A	155	THR
1	A	160	ASP
1	A	174	GLU
1	A	182	VAL
1	A	194	LEU
1	A	197	ASN
1	A	203	SER
1	A	208	THR
1	A	213	SER
1	A	214	THR
1	A	219	THR
1	A	226	LEU
1	A	228	SER
1	A	236	LEU
1	A	263	ARG
1	A	264	SER
1	A	277	CYS
1	A	283	THR
1	A	302	ILE
1	A	315	VAL
1	A	316	LEU
1	A	318	THR
1	A	320	LEU
1	A	323	VAL
2	a	19	ASP
2	a	22	TYR
2	a	26	HIS
2	a	29	ASP
2	a	39	GLU
2	a	58	LYS

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Mol	Chain	Res	Type
2	a	59	MET
2	a	61	THR
2	a	64	GLU
2	a	71	SER
2	a	72	ASN
2	a	83	LYS
2	a	121	LYS
2	a	130	VAL
2	a	145	ASP
2	a	148	CYS
2	a	151	SER
2	a	156	THR
2	a	164	GLU
2	a	171	ASN
1	B	18	HIS
1	B	22	SER
1	B	23	THR
1	B	28	THR
1	B	30	LEU
1	B	43	LEU
1	B	45	LYS
1	B	51	LEU
1	B	53(A)	LEU
1	B	56	ILE
1	B	78	ARG
1	B	80	LEU
1	B	81(A)	VAL
1	B	85	SER
1	B	101	SER
1	B	104	ASP
1	B	108	LEU
1	B	109	LYS
1	B	111	LEU
1	B	114	SER
1	B	116(C)	GLU
1	B	118	VAL
1	B	123	LYS
1	B	144	ASN
1	B	146	SER
1	B	154	LEU
1	B	155	THR
1	B	160	ASP

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Mol	Chain	Res	Type
1	B	171	THR
1	B	174	GLU
1	B	182	VAL
1	B	194	LEU
1	B	197	ASN
1	B	198	VAL
1	B	203	SER
1	B	208	THR
1	B	213	SER
1	B	214	THR
1	B	219	THR
1	B	226	LEU
1	B	236	LEU
1	B	264	SER
1	B	277	CYS
1	B	279	THR
1	B	283	THR
1	B	297	VAL
1	B	301	THR
1	B	302	ILE
1	B	309	VAL
1	B	315	VAL
1	B	316	LEU
1	B	318	THR
1	B	320	LEU
1	B	323	VAL
2	b	2	LEU
2	b	19	ASP
2	b	25	HIS
2	b	26	HIS
2	b	29	ASP
2	b	39	GLU
2	b	56	ILE
2	b	66	VAL
2	b	71	SER
2	b	72	ASN
2	b	74	GLU
2	b	83	LYS
2	b	121	LYS
2	b	145	ASP
2	b	148	CYS
2	b	150	ASN

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Mol	Chain	Res	Type
2	b	151	SER
2	b	153	LYS
2	b	156	THR
2	b	164	GLU
2	b	168	LEU
1	C	23	THR
1	C	25	LYS
1	C	30	LEU
1	C	32	ARG
1	C	54	ASN
1	C	56	ILE
1	C	63	ASP
1	C	65	SER
1	C	80	LEU
1	C	81(A)	VAL
1	C	96	LEU
1	C	101	SER
1	C	116(B)	PHE
1	C	125	ASP
1	C	133	THR
1	C	146	SER
1	C	154	LEU
1	C	155	THR
1	C	159	SER
1	C	182	VAL
1	C	187	ASP
1	C	194	LEU
1	C	197	ASN
1	C	203	SER
1	C	206	THR
1	C	208	THR
1	C	209	LEU
1	C	214	THR
1	C	219	THR
1	C	226	LEU
1	C	233	SER
1	C	236	LEU
1	C	273	THR
1	C	277	CYS
1	C	278	GLU
1	C	283	THR
1	C	285	LEU

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Mol	Chain	Res	Type
1	C	295	HIS
1	C	307	ARG
1	C	311	SER
1	C	312	GLU
1	C	315	VAL
1	C	316	LEU
1	C	320	LEU
1	C	323	VAL
2	c	19	ASP
2	c	26	HIS
2	c	59	MET
2	c	61	THR
2	c	64	GLU
2	c	66	VAL
2	c	71	SER
2	c	72	ASN
2	c	73	LEU
2	c	113	SER
2	c	148	CYS
2	c	164	GLU
1	D	21	ASN
1	D	22	SER
1	D	23	THR
1	D	25	LYS
1	D	29	ILE
1	D	30	LEU
1	D	32	ARG
1	D	45	LYS
1	D	54	ASN
1	D	56	ILE
1	D	63	ASP
1	D	65	SER
1	D	80	LEU
1	D	81(A)	VAL
1	D	101	SER
1	D	116(B)	PHE
1	D	133	THR
1	D	136	SER
1	D	146	SER
1	D	154	LEU
1	D	155	THR
1	D	163	VAL

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Mol	Chain	Res	Type
1	D	187	ASP
1	D	197	ASN
1	D	206	THR
1	D	208	THR
1	D	214	THR
1	D	219	THR
1	D	236	LEU
1	D	239	MET
1	D	242	THR
1	D	265	SER
1	D	273	THR
1	D	277	CYS
1	D	278	GLU
1	D	279	THR
1	D	291	THR
1	D	295	HIS
1	D	301	THR
1	D	307	ARG
1	D	309	VAL
1	D	311	SER
1	D	312	GLU
1	D	315	VAL
1	D	316	LEU
1	D	320	LEU
1	D	323	VAL
2	d	19	ASP
2	d	26	HIS
2	d	59	MET
2	d	63	PHE
2	d	66	VAL
2	d	69	GLU
2	d	73	LEU
2	d	74	GLU
2	d	80	LEU
2	d	113	SER
2	d	148	CYS
2	d	164	GLU
1	E	12	GLN
1	E	18	HIS
1	E	30	LEU
1	E	32	ARG
1	E	33	ASN

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Mol	Chain	Res	Type
1	E	54	ASN
1	E	56	ILE
1	E	63	ASP
1	E	65	SER
1	E	80	LEU
1	E	81(A)	VAL
1	E	96	LEU
1	E	101	SER
1	E	111	LEU
1	E	113	SER
1	E	116(B)	PHE
1	E	133	THR
1	E	136	SER
1	E	146	SER
1	E	154	LEU
1	E	155	THR
1	E	163	VAL
1	E	187	ASP
1	E	194	LEU
1	E	203	SER
1	E	206	THR
1	E	208	THR
1	E	209	LEU
1	E	213	SER
1	E	214	THR
1	E	219	THR
1	E	230	MET
1	E	236	LEU
1	E	242	THR
1	E	265	SER
1	E	273	THR
1	E	277	CYS
1	E	278	GLU
1	E	291	THR
1	E	295	HIS
1	E	307	ARG
1	E	309	VAL
1	E	315	VAL
1	E	316	LEU
1	E	320	LEU
1	E	323	VAL
2	e	19	ASP

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Mol	Chain	Res	Type
2	e	32	SER
2	e	59	MET
2	e	64	GLU
2	e	66	VAL
2	e	69	GLU
2	e	71	SER
2	e	72	ASN
2	e	73	LEU
2	e	74	GLU
2	e	84	MET
2	e	113	SER
2	e	147	GLU
2	e	148	CYS
2	e	164	GLU
1	F	22	SER
1	F	30	LEU
1	F	32	ARG
1	F	43	LEU
1	F	45	LYS
1	F	53(A)	LEU
1	F	65	SER
1	F	78	ARG
1	F	81(A)	VAL
1	F	89	GLU
1	F	101	SER
1	F	102	PHE
1	F	114	SER
1	F	116(B)	PHE
1	F	132	THR
1	F	133	THR
1	F	137	ARG
1	F	142	SER
1	F	146	SER
1	F	154	LEU
1	F	155	THR
1	F	159	SER
1	F	189	THR
1	F	194	LEU
1	F	197	ASN
1	F	198	VAL
1	F	203	SER
1	F	208	THR

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Mol	Chain	Res	Type
1	F	210	ASN
1	F	212	ARG
1	F	213	SER
1	F	214	THR
1	F	217	ILE
1	F	219	THR
1	F	226	LEU
1	F	236	LEU
1	F	242	THR
1	F	261	SER
1	F	265	SER
1	F	273	THR
1	F	274	LEU
1	F	275	GLU
1	F	279	THR
1	F	290	THR
1	F	297	VAL
1	F	301	THR
1	F	309	VAL
1	F	315	VAL
1	F	316	LEU
1	F	320	LEU
1	F	326	ILE
2	f	19	ASP
2	f	26	HIS
2	f	59	MET
2	f	60	ASN
2	f	64	GLU
2	f	66	VAL
2	f	71	SER
2	f	72	ASN
2	f	73	LEU
2	f	74	GLU
2	f	84	MET
2	f	113	SER
2	f	127	ARG
2	f	148	CYS
2	f	164	GLU
1	G	12	GLN
1	G	13	ILE
1	G	25	LYS
1	G	30	LEU

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Mol	Chain	Res	Type
1	G	32	ARG
1	G	43	LEU
1	G	53(A)	LEU
1	G	65	SER
1	G	81(A)	VAL
1	G	89	GLU
1	G	101	SER
1	G	114	SER
1	G	116(B)	PHE
1	G	132	THR
1	G	133	THR
1	G	137	ARG
1	G	142	SER
1	G	146	SER
1	G	155	THR
1	G	189	THR
1	G	194	LEU
1	G	197	ASN
1	G	208	THR
1	G	210	ASN
1	G	212	ARG
1	G	213	SER
1	G	214	THR
1	G	217	ILE
1	G	219	THR
1	G	226	LEU
1	G	236	LEU
1	G	270	THR
1	G	273	THR
1	G	274	LEU
1	G	275	GLU
1	G	279	THR
1	G	297	VAL
1	G	301	THR
1	G	307	ARG
1	G	309	VAL
1	G	315	VAL
1	G	316	LEU
1	G	320	LEU
1	G	323	VAL
1	G	326	ILE
2	g	19	ASP

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Mol	Chain	Res	Type
2	g	26	HIS
2	g	59	MET
2	g	61	THR
2	g	62	GLN
2	g	66	VAL
2	g	69	GLU
2	g	72	ASN
2	g	73	LEU
2	g	80	LEU
2	g	147	GLU
2	g	148	CYS
2	g	164	GLU
1	H	13	ILE
1	H	30	LEU
1	H	32	ARG
1	H	53(A)	LEU
1	H	65	SER
1	H	81(A)	VAL
1	H	89	GLU
1	H	97	CYS
1	H	101	SER
1	H	102	PHE
1	H	114	SER
1	H	132	THR
1	H	133	THR
1	H	137	ARG
1	H	142	SER
1	H	146	SER
1	H	154	LEU
1	H	155	THR
1	H	159	SER
1	H	182	VAL
1	H	187	ASP
1	H	189	THR
1	H	194	LEU
1	H	197	ASN
1	H	203	SER
1	H	208	THR
1	H	210	ASN
1	H	213	SER
1	H	214	THR
1	H	217	ILE

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Mol	Chain	Res	Type
1	H	219	THR
1	H	236	LEU
1	H	261	SER
1	H	265	SER
1	H	273	THR
1	H	274	LEU
1	H	279	THR
1	H	291	THR
1	H	297	VAL
1	H	301	THR
1	H	307	ARG
1	H	309	VAL
1	H	315	VAL
1	H	316	LEU
1	H	320	LEU
1	H	323	VAL
1	H	326	ILE
1	H	327	GLU
2	h	19	ASP
2	h	21	TRP
2	h	26	HIS
2	h	32	SER
2	h	49	THR
2	h	59	MET
2	h	66	VAL
2	h	69	GLU
2	h	72	ASN
2	h	73	LEU
2	h	74	GLU
2	h	113	SER
2	h	127	ARG
2	h	151	SER
2	h	164	GLU
1	I	11	ASP
1	I	18	HIS
1	I	29	ILE
1	I	30	LEU
1	I	32	ARG
1	I	48	ASN
1	I	53(A)	LEU
1	I	65	SER
1	I	81(A)	VAL

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Mol	Chain	Res	Type
1	I	89	GLU
1	I	101	SER
1	I	102	PHE
1	I	114	SER
1	I	132	THR
1	I	133	THR
1	I	137	ARG
1	I	146	SER
1	I	155	THR
1	I	187	ASP
1	I	189	THR
1	I	194	LEU
1	I	197	ASN
1	I	203	SER
1	I	207	SER
1	I	208	THR
1	I	210	ASN
1	I	212	ARG
1	I	214	THR
1	I	217	ILE
1	I	219	THR
1	I	226	LEU
1	I	236	LEU
1	I	261	SER
1	I	264	SER
1	I	265	SER
1	I	270	THR
1	I	273	THR
1	I	274	LEU
1	I	275	GLU
1	I	279	THR
1	I	297	VAL
1	I	301	THR
1	I	307	ARG
1	I	316	LEU
1	I	320	LEU
1	I	323	VAL
1	I	326	ILE
2	i	19	ASP
2	i	26	HIS
2	i	27	SER
2	i	56	ILE

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Mol	Chain	Res	Type
2	i	59	MET
2	i	64	GLU
2	i	66	VAL
2	i	73	LEU
2	i	74	GLU
2	i	80	LEU
2	i	127	ARG
2	i	147	GLU
2	i	148	CYS
2	i	164	GLU
3	J	3	GLN
3	J	4	LEU
3	J	5	VAL
3	J	6	GLU
3	J	10	GLU
3	J	12	LYS
3	J	21	SER
3	J	23	LYS
3	J	32	HIS
3	J	38	ARG
3	J	48	VAL
3	J	70	THR
3	J	72	ASP
3	J	74	SER
3	J	79	TYR
3	J	80	MET
3	J	85	GLU
3	J	94	ARG
3	J	97	SER
3	J	100(B)	TRP
3	J	101	ASP
4	K	1	ASP
4	K	4	LEU
4	K	5	THR
4	K	7	SER
4	K	18	ARG
4	K	19	VAL
4	K	20	THR
4	K	24	GLN
4	K	29	ILE
4	K	39	LYS
4	K	42	LYS

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Mol	Chain	Res	Type
4	K	45	ASN
4	K	48	ILE
4	K	55	LYS
4	K	61	ARG
4	K	63	ARG
4	K	65	SER
4	K	69	THR
4	K	70	ASP
4	K	78	LEU
4	K	79	GLN
4	K	85	THR
4	K	90	GLN
4	K	97	THR
4	K	103	ARG
4	K	104	LEU
3	L	4	LEU
3	L	17	SER
3	L	28	THR
3	L	43	GLN
3	L	57	SER
3	L	74	SER
3	L	75	THR
3	L	76	SER
3	L	83	THR
3	L	85	GLU
3	L	97	SER
3	L	107	THR
3	L	110	THR
3	L	116	THR
3	L	117	LYS
3	L	138	LEU
3	L	151	THR
3	L	164	HIS
3	L	169	VAL
3	L	170	LEU
3	L	172	SER
3	L	173	SER
3	L	177	SER
3	L	178	LEU
3	L	179	SER
3	L	182	VAL
3	L	183	THR

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Mol	Chain	Res	Type
3	L	186	SER
3	L	191	THR
3	L	195	ILE
3	L	197	ASN
3	L	198	VAL
3	L	205	THR
3	L	210	ARG
4	M	3	GLN
4	M	5	THR
4	M	7	SER
4	M	22	THR
4	M	26	SER
4	M	33	LEU
4	M	52	SER
4	M	63	ARG
4	M	65	SER
4	M	69	THR
4	M	72	THR
4	M	77	SER
4	M	78	LEU
4	M	83	ILE
4	M	90	GLN
4	M	94	LEU
4	M	97	THR
4	M	104	LEU
4	M	105	GLU
4	M	107	LYS
4	M	110	VAL
4	M	117	ILE
4	M	150	VAL
4	M	155	GLN
4	M	181	LEU
4	M	182	SER
4	M	202	SER
4	M	206	THR
4	M	207	LYS
4	M	208	SER
4	M	213	GLU
4	M	214	CYS
3	N	4	LEU
3	N	11	VAL
3	N	28	THR

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Mol	Chain	Res	Type
3	N	31	THR
3	N	43	GLN
3	N	53	ILE
3	N	57	SER
3	N	62	LYS
3	N	70	THR
3	N	74	SER
3	N	75	THR
3	N	76	SER
3	N	83	THR
3	N	85	GLU
3	N	110	THR
3	N	116	THR
3	N	117	LYS
3	N	120	SER
3	N	128	SER
3	N	130	SER
3	N	131	THR
3	N	132	SER
3	N	138	LEU
3	N	151	THR
3	N	156	SER
3	N	167	PRO
3	N	169	VAL
3	N	170	LEU
3	N	173	SER
3	N	177	SER
3	N	178	LEU
3	N	179	SER
3	N	182	VAL
3	N	184	VAL
3	N	186	SER
3	N	189	LEU
3	N	191	THR
3	N	195	ILE
3	N	197	ASN
3	N	210	ARG
3	N	214	LYS
3	N	215	SER
3	N	216	CYS
4	O	3	GLN
4	O	5	THR

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Mol	Chain	Res	Type
4	O	7	SER
4	O	11	LEU
4	O	20	THR
4	O	22	THR
4	O	26	SER
4	O	52	SER
4	O	60	SER
4	O	63	ARG
4	O	65	SER
4	O	74	THR
4	O	76	SER
4	O	77	SER
4	O	78	LEU
4	O	81	GLU
4	O	85	THR
4	O	90	GLN
4	O	91	TYR
4	O	94	LEU
4	O	97	THR
4	O	104	LEU
4	O	107	LYS
4	O	127	SER
4	O	132	VAL
4	O	142	ARG
4	O	150	VAL
4	O	155	GLN
4	O	164	THR
4	O	180	THR
4	O	182	SER
4	O	194	CYS
4	O	197	THR
4	O	201	LEU
4	O	202	SER
4	O	207	LYS
4	O	208	SER
4	O	214	CYS
3	P	2	VAL
3	P	6	GLU
3	P	7	SER
3	P	11	VAL
3	P	21	SER
3	P	25	SER

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Mol	Chain	Res	Type
3	P	28	THR
3	P	33	VAL
3	P	61	GLN
3	P	66	ARG
3	P	68	THR
3	P	70	THR
3	P	75	THR
3	P	83	THR
3	P	97	SER
3	P	110	THR
3	P	116	THR
3	P	117	LYS
3	P	156	SER
3	P	160	THR
3	P	161	SER
3	P	169	VAL
3	P	170	LEU
3	P	173	SER
3	P	177	SER
3	P	178	LEU
4	Q	5	THR
4	Q	11	LEU
4	Q	14	SER
4	Q	18	ARG
4	Q	19	VAL
4	Q	26	SER
4	Q	30	ARG
4	Q	52	SER
4	Q	60	SER
4	Q	63	ARG
4	Q	65	SER
4	Q	67	SER
4	Q	69	THR
4	Q	74	THR
4	Q	77	SER
4	Q	81	GLU
4	Q	85	THR
4	Q	90	GLN
4	Q	94	LEU
4	Q	109	THR
4	Q	132	VAL
4	Q	133	VAL

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Mol	Chain	Res	Type
4	Q	135	LEU
4	Q	138	ASN
4	Q	142	ARG
4	Q	166	GLN
4	Q	174	SER
4	Q	175	LEU
4	Q	176	SER
4	Q	197	THR
4	Q	199	GLN
4	Q	201	LEU
3	R	1	GLU
3	R	2	VAL
3	R	6	GLU
3	R	7	SER
3	R	11	VAL
3	R	17	SER
3	R	25	SER
3	R	28	THR
3	R	33	VAL
3	R	61	GLN
3	R	64	GLN
3	R	66	ARG
3	R	68	THR
3	R	70	THR
3	R	75	THR
3	R	83	THR
3	R	97	SER
3	R	110	THR
3	R	113	SER
3	R	115	SER
3	R	116	THR
3	R	117	LYS
3	R	135	THR
3	R	140	CYS
3	R	151	THR
3	R	153	SER
3	R	154	TRP
3	R	161	SER
3	R	164	HIS
3	R	169	VAL
3	R	170	LEU
3	R	173	SER

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Mol	Chain	Res	Type
3	R	179	SER
3	R	182	VAL
3	R	187	SER
3	R	189	LEU
3	R	191	THR
3	R	192	GLN
3	R	196	CYS
3	R	197	ASN
3	R	209	LYS
4	S	5	THR
4	S	11	LEU
4	S	14	SER
4	S	18	ARG
4	S	19	VAL
4	S	21	ILE
4	S	26	SER
4	S	52	SER
4	S	60	SER
4	S	61	ARG
4	S	63	ARG
4	S	65	SER
4	S	74	THR
4	S	77	SER
4	S	78	LEU
4	S	81	GLU
4	S	85	THR
4	S	90	GLN
4	S	94	LEU
4	S	105	GLU
4	S	107	LYS
4	S	109	THR
4	S	129	THR
4	S	132	VAL
4	S	133	VAL
4	S	152	ASN
4	S	154	LEU
4	S	155	GLN
4	S	156	SER
4	S	158	ASN
4	S	162	SER
4	S	168	SER
4	S	169	LYS

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Mol	Chain	Res	Type
4	S	180	THR
4	S	188	LYS
4	S	202	SER
4	S	207	LYS
3	T	2	VAL
3	T	6	GLU
3	T	7	SER
3	T	11	VAL
3	T	17	SER
3	T	25	SER
3	T	28	THR
3	T	33	VAL
3	T	61	GLN
3	T	66	ARG
3	T	68	THR
3	T	70	THR
3	T	75	THR
3	T	81	GLU
3	T	83	THR
3	T	97	SER
3	T	99	SER
3	T	110	THR
3	T	115	SER
3	T	116	THR
3	T	117	LYS
3	T	127	SER
3	T	140	CYS
3	T	150	VAL
3	T	153	SER
3	T	160	THR
3	T	169	VAL
3	T	172	SER
3	T	173	SER
3	T	182	VAL
3	T	183	THR
3	T	184	VAL
3	T	187	SER
3	T	192	GLN
3	T	194	TYR
3	T	198	VAL
3	T	205	THR
3	T	212	GLU

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Mol	Chain	Res	Type
4	U	5	THR
4	U	11	LEU
4	U	14	SER
4	U	18	ARG
4	U	19	VAL
4	U	20	THR
4	U	26	SER
4	U	52	SER
4	U	60	SER
4	U	61	ARG
4	U	63	ARG
4	U	72	THR
4	U	74	THR
4	U	77	SER
4	U	81	GLU
4	U	83	ILE
4	U	85	THR
4	U	90	GLN
4	U	94	LEU
4	U	97	THR
4	U	107	LYS
4	U	109	THR
4	U	114	SER
4	U	122	ASP
4	U	123	GLU
4	U	125	LEU
4	U	129	THR
4	U	131	SER
4	U	138	ASN
4	U	142	ARG
4	U	145	LYS
4	U	152	ASN
4	U	155	GLN
4	U	156	SER
4	U	168	SER
4	U	170	ASP
4	U	172	THR
4	U	174	SER
4	U	175	LEU
4	U	176	SER
4	U	182	SER
4	U	183	LYS

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Mol	Chain	Res	Type
4	U	190	LYS
4	U	201	LEU
4	U	203	SER
4	U	208	SER
4	U	210	ASN
3	V	2	VAL
3	V	7	SER
3	V	11	VAL
3	V	16	SER
3	V	17	SER
3	V	21	SER
3	V	25	SER
3	V	28	THR
3	V	33	VAL
3	V	61	GLN
3	V	64	GLN
3	V	66	ARG
3	V	68	THR
3	V	70	THR
3	V	75	THR
3	V	83	THR
3	V	92	CYS
3	V	97	SER
3	V	110	THR
4	W	5	THR
4	W	11	LEU
4	W	14	SER
4	W	18	ARG
4	W	19	VAL
4	W	26	SER
4	W	30	ARG
4	W	52	SER
4	W	60	SER
4	W	61	ARG
4	W	63	ARG
4	W	67	SER
4	W	74	THR
4	W	77	SER
4	W	78	LEU
4	W	81	GLU
4	W	85	THR
4	W	90	GLN

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Mol	Chain	Res	Type
4	W	94	LEU
3	X	6	GLU
3	X	7	SER
3	X	10	GLU
3	X	12	LYS
3	X	28	THR
3	X	31	THR
3	X	48	VAL
3	X	53	ILE
3	X	62	LYS
3	X	64	GLN
3	X	68	THR
3	X	70	THR
3	X	77	THR
3	X	83	THR
3	X	85	GLU
3	X	87	THR
3	X	97	SER
3	X	111	VAL
3	X	115	SER
3	X	117	LYS
3	X	142	VAL
3	X	146	PHE
3	X	148	GLU
3	X	150	VAL
3	X	169	VAL
3	X	170	LEU
3	X	171	GLN
3	X	180	SER
3	X	204	ASN
3	X	207	VAL
4	Y	5	THR
4	Y	9	SER
4	Y	11	LEU
4	Y	14	SER
4	Y	18	ARG
4	Y	19	VAL
4	Y	26	SER
4	Y	52	SER
4	Y	60	SER
4	Y	61	ARG
4	Y	63	ARG

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Mol	Chain	Res	Type
4	Y	65	SER
4	Y	74	THR
4	Y	77	SER
4	Y	78	LEU
4	Y	81	GLU
4	Y	83	ILE
4	Y	90	GLN
4	Y	94	LEU
4	Y	105	GLU
3	Z	4	LEU
3	Z	6	GLU
3	Z	7	SER
3	Z	10	GLU
3	Z	12	LYS
3	Z	28	THR
3	Z	31	THR
3	Z	48	VAL
3	Z	57	SER
3	Z	62	LYS
3	Z	64	GLN
3	Z	68	THR
3	Z	70	THR
3	Z	83	THR
3	Z	84	SER
3	Z	87	THR
3	Z	89	VAL
3	Z	97	SER
3	Z	111	VAL
3	Z	113	SER
3	Z	115	SER
3	Z	117	LYS
3	Z	121	VAL
3	Z	146	PHE
3	Z	150	VAL
3	Z	164	HIS
3	Z	170	LEU
3	Z	171	GLN
3	Z	195	ILE
3	Z	197	ASN
4	z	5	THR
4	z	11	LEU
4	z	14	SER

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Mol	Chain	Res	Type
4	z	18	ARG
4	z	19	VAL
4	z	21	ILE
4	z	26	SER
4	z	60	SER
4	z	61	ARG
4	z	63	ARG
4	z	65	SER
4	z	67	SER
4	z	69	THR
4	z	74	THR
4	z	77	SER
4	z	78	LEU
4	z	81	GLU
4	z	85	THR
4	z	90	GLN
4	z	94	LEU
4	z	156	SER
4	z	158	ASN
4	z	159	SER
4	z	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	25	HIS
2	a	171	ASN
1	B	295	HIS
2	b	26	HIS
2	b	171	ASN
1	C	295	HIS
1	C	298	HIS
1	C	325	GLN
2	c	125	GLN
1	D	295	HIS
2	d	114	ASN
1	E	33	ASN
1	E	47	HIS
1	E	129	GLN
1	E	295	HIS
2	e	26	HIS
1	G	103	ASN

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Mol	Chain	Res	Type
1	H	295	HIS
2	h	30	GLN
2	h	125	GLN
1	I	295	HIS
2	i	125	GLN
4	K	34	ASN
3	N	171	GLN
4	O	90	GLN
4	O	155	GLN
4	Q	90	GLN
3	R	39	GLN
3	R	171	GLN
4	S	24	GLN
4	S	38	GLN
4	S	90	GLN
4	S	155	GLN
3	V	39	GLN
4	W	38	GLN
4	Y	90	GLN
4	z	24	GLN
4	z	90	GLN

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)

24 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	$\#\|Z\| > 2$
5	NAG	j	1	5,1	14,14,15	0.54	0	17,19,21	1.24	2 (11%)
5	NAG	j	2	5	14,14,15	0.61	0	17,19,21	0.82	0
5	NAG	k	1	5,1	14,14,15	0.52	0	17,19,21	1.07	1 (5%)
5	NAG	k	2	5	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
6	NAG	l	1	6,1	14,14,15	0.60	0	17,19,21	1.72	3 (17%)
6	NAG	l	2	6	14,14,15	0.52	0	17,19,21	0.98	0
6	BMA	l	3	6	11,11,12	0.55	0	15,15,17	1.12	1 (6%)
5	NAG	m	1	5,1	14,14,15	0.48	0	17,19,21	1.09	2 (11%)
5	NAG	m	2	5	14,14,15	0.57	0	17,19,21	0.65	0
5	NAG	n	1	5,1	14,14,15	0.62	0	17,19,21	1.52	3 (17%)
5	NAG	n	2	5	14,14,15	0.58	0	17,19,21	0.96	0
5	NAG	o	1	5,1	14,14,15	0.62	0	17,19,21	1.68	3 (17%)
5	NAG	o	2	5	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
6	NAG	p	1	6,1	14,14,15	0.62	0	17,19,21	1.06	1 (5%)
6	NAG	p	2	6	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
6	BMA	p	3	6	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
5	NAG	q	1	5,1	14,14,15	0.50	0	17,19,21	1.02	1 (5%)
5	NAG	q	2	5	14,14,15	0.56	0	17,19,21	0.83	0
5	NAG	r	1	5,1	14,14,15	0.49	0	17,19,21	1.39	1 (5%)
5	NAG	r	2	5	14,14,15	0.52	0	17,19,21	0.77	1 (5%)
5	NAG	s	1	5,1	14,14,15	0.48	0	17,19,21	1.29	1 (5%)
5	NAG	s	2	5	14,14,15	0.51	0	17,19,21	0.64	0
5	NAG	t	1	5,1	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
5	NAG	t	2	5	14,14,15	0.48	0	17,19,21	1.19	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	j	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	j	2	5	-	4/6/23/26	0/1/1/1
5	NAG	k	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
6	NAG	l	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	l	3	6	-	2/2/19/22	0/1/1/1
5	NAG	m	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	2/6/23/26	0/1/1/1
5	NAG	n	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	n	2	5	-	4/6/23/26	0/1/1/1
5	NAG	o	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
6	NAG	p	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	p	2	6	-	2/6/23/26	0/1/1/1
6	BMA	p	3	6	-	2/2/19/22	0/1/1/1
5	NAG	q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	r	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	r	2	5	-	2/6/23/26	0/1/1/1
5	NAG	s	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	NAG	t	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	1	NAG	C2-N2-C7	-5.22	115.90	122.90
5	o	1	NAG	C2-N2-C7	-5.03	116.16	122.90
5	n	1	NAG	C2-N2-C7	4.00	128.27	122.90
5	r	1	NAG	C3-C4-C5	3.67	116.89	110.23
5	j	1	NAG	C1-O5-C5	3.29	116.59	112.19
6	l	3	BMA	O5-C5-C6	3.28	114.05	107.66
5	o	2	NAG	C1-O5-C5	3.12	116.37	112.19
6	p	2	NAG	C2-N2-C7	-2.85	119.08	122.90
5	k	1	NAG	C1-O5-C5	2.79	115.92	112.19
6	p	1	NAG	C2-N2-C7	-2.77	119.19	122.90
5	t	1	NAG	O5-C1-C2	-2.74	107.05	111.29
6	l	1	NAG	O5-C1-C2	-2.61	107.25	111.29
5	t	2	NAG	C1-O5-C5	2.49	115.52	112.19
5	m	1	NAG	O5-C5-C6	2.47	112.46	107.66
6	p	3	BMA	C1-C2-C3	2.44	113.20	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	1	NAG	O7-C7-C8	-2.40	117.78	122.05
5	s	1	NAG	O5-C5-C6	2.38	112.29	107.66
6	l	1	NAG	C3-C4-C5	2.35	114.49	110.23
6	p	3	BMA	C1-O5-C5	2.25	115.21	112.19
5	t	2	NAG	O5-C5-C6	2.21	111.97	107.66
5	m	1	NAG	C4-C3-C2	-2.21	107.78	111.02
5	r	2	NAG	C2-N2-C7	-2.16	120.01	122.90
5	o	1	NAG	O5-C1-C2	-2.15	107.96	111.29
5	k	2	NAG	C1-O5-C5	2.14	115.06	112.19
5	q	1	NAG	O5-C5-C6	2.13	111.81	107.66
5	o	1	NAG	O7-C7-N2	-2.09	118.29	121.98
5	j	1	NAG	C2-N2-C7	-2.08	120.11	122.90
5	n	1	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	k	1	NAG	C8-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	o	1	NAG	C8-C7-N2-C2
5	o	1	NAG	O7-C7-N2-C2
5	q	1	NAG	C8-C7-N2-C2
5	q	1	NAG	O7-C7-N2-C2
5	r	1	NAG	C8-C7-N2-C2
5	r	1	NAG	O7-C7-N2-C2
5	s	2	NAG	C8-C7-N2-C2
5	s	2	NAG	O7-C7-N2-C2
5	t	1	NAG	C8-C7-N2-C2
5	t	1	NAG	O7-C7-N2-C2
6	l	1	NAG	C8-C7-N2-C2
6	l	1	NAG	O7-C7-N2-C2
6	p	1	NAG	C8-C7-N2-C2
6	p	1	NAG	O7-C7-N2-C2
5	m	1	NAG	O5-C5-C6-O6
6	p	3	BMA	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
5	r	1	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
6	l	3	BMA	O5-C5-C6-O6
5	m	1	NAG	C4-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6

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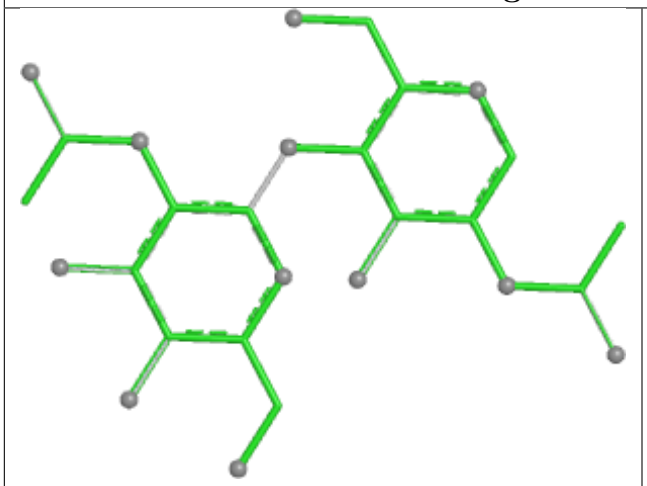
Mol	Chain	Res	Type	Atoms
5	r	1	NAG	C4-C5-C6-O6
6	l	3	BMA	C4-C5-C6-O6
6	p	3	BMA	C4-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
5	m	2	NAG	C4-C5-C6-O6
5	j	1	NAG	C8-C7-N2-C2
5	r	2	NAG	C8-C7-N2-C2
5	r	2	NAG	O7-C7-N2-C2
6	p	2	NAG	C8-C7-N2-C2
6	p	2	NAG	O7-C7-N2-C2
6	p	1	NAG	C4-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
5	j	2	NAG	C8-C7-N2-C2
5	n	2	NAG	C8-C7-N2-C2
5	j	1	NAG	O7-C7-N2-C2
5	j	2	NAG	O7-C7-N2-C2
5	n	2	NAG	O7-C7-N2-C2
6	l	2	NAG	C8-C7-N2-C2
6	p	1	NAG	O5-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
6	l	2	NAG	O7-C7-N2-C2
5	o	2	NAG	C8-C7-N2-C2
5	k	2	NAG	O5-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	n	1	NAG	C4-C5-C6-O6
5	o	2	NAG	O7-C7-N2-C2
5	t	2	NAG	C8-C7-N2-C2
5	t	2	NAG	O7-C7-N2-C2
5	n	1	NAG	O5-C5-C6-O6
5	r	1	NAG	C3-C2-N2-C7

There are no ring outliers.

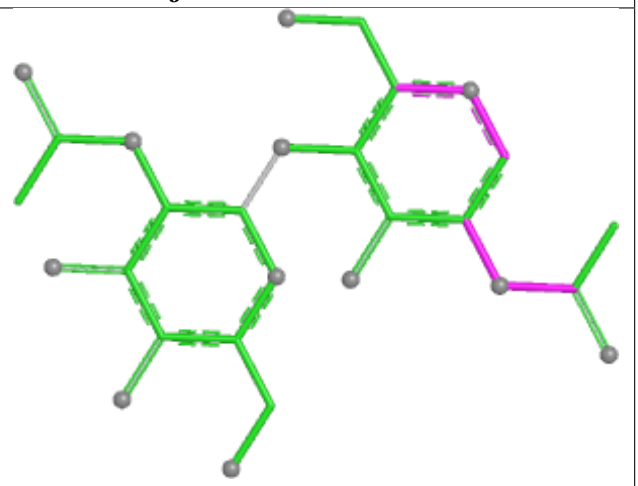
No monomer is involved in short contacts.

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

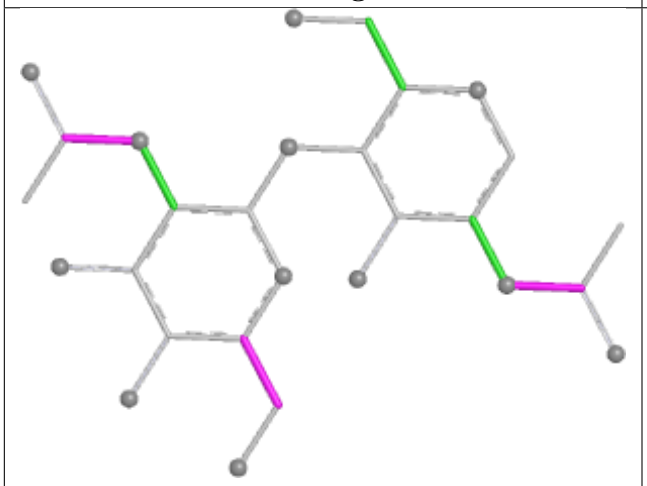
Oligosaccharide Chain j



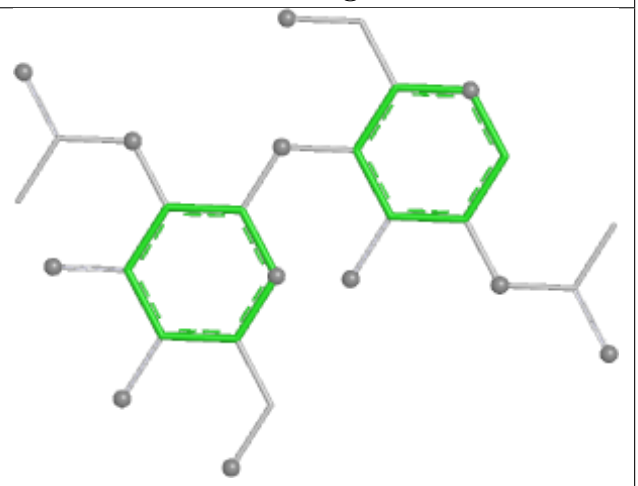
Bond lengths



Bond angles

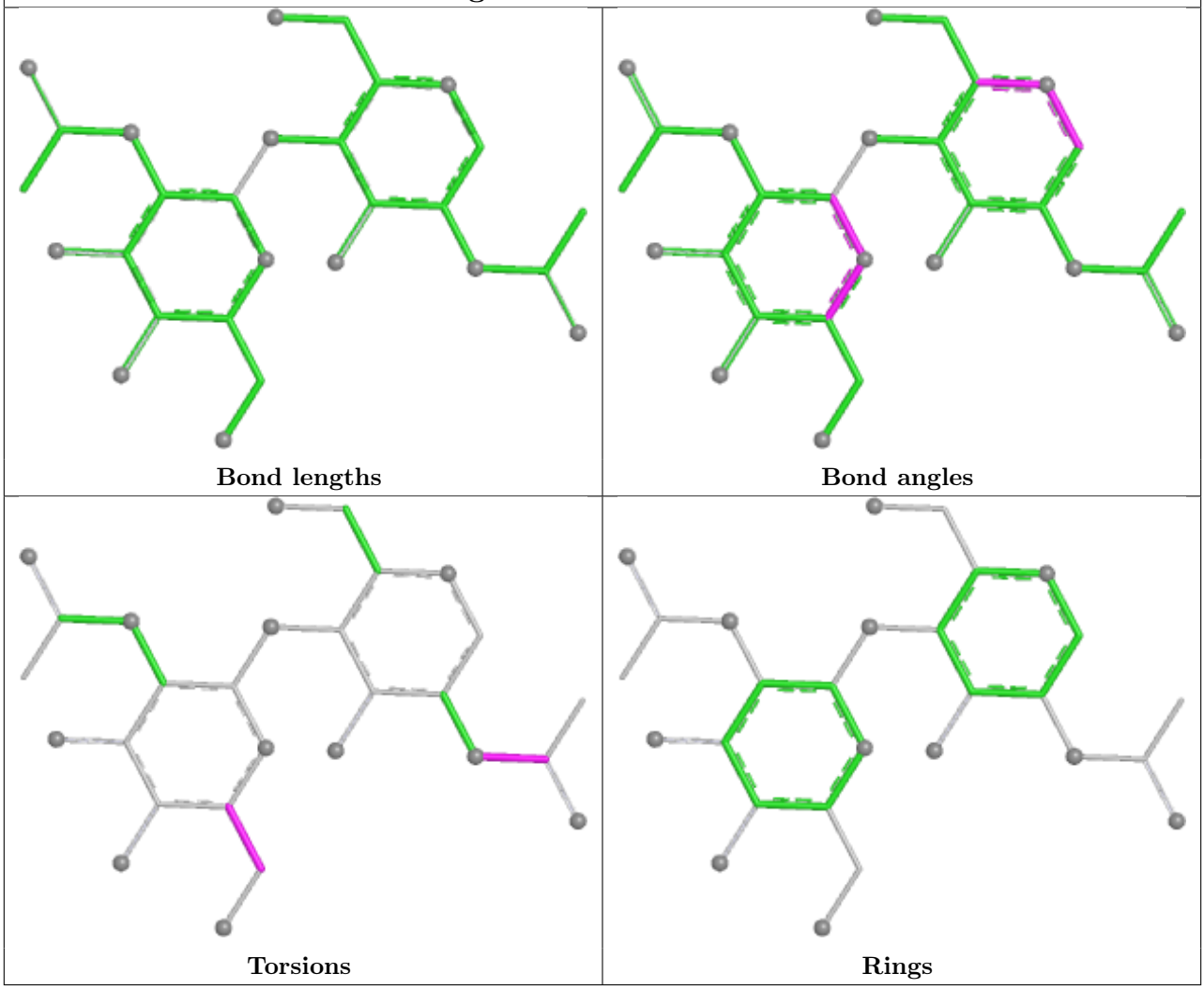


Torsions

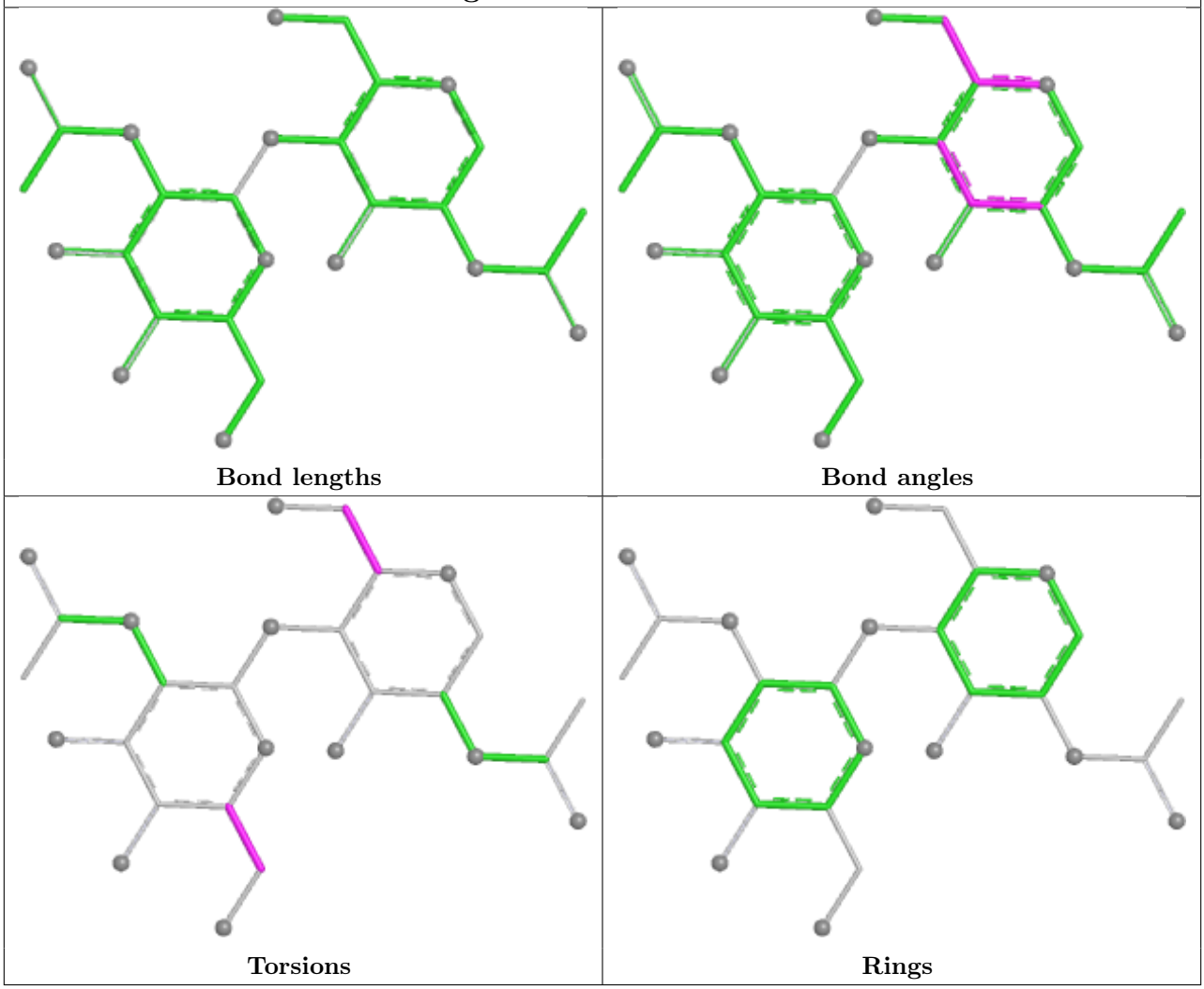


Rings

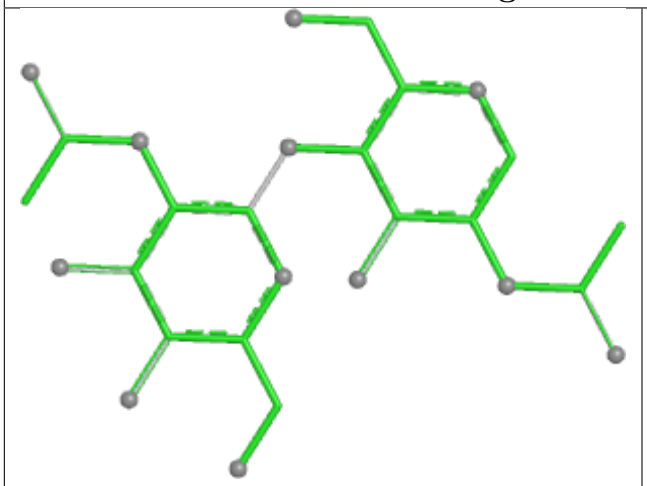
Oligosaccharide Chain k



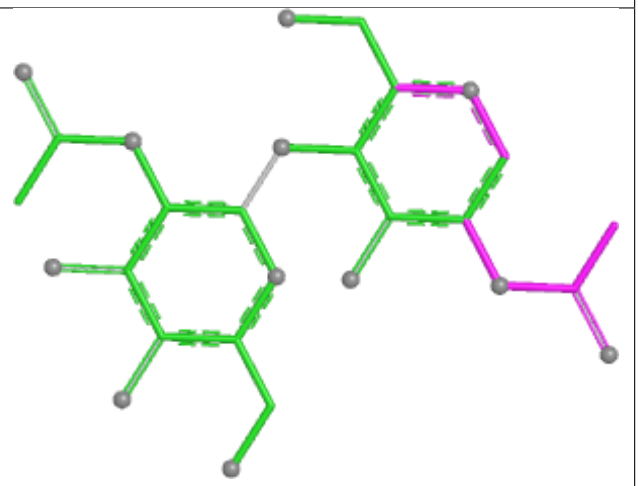
Oligosaccharide Chain m



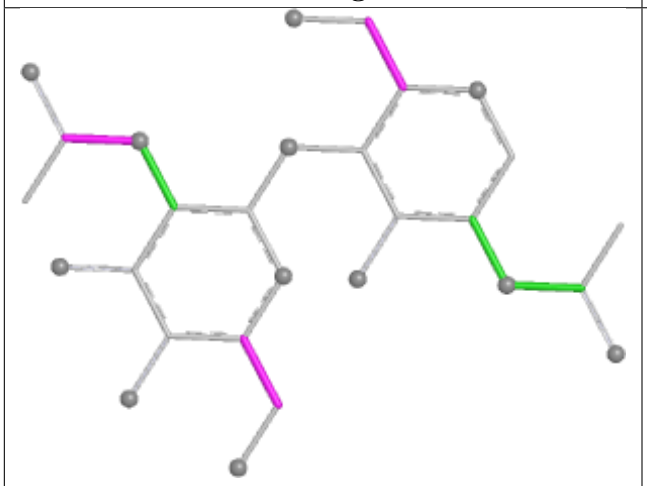
Oligosaccharide Chain n



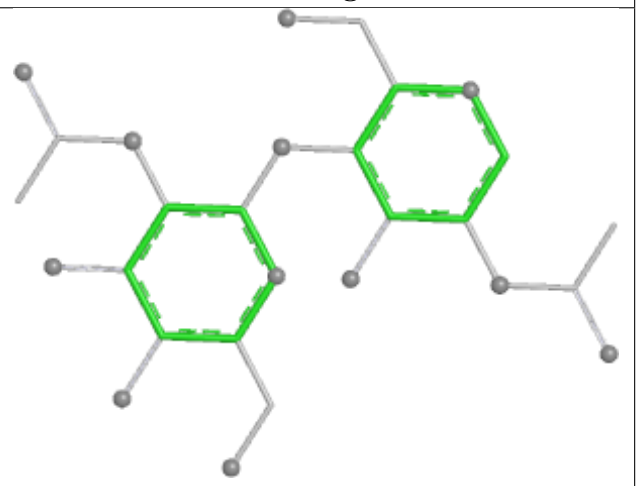
Bond lengths



Bond angles

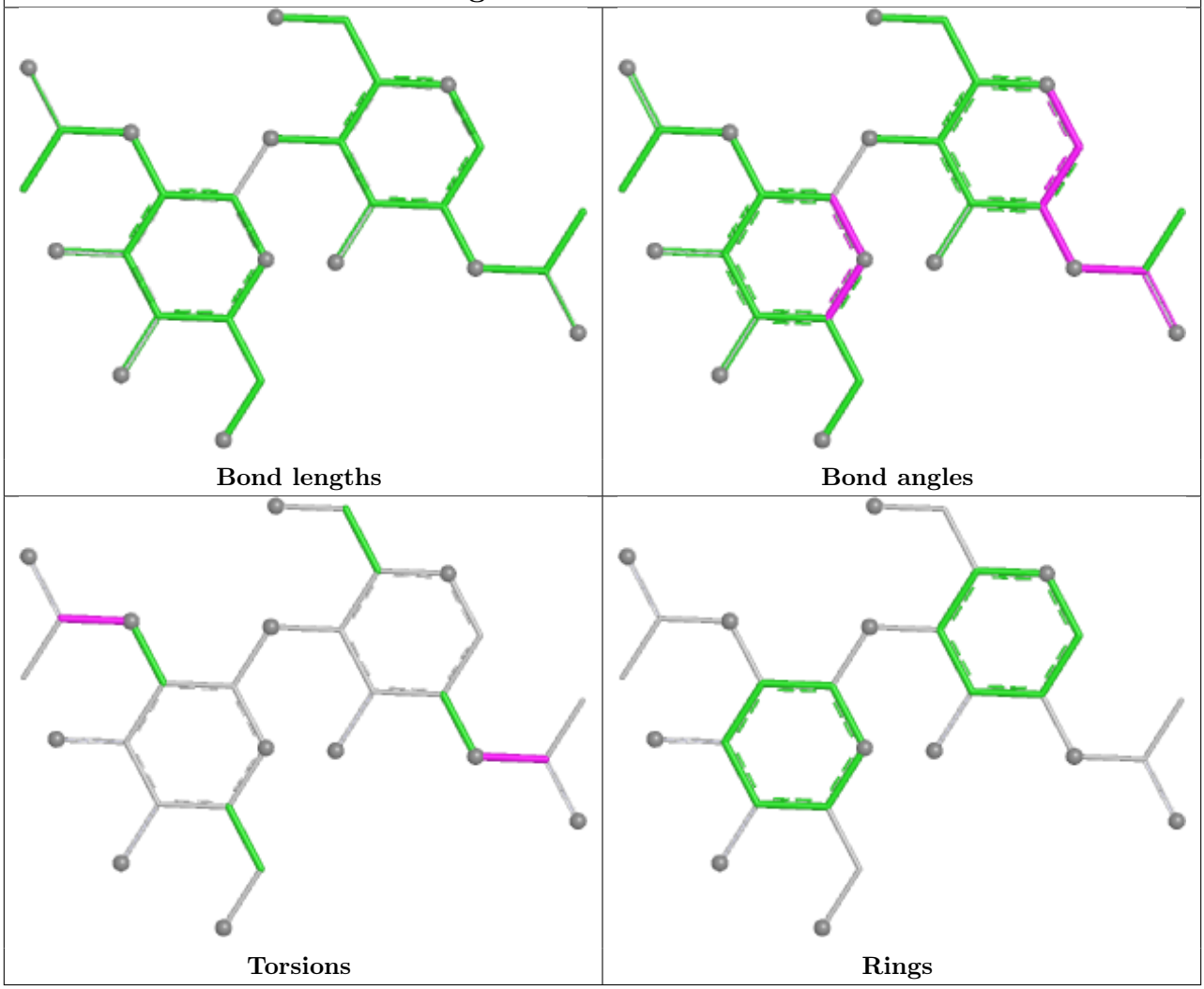


Torsions

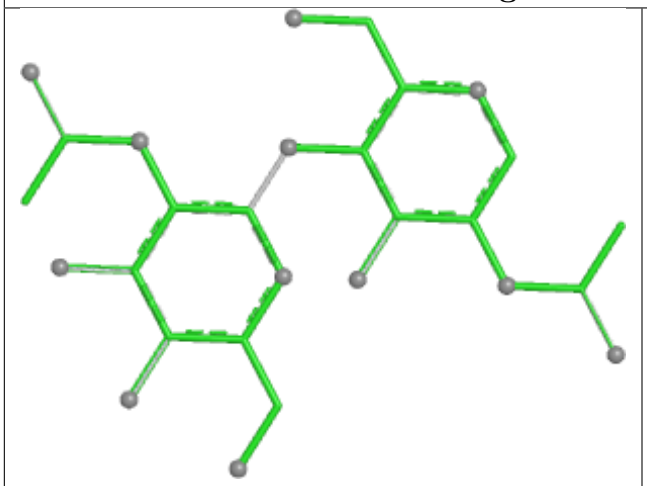


Rings

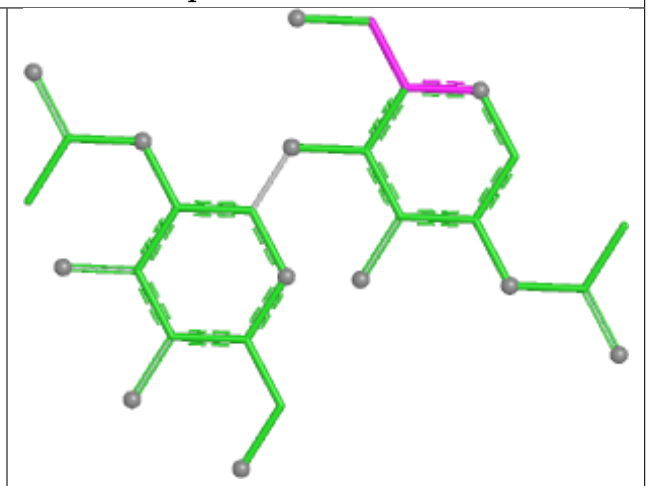
Oligosaccharide Chain o



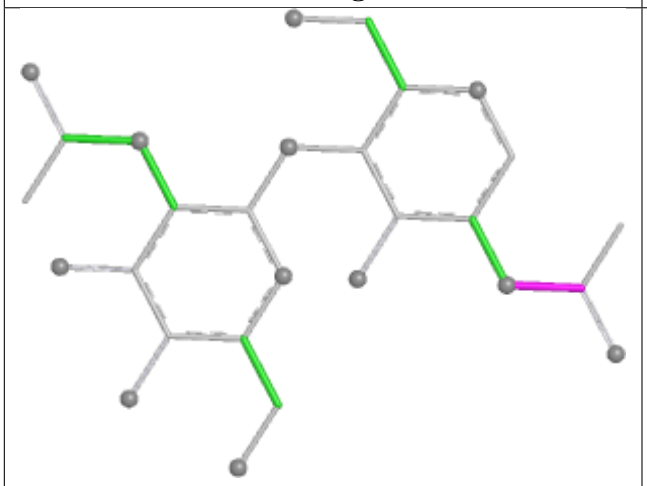
Oligosaccharide Chain q



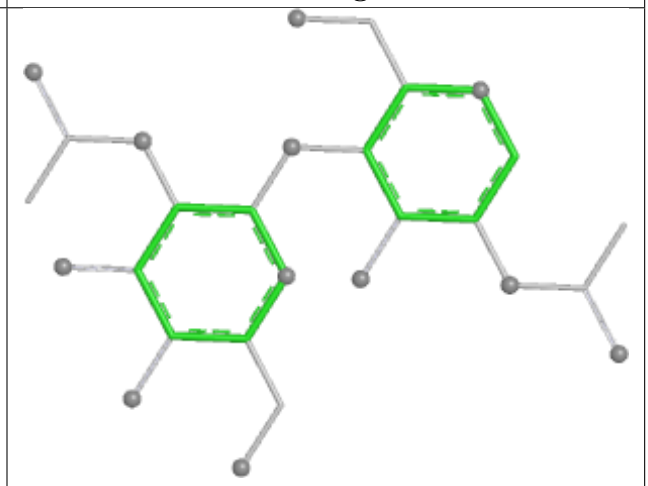
Bond lengths



Bond angles

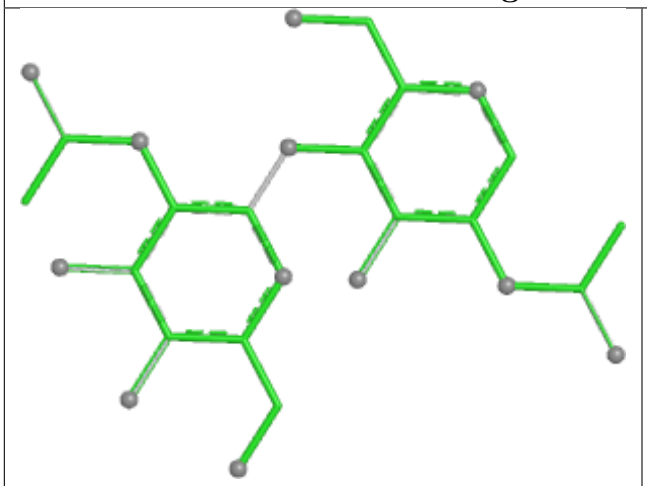


Torsions

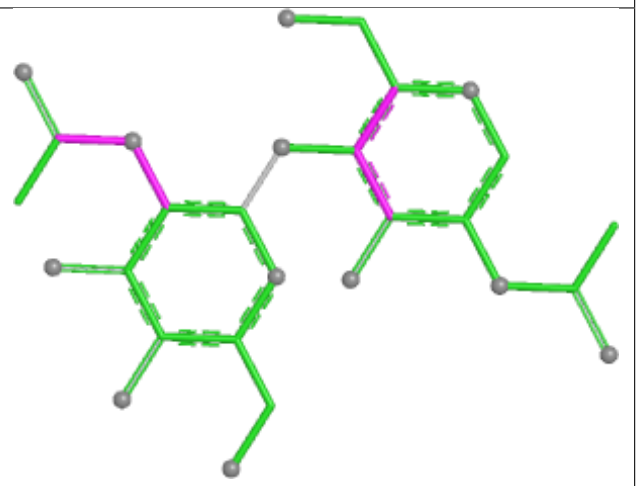


Rings

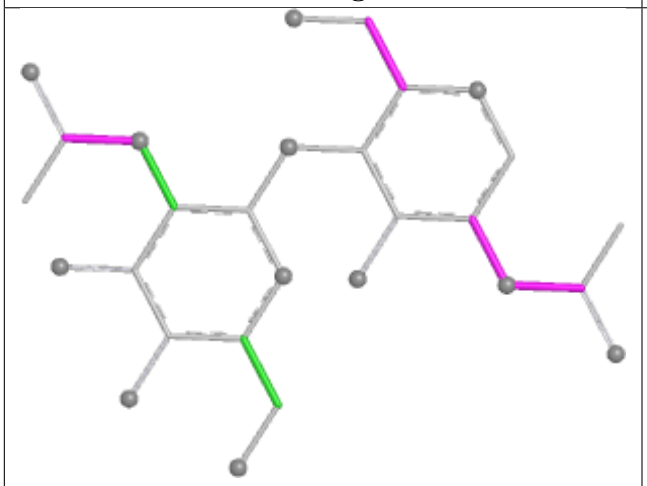
Oligosaccharide Chain r



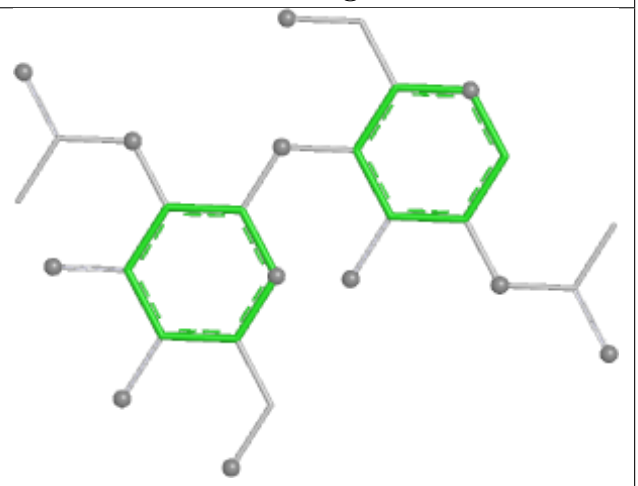
Bond lengths



Bond angles

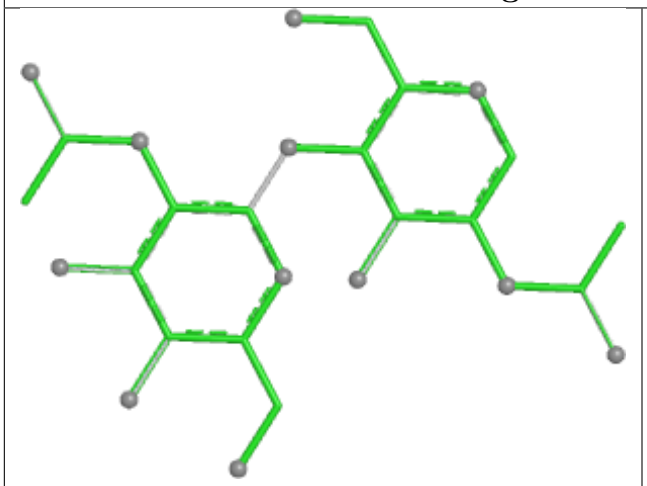


Torsions

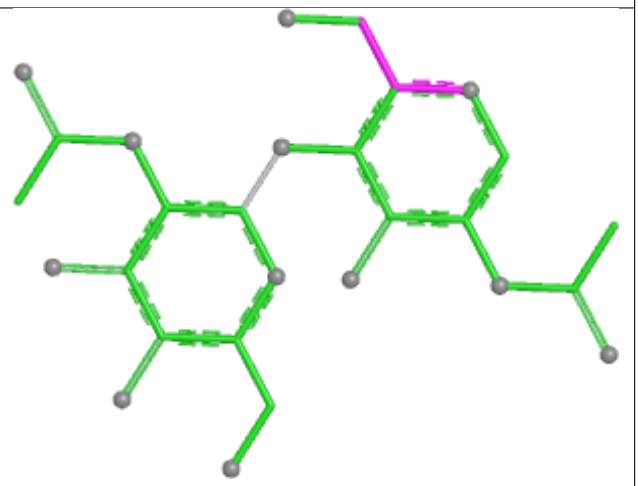


Rings

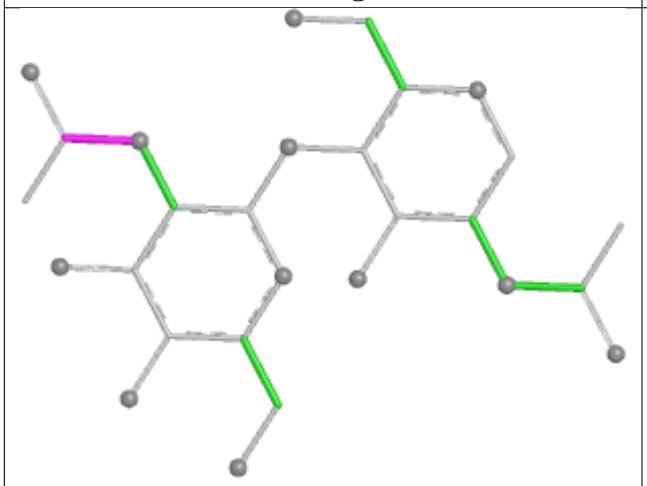
Oligosaccharide Chain s



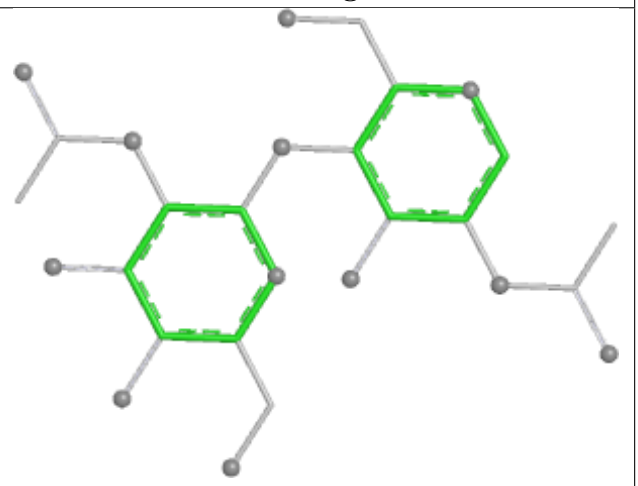
Bond lengths



Bond angles

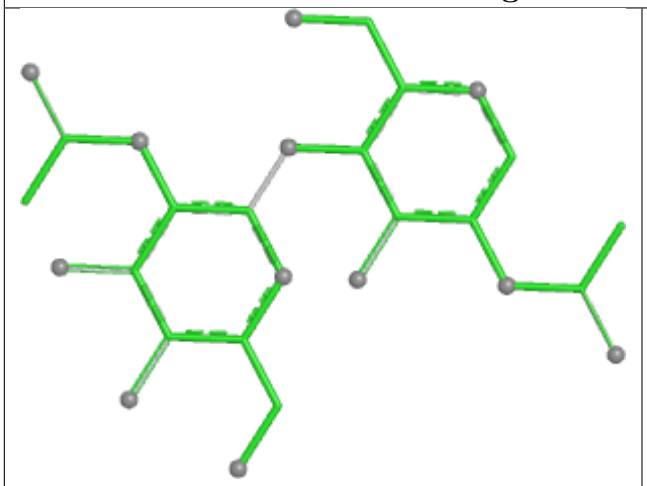


Torsions

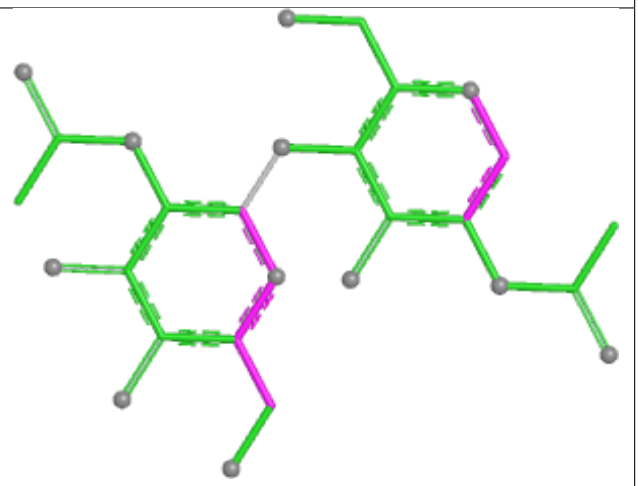


Rings

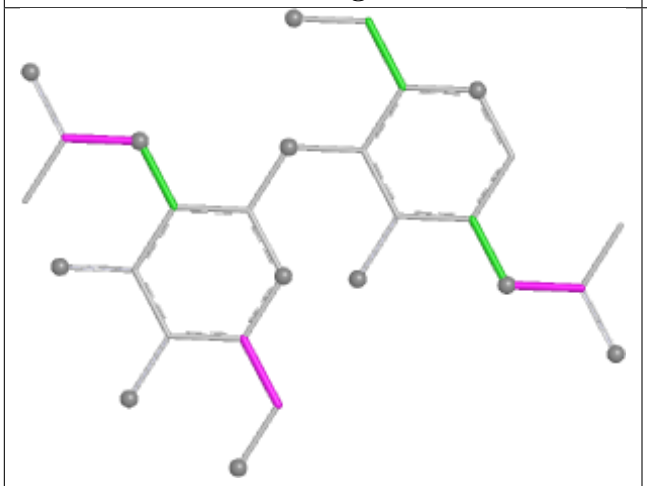
Oligosaccharide Chain t



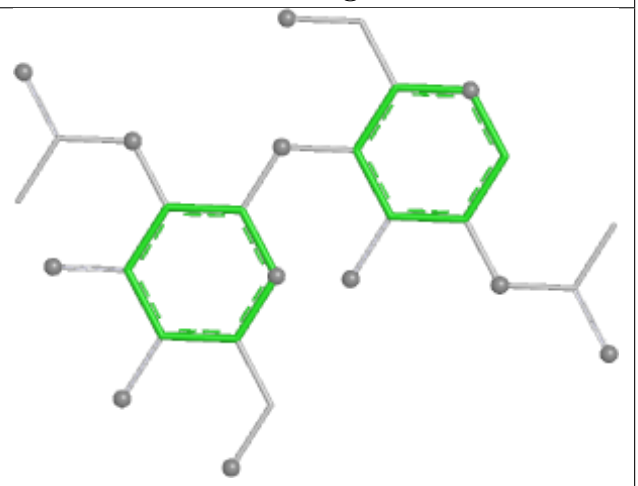
Bond lengths



Bond angles

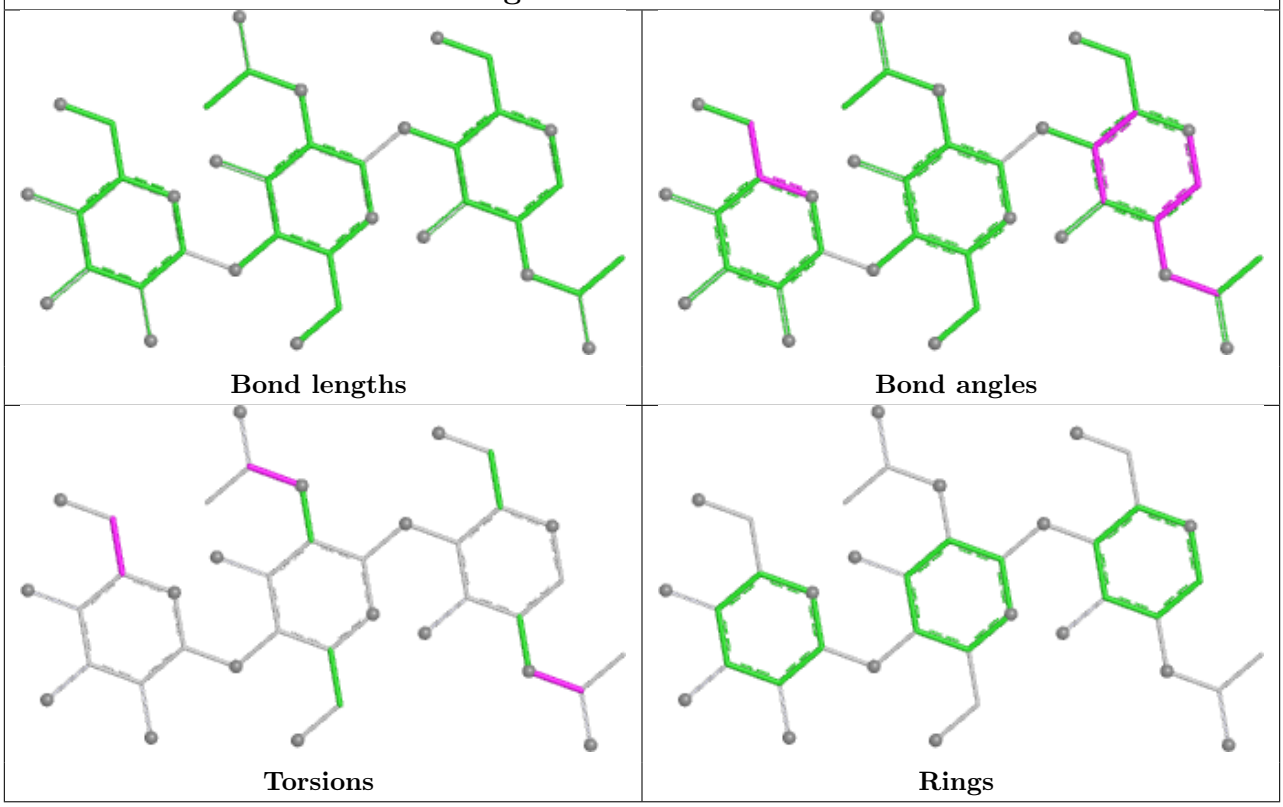


Torsions

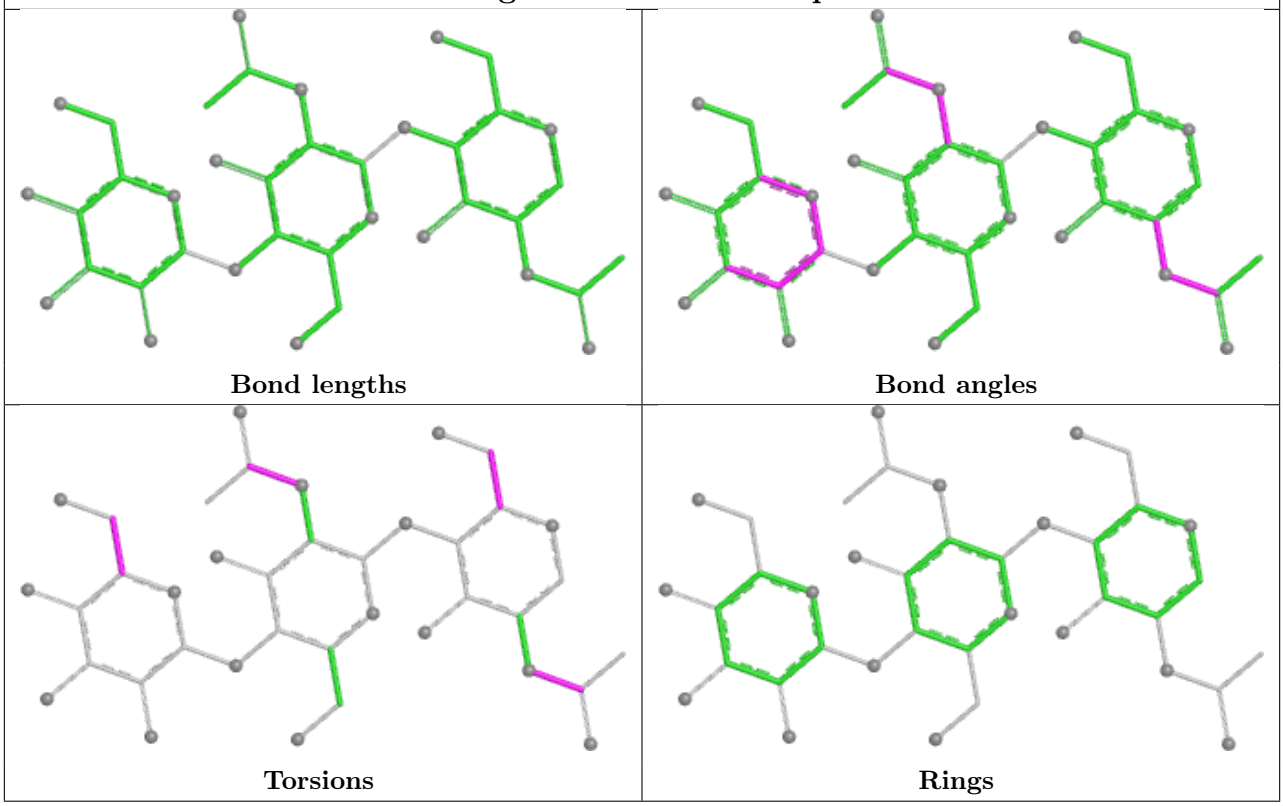


Rings

Oligosaccharide Chain l



Oligosaccharide Chain p



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	$\#\|Z\| > 2$
7	NAG	A	403	1	14,14,15	0.49	0	17,19,21	1.31	1 (5%)
7	NAG	E	401	1	14,14,15	0.51	0	17,19,21	1.32	3 (17%)
7	NAG	C	404	1	14,14,15	1.78	2 (14%)	17,19,21	2.66	4 (23%)
7	NAG	F	403	1	14,14,15	0.37	0	17,19,21	1.17	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	403	1	-	2/6/23/26	0/1/1/1
7	NAG	E	401	1	-	2/6/23/26	0/1/1/1
7	NAG	C	404	1	-	3/6/23/26	0/1/1/1
7	NAG	F	403	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	404	NAG	C1-C2	4.18	1.58	1.52
7	C	404	NAG	O5-C5	3.84	1.50	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	404	NAG	C1-O5-C5	9.78	125.29	112.19
7	A	403	NAG	C1-O5-C5	3.68	117.12	112.19
7	F	403	NAG	C1-O5-C5	3.35	116.67	112.19
7	E	401	NAG	C1-O5-C5	2.97	116.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	404	NAG	C1-C2-N2	-2.35	106.72	110.43
7	E	401	NAG	C2-N2-C7	-2.31	119.81	122.90
7	C	404	NAG	O5-C1-C2	2.27	114.81	111.29
7	C	404	NAG	C4-C3-C2	-2.26	107.71	111.02
7	E	401	NAG	O5-C1-C2	-2.07	108.09	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	403	NAG	O7-C7-N2-C2
7	A	403	NAG	C8-C7-N2-C2
7	C	404	NAG	O5-C5-C6-O6
7	C	404	NAG	C8-C7-N2-C2
7	F	403	NAG	C8-C7-N2-C2
7	C	404	NAG	O7-C7-N2-C2
7	E	401	NAG	C8-C7-N2-C2
7	F	403	NAG	O7-C7-N2-C2
7	E	401	NAG	O7-C7-N2-C2

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	323/327 (98%)	-0.34	0	100	100	20, 53, 91, 130	0
1	B	319/327 (97%)	-0.18	2 (0%)	89	83	25, 60, 101, 142	0
1	C	324/327 (99%)	-0.25	2 (0%)	89	83	21, 58, 98, 133	0
1	D	324/327 (99%)	-0.20	2 (0%)	89	83	38, 66, 99, 168	0
1	E	323/327 (98%)	-0.25	1 (0%)	94	92	45, 68, 97, 125	0
1	F	324/327 (99%)	-0.07	4 (1%)	79	67	45, 76, 107, 138	0
1	G	324/327 (99%)	0.17	5 (1%)	73	61	46, 82, 124, 162	0
1	H	325/327 (99%)	-0.40	0	100	100	31, 53, 82, 122	0
1	I	324/327 (99%)	-0.13	1 (0%)	94	92	42, 75, 107, 127	0
2	a	171/174 (98%)	-0.02	3 (1%)	68	55	25, 75, 130, 168	0
2	b	167/174 (95%)	0.02	5 (2%)	50	34	24, 79, 138, 179	0
2	c	172/174 (98%)	-0.02	3 (1%)	70	57	30, 79, 134, 176	0
2	d	172/174 (98%)	0.32	8 (4%)	31	19	43, 91, 149, 196	0
2	e	172/174 (98%)	-0.05	5 (2%)	51	36	38, 69, 123, 176	0
2	f	172/174 (98%)	-0.03	4 (2%)	60	47	46, 74, 125, 195	0
2	g	172/174 (98%)	0.09	5 (2%)	51	36	43, 81, 145, 169	0
2	h	167/174 (95%)	-0.28	0	100	100	35, 49, 85, 134	0
2	i	172/174 (98%)	-0.26	2 (1%)	79	67	33, 55, 122, 187	0
3	J	115/223 (51%)	0.68	11 (9%)	8	4	46, 94, 132, 166	0
3	L	212/223 (95%)	-0.33	1 (0%)	91	86	20, 38, 99, 134	0
3	N	223/223 (100%)	-0.37	1 (0%)	92	89	14, 28, 73, 129	0
3	P	161/223 (72%)	0.40	16 (9%)	7	4	52, 90, 147, 172	0
3	R	214/223 (95%)	0.17	7 (3%)	46	30	45, 83, 114, 128	0
3	T	213/223 (95%)	0.76	26 (12%)	4	2	62, 107, 153, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	V	117/223 (52%)	1.22	22 (18%) 1 1	66, 122, 174, 221	0
3	X	164/223 (73%)	0.16	13 (7%) 12 6	35, 67, 110, 147	0
3	Z	167/223 (74%)	0.05	8 (4%) 30 18	59, 95, 128, 180	0
4	K	106/214 (49%)	0.48	9 (8%) 10 6	63, 111, 145, 173	0
4	M	214/214 (100%)	-0.21	1 (0%) 91 86	19, 42, 96, 150	0
4	O	214/214 (100%)	-0.50	0 100 100	16, 30, 52, 70	0
4	Q	157/214 (73%)	0.33	19 (12%) 4 2	49, 90, 134, 161	0
4	S	211/214 (98%)	0.00	4 (1%) 66 53	52, 77, 123, 185	0
4	U	211/214 (98%)	0.46	10 (4%) 31 19	66, 104, 140, 162	0
4	W	105/214 (49%)	0.05	1 (0%) 82 72	57, 88, 125, 148	0
4	Y	109/214 (50%)	-0.41	0 100 100	36, 51, 76, 98	0
4	z	119/214 (55%)	0.46	6 (5%) 28 16	61, 98, 140, 161	0
All	All	7479/8442 (88%)	-0.02	207 (2%) 53 37	14, 70, 129, 233	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	134	CYS	7.3
3	T	185	PRO	6.4
3	T	180	SER	6.3
3	T	183	THR	5.8
3	V	48	VAL	5.6
1	D	9	PRO	5.5
3	J	105	GLN	5.4
3	T	82	LEU	5.1
3	J	90	TYR	5.1
4	S	154	LEU	4.9
3	T	140	CYS	4.7
4	Q	113	PRO	4.5
3	P	142	VAL	4.4
4	Q	135	LEU	4.4
4	K	80	PRO	4.4
3	X	199	ASN	4.2
3	T	184	VAL	4.2
3	Z	141	LEU	4.2
3	V	82	LEU	4.1
3	V	82(A)	THR	4.1
3	T	186	SER	4.0

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Mol	Chain	Res	Type	RSRZ
4	Q	137	ASN	4.0
3	P	180	SER	4.0
3	J	34	PHE	4.0
3	V	8	GLY	4.0
3	X	174	GLY	3.9
3	V	45	LEU	3.9
2	f	59	MET	3.8
1	G	144	ASN	3.8
2	d	27	SER	3.7
3	T	150	VAL	3.7
2	d	33	GLY	3.7
4	Q	200	GLY	3.7
3	X	141	LEU	3.6
2	f	65	ALA	3.6
3	V	41	PRO	3.6
3	X	172	SER	3.6
2	c	65	ALA	3.6
3	T	136	ALA	3.6
3	V	49	GLY	3.6
2	d	26	HIS	3.5
2	g	32	SER	3.5
2	b	65	ALA	3.4
1	F	325	GLN	3.4
4	Q	160	GLN	3.4
3	P	119	PRO	3.4
3	V	80	MET	3.4
2	e	61	THR	3.4
3	V	75	THR	3.4
3	X	179	SER	3.4
3	X	170	LEU	3.3
2	b	27	SER	3.3
2	d	65	ALA	3.3
2	e	63	PHE	3.3
2	e	62	GLN	3.3
4	K	42	LYS	3.2
3	T	138	LEU	3.2
4	z	62	PHE	3.2
3	V	81	GLU	3.1
4	Q	203	SER	3.1
3	T	145	TYR	3.1
3	T	80	MET	3.1
3	Z	121	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	T	141	LEU	3.1
1	E	325	GLN	3.1
1	F	288	ILE	3.1
3	V	7	SER	3.1
2	f	63	PHE	3.0
2	a	33	GLY	3.0
3	V	42	GLY	3.0
3	P	146	PHE	3.0
3	P	145	TYR	3.0
4	K	41	GLY	3.0
4	U	67	SER	3.0
3	X	142	VAL	2.9
4	U	134	CYS	2.9
3	J	104	GLY	2.9
3	R	181	VAL	2.9
4	U	63	ARG	2.9
2	c	60	ASN	2.9
3	X	171	GLN	2.9
3	T	211	VAL	2.9
3	T	137	ALA	2.8
4	Q	136	LEU	2.8
4	U	135	LEU	2.8
4	z	178	THR	2.8
3	V	86	ASP	2.8
4	Q	114	SER	2.7
3	T	181	VAL	2.7
3	T	189	LEU	2.7
3	J	41	PRO	2.7
4	U	116	PHE	2.7
4	Q	139	PHE	2.7
1	G	55	GLY	2.7
3	J	103	TRP	2.7
3	T	155	ASN	2.7
3	R	183	THR	2.7
2	d	64	GLU	2.7
3	J	95	GLY	2.6
3	R	174	GLY	2.6
4	K	45	ASN	2.6
2	g	35	ALA	2.6
3	R	125	ALA	2.6
2	i	65	ALA	2.6
4	Q	110	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
4	Q	133	VAL	2.6
3	P	160	THR	2.6
3	P	181	VAL	2.6
4	Q	199	GLN	2.6
1	G	326	ILE	2.5
3	P	173	SER	2.5
3	P	159	LEU	2.5
2	g	29	ASP	2.5
4	Q	80	PRO	2.5
4	M	119	PRO	2.5
3	X	120	SER	2.5
3	Z	179	SER	2.5
1	B	205	GLY	2.5
3	Z	198	VAL	2.5
4	S	153	ALA	2.5
3	V	63	PHE	2.5
2	g	168	LEU	2.5
3	V	27	GLY	2.5
4	S	135	LEU	2.4
3	T	18	VAL	2.4
3	T	154	TRP	2.4
1	C	276	ASN	2.4
3	P	177	SER	2.4
3	X	180	SER	2.4
2	g	62	GLN	2.4
1	G	137	ARG	2.4
3	R	145	TYR	2.4
4	U	12	SER	2.4
3	X	150	VAL	2.4
4	z	47	LEU	2.4
2	i	59	MET	2.4
3	Z	144	ASP	2.3
4	U	51	ALA	2.3
3	T	68	THR	2.3
2	e	29	ASP	2.3
3	P	161	SER	2.3
4	z	57	GLY	2.3
2	f	64	GLU	2.3
3	Z	123	PRO	2.3
1	C	277	CYS	2.3
3	T	120	SER	2.3
2	d	32	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	V	82(B)	SER	2.3
4	K	36	TYR	2.3
3	J	107	THR	2.3
3	T	112	SER	2.3
3	V	68	THR	2.3
4	K	17	ASP	2.3
1	D	326	ILE	2.3
3	V	11	VAL	2.3
3	V	20	VAL	2.3
4	K	62	PHE	2.3
4	Q	178	THR	2.2
3	Z	120	SER	2.2
4	U	179	LEU	2.2
1	I	244	ASN	2.2
3	T	193	THR	2.2
3	P	112	SER	2.2
2	e	1	GLY	2.2
3	P	179	SER	2.2
3	X	178	LEU	2.2
2	d	139	GLU	2.2
2	a	63	PHE	2.2
3	R	165	THR	2.2
3	V	9	ALA	2.2
4	S	181	LEU	2.2
3	P	115	SER	2.2
4	Q	177	SER	2.2
3	J	100(C)	PHE	2.1
4	U	193	ALA	2.1
4	z	56	THR	2.1
1	B	304	GLU	2.1
1	F	25	LYS	2.1
3	J	7	SER	2.1
2	b	144	CYS	2.1
4	Q	201	LEU	2.1
4	z	21	ILE	2.1
3	T	149	PRO	2.1
3	L	125	ALA	2.1
3	P	178	LEU	2.1
1	F	9	PRO	2.1
4	K	44	PRO	2.1
1	G	277	CYS	2.1
3	X	173	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	158	ASP	2.1
3	N	133	GLY	2.1
3	V	101	ASP	2.1
3	V	51	PHE	2.1
2	d	113	SER	2.1
4	W	80	PRO	2.0
3	Z	122	PHE	2.0
2	b	159	TYR	2.0
3	P	176	TYR	2.0
2	c	62	GLN	2.0
3	R	182	VAL	2.0
3	T	147	PRO	2.0
4	Q	109	THR	2.0
3	J	3	GLN	2.0
4	Q	111	ALA	2.0
4	K	57	GLY	2.0
4	U	178	THR	2.0
2	a	62	GLN	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(Å^2)	Q<0.9
6	BMA	l	3	11/12	0.61	0.31	109,140,145,148	0
5	NAG	s	2	14/15	0.72	0.46	148,157,164,167	0
5	NAG	o	2	14/15	0.81	0.30	97,113,122,124	0
5	NAG	t	2	14/15	0.82	0.22	82,103,118,122	0
5	NAG	n	2	14/15	0.83	0.25	101,113,121,122	0
5	NAG	k	2	14/15	0.84	0.22	125,133,136,140	0
5	NAG	j	2	14/15	0.85	0.26	90,107,119,121	0
6	BMA	p	3	11/12	0.85	0.15	117,121,132,137	0
5	NAG	r	2	14/15	0.86	0.34	94,108,128,135	0
6	NAG	l	2	14/15	0.86	0.34	88,117,138,139	0

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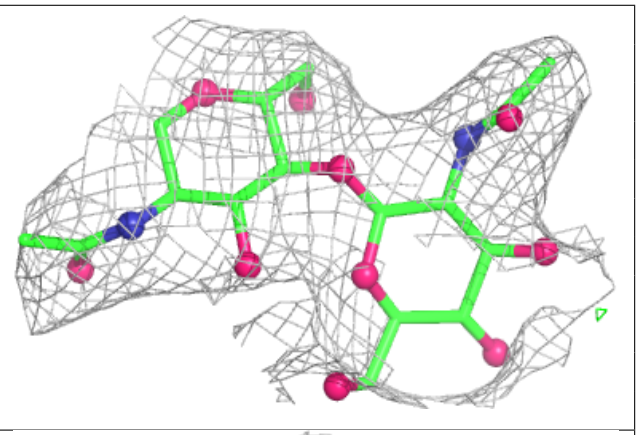
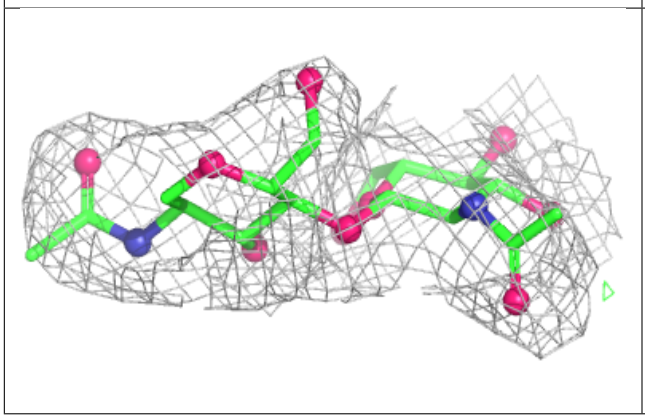
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	s	1	14/15	0.86	0.26	88,112,125,131	0
5	NAG	k	1	14/15	0.86	0.17	63,92,107,114	0
5	NAG	q	2	14/15	0.88	0.41	98,107,122,125	0
6	NAG	p	2	14/15	0.88	0.18	93,112,127,132	0
5	NAG	m	2	14/15	0.88	0.17	85,111,119,120	0
5	NAG	o	1	14/15	0.89	0.26	60,82,88,96	0
5	NAG	n	1	14/15	0.91	0.17	60,86,97,102	0
5	NAG	q	1	14/15	0.92	0.14	50,75,92,93	0
6	NAG	l	1	14/15	0.92	0.29	56,81,94,108	0
6	NAG	p	1	14/15	0.93	0.18	84,97,101,102	0
5	NAG	m	1	14/15	0.93	0.10	61,84,89,97	0
5	NAG	t	1	14/15	0.93	0.22	68,81,87,88	0
5	NAG	j	1	14/15	0.94	0.24	72,88,97,98	0
5	NAG	r	1	14/15	0.95	0.17	61,80,90,101	0

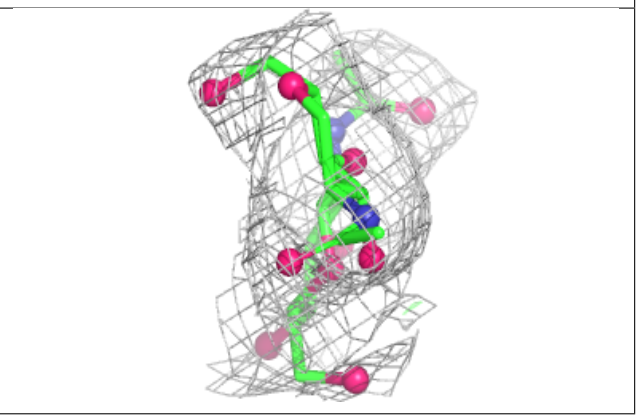
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain j:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

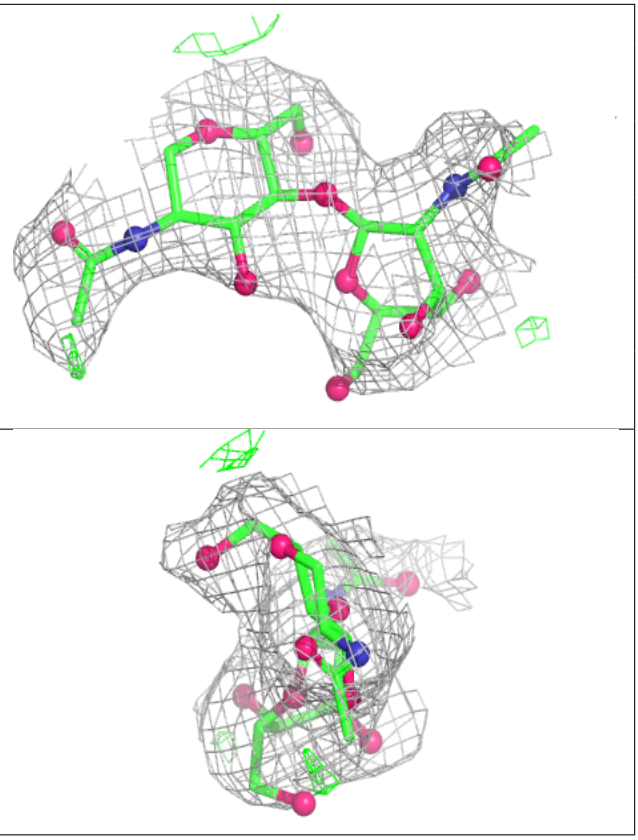






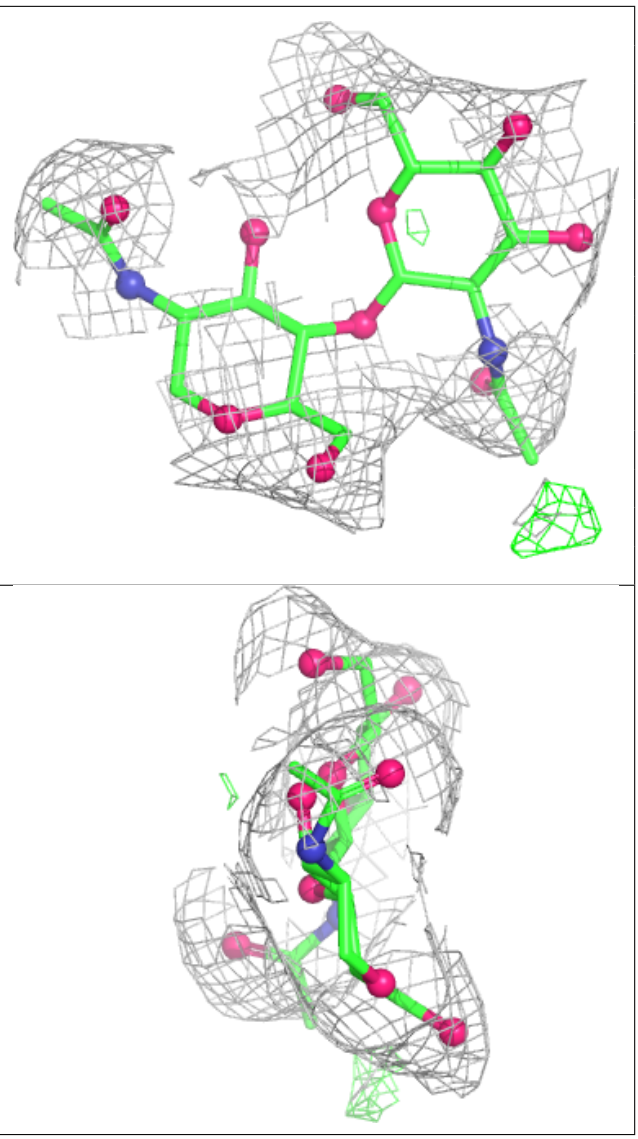
Electron density around Chain k:

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



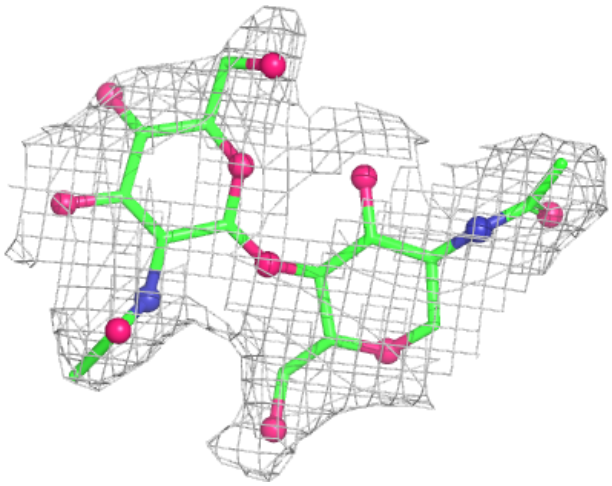
Electron density around Chain m:

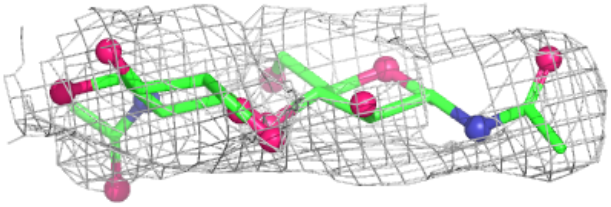
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

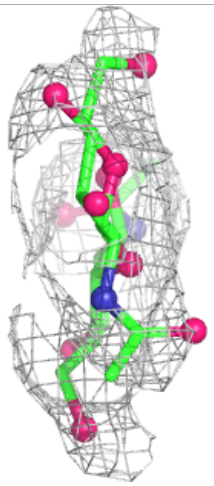


Electron density around Chain n:

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

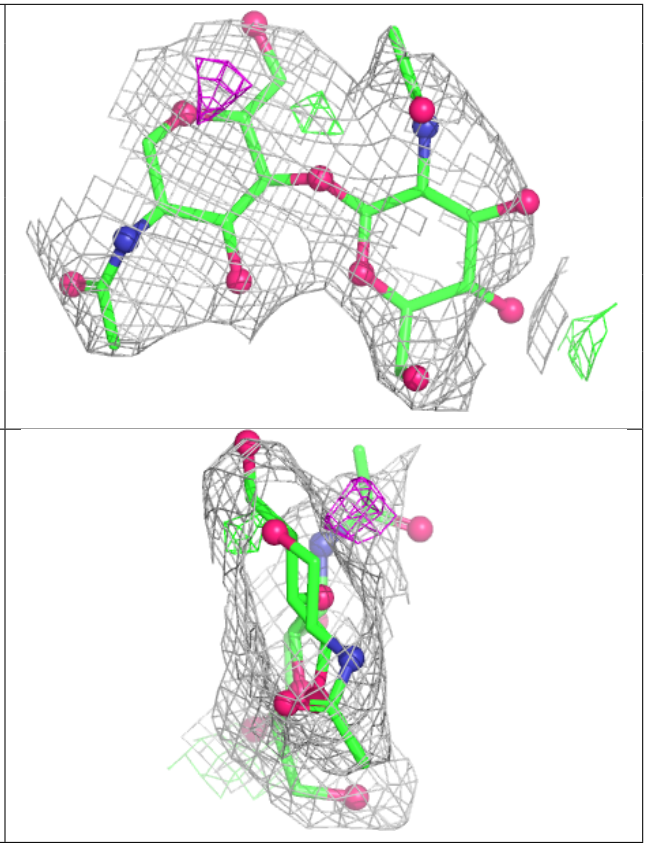


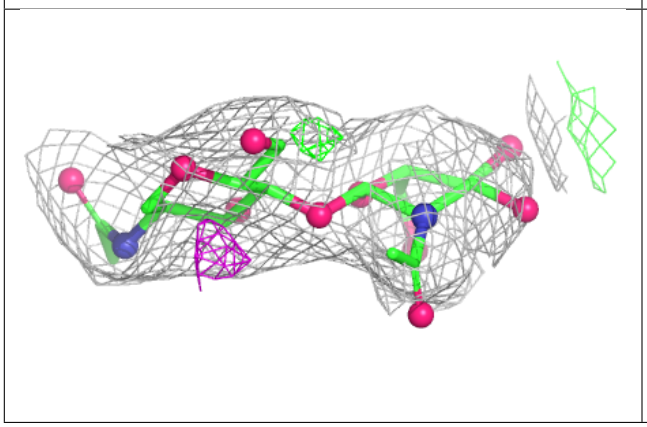




Electron density around Chain o:

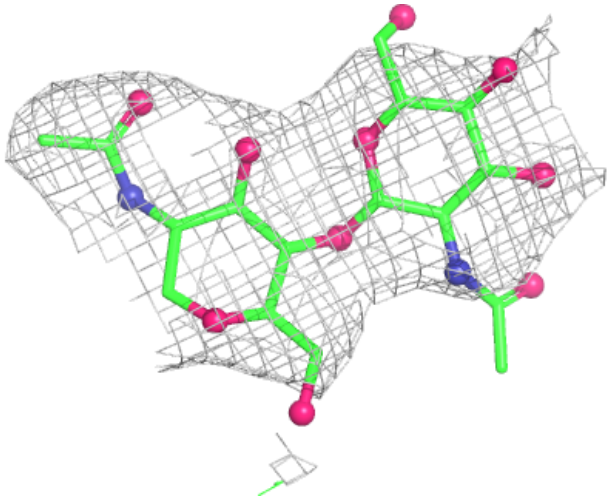
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

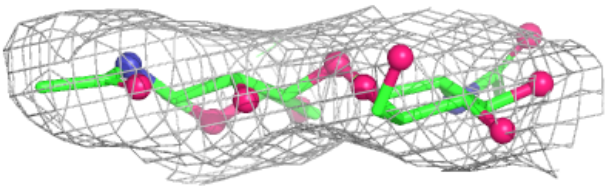


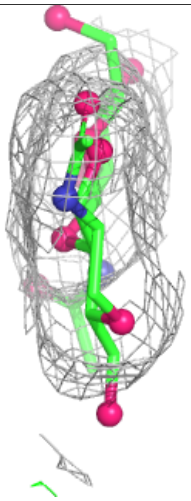


Electron density around Chain q:

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

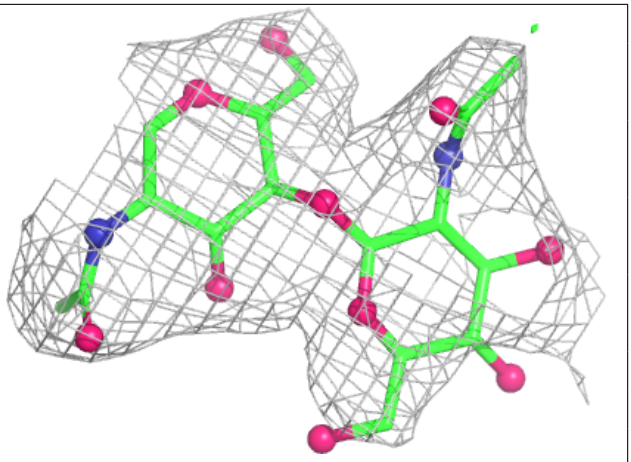


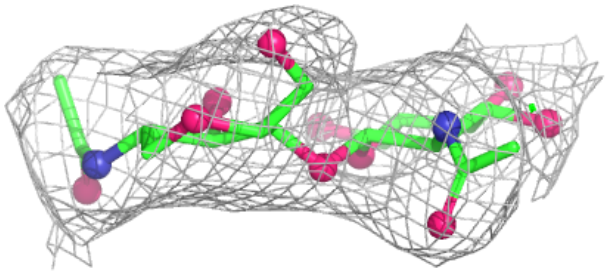


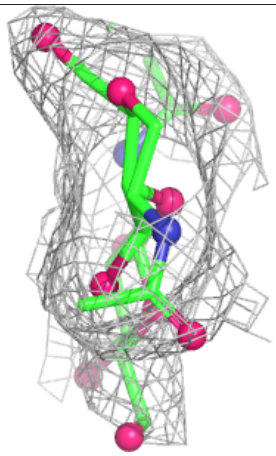


Electron density around Chain r:

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

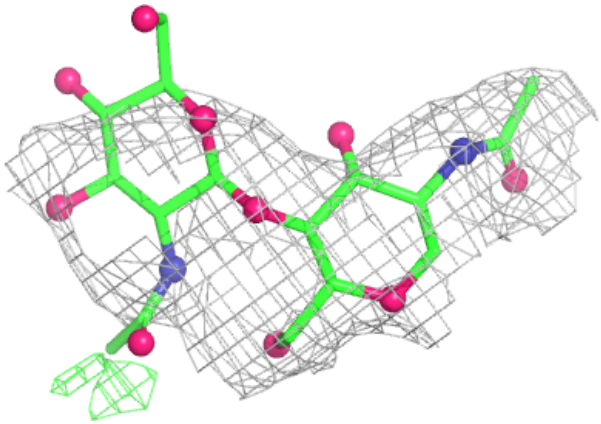


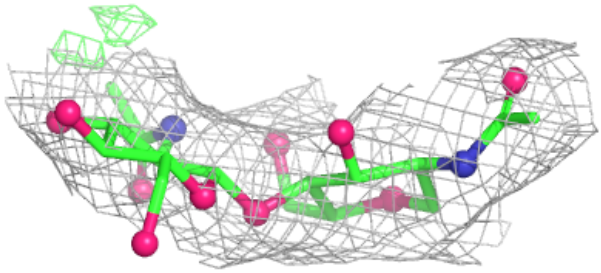


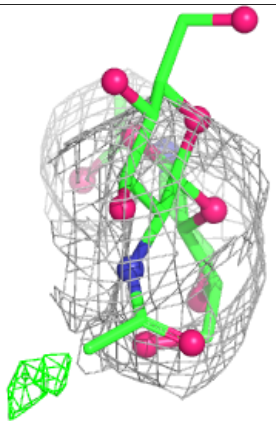


Electron density around Chain s:

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

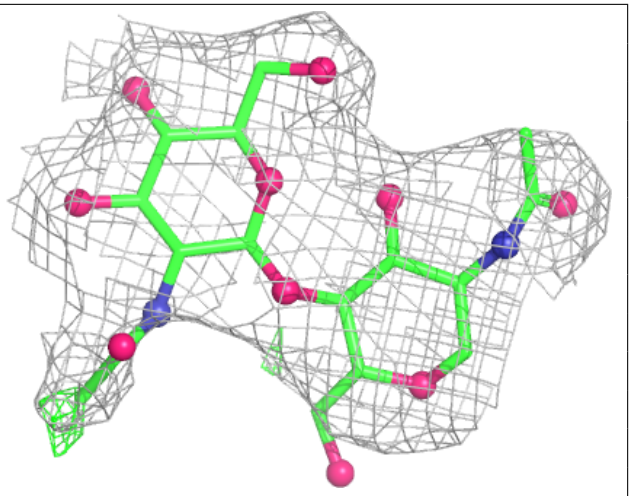


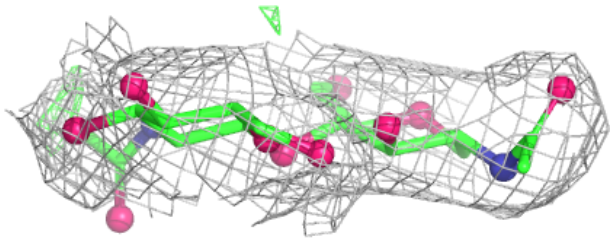


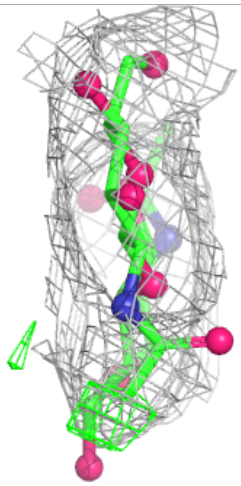


Electron density around Chain t:

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

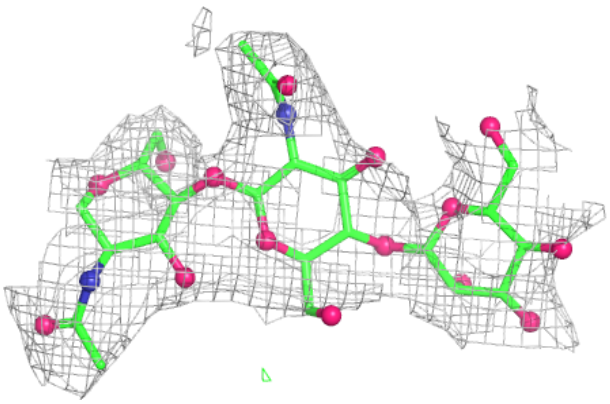


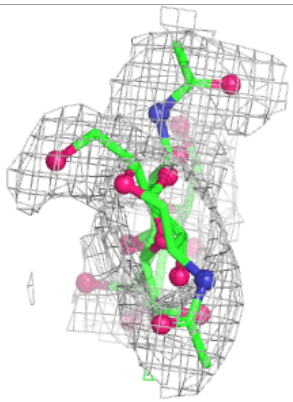




Electron density around Chain l:

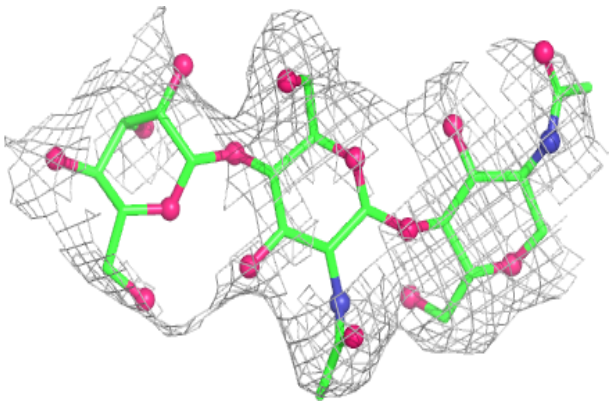
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

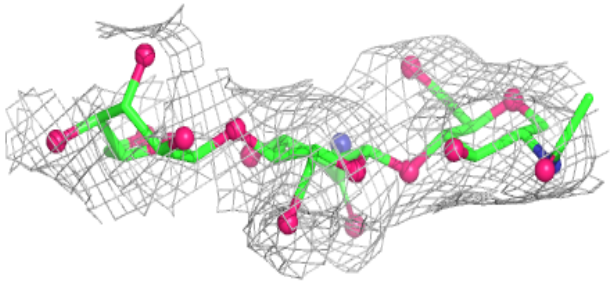


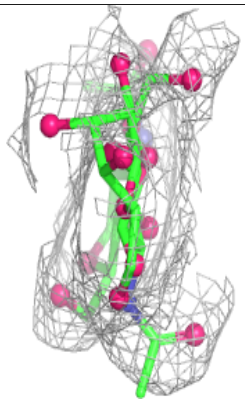


Electron density around Chain p:

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







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(Å^2)	Q<0.9
7	NAG	C	404	14/15	0.75	0.37	116,126,129,130	0
7	NAG	E	401	14/15	0.79	0.24	80,99,105,113	0
7	NAG	A	403	14/15	0.90	0.32	75,97,108,109	0
7	NAG	F	403	14/15	0.93	0.24	68,81,94,96	0

6.5 Other polymers (i)

There are no such residues in this entry.