wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 01:24 AM EDT

PDB ID	:	2FK0
Title	:	Crystal Structure of a H5N1 influenza virus hemagglutinin.
Authors	:	Stevens, J.; Wilson, I.A.
Deposited on	:	2006-01-03
Resolution	:	2.95 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:

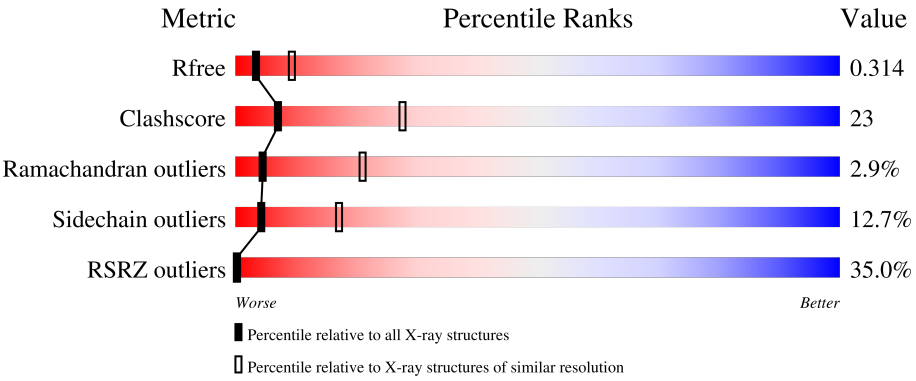
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	334	15% 61% 29% 6%
1	C	334	13% 60% 31%
1	E	334	14% 56% 34% 6%
1	G	334	13% 58% 32% 6%
1	I	334	15% 57% 32% 7%

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Mol	Chain	Length	Quality of chain
1	K	334	18% 57% 33% 5%
1	M	334	46% 43% 42% 11%
1	O	334	42% 41% 42% 11%
1	Q	334	68% 46% 41% 8%
2	B	181	39% 70% 22%
2	D	181	49% 70% 23%
2	F	181	41% 64% 28%
2	H	181	50% 65% 27%
2	J	181	46% 71% 21%
2	L	181	49% 72% 20%
2	N	181	38% 48% 34% 13%
2	P	181	36% 45% 38% 12%
2	R	181	67% 46% 38% 10%
3	S	2	100%
3	U	2	50% 50%
3	V	2	100%
3	W	2	100%
3	Y	2	100%
3	a	2	100%
3	b	2	100%
3	c	2	100%
3	d	2	100%
3	e	2	100%
3	f	2	100%
3	g	2	100%

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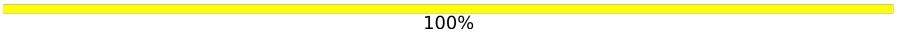
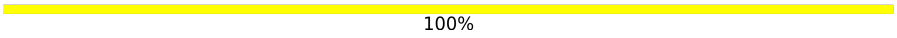
Mol	Chain	Length	Quality of chain
3	h	2	
4	T	3	
4	X	3	
4	Z	3	

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
3	NAG	S	1	-	-	-	X
3	NAG	S	2	-	-	-	X
3	NAG	U	1	-	-	-	X
3	NAG	U	2	-	-	-	X
3	NAG	V	1	X	-	-	-
3	NAG	V	2	-	-	-	X
3	NAG	W	2	-	-	-	X
3	NAG	Y	2	-	-	-	X
3	NAG	a	1	-	-	-	X
3	NAG	a	2	-	-	-	X
3	NAG	b	1	X	-	-	-
3	NAG	b	2	-	-	-	X
3	NAG	c	1	-	-	-	X
3	NAG	c	2	-	-	-	X
3	NAG	d	1	X	-	-	-
3	NAG	d	2	-	-	-	X
3	NAG	e	1	-	-	-	X
3	NAG	e	2	-	-	-	X
3	NAG	f	1	X	-	-	X
3	NAG	g	1	-	-	-	X
3	NAG	g	2	-	-	-	X
3	NAG	h	1	X	-	-	X
3	NAG	h	2	-	-	-	X
4	NAG	T	1	X	-	-	-
4	NAG	T	2	-	-	-	X
4	BMA	T	3	-	-	-	X
4	NAG	X	1	X	-	-	-
4	BMA	X	3	-	-	-	X
4	BMA	Z	3	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36202 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	C	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	G	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	I	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	K	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	M	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	O	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	Q	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	cloning artifact	GB 50296053
A	8	ASP	-	cloning artifact	GB 50296053
A	9	PRO	-	cloning artifact	GB 50296053
A	10	GLY	-	cloning artifact	GB 50296053
C	7	ALA	-	cloning artifact	GB 50296053
C	8	ASP	-	cloning artifact	GB 50296053
C	9	PRO	-	cloning artifact	GB 50296053
C	10	GLY	-	cloning artifact	GB 50296053
E	7	ALA	-	cloning artifact	GB 50296053
E	8	ASP	-	cloning artifact	GB 50296053
E	9	PRO	-	cloning artifact	GB 50296053

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	cloning artifact	GB 50296053
G	7	ALA	-	cloning artifact	GB 50296053
G	8	ASP	-	cloning artifact	GB 50296053
G	9	PRO	-	cloning artifact	GB 50296053
G	10	GLY	-	cloning artifact	GB 50296053
I	7	ALA	-	cloning artifact	GB 50296053
I	8	ASP	-	cloning artifact	GB 50296053
I	9	PRO	-	cloning artifact	GB 50296053
I	10	GLY	-	cloning artifact	GB 50296053
K	7	ALA	-	cloning artifact	GB 50296053
K	8	ASP	-	cloning artifact	GB 50296053
K	9	PRO	-	cloning artifact	GB 50296053
K	10	GLY	-	cloning artifact	GB 50296053
M	7	ALA	-	cloning artifact	GB 50296053
M	8	ASP	-	cloning artifact	GB 50296053
M	9	PRO	-	cloning artifact	GB 50296053
M	10	GLY	-	cloning artifact	GB 50296053
O	7	ALA	-	cloning artifact	GB 50296053
O	8	ASP	-	cloning artifact	GB 50296053
O	9	PRO	-	cloning artifact	GB 50296053
O	10	GLY	-	cloning artifact	GB 50296053
Q	7	ALA	-	cloning artifact	GB 50296053
Q	8	ASP	-	cloning artifact	GB 50296053
Q	9	PRO	-	cloning artifact	GB 50296053
Q	10	GLY	-	cloning artifact	GB 50296053

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	H	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	J	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	L	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	N	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	R	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	cloning artifact	GB 58618438
B	176	GLY	-	cloning artifact	GB 58618438
B	177	ARG	-	cloning artifact	GB 58618438
B	178	LEU	-	cloning artifact	GB 58618438
B	179	VAL	-	cloning artifact	GB 58618438
B	180	PRO	-	cloning artifact	GB 58618438
B	181	ARG	-	cloning artifact	GB 58618438
D	175	SER	-	cloning artifact	GB 58618438
D	176	GLY	-	cloning artifact	GB 58618438
D	177	ARG	-	cloning artifact	GB 58618438
D	178	LEU	-	cloning artifact	GB 58618438
D	179	VAL	-	cloning artifact	GB 58618438
D	180	PRO	-	cloning artifact	GB 58618438
D	181	ARG	-	cloning artifact	GB 58618438
F	175	SER	-	cloning artifact	GB 58618438
F	176	GLY	-	cloning artifact	GB 58618438
F	177	ARG	-	cloning artifact	GB 58618438
F	178	LEU	-	cloning artifact	GB 58618438
F	179	VAL	-	cloning artifact	GB 58618438
F	180	PRO	-	cloning artifact	GB 58618438
F	181	ARG	-	cloning artifact	GB 58618438
H	175	SER	-	cloning artifact	GB 58618438
H	176	GLY	-	cloning artifact	GB 58618438
H	177	ARG	-	cloning artifact	GB 58618438
H	178	LEU	-	cloning artifact	GB 58618438
H	179	VAL	-	cloning artifact	GB 58618438
H	180	PRO	-	cloning artifact	GB 58618438
H	181	ARG	-	cloning artifact	GB 58618438
J	175	SER	-	cloning artifact	GB 58618438
J	176	GLY	-	cloning artifact	GB 58618438
J	177	ARG	-	cloning artifact	GB 58618438
J	178	LEU	-	cloning artifact	GB 58618438
J	179	VAL	-	cloning artifact	GB 58618438
J	180	PRO	-	cloning artifact	GB 58618438

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Chain	Residue	Modelled	Actual	Comment	Reference
J	181	ARG	-	cloning artifact	GB 58618438
L	175	SER	-	cloning artifact	GB 58618438
L	176	GLY	-	cloning artifact	GB 58618438
L	177	ARG	-	cloning artifact	GB 58618438
L	178	LEU	-	cloning artifact	GB 58618438
L	179	VAL	-	cloning artifact	GB 58618438
L	180	PRO	-	cloning artifact	GB 58618438
L	181	ARG	-	cloning artifact	GB 58618438
N	175	SER	-	cloning artifact	GB 58618438
N	176	GLY	-	cloning artifact	GB 58618438
N	177	ARG	-	cloning artifact	GB 58618438
N	178	LEU	-	cloning artifact	GB 58618438
N	179	VAL	-	cloning artifact	GB 58618438
N	180	PRO	-	cloning artifact	GB 58618438
N	181	ARG	-	cloning artifact	GB 58618438
P	175	SER	-	cloning artifact	GB 58618438
P	176	GLY	-	cloning artifact	GB 58618438
P	177	ARG	-	cloning artifact	GB 58618438
P	178	LEU	-	cloning artifact	GB 58618438
P	179	VAL	-	cloning artifact	GB 58618438
P	180	PRO	-	cloning artifact	GB 58618438
P	181	ARG	-	cloning artifact	GB 58618438
R	175	SER	-	cloning artifact	GB 58618438
R	176	GLY	-	cloning artifact	GB 58618438
R	177	ARG	-	cloning artifact	GB 58618438
R	178	LEU	-	cloning artifact	GB 58618438
R	179	VAL	-	cloning artifact	GB 58618438
R	180	PRO	-	cloning artifact	GB 58618438
R	181	ARG	-	cloning artifact	GB 58618438

- Molecule 3 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
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

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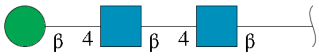
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	h	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



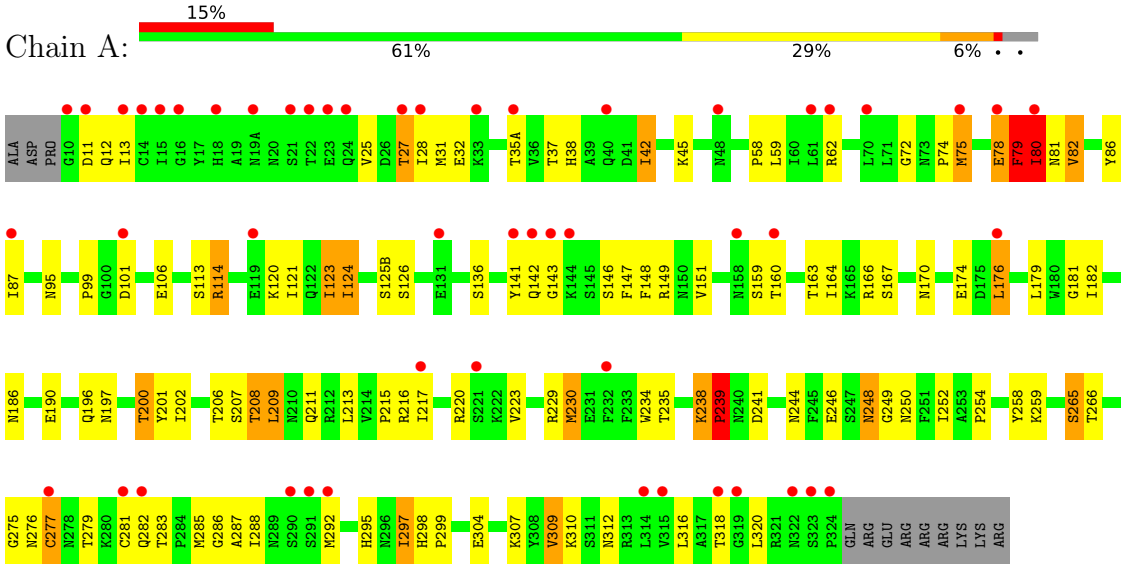
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			

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.

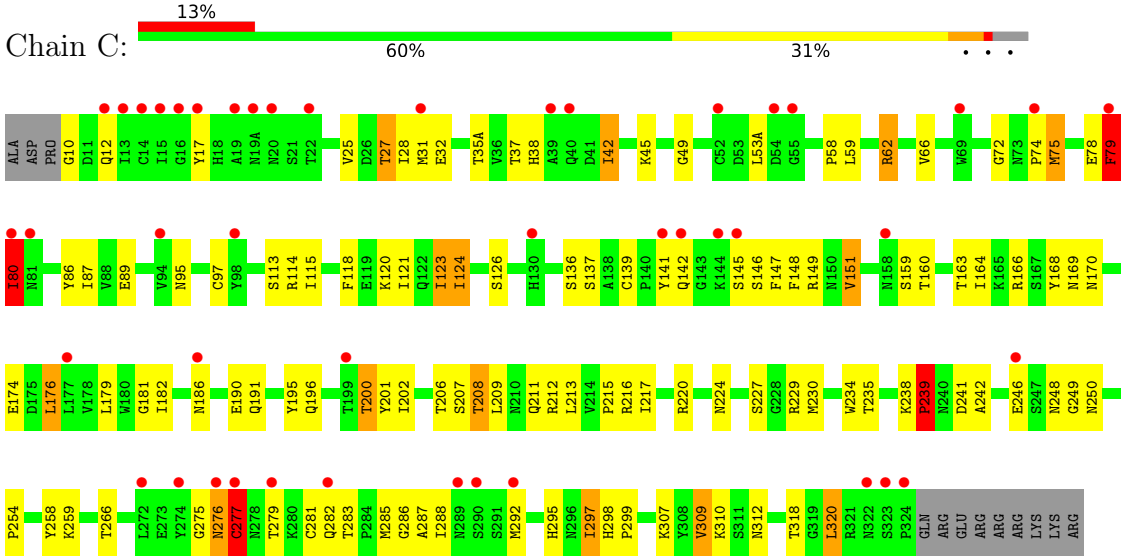
- Molecule 1: hemagglutinin

Chain A:



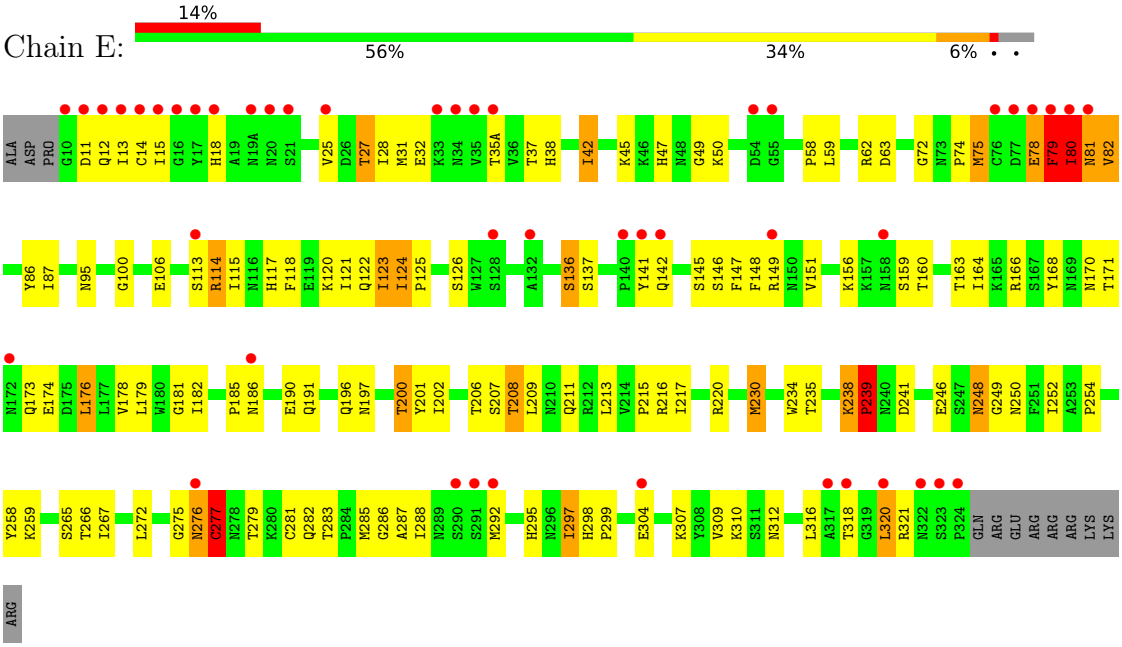
- Molecule 1: hemagglutinin

Chain C:



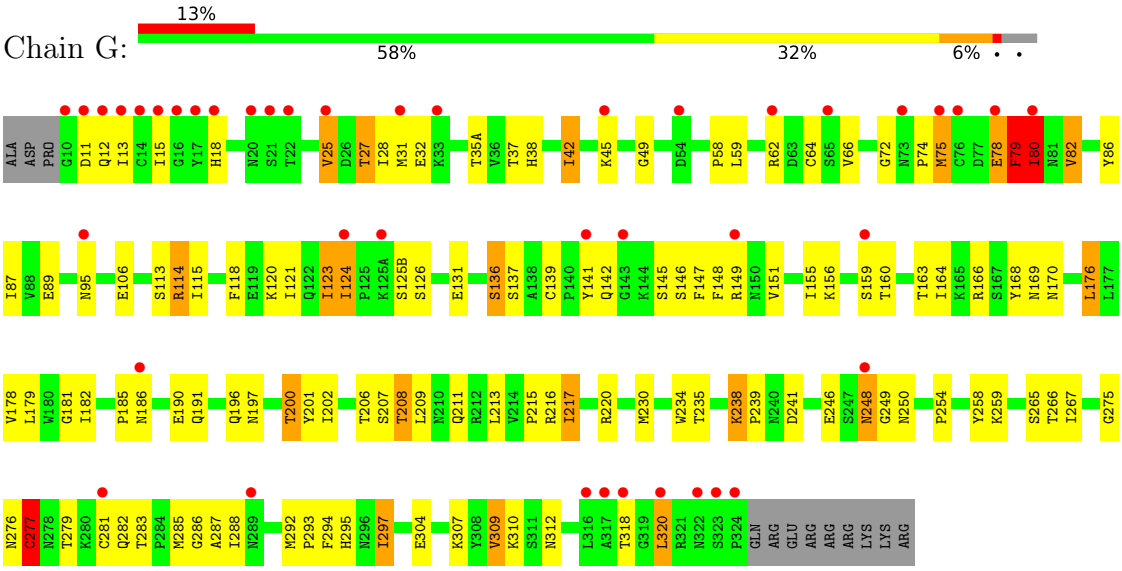
- Molecule 1: hemagglutinin

Chain E:



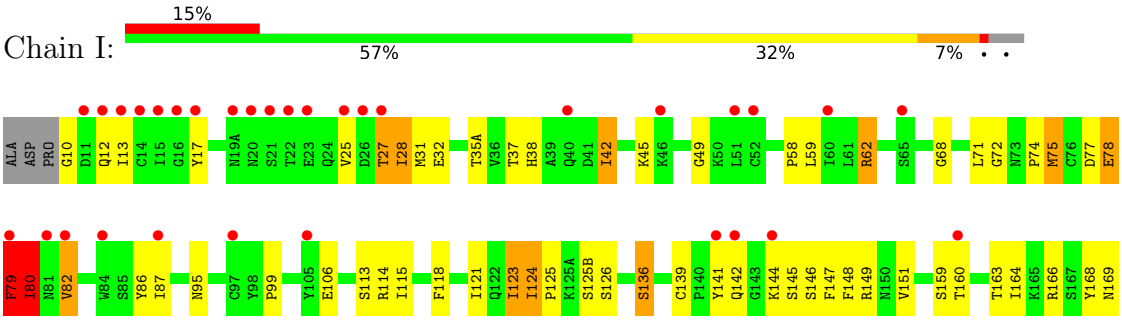
• Molecule 1: hemagglutinin

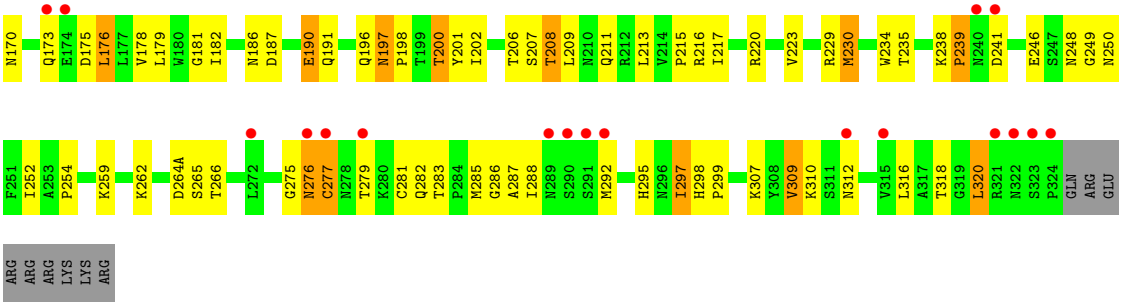
Chain G:



• Molecule 1: hemagglutinin

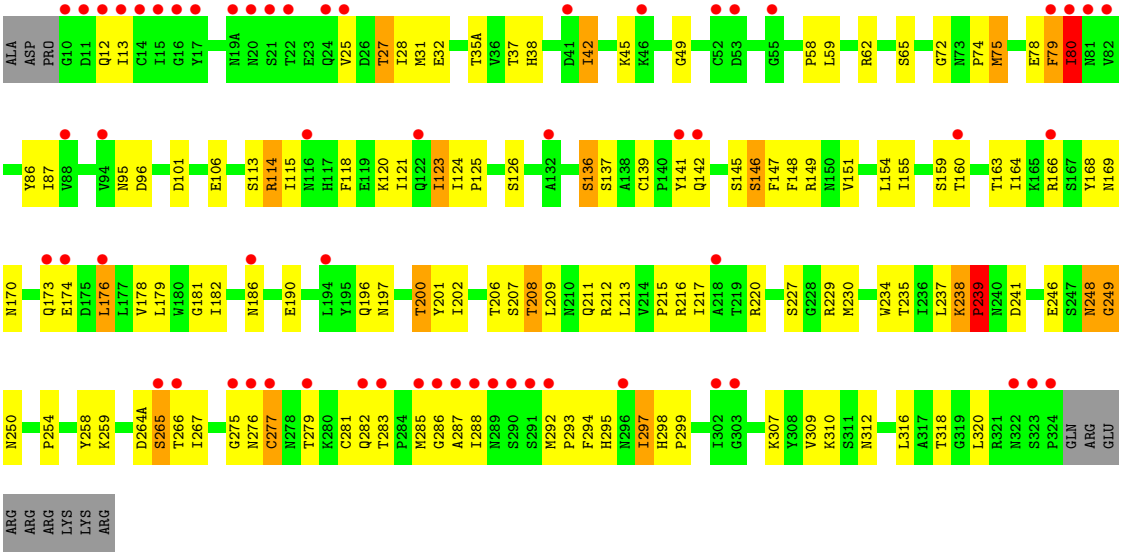
Chain I:





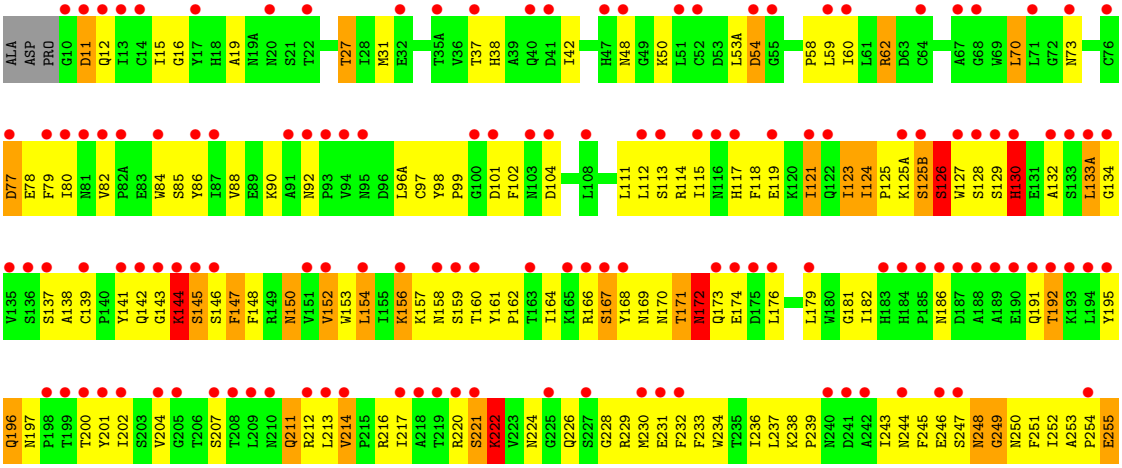
• Molecule 1: hemagglutinin

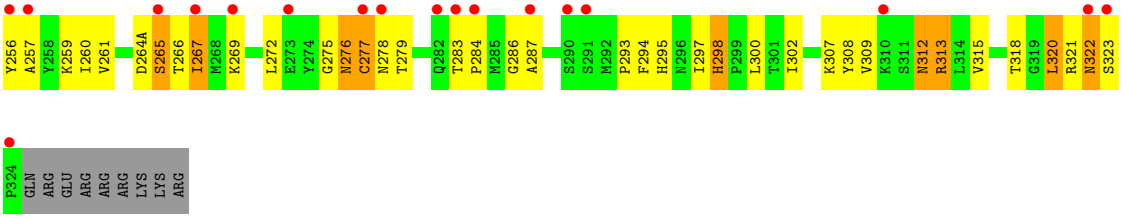
Chain K:



• Molecule 1: hemagglutinin

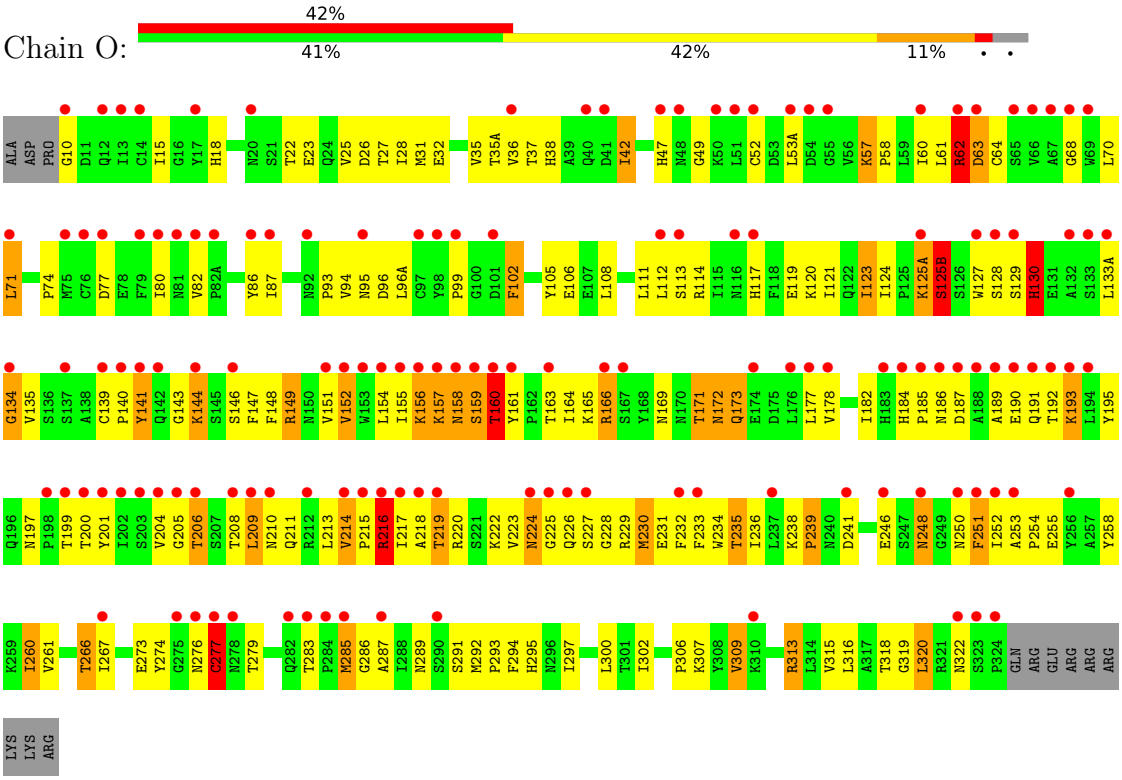
Chain M:





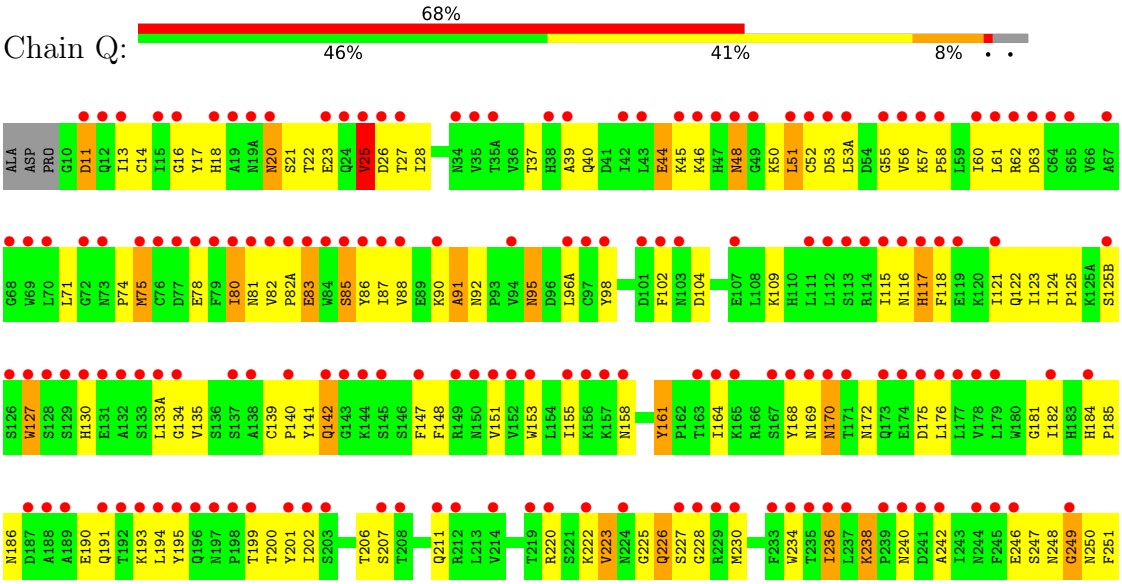
• Molecule 1: hemagglutinin

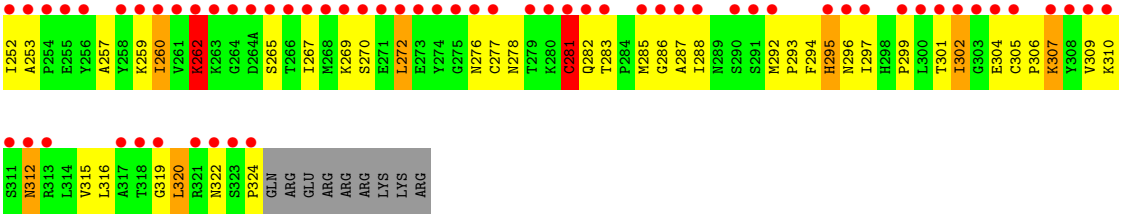
Chain O:



• Molecule 1: hemagglutinin

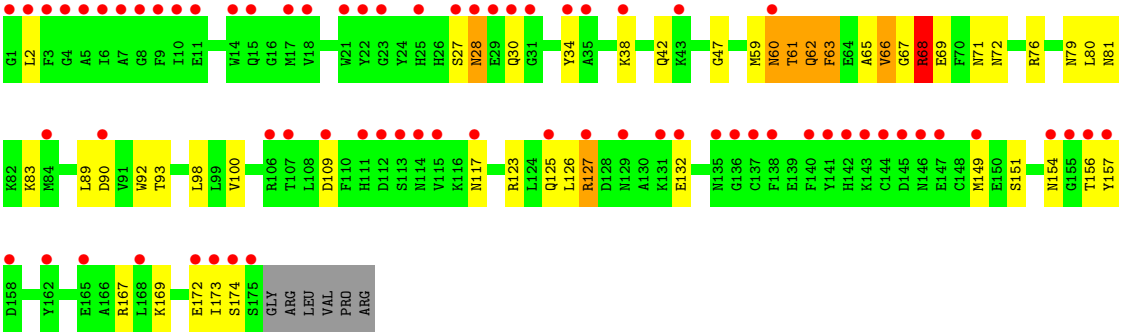
Chain Q:





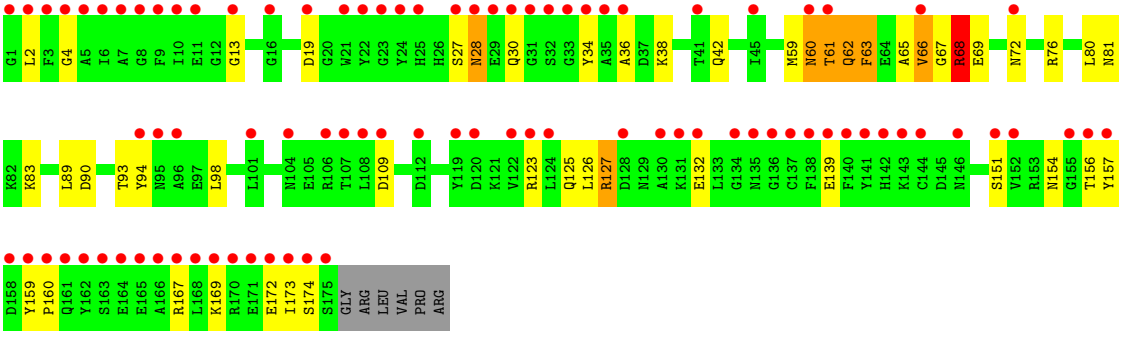
• Molecule 2: hemagglutinin

Chain B:



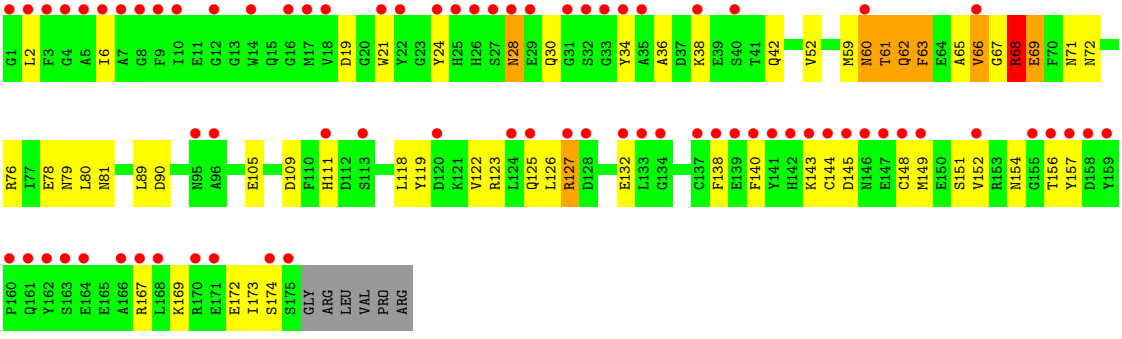
• Molecule 2: hemagglutinin

Chain D:



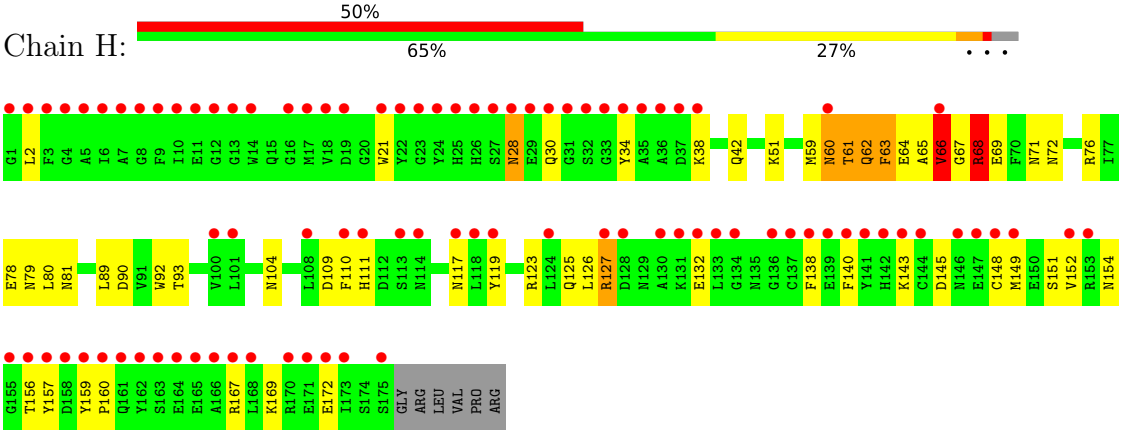
• Molecule 2: hemagglutinin

Chain F:



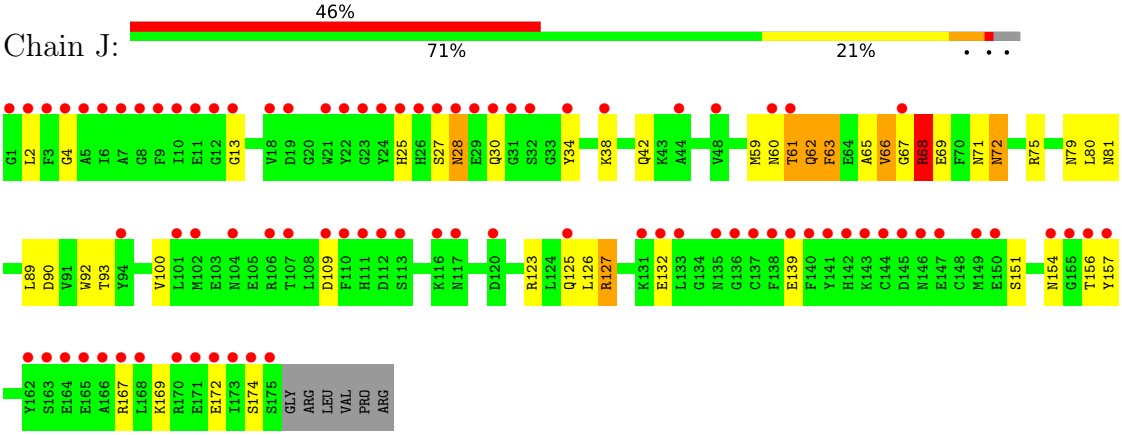
• Molecule 2: hemagglutinin

Chain H:



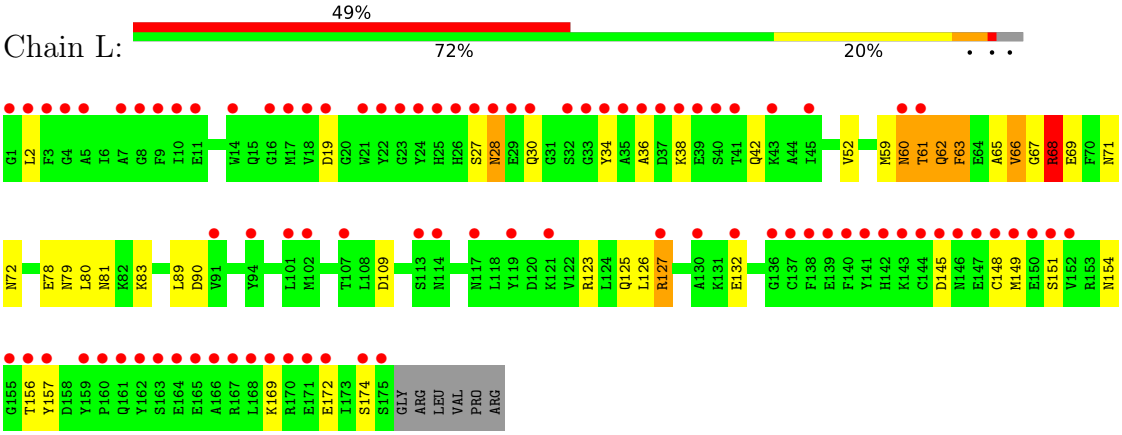
• Molecule 2: hemagglutinin

Chain J:



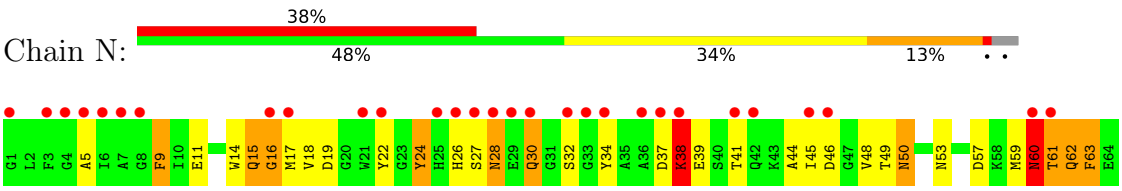
• Molecule 2: hemagglutinin

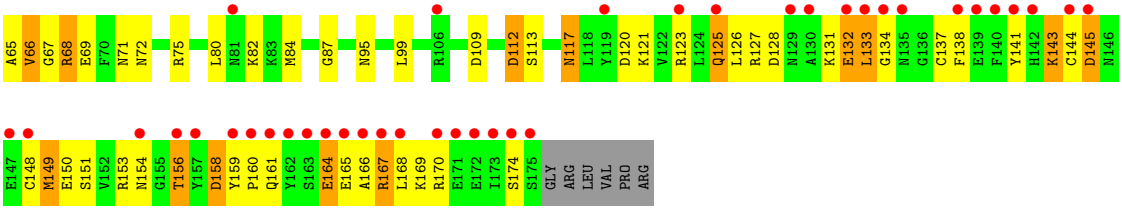
Chain L:



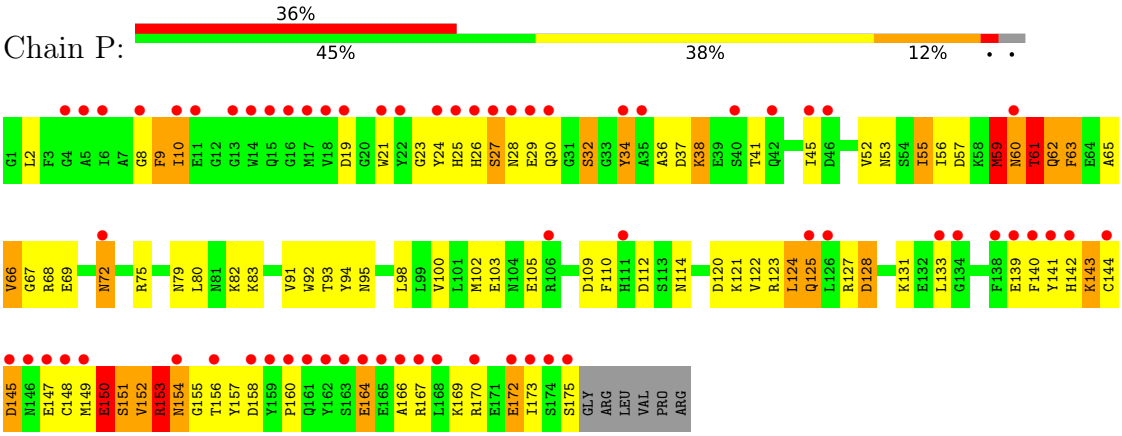
• Molecule 2: hemagglutinin

Chain N:

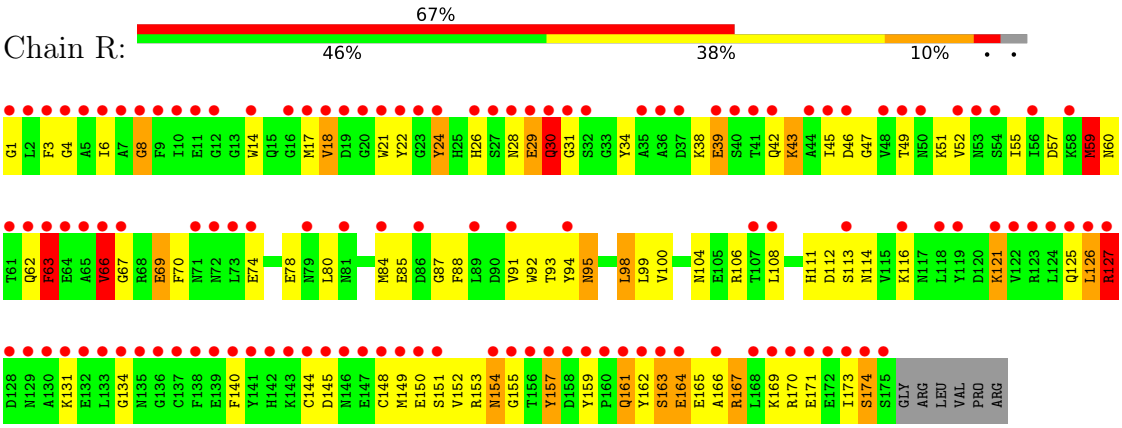




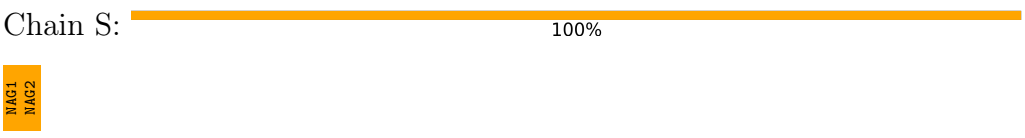
• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin



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



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

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

Chain V: 100%

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

Chain W: 100%

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

Chain Y: 100%

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

Chain a: 100%

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

Chain b: 100%

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

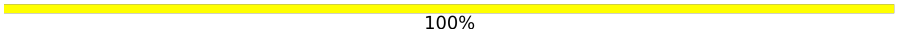
Chain c: 100%

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

Chain d: 100%

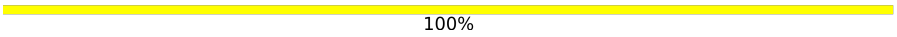
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



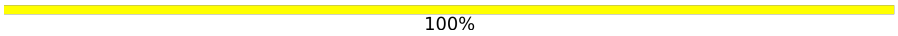
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



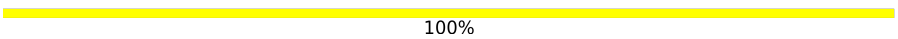
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



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

Chain h:

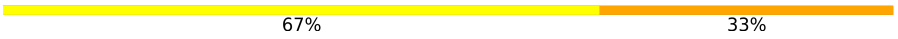


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

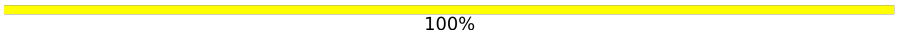
Chain T:

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

Chain X:



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

Chain Z: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	197.94Å 197.94Å 134.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	171.50 – 2.95 49.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (171.50-2.95) 98.9 (49.49-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.319 0.266 , 0.314	Depositor DCC
R_{free} test set	1233 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 98.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	36202	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% 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	0.76	0/2615	0.83	3/3551 (0.1%)
1	C	0.84	3/2615 (0.1%)	0.87	2/3551 (0.1%)
1	E	0.84	1/2615 (0.0%)	0.87	4/3551 (0.1%)
1	G	0.84	3/2615 (0.1%)	0.85	3/3551 (0.1%)
1	I	0.80	2/2615 (0.1%)	0.85	4/3551 (0.1%)
1	K	0.79	1/2615 (0.0%)	0.83	2/3551 (0.1%)
1	M	1.12	21/2615 (0.8%)	0.87	5/3551 (0.1%)
1	O	1.49	22/2615 (0.8%)	0.91	9/3551 (0.3%)
1	Q	0.65	2/2615 (0.1%)	0.70	0/3551
2	B	0.67	0/1443	0.70	3/1939 (0.2%)
2	D	0.68	0/1443	0.71	3/1939 (0.2%)
2	F	0.70	3/1443 (0.2%)	0.71	3/1939 (0.2%)
2	H	0.67	1/1443 (0.1%)	0.70	3/1939 (0.2%)
2	J	0.64	0/1443	0.68	2/1939 (0.1%)
2	L	0.67	1/1443 (0.1%)	0.67	2/1939 (0.1%)
2	N	1.29	7/1443 (0.5%)	0.86	5/1939 (0.3%)
2	P	1.38	13/1443 (0.9%)	0.88	5/1939 (0.3%)
2	R	0.74	5/1443 (0.3%)	0.69	0/1939
All	All	0.91	85/36522 (0.2%)	0.81	58/49410 (0.1%)

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	2
1	C	0	2
1	E	0	2
1	G	0	2
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	3
1	M	0	1
1	O	0	3
1	Q	0	1
2	B	0	3
2	D	0	3
2	F	0	3
2	H	0	3
2	J	0	2
2	L	0	3
2	N	0	2
2	P	0	2
All	All	0	38

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	125(B)	SER	CB-OG	34.55	1.87	1.42
2	N	38	LYS	CE-NZ	31.98	2.29	1.49
2	P	143	LYS	CE-NZ	27.78	2.18	1.49
1	O	157	LYS	CD-CE	22.51	2.07	1.51
1	O	130	HIS	CE1-NE2	20.34	1.79	1.32

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	38	LYS	CD-CE-NZ	-14.03	79.42	111.70
1	M	166	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	O	125(A)	LYS	CD-CE-NZ	-11.74	84.70	111.70
1	M	154	LEU	CB-CG-CD2	11.21	130.05	111.00
2	P	143	LYS	CD-CE-NZ	-10.31	87.98	111.70

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ASN	Peptide
1	A	276	ASN	Peptide
2	B	60	ASN	Peptide
2	B	61	THR	Peptide
2	B	68	ARG	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	2553	0	2496	118	2
1	C	2553	0	2496	118	3
1	E	2553	0	2496	169	0
1	G	2553	0	2496	131	3
1	I	2553	0	2496	139	0
1	K	2553	0	2496	117	2
1	M	2553	0	2496	166	0
1	O	2553	0	2496	190	0
1	Q	2553	0	2498	132	0
2	B	1416	0	1320	48	0
2	D	1416	0	1320	46	0
2	F	1416	0	1320	72	0
2	H	1416	0	1320	60	0
2	J	1416	0	1320	42	0
2	L	1416	0	1320	39	0
2	N	1416	0	1320	75	0
2	P	1416	0	1320	82	0
2	R	1416	0	1320	77	0
3	S	28	0	25	1	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	Y	28	0	25	2	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
4	T	39	0	34	3	0
4	X	39	0	34	3	0
4	Z	39	0	34	0	0
All	All	36202	0	34773	1618	5

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 23.

The worst 5 of 1618 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:LEU:CG	1:M:154:LEU:CD1	1.79	1.60
1:M:130:HIS:CG	1:M:130:HIS:ND1	1.71	1.54
1:M:130:HIS:CE1	1:M:130:HIS:NE2	1.75	1.53
1:O:125(A):LYS:CE	1:O:125(A):LYS:CD	1.83	1.52
2:P:143:LYS:CD	2:P:143:LYS:CE	1.86	1.51

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE2	1:K:142:GLN:OE1[3_455]	1.69	0.51
1:C:142:GLN:OE1	1:G:78:GLU:OE2[2_555]	1.87	0.33
1:C:79:PHE:CE2	1:G:125(B):SER:C[2_555]	1.94	0.26
1:C:142:GLN:OE1	1:G:149:ARG:NH1[2_555]	2.17	0.03
1:A:125(B):SER:C	1:K:79:PHE:CE2[3_455]	2.18	0.02

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	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	8 32
1	C	320/334 (96%)	290 (91%)	26 (8%)	4 (1%)	12 41
1	E	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	8 32
1	G	320/334 (96%)	285 (89%)	31 (10%)	4 (1%)	12 41
1	I	320/334 (96%)	285 (89%)	29 (9%)	6 (2%)	8 32
1	K	320/334 (96%)	287 (90%)	28 (9%)	5 (2%)	9 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	320/334 (96%)	255 (80%)	52 (16%)	13 (4%)	3 13
1	O	320/334 (96%)	248 (78%)	57 (18%)	15 (5%)	2 11
1	Q	320/334 (96%)	237 (74%)	63 (20%)	20 (6%)	1 6
2	B	173/181 (96%)	161 (93%)	10 (6%)	2 (1%)	13 43
2	D	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	13 43
2	F	173/181 (96%)	162 (94%)	9 (5%)	2 (1%)	13 43
2	H	173/181 (96%)	162 (94%)	8 (5%)	3 (2%)	9 34
2	J	173/181 (96%)	163 (94%)	8 (5%)	2 (1%)	13 43
2	L	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	13 43
2	N	173/181 (96%)	132 (76%)	35 (20%)	6 (4%)	3 17
2	P	173/181 (96%)	126 (73%)	37 (21%)	10 (6%)	1 7
2	R	173/181 (96%)	124 (72%)	29 (17%)	20 (12%)	0 1
All	All	4437/4635 (96%)	3823 (86%)	486 (11%)	128 (3%)	4 21

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	127	ARG
2	D	60	ASN
2	D	127	ARG
1	E	80	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	289/300 (96%)	257 (89%)	32 (11%)	6 22
1	C	289/300 (96%)	260 (90%)	29 (10%)	7 26
1	E	289/300 (96%)	257 (89%)	32 (11%)	6 22
1	G	289/300 (96%)	258 (89%)	31 (11%)	6 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	289/300 (96%)	256 (89%)	33 (11%)	5 21
1	K	289/300 (96%)	255 (88%)	34 (12%)	5 20
1	M	289/300 (96%)	239 (83%)	50 (17%)	2 8
1	O	289/300 (96%)	246 (85%)	43 (15%)	3 12
1	Q	289/300 (96%)	238 (82%)	51 (18%)	2 8
2	B	149/155 (96%)	135 (91%)	14 (9%)	8 29
2	D	149/155 (96%)	135 (91%)	14 (9%)	8 29
2	F	149/155 (96%)	135 (91%)	14 (9%)	8 29
2	H	149/155 (96%)	134 (90%)	15 (10%)	7 26
2	J	149/155 (96%)	135 (91%)	14 (9%)	8 29
2	L	149/155 (96%)	135 (91%)	14 (9%)	8 29
2	N	149/155 (96%)	121 (81%)	28 (19%)	1 7
2	P	149/155 (96%)	121 (81%)	28 (19%)	1 7
2	R	149/155 (96%)	125 (84%)	24 (16%)	2 10
All	All	3942/4095 (96%)	3442 (87%)	500 (13%)	4 17

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	35(A)	THR
1	Q	118	PHE
1	M	92	ASN
1	Q	75	MET
1	Q	315	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	53	ASN
2	R	28	ASN
2	P	117	ASN
1	Q	122	GLN
2	R	114	ASN

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)

35 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	$\#\|Z\| > 2$
3	NAG	S	1	1,3	14,14,15	0.64	0	17,19,21	1.47	3 (17%)
3	NAG	S	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.07	2 (11%)
4	NAG	T	1	4,1	14,14,15	0.72	0	17,19,21	1.77	3 (17%)
4	NAG	T	2	4	14,14,15	0.76	0	17,19,21	1.85	5 (29%)
4	BMA	T	3	4	11,11,12	0.69	0	15,15,17	1.43	2 (13%)
3	NAG	U	1	1,3	14,14,15	0.69	0	17,19,21	2.74	7 (41%)
3	NAG	U	2	3	14,14,15	0.63	0	17,19,21	1.64	3 (17%)
3	NAG	V	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	2.34	6 (35%)
3	NAG	V	2	3	14,14,15	0.60	0	17,19,21	1.77	4 (23%)
3	NAG	W	1	1,3	14,14,15	0.58	0	17,19,21	1.83	5 (29%)
3	NAG	W	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.76	3 (17%)
4	NAG	X	1	4,1	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
4	NAG	X	2	4	14,14,15	0.59	0	17,19,21	1.38	3 (17%)
4	BMA	X	3	4	11,11,12	0.86	0	15,15,17	2.57	4 (26%)
3	NAG	Y	1	1,3	14,14,15	0.66	0	17,19,21	1.25	1 (5%)
3	NAG	Y	2	3	14,14,15	1.00	1 (7%)	17,19,21	1.51	2 (11%)
4	NAG	Z	1	4,1	14,14,15	0.79	0	17,19,21	2.44	5 (29%)
4	NAG	Z	2	4	14,14,15	0.75	0	17,19,21	1.49	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	Z	3	4	11,11,12	0.56	0	15,15,17	2.49	2 (13%)
3	NAG	a	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	2.88	8 (47%)
3	NAG	a	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.63	4 (23%)
3	NAG	b	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	1.57	5 (29%)
3	NAG	b	2	3	14,14,15	0.66	0	17,19,21	1.57	4 (23%)
3	NAG	c	1	1,3	14,14,15	0.77	0	17,19,21	2.24	5 (29%)
3	NAG	c	2	3	14,14,15	1.03	1 (7%)	17,19,21	2.74	6 (35%)
3	NAG	d	1	1,3	14,14,15	0.71	0	17,19,21	1.83	4 (23%)
3	NAG	d	2	3	14,14,15	0.53	0	17,19,21	1.35	2 (11%)
3	NAG	e	1	1,3	14,14,15	0.82	0	17,19,21	1.69	4 (23%)
3	NAG	e	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.17	1 (5%)
3	NAG	f	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	1.89	4 (23%)
3	NAG	f	2	3	14,14,15	0.88	0	17,19,21	2.04	5 (29%)
3	NAG	g	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	2.03	6 (35%)
3	NAG	g	2	3	14,14,15	1.21	1 (7%)	17,19,21	1.90	4 (23%)
3	NAG	h	1	1,3	14,14,15	0.73	0	17,19,21	2.63	7 (41%)
3	NAG	h	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.36	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
3	NAG	S	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
4	NAG	T	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	4/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	4/6/23/26	0/1/1/1
4	NAG	X	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	5/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	c	2	3	-	1/6/23/26	0/1/1/1
3	NAG	d	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	3/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	g	2	3	-	5/6/23/26	0/1/1/1
3	NAG	h	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	5/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	NAG	C1-C2	3.66	1.57	1.52
3	S	2	NAG	C1-C2	2.81	1.56	1.52
3	e	2	NAG	C1-C2	2.73	1.56	1.52
3	Y	2	NAG	C1-C2	2.73	1.56	1.52
3	g	1	NAG	C1-C2	2.72	1.56	1.52

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	3	BMA	C1-O5-C5	8.68	123.95	112.19
3	U	1	NAG	C1-O5-C5	8.51	123.73	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1	NAG	C1-O5-C5	8.22	123.33	112.19
4	X	3	BMA	C1-C2-C3	6.55	117.71	109.67
4	Z	1	NAG	O5-C1-C2	-6.39	101.19	111.29

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	V	1	NAG	C1
3	b	1	NAG	C1
3	d	1	NAG	C1
3	f	1	NAG	C1
3	h	1	NAG	C1

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C8-C7-N2-C2

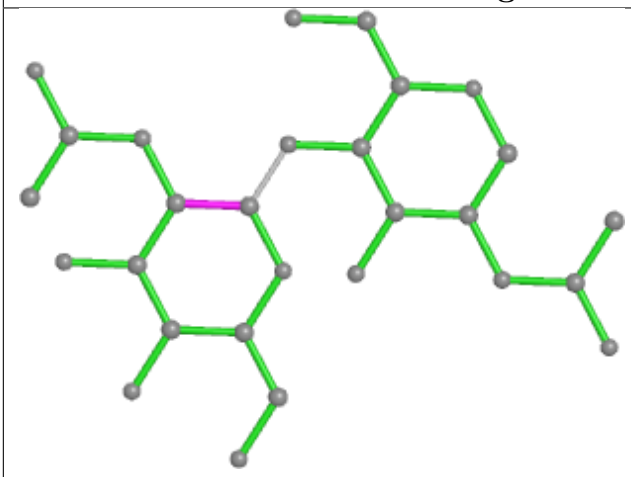
There are no ring outliers.

8 monomers are involved in 10 short contacts:

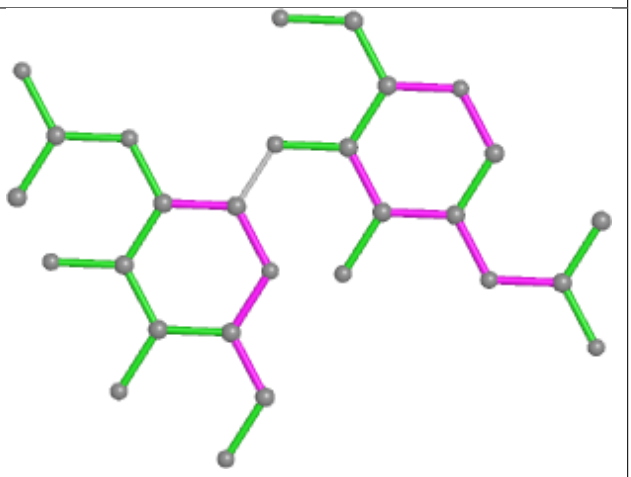
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	1	NAG	1	0
3	S	1	NAG	1	0
3	U	1	NAG	1	0
3	Y	2	NAG	2	0
3	S	2	NAG	1	0
3	Y	1	NAG	2	0
4	T	2	NAG	3	0
4	X	3	BMA	3	0

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

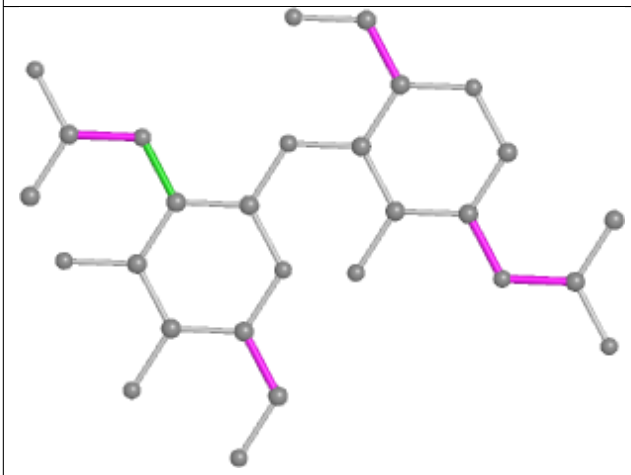
Oligosaccharide Chain S



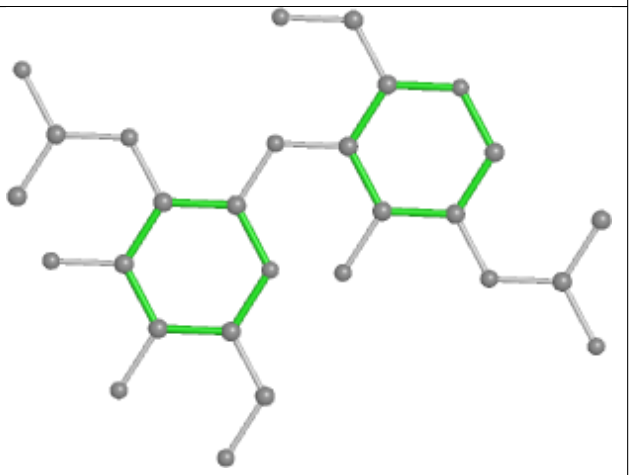
Bond lengths



Bond angles

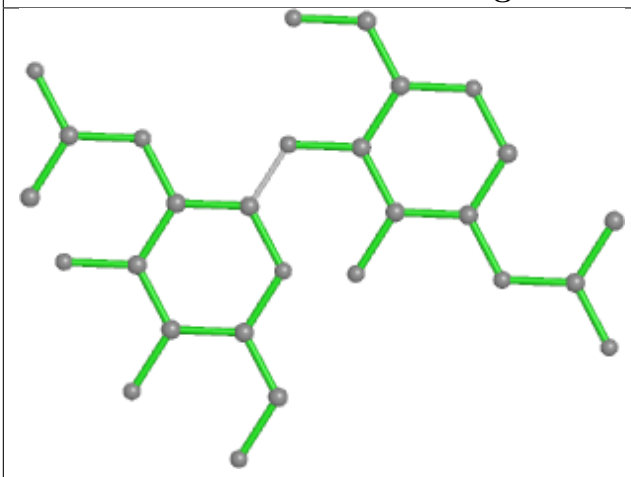


Torsions

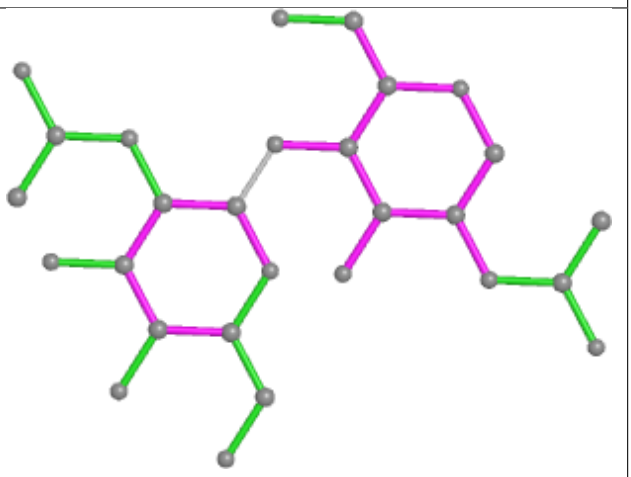


Rings

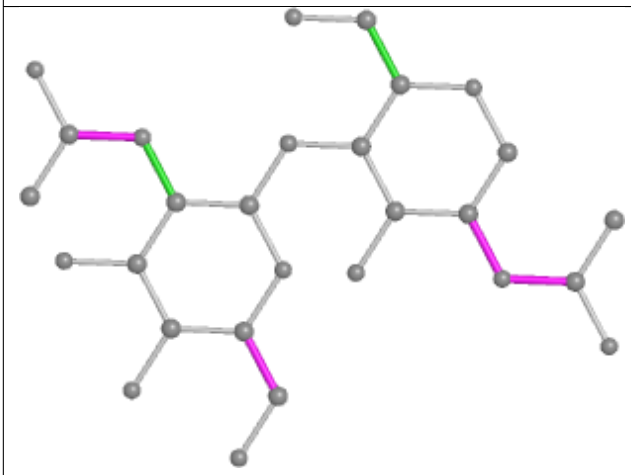
Oligosaccharide Chain U



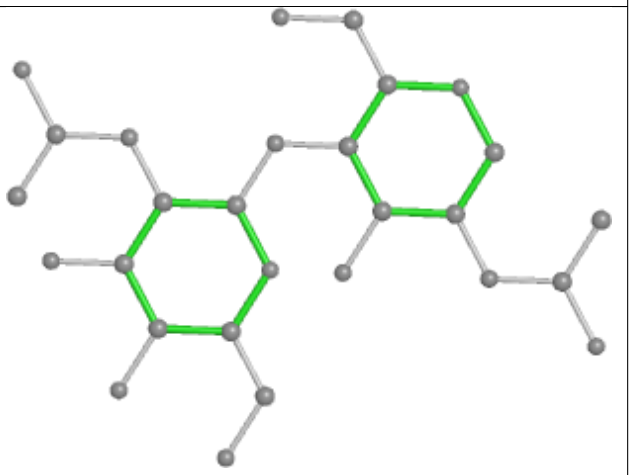
Bond lengths



Bond angles

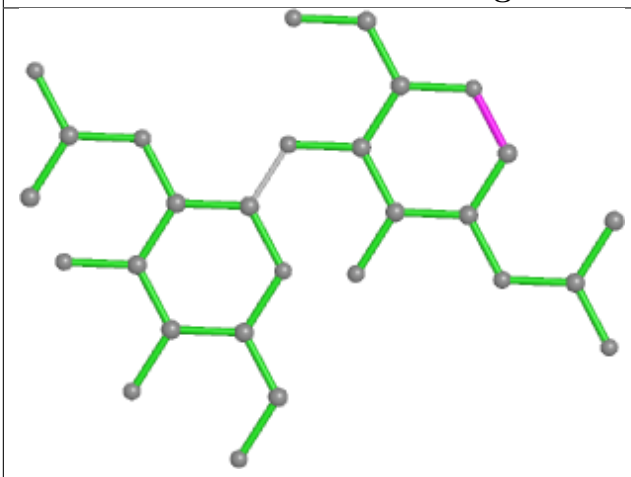


Torsions

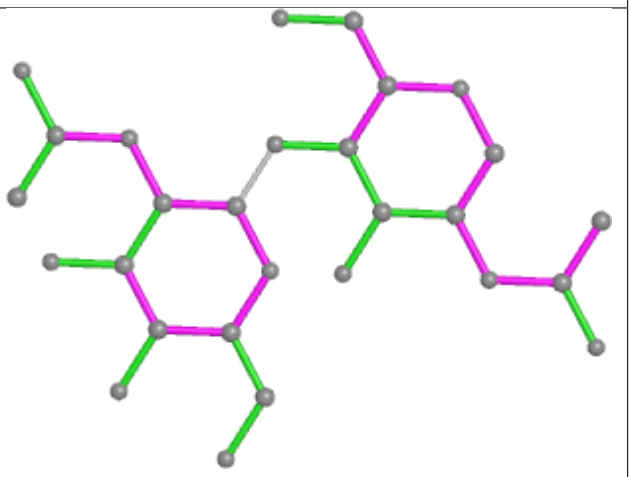


Rings

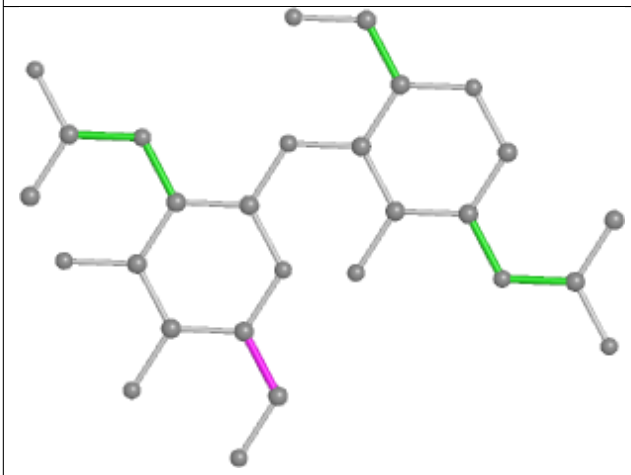
Oligosaccharide Chain V



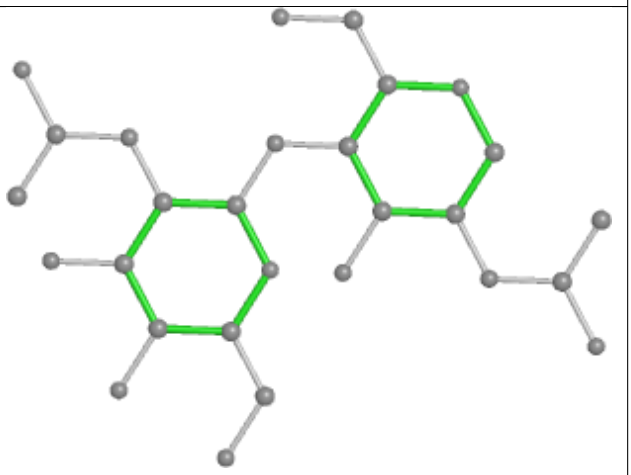
Bond lengths



Bond angles

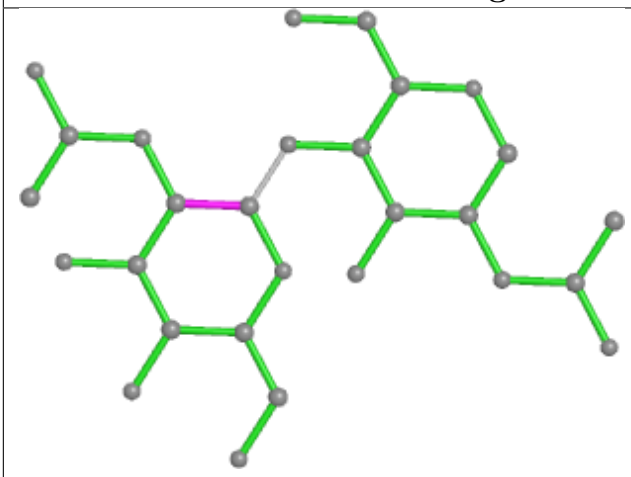


Torsions

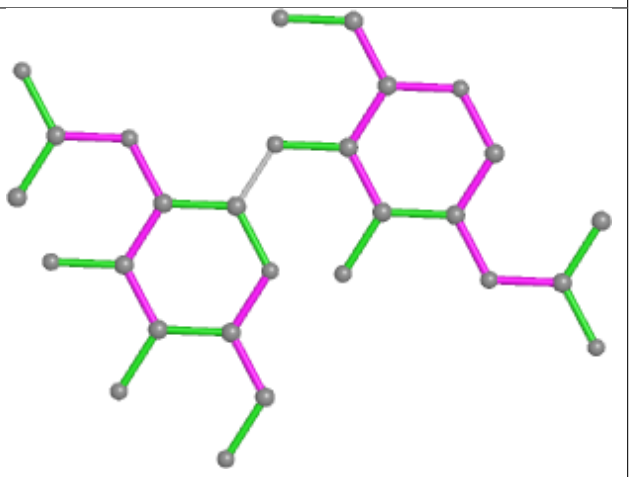


Rings

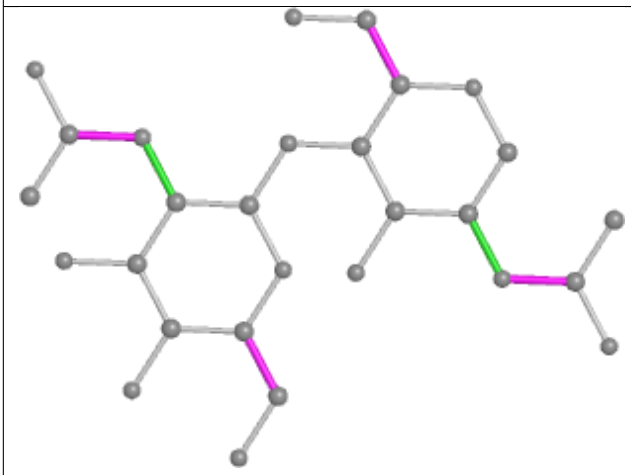
Oligosaccharide Chain W



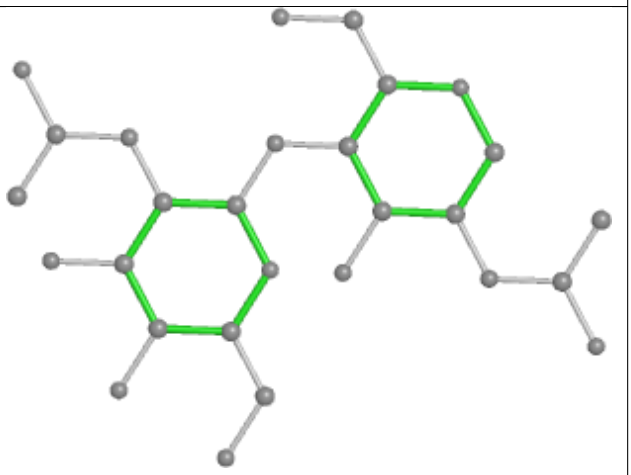
Bond lengths



Bond angles

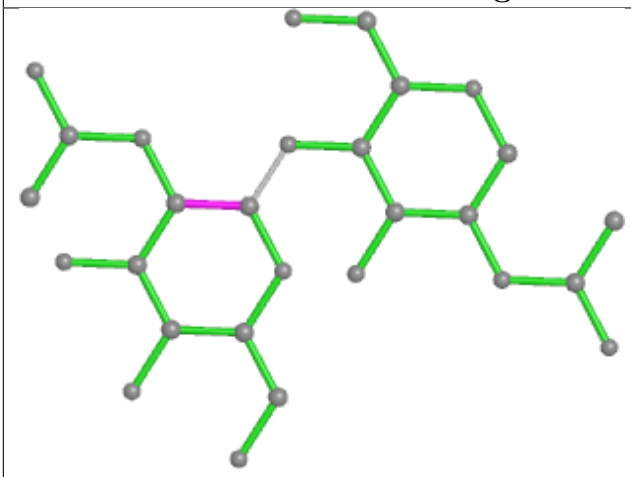


Torsions

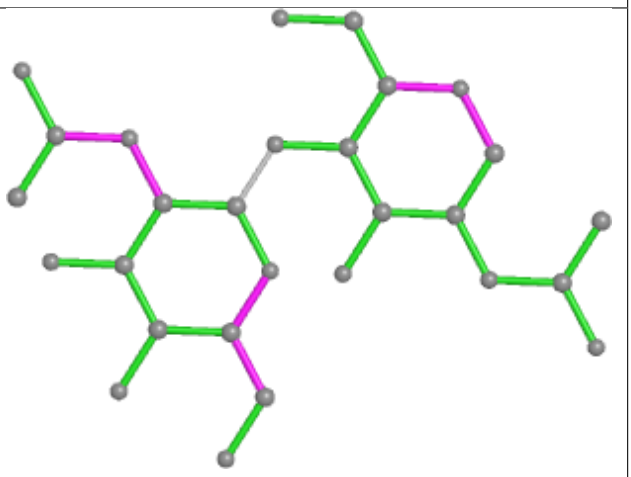


Rings

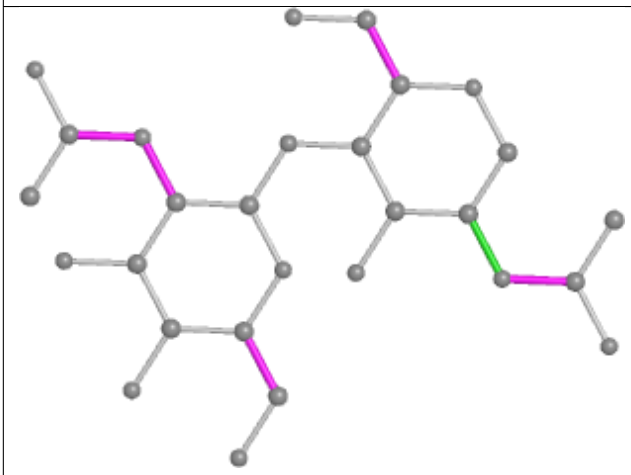
Oligosaccharide Chain Y



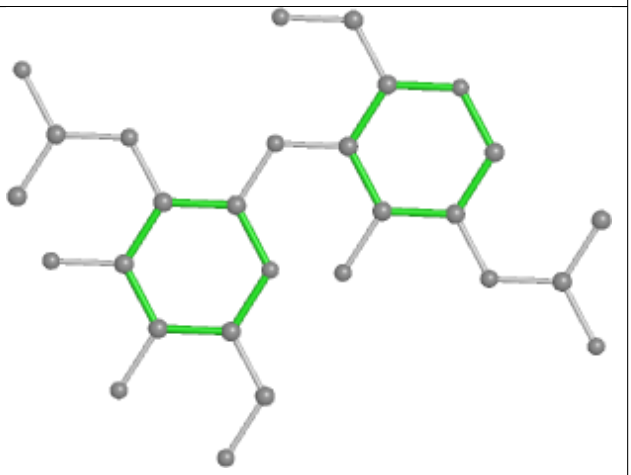
Bond lengths



Bond angles

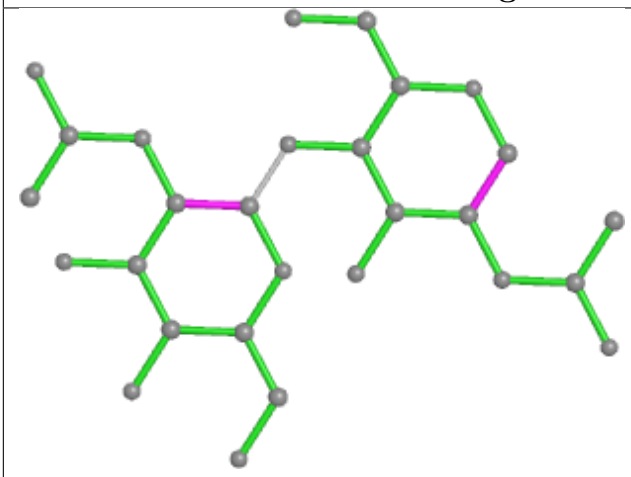


Torsions

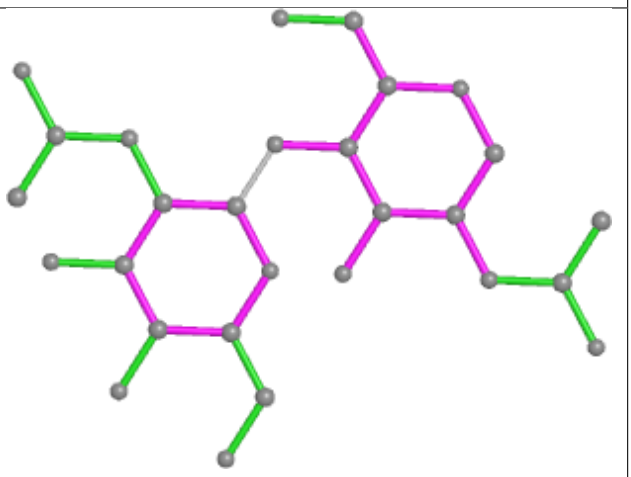


Rings

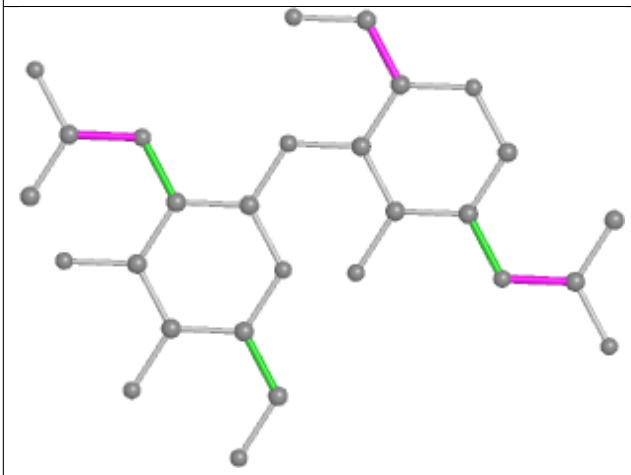
Oligosaccharide Chain a



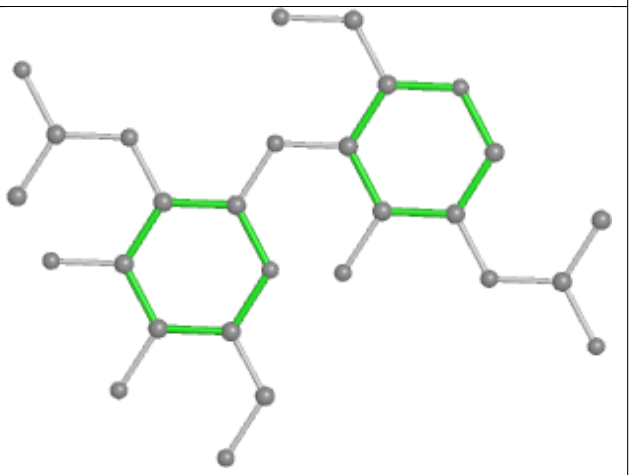
Bond lengths



Bond angles

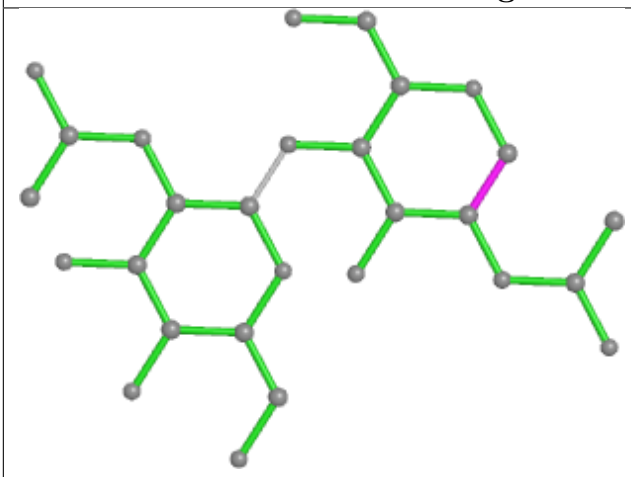


Torsions

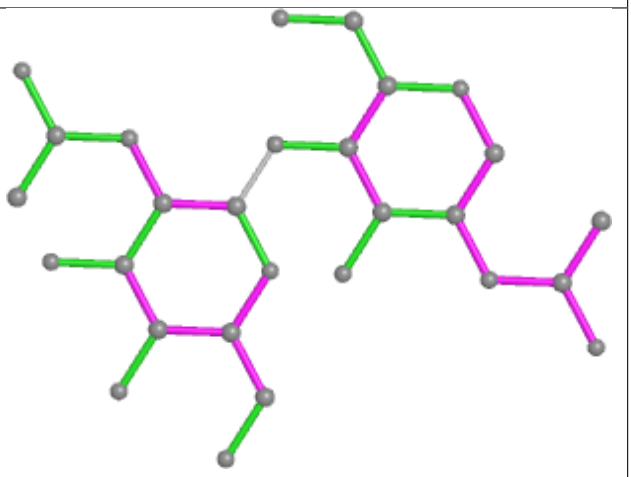


Rings

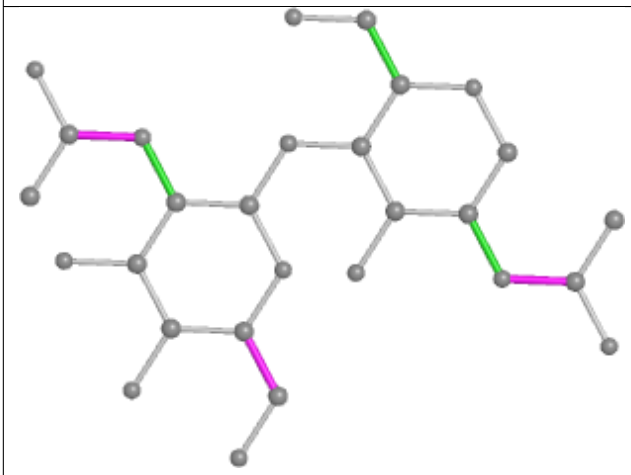
Oligosaccharide Chain b



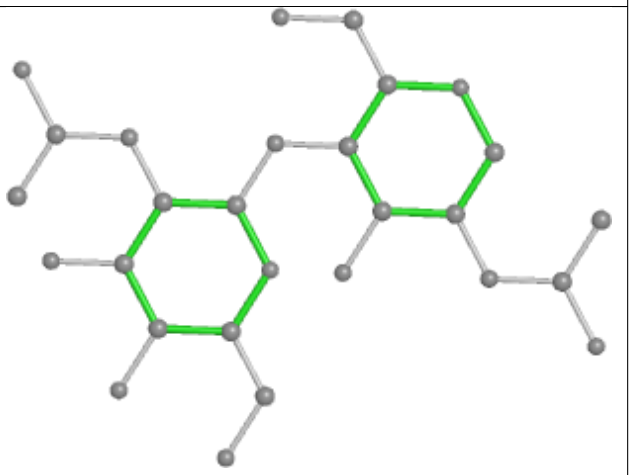
Bond lengths



Bond angles

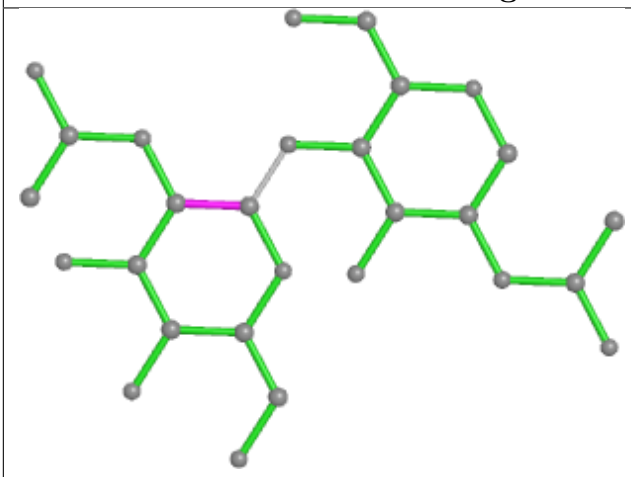


Torsions

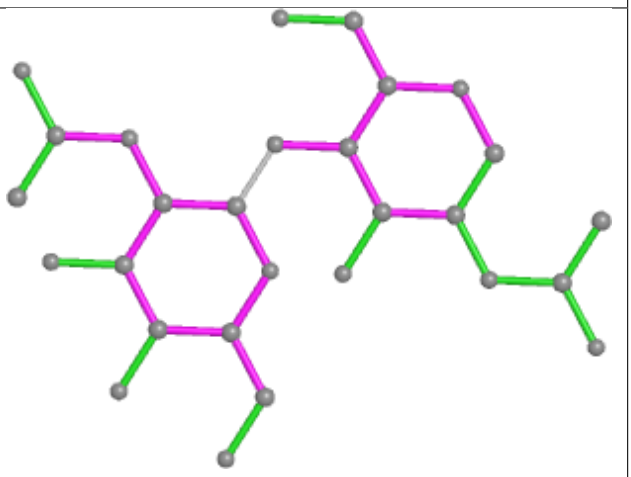


Rings

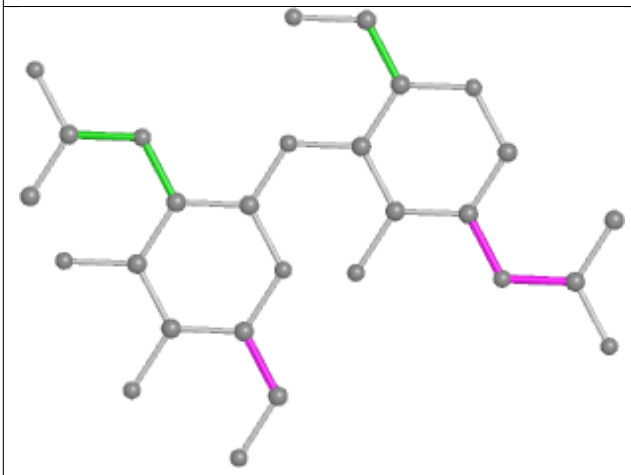
Oligosaccharide Chain c



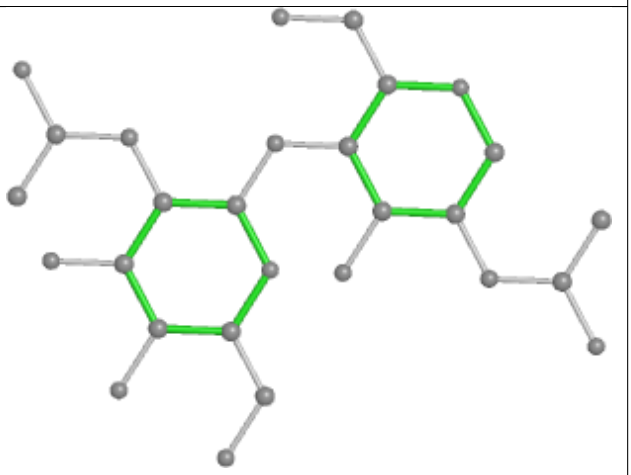
Bond lengths



Bond angles

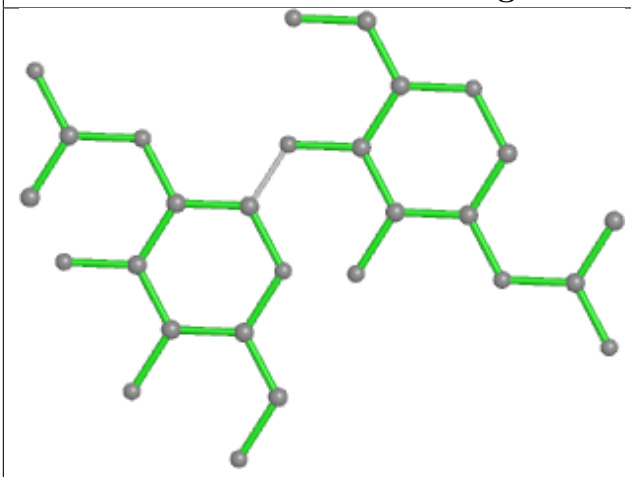


Torsions

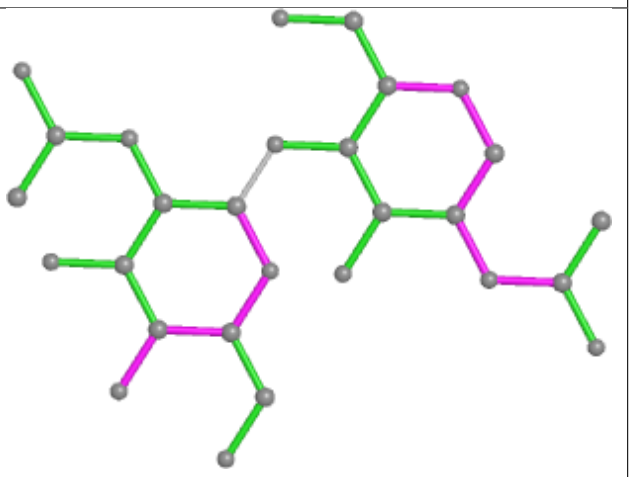


Rings

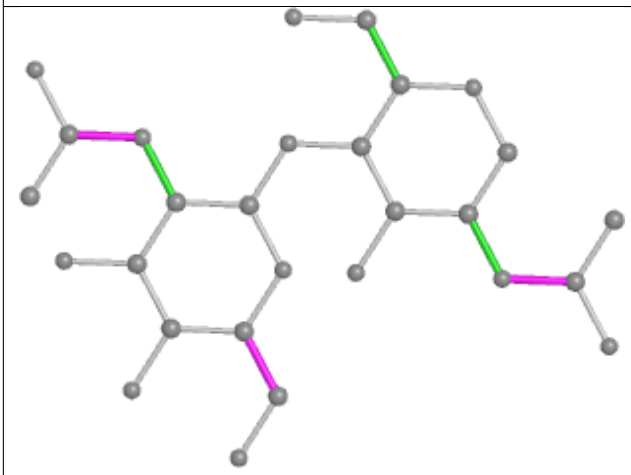
Oligosaccharide Chain d



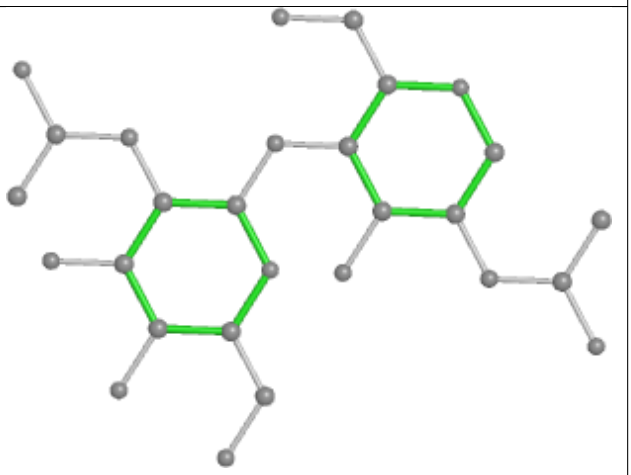
Bond lengths



Bond angles

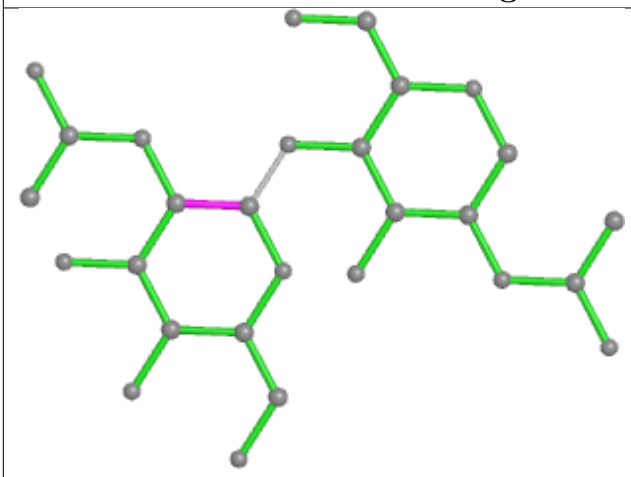


Torsions

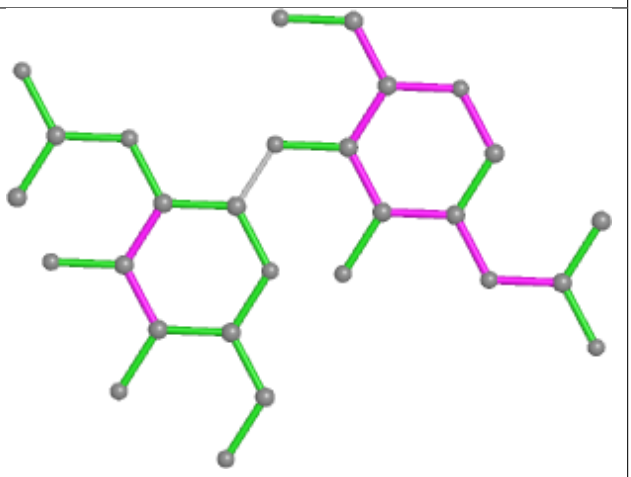


Rings

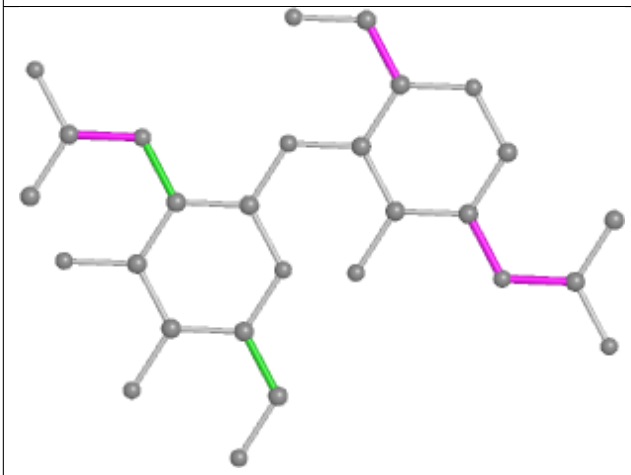
Oligosaccharide Chain e



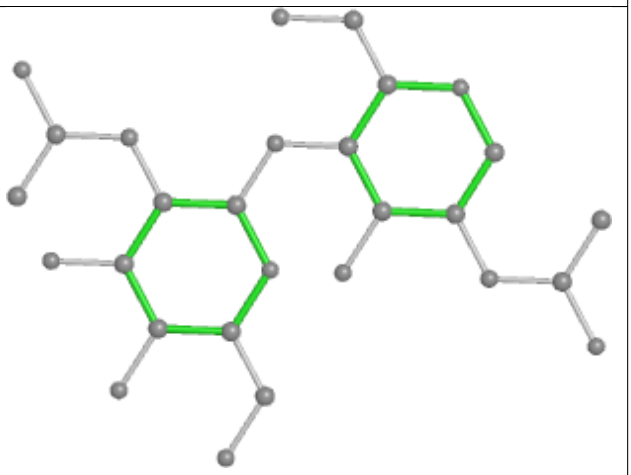
Bond lengths



Bond angles

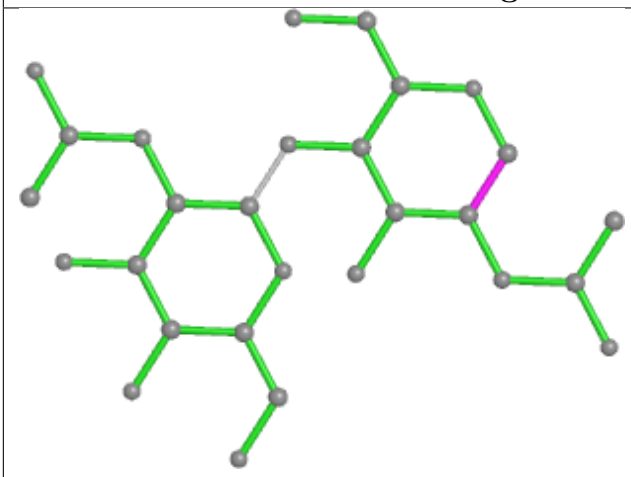


Torsions

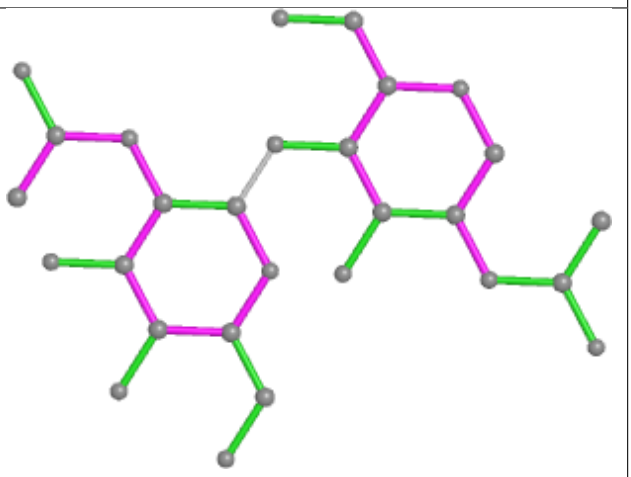


Rings

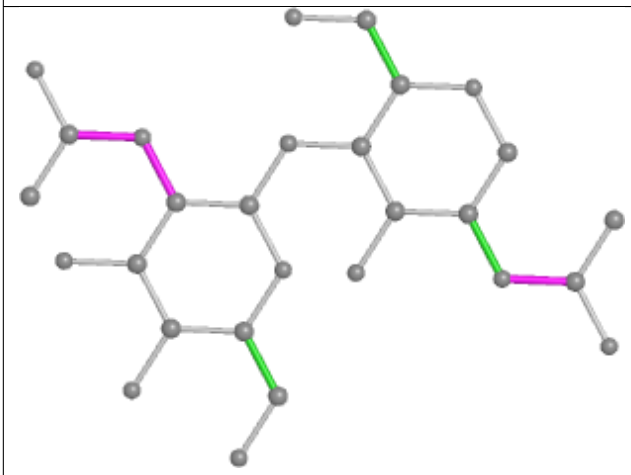
Oligosaccharide Chain f



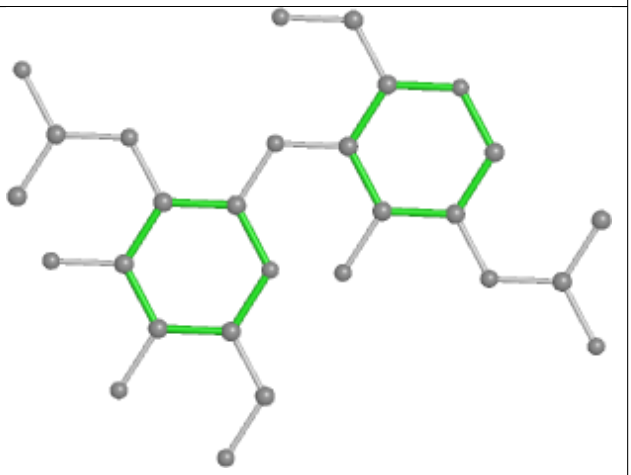
Bond lengths



Bond angles

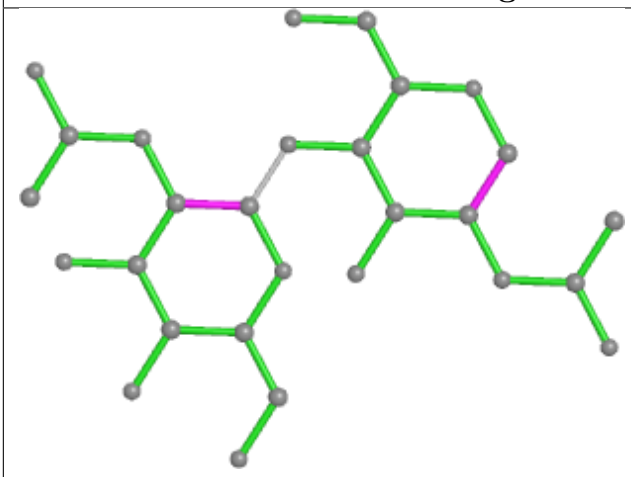


Torsions

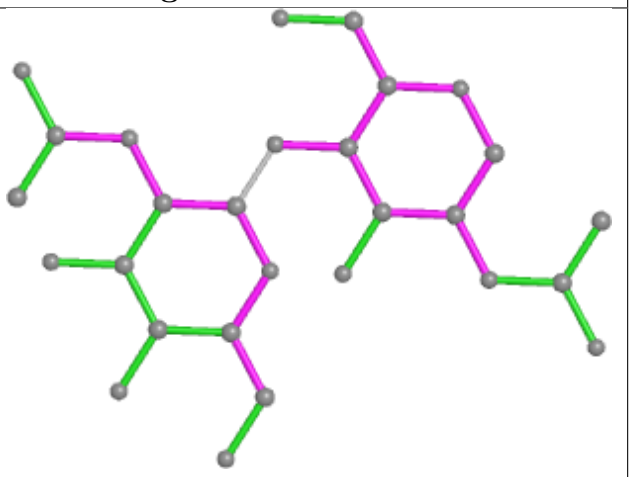


Rings

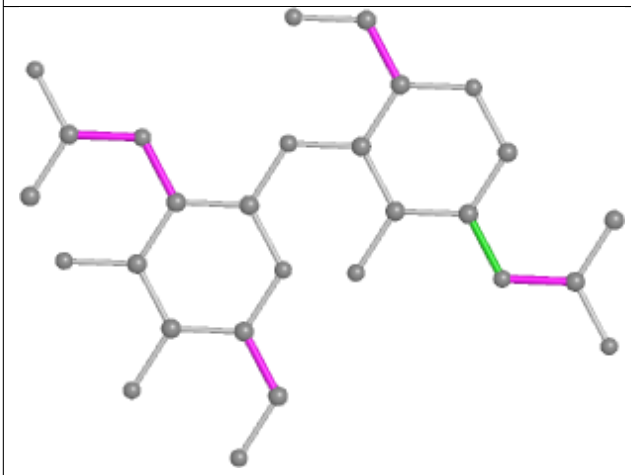
Oligosaccharide Chain g



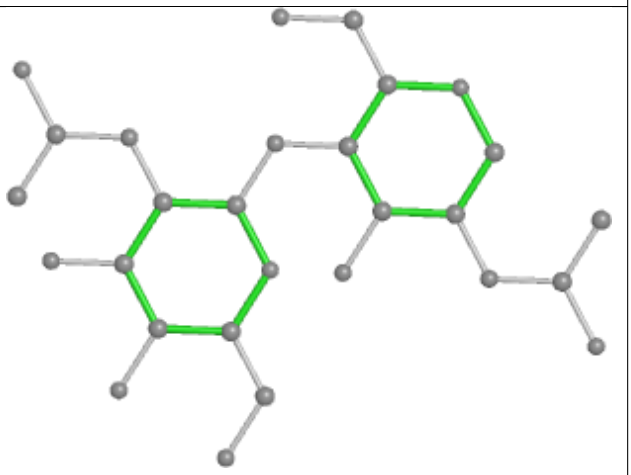
Bond lengths



Bond angles

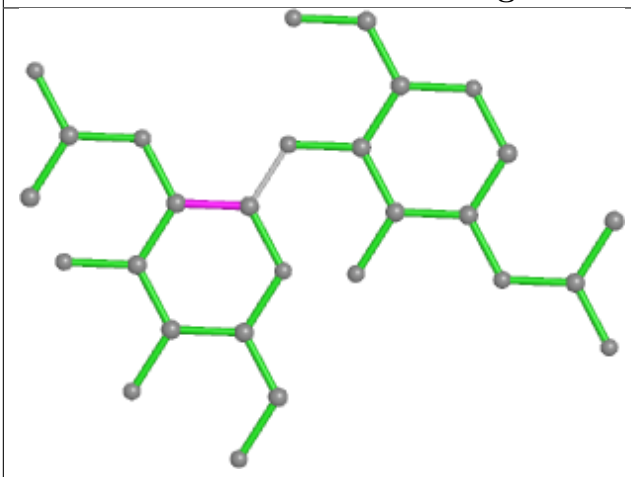


Torsions

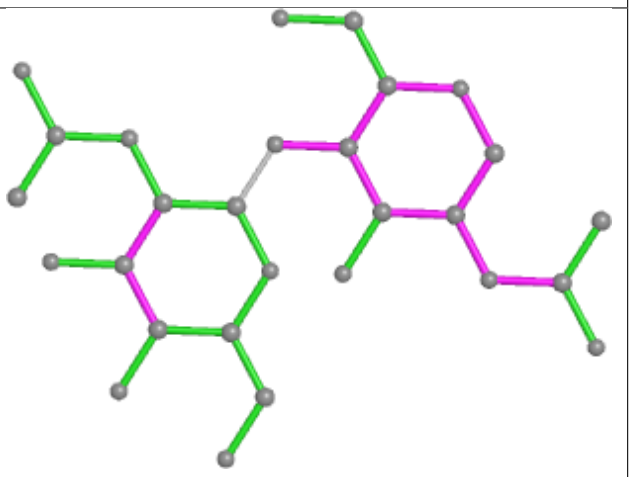


Rings

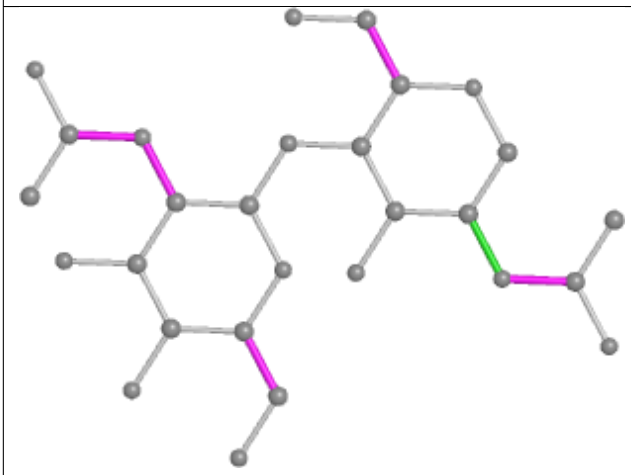
Oligosaccharide Chain h



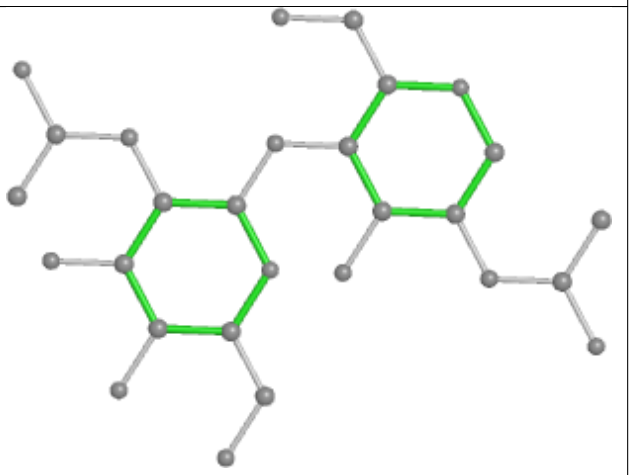
Bond lengths



Bond angles

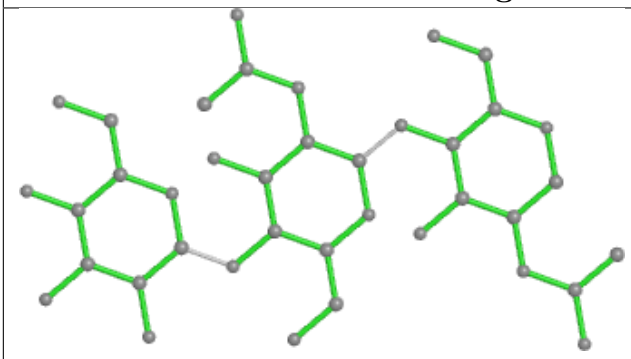


Torsions

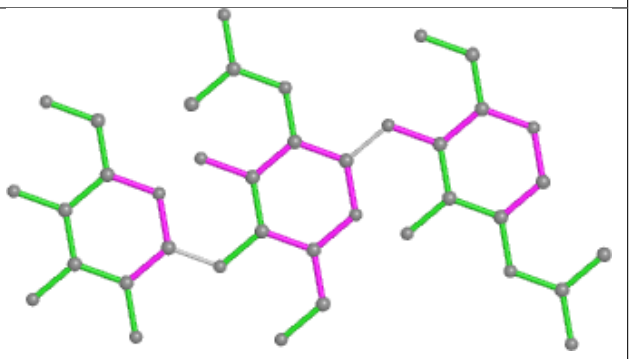


Rings

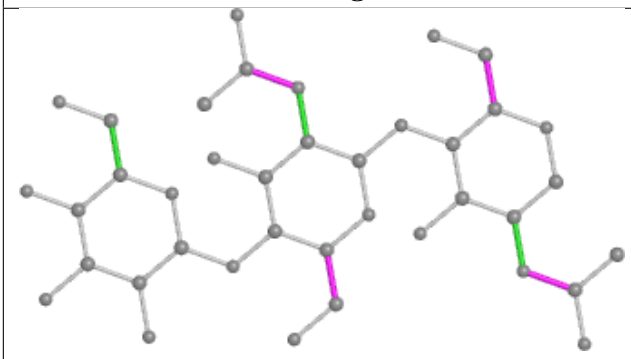
Oligosaccharide Chain T



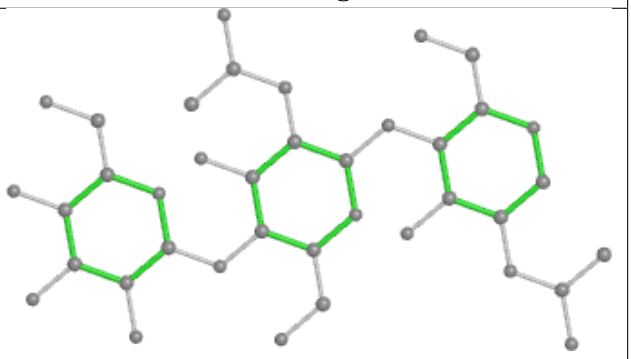
Bond lengths



Bond angles

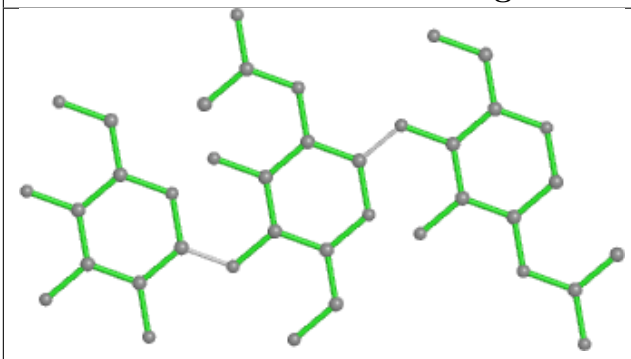


Torsions

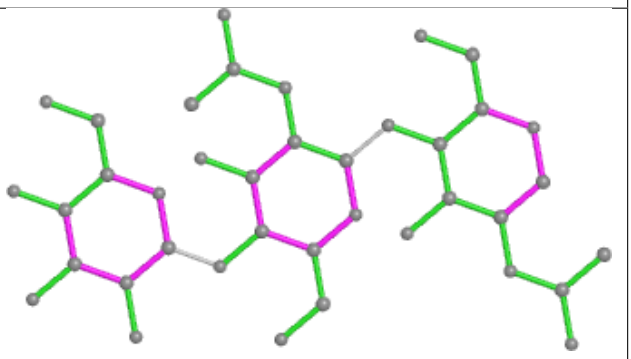


Rings

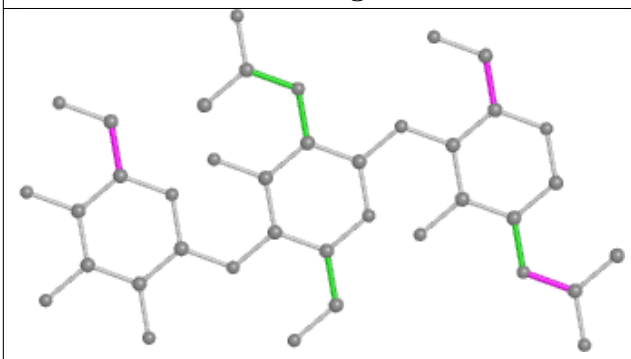
Oligosaccharide Chain X



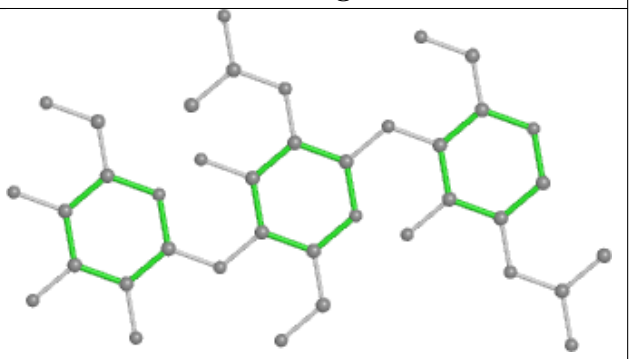
Bond lengths



Bond angles

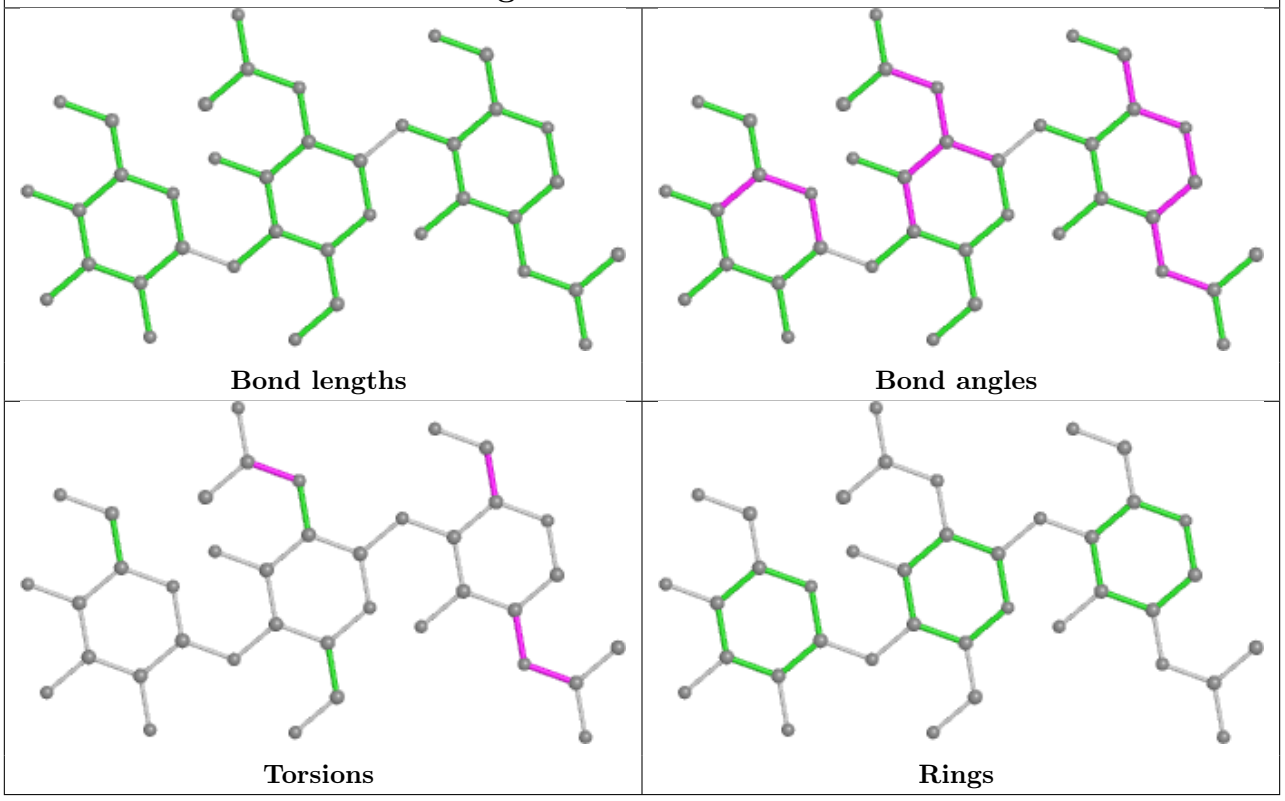


Torsions



Rings

Oligosaccharide Chain Z



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	322/334 (96%)	1.28	51 (15%)	2	1	70, 71, 72, 73	0
1	C	322/334 (96%)	1.19	45 (13%)	2	1	70, 71, 72, 73	0
1	E	322/334 (96%)	1.35	46 (14%)	2	1	70, 71, 72, 73	0
1	G	322/334 (96%)	1.30	42 (13%)	3	2	70, 71, 72, 73	0
1	I	322/334 (96%)	1.28	50 (15%)	2	1	70, 71, 72, 73	0
1	K	322/334 (96%)	1.38	60 (18%)	1	0	70, 71, 72, 74	0
1	M	322/334 (96%)	2.22	153 (47%)	0	0	54, 67, 75, 84	0
1	O	322/334 (96%)	2.08	140 (43%)	0	0	57, 68, 76, 83	0
1	Q	322/334 (96%)	3.58	228 (70%)	0	0	63, 72, 81, 86	0
2	B	175/181 (96%)	2.27	70 (40%)	0	0	70, 71, 72, 73	0
2	D	175/181 (96%)	2.62	89 (50%)	0	0	70, 71, 72, 73	0
2	F	175/181 (96%)	2.56	75 (42%)	0	0	70, 71, 72, 73	0
2	H	175/181 (96%)	2.81	90 (51%)	0	0	70, 71, 72, 73	0
2	J	175/181 (96%)	2.54	84 (48%)	0	0	70, 71, 72, 73	0
2	L	175/181 (96%)	2.80	88 (50%)	0	0	70, 71, 72, 73	0
2	N	175/181 (96%)	2.06	68 (38%)	0	0	55, 71, 82, 87	0
2	P	175/181 (96%)	2.13	65 (37%)	0	0	58, 68, 80, 82	0
2	R	175/181 (96%)	3.94	122 (69%)	0	0	60, 70, 85, 87	0
All	All	4473/4635 (96%)	2.06	1566 (35%)	0	0	54, 71, 77, 87	0

The worst 5 of 1566 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	134	GLY	20.5
1	G	324	PRO	20.3
1	I	16	GLY	18.5

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Mol	Chain	Res	Type	RSRZ
1	Q	324	PRO	18.4
1	Q	323	SER	15.6

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	g	2	14/15	0.10	0.66	115,117,118,118	0
3	NAG	W	2	14/15	0.29	0.49	108,111,113,113	0
4	BMA	T	3	11/12	0.32	0.57	96,100,101,102	0
3	NAG	h	2	14/15	0.44	0.52	104,106,111,112	0
3	NAG	c	2	14/15	0.47	0.43	109,112,114,115	0
4	BMA	X	3	11/12	0.48	0.47	105,106,107,107	0
4	BMA	Z	3	11/12	0.50	0.60	94,96,97,97	0
3	NAG	f	2	14/15	0.51	0.34	92,93,94,94	0
3	NAG	e	2	14/15	0.59	0.62	109,110,110,110	0
3	NAG	g	1	14/15	0.60	0.41	99,104,107,113	0
3	NAG	a	2	14/15	0.60	0.70	107,108,109,110	0
4	NAG	X	2	14/15	0.61	0.39	94,97,100,103	0
3	NAG	c	1	14/15	0.61	0.45	90,97,100,106	0
3	NAG	S	2	14/15	0.61	0.56	97,100,103,104	0
3	NAG	Y	2	14/15	0.62	0.46	103,106,107,108	0
3	NAG	a	1	14/15	0.62	0.42	90,97,100,103	0
4	NAG	Z	2	14/15	0.65	0.36	82,85,88,91	0
3	NAG	h	1	14/15	0.67	0.49	87,91,94,99	0
3	NAG	b	2	14/15	0.69	0.44	82,85,88,88	0
3	NAG	S	1	14/15	0.69	0.48	87,93,97,98	0
4	NAG	T	2	14/15	0.70	0.41	80,84,88,92	0
3	NAG	W	1	14/15	0.70	0.36	87,91,96,102	0
3	NAG	U	2	14/15	0.71	0.51	94,95,97,97	0
3	NAG	V	1	14/15	0.72	0.34	70,73,77,78	0
3	NAG	e	1	14/15	0.72	0.52	92,98,102,105	0

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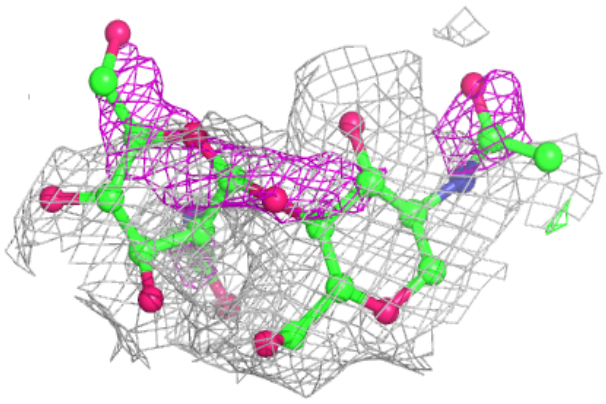
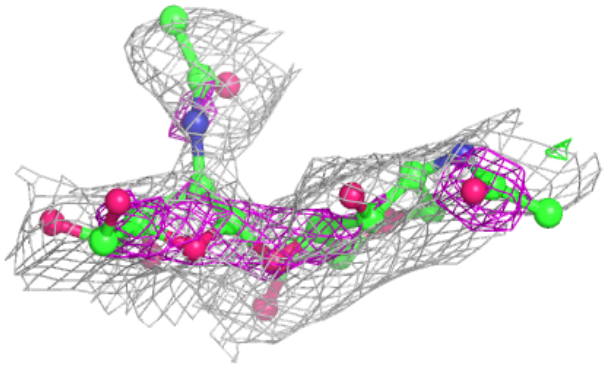
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	d	2	14/15	0.75	0.48	82,84,85,87	0
3	NAG	V	2	14/15	0.75	0.52	80,82,86,86	0
3	NAG	U	1	14/15	0.77	0.43	85,91,92,94	0
3	NAG	f	1	14/15	0.78	0.41	82,85,87,89	0
3	NAG	b	1	14/15	0.78	0.31	64,72,76,79	0
3	NAG	Y	1	14/15	0.79	0.35	87,91,94,100	0
4	NAG	X	1	14/15	0.81	0.33	79,81,84,89	0
3	NAG	d	1	14/15	0.83	0.30	61,71,74,80	0
4	NAG	Z	1	14/15	0.85	0.23	67,69,73,78	0
4	NAG	T	1	14/15	0.87	0.20	57,64,69,75	0

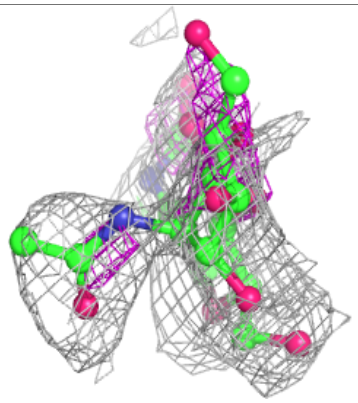
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

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

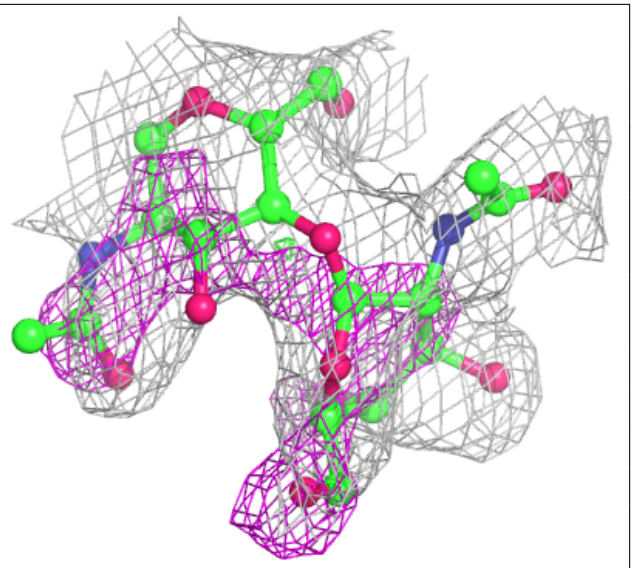


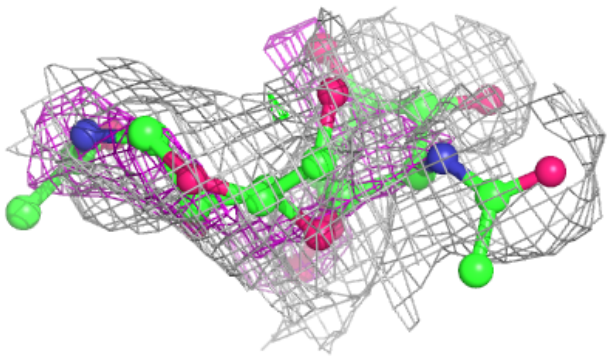


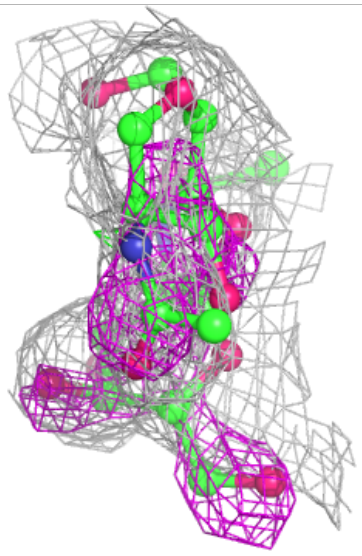


Electron density around Chain U:

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

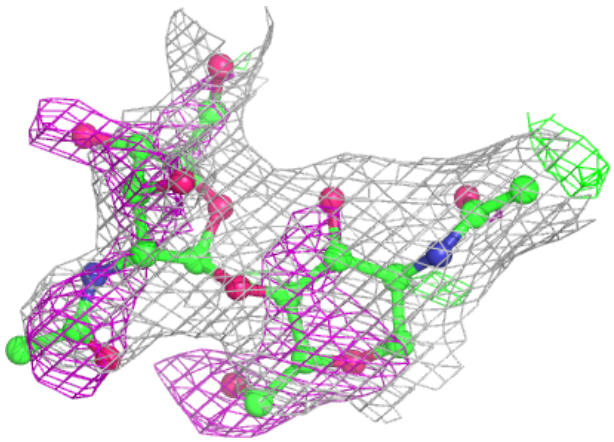


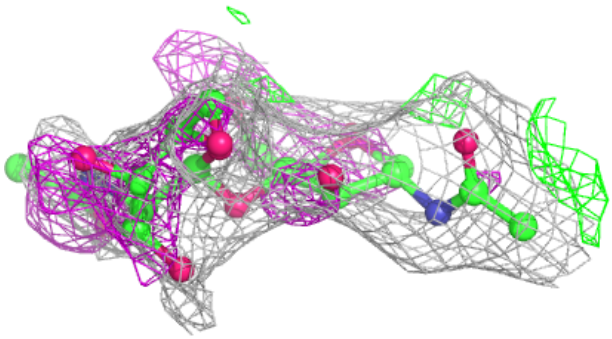


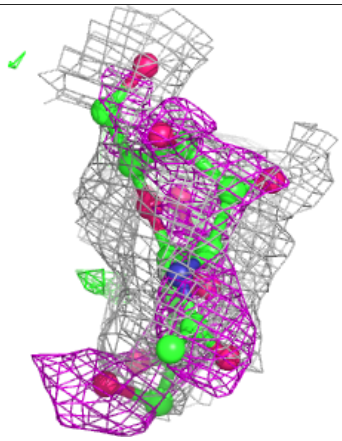


Electron density around Chain V:

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

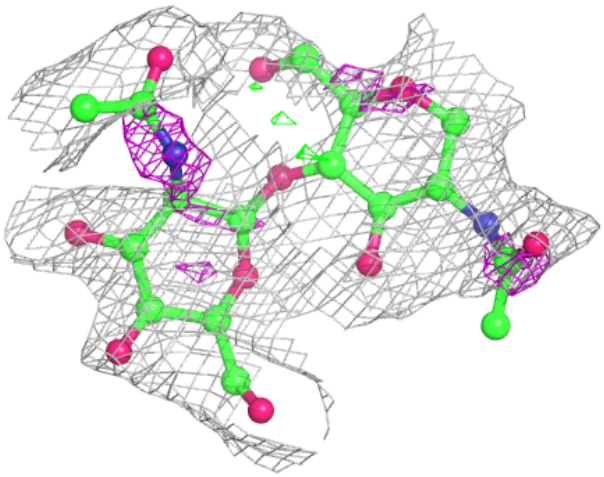


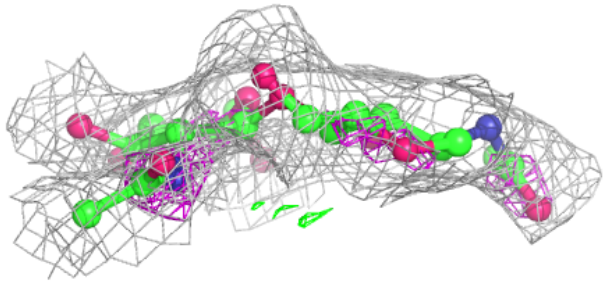


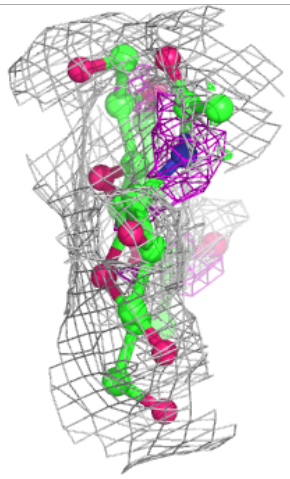


Electron density around Chain W:

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

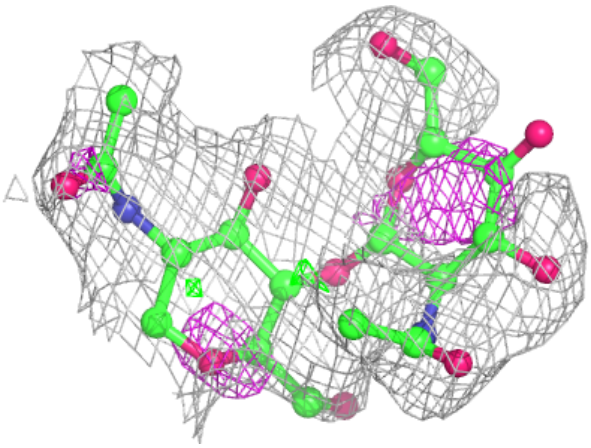


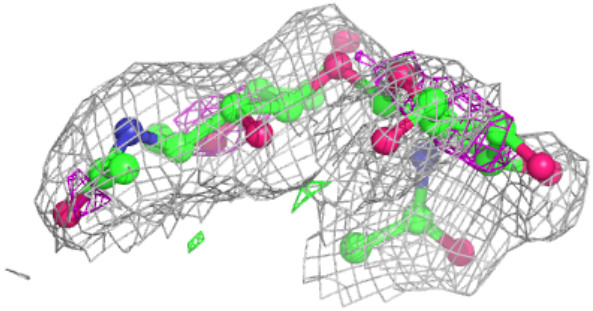


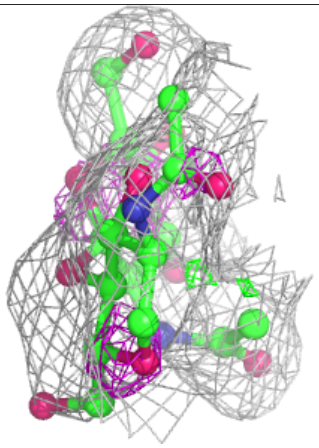


Electron density around Chain Y:

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

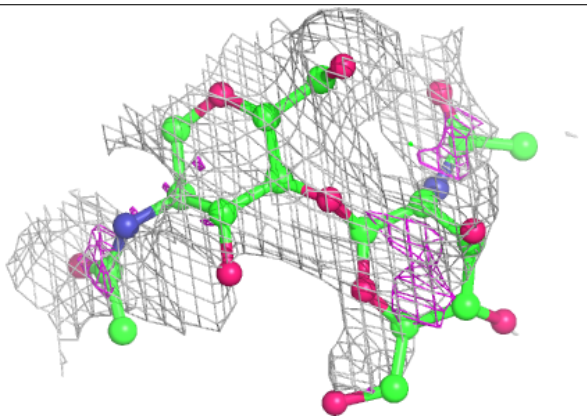


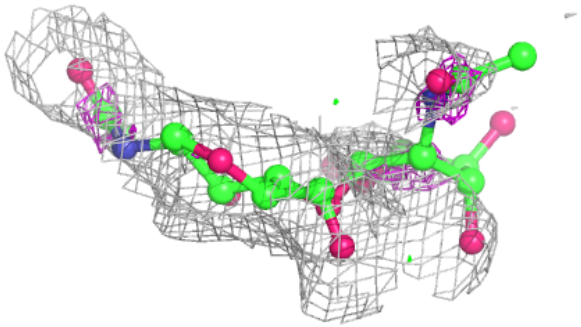


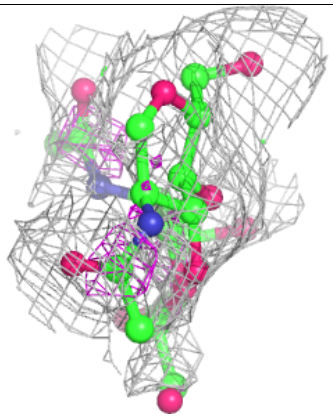


Electron density around Chain a:

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

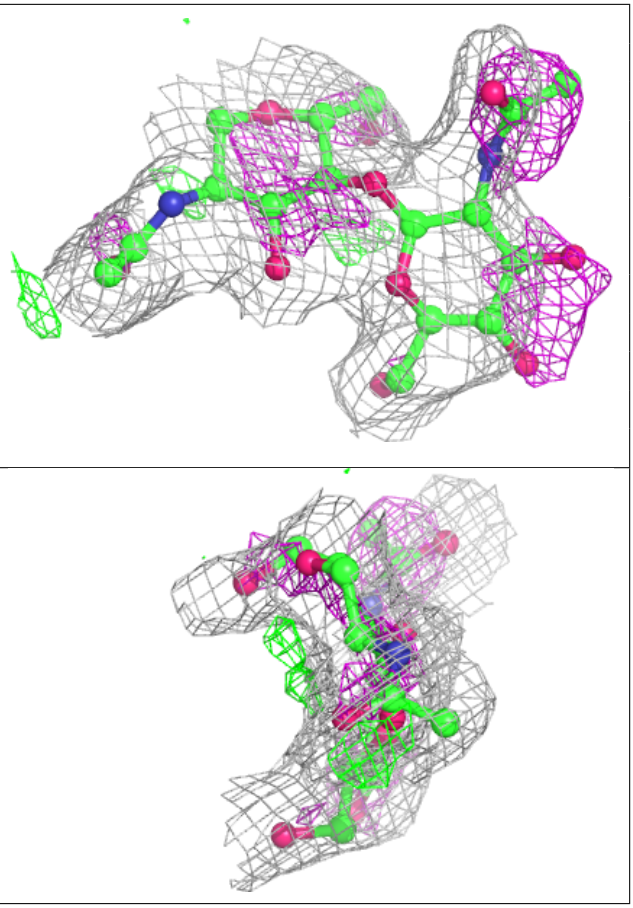


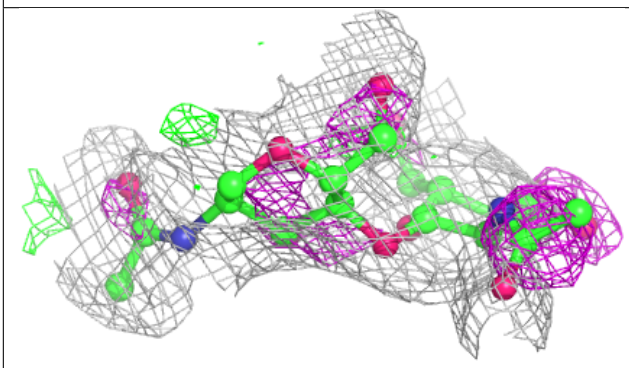




Electron density around Chain b:

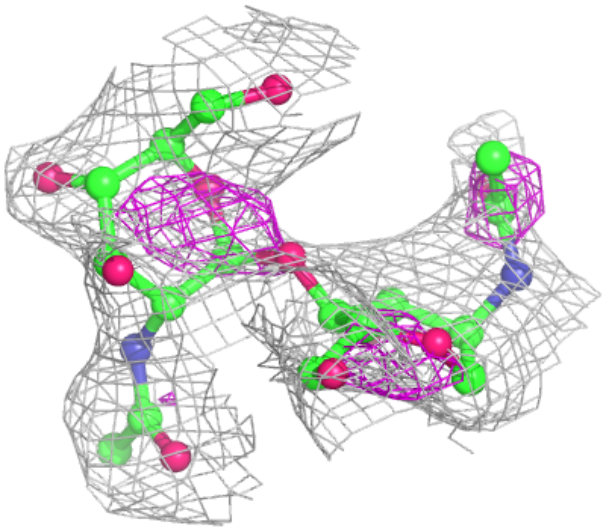
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

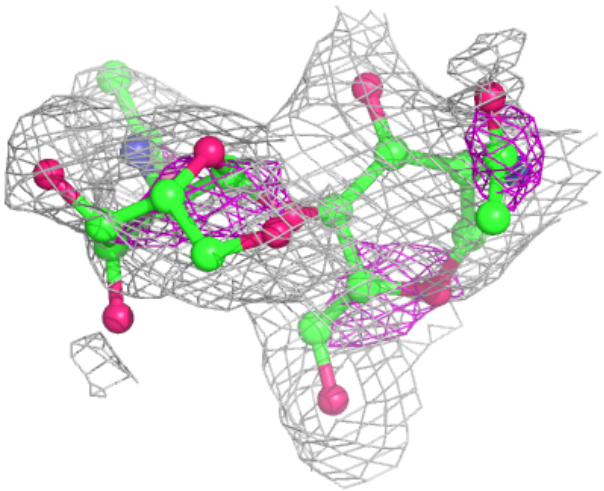


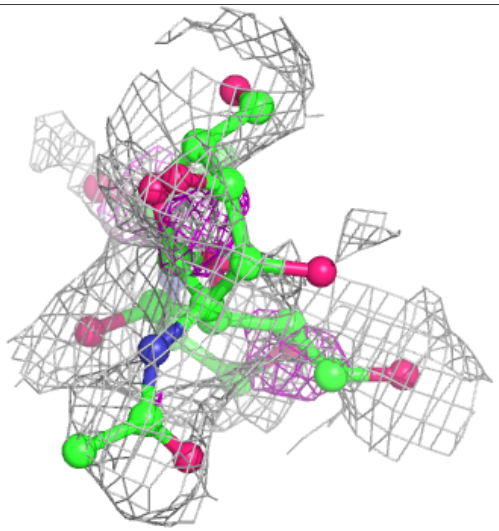


Electron density around Chain c:

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

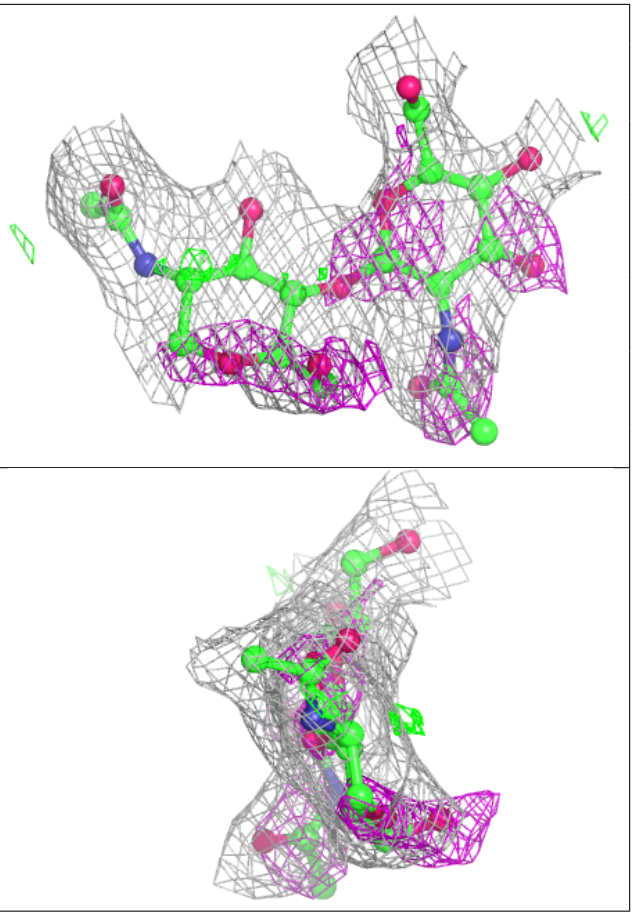






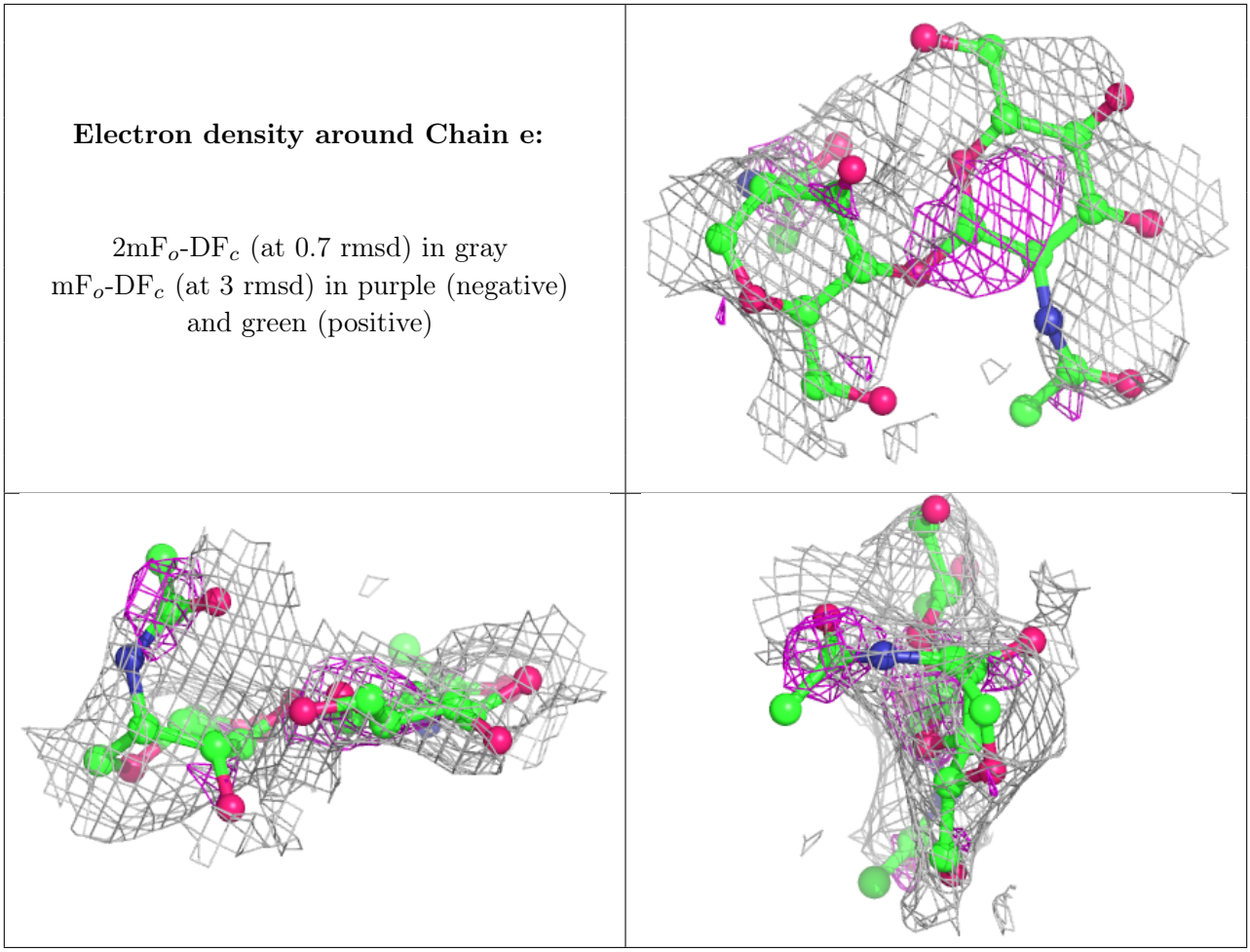
Electron density around Chain d:

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



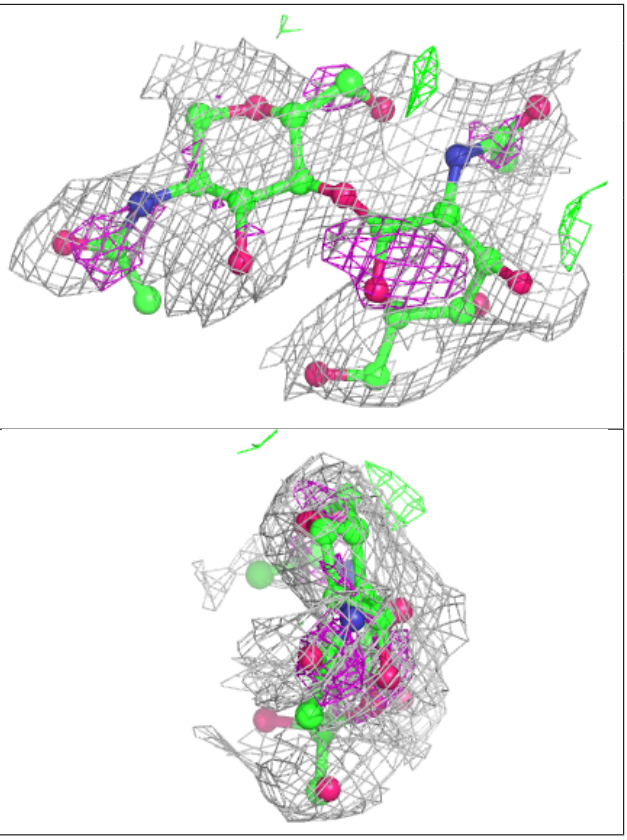
Electron density around Chain e:

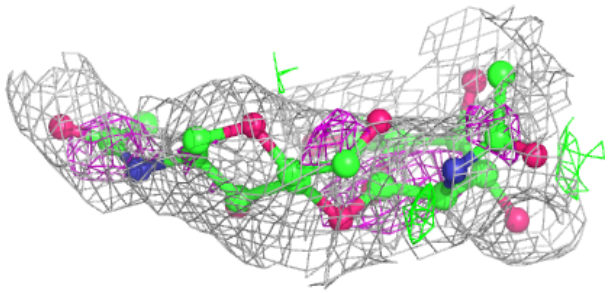
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain f:

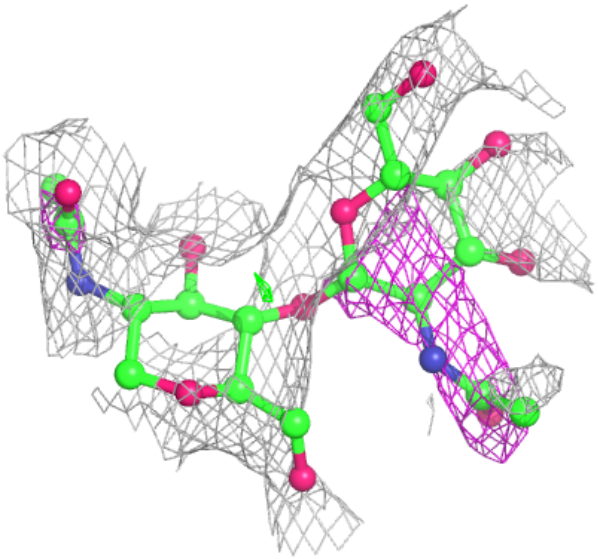
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

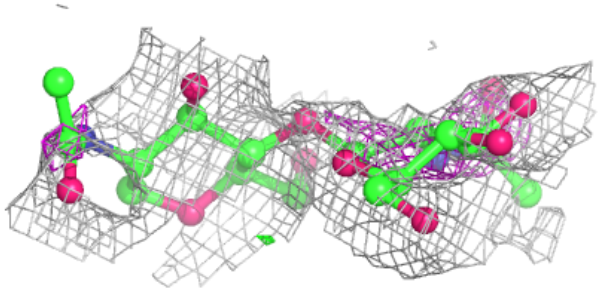


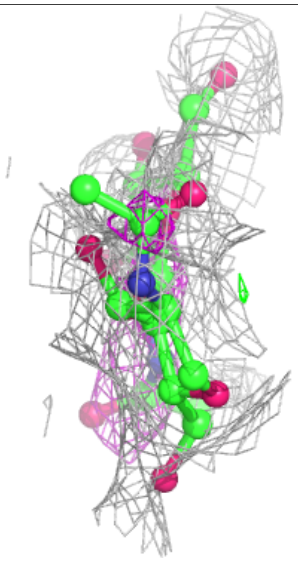


Electron density around Chain g:

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

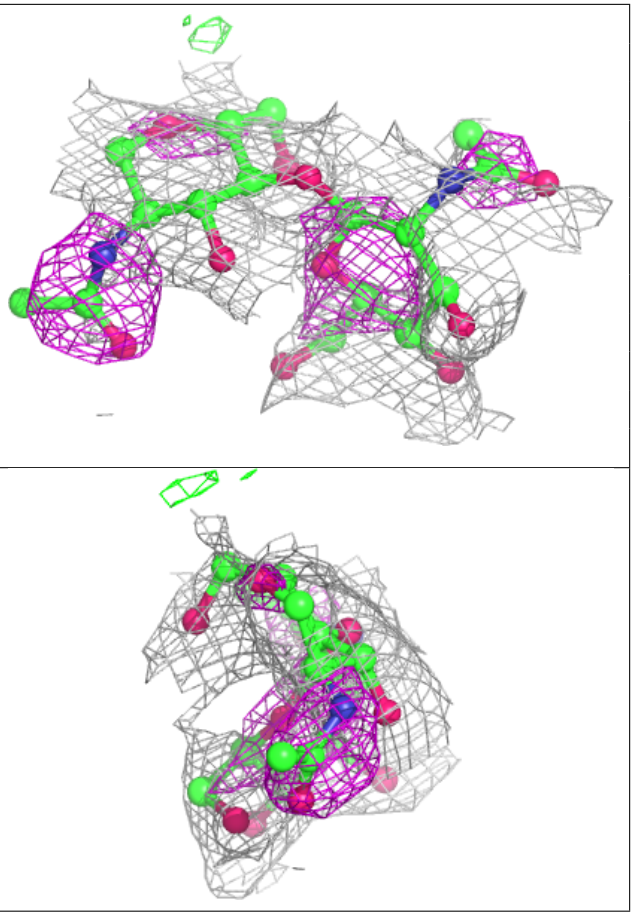






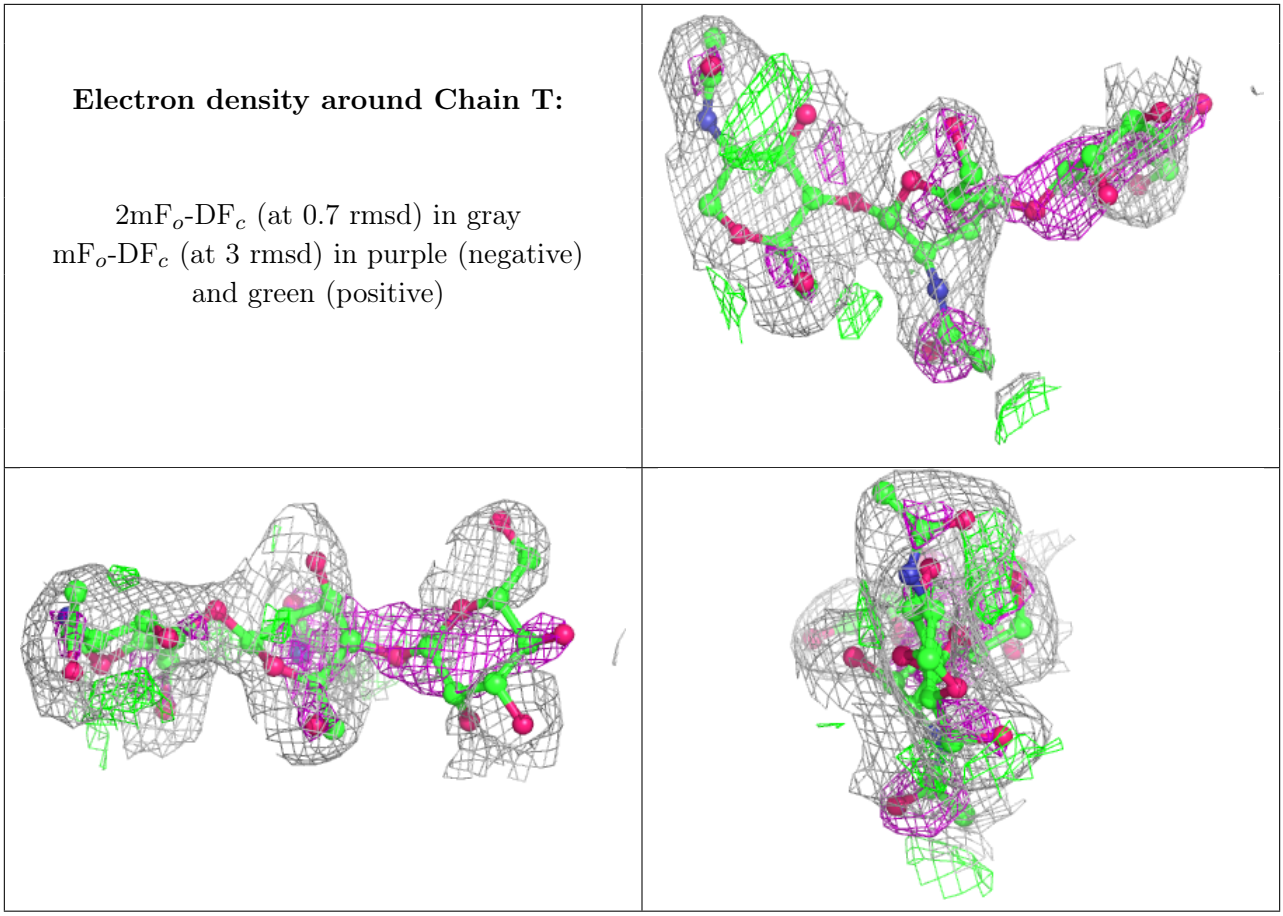
Electron density around Chain h:

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



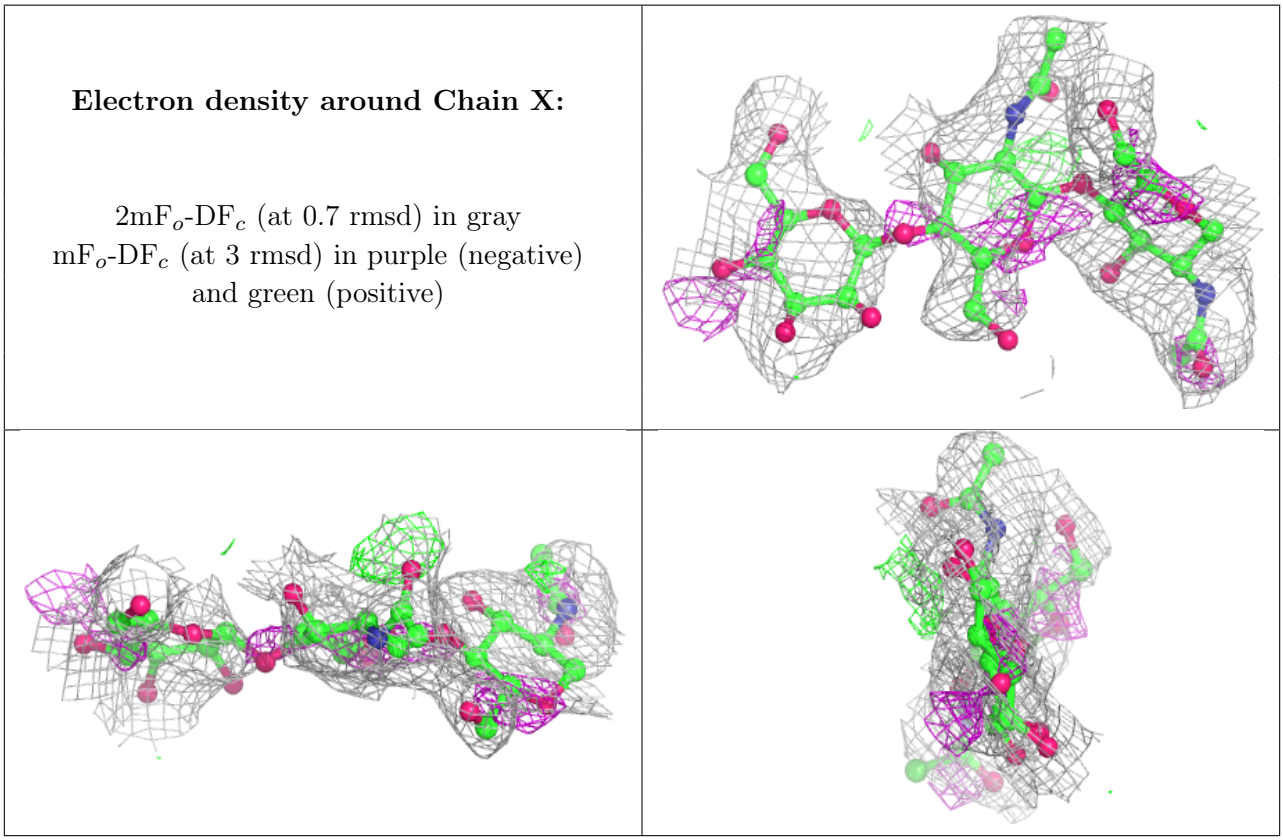
Electron density around Chain T:

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



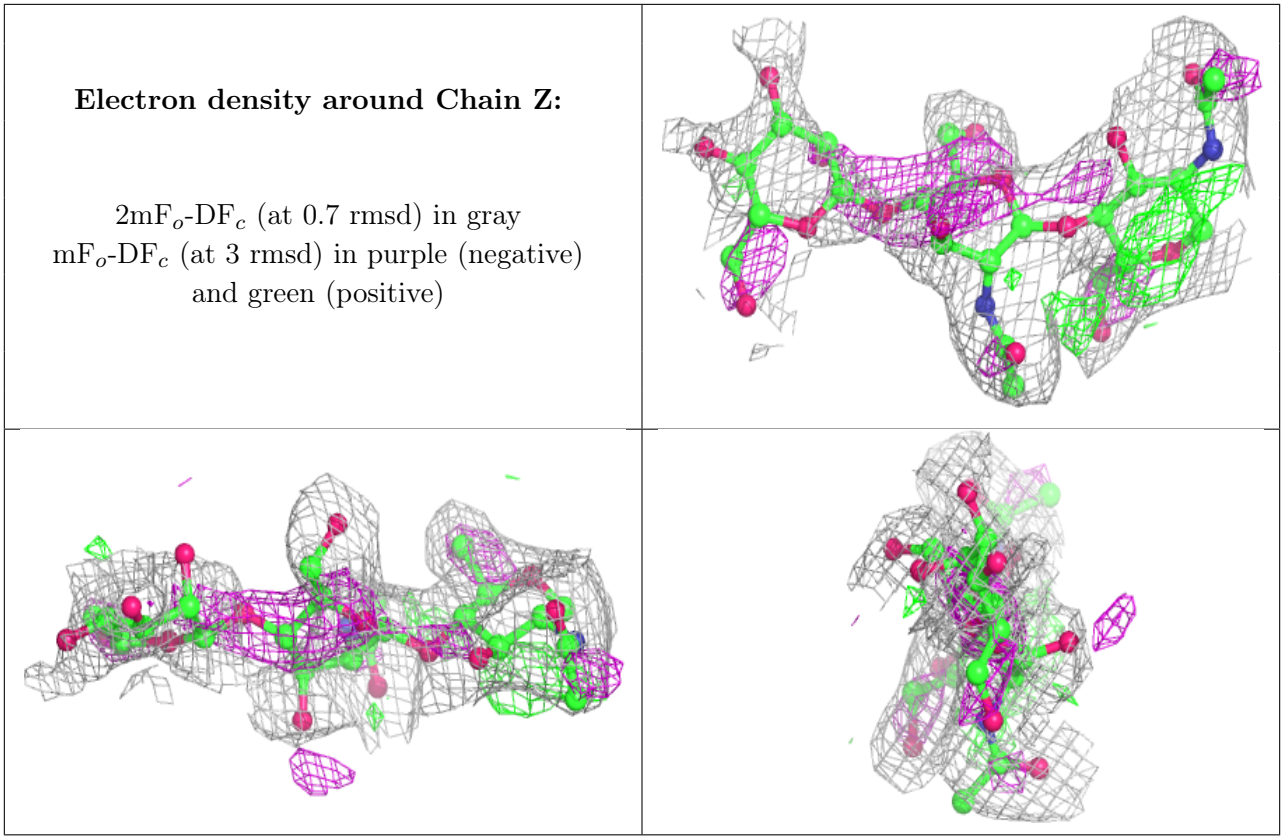
Electron density around Chain X:

$2mF_o$-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 Z:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.