wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 04:51 AM EDT

PDB ID	:	5W08
Title	:	A/Texas/50/2012(H3N2) Influenza hemagglutinin in complex with K03.12 Fab
Authors	:	McCarthy, K.R.; Harrison, S.C.
Deposited on	:	2017-05-30
Resolution	:	2.60 Å(reported)

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

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

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

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

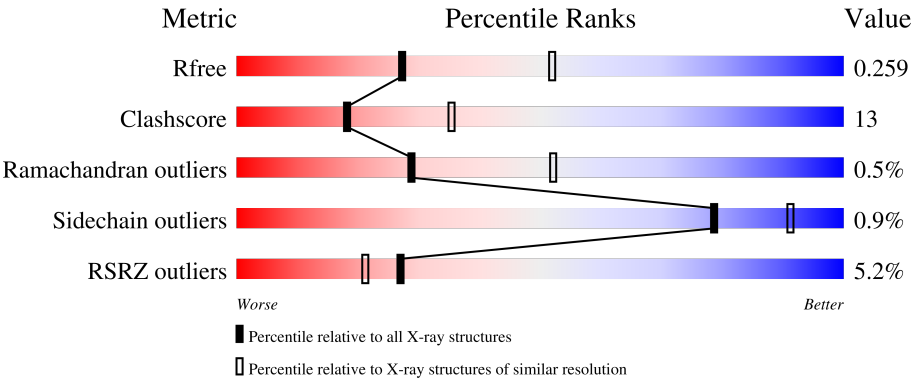
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	291	3% 72% 21% • 7%
1	B	291	2% 74% 20% • 6%
1	C	291	3% 66% 27% 7%
1	D	291	4% 73% 21% 6%
1	E	291	2% 72% 21% • 6%

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Mol	Chain	Length	Quality of chain
1	F	291	8% 68% 26% 6%
2	G	244	78% 19%
2	I	244	77% 20%
2	K	244	77% 19%
2	M	244	6% 81% 15%
2	O	244	6% 80% 15%
2	Q	244	7% 79% 16%
3	H	214	6% 84% 14%
3	J	214	7% 82% 18%
3	L	214	8% 74% 24%
3	N	214	8% 80% 17%
3	P	214	7% 85% 14%
3	R	214	10% 76% 22%
4	S	2	100%
4	V	2	50% 50%
4	W	2	50% 50%
4	Y	2	50% 50%
4	Z	2	50% 50%
5	T	3	67% 33%
5	U	3	33% 67%
5	X	3	100%
5	a	3	33% 67%
5	b	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
4	NAG	Z	2	-	-	-	X
5	NAG	T	1	-	-	X	-
5	BMA	T	3	-	-	-	X
5	BMA	U	3	-	-	-	X
5	BMA	a	3	-	-	-	X
5	BMA	b	3	-	-	-	X
6	NAG	A	406	-	-	X	-
6	NAG	A	407	-	-	-	X
6	NAG	C	401	-	-	-	X
6	NAG	D	405	-	-	X	X
6	NAG	D	406	-	-	X	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 34382 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
1	A	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	B	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			
1	C	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	D	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	E	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	F	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP R4L1D1
A	321	ALA	-	expression tag	UNP R4L1D1
A	322	LEU	-	expression tag	UNP R4L1D1
A	323	GLU	-	expression tag	UNP R4L1D1
A	324	VAL	-	expression tag	UNP R4L1D1
A	325	LEU	-	expression tag	UNP R4L1D1
A	326	PHE	-	expression tag	UNP R4L1D1
A	327	GLN	-	expression tag	UNP R4L1D1
B	320	GLY	-	expression tag	UNP R4L1D1
B	321	ALA	-	expression tag	UNP R4L1D1
B	322	LEU	-	expression tag	UNP R4L1D1
B	323	GLU	-	expression tag	UNP R4L1D1
B	324	VAL	-	expression tag	UNP R4L1D1
B	325	LEU	-	expression tag	UNP R4L1D1
B	326	PHE	-	expression tag	UNP R4L1D1
B	327	GLN	-	expression tag	UNP R4L1D1
C	320	GLY	-	expression tag	UNP R4L1D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	321	ALA	-	expression tag	UNP R4L1D1
C	322	LEU	-	expression tag	UNP R4L1D1
C	323	GLU	-	expression tag	UNP R4L1D1
C	324	VAL	-	expression tag	UNP R4L1D1
C	325	LEU	-	expression tag	UNP R4L1D1
C	326	PHE	-	expression tag	UNP R4L1D1
C	327	GLN	-	expression tag	UNP R4L1D1
D	320	GLY	-	expression tag	UNP R4L1D1
D	321	ALA	-	expression tag	UNP R4L1D1
D	322	LEU	-	expression tag	UNP R4L1D1
D	323	GLU	-	expression tag	UNP R4L1D1
D	324	VAL	-	expression tag	UNP R4L1D1
D	325	LEU	-	expression tag	UNP R4L1D1
D	326	PHE	-	expression tag	UNP R4L1D1
D	327	GLN	-	expression tag	UNP R4L1D1
E	320	GLY	-	expression tag	UNP R4L1D1
E	321	ALA	-	expression tag	UNP R4L1D1
E	322	LEU	-	expression tag	UNP R4L1D1
E	323	GLU	-	expression tag	UNP R4L1D1
E	324	VAL	-	expression tag	UNP R4L1D1
E	325	LEU	-	expression tag	UNP R4L1D1
E	326	PHE	-	expression tag	UNP R4L1D1
E	327	GLN	-	expression tag	UNP R4L1D1
F	320	GLY	-	expression tag	UNP R4L1D1
F	321	ALA	-	expression tag	UNP R4L1D1
F	322	LEU	-	expression tag	UNP R4L1D1
F	323	GLU	-	expression tag	UNP R4L1D1
F	324	VAL	-	expression tag	UNP R4L1D1
F	325	LEU	-	expression tag	UNP R4L1D1
F	326	PHE	-	expression tag	UNP R4L1D1
F	327	GLN	-	expression tag	UNP R4L1D1

- Molecule 2 is a protein called K03.12 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	236	Total	C	N	O	S	0	0	0
			1790	1132	300	349	9			
2	I	238	Total	C	N	O	S	0	0	0
			1807	1142	303	353	9			
2	K	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	M	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	Q	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	239	HIS	-	expression tag	UNP S6C4S0
G	240	HIS	-	expression tag	UNP S6C4S0
G	241	HIS	-	expression tag	UNP S6C4S0
G	242	HIS	-	expression tag	UNP S6C4S0
G	243	HIS	-	expression tag	UNP S6C4S0
G	244	HIS	-	expression tag	UNP S6C4S0
I	239	HIS	-	expression tag	UNP S6C4S0
I	240	HIS	-	expression tag	UNP S6C4S0
I	241	HIS	-	expression tag	UNP S6C4S0
I	242	HIS	-	expression tag	UNP S6C4S0
I	243	HIS	-	expression tag	UNP S6C4S0
I	244	HIS	-	expression tag	UNP S6C4S0
K	239	HIS	-	expression tag	UNP S6C4S0
K	240	HIS	-	expression tag	UNP S6C4S0
K	241	HIS	-	expression tag	UNP S6C4S0
K	242	HIS	-	expression tag	UNP S6C4S0
K	243	HIS	-	expression tag	UNP S6C4S0
K	244	HIS	-	expression tag	UNP S6C4S0
M	239	HIS	-	expression tag	UNP S6C4S0
M	240	HIS	-	expression tag	UNP S6C4S0
M	241	HIS	-	expression tag	UNP S6C4S0
M	242	HIS	-	expression tag	UNP S6C4S0
M	243	HIS	-	expression tag	UNP S6C4S0
M	244	HIS	-	expression tag	UNP S6C4S0
O	239	HIS	-	expression tag	UNP S6C4S0
O	240	HIS	-	expression tag	UNP S6C4S0
O	241	HIS	-	expression tag	UNP S6C4S0
O	242	HIS	-	expression tag	UNP S6C4S0
O	243	HIS	-	expression tag	UNP S6C4S0
O	244	HIS	-	expression tag	UNP S6C4S0
Q	239	HIS	-	expression tag	UNP S6C4S0
Q	240	HIS	-	expression tag	UNP S6C4S0
Q	241	HIS	-	expression tag	UNP S6C4S0
Q	242	HIS	-	expression tag	UNP S6C4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	243	HIS	-	expression tag	UNP S6C4S0
Q	244	HIS	-	expression tag	UNP S6C4S0

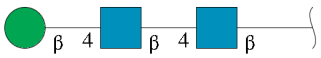
- Molecule 3 is a protein called K03.12 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1561	973	258	325	5			
3	J	213	Total	C	N	O	S	0	0	0
			1568	978	259	326	5			
3	L	211	Total	C	N	O	S	0	0	0
			1555	970	257	324	4			
3	N	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	P	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	R	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			

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

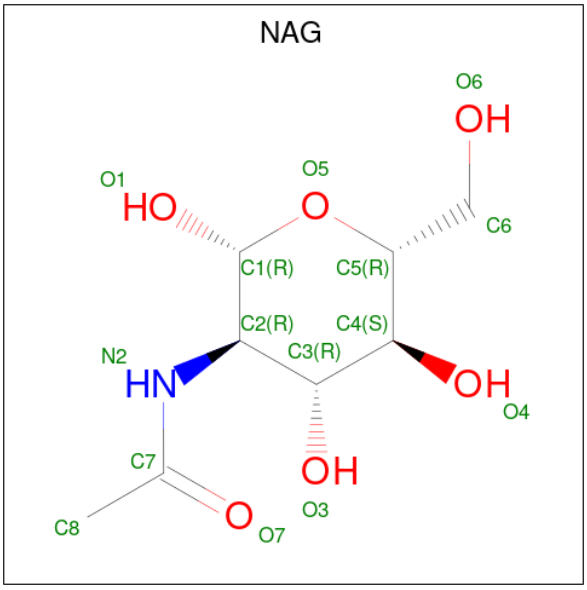
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	T	3	Total C N O 39 22 2 15	0	0	0
5	U	3	Total C N O 39 22 2 15	0	0	0
5	X	3	Total C N O 39 22 2 15	0	0	0
5	a	3	Total C N O 39 22 2 15	0	0	0
5	b	3	Total C N O 39 22 2 15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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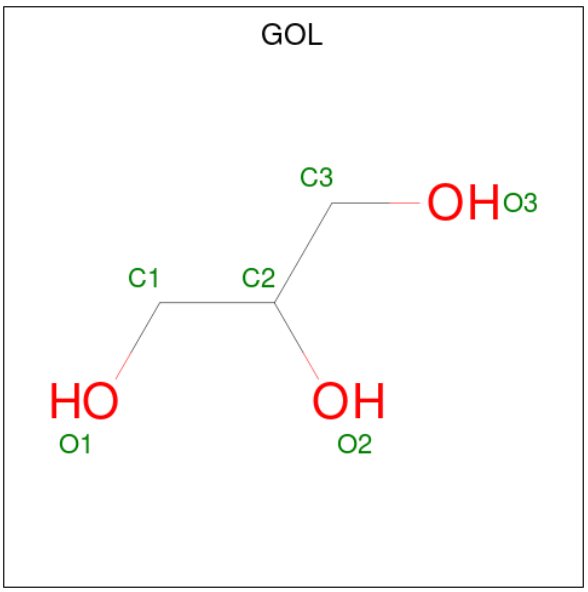
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 6 3 3	0	0

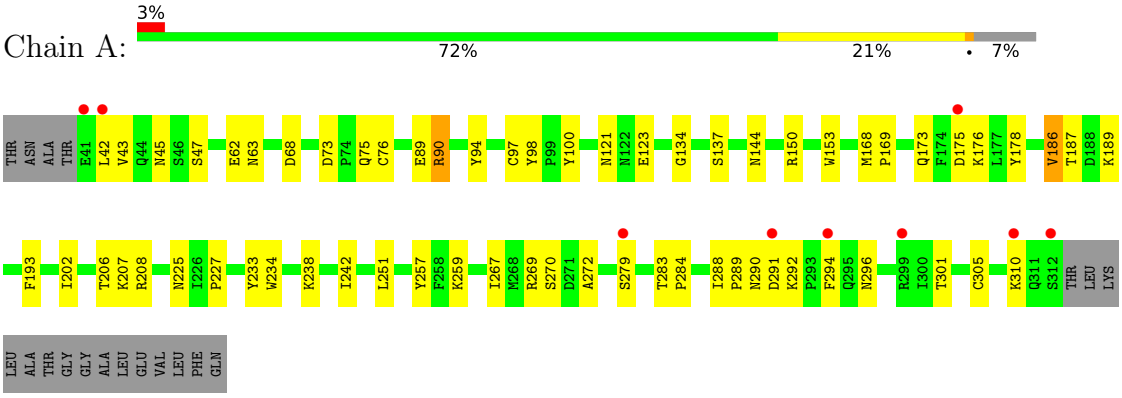
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	58	Total O 58 58	0	0
8	B	79	Total O 79 79	0	0
8	C	48	Total O 48 48	0	0
8	D	49	Total O 49 49	0	0
8	E	46	Total O 46 46	0	0
8	F	37	Total O 37 37	0	0
8	G	45	Total O 45 45	0	0
8	H	41	Total O 41 41	0	0
8	I	55	Total O 55 55	0	0
8	J	43	Total O 43 43	0	0
8	K	29	Total O 29 29	0	0
8	L	23	Total O 23 23	0	0
8	M	28	Total O 28 28	0	0
8	N	40	Total O 40 40	0	0
8	O	30	Total O 30 30	0	0
8	P	22	Total O 22 22	0	0
8	Q	24	Total O 24 24	0	0
8	R	25	Total O 25 25	0	0

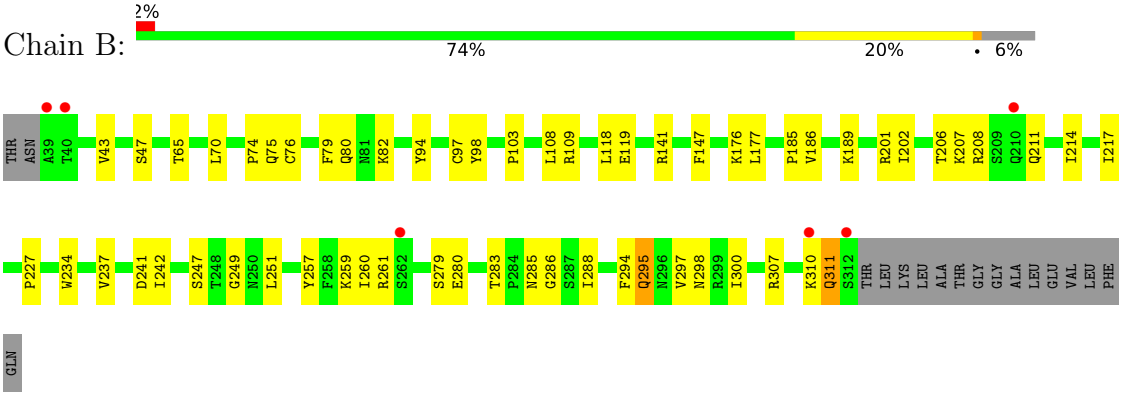
3 Residue-property plots (i)

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.

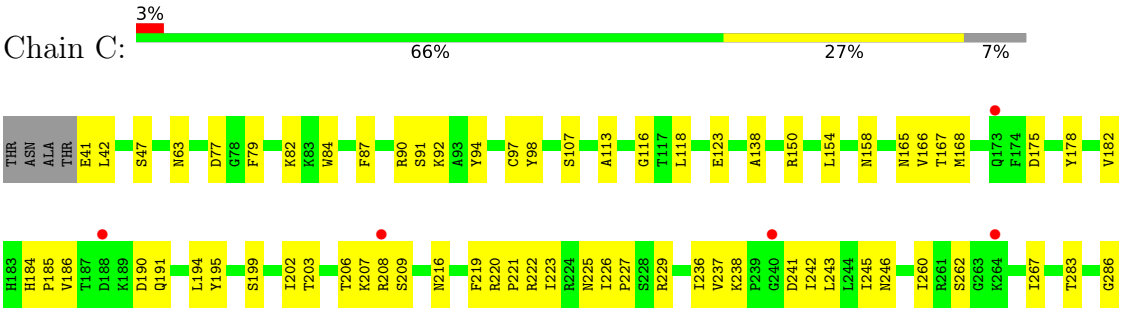
• Molecule 1: Hemagglutinin HA1

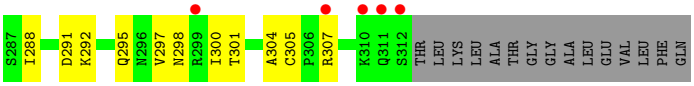


• Molecule 1: Hemagglutinin HA1

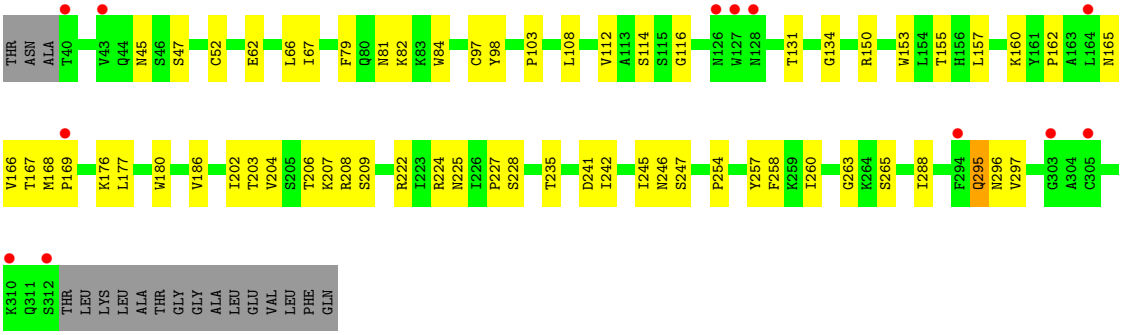


• Molecule 1: Hemagglutinin HA1

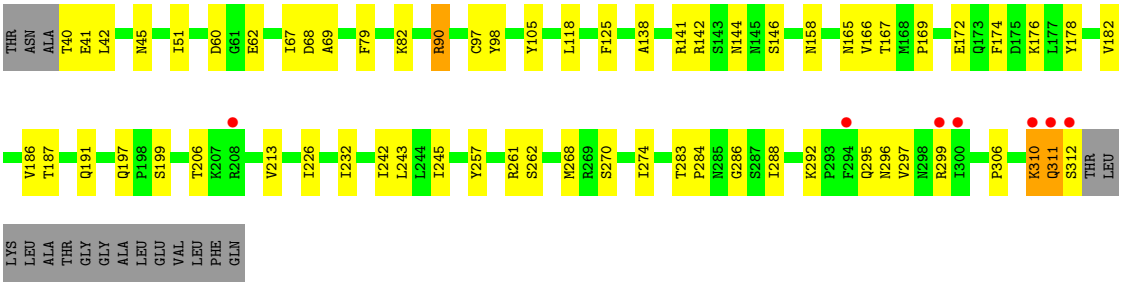




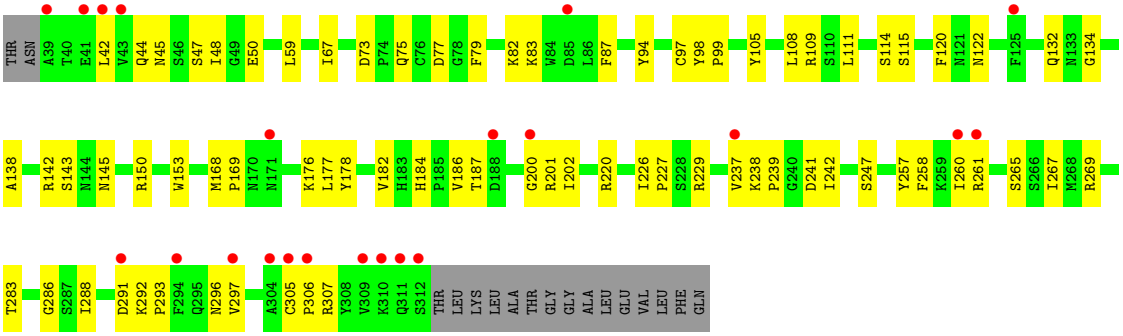
• Molecule 1: Hemagglutinin HA1



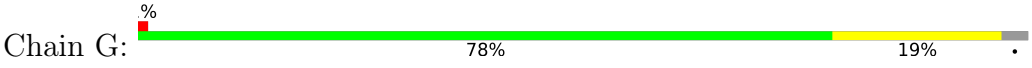
• Molecule 1: Hemagglutinin HA1

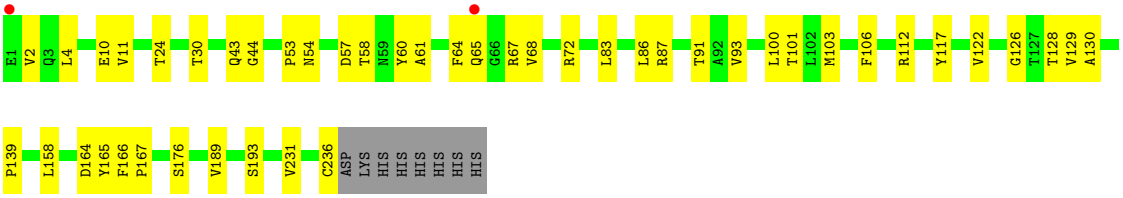


• Molecule 1: Hemagglutinin HA1

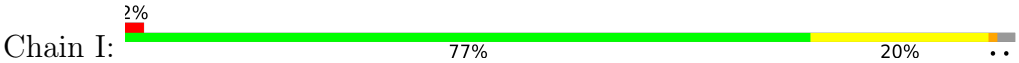


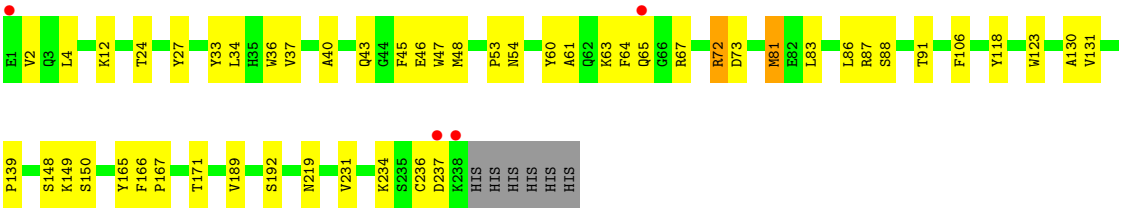
• Molecule 2: K03.12 antibody heavy chain



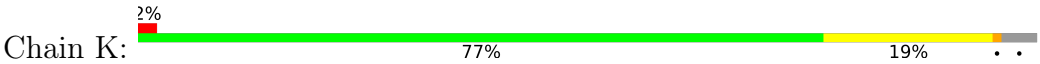


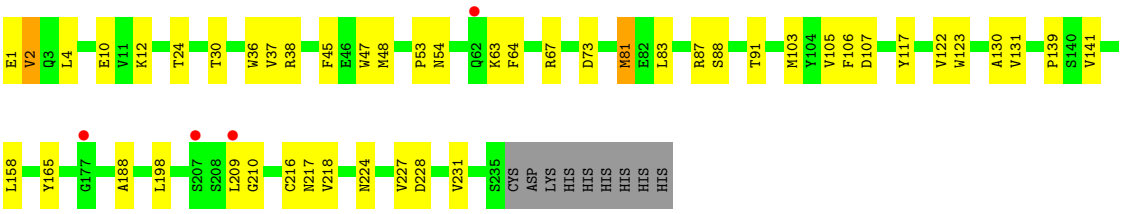
• Molecule 2: K03.12 antibody heavy chain



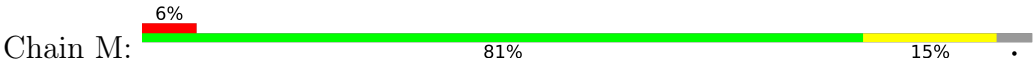


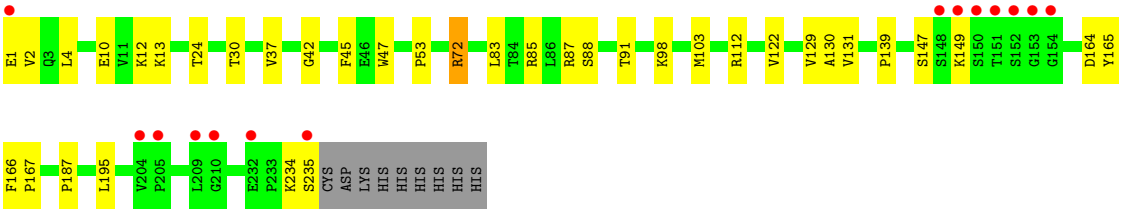
• Molecule 2: K03.12 antibody heavy chain



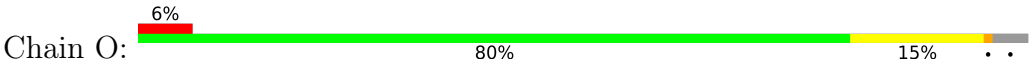


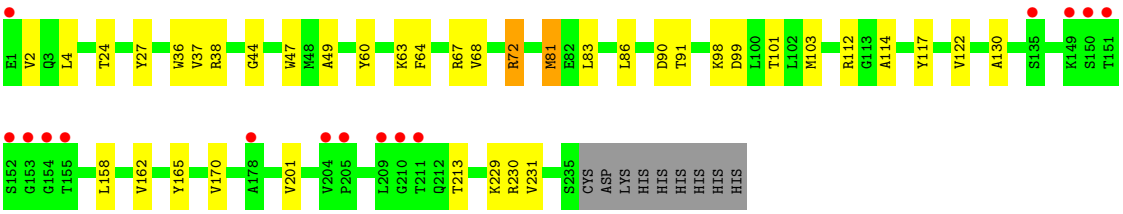
• Molecule 2: K03.12 antibody heavy chain





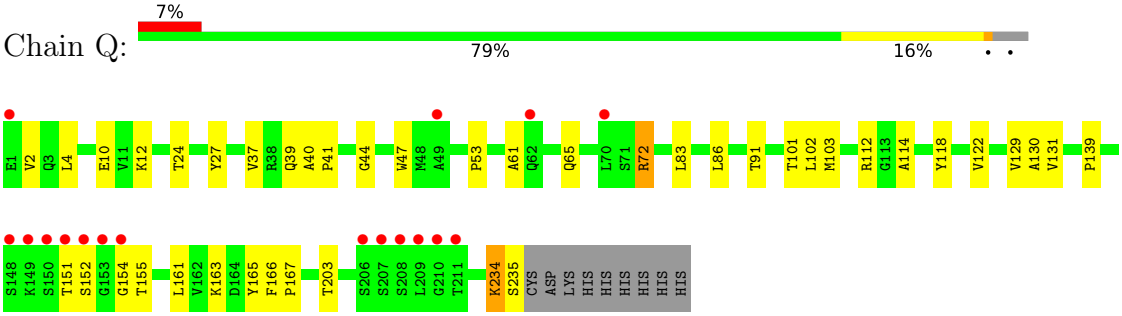
• Molecule 2: K03.12 antibody heavy chain





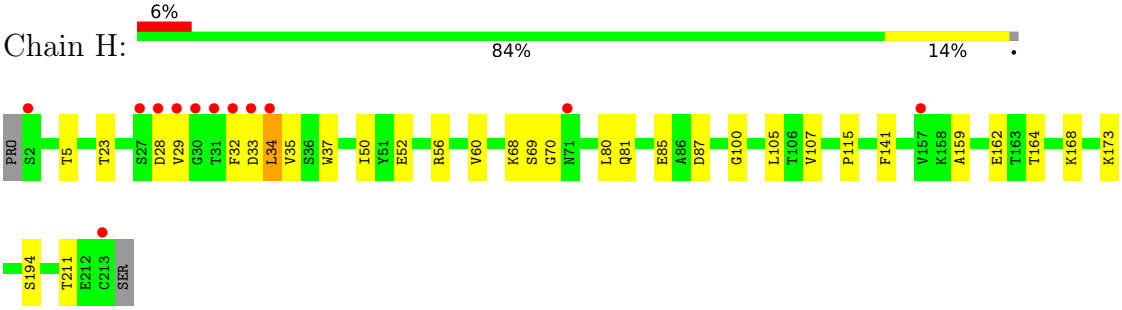
• Molecule 2: K03.12 antibody heavy chain

Chain Q:



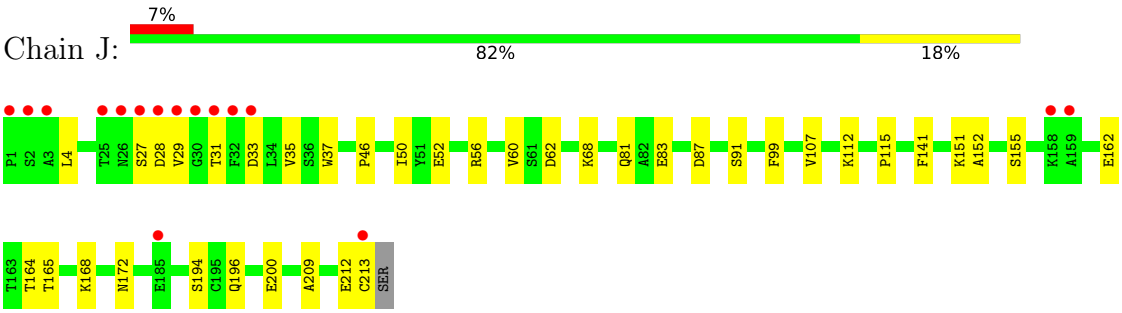
• Molecule 3: K03.12 antibody light chain

Chain H:



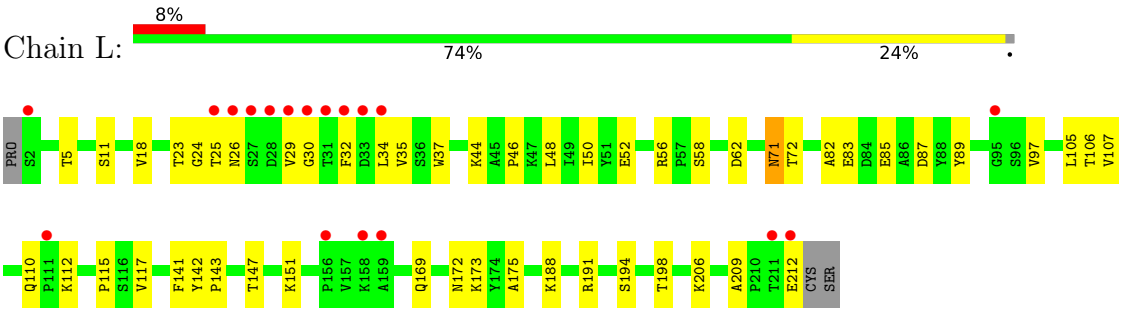
• Molecule 3: K03.12 antibody light chain

Chain J:



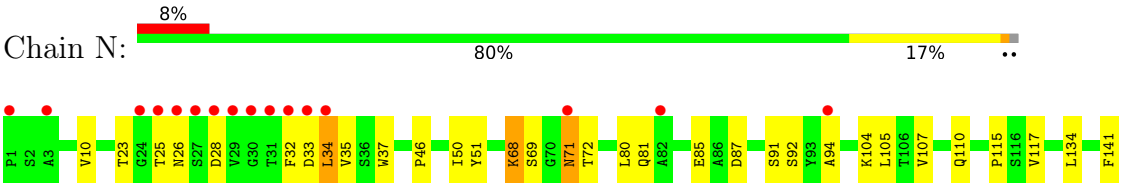
• Molecule 3: K03.12 antibody light chain

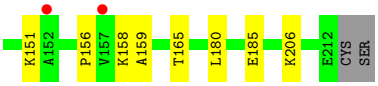
Chain L:



• Molecule 3: K03.12 antibody light chain

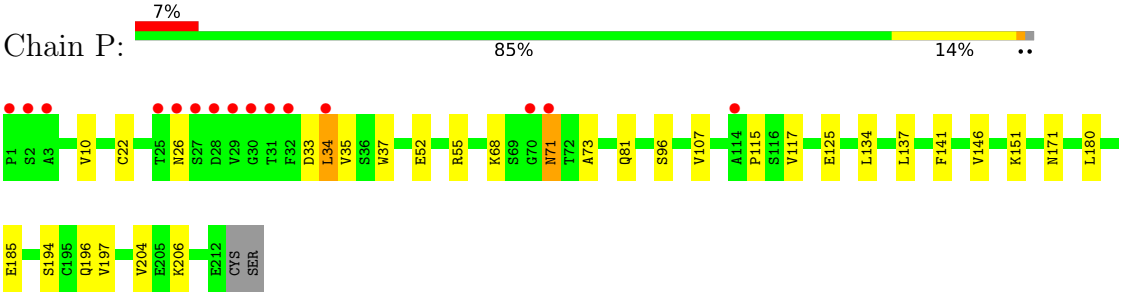
Chain N:





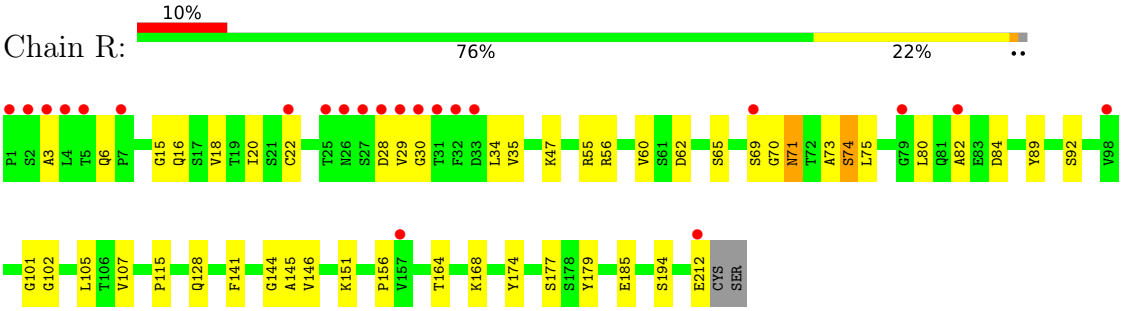
• Molecule 3: K03.12 antibody light chain

Chain P:



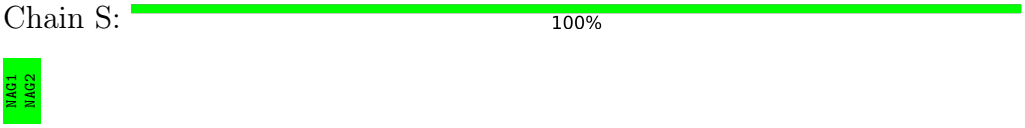
• Molecule 3: K03.12 antibody light chain

Chain R:



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

Chain S:



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

Chain V:

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

Chain W:

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

Chain Y:

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

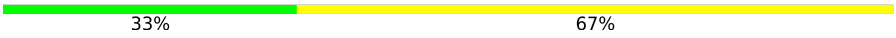
Chain Z:

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

Chain T:

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

Chain U:



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

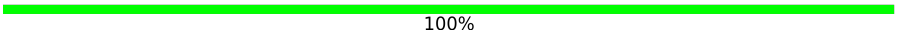
Chain X:

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

Chain a:

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

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.80Å 325.12Å 156.99Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	49.41 – 2.60 49.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.41-2.60) 99.2 (49.41-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.240 , 0.262 0.238 , 0.259	Depositor DCC
R_{free} test set	9069 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	34382	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.36	0/2213	0.50	0/3006
1	B	0.26	0/2225	0.48	0/3023
1	C	0.30	0/2213	0.50	0/3006
1	D	0.26	0/2220	0.47	0/3016
1	E	0.27	0/2220	0.50	0/3016
1	F	0.27	0/2225	0.52	0/3023
2	G	0.28	0/1837	0.52	0/2506
2	I	0.28	0/1854	0.52	0/2528
2	K	0.27	0/1831	0.50	0/2498
2	M	0.27	0/1831	0.51	0/2498
2	O	0.27	0/1831	0.50	0/2498
2	Q	0.27	0/1831	0.50	0/2498
3	H	0.33	0/1597	0.51	0/2178
3	J	0.27	0/1605	0.51	0/2189
3	L	0.33	0/1591	0.55	0/2170
3	N	0.27	0/1599	0.51	0/2181
3	P	0.28	0/1599	0.51	0/2181
3	R	0.30	0/1599	0.53	0/2181
All	All	0.29	0/33921	0.51	0/46196

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2159	0	2106	74	0
1	B	2171	0	2118	58	0
1	C	2159	0	2105	85	0
1	D	2166	0	2112	48	0
1	E	2166	0	2113	68	0
1	F	2171	0	2117	80	0
2	G	1790	0	1735	33	0
2	I	1807	0	1752	44	0
2	K	1784	0	1731	45	0
2	M	1784	0	1731	29	0
2	O	1784	0	1731	33	0
2	Q	1784	0	1731	36	0
3	H	1561	0	1505	31	0
3	J	1568	0	1515	37	0
3	L	1555	0	1501	51	0
3	N	1562	0	1511	40	0
3	P	1562	0	1511	27	0
3	R	1562	0	1511	48	0
4	S	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	5	0
4	Y	28	0	25	1	0
4	Z	28	0	25	3	0
5	T	39	0	34	21	0
5	U	39	0	34	7	0
5	X	39	0	34	2	0
5	a	39	0	34	0	0
5	b	39	0	34	0	0
6	A	42	0	39	17	0
6	B	14	0	13	1	0
6	C	42	0	39	1	0
6	D	42	0	39	15	0
6	E	42	0	39	4	0
6	F	42	0	39	1	0
7	I	6	0	8	0	0
8	A	58	0	0	30	0
8	B	79	0	0	35	0
8	C	48	0	0	24	0
8	D	49	0	0	11	0
8	E	46	0	0	33	0
8	F	37	0	0	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	45	0	0	11	1
8	H	41	0	0	13	1
8	I	55	0	0	12	0
8	J	43	0	0	15	0
8	K	29	0	0	22	0
8	L	23	0	0	20	0
8	M	28	0	0	11	0
8	N	40	0	0	14	0
8	O	30	0	0	8	0
8	P	22	0	0	10	0
8	Q	24	0	0	13	0
8	R	25	0	0	12	0
All	All	34382	0	32647	889	1

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 13.

The worst 5 of 889 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:A:63:ASN:HD21	5:T:1:NAG:C2	1.17	1.52
1:A:144:ASN:HD21	6:A:406:NAG:C1	1.21	1.49
1:C:220:ARG:CB	1:C:229:ARG:HH12	1.31	1.44
1:A:63:ASN:HD21	5:T:1:NAG:C1	1.41	1.32
1:A:144:ASN:ND2	6:A:406:NAG:C1	1.91	1.28

All (1) 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)
8:G:334:HOH:O	8:H:338:HOH:O[1_455]	1.91	0.29

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	270/291 (93%)	255 (94%)	14 (5%)	1 (0%)	34	57
1	B	272/291 (94%)	259 (95%)	12 (4%)	1 (0%)	34	57
1	C	270/291 (93%)	257 (95%)	13 (5%)	0	100	100
1	D	271/291 (93%)	258 (95%)	13 (5%)	0	100	100
1	E	271/291 (93%)	256 (94%)	13 (5%)	2 (1%)	22	43
1	F	272/291 (94%)	257 (94%)	15 (6%)	0	100	100
2	G	234/244 (96%)	228 (97%)	6 (3%)	0	100	100
2	I	236/244 (97%)	228 (97%)	8 (3%)	0	100	100
2	K	233/244 (96%)	227 (97%)	5 (2%)	1 (0%)	34	57
2	M	233/244 (96%)	227 (97%)	6 (3%)	0	100	100
2	O	233/244 (96%)	227 (97%)	6 (3%)	0	100	100
2	Q	233/244 (96%)	225 (97%)	6 (3%)	2 (1%)	17	35
3	H	210/214 (98%)	199 (95%)	10 (5%)	1 (0%)	29	52
3	J	211/214 (99%)	196 (93%)	14 (7%)	1 (0%)	29	52
3	L	209/214 (98%)	194 (93%)	11 (5%)	4 (2%)	8	15
3	N	210/214 (98%)	194 (92%)	15 (7%)	1 (0%)	29	52
3	P	210/214 (98%)	197 (94%)	11 (5%)	2 (1%)	15	32
3	R	210/214 (98%)	188 (90%)	16 (8%)	6 (3%)	4	7
All	All	4288/4494 (95%)	4072 (95%)	194 (4%)	22 (0%)	29	52

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
3	H	34	LEU
3	L	26	ASN
3	N	34	LEU
2	Q	154	GLY

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	244/258 (95%)	242 (99%)	2 (1%)	81	92
1	B	245/258 (95%)	243 (99%)	2 (1%)	81	92
1	C	244/258 (95%)	244 (100%)	0	100	100
1	D	245/258 (95%)	244 (100%)	1 (0%)	91	97
1	E	245/258 (95%)	244 (100%)	1 (0%)	91	97
1	F	245/258 (95%)	245 (100%)	0	100	100
2	G	197/205 (96%)	195 (99%)	2 (1%)	76	90
2	I	199/205 (97%)	196 (98%)	3 (2%)	65	83
2	K	196/205 (96%)	193 (98%)	3 (2%)	65	83
2	M	196/205 (96%)	192 (98%)	4 (2%)	55	78
2	O	196/205 (96%)	194 (99%)	2 (1%)	76	90
2	Q	196/205 (96%)	195 (100%)	1 (0%)	88	96
3	H	176/178 (99%)	175 (99%)	1 (1%)	86	95
3	J	177/178 (99%)	176 (99%)	1 (1%)	86	95
3	L	175/178 (98%)	174 (99%)	1 (1%)	86	95
3	N	176/178 (99%)	173 (98%)	3 (2%)	60	81
3	P	176/178 (99%)	172 (98%)	4 (2%)	50	75
3	R	176/178 (99%)	175 (99%)	1 (1%)	86	95
All	All	3704/3846 (96%)	3672 (99%)	32 (1%)	78	91

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	71	ASN
3	P	171	ASN
3	J	87	ASP
2	I	234	LYS
2	Q	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	6	GLN

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Mol	Chain	Res	Type
3	R	71	ASN
3	R	169	GLN
1	D	165	ASN
1	E	158	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)

25 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	S	1	4,1	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	S	2	4	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	T	1	5	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	T	2	5	14,14,15	0.29	0	17,19,21	0.62	0
5	BMA	T	3	5	11,11,12	0.28	0	15,15,17	0.64	0
5	NAG	U	1	5,1	14,14,15	0.30	0	17,19,21	0.61	0
5	NAG	U	2	5	14,14,15	0.30	0	17,19,21	0.63	0
5	BMA	U	3	5	11,11,12	0.26	0	15,15,17	0.64	0
4	NAG	V	1	4,1	14,14,15	0.93	1 (7%)	17,19,21	1.32	1 (5%)
4	NAG	V	2	4	14,14,15	0.40	0	17,19,21	0.55	0
4	NAG	W	1	4,1	14,14,15	0.35	0	17,19,21	0.43	0
4	NAG	W	2	4	14,14,15	0.51	0	17,19,21	0.43	0
5	NAG	X	1	5,1	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
5	NAG	X	2	5	14,14,15	0.43	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	X	3	5	11,11,12	0.91	1 (9%)	15,15,17	0.85	0
4	NAG	Y	1	4,1	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	Y	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	Z	1	4,1	14,14,15	0.42	0	17,19,21	0.62	0
4	NAG	Z	2	4	14,14,15	0.28	0	17,19,21	0.33	0
5	NAG	a	1	5,1	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
5	NAG	a	2	5	14,14,15	0.43	0	17,19,21	0.92	0
5	BMA	a	3	5	11,11,12	0.32	0	15,15,17	1.14	2 (13%)
5	NAG	b	1	5,1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	b	2	5	14,14,15	0.29	0	17,19,21	0.40	0
5	BMA	b	3	5	11,11,12	0.71	0	15,15,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
5	NAG	T	1	5	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	NAG	O5-C1	3.36	1.49	1.43
5	X	3	BMA	C1-C2	2.55	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	V	1	NAG	C1-O5-C5	5.24	119.30	112.19
5	X	2	NAG	C2-N2-C7	2.50	126.46	122.90
5	a	3	BMA	C3-C4-C5	2.20	114.17	110.24
5	X	1	NAG	C1-O5-C5	2.16	115.12	112.19
5	a	3	BMA	C1-O5-C5	-2.02	109.46	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
5	U	1	NAG	C1-C2-N2-C7
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	1	NAG	3	0
5	X	1	NAG	1	0
5	X	2	NAG	1	0
5	T	1	NAG	21	0
5	U	1	NAG	2	0
4	W	2	NAG	5	0

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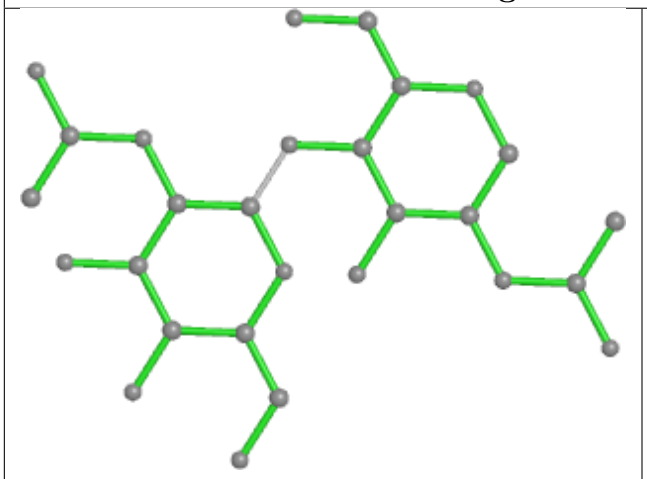
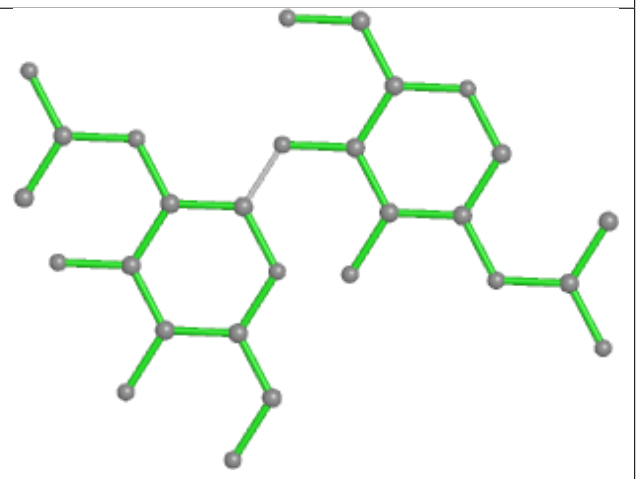
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	2	NAG	5	0
4	Y	2	NAG	1	0
5	X	3	BMA	1	0

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

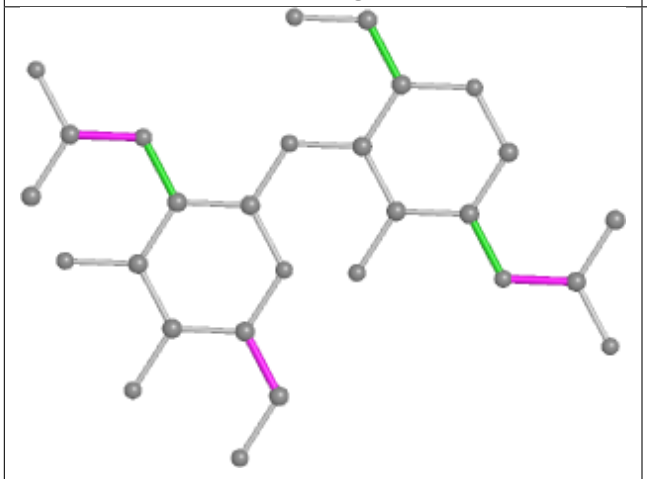
Oligosaccharide Chain S



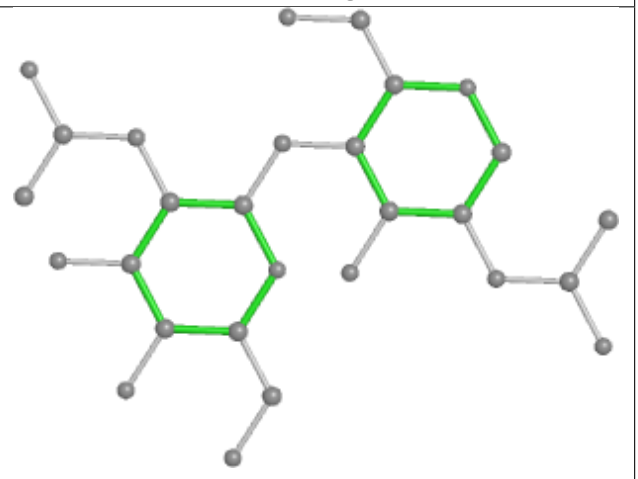
Bond lengths



Bond angles

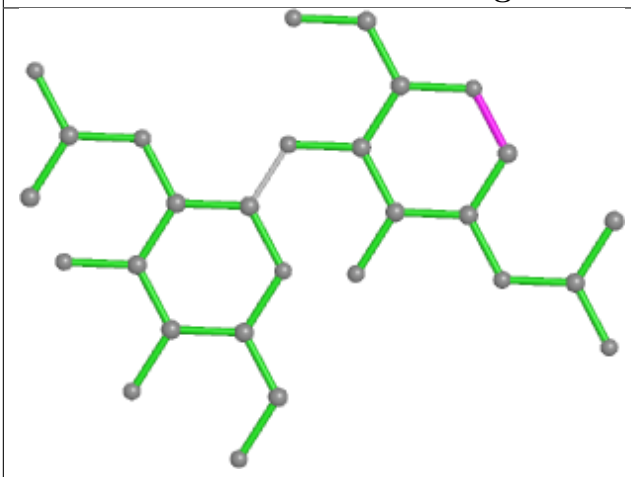


Torsions

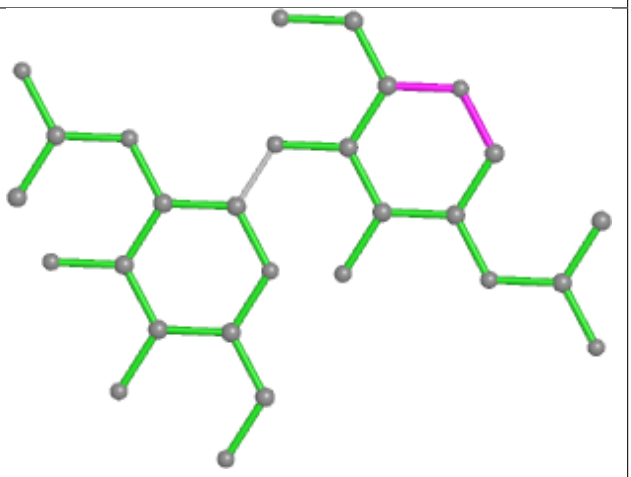


Rings

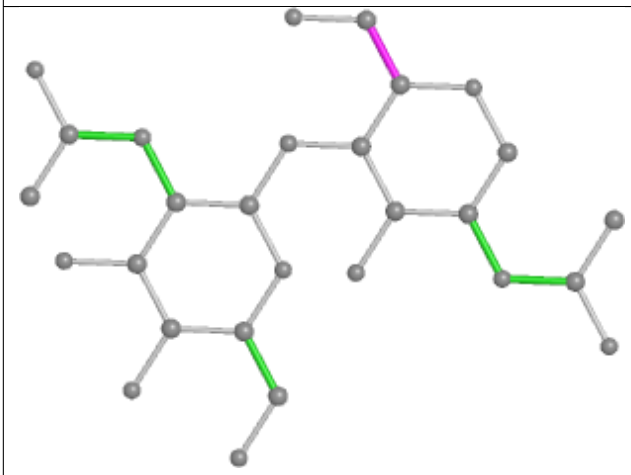
Oligosaccharide Chain V



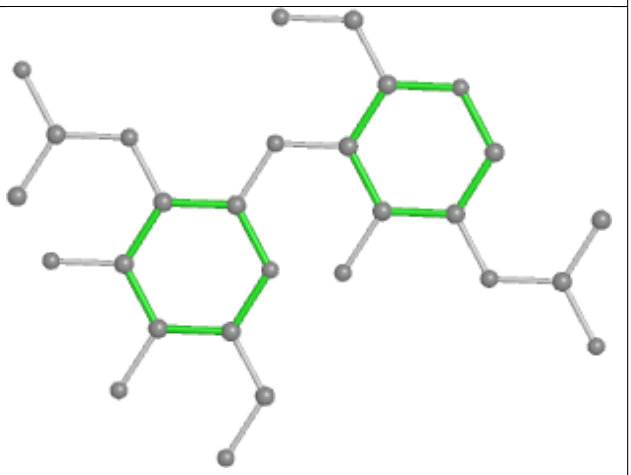
Bond lengths



Bond angles

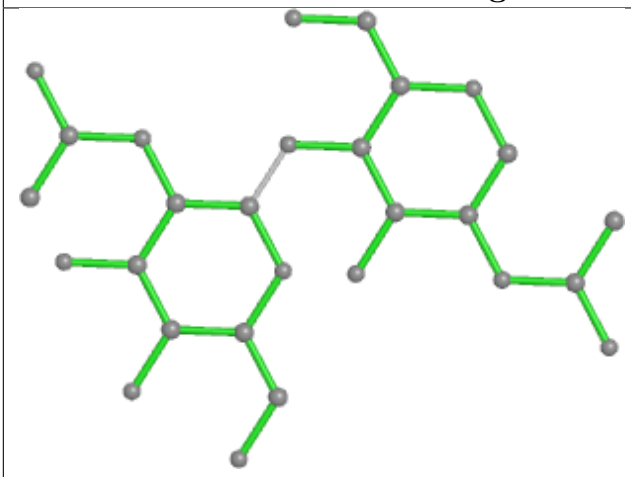


Torsions

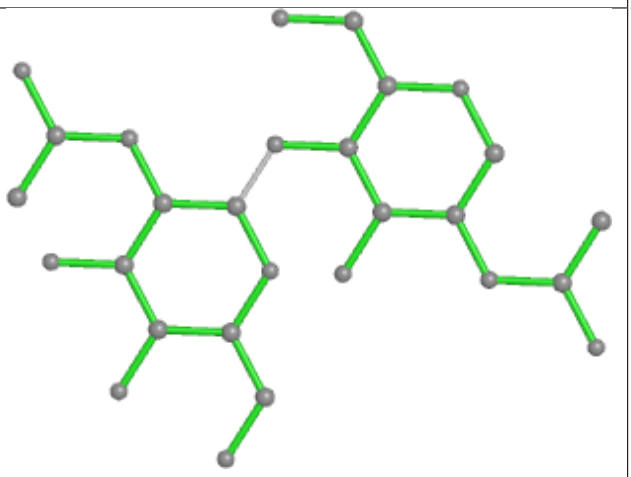


Rings

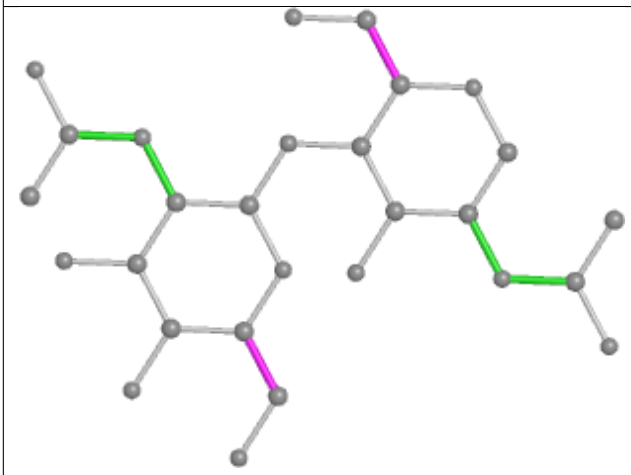
Oligosaccharide Chain W



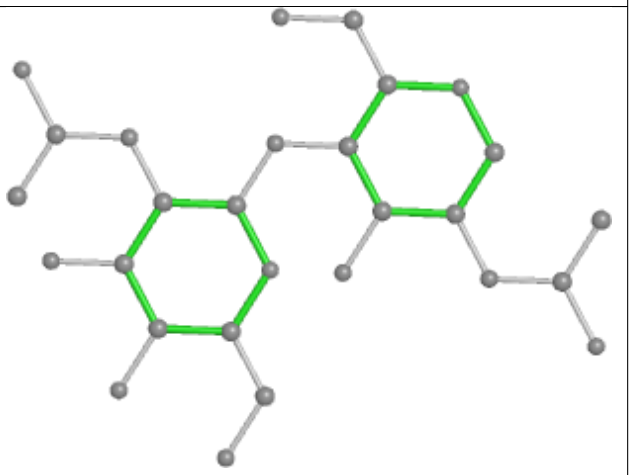
Bond lengths



Bond angles

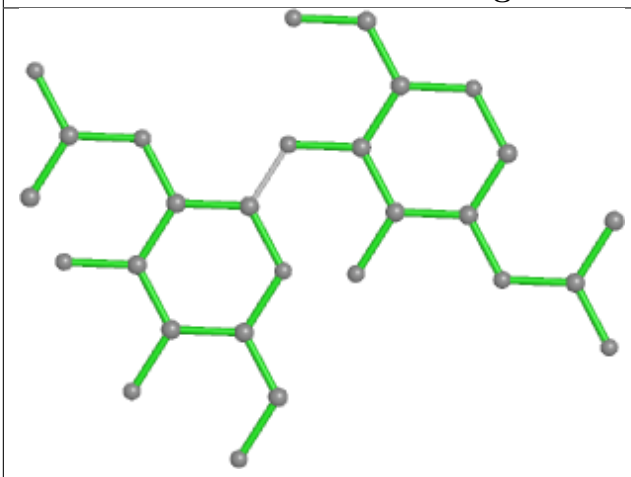


Torsions

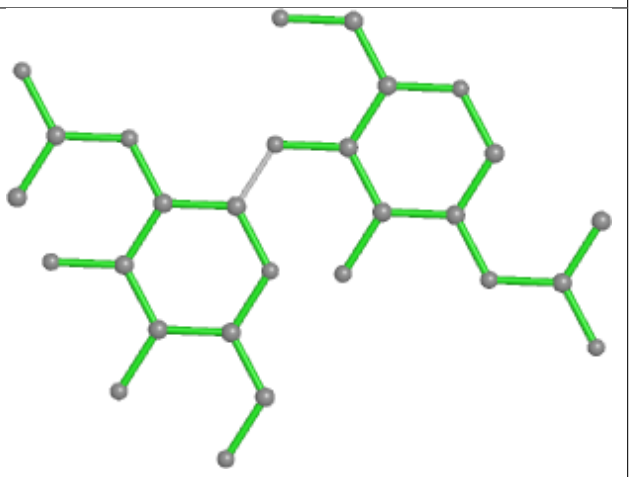


Rings

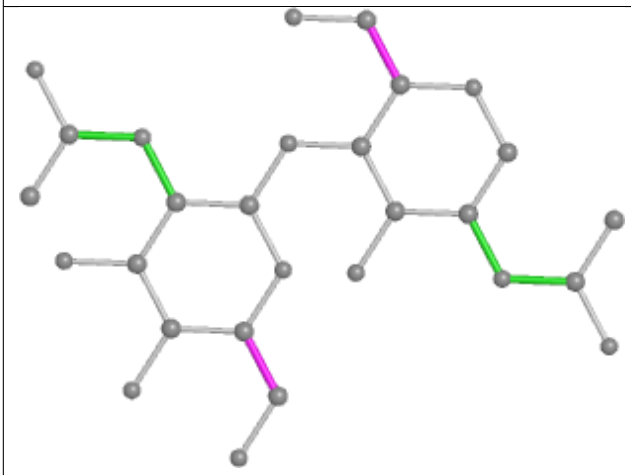
Oligosaccharide Chain Y



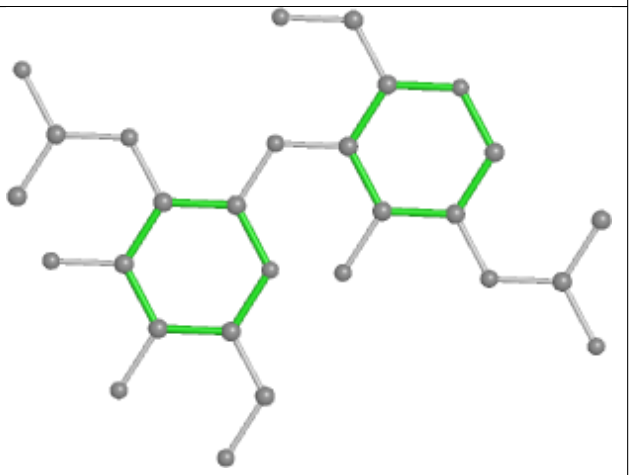
Bond lengths



Bond angles

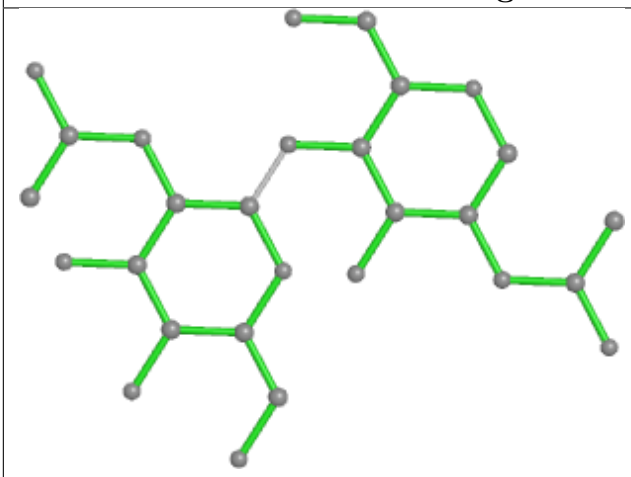


Torsions

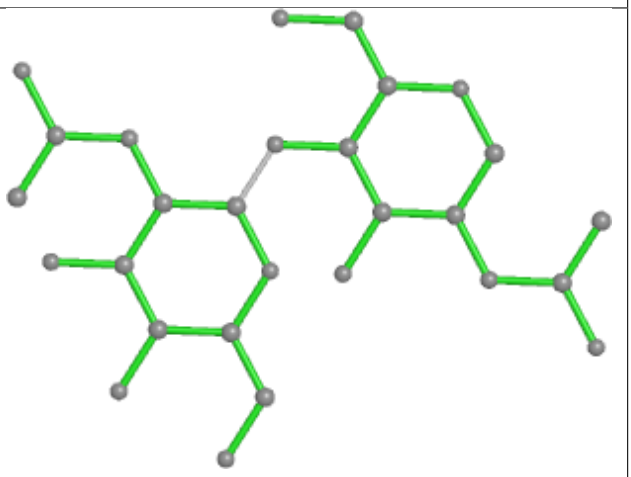


Rings

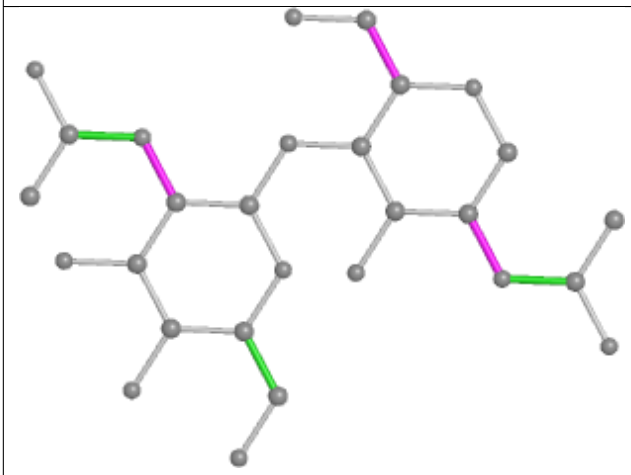
Oligosaccharide Chain Z



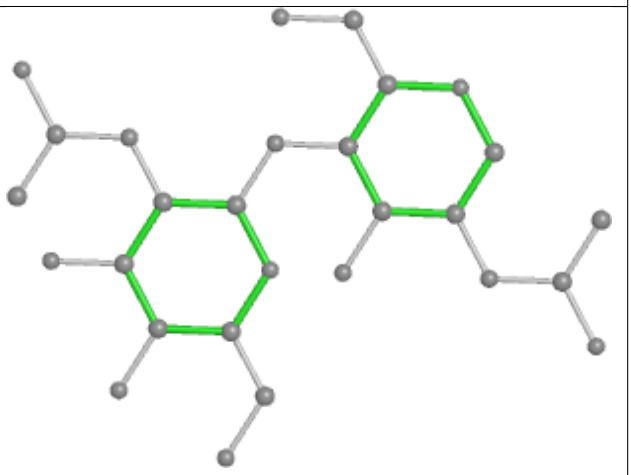
Bond lengths



Bond angles

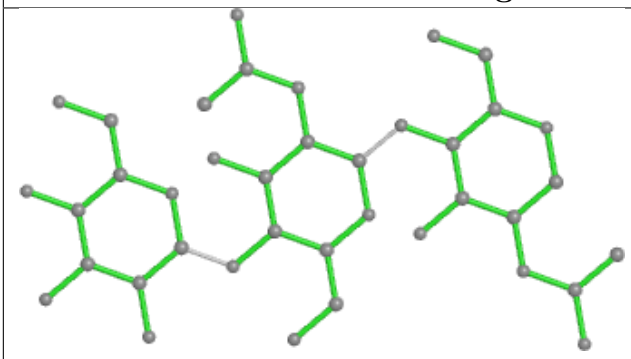


Torsions

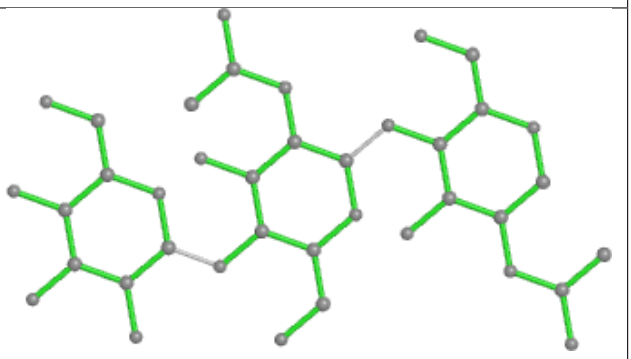


Rings

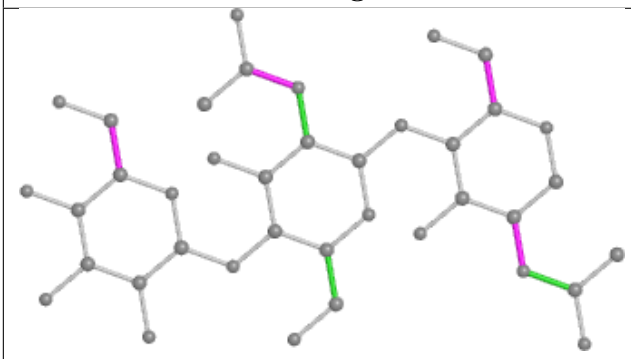
Oligosaccharide Chain T



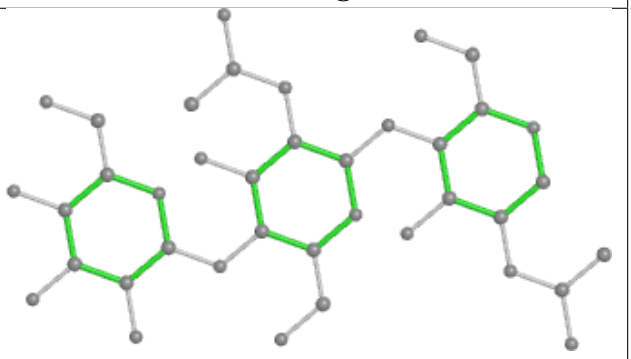
Bond lengths



Bond angles

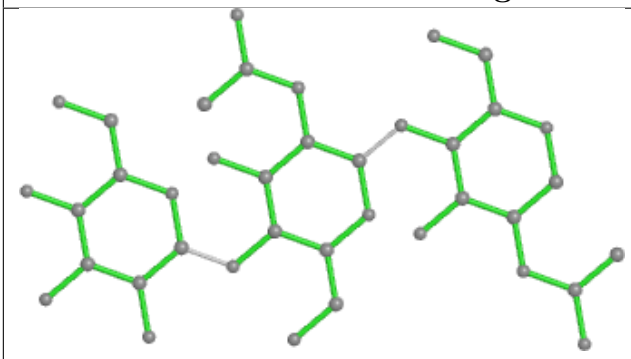


Torsions

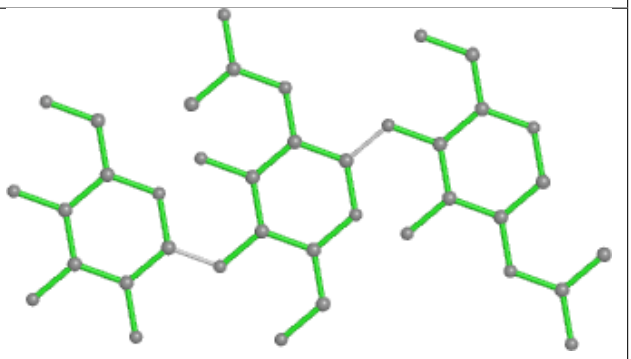


Rings

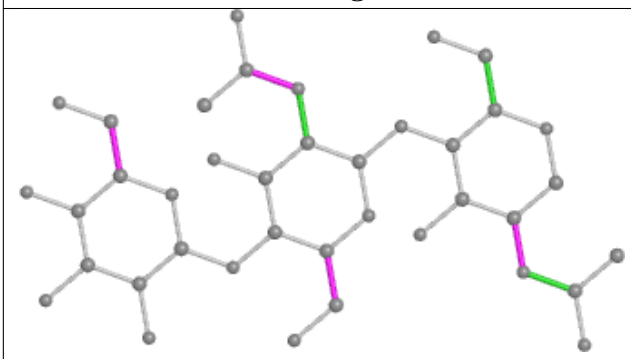
Oligosaccharide Chain U



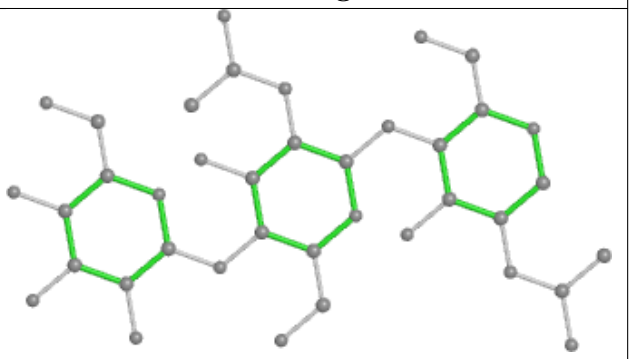
Bond lengths



Bond angles

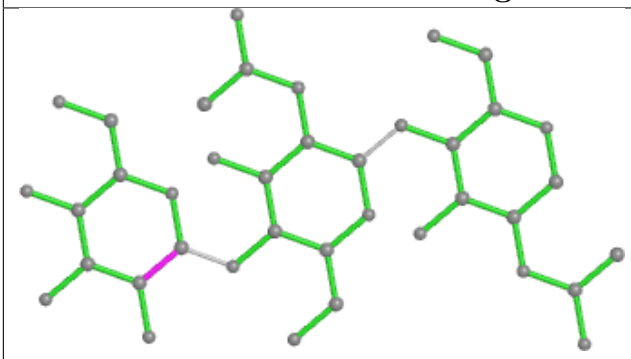


Torsions

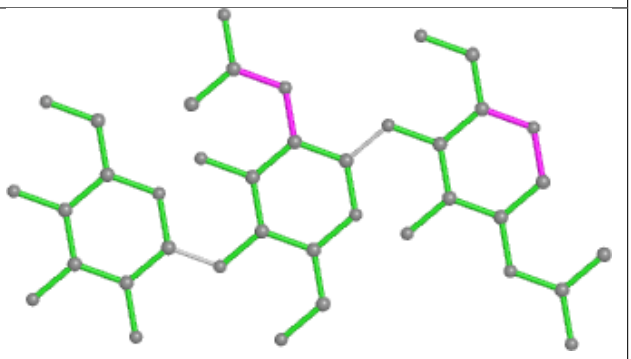


Rings

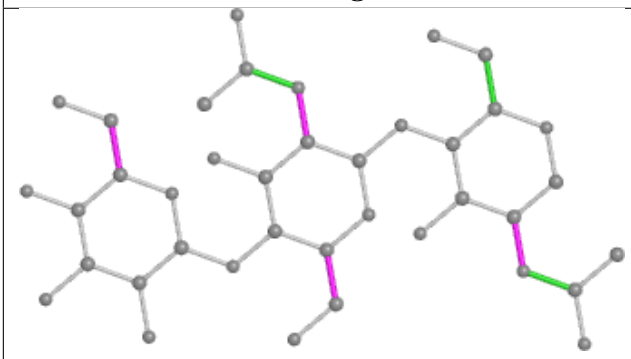
Oligosaccharide Chain X



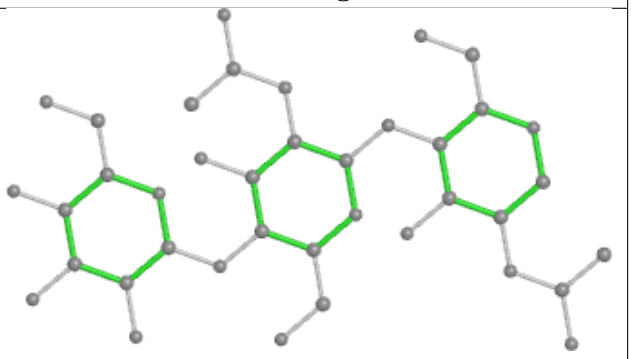
Bond lengths



Bond angles

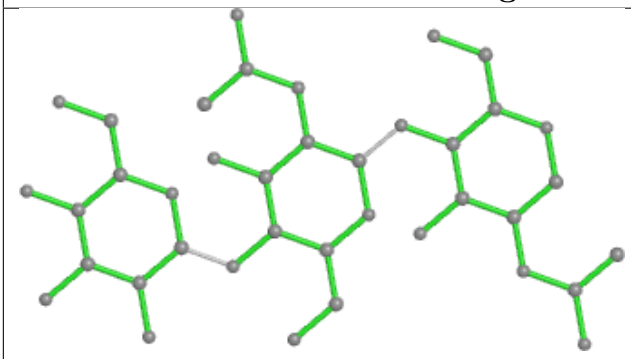


Torsions

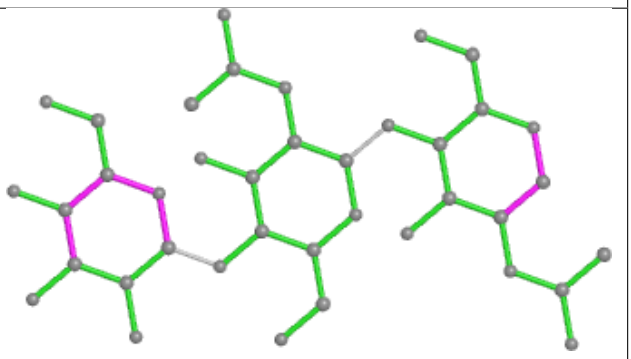


Rings

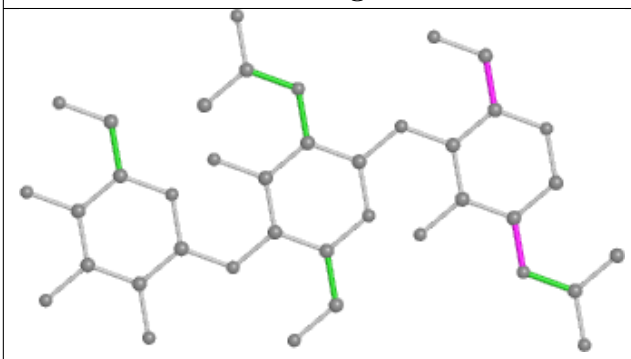
Oligosaccharide Chain a



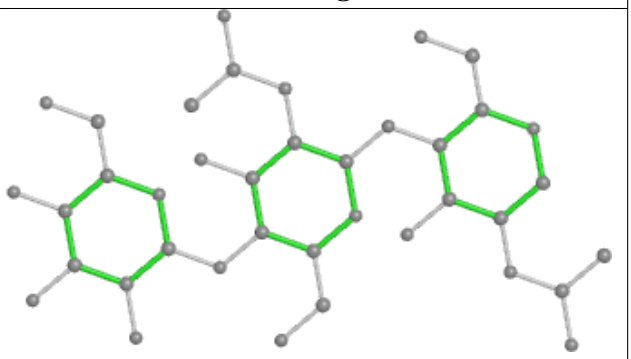
Bond lengths



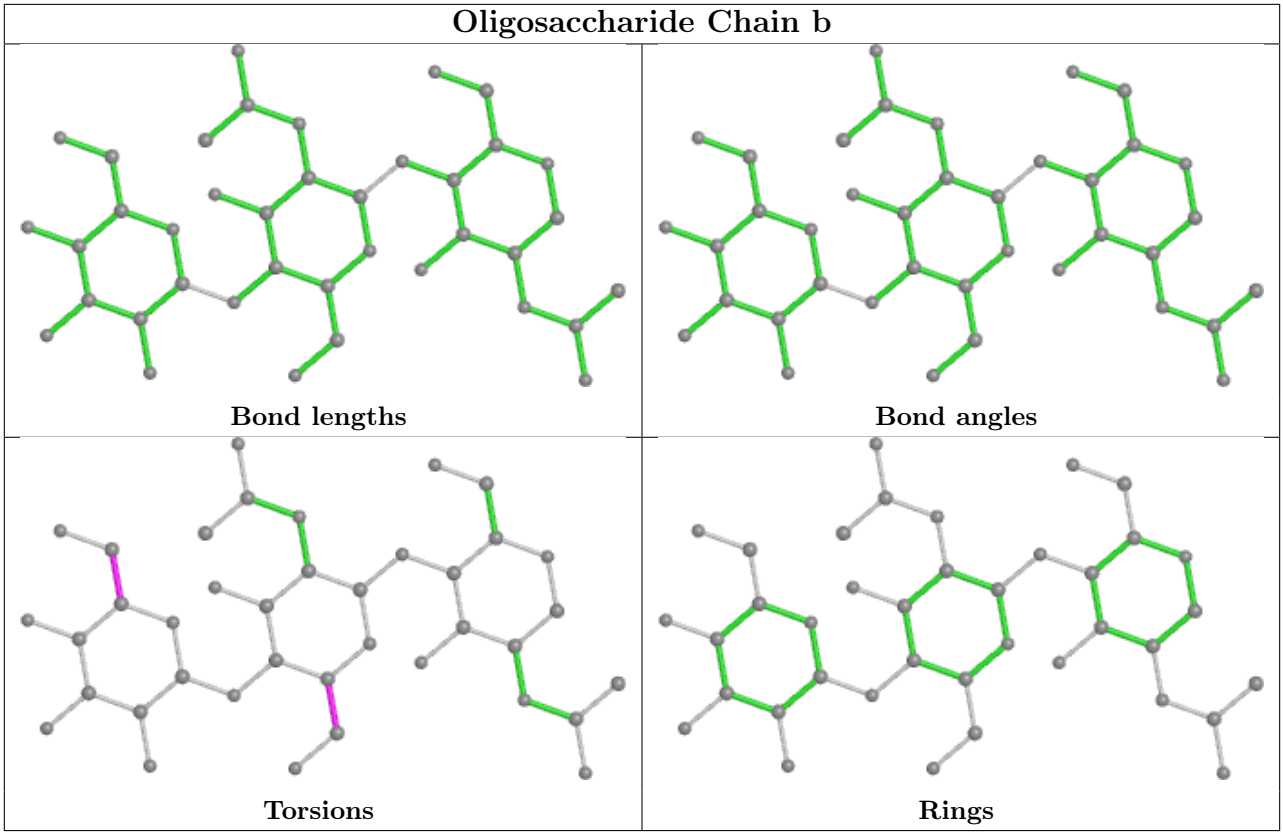
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
6	NAG	D	405	1	14,14,15	0.41	0	17,19,21	1.35	4 (23%)
6	NAG	A	406	-	14,14,15	0.28	0	17,19,21	0.62	0
7	GOL	I	301	-	5,5,5	0.38	0	5,5,5	0.34	0
6	NAG	C	405	1	14,14,15	0.66	1 (7%)	17,19,21	0.64	0
6	NAG	A	408	1	14,14,15	0.37	0	17,19,21	0.76	0
6	NAG	C	401	1	14,14,15	0.29	0	17,19,21	0.42	0
6	NAG	C	406	1	14,14,15	0.32	0	17,19,21	0.65	0
6	NAG	A	407	1	14,14,15	0.31	0	17,19,21	0.60	0
6	NAG	E	405	1	14,14,15	0.88	1 (7%)	17,19,21	1.42	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	D	407	1	14,14,15	0.35	0	17,19,21	0.87	0
6	NAG	B	408	1	14,14,15	1.23	2 (14%)	17,19,21	1.79	5 (29%)
6	NAG	F	404	1	14,14,15	0.34	0	17,19,21	0.73	0
6	NAG	F	406	1	14,14,15	0.35	0	17,19,21	0.74	0
6	NAG	E	406	1	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
6	NAG	E	404	1	14,14,15	0.58	0	17,19,21	0.44	0
6	NAG	D	406	1	14,14,15	0.23	0	17,19,21	1.08	2 (11%)
6	NAG	F	405	1	14,14,15	0.41	0	17,19,21	1.40	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
6	NAG	D	405	1	-	4/6/23/26	0/1/1/1
6	NAG	A	406	-	-	1/6/23/26	0/1/1/1
7	GOL	I	301	-	-	2/4/4/4	-
6	NAG	C	405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	408	1	-	4/6/23/26	0/1/1/1
6	NAG	C	401	1	-	0/6/23/26	0/1/1/1
6	NAG	C	406	1	-	2/6/23/26	0/1/1/1
6	NAG	A	407	1	-	1/6/23/26	0/1/1/1
6	NAG	E	405	1	-	3/6/23/26	0/1/1/1
6	NAG	D	407	1	-	4/6/23/26	0/1/1/1
6	NAG	B	408	1	-	5/6/23/26	0/1/1/1
6	NAG	F	404	1	-	2/6/23/26	0/1/1/1
6	NAG	F	406	1	-	3/6/23/26	0/1/1/1
6	NAG	E	406	1	-	3/6/23/26	0/1/1/1
6	NAG	E	404	1	-	0/6/23/26	0/1/1/1
6	NAG	D	406	1	-	4/6/23/26	0/1/1/1
6	NAG	F	405	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	408	NAG	O5-C1	-3.63	1.37	1.43
6	E	405	NAG	O5-C1	2.67	1.48	1.43
6	C	405	NAG	C1-C2	2.22	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	408	NAG	C1-C2	2.17	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	405	NAG	C1-O5-C5	5.18	119.21	112.19
6	B	408	NAG	C2-N2-C7	4.81	129.75	122.90
6	E	405	NAG	C2-N2-C7	4.17	128.85	122.90
6	B	408	NAG	C4-C3-C2	3.25	115.79	111.02
6	E	405	NAG	C1-C2-N2	3.09	115.76	110.49

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	NAG	O7-C7-N2-C2
6	C	406	NAG	C3-C2-N2-C7
6	D	405	NAG	C3-C2-N2-C7
6	D	405	NAG	C8-C7-N2-C2
6	D	405	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	405	NAG	8	0
6	A	406	NAG	11	0
6	A	408	NAG	2	0
6	C	406	NAG	1	0
6	A	407	NAG	4	0
6	E	405	NAG	1	0
6	B	408	NAG	1	0
6	F	406	NAG	1	0
6	E	406	NAG	3	0
6	D	406	NAG	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	272/291 (93%)	0.35	9 (3%) 46 39	23, 49, 83, 116	0
1	B	274/291 (94%)	0.26	6 (2%) 62 56	26, 45, 82, 134	0
1	C	272/291 (93%)	0.40	10 (3%) 41 34	28, 62, 97, 136	0
1	D	273/291 (93%)	0.41	12 (4%) 34 27	35, 57, 95, 156	0
1	E	273/291 (93%)	0.30	7 (2%) 56 50	29, 59, 96, 141	0
1	F	274/291 (94%)	0.64	22 (8%) 12 9	39, 73, 111, 206	0
2	G	236/244 (96%)	0.25	2 (0%) 86 84	26, 44, 72, 139	0
2	I	238/244 (97%)	0.23	4 (1%) 70 66	25, 44, 72, 156	0
2	K	235/244 (96%)	0.36	4 (1%) 70 66	35, 57, 85, 110	0
2	M	235/244 (96%)	0.38	14 (5%) 21 16	33, 49, 90, 158	0
2	O	235/244 (96%)	0.49	15 (6%) 19 14	34, 52, 87, 159	0
2	Q	235/244 (96%)	0.63	17 (7%) 15 11	41, 63, 108, 153	0
3	H	212/214 (99%)	0.42	12 (5%) 23 18	29, 47, 112, 200	0
3	J	213/214 (99%)	0.49	16 (7%) 14 10	22, 44, 121, 182	0
3	L	211/214 (98%)	0.70	18 (8%) 10 7	40, 66, 119, 156	0
3	N	212/214 (99%)	0.49	18 (8%) 10 7	33, 54, 133, 167	0
3	P	212/214 (99%)	0.53	15 (7%) 16 11	38, 62, 116, 160	0
3	R	212/214 (99%)	0.85	22 (10%) 6 4	45, 81, 143, 166	0
All	All	4324/4494 (96%)	0.45	223 (5%) 27 21	22, 56, 105, 206	0

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	31	THR	10.0
3	P	1	PRO	9.8
3	R	29	VAL	9.4

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Mol	Chain	Res	Type	RSRZ
3	R	1	PRO	9.3
3	R	2	SER	9.0

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)

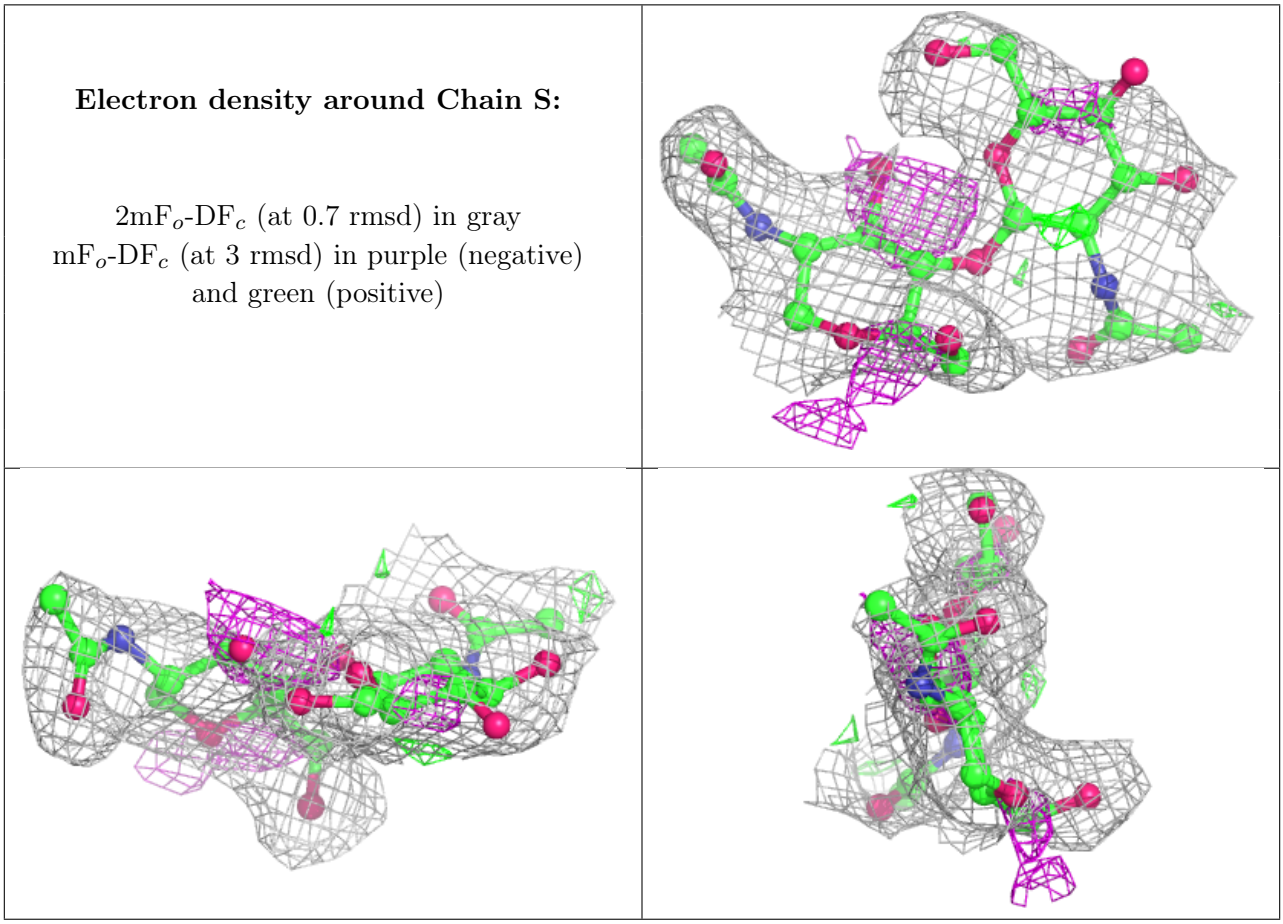
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	T	3	11/12	0.58	0.46	75,77,77,78	0
5	BMA	U	3	11/12	0.63	0.42	71,73,74,74	0
5	NAG	X	1	14/15	0.63	0.38	50,52,55,60	0
4	NAG	Z	2	14/15	0.67	0.41	69,71,72,73	0
5	BMA	b	3	11/12	0.69	0.48	72,73,74,74	0
5	BMA	a	3	11/12	0.70	0.47	75,76,77,77	0
4	NAG	W	1	14/15	0.71	0.35	47,52,54,58	0
5	NAG	b	2	14/15	0.72	0.31	61,66,68,70	0
4	NAG	S	2	14/15	0.73	0.30	63,67,68,68	0
5	NAG	U	1	14/15	0.79	0.27	46,47,50,55	0
5	BMA	X	3	11/12	0.80	0.43	75,77,77,77	0
5	NAG	T	2	14/15	0.81	0.39	63,68,70,73	0
5	NAG	U	2	14/15	0.81	0.36	60,64,66,68	0
5	NAG	a	2	14/15	0.82	0.35	63,67,69,72	0
5	NAG	a	1	14/15	0.83	0.21	44,49,52,57	0
4	NAG	W	2	14/15	0.84	0.37	61,65,66,66	0
4	NAG	Y	2	14/15	0.85	0.35	58,61,62,62	0
4	NAG	S	1	14/15	0.86	0.29	44,49,53,58	0
5	NAG	T	1	14/15	0.87	0.26	45,46,51,57	0
5	NAG	X	2	14/15	0.87	0.40	65,70,71,73	0
4	NAG	Z	1	14/15	0.87	0.31	58,64,65,67	0
4	NAG	V	2	14/15	0.87	0.27	54,57,58,59	0
5	NAG	b	1	14/15	0.88	0.22	46,48,51,56	0
4	NAG	V	1	14/15	0.90	0.18	38,44,46,51	0
4	NAG	Y	1	14/15	0.90	0.23	45,47,49,54	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.

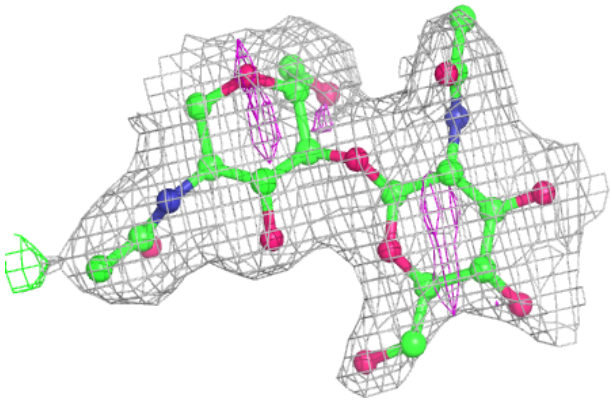
Electron density around Chain S:

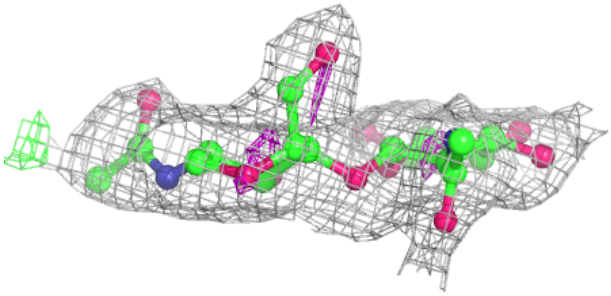
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

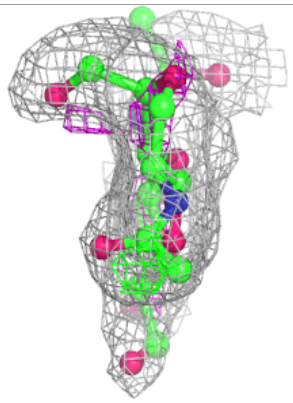


Electron density around Chain V:

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

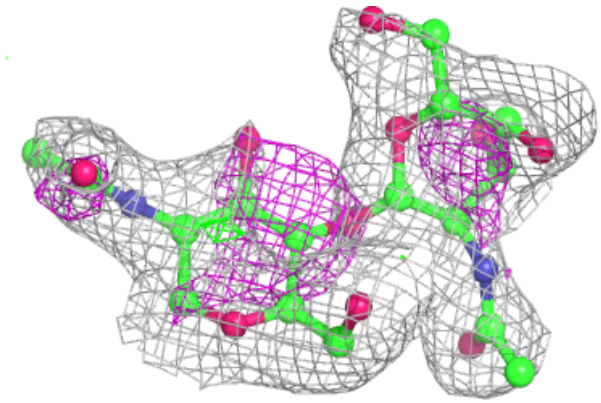


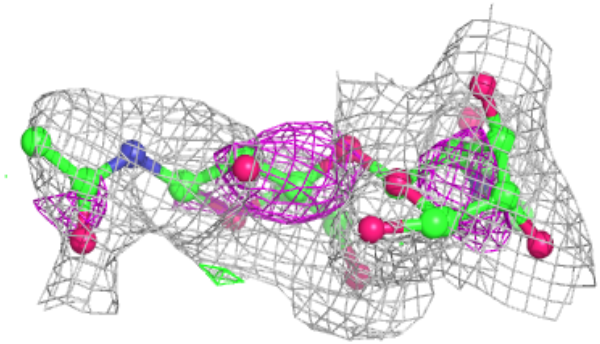


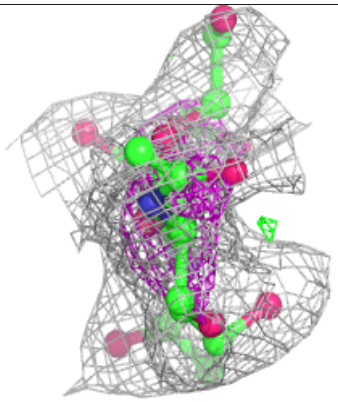


Electron density around Chain W:

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

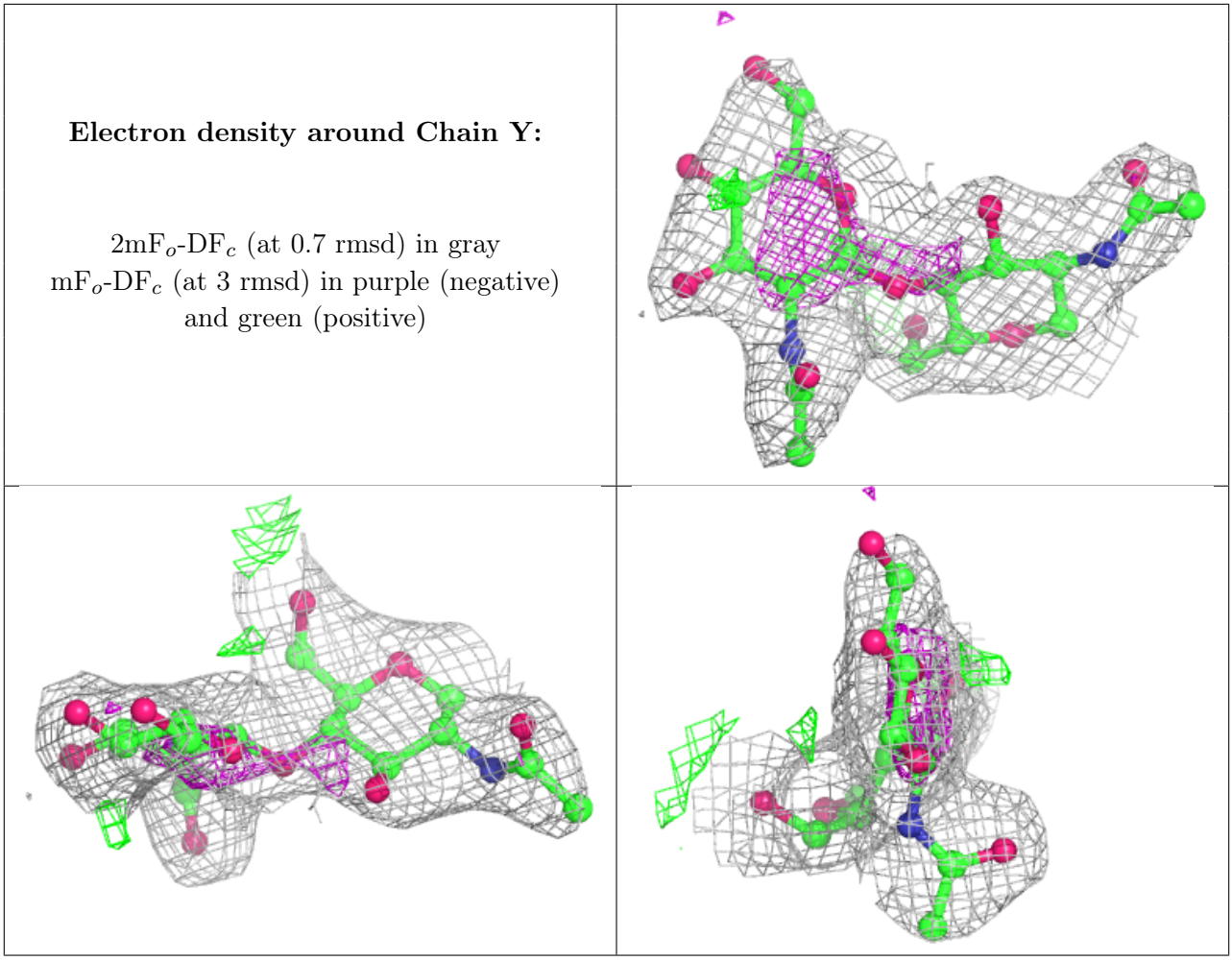






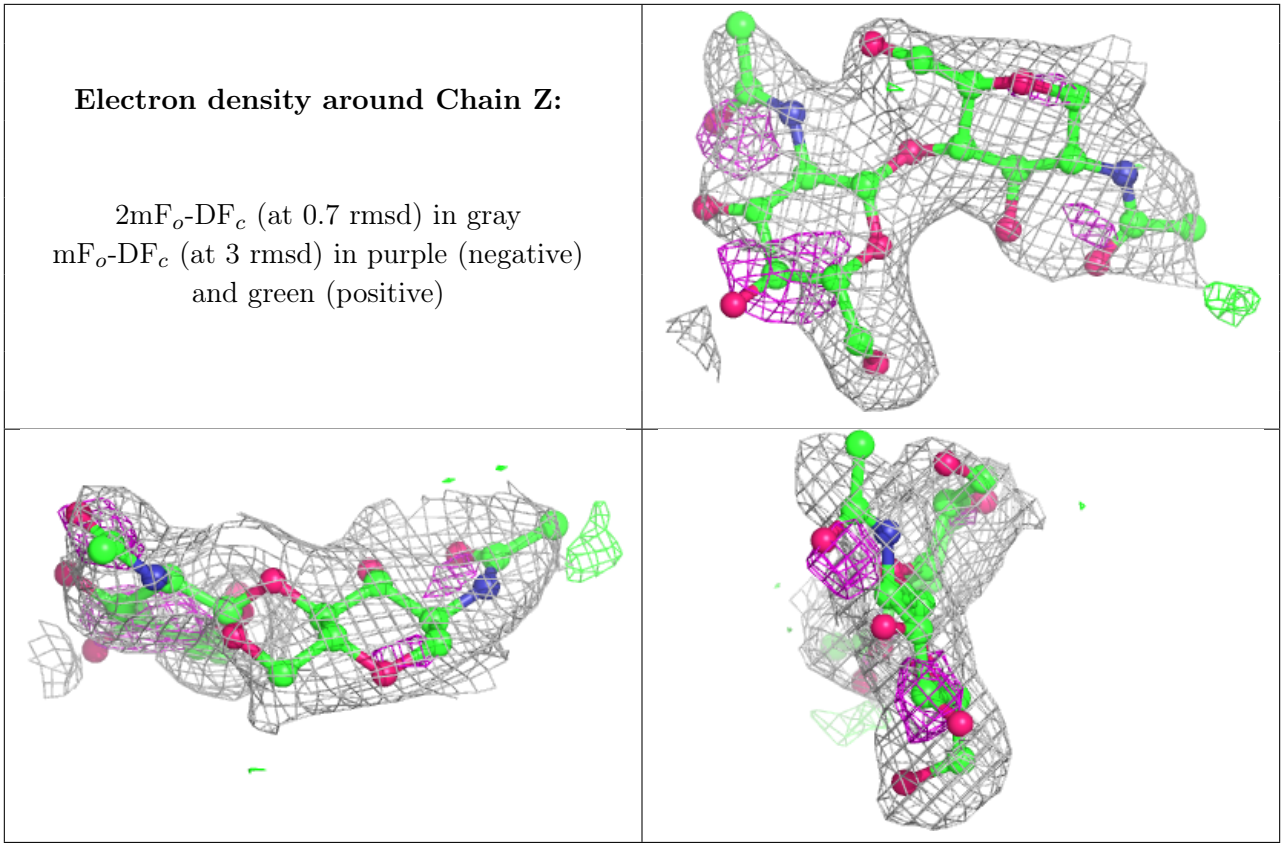
Electron density around Chain Y:

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



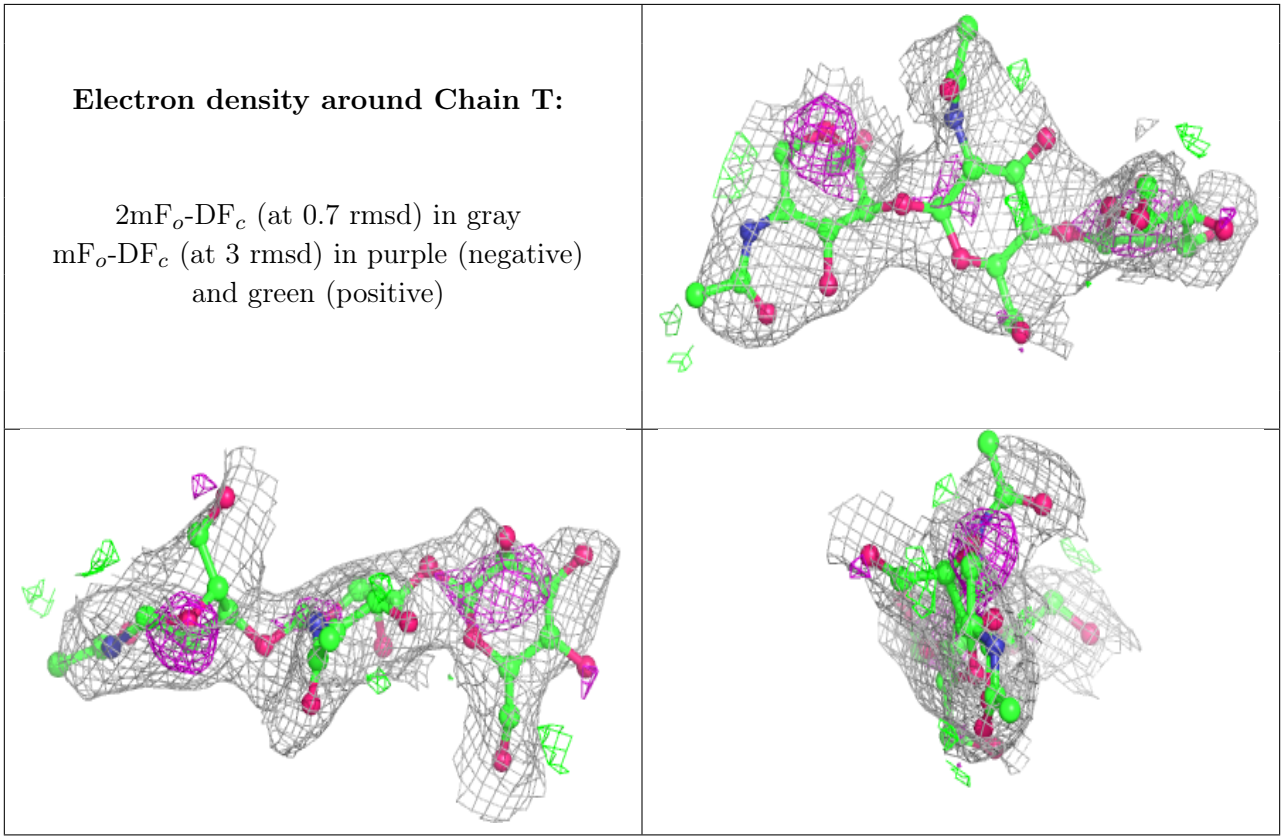
Electron density around Chain Z:

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



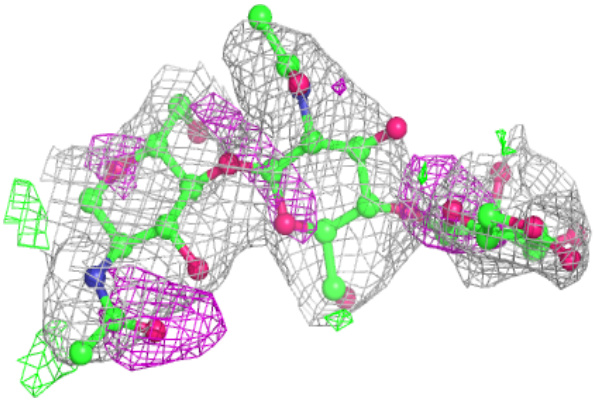
Electron density around Chain T:

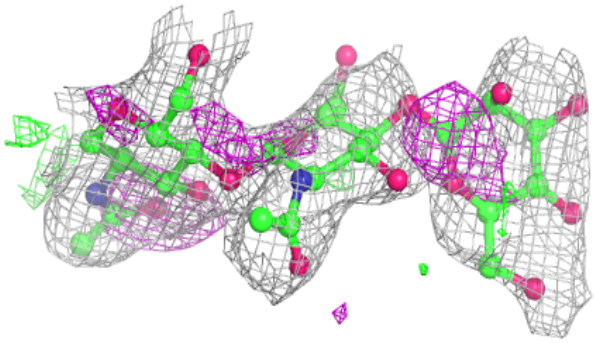
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

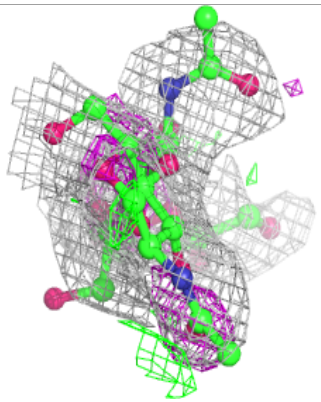


Electron density around Chain U:

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

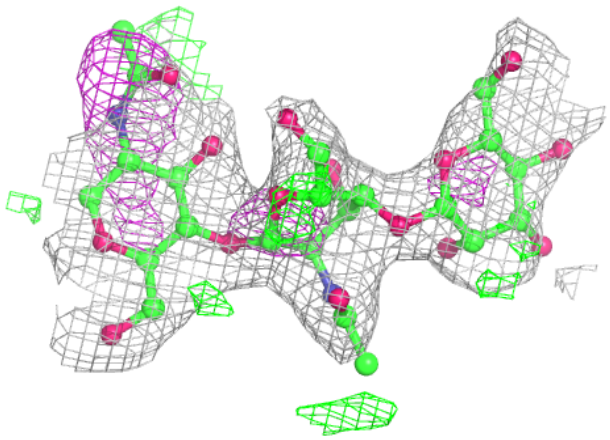


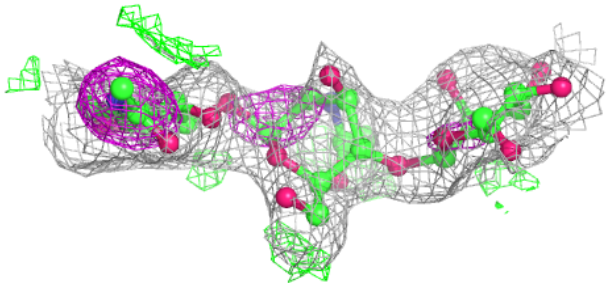


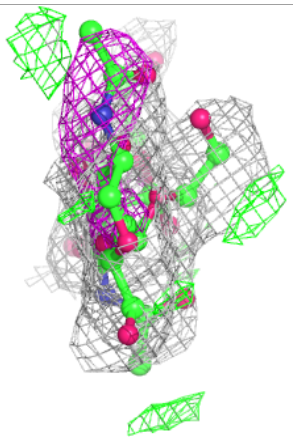


Electron density around Chain X:

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

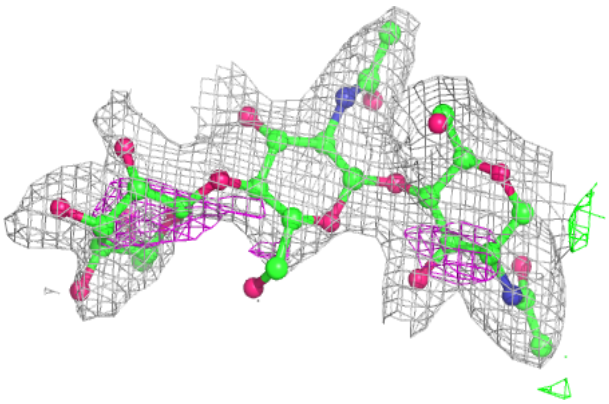


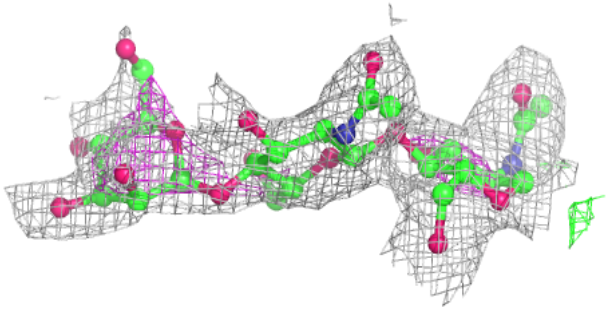


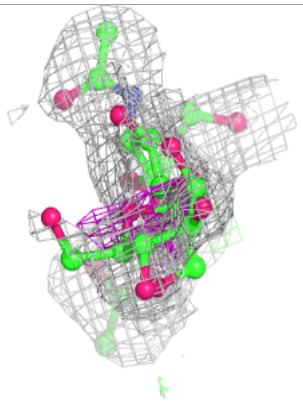


Electron density around Chain a:

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

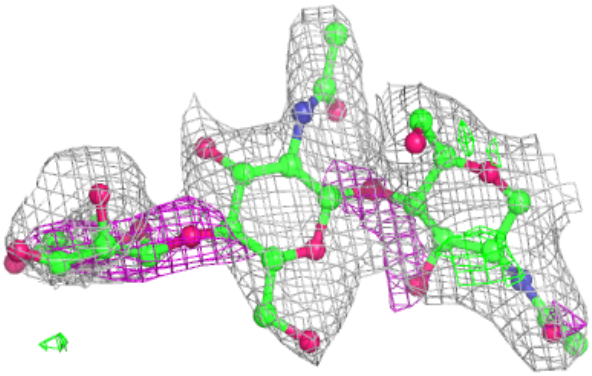


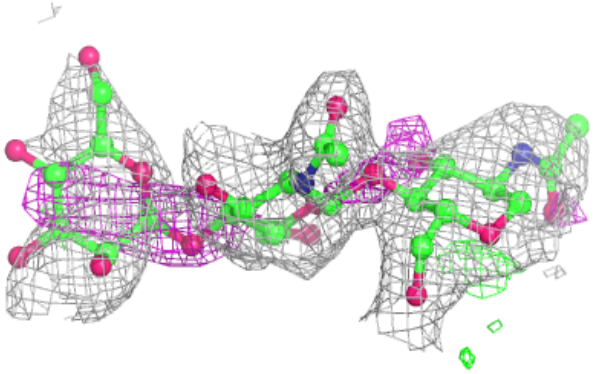


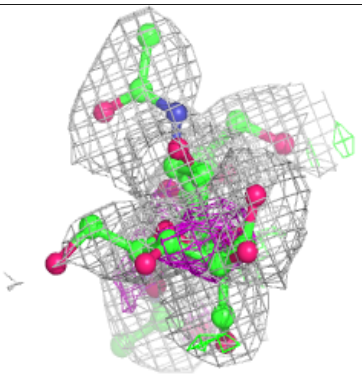


Electron density around Chain b:

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







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, 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
6	NAG	D	405	14/15	0.57	0.62	43,47,49,50	0
6	NAG	F	405	14/15	0.62	0.32	46,46,49,49	0
6	NAG	A	408	14/15	0.63	0.33	41,46,47,47	0
6	NAG	D	406	14/15	0.74	0.46	43,47,52,53	0
6	NAG	C	401	14/15	0.74	0.40	46,50,53,53	0
6	NAG	E	405	14/15	0.76	0.32	46,50,52,52	0
6	NAG	C	405	14/15	0.77	0.38	50,52,54,55	0
6	NAG	A	407	14/15	0.79	0.55	45,50,53,54	0
6	NAG	D	407	14/15	0.80	0.32	42,46,48,48	0
6	NAG	C	406	14/15	0.81	0.30	38,43,45,46	0
6	NAG	E	404	14/15	0.83	0.29	40,44,48,51	0
6	NAG	B	408	14/15	0.84	0.35	48,52,55,56	0
6	NAG	A	406	14/15	0.85	0.30	43,46,48,49	0
6	NAG	F	406	14/15	0.85	0.41	37,39,40,41	0
6	NAG	E	406	14/15	0.86	0.39	41,47,48,49	0
6	NAG	F	404	14/15	0.86	0.31	41,45,47,49	0
7	GOL	I	301	6/6	0.89	0.24	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.