Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:58 PM EST

PDB ID	:	7LU9
EMDB ID	:	EMD-23518
Title	:	Cryo-EM structure of DH851.3 bound to HIV-1 CH505 Env
Authors	:	Manne, K.; Edwards, R.J.; Acharya, P.
Deposited on	:	2021-02-21
Resolution	:	5.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

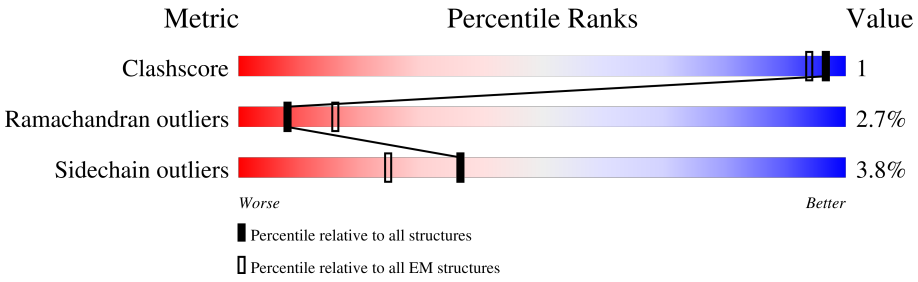
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	j	210	57% 93% 6%
1	k	210	38% 95% .
1	r	210	41% 91% 8%
2	i	228	46% 90% 10%
2	l	228	31% 92% 7% .
2	q	228	43% 92% 7% .
3	h	222	37% 93% 6%
3	m	222	43% 91% 8% .

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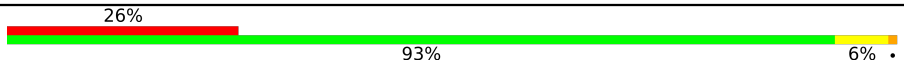
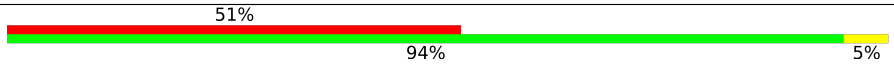
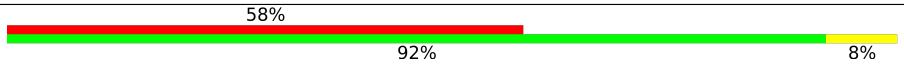
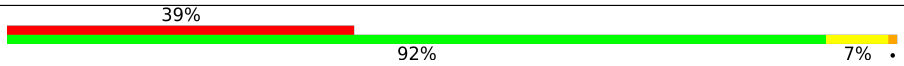
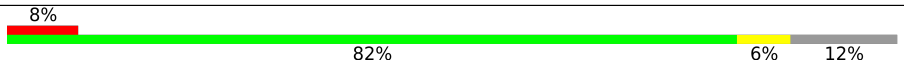
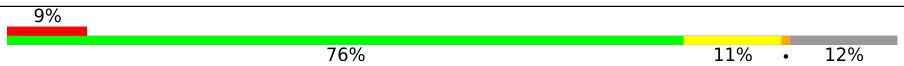
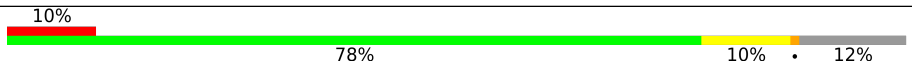
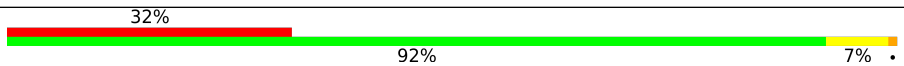
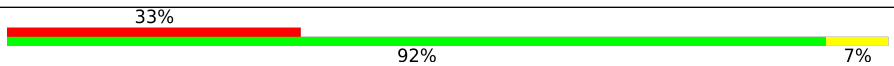
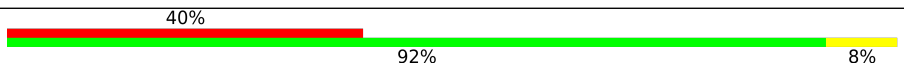
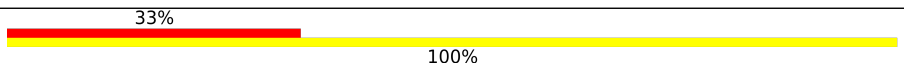
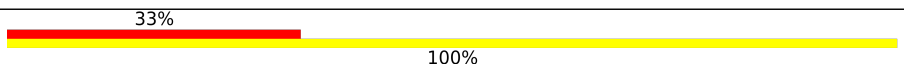
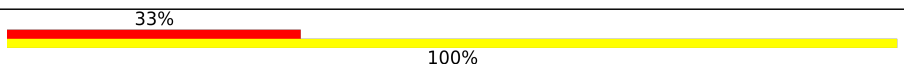
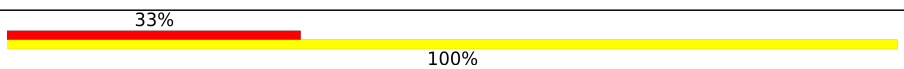
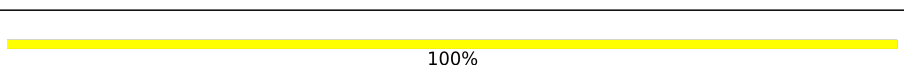
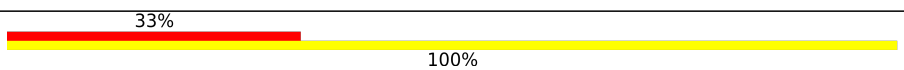
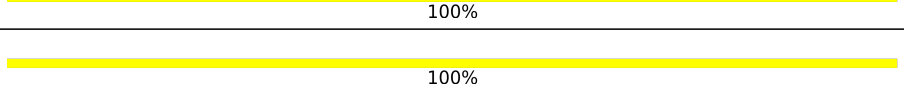
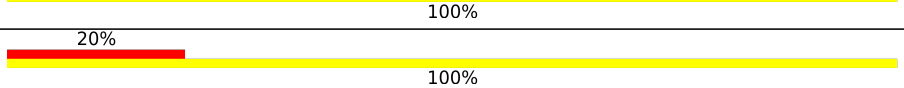
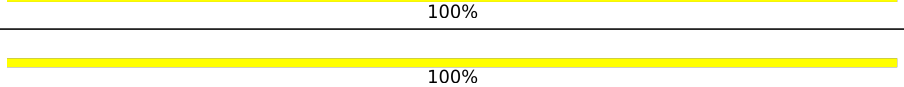
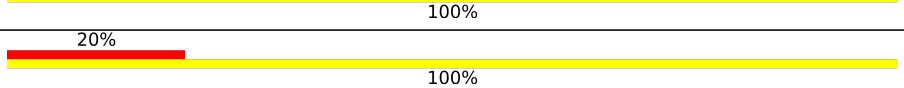
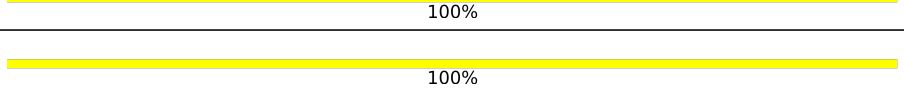
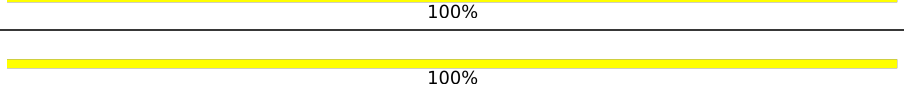
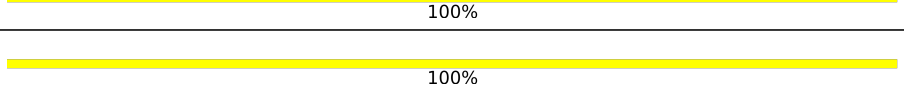
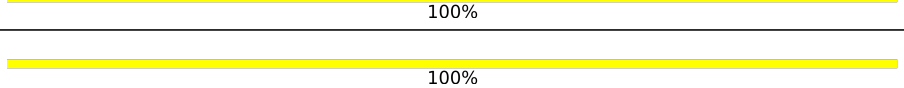
Mol	Chain	Length	Quality of chain
3	p	222	
4	g	207	
4	n	207	
4	o	207	
5	a	153	
5	b	153	
5	c	153	
6	d	461	
6	e	461	
6	f	461	
7	A	3	
7	E	3	
7	H	3	
7	L	3	
7	O	3	
7	S	3	
8	B	5	
8	F	5	
8	I	5	
8	M	5	
8	P	5	
8	T	5	
9	C	6	
9	J	6	
9	Q	6	

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Mol	Chain	Length	Quality of chain
10	D	4	25% 100%
10	K	4	100%
10	R	4	100%
11	G	2	100% 100%
11	N	2	50% 100%
11	U	2	50% 100%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 34626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DH851.3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	209	Total	C	N	O	S	0	0
			1546	962	258	320	6		
1	j	209	Total	C	N	O	S	0	0
			1546	962	258	320	6		
1	r	209	Total	C	N	O	S	0	0
			1546	962	258	320	6		

- Molecule 2 is a protein called DH851.3 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	228	Total	C	N	O	S	0	0
			1719	1090	287	335	7		
2	i	228	Total	C	N	O	S	0	0
			1719	1090	287	335	7		
2	q	228	Total	C	N	O	S	0	0
			1719	1090	287	335	7		

- Molecule 3 is a protein called DH851.3 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	222	Total	C	N	O	S	0	0
			1681	1067	280	328	6		
3	h	222	Total	C	N	O	S	0	0
			1681	1067	280	328	6		
3	p	222	Total	C	N	O	S	0	0
			1681	1067	280	328	6		

- Molecule 4 is a protein called DH851.3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	206	Total	C	N	O	S	0	0
			1526	951	255	315	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	206	Total	C	N	O	S	0	0
			1526	951	255	315	5		
4	o	206	Total	C	N	O	S	0	0
			1526	951	255	315	5		

- Molecule 5 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	135	Total	C	N	O	S	0	0
			1069	678	185	200	6		
5	b	135	Total	C	N	O	S	0	0
			1069	678	185	200	6		
5	c	135	Total	C	N	O	S	0	0
			1069	678	185	200	6		

- Molecule 6 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	461	Total	C	N	O	S	0	0
			3631	2277	635	690	29		
6	e	461	Total	C	N	O	S	0	0
			3631	2277	635	690	29		
6	f	461	Total	C	N	O	S	0	0
			3631	2277	635	690	29		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	32	GLU	-	expression tag	UNP M4M097
d	33	ASN	-	expression tag	UNP M4M097
d	34	LEU	-	expression tag	UNP M4M097
d	316	TRP	ALA	conflict	UNP M4M097
d	490	LYS	GLU	conflict	UNP M4M097
d	491	ILE	VAL	conflict	UNP M4M097
d	492	GLU	LYS	conflict	UNP M4M097
d	500	ARG	ASN	conflict	UNP M4M097
d	501	CYS	ALA	conflict	UNP M4M097
d	502	LYS	ARG	conflict	UNP M4M097
e	32	GLU	-	expression tag	UNP M4M097
e	33	ASN	-	expression tag	UNP M4M097
e	34	LEU	-	expression tag	UNP M4M097
e	316	TRP	ALA	conflict	UNP M4M097

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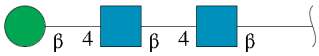
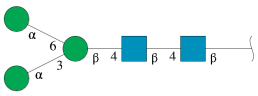
Chain	Residue	Modelled	Actual	Comment	Reference
e	490	LYS	GLU	conflict	UNP M4M097
e	491	ILE	VAL	conflict	UNP M4M097
e	492	GLU	LYS	conflict	UNP M4M097
e	500	ARG	ASN	conflict	UNP M4M097
e	501	CYS	ALA	conflict	UNP M4M097
e	502	LYS	ARG	conflict	UNP M4M097
f	32	GLU	-	expression tag	UNP M4M097
f	33	ASN	-	expression tag	UNP M4M097
f	34	LEU	-	expression tag	UNP M4M097
f	316	TRP	ALA	conflict	UNP M4M097
f	490	LYS	GLU	conflict	UNP M4M097
f	491	ILE	VAL	conflict	UNP M4M097
f	492	GLU	LYS	conflict	UNP M4M097
f	500	ARG	ASN	conflict	UNP M4M097
f	501	CYS	ALA	conflict	UNP M4M097
f	502	LYS	ARG	conflict	UNP M4M097

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



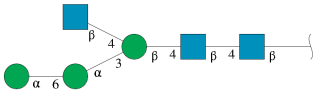
Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	E	3	Total	C	N	O	0	0
			39	22	2	15		
7	H	3	Total	C	N	O	0	0
			39	22	2	15		
7	L	3	Total	C	N	O	0	0
			39	22	2	15		
7	O	3	Total	C	N	O	0	0
			39	22	2	15		
7	S	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	B	5	Total	C	N	O	0	0
			61	34	2	25		
8	F	5	Total	C	N	O	0	0
			61	34	2	25		
8	I	5	Total	C	N	O	0	0
			61	34	2	25		
8	M	5	Total	C	N	O	0	0
			61	34	2	25		
8	P	5	Total	C	N	O	0	0
			61	34	2	25		
8	T	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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				AltConf	Trace
9	C	6	Total	C	N	O	0	0
			75	42	3	30		
9	J	6	Total	C	N	O	0	0
			75	42	3	30		
9	Q	6	Total	C	N	O	0	0
			75	42	3	30		

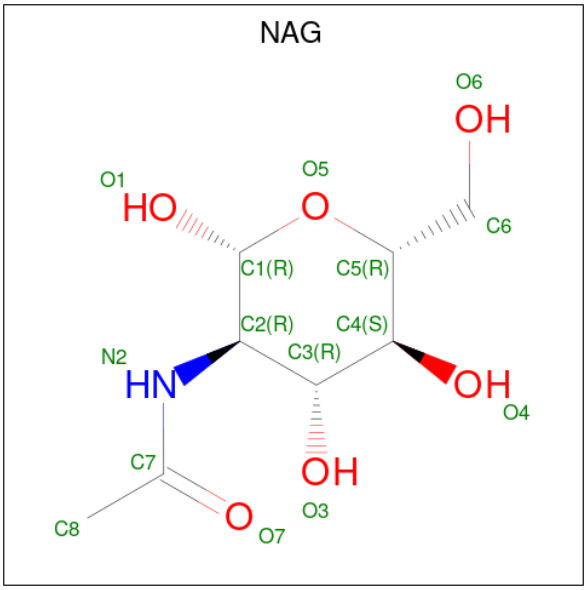
- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	D	4	Total C N O 53 30 3 20	0	0
10	K	4	Total C N O 53 30 3 20	0	0
10	R	4	Total C N O 53 30 3 20	0	0

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	G	2	Total C N O 28 16 2 10	0	0
11	N	2	Total C N O 28 16 2 10	0	0
11	U	2	Total C N O 28 16 2 10	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



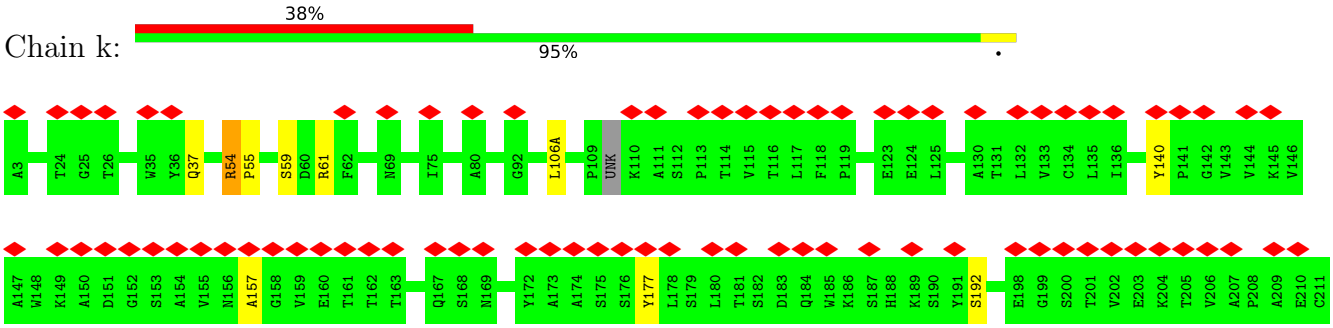
Mol	Chain	Residues	Atoms				AltConf
12	a	1	Total	C	N	O	0
			14	8	1	5	
12	b	1	Total	C	N	O	0
			14	8	1	5	
12	c	1	Total	C	N	O	0
			14	8	1	5	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

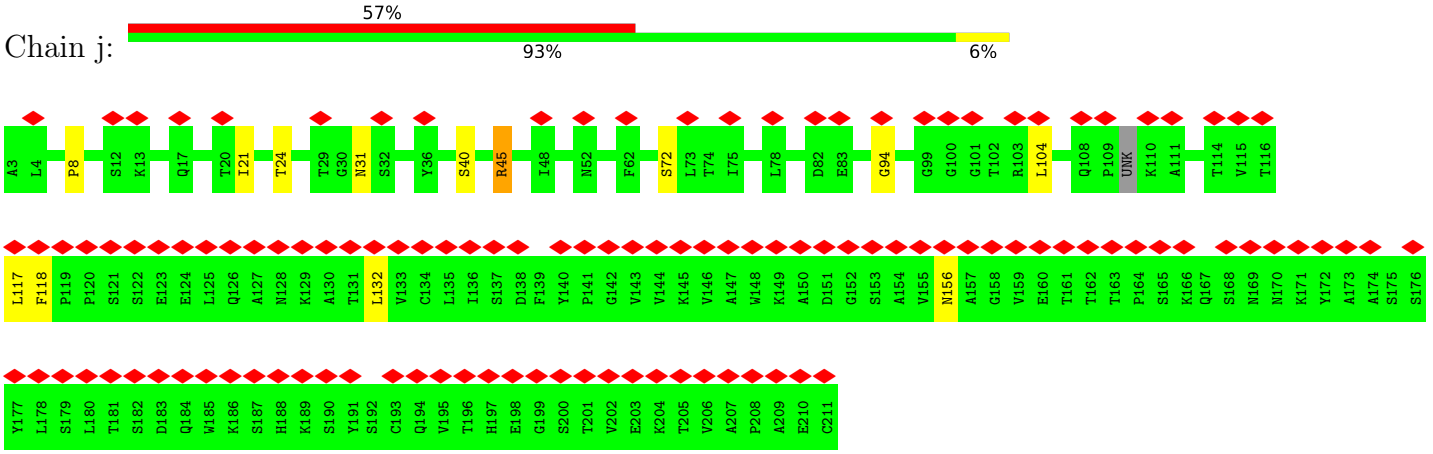
• Molecule 1: DH851.3 light chain

Chain k:



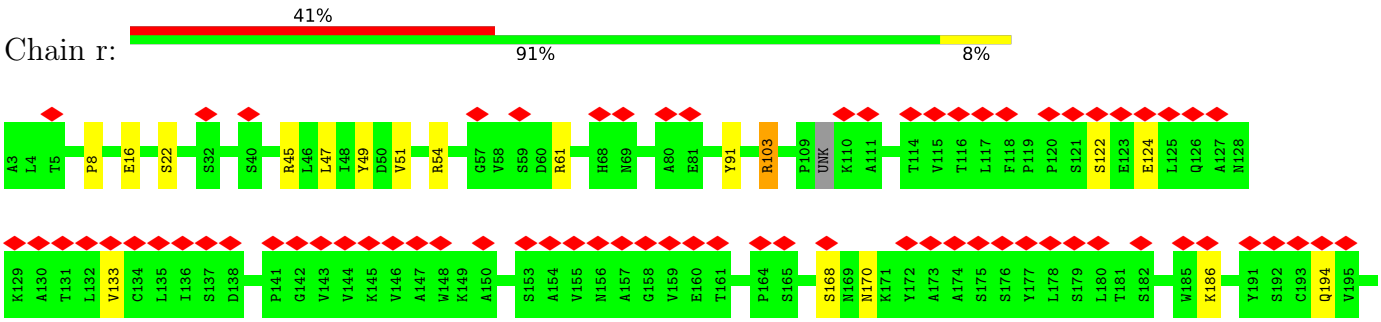
• Molecule 1: DH851.3 light chain

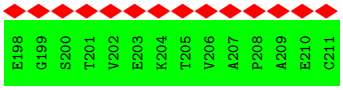
Chain j:



• Molecule 1: DH851.3 light chain

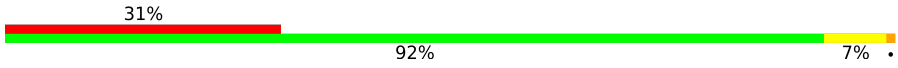
Chain r:

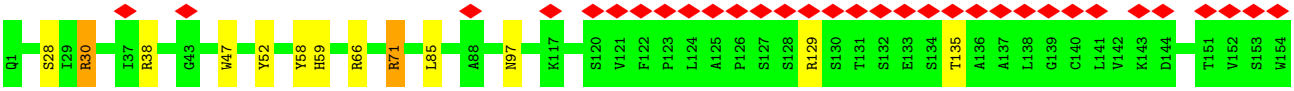


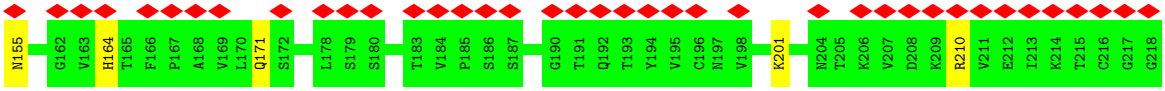


• Molecule 2: DH851.3 heavy chain

Chain l:

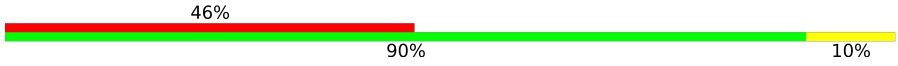


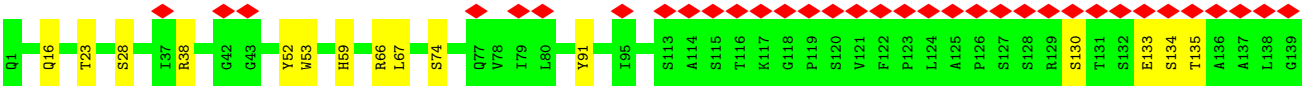


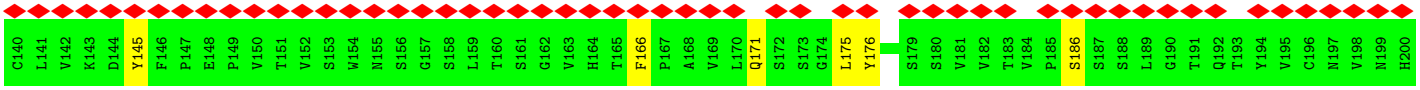


• Molecule 2: DH851.3 heavy chain

Chain i:

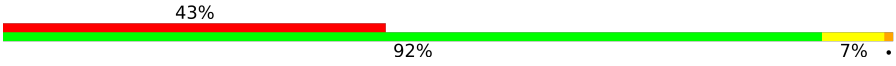


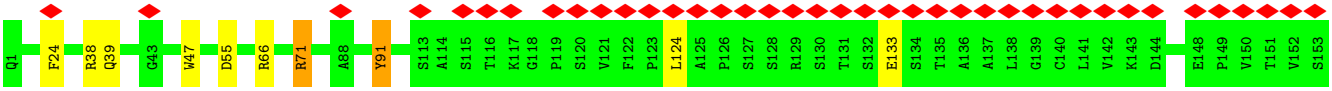


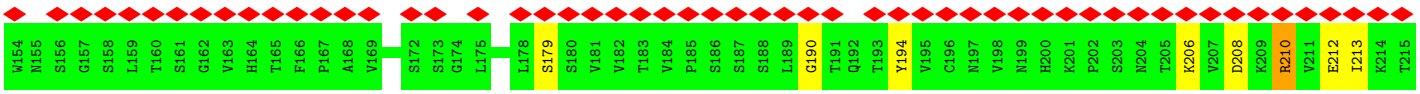


• Molecule 2: DH851.3 heavy chain

Chain q:

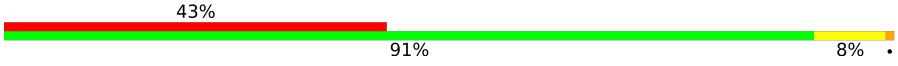


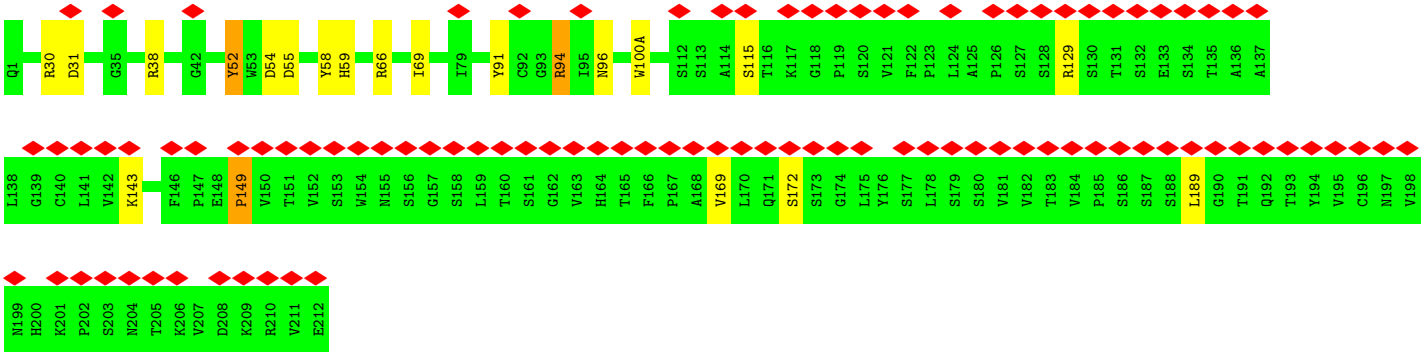




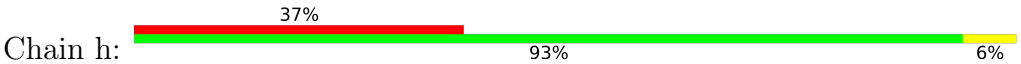
• Molecule 3: DH851.3 heavy chain

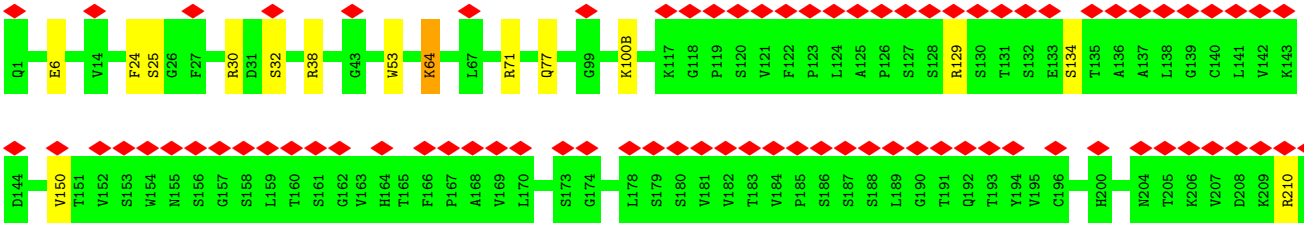
Chain m:



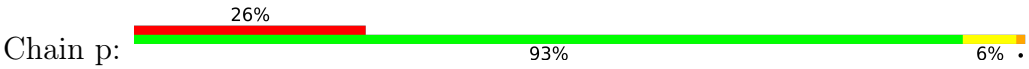


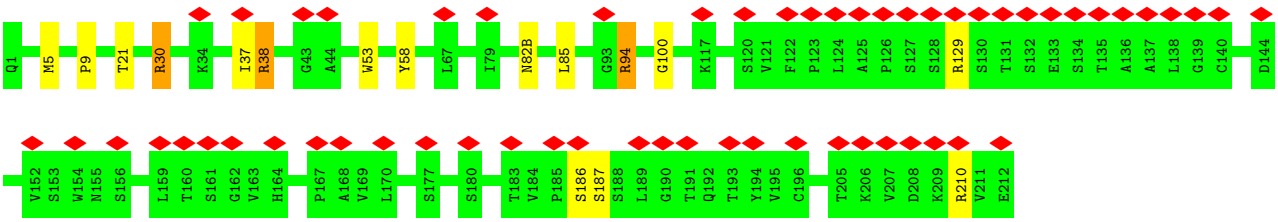
• Molecule 3: DH851.3 heavy chain



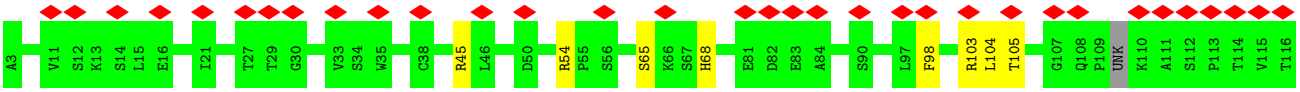


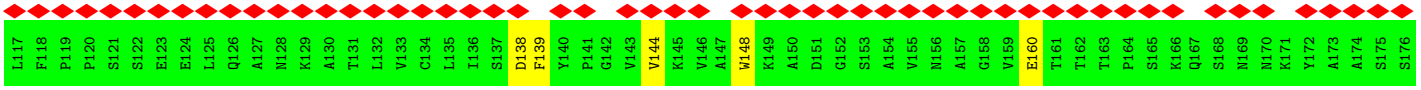
• Molecule 3: DH851.3 heavy chain

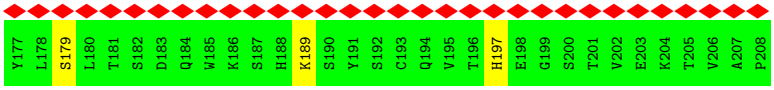




• Molecule 4: DH851.3 light chain

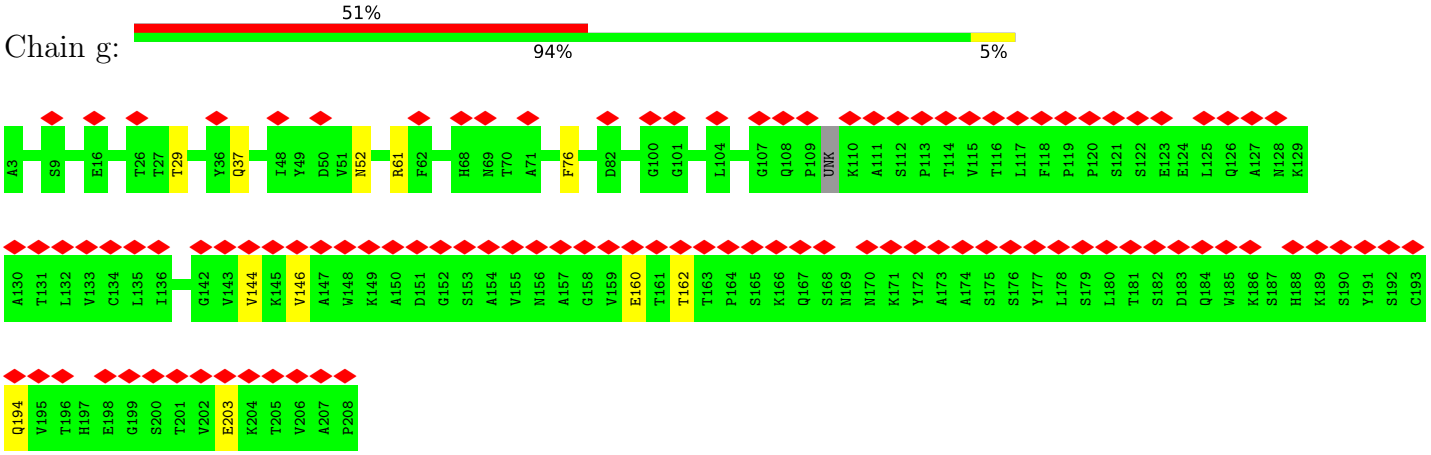






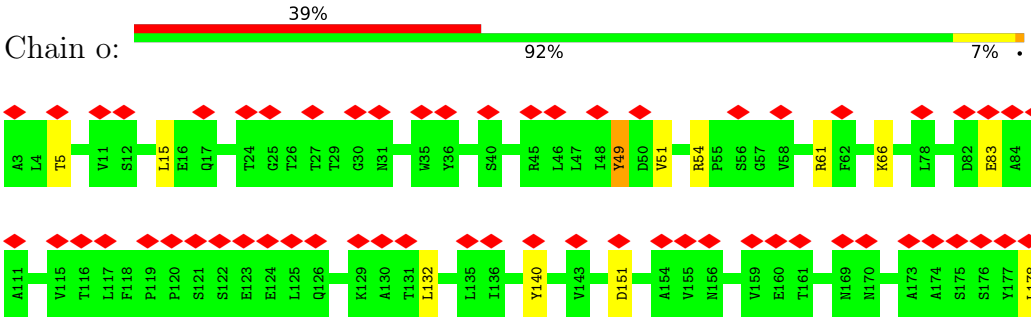
• Molecule 4: DH851.3 light chain

Chain g:



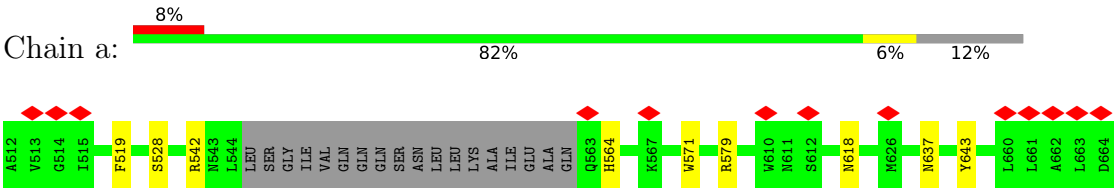
• Molecule 4: DH851.3 light chain

Chain o:



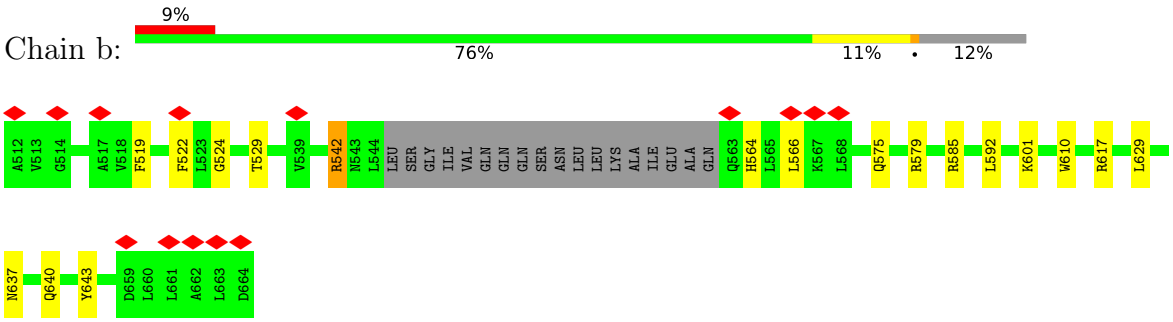
• Molecule 5: Envelope glycoprotein gp41

Chain a:



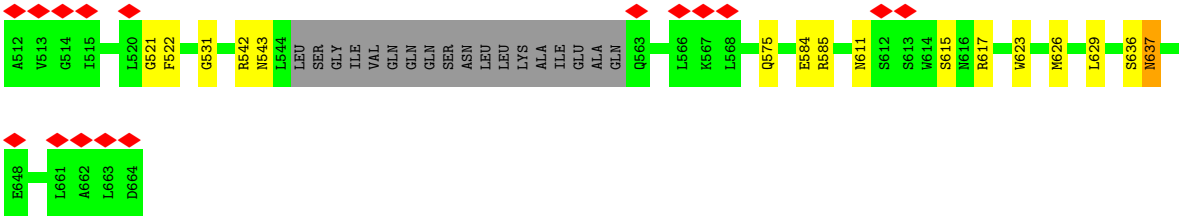
• Molecule 5: Envelope glycoprotein gp41

Chain b:

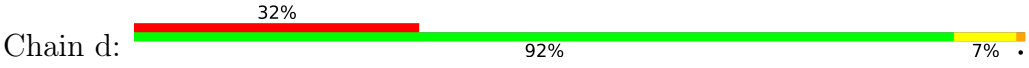


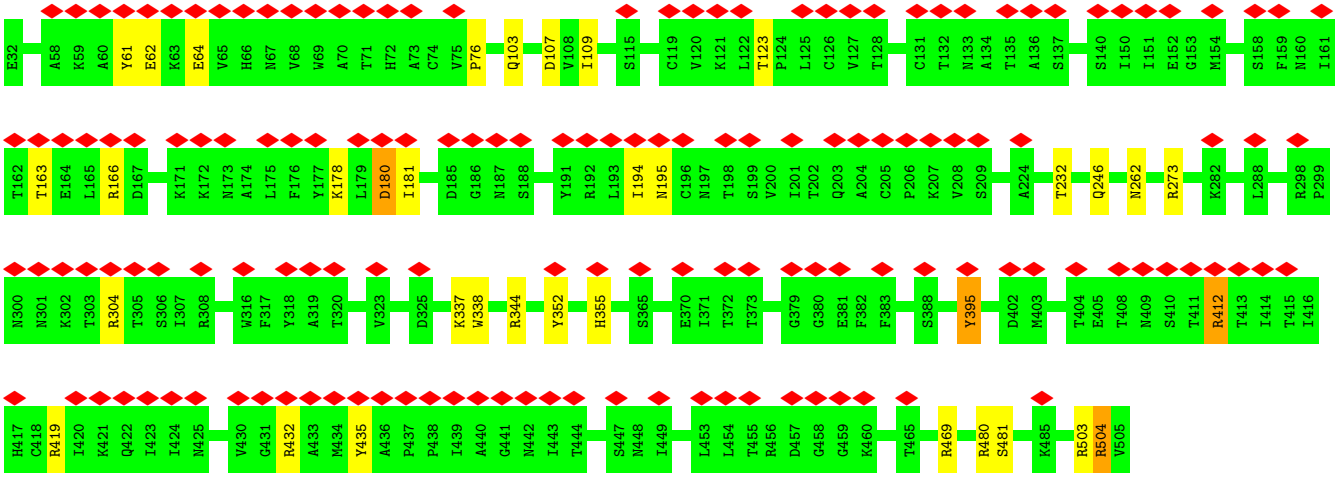
• Molecule 5: Envelope glycoprotein gp41

Chain c:

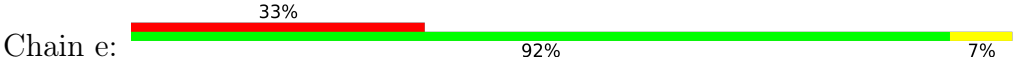


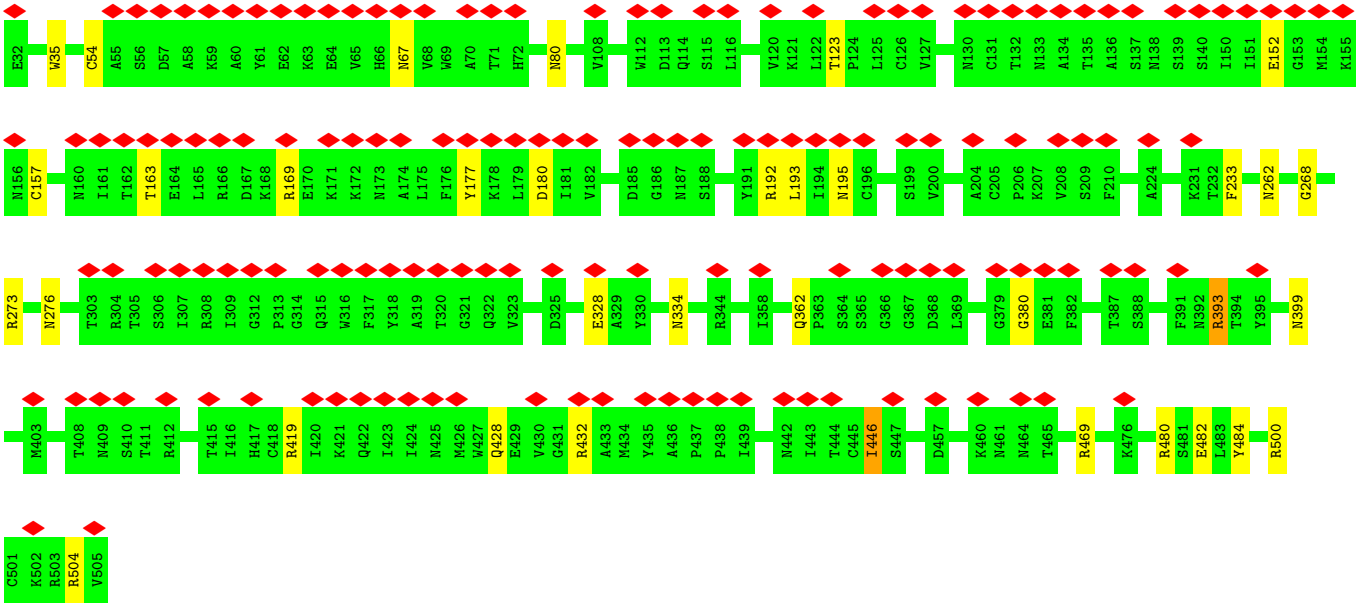
• Molecule 6: Envelope glycoprotein gp120





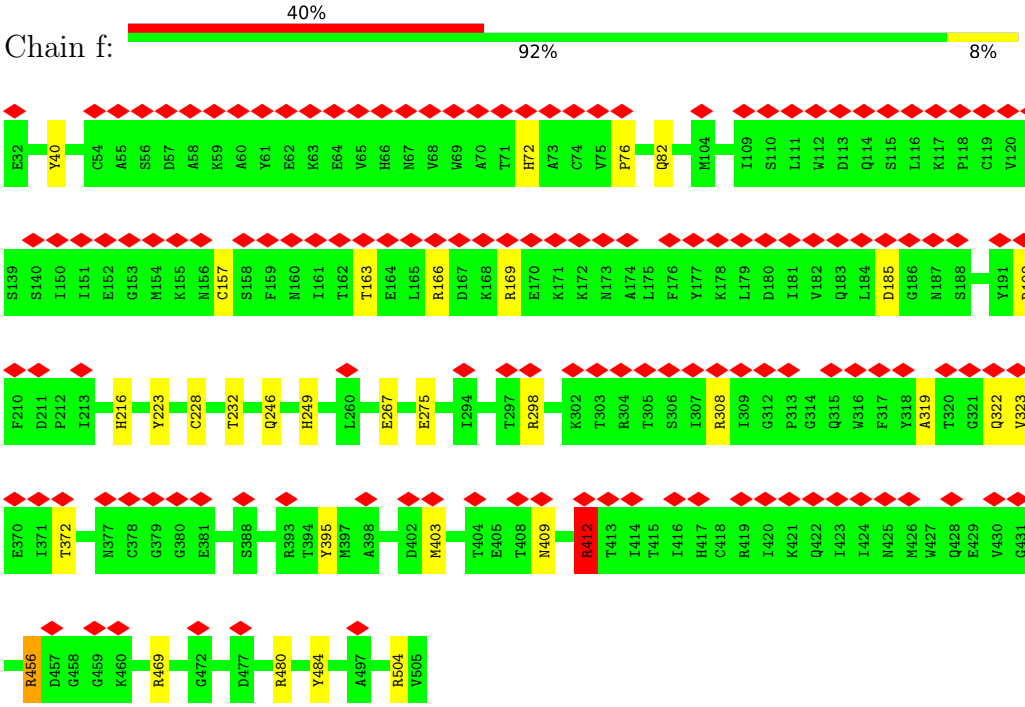
• Molecule 6: Envelope glycoprotein gp120





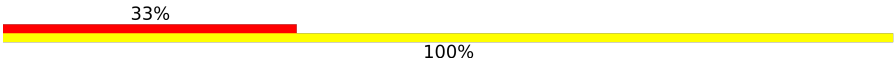
• Molecule 6: Envelope glycoprotein gp120

Chain f:



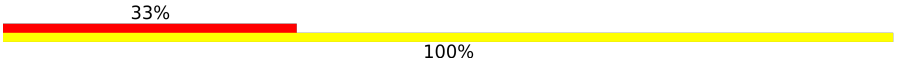
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



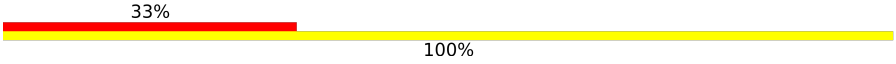
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



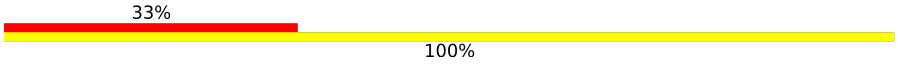
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



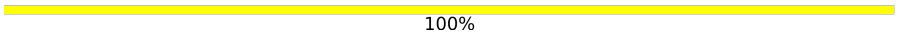
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



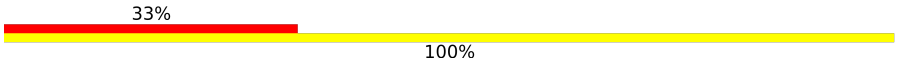
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



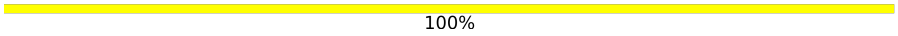
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



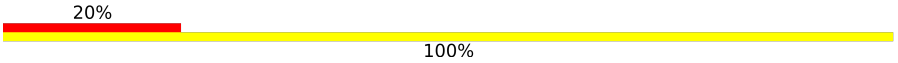
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



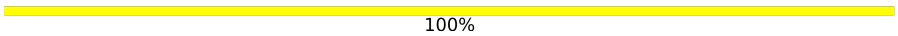
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



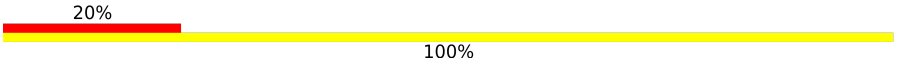
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



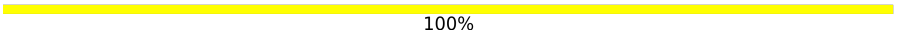
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain P:

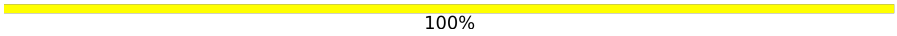


• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

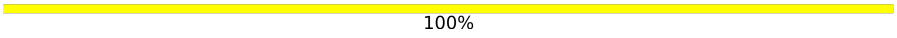
• Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



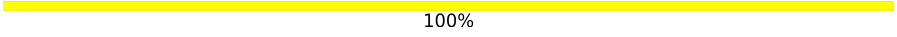
• Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



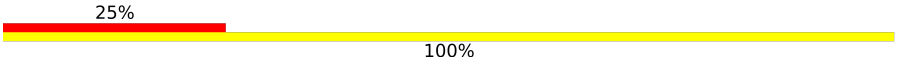
• Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



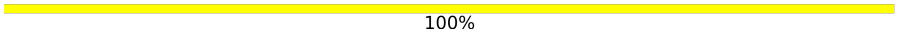
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



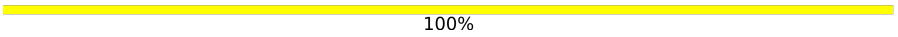
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.476	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	150.3765, 237.82948, 247.428	wwPDB
Map dimensions	232, 223, 141	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0665, 1.0665, 1.0665	Depositor

5 Model quality

5.1 Standard geometry

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

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	j	0.69	0/1579	1.06	1/2147 (0.0%)
1	k	0.67	0/1579	1.06	4/2147 (0.2%)
1	r	0.68	0/1579	1.05	4/2147 (0.2%)
2	i	0.68	0/1762	1.05	4/2407 (0.2%)
2	l	0.66	0/1762	1.06	6/2407 (0.2%)
2	q	0.66	0/1762	1.10	5/2407 (0.2%)
3	h	0.66	0/1724	1.05	4/2357 (0.2%)
3	m	0.70	0/1724	1.08	6/2357 (0.3%)
3	p	0.67	0/1724	1.06	4/2357 (0.2%)
4	g	0.66	0/1559	0.97	1/2120 (0.0%)
4	n	0.69	0/1559	1.09	3/2120 (0.1%)
4	o	0.68	0/1559	1.04	4/2120 (0.2%)
5	a	0.62	0/1088	1.04	3/1474 (0.2%)
5	b	0.62	0/1088	1.08	5/1474 (0.3%)
5	c	0.63	0/1088	1.05	2/1474 (0.1%)
6	d	0.67	0/3707	1.05	13/5033 (0.3%)
6	e	0.68	0/3707	1.06	10/5033 (0.2%)
6	f	0.67	0/3707	1.03	13/5033 (0.3%)
All	All	0.67	0/34257	1.05	92/46614 (0.2%)

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	r	0	3
2	i	0	4
2	l	0	3
2	q	0	1
3	h	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	m	0	2
3	p	0	1
4	o	0	1
5	b	0	1
6	d	0	3
6	e	0	2
6	f	0	5
All	All	0	27

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	k	54	ARG	NE-CZ-NH2	9.11	124.86	120.30
2	q	66	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	r	103	ARG	NE-CZ-NH1	8.20	124.40	120.30
4	o	61	ARG	NE-CZ-NH1	7.79	124.19	120.30
6	e	480	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	l	30	ARG	NE-CZ-NH1	7.53	124.06	120.30
3	m	66	ARG	NE-CZ-NH1	7.43	124.01	120.30
5	c	585	ARG	NE-CZ-NH1	7.37	123.99	120.30
3	p	30	ARG	NE-CZ-NH2	7.35	123.98	120.30
6	d	480	ARG	NE-CZ-NH1	7.34	123.97	120.30
3	m	129	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	j	45	ARG	NE-CZ-NH1	7.11	123.86	120.30
2	q	91	TYR	CB-CG-CD2	-7.10	116.74	121.00
6	e	504	ARG	NE-CZ-NH1	7.09	123.84	120.30
6	d	503	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	q	38	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	k	61	ARG	NE-CZ-NH1	7.03	123.81	120.30
4	n	45	ARG	NE-CZ-NH1	7.00	123.80	120.30
6	e	419	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	l	66	ARG	NE-CZ-NH1	6.89	123.75	120.30
4	n	103	ARG	NE-CZ-NH1	6.74	123.67	120.30
6	d	469	ARG	NE-CZ-NH1	6.73	123.67	120.30
6	d	412	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	r	45	ARG	NE-CZ-NH1	6.69	123.65	120.30
6	e	500	ARG	NE-CZ-NH2	6.68	123.64	120.30
6	d	166	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	k	54	ARG	CD-NE-CZ	6.58	132.81	123.60
2	i	145	TYR	CB-CG-CD1	-6.57	117.06	121.00
6	d	504	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	412	ARG	NE-CZ-NH2	6.53	123.56	120.30
5	b	579	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	i	38	ARG	NE-CZ-NH1	6.32	123.46	120.30
6	e	480	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	r	54	ARG	NE-CZ-NH2	6.27	123.43	120.30
6	d	480	ARG	NE-CZ-NH2	-6.24	117.18	120.30
3	p	210	ARG	NE-CZ-NH1	6.20	123.40	120.30
6	d	344	ARG	NE-CZ-NH2	6.20	123.40	120.30
5	a	542	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	l	210	ARG	NE-CZ-NH1	6.15	123.38	120.30
6	f	504	ARG	NE-CZ-NH1	6.14	123.37	120.30
6	f	432	ARG	NE-CZ-NH2	6.12	123.36	120.30
6	e	469	ARG	NE-CZ-NH1	6.12	123.36	120.30
6	d	273	ARG	NE-CZ-NH1	6.09	123.35	120.30
6	e	273	ARG	NE-CZ-NH1	6.05	123.33	120.30
3	m	30	ARG	NE-CZ-NH2	6.04	123.32	120.30
6	f	298	ARG	NE-CZ-NH1	6.01	123.31	120.30
5	b	643	TYR	CB-CG-CD2	-6.00	117.40	121.00
6	f	169	ARG	NE-CZ-NH2	5.97	123.28	120.30
6	e	432	ARG	NE-CZ-NH2	5.96	123.28	120.30
3	m	94	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	q	71	ARG	NE-CZ-NH2	5.84	123.22	120.30
3	h	210	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	h	38	ARG	NE-CZ-NH1	5.74	123.17	120.30
3	p	38	ARG	NE-CZ-NH1	5.73	123.17	120.30
3	m	38	ARG	NE-CZ-NH1	5.71	123.16	120.30
5	b	585	ARG	NE-CZ-NH1	5.63	123.12	120.30
5	a	643	TYR	CB-CG-CD2	-5.62	117.63	121.00
4	n	54	ARG	NE-CZ-NH2	5.60	123.10	120.30
6	f	469	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	p	94	ARG	NE-CZ-NH1	5.56	123.08	120.30
6	f	327	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	q	38	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	e	169	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	r	61	ARG	NE-CZ-NH1	5.50	123.05	120.30
6	e	192	ARG	NE-CZ-NH1	5.50	123.05	120.30
6	d	432	ARG	NE-CZ-NH2	5.49	123.05	120.30
3	h	30	ARG	NE-CZ-NH2	5.43	123.01	120.30
6	f	344	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	k	177	TYR	CB-CG-CD2	-5.42	117.75	121.00
4	o	54	ARG	NE-CZ-NH2	5.38	122.99	120.30
6	d	469	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	66	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	m	52	TYR	CB-CG-CD1	-5.37	117.78	121.00
5	c	617	ARG	NE-CZ-NH2	5.35	122.97	120.30
6	f	166	ARG	NE-CZ-NH2	5.28	122.94	120.30
6	d	419	ARG	NE-CZ-NH1	5.23	122.92	120.30
5	b	542	ARG	NE-CZ-NH1	5.22	122.91	120.30
4	g	61	ARG	NE-CZ-NH1	5.21	122.90	120.30
5	b	617	ARG	NE-CZ-NH2	5.19	122.89	120.30
4	o	49	TYR	CB-CG-CD2	-5.18	117.89	121.00
6	f	395	TYR	CB-CG-CD1	-5.18	117.89	121.00
6	f	456	ARG	NE-CZ-NH1	5.17	122.88	120.30
6	f	192	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	l	71	ARG	NE-CZ-NH2	5.15	122.87	120.30
3	h	129	ARG	NE-CZ-NH2	5.13	122.86	120.30
6	f	308	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	l	38	ARG	NE-CZ-NH1	5.09	122.85	120.30
5	a	579	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	l	129	ARG	NE-CZ-NH2	5.05	122.83	120.30
6	d	412	ARG	NE-CZ-NH1	-5.03	117.79	120.30
4	o	103	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	i	210	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	b	629	LEU	Peptide
6	d	352	TYR	Sidechain
6	d	395	TYR	Sidechain
6	d	61	TYR	Sidechain
6	e	177	TYR	Sidechain
6	e	393	ARG	Sidechain
6	f	223	TYR	Sidechain
6	f	249	HIS	Sidechain
6	f	40	TYR	Sidechain
6	f	456	ARG	Sidechain
6	f	484	TYR	Sidechain
3	h	71	ARG	Peptide
2	i	175	LEU	Peptide
2	i	176	TYR	Sidechain
2	i	52	TYR	Sidechain
2	i	67	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	l	30	ARG	Sidechain
2	l	52	TYR	Sidechain
2	l	58	TYR	Sidechain
3	m	59	HIS	Sidechain
3	m	91	TYR	Sidechain
4	o	91	TYR	Sidechain
3	p	38	ARG	Sidechain
2	q	133	GLU	Peptide
1	r	22	SER	Peptide
1	r	49	TYR	Sidechain
1	r	91	TYR	Sidechain

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	j	1546	0	1489	0	0
1	k	1546	0	1489	0	0
1	r	1546	0	1489	0	0
2	i	1719	0	1701	0	0
2	l	1719	0	1701	0	0
2	q	1719	0	1701	0	0
3	h	1681	0	1659	0	0
3	m	1681	0	1659	0	0
3	p	1681	0	1659	0	0
4	g	1526	0	1473	0	0
4	n	1526	0	1473	0	0
4	o	1526	0	1473	0	0
5	a	1069	0	1055	0	0
5	b	1069	0	1055	0	0
5	c	1069	0	1055	0	0
6	d	3631	0	3582	0	0
6	e	3631	0	3582	0	0
6	f	3631	0	3582	0	0
7	A	39	0	34	0	0
7	E	39	0	34	0	0
7	H	39	0	34	0	0
7	L	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	39	0	34	0	0
7	S	39	0	34	0	0
8	B	61	0	52	0	0
8	F	61	0	52	0	0
8	I	61	0	52	0	0
8	M	61	0	52	0	0
8	P	61	0	52	0	0
8	T	61	0	52	0	0
9	C	75	0	64	0	0
9	J	75	0	64	0	0
9	Q	75	0	64	0	0
10	D	53	0	46	0	0
10	K	53	0	46	0	0
10	R	53	0	46	0	0
11	G	28	0	25	0	0
11	N	28	0	25	0	0
11	U	28	0	25	0	0
12	a	14	0	13	0	0
12	b	14	0	13	0	0
12	c	14	0	13	0	0
All	All	34626	0	33837	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	j	205/210 (98%)	166 (81%)	34 (17%)	5 (2%)	6 33
1	k	205/210 (98%)	161 (78%)	40 (20%)	4 (2%)	7 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	r	205/210 (98%)	167 (82%)	31 (15%)	7 (3%)	3 26
2	i	226/228 (99%)	188 (83%)	32 (14%)	6 (3%)	5 31
2	l	226/228 (99%)	203 (90%)	21 (9%)	2 (1%)	17 56
2	q	226/228 (99%)	184 (81%)	38 (17%)	4 (2%)	8 40
3	h	220/222 (99%)	195 (89%)	20 (9%)	5 (2%)	6 34
3	m	220/222 (99%)	182 (83%)	30 (14%)	8 (4%)	3 25
3	p	220/222 (99%)	196 (89%)	17 (8%)	7 (3%)	4 26
4	g	202/207 (98%)	171 (85%)	26 (13%)	5 (2%)	5 32
4	n	202/207 (98%)	160 (79%)	35 (17%)	7 (4%)	3 25
4	o	202/207 (98%)	169 (84%)	28 (14%)	5 (2%)	5 32
5	a	131/153 (86%)	112 (86%)	16 (12%)	3 (2%)	6 34
5	b	131/153 (86%)	107 (82%)	18 (14%)	6 (5%)	2 21
5	c	131/153 (86%)	111 (85%)	14 (11%)	6 (5%)	2 21
6	d	459/461 (100%)	395 (86%)	49 (11%)	15 (3%)	4 26
6	e	459/461 (100%)	386 (84%)	61 (13%)	12 (3%)	5 31
6	f	459/461 (100%)	379 (83%)	69 (15%)	11 (2%)	6 33
All	All	4329/4443 (97%)	3632 (84%)	579 (13%)	118 (3%)	8 31

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	k	157	ALA
3	m	143	LYS
1	j	31	ASN
4	o	15	LEU
2	q	213	ILE
5	b	637	ASN
5	c	637	ASN
4	n	189	LYS
4	g	29	THR
4	g	76	PHE
4	g	146	VAL
4	g	160	GLU
2	i	53	TRP
2	i	130	SER
1	j	40	SER

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Mol	Chain	Res	Type
1	j	132	LEU
4	o	151	ASP
3	p	30	ARG
3	p	53	TRP
3	p	129	ARG
2	q	55	ASP
5	a	528	SER
5	a	564	HIS
6	d	62	GLU
6	d	163	THR
6	d	181	ILE
6	d	481	SER
5	b	566	LEU
6	e	163	THR
6	e	446	ILE
5	c	531	GLY
6	f	72	HIS
6	f	323	VAL
2	l	155	ASN
3	m	31	ASP
3	m	115	SER
4	n	104	LEU
4	n	148	TRP
3	h	25	SER
2	i	166	PHE
4	o	5	THR
4	o	51	VAL
3	p	9	PRO
1	r	168	SER
5	a	618	ASN
6	d	103	GLN
6	d	262	ASN
6	d	355	HIS
5	b	519	PHE
5	b	524	GLY
5	b	564	HIS
6	e	276	ASN
6	e	399	ASN
6	f	163	THR
6	f	232	THR
1	k	59	SER
1	k	192	SER

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Mol	Chain	Res	Type
2	l	201	LYS
3	m	54	ASP
3	m	172	SER
4	n	68	HIS
4	g	52	ASN
3	h	32	SER
3	h	100(B)	LYS
3	h	134	SER
2	i	186	SER
4	o	83	GLU
3	p	186	SER
1	r	51	VAL
1	r	103	ARG
1	r	122	SER
6	d	76	PRO
6	d	178	LYS
6	d	412	ARG
6	e	152	GLU
6	e	233	PHE
6	e	482	GLU
5	c	615	SER
5	c	629	LEU
6	f	185	ASP
6	f	322	GLN
6	f	409	ASN
3	m	55	ASP
4	n	65	SER
4	n	179	SER
4	n	197	HIS
2	i	134	SER
3	p	187	SER
6	d	123	THR
6	d	304	ARG
6	d	395	TYR
6	d	504	ARG
5	b	601	LYS
6	f	319	ALA
6	f	412	ARG
1	k	55	PRO
2	i	16	GLN
2	q	210	ARG
1	r	8	PRO

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Mol	Chain	Res	Type
1	r	133	VAL
1	r	170	ASN
6	d	180	ASP
6	e	334	ASN
5	c	636	SER
6	f	76	PRO
6	f	123	THR
3	p	100	GLY
2	q	190	GLY
6	e	380	GLY
1	j	94	GLY
6	e	80	ASN
5	c	521	GLY
3	h	64	LYS
6	e	268	GLY
1	j	8	PRO
6	e	123	THR
3	m	169	VAL
3	m	149	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	j	174/175 (99%)	166 (95%)	8 (5%)	27	53
1	k	174/175 (99%)	170 (98%)	4 (2%)	50	70
1	r	174/175 (99%)	169 (97%)	5 (3%)	42	64
2	i	196/197 (100%)	188 (96%)	8 (4%)	30	55
2	l	196/197 (100%)	187 (95%)	9 (5%)	27	53
2	q	196/197 (100%)	184 (94%)	12 (6%)	18	45
3	h	192/193 (100%)	186 (97%)	6 (3%)	40	62
3	m	192/193 (100%)	184 (96%)	8 (4%)	30	54
3	p	192/193 (100%)	185 (96%)	7 (4%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	g	172/173 (99%)	167 (97%)	5 (3%)	42	64
4	n	172/173 (99%)	166 (96%)	6 (4%)	36	60
4	o	172/173 (99%)	164 (95%)	8 (5%)	26	52
5	a	114/129 (88%)	111 (97%)	3 (3%)	46	67
5	b	114/129 (88%)	107 (94%)	7 (6%)	18	45
5	c	114/129 (88%)	105 (92%)	9 (8%)	12	37
6	d	413/413 (100%)	402 (97%)	11 (3%)	44	65
6	e	413/413 (100%)	399 (97%)	14 (3%)	37	60
6	f	413/413 (100%)	400 (97%)	13 (3%)	40	62
All	All	3783/3840 (98%)	3640 (96%)	143 (4%)	36	57

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	37	GLN
1	k	54	ARG
1	k	106(A)	LEU
1	k	140	TYR
2	l	28	SER
2	l	47	TRP
2	l	59	HIS
2	l	71	ARG
2	l	85	LEU
2	l	97	ASN
2	l	135	THR
2	l	164	HIS
2	l	171	GLN
3	m	52	TYR
3	m	58	TYR
3	m	69	ILE
3	m	94	ARG
3	m	96	ASN
3	m	100(A)	TRP
3	m	149	PRO
3	m	189	LEU
4	n	98	PHE
4	n	105	THR
4	n	138	ASP
4	n	139	PHE

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Mol	Chain	Res	Type
4	n	144	VAL
4	n	160	GLU
4	g	37	GLN
4	g	144	VAL
4	g	162	THR
4	g	194	GLN
4	g	203	GLU
3	h	6	GLU
3	h	24	PHE
3	h	53	TRP
3	h	64	LYS
3	h	77	GLN
3	h	150	VAL
2	i	23	THR
2	i	28	SER
2	i	59	HIS
2	i	74	SER
2	i	91	TYR
2	i	133	GLU
2	i	135	THR
2	i	171	GLN
1	j	21	ILE
1	j	24	THR
1	j	45	ARG
1	j	72	SER
1	j	104	LEU
1	j	117	LEU
1	j	118	PHE
1	j	156	ASN
4	o	49	TYR
4	o	66	LYS
4	o	103	ARG
4	o	132	LEU
4	o	140	TYR
4	o	178	LEU
4	o	189	LYS
4	o	194	GLN
3	p	5	MET
3	p	21	THR
3	p	37	ILE
3	p	58	TYR
3	p	82(B)	ASN

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Mol	Chain	Res	Type
3	p	85	LEU
3	p	94	ARG
2	q	24	PHE
2	q	39	GLN
2	q	47	TRP
2	q	71	ARG
2	q	91	TYR
2	q	124	LEU
2	q	179	SER
2	q	194	TYR
2	q	206	LYS
2	q	208	ASP
2	q	210	ARG
2	q	212	GLU
1	r	16	GLU
1	r	47	LEU
1	r	124	GLU
1	r	186	LYS
1	r	194	GLN
5	a	519	PHE
5	a	571	TRP
5	a	637	ASN
6	d	64	GLU
6	d	107	ASP
6	d	109	ILE
6	d	180	ASP
6	d	194	ILE
6	d	195	ASN
6	d	232	THR
6	d	246	GLN
6	d	337	LYS
6	d	338	TRP
6	d	435	TYR
5	b	522	PHE
5	b	529	THR
5	b	542	ARG
5	b	575	GLN
5	b	592	LEU
5	b	610	TRP
5	b	640	GLN
6	e	35	TRP
6	e	54	CYS

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Mol	Chain	Res	Type
6	e	67	ASN
6	e	157	CYS
6	e	180	ASP
6	e	193	LEU
6	e	195	ASN
6	e	262	ASN
6	e	328	GLU
6	e	362	GLN
6	e	393	ARG
6	e	428	GLN
6	e	446	ILE
6	e	484	TYR
5	c	522	PHE
5	c	542	ARG
5	c	543	ASN
5	c	575	GLN
5	c	584	GLU
5	c	611	ASN
5	c	623	TRP
5	c	626	MET
5	c	637	ASN
6	f	82	GLN
6	f	157	CYS
6	f	195	ASN
6	f	216	HIS
6	f	228	CYS
6	f	246	GLN
6	f	267	GLU
6	f	275	GLU
6	f	350	LYS
6	f	372	THR
6	f	403	MET
6	f	412	ARG
6	f	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	g	69	ASN
3	h	97	ASN
1	r	68	HIS
6	e	103	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

84 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	$\#\|Z\| > 2$
7	NAG	A	1	7,5	14,14,15	1.38	3 (21%)	17,19,21	0.90	0
7	NAG	A	2	7	14,14,15	1.43	3 (21%)	17,19,21	1.05	1 (5%)
7	BMA	A	3	7	11,11,12	1.36	2 (18%)	15,15,17	0.92	1 (6%)
8	NAG	B	1	8,6	14,14,15	1.17	2 (14%)	17,19,21	1.46	1 (5%)
8	NAG	B	2	8	14,14,15	1.56	3 (21%)	17,19,21	1.31	2 (11%)
8	BMA	B	3	8	11,11,12	1.34	1 (9%)	15,15,17	1.29	2 (13%)
8	MAN	B	4	8	11,11,12	1.33	2 (18%)	15,15,17	1.70	3 (20%)
8	MAN	B	5	8	11,11,12	1.23	2 (18%)	15,15,17	1.44	1 (6%)
9	NAG	C	1	6,9	14,14,15	1.17	2 (14%)	17,19,21	0.82	0
9	NAG	C	2	9	14,14,15	1.40	2 (14%)	17,19,21	1.14	1 (5%)
9	BMA	C	3	9	11,11,12	1.88	3 (27%)	15,15,17	1.66	3 (20%)
9	MAN	C	4	9	11,11,12	1.33	2 (18%)	15,15,17	1.54	2 (13%)
9	MAN	C	5	9	11,11,12	1.19	2 (18%)	15,15,17	1.40	1 (6%)
9	NAG	C	6	9	14,14,15	1.49	2 (14%)	17,19,21	1.93	4 (23%)
10	NAG	D	1	10,6	14,14,15	1.38	2 (14%)	17,19,21	0.88	0
10	NAG	D	2	10	14,14,15	1.56	4 (28%)	17,19,21	1.11	1 (5%)
10	BMA	D	3	10	11,11,12	1.44	3 (27%)	15,15,17	1.03	0
10	NAG	D	4	10	14,14,15	1.32	2 (14%)	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	E	1	6,7	14,14,15	1.26	2 (14%)	17,19,21	0.96	1 (5%)
7	NAG	E	2	7	14,14,15	1.48	4 (28%)	17,19,21	0.93	1 (5%)
7	BMA	E	3	7	11,11,12	1.30	2 (18%)	15,15,17	0.80	1 (6%)
8	NAG	F	1	8,6	14,14,15	1.34	4 (28%)	17,19,21	0.81	0
8	NAG	F	2	8	14,14,15	1.30	2 (14%)	17,19,21	0.91	0
8	BMA	F	3	8	11,11,12	1.53	2 (18%)	15,15,17	1.04	1 (6%)
8	MAN	F	4	8	11,11,12	1.26	2 (18%)	15,15,17	0.93	1 (6%)
8	MAN	F	5	8	11,11,12	1.41	2 (18%)	15,15,17	1.63	2 (13%)
11	NAG	G	1	6,11	14,14,15	1.35	3 (21%)	17,19,21	0.88	1 (5%)
11	NAG	G	2	11	14,14,15	1.23	2 (14%)	17,19,21	1.10	1 (5%)
7	NAG	H	1	7,5	14,14,15	1.35	3 (21%)	17,19,21	1.51	2 (11%)
7	NAG	H	2	7	14,14,15	1.38	4 (28%)	17,19,21	1.26	1 (5%)
7	BMA	H	3	7	11,11,12	1.30	2 (18%)	15,15,17	0.87	0
8	NAG	I	1	8,6	14,14,15	1.41	3 (21%)	17,19,21	0.96	1 (5%)
8	NAG	I	2	8	14,14,15	1.57	4 (28%)	17,19,21	1.51	1 (5%)
8	BMA	I	3	8	11,11,12	1.46	2 (18%)	15,15,17	0.81	0
8	MAN	I	4	8	11,11,12	1.36	2 (18%)	15,15,17	1.69	2 (13%)
8	MAN	I	5	8	11,11,12	1.11	1 (9%)	15,15,17	1.17	2 (13%)
9	NAG	J	1	6,9	14,14,15	1.30	2 (14%)	17,19,21	0.96	1 (5%)
9	NAG	J	2	9	14,14,15	1.55	3 (21%)	17,19,21	1.26	2 (11%)
9	BMA	J	3	9	11,11,12	2.09	5 (45%)	15,15,17	1.97	6 (40%)
9	MAN	J	4	9	11,11,12	1.35	2 (18%)	15,15,17	1.80	1 (6%)
9	MAN	J	5	9	11,11,12	1.18	2 (18%)	15,15,17	1.93	4 (26%)
9	NAG	J	6	9	14,14,15	1.65	3 (21%)	17,19,21	1.94	3 (17%)
10	NAG	K	1	10,6	14,14,15	1.26	2 (14%)	17,19,21	0.95	1 (5%)
10	NAG	K	2	10	14,14,15	1.53	4 (28%)	17,19,21	0.90	1 (5%)
10	BMA	K	3	10	11,11,12	1.38	2 (18%)	15,15,17	1.43	2 (13%)
10	NAG	K	4	10	14,14,15	1.27	2 (14%)	17,19,21	1.01	1 (5%)
7	NAG	L	1	6,7	14,14,15	1.36	2 (14%)	17,19,21	1.06	1 (5%)
7	NAG	L	2	7	14,14,15	1.37	3 (21%)	17,19,21	0.76	0
7	BMA	L	3	7	11,11,12	1.35	2 (18%)	15,15,17	1.06	1 (6%)
8	NAG	M	1	8,6	14,14,15	1.07	1 (7%)	17,19,21	1.08	0
8	NAG	M	2	8	14,14,15	1.10	1 (7%)	17,19,21	0.74	0
8	BMA	M	3	8	11,11,12	1.50	3 (27%)	15,15,17	1.33	2 (13%)
8	MAN	M	4	8	11,11,12	1.40	2 (18%)	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	M	5	8	11,11,12	1.28	2 (18%)	15,15,17	1.37	2 (13%)
11	NAG	N	1	6,11	14,14,15	1.31	2 (14%)	17,19,21	1.45	4 (23%)
11	NAG	N	2	11	14,14,15	1.24	2 (14%)	17,19,21	1.06	1 (5%)
7	NAG	O	1	7,5	14,14,15	1.31	2 (14%)	17,19,21	1.25	2 (11%)
7	NAG	O	2	7	14,14,15	1.64	4 (28%)	17,19,21	1.74	1 (5%)
7	BMA	O	3	7	11,11,12	1.39	2 (18%)	15,15,17	0.92	1 (6%)
8	NAG	P	1	8,6	14,14,15	1.16	2 (14%)	17,19,21	1.67	2 (11%)
8	NAG	P	2	8	14,14,15	1.38	4 (28%)	17,19,21	1.23	1 (5%)
8	BMA	P	3	8	11,11,12	1.24	2 (18%)	15,15,17	1.35	3 (20%)
8	MAN	P	4	8	11,11,12	1.19	2 (18%)	15,15,17	1.22	2 (13%)
8	MAN	P	5	8	11,11,12	1.35	2 (18%)	15,15,17	0.91	1 (6%)
9	NAG	Q	1	6,9	14,14,15	1.07	1 (7%)	17,19,21	0.71	0
9	NAG	Q	2	9	14,14,15	1.26	2 (14%)	17,19,21	1.10	1 (5%)
9	BMA	Q	3	9	11,11,12	1.89	4 (36%)	15,15,17	1.49	2 (13%)
9	MAN	Q	4	9	11,11,12	1.37	2 (18%)	15,15,17	1.70	2 (13%)
9	MAN	Q	5	9	11,11,12	1.26	2 (18%)	15,15,17	1.48	2 (13%)
9	NAG	Q	6	9	14,14,15	1.44	3 (21%)	17,19,21	1.77	2 (11%)
10	NAG	R	1	10,6	14,14,15	1.36	2 (14%)	17,19,21	0.91	0
10	NAG	R	2	10	14,14,15	1.39	2 (14%)	17,19,21	1.44	1 (5%)
10	BMA	R	3	10	11,11,12	1.40	3 (27%)	15,15,17	0.83	0
10	NAG	R	4	10	14,14,15	1.27	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	S	1	6,7	14,14,15	1.34	3 (21%)	17,19,21	0.66	0
7	NAG	S	2	7	14,14,15	1.40	4 (28%)	17,19,21	0.84	1 (5%)
7	BMA	S	3	7	11,11,12	1.32	2 (18%)	15,15,17	0.91	1 (6%)
8	NAG	T	1	8,6	14,14,15	1.33	3 (21%)	17,19,21	0.84	1 (5%)
8	NAG	T	2	8	14,14,15	1.38	3 (21%)	17,19,21	1.01	1 (5%)
8	BMA	T	3	8	11,11,12	1.50	2 (18%)	15,15,17	1.25	2 (13%)
8	MAN	T	4	8	11,11,12	1.39	2 (18%)	15,15,17	0.98	1 (6%)
8	MAN	T	5	8	11,11,12	1.40	2 (18%)	15,15,17	0.89	0
11	NAG	U	1	6,11	14,14,15	1.42	3 (21%)	17,19,21	1.54	3 (17%)
11	NAG	U	2	11	14,14,15	1.36	2 (14%)	17,19,21	0.89	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	A	2	7	-	0/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
8	NAG	B	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	B	2	8	-	0/6/23/26	0/1/1/1
8	BMA	B	3	8	-	1/2/19/22	0/1/1/1
8	MAN	B	4	8	-	0/2/19/22	0/1/1/1
8	MAN	B	5	8	-	0/2/19/22	0/1/1/1
9	NAG	C	1	6,9	-	0/6/23/26	0/1/1/1
9	NAG	C	2	9	-	0/6/23/26	0/1/1/1
9	BMA	C	3	9	-	0/2/19/22	0/1/1/1
9	MAN	C	4	9	-	1/2/19/22	0/1/1/1
9	MAN	C	5	9	-	1/2/19/22	0/1/1/1
9	NAG	C	6	9	-	2/6/23/26	0/1/1/1
10	NAG	D	1	10,6	-	2/6/23/26	0/1/1/1
10	NAG	D	2	10	-	0/6/23/26	0/1/1/1
10	BMA	D	3	10	-	0/2/19/22	0/1/1/1
10	NAG	D	4	10	-	2/6/23/26	0/1/1/1
7	NAG	E	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	0/6/23/26	0/1/1/1
7	BMA	E	3	7	-	0/2/19/22	0/1/1/1
8	NAG	F	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1
8	MAN	F	4	8	-	0/2/19/22	0/1/1/1
8	MAN	F	5	8	-	0/2/19/22	0/1/1/1
11	NAG	G	1	6,11	-	1/6/23/26	0/1/1/1
11	NAG	G	2	11	-	0/6/23/26	0/1/1/1
7	NAG	H	1	7,5	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	6,9	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	1/2/19/22	0/1/1/1
9	MAN	J	5	9	-	1/2/19/22	0/1/1/1
9	NAG	J	6	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	K	1	10,6	-	0/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	NAG	K	4	10	-	2/6/23/26	0/1/1/1
7	NAG	L	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	1/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1
8	MAN	M	5	8	-	0/2/19/22	0/1/1/1
11	NAG	N	1	6,11	-	1/6/23/26	0/1/1/1
11	NAG	N	2	11	-	0/6/23/26	0/1/1/1
7	NAG	O	1	7,5	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
8	NAG	P	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	BMA	P	3	8	-	0/2/19/22	0/1/1/1
8	MAN	P	4	8	-	0/2/19/22	0/1/1/1
8	MAN	P	5	8	-	0/2/19/22	0/1/1/1
9	NAG	Q	1	6,9	-	1/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Q	4	9	-	1/2/19/22	0/1/1/1
9	MAN	Q	5	9	-	1/2/19/22	0/1/1/1
9	NAG	Q	6	9	-	0/6/23/26	0/1/1/1
10	NAG	R	1	10,6	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	0/2/19/22	0/1/1/1
10	NAG	R	4	10	-	2/6/23/26	0/1/1/1
7	NAG	S	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	8,6	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
11	NAG	U	1	6,11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	U	2	11	-	0/6/23/26	0/1/1/1

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	3	BMA	O4-C4	3.93	1.52	1.43
9	J	6	NAG	O5-C5	3.72	1.51	1.43
9	J	6	NAG	O5-C1	3.65	1.49	1.43
9	C	3	BMA	O3-C3	3.57	1.51	1.43
9	J	3	BMA	O3-C3	3.41	1.51	1.43
9	C	6	NAG	O5-C5	3.41	1.50	1.43
9	J	2	NAG	O5-C5	3.36	1.50	1.43
7	O	2	NAG	C1-C2	3.33	1.57	1.52
8	I	2	NAG	C1-C2	3.32	1.57	1.52
9	Q	3	BMA	O3-C3	3.31	1.50	1.43
9	J	2	NAG	O4-C4	3.27	1.50	1.43
8	B	2	NAG	O4-C4	3.25	1.50	1.43
9	C	2	NAG	O5-C5	3.21	1.49	1.43
9	Q	6	NAG	O5-C5	3.08	1.49	1.43
9	Q	3	BMA	O4-C4	3.05	1.50	1.43
9	Q	6	NAG	O5-C1	3.03	1.48	1.43
9	C	3	BMA	O4-C4	3.00	1.50	1.43
8	I	1	NAG	O5-C5	2.97	1.49	1.43
9	C	6	NAG	O5-C1	2.97	1.48	1.43
8	P	5	MAN	O5-C5	2.94	1.49	1.43
8	I	4	MAN	O5-C1	2.93	1.48	1.43
7	H	1	NAG	O5-C5	2.92	1.49	1.43
8	T	5	MAN	O5-C5	2.92	1.49	1.43
11	U	2	NAG	O5-C5	2.91	1.49	1.43
8	T	3	BMA	O3-C3	2.91	1.49	1.43
8	F	3	BMA	O3-C3	2.90	1.49	1.43
10	D	4	NAG	O5-C5	2.89	1.49	1.43
8	I	2	NAG	O5-C1	2.89	1.48	1.43
8	M	4	MAN	O5-C5	2.87	1.49	1.43
10	D	1	NAG	O4-C4	2.87	1.49	1.43
8	I	3	BMA	O3-C3	2.85	1.49	1.43
7	L	3	BMA	O5-C5	2.84	1.49	1.43
10	D	1	NAG	O5-C5	2.84	1.49	1.43
9	Q	2	NAG	O5-C5	2.83	1.49	1.43
7	O	2	NAG	O5-C1	2.82	1.48	1.43
8	F	4	MAN	O5-C5	2.82	1.49	1.43
8	B	4	MAN	O5-C5	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	4	MAN	O5-C5	2.81	1.49	1.43
10	K	2	NAG	O4-C4	2.81	1.49	1.43
9	C	2	NAG	O4-C4	2.80	1.49	1.43
7	O	3	BMA	O5-C5	2.80	1.49	1.43
10	R	2	NAG	O4-C4	2.79	1.49	1.43
8	P	4	MAN	O5-C5	2.77	1.49	1.43
8	B	2	NAG	O5-C5	2.77	1.49	1.43
8	T	2	NAG	O5-C5	2.76	1.49	1.43
9	Q	4	MAN	O5-C1	2.75	1.48	1.43
8	B	1	NAG	O4-C4	2.74	1.49	1.43
9	Q	5	MAN	O5-C5	2.74	1.49	1.43
7	A	1	NAG	O5-C5	2.72	1.48	1.43
8	B	5	MAN	O5-C5	2.71	1.48	1.43
9	C	5	MAN	O5-C1	2.71	1.48	1.43
10	D	2	NAG	O4-C4	2.71	1.49	1.43
7	E	2	NAG	O5-C5	2.71	1.48	1.43
7	E	3	BMA	O5-C5	2.70	1.48	1.43
7	E	1	NAG	O5-C5	2.70	1.48	1.43
7	A	2	NAG	O5-C5	2.70	1.48	1.43
10	R	4	NAG	O5-C5	2.70	1.48	1.43
11	U	1	NAG	O5-C5	2.70	1.48	1.43
8	F	5	MAN	O5-C5	2.69	1.48	1.43
8	F	2	NAG	O5-C5	2.68	1.48	1.43
7	A	3	BMA	O5-C5	2.68	1.48	1.43
10	D	2	NAG	C1-C2	2.68	1.56	1.52
9	J	1	NAG	O4-C4	2.67	1.49	1.43
7	S	3	BMA	O5-C5	2.67	1.48	1.43
9	C	1	NAG	O5-C5	2.67	1.48	1.43
9	Q	2	NAG	O4-C4	2.66	1.49	1.43
7	S	2	NAG	O5-C5	2.66	1.48	1.43
8	B	3	BMA	O3-C3	2.66	1.49	1.43
11	G	2	NAG	O5-C1	2.65	1.47	1.43
10	K	1	NAG	O4-C4	2.64	1.49	1.43
9	J	3	BMA	O5-C5	2.63	1.48	1.43
7	O	1	NAG	O4-C4	2.63	1.49	1.43
10	K	4	NAG	O5-C5	2.63	1.48	1.43
9	J	5	MAN	O5-C1	2.62	1.47	1.43
8	F	3	BMA	O5-C5	2.61	1.48	1.43
11	N	1	NAG	C1-C2	2.60	1.56	1.52
8	M	3	BMA	O3-C3	2.60	1.49	1.43
7	O	2	NAG	O5-C5	2.59	1.48	1.43
8	I	1	NAG	O4-C4	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	5	MAN	O5-C1	2.58	1.47	1.43
7	H	3	BMA	O5-C5	2.58	1.48	1.43
10	K	3	BMA	O4-C4	2.57	1.49	1.43
10	D	3	BMA	O5-C5	2.57	1.48	1.43
8	M	1	NAG	O5-C5	2.56	1.48	1.43
8	P	2	NAG	O5-C5	2.55	1.48	1.43
7	A	1	NAG	O4-C4	2.55	1.49	1.43
9	Q	4	MAN	O5-C5	2.55	1.48	1.43
10	R	3	BMA	O5-C5	2.54	1.48	1.43
9	C	1	NAG	O4-C4	2.54	1.49	1.43
10	R	1	NAG	O4-C4	2.54	1.49	1.43
8	T	1	NAG	O5-C5	2.52	1.48	1.43
8	F	1	NAG	O5-C5	2.52	1.48	1.43
10	D	2	NAG	O5-C1	2.52	1.47	1.43
7	O	1	NAG	O5-C5	2.52	1.48	1.43
8	B	4	MAN	O5-C1	2.51	1.47	1.43
8	F	5	MAN	O5-C1	2.51	1.47	1.43
11	U	1	NAG	O4-C4	2.51	1.48	1.43
7	S	1	NAG	O5-C5	2.50	1.48	1.43
10	D	2	NAG	O5-C5	2.50	1.48	1.43
7	E	2	NAG	O5-C1	2.50	1.47	1.43
10	K	2	NAG	O5-C1	2.50	1.47	1.43
8	M	5	MAN	O5-C1	2.50	1.47	1.43
7	L	1	NAG	O5-C5	2.50	1.48	1.43
8	M	3	BMA	O5-C5	2.50	1.48	1.43
8	I	4	MAN	O5-C5	2.49	1.48	1.43
8	T	2	NAG	O4-C4	2.49	1.48	1.43
9	Q	3	BMA	O5-C5	2.49	1.48	1.43
8	B	2	NAG	O5-C1	2.48	1.47	1.43
8	M	5	MAN	O5-C5	2.47	1.48	1.43
7	L	1	NAG	O4-C4	2.47	1.48	1.43
11	G	1	NAG	C1-C2	2.46	1.56	1.52
11	N	1	NAG	O4-C4	2.46	1.48	1.43
7	H	2	NAG	O5-C5	2.46	1.48	1.43
10	K	2	NAG	C1-C2	2.46	1.56	1.52
11	N	2	NAG	O5-C5	2.45	1.48	1.43
8	P	3	BMA	O3-C3	2.45	1.48	1.43
10	D	3	BMA	O4-C4	2.44	1.48	1.43
9	C	4	MAN	O5-C5	2.44	1.48	1.43
8	T	5	MAN	O5-C1	2.44	1.47	1.43
10	K	1	NAG	O5-C5	2.43	1.48	1.43
8	M	4	MAN	O5-C1	2.43	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	1	NAG	O4-C4	2.43	1.48	1.43
9	J	4	MAN	O5-C5	2.43	1.48	1.43
9	J	1	NAG	O5-C5	2.42	1.48	1.43
8	T	1	NAG	C1-C2	2.42	1.55	1.52
7	H	2	NAG	O5-C1	2.41	1.47	1.43
9	J	4	MAN	O5-C1	2.40	1.47	1.43
8	T	4	MAN	O5-C1	2.40	1.47	1.43
7	L	2	NAG	O4-C4	2.39	1.48	1.43
11	G	1	NAG	O4-C4	2.39	1.48	1.43
7	O	2	NAG	O4-C4	2.39	1.48	1.43
11	U	2	NAG	O5-C1	2.39	1.47	1.43
7	A	2	NAG	O4-C4	2.38	1.48	1.43
8	P	2	NAG	C1-C2	2.37	1.55	1.52
9	J	5	MAN	O5-C5	2.36	1.48	1.43
7	A	2	NAG	O5-C1	2.36	1.47	1.43
7	L	2	NAG	O5-C5	2.35	1.48	1.43
9	C	4	MAN	O5-C1	2.35	1.47	1.43
9	Q	5	MAN	O5-C1	2.34	1.47	1.43
10	R	1	NAG	O5-C5	2.34	1.48	1.43
10	K	2	NAG	O5-C5	2.33	1.48	1.43
10	K	3	BMA	O5-C5	2.32	1.48	1.43
7	E	2	NAG	O4-C4	2.32	1.48	1.43
7	S	3	BMA	O5-C1	2.31	1.47	1.43
8	I	3	BMA	O5-C5	2.30	1.48	1.43
7	L	3	BMA	O5-C1	2.30	1.47	1.43
7	O	3	BMA	O5-C1	2.30	1.47	1.43
9	C	5	MAN	O5-C5	2.29	1.48	1.43
9	C	3	BMA	O5-C5	2.29	1.48	1.43
10	R	2	NAG	O5-C5	2.29	1.48	1.43
8	B	5	MAN	O5-C1	2.29	1.47	1.43
8	B	1	NAG	O5-C5	2.27	1.48	1.43
7	H	3	BMA	O5-C1	2.27	1.47	1.43
11	N	2	NAG	O5-C1	2.27	1.47	1.43
7	H	1	NAG	O4-C4	2.27	1.48	1.43
7	E	2	NAG	C1-C2	2.26	1.55	1.52
7	S	2	NAG	O5-C1	2.26	1.47	1.43
7	E	3	BMA	O5-C1	2.24	1.47	1.43
8	P	1	NAG	O5-C5	2.24	1.48	1.43
8	M	3	BMA	O5-C1	2.24	1.47	1.43
11	G	1	NAG	O5-C5	2.24	1.48	1.43
10	R	3	BMA	O5-C1	2.24	1.47	1.43
7	H	2	NAG	O4-C4	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4	MAN	O5-C1	2.22	1.47	1.43
9	J	6	NAG	C1-C2	2.22	1.55	1.52
8	P	4	MAN	O5-C1	2.22	1.47	1.43
8	F	2	NAG	O4-C4	2.22	1.48	1.43
7	L	2	NAG	O5-C1	2.22	1.47	1.43
8	F	1	NAG	O5-C1	2.22	1.47	1.43
8	F	1	NAG	O4-C4	2.21	1.48	1.43
7	S	2	NAG	O4-C4	2.21	1.48	1.43
8	M	2	NAG	O5-C5	2.19	1.47	1.43
10	D	4	NAG	O5-C1	2.19	1.47	1.43
7	A	3	BMA	O5-C1	2.19	1.47	1.43
7	S	1	NAG	O4-C4	2.18	1.48	1.43
8	F	1	NAG	C1-C2	2.17	1.55	1.52
11	U	1	NAG	C1-C2	2.16	1.55	1.52
8	T	3	BMA	O5-C5	2.15	1.47	1.43
8	P	2	NAG	O5-C1	2.15	1.47	1.43
9	J	3	BMA	C2-C3	2.14	1.55	1.52
10	R	3	BMA	O4-C4	2.12	1.48	1.43
7	A	1	NAG	O5-C1	2.12	1.47	1.43
8	I	5	MAN	O5-C5	2.11	1.47	1.43
8	P	2	NAG	O4-C4	2.11	1.47	1.43
11	G	2	NAG	O5-C5	2.11	1.47	1.43
10	D	3	BMA	O5-C1	2.10	1.47	1.43
9	J	2	NAG	O5-C1	2.10	1.47	1.43
8	I	2	NAG	O5-C5	2.09	1.47	1.43
8	T	2	NAG	O5-C1	2.09	1.47	1.43
7	S	1	NAG	C1-C2	2.08	1.55	1.52
8	T	1	NAG	O4-C4	2.07	1.47	1.43
7	E	1	NAG	O4-C4	2.06	1.47	1.43
7	H	1	NAG	O5-C1	2.05	1.47	1.43
9	Q	3	BMA	C2-C3	2.05	1.55	1.52
9	J	3	BMA	C4-C3	2.05	1.57	1.52
9	Q	6	NAG	C1-C2	2.04	1.55	1.52
9	Q	1	NAG	O5-C5	2.04	1.47	1.43
8	P	3	BMA	O5-C5	2.03	1.47	1.43
10	K	4	NAG	C1-C2	2.03	1.55	1.52
8	I	2	NAG	O4-C4	2.03	1.47	1.43
7	S	2	NAG	C1-C2	2.03	1.55	1.52
8	I	1	NAG	C1-C2	2.03	1.55	1.52
7	H	2	NAG	C1-C2	2.01	1.55	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	2	NAG	C1-O5-C5	6.52	121.02	112.19
9	J	6	NAG	C1-O5-C5	6.17	120.55	112.19
9	J	4	MAN	C1-O5-C5	5.96	120.27	112.19
9	Q	6	NAG	C1-O5-C5	5.42	119.54	112.19
9	Q	4	MAN	C1-O5-C5	5.40	119.52	112.19
10	R	2	NAG	C1-O5-C5	5.33	119.41	112.19
8	P	1	NAG	C1-O5-C5	5.26	119.32	112.19
8	I	2	NAG	C1-O5-C5	5.07	119.06	112.19
8	F	5	MAN	C1-O5-C5	5.04	119.03	112.19
9	J	5	MAN	C1-O5-C5	5.02	119.00	112.19
9	C	6	NAG	O5-C1-C2	-4.81	103.69	111.29
7	H	1	NAG	C1-O5-C5	4.81	118.71	112.19
9	C	6	NAG	C1-O5-C5	4.81	118.71	112.19
8	B	5	MAN	C1-O5-C5	4.71	118.57	112.19
7	H	2	NAG	C1-O5-C5	4.67	118.52	112.19
9	C	4	MAN	C1-O5-C5	4.55	118.35	112.19
8	P	2	NAG	C1-O5-C5	4.54	118.34	112.19
8	B	1	NAG	C1-O5-C5	4.30	118.01	112.19
9	C	5	MAN	C1-O5-C5	4.28	118.00	112.19
8	B	4	MAN	C1-C2-C3	4.17	114.79	109.67
8	I	4	MAN	C1-C2-C3	4.05	114.64	109.67
9	J	3	BMA	C3-C4-C5	-3.91	103.26	110.24
9	J	3	BMA	C1-C2-C3	3.86	114.42	109.67
8	B	4	MAN	C1-O5-C5	3.86	117.42	112.19
9	Q	6	NAG	O5-C1-C2	-3.79	105.31	111.29
8	B	2	NAG	C1-O5-C5	3.78	117.32	112.19
7	A	2	NAG	C1-O5-C5	3.71	117.22	112.19
11	G	2	NAG	C1-O5-C5	3.69	117.19	112.19
9	C	3	BMA	C1-C2-C3	3.63	114.13	109.67
8	M	3	BMA	C1-O5-C5	3.63	117.11	112.19
11	N	2	NAG	C1-O5-C5	3.57	117.03	112.19
10	D	2	NAG	C1-O5-C5	3.57	117.02	112.19
9	C	2	NAG	O5-C1-C2	-3.56	105.67	111.29
10	K	3	BMA	C1-O5-C5	3.54	116.99	112.19
9	Q	5	MAN	C1-O5-C5	3.49	116.92	112.19
9	J	2	NAG	C1-O5-C5	3.41	116.81	112.19
11	U	1	NAG	C1-O5-C5	3.37	116.76	112.19
8	M	5	MAN	C1-C2-C3	3.33	113.77	109.67
7	O	1	NAG	C3-C4-C5	3.32	116.17	110.24
11	U	1	NAG	O4-C4-C3	-3.28	102.77	110.35
9	Q	5	MAN	C1-C2-C3	3.27	113.68	109.67
9	Q	3	BMA	C3-C4-C5	-3.20	104.53	110.24
8	T	4	MAN	C1-O5-C5	3.10	116.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	4	MAN	C1-O5-C5	3.03	116.30	112.19
8	P	1	NAG	C4-C3-C2	3.03	115.46	111.02
7	L	3	BMA	C1-O5-C5	2.93	116.16	112.19
8	M	5	MAN	C1-O5-C5	2.92	116.14	112.19
8	T	2	NAG	C1-O5-C5	2.92	116.14	112.19
9	Q	2	NAG	O5-C1-C2	-2.91	106.69	111.29
8	P	5	MAN	C1-O5-C5	2.91	116.13	112.19
10	K	4	NAG	C1-O5-C5	2.88	116.10	112.19
9	J	5	MAN	C1-C2-C3	2.87	113.19	109.67
8	F	5	MAN	C1-C2-C3	2.84	113.16	109.67
9	J	6	NAG	O5-C1-C2	-2.83	106.82	111.29
10	K	3	BMA	C1-C2-C3	2.77	113.07	109.67
7	E	2	NAG	C1-O5-C5	2.76	115.93	112.19
8	F	3	BMA	C1-O5-C5	2.76	115.92	112.19
9	J	2	NAG	O5-C1-C2	-2.71	107.01	111.29
9	J	3	BMA	O5-C1-C2	-2.69	106.62	110.77
9	Q	4	MAN	C1-C2-C3	2.67	112.95	109.67
9	J	5	MAN	O3-C3-C4	-2.66	104.20	110.35
9	J	5	MAN	C2-C3-C4	2.57	115.34	110.89
7	L	1	NAG	O5-C1-C2	-2.56	107.24	111.29
10	D	4	NAG	C1-O5-C5	2.55	115.65	112.19
8	P	3	BMA	C3-C4-C5	2.53	114.76	110.24
8	I	4	MAN	C1-O5-C5	2.53	115.61	112.19
7	O	3	BMA	C1-O5-C5	2.52	115.60	112.19
10	R	4	NAG	C1-O5-C5	2.52	115.60	112.19
8	T	1	NAG	C1-O5-C5	2.51	115.59	112.19
7	A	3	BMA	C1-O5-C5	2.50	115.59	112.19
11	N	1	NAG	C1-C2-N2	-2.50	106.22	110.49
10	K	1	NAG	O5-C1-C2	-2.49	107.36	111.29
8	I	5	MAN	C1-C2-C3	2.46	112.69	109.67
7	S	3	BMA	C1-O5-C5	2.45	115.52	112.19
8	M	4	MAN	C1-O5-C5	2.45	115.51	112.19
9	C	6	NAG	C1-C2-N2	2.41	114.60	110.49
9	C	3	BMA	O4-C4-C3	2.40	115.91	110.35
8	I	1	NAG	O4-C4-C5	2.39	115.24	109.30
7	H	1	NAG	O4-C4-C5	2.39	115.23	109.30
11	G	1	NAG	C1-O5-C5	2.38	115.42	112.19
8	B	3	BMA	O3-C3-C4	-2.37	104.87	110.35
8	P	3	BMA	O3-C3-C4	-2.34	104.93	110.35
8	T	3	BMA	O5-C1-C2	-2.34	107.16	110.77
9	C	3	BMA	O5-C1-C2	-2.34	107.16	110.77
9	J	1	NAG	C4-C3-C2	2.31	114.41	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	3	BMA	O3-C3-C4	2.30	115.67	110.35
7	O	1	NAG	C4-C3-C2	2.29	114.38	111.02
8	B	2	NAG	C3-C4-C5	-2.29	106.15	110.24
8	P	4	MAN	O4-C4-C3	-2.29	105.06	110.35
9	J	3	BMA	O4-C4-C3	2.27	115.59	110.35
8	I	5	MAN	C6-C5-C4	2.26	118.31	113.00
11	N	1	NAG	C2-N2-C7	2.26	126.12	122.90
7	S	2	NAG	C1-O5-C5	2.25	115.25	112.19
11	N	1	NAG	O4-C4-C5	-2.25	103.70	109.30
8	T	3	BMA	O6-C6-C5	-2.22	103.68	111.29
11	N	1	NAG	C1-O5-C5	2.18	115.14	112.19
8	F	4	MAN	C1-O5-C5	2.15	115.11	112.19
9	C	4	MAN	C1-C2-C3	2.14	112.30	109.67
11	U	2	NAG	C1-O5-C5	2.14	115.09	112.19
8	P	3	BMA	C1-O5-C5	2.13	115.08	112.19
10	K	2	NAG	C1-O5-C5	2.10	115.03	112.19
8	M	3	BMA	C3-C4-C5	2.09	113.97	110.24
8	B	3	BMA	C1-O5-C5	2.09	115.02	112.19
9	J	3	BMA	C1-O5-C5	2.08	115.01	112.19
9	C	6	NAG	O4-C4-C3	-2.07	105.56	110.35
8	B	4	MAN	O2-C2-C3	-2.07	105.99	110.14
9	J	6	NAG	C3-C4-C5	-2.07	106.55	110.24
7	E	1	NAG	O5-C1-C2	-2.07	108.02	111.29
7	E	3	BMA	C1-O5-C5	2.05	114.97	112.19
11	U	1	NAG	C4-C3-C2	2.02	113.98	111.02
9	J	3	BMA	C6-C5-C4	2.01	117.71	113.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1	NAG	C1-C2-N2-C7
9	Q	3	BMA	O5-C5-C6-O6
9	Q	3	BMA	C4-C5-C6-O6
9	Q	4	MAN	O5-C5-C6-O6
9	J	6	NAG	O5-C5-C6-O6
9	C	6	NAG	O5-C5-C6-O6
9	Q	5	MAN	O5-C5-C6-O6
9	C	5	MAN	O5-C5-C6-O6
9	J	4	MAN	O5-C5-C6-O6
9	J	5	MAN	O5-C5-C6-O6
9	C	4	MAN	O5-C5-C6-O6

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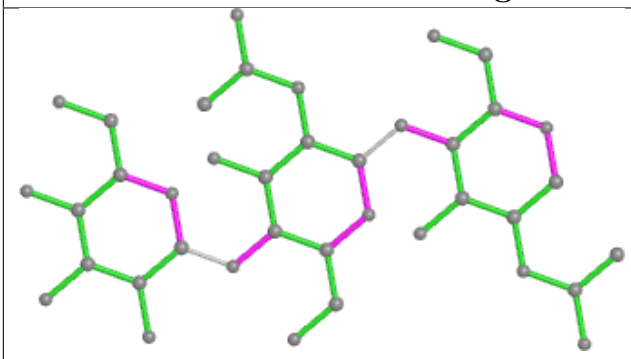
Mol	Chain	Res	Type	Atoms
9	J	6	NAG	C3-C2-N2-C7
10	D	1	NAG	C4-C5-C6-O6
11	N	1	NAG	C1-C2-N2-C7
8	F	1	NAG	C3-C2-N2-C7
8	I	1	NAG	C3-C2-N2-C7
9	C	6	NAG	C3-C2-N2-C7
10	D	4	NAG	C3-C2-N2-C7
10	K	4	NAG	C3-C2-N2-C7
11	G	1	NAG	C3-C2-N2-C7
11	U	1	NAG	C3-C2-N2-C7
10	D	1	NAG	O5-C5-C6-O6
8	B	3	BMA	C4-C5-C6-O6
8	T	1	NAG	C1-C2-N2-C7
8	M	3	BMA	C4-C5-C6-O6
11	U	1	NAG	C1-C2-N2-C7
9	Q	1	NAG	O5-C5-C6-O6
10	R	4	NAG	C1-C2-N2-C7
8	P	1	NAG	C1-C2-N2-C7
8	T	1	NAG	C3-C2-N2-C7
10	R	4	NAG	C3-C2-N2-C7
10	D	4	NAG	C1-C2-N2-C7
7	A	1	NAG	C4-C5-C6-O6
10	K	4	NAG	C1-C2-N2-C7

There are no ring outliers.

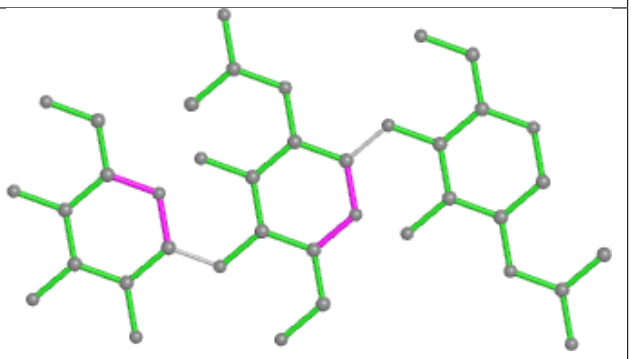
No monomer is involved in short contacts.

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

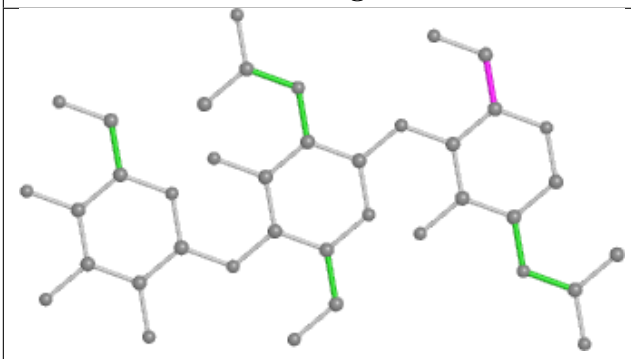
Oligosaccharide Chain A



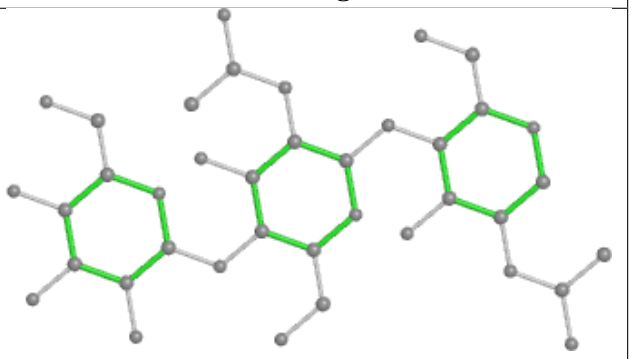
Bond lengths



Bond angles

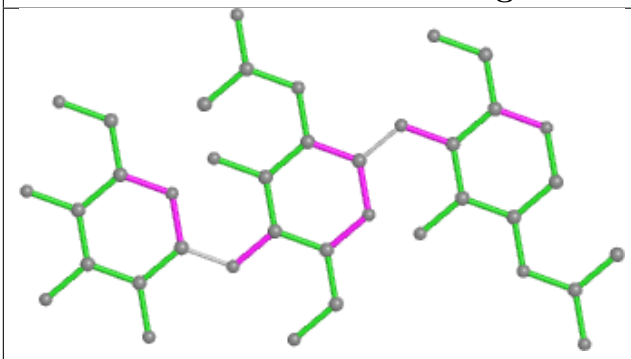


Torsions

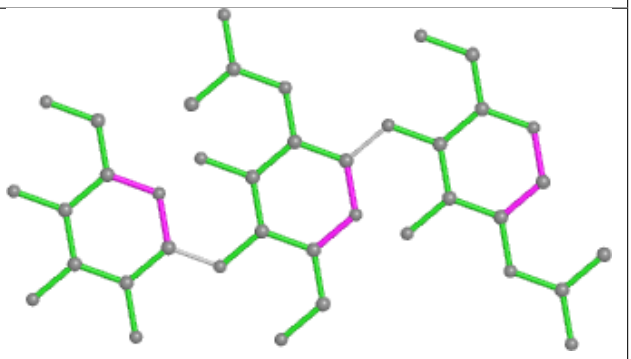


Rings

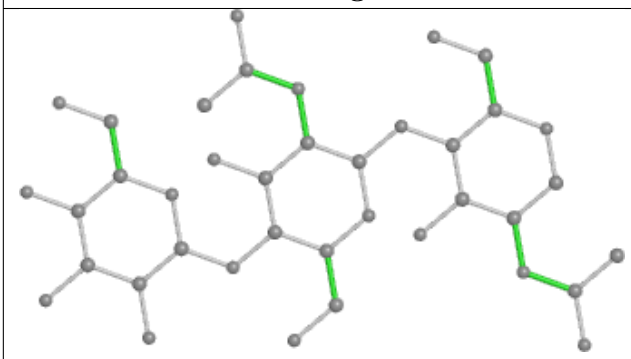
Oligosaccharide Chain E



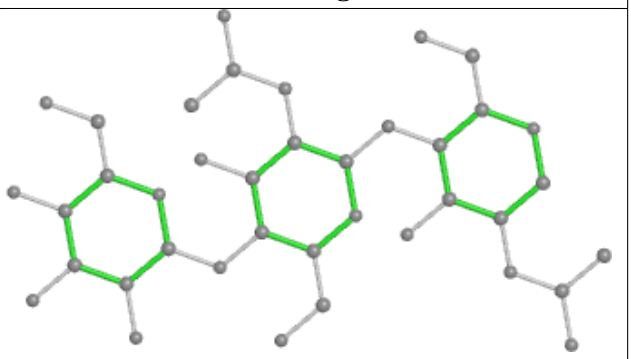
Bond lengths



Bond angles

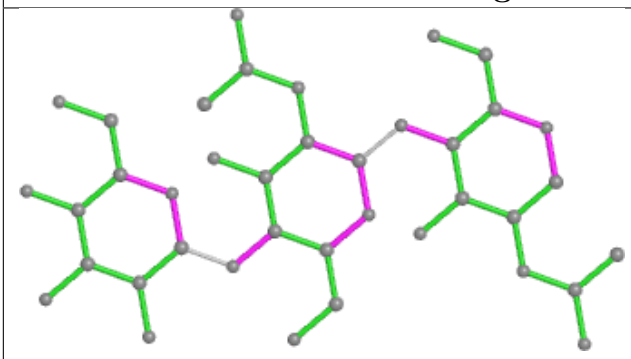


Torsions

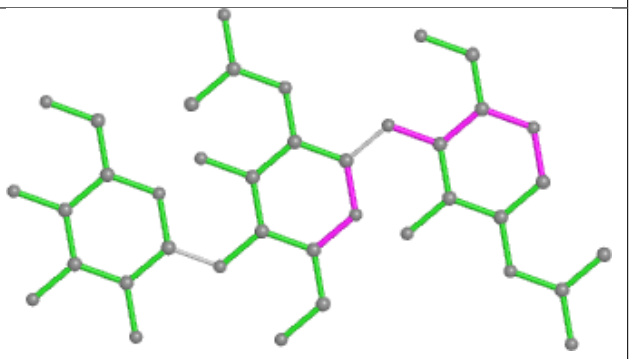


Rings

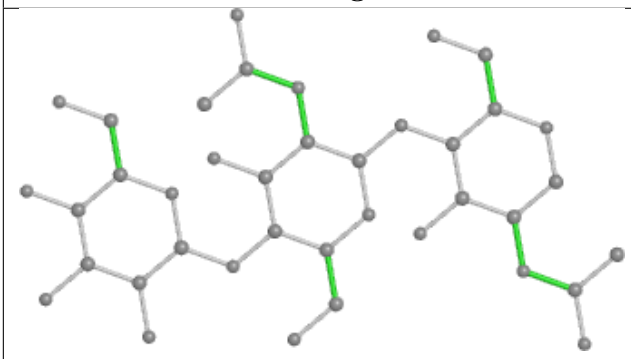
Oligosaccharide Chain H



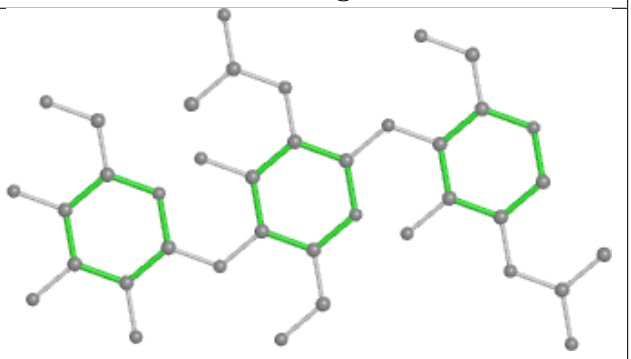
Bond lengths



Bond angles

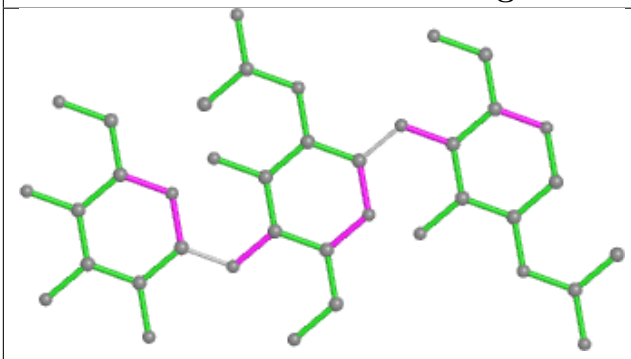


Torsions

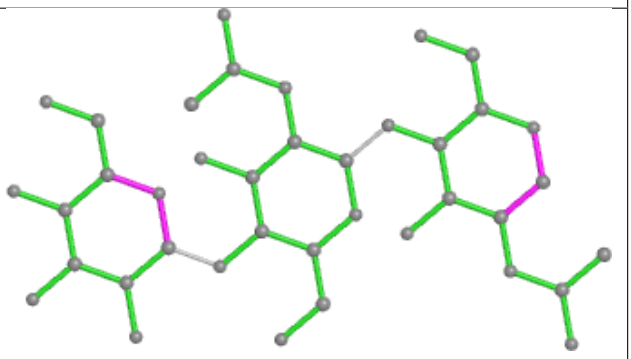


Rings

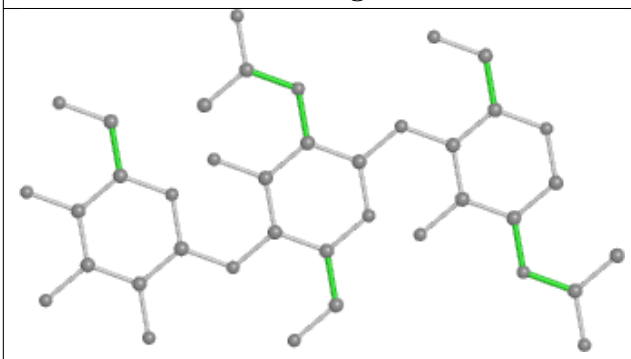
Oligosaccharide Chain L



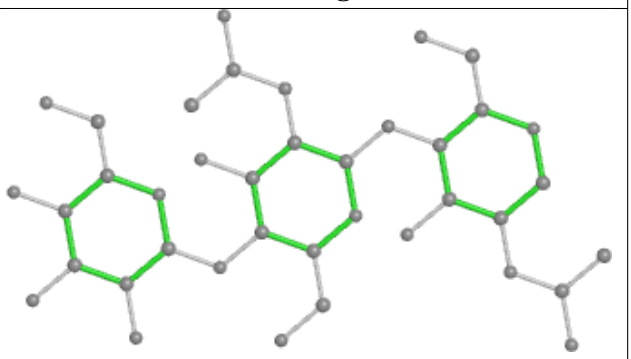
Bond lengths



Bond angles

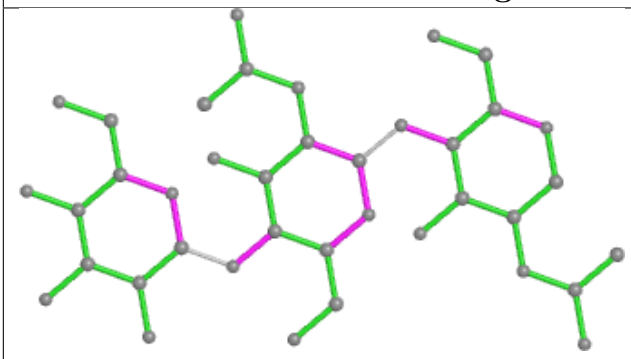


Torsions

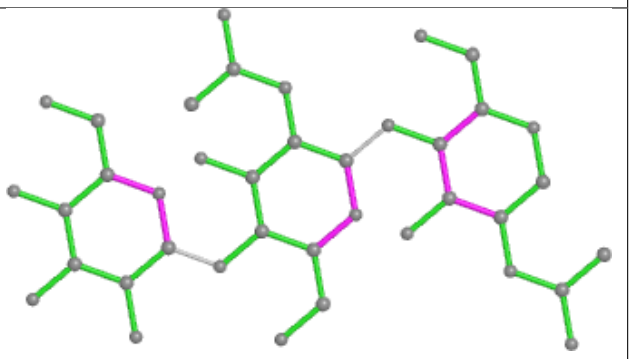


Rings

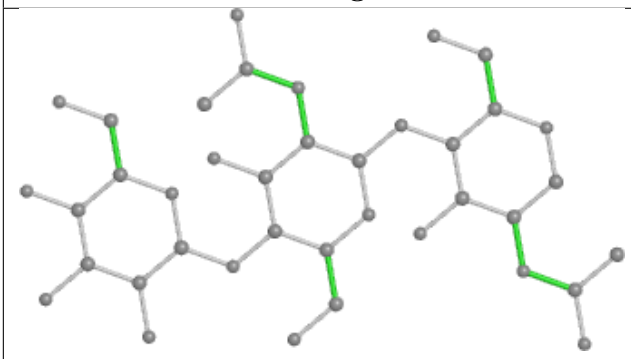
Oligosaccharide Chain O



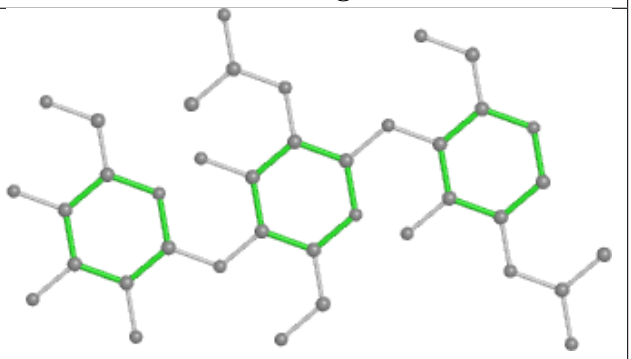
Bond lengths



Bond angles

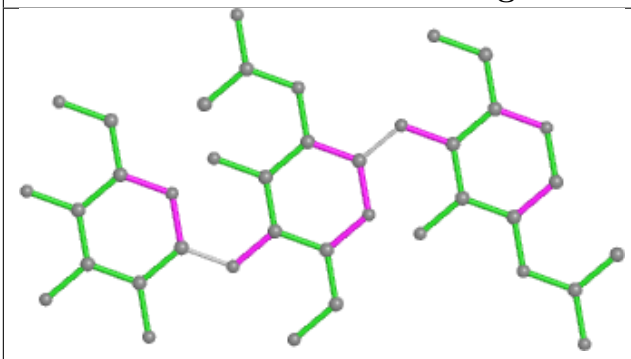


Torsions

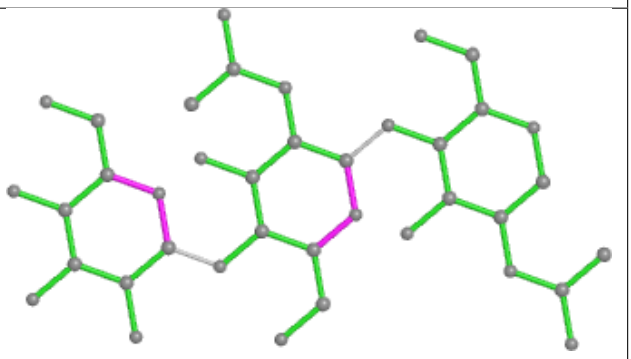


Rings

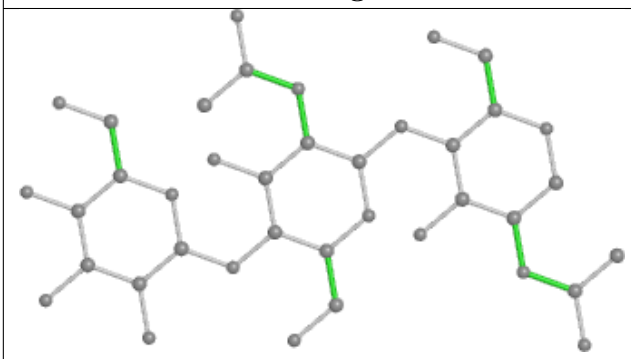
Oligosaccharide Chain S



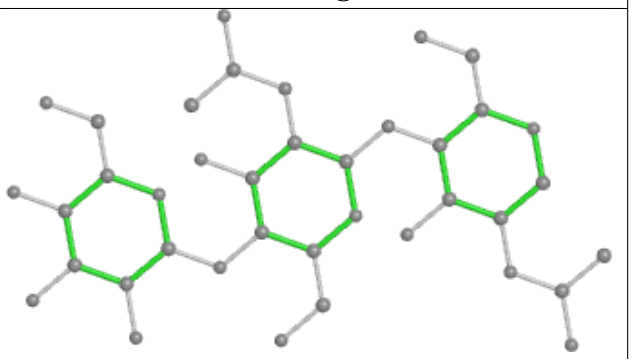
Bond lengths



Bond angles

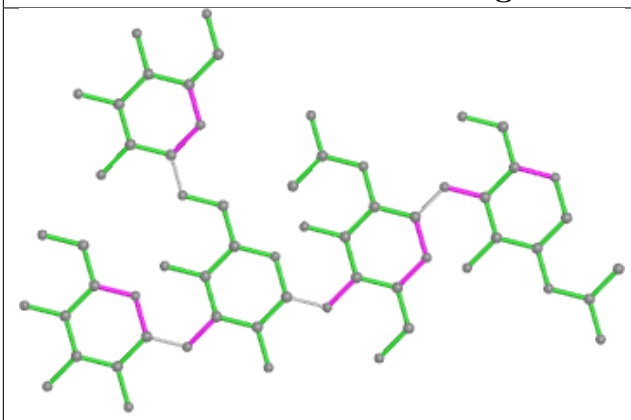


Torsions

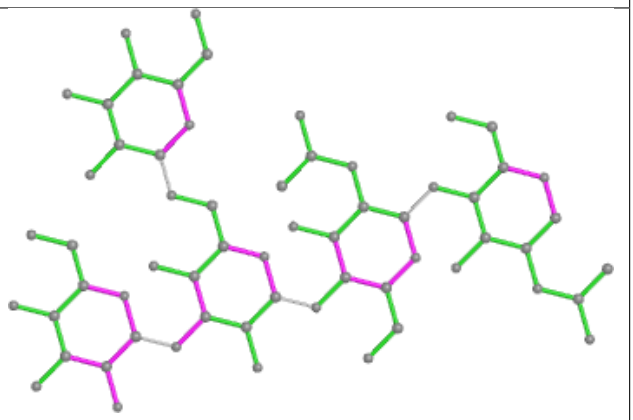


Rings

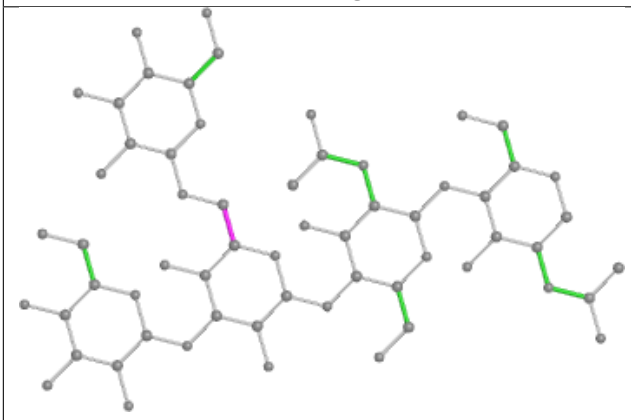
Oligosaccharide Chain B



Bond lengths



Bond angles



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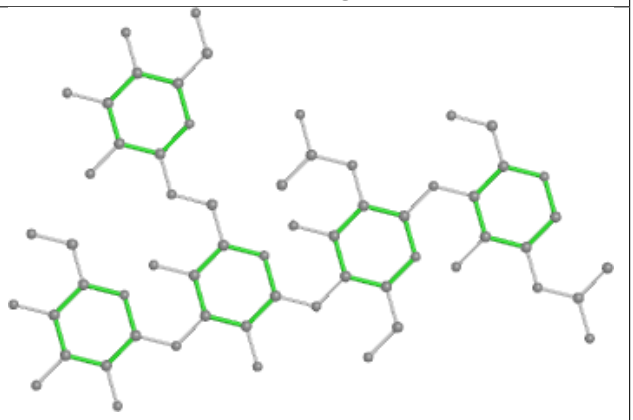
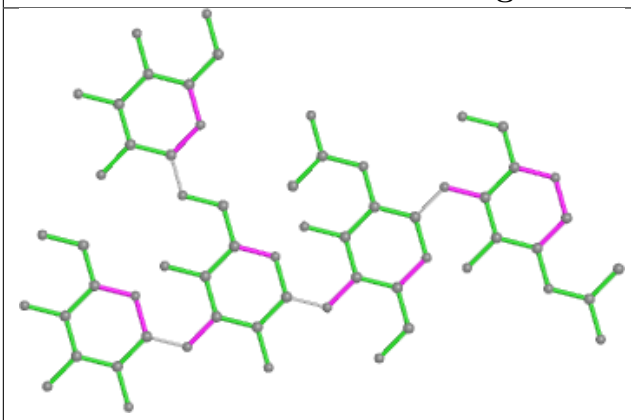
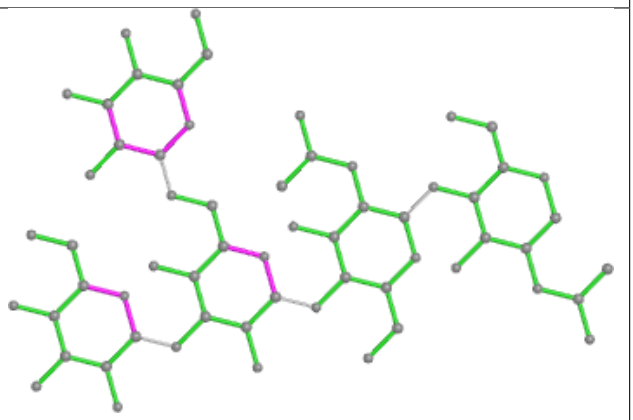


Rings

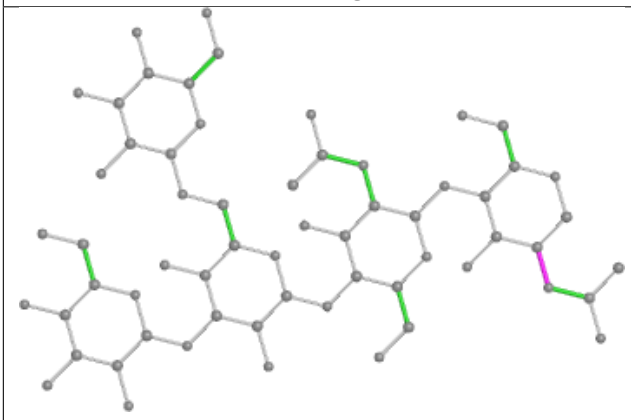
Oligosaccharide Chain F



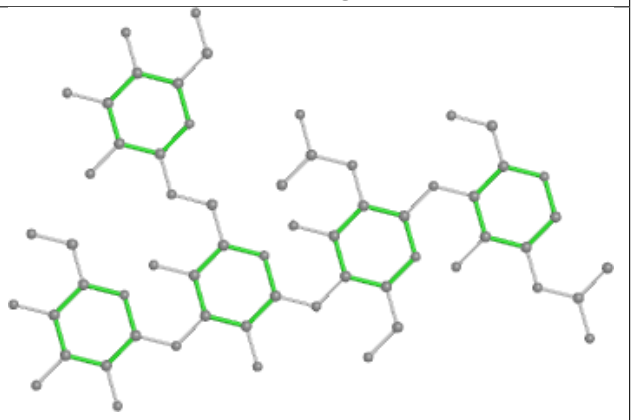
Bond lengths



Bond angles

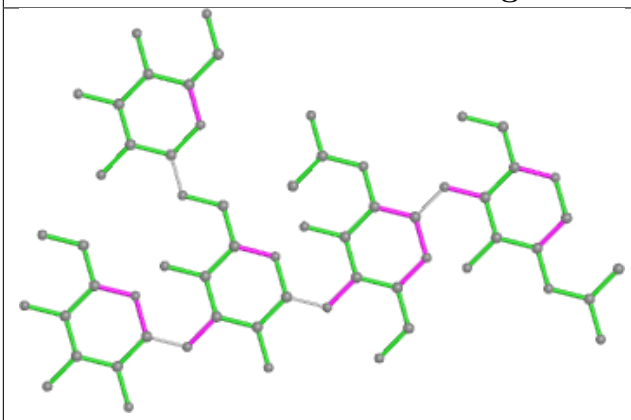


Torsions

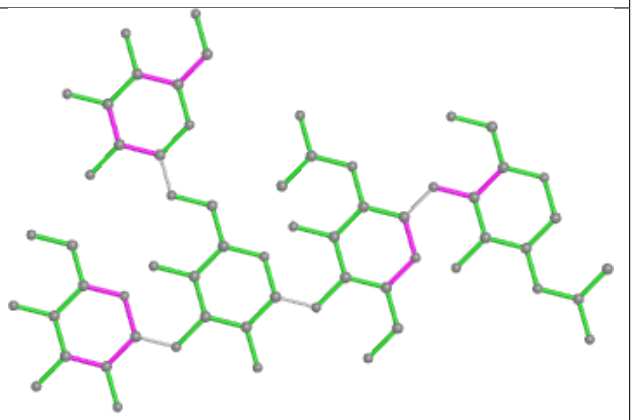


Rings

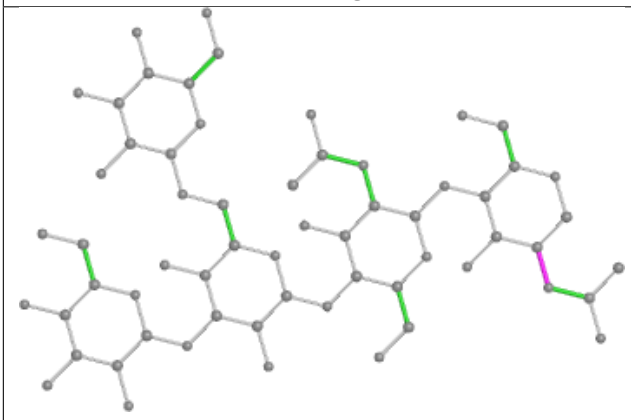
Oligosaccharide Chain I



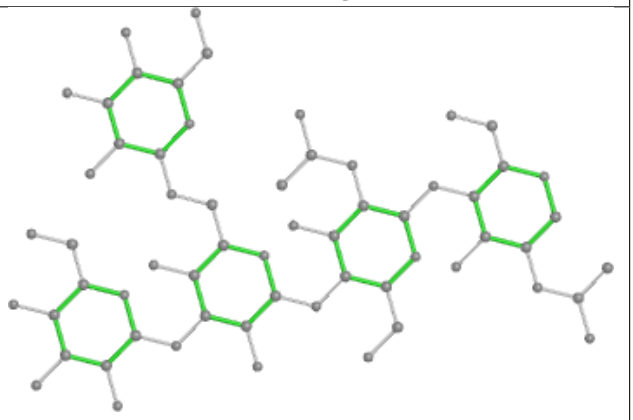
Bond lengths



Bond angles

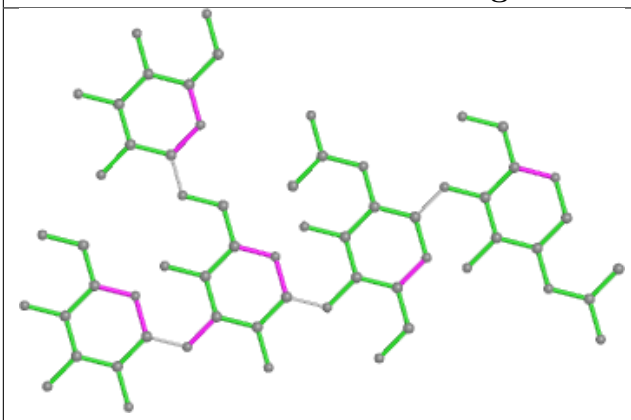


Torsions

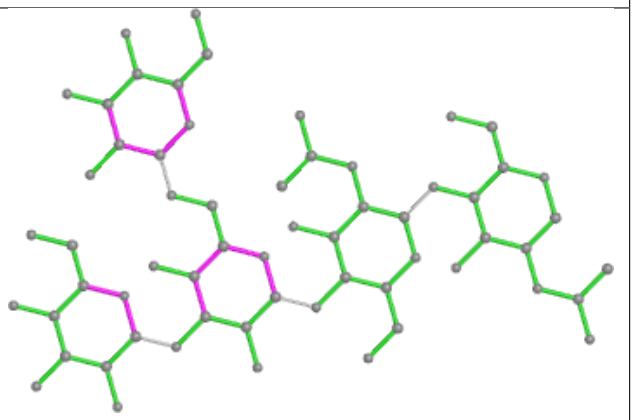


Rings

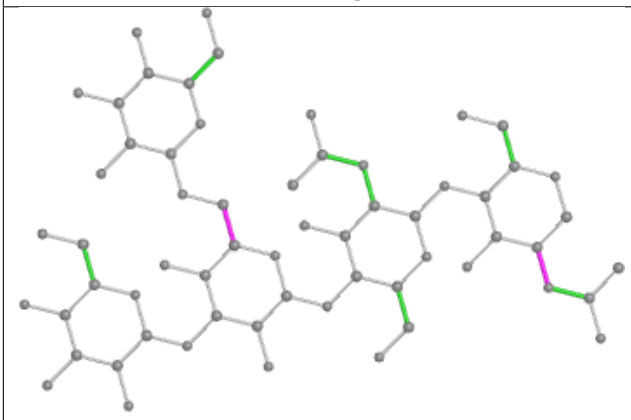
Oligosaccharide Chain M



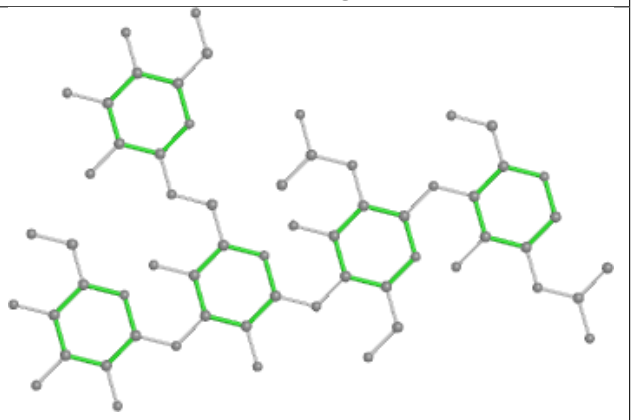
Bond lengths



Bond angles

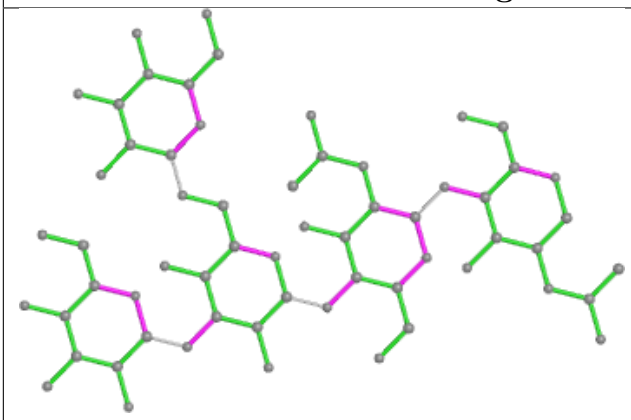


Torsions

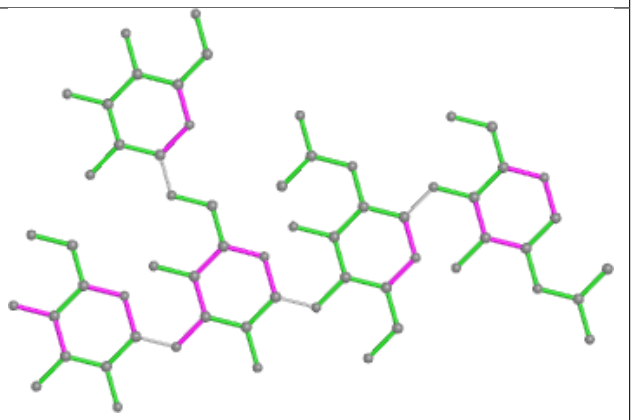


Rings

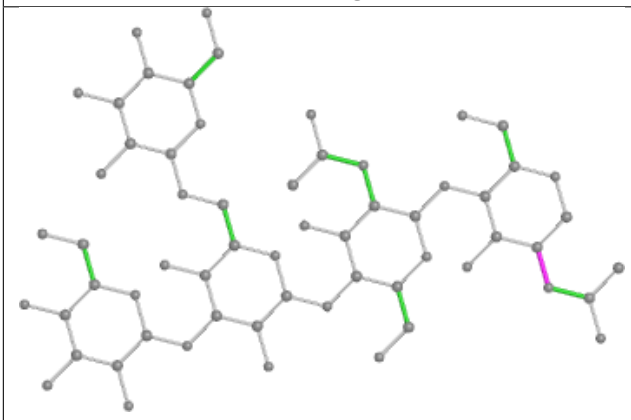
Oligosaccharide Chain P



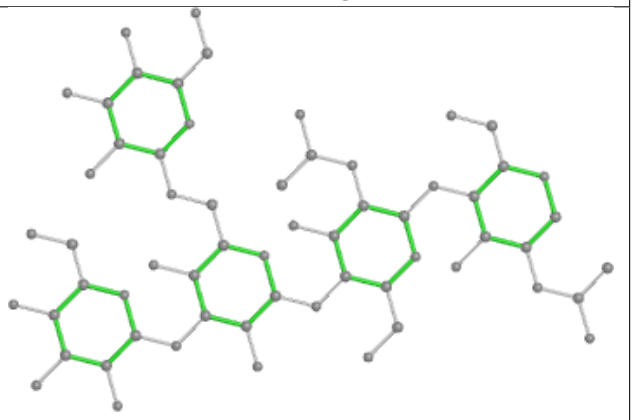
Bond lengths



Bond angles

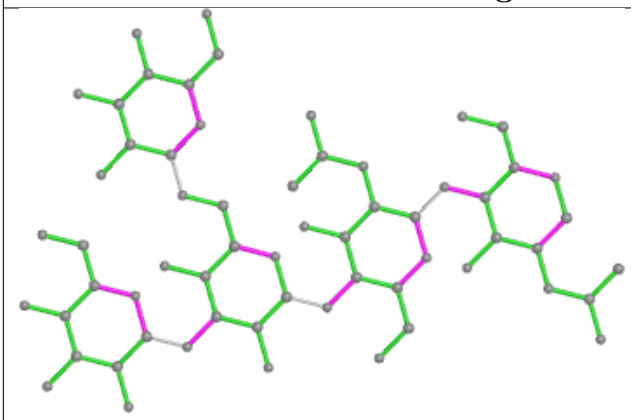


Torsions

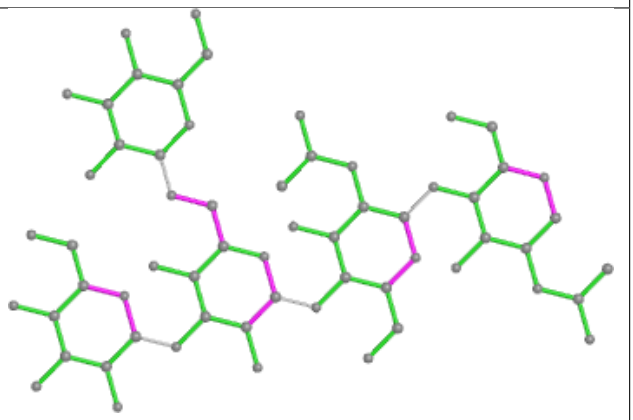


Rings

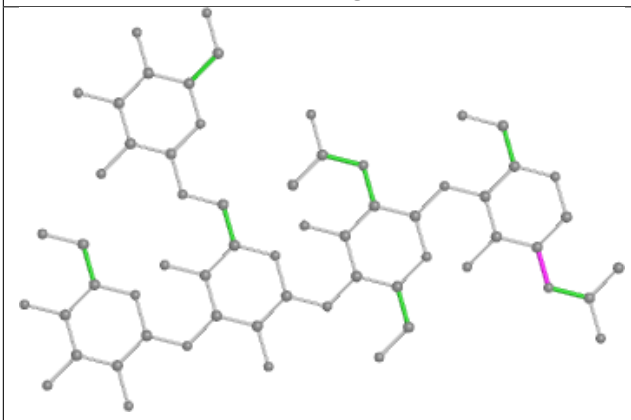
Oligosaccharide Chain T



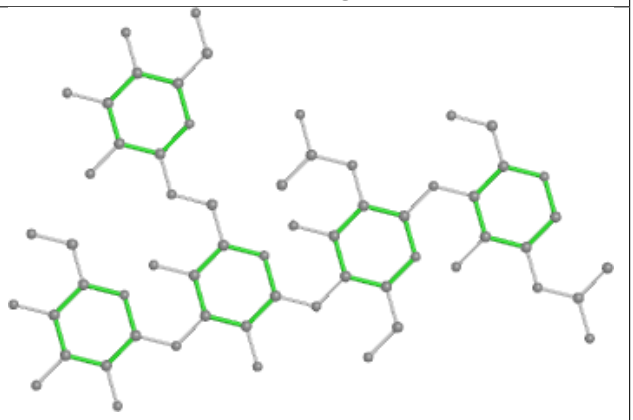
Bond lengths



Bond angles

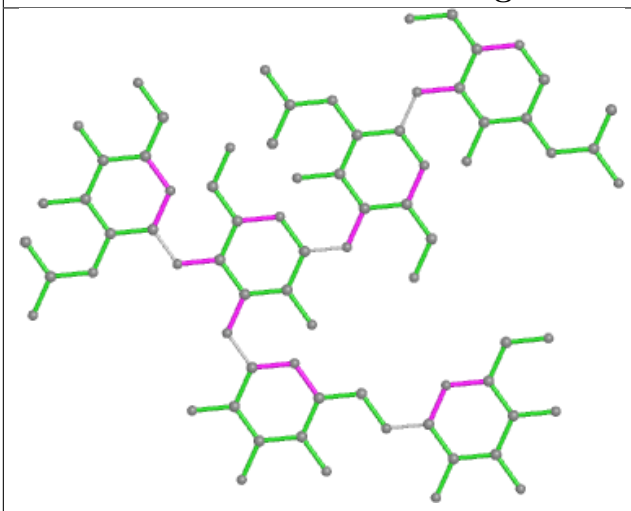


Torsions

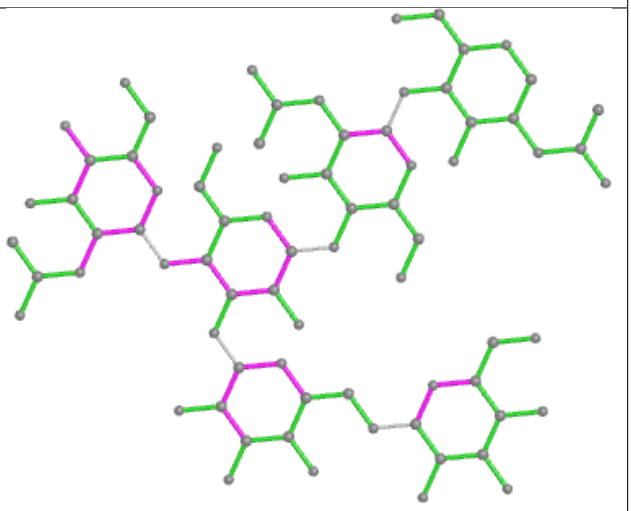


Rings

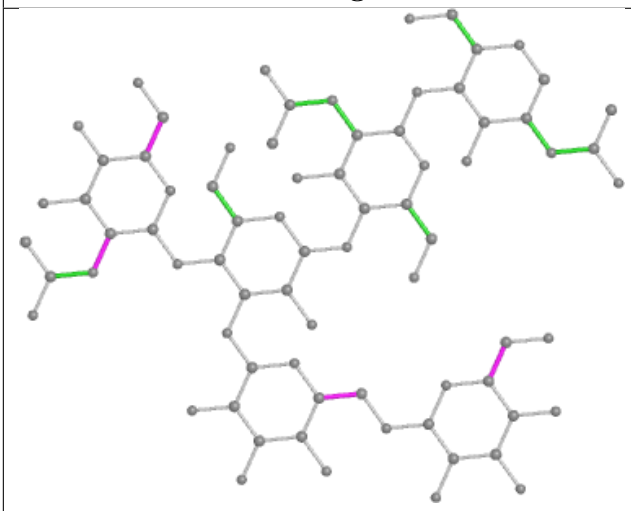
Oligosaccharide Chain C



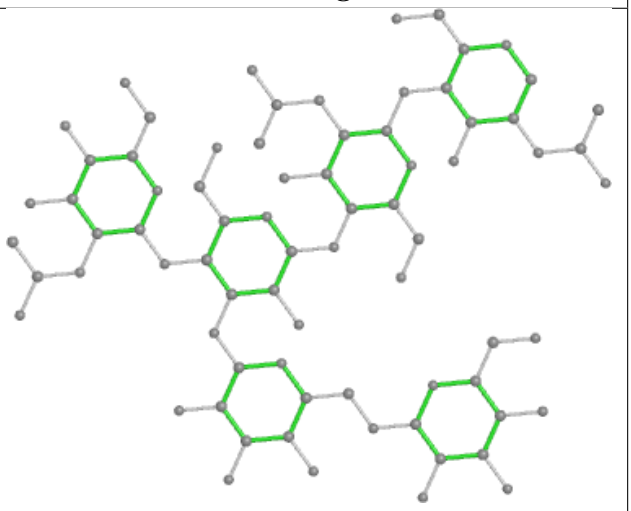
Bond lengths



Bond angles

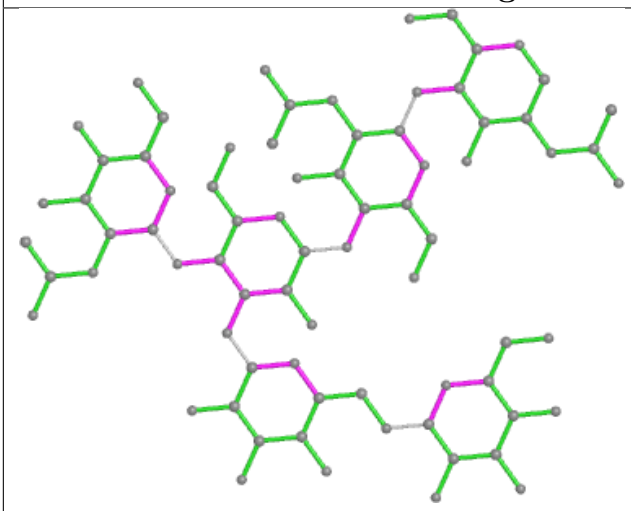


Torsions

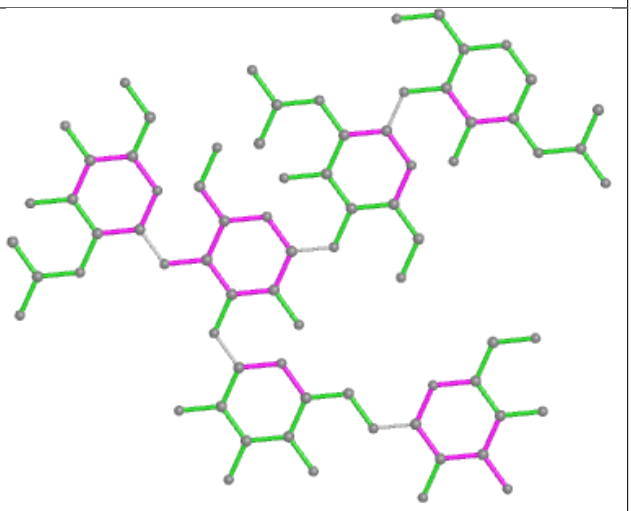


Rings

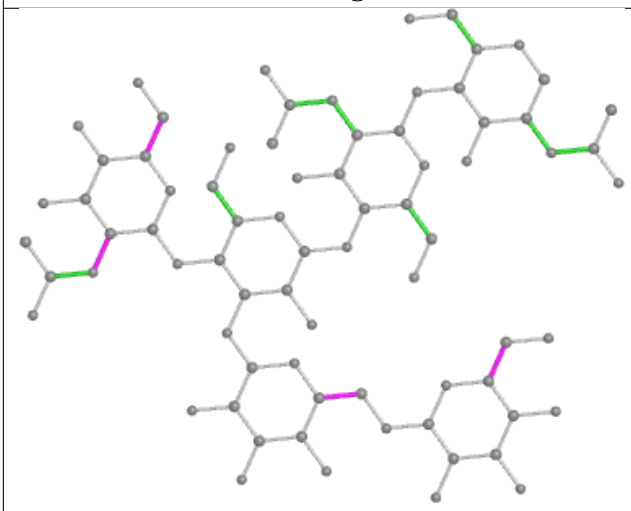
Oligosaccharide Chain J



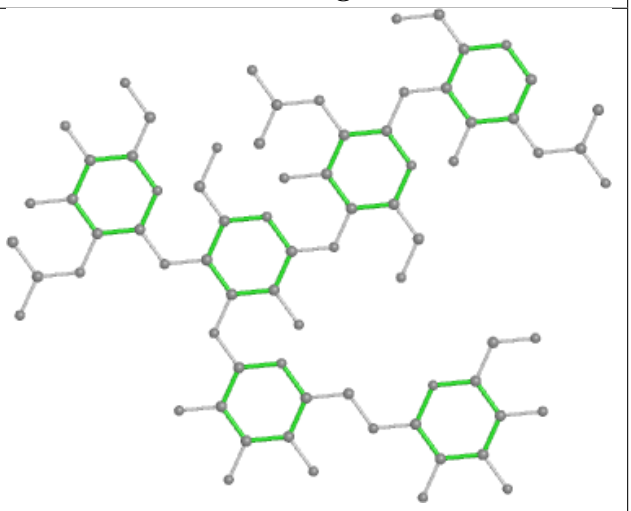
Bond lengths



Bond angles

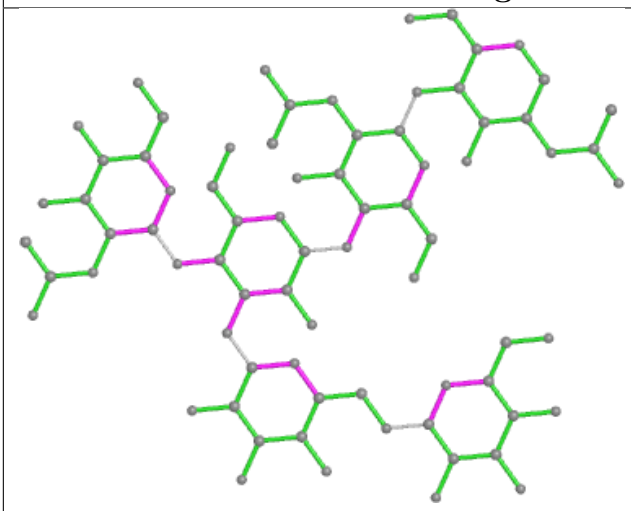


Torsions

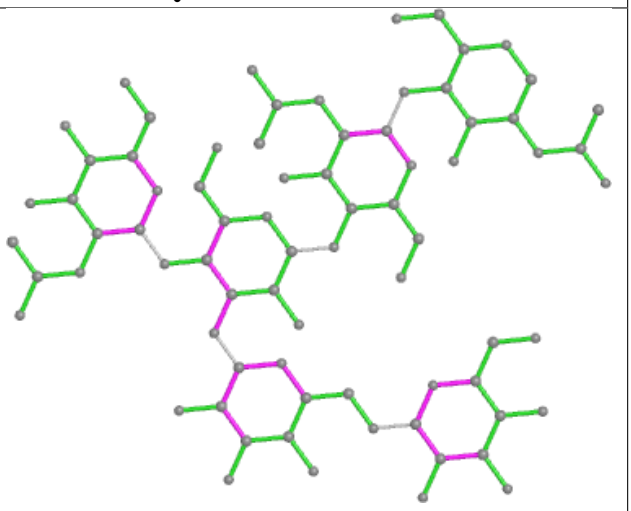


Rings

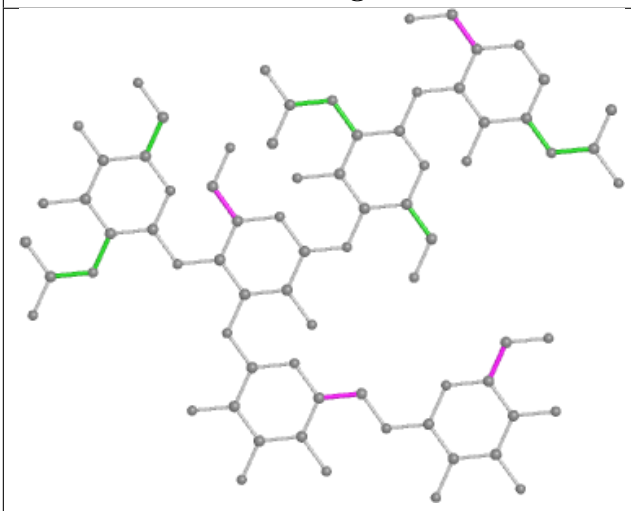
Oligosaccharide Chain Q



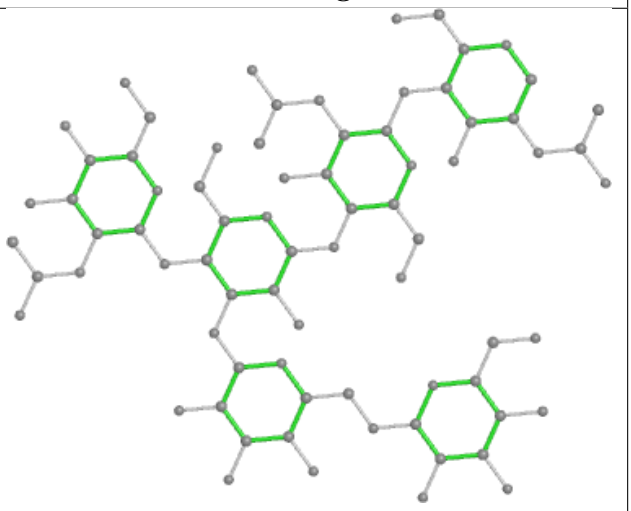
Bond lengths



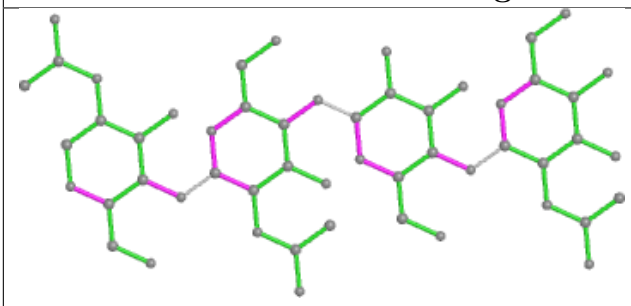
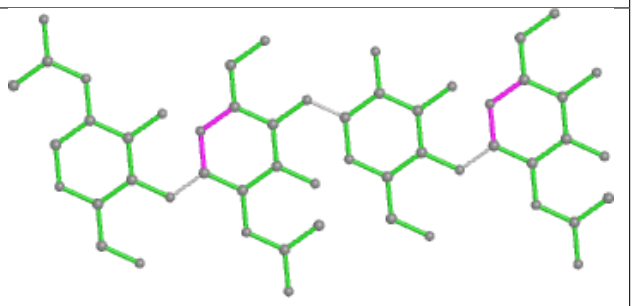
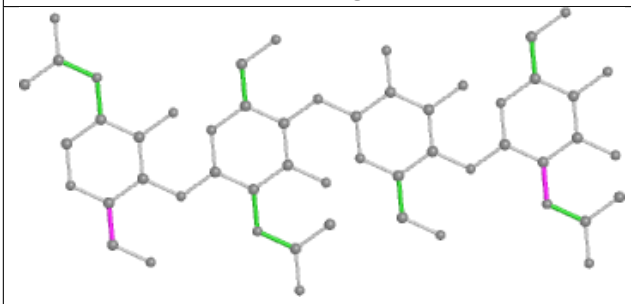
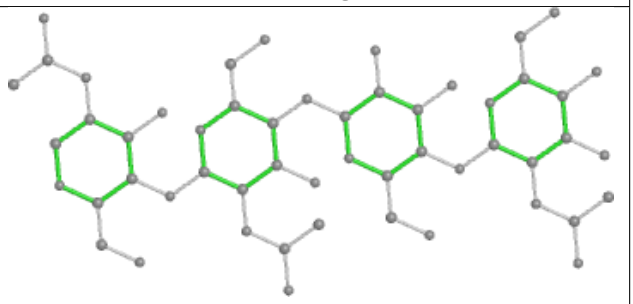
Bond angles

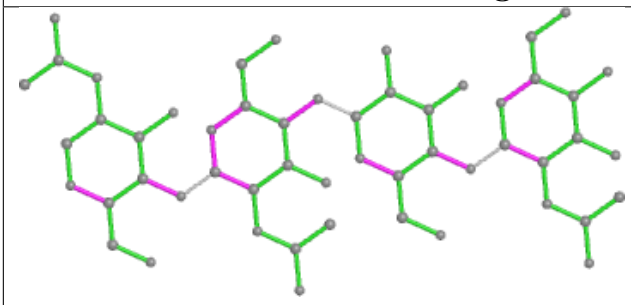
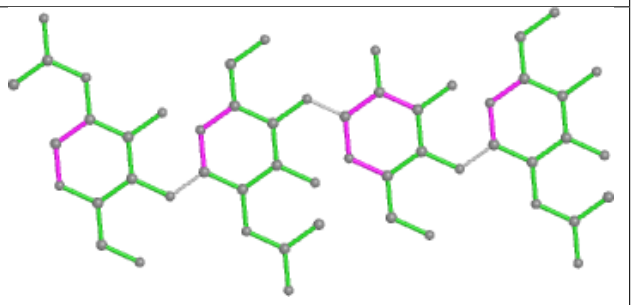
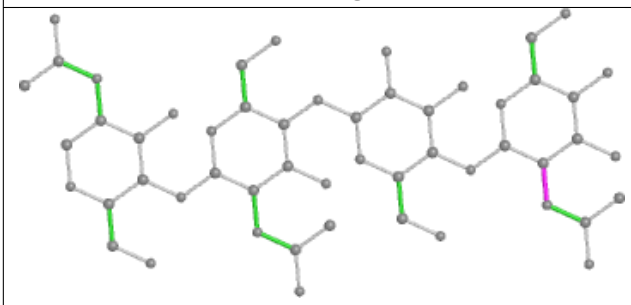
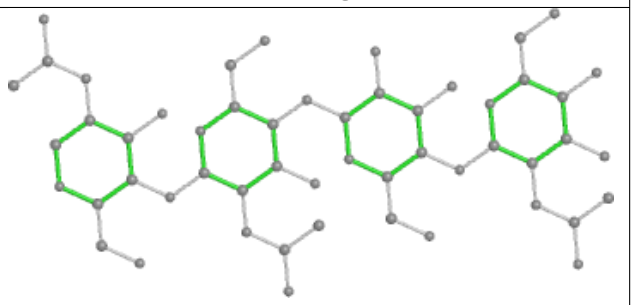


Torsions

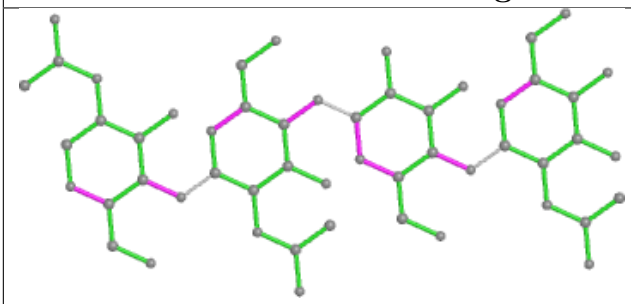


Rings

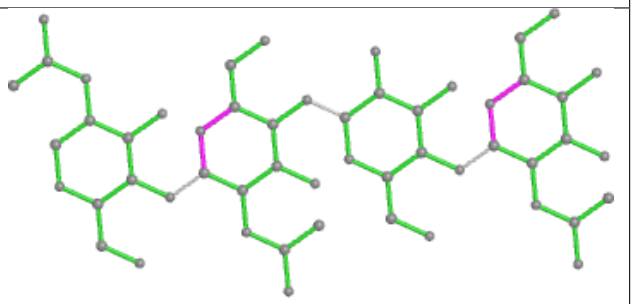
Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

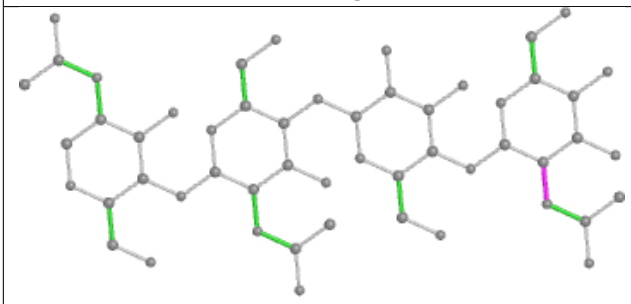
Oligosaccharide Chain R



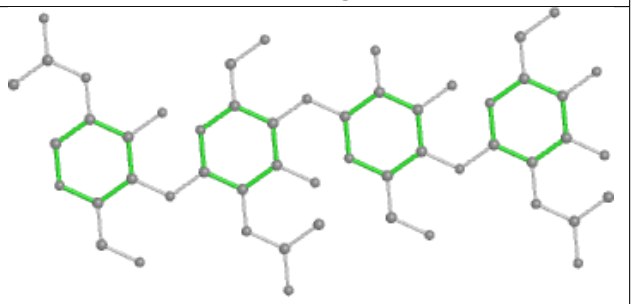
Bond lengths



Bond angles

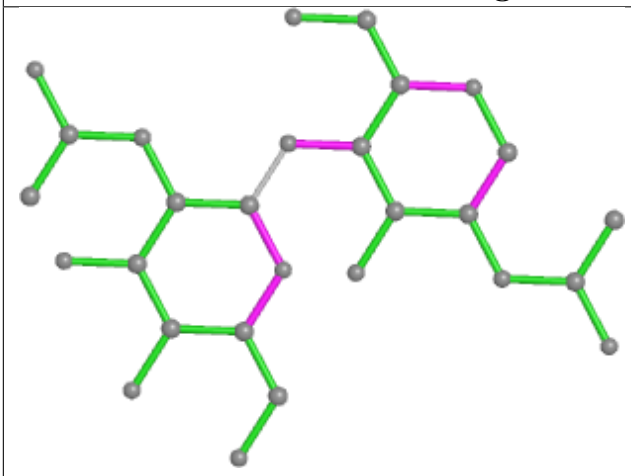


Torsions

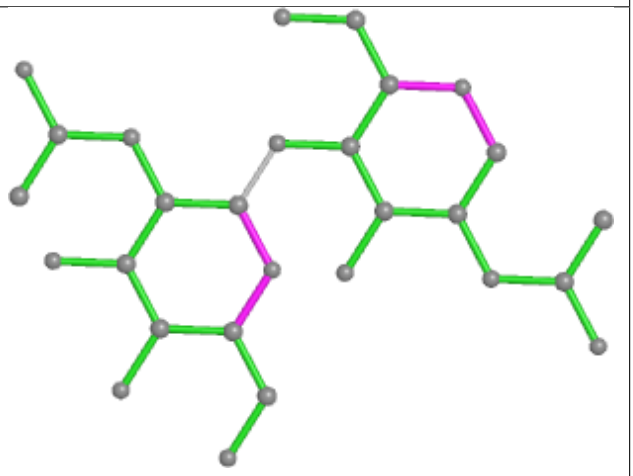


Rings

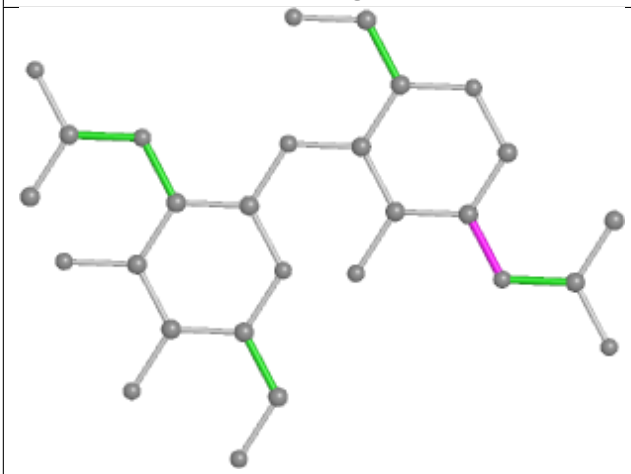
Oligosaccharide Chain G



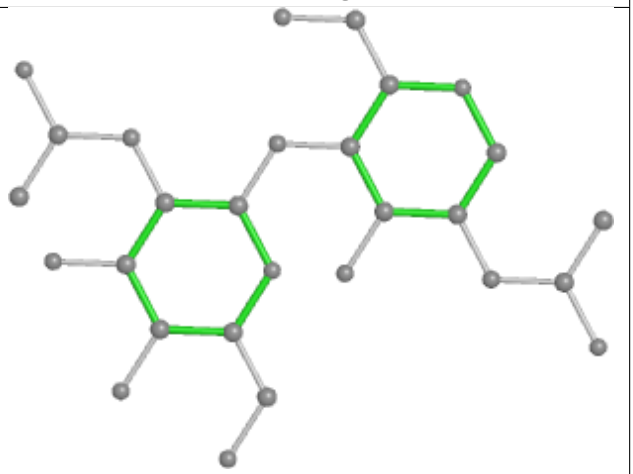
Bond lengths



Bond angles

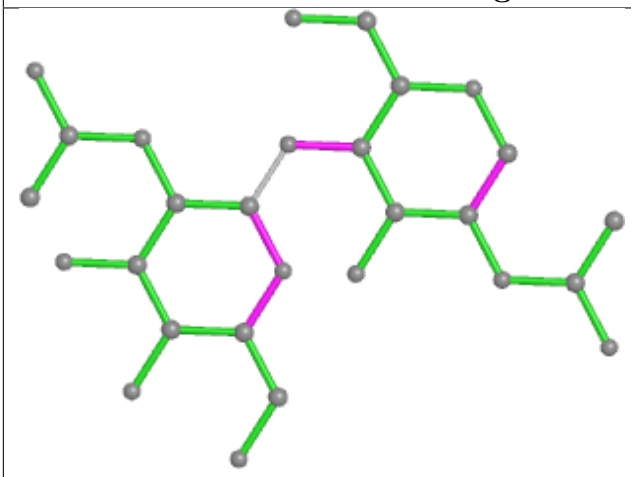


Torsions

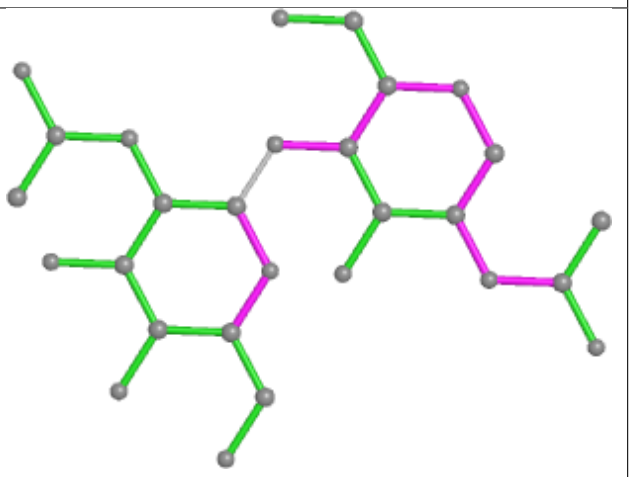


Rings

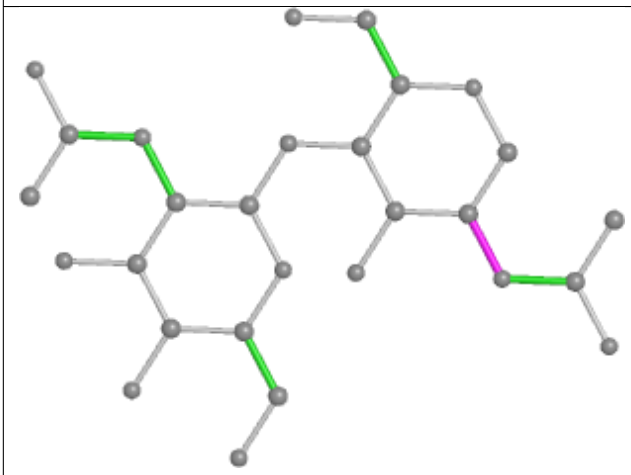
Oligosaccharide Chain N



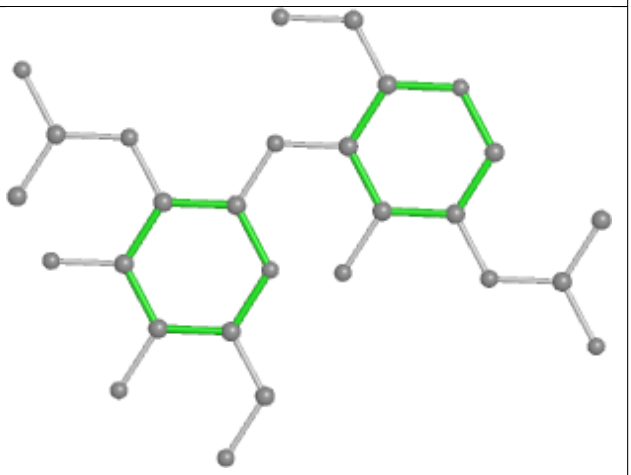
Bond lengths



Bond angles

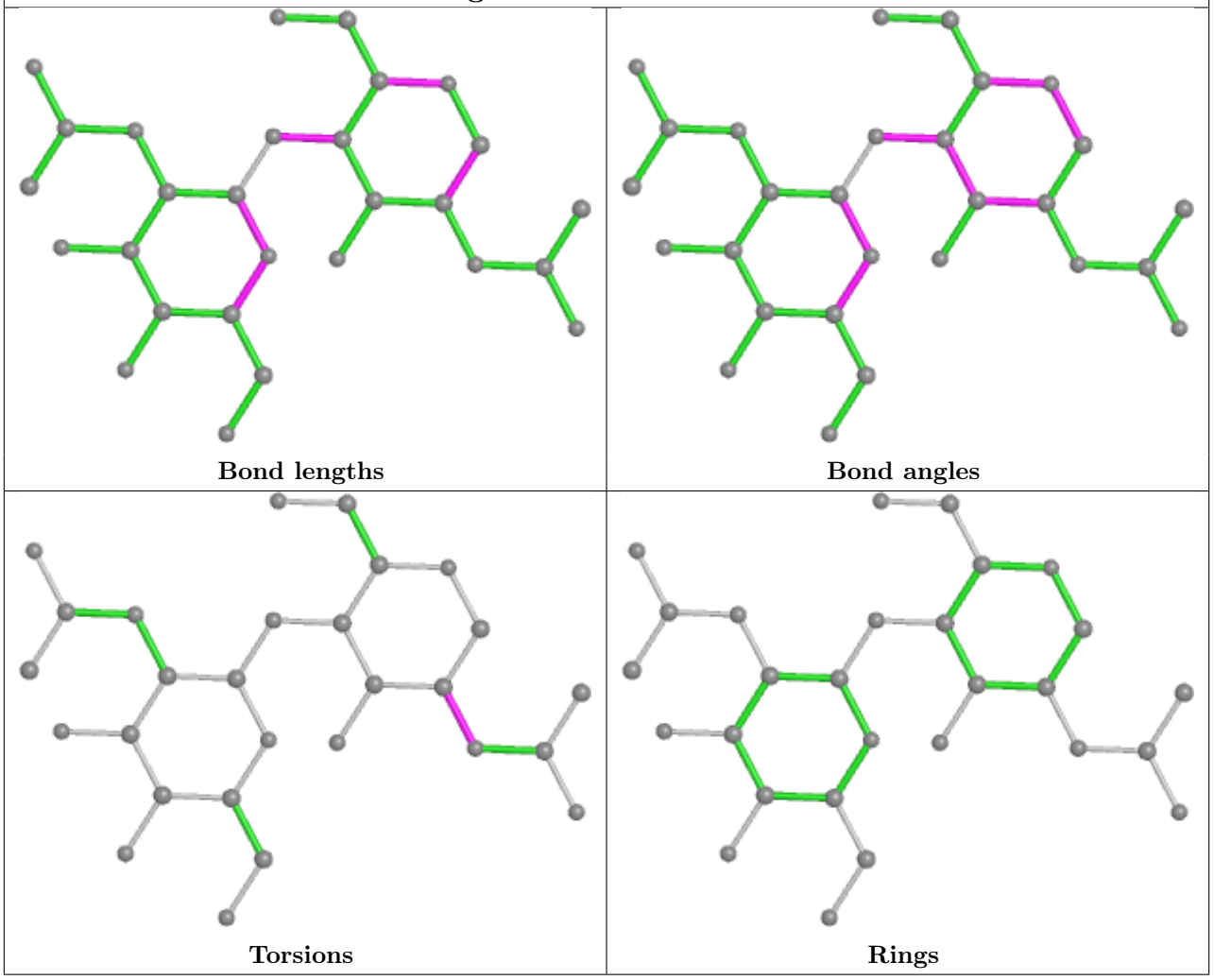


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
12	NAG	c	701	5	14,14,15	1.16	2 (14%)	17,19,21	1.41	2 (11%)
12	NAG	b	701	5	14,14,15	1.17	1 (7%)	17,19,21	0.81	0
12	NAG	a	701	5	14,14,15	1.30	2 (14%)	17,19,21	0.81	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
12	NAG	c	701	5	-	1/6/23/26	0/1/1/1
12	NAG	b	701	5	-	2/6/23/26	0/1/1/1
12	NAG	a	701	5	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	701	NAG	O5-C5	3.15	1.49	1.43
12	b	701	NAG	O5-C5	2.52	1.48	1.43
12	c	701	NAG	O5-C5	2.25	1.48	1.43
12	c	701	NAG	C1-C2	2.15	1.55	1.52
12	a	701	NAG	O5-C1	2.10	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	c	701	NAG	C2-N2-C7	3.31	127.62	122.90
12	c	701	NAG	C1-C2-N2	2.71	115.12	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	c	701	NAG	C1-C2-N2-C7
12	b	701	NAG	C1-C2-N2-C7
12	a	701	NAG	C3-C2-N2-C7
12	b	701	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

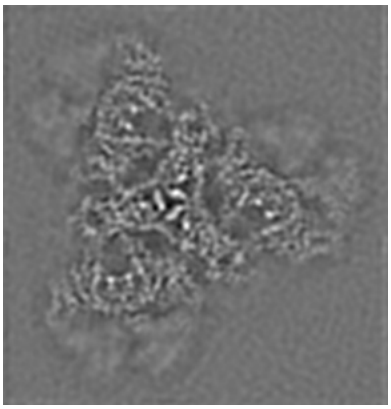
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23518. These allow visual inspection of the internal detail of the map and identification of artifacts.

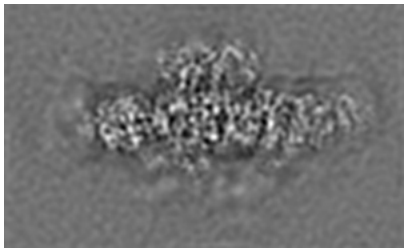
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

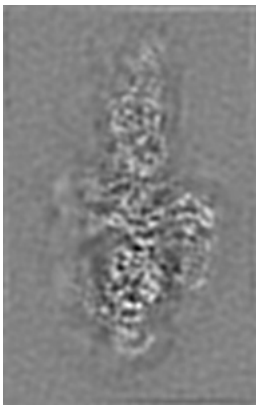
6.1.1 Primary map



X

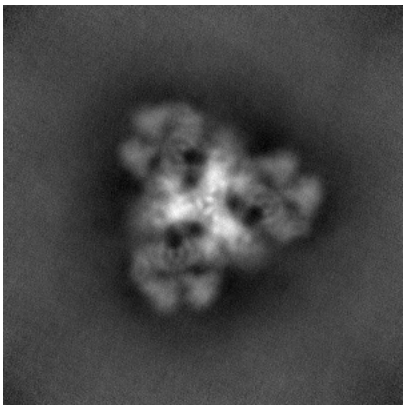


Y

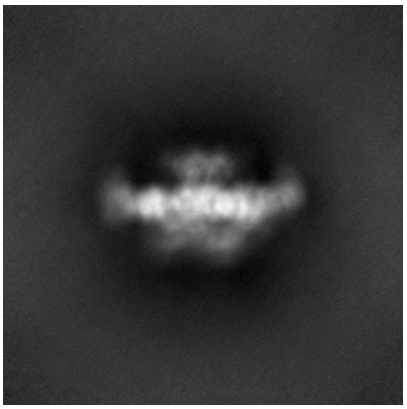


Z

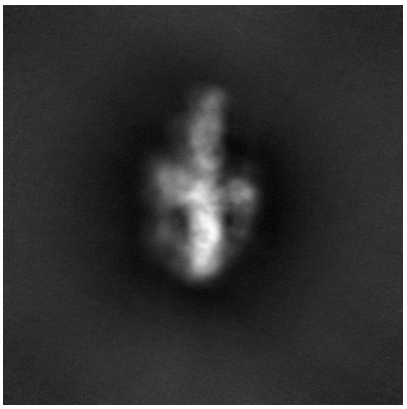
6.1.2 Raw map



X



Y

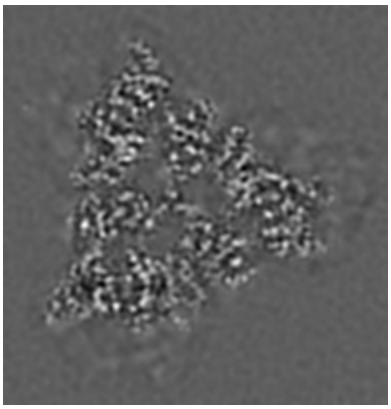


Z

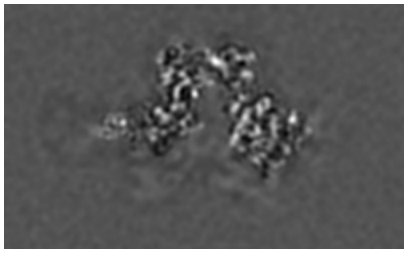
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

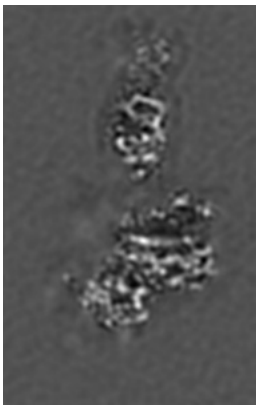
6.2.1 Primary map



X Index: 70

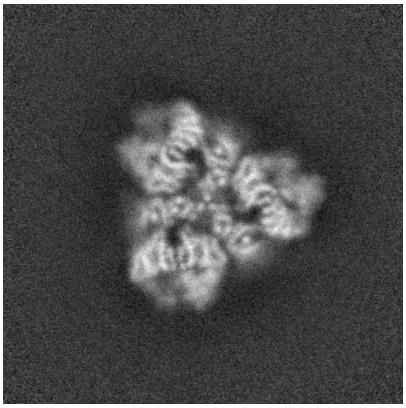


Y Index: 111

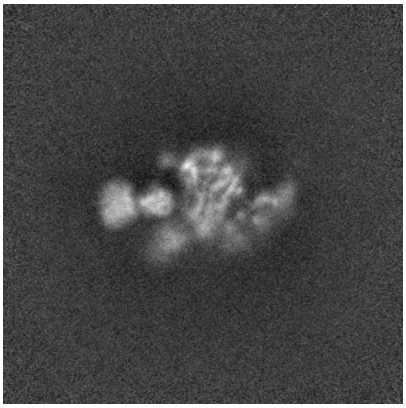


Z Index: 116

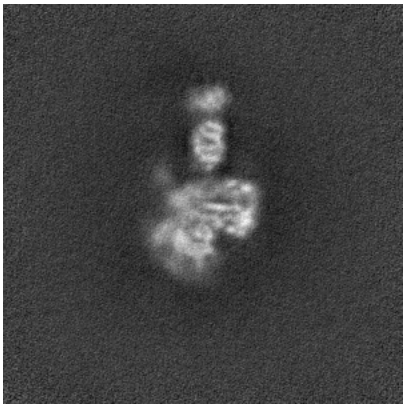
6.2.2 Raw map



X Index: 192



Y Index: 192

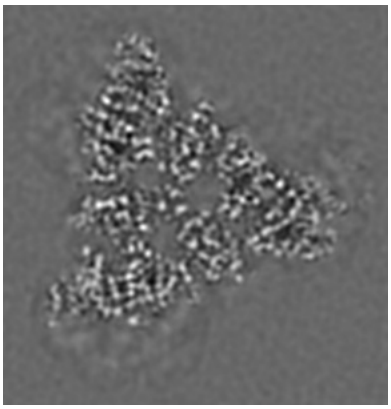


Z Index: 192

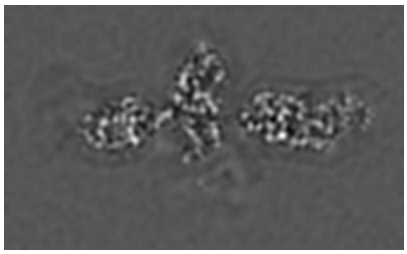
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

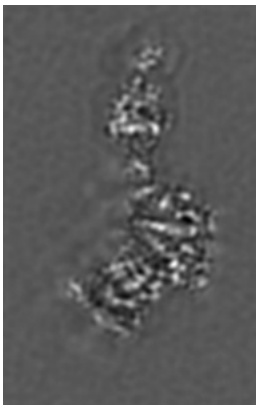
6.3.1 Primary map



X Index: 75

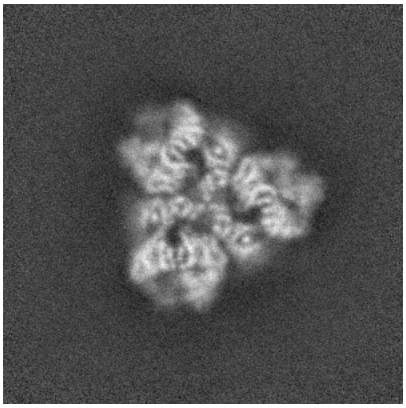


Y Index: 73

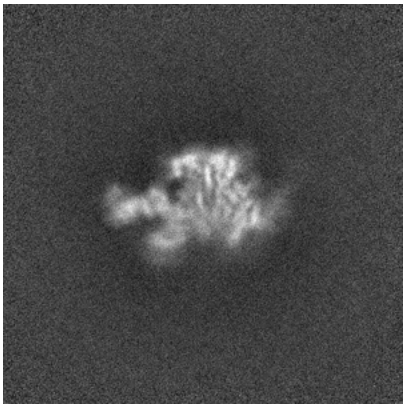


Z Index: 110

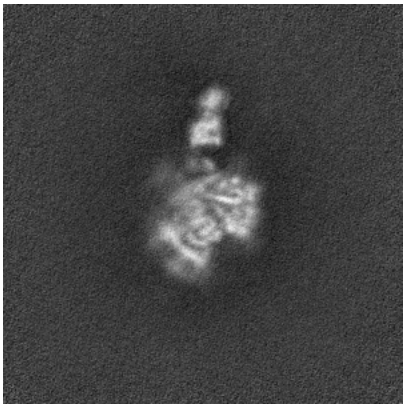
6.3.2 Raw map



X Index: 191



Y Index: 201



Z Index: 185

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

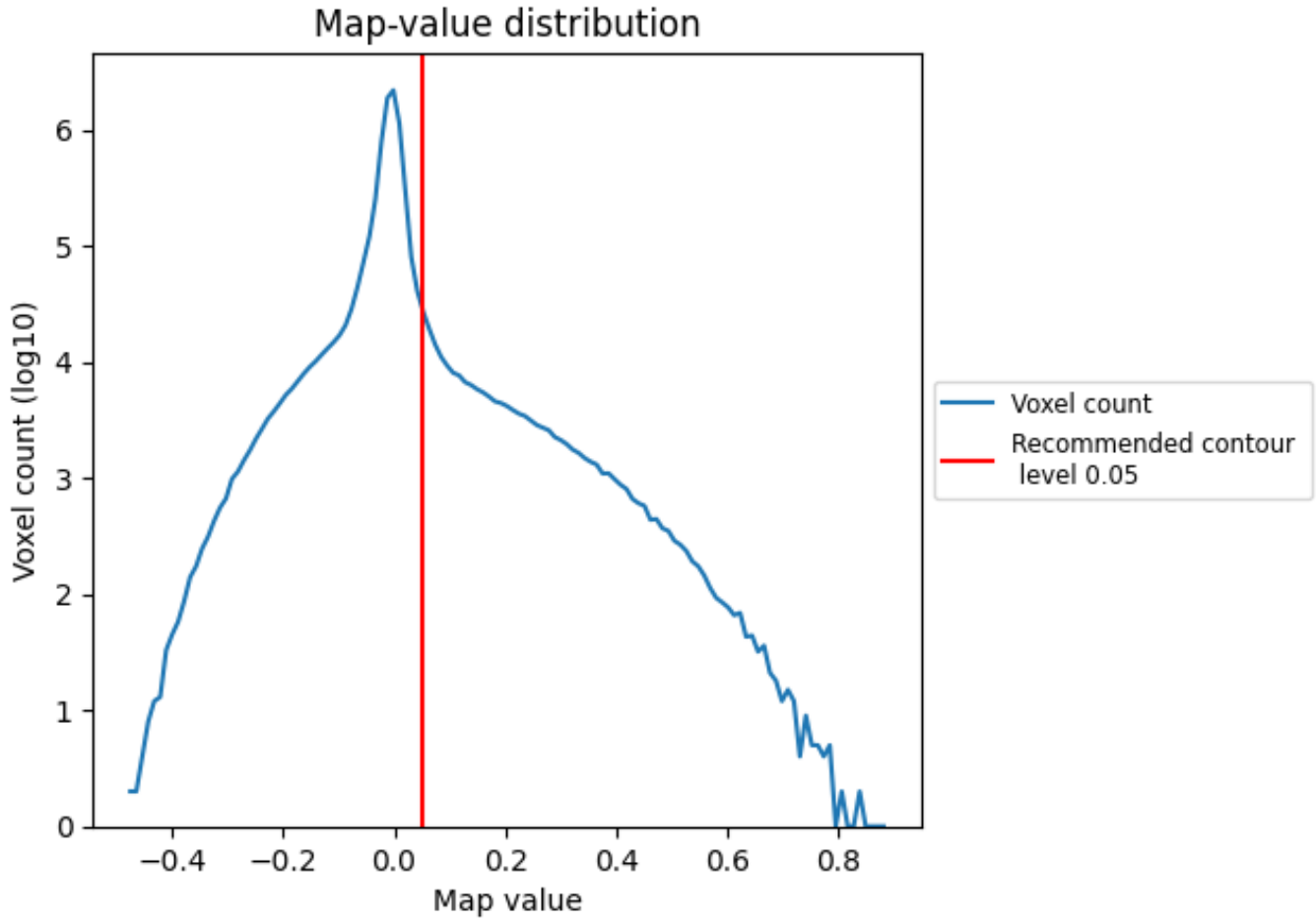
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

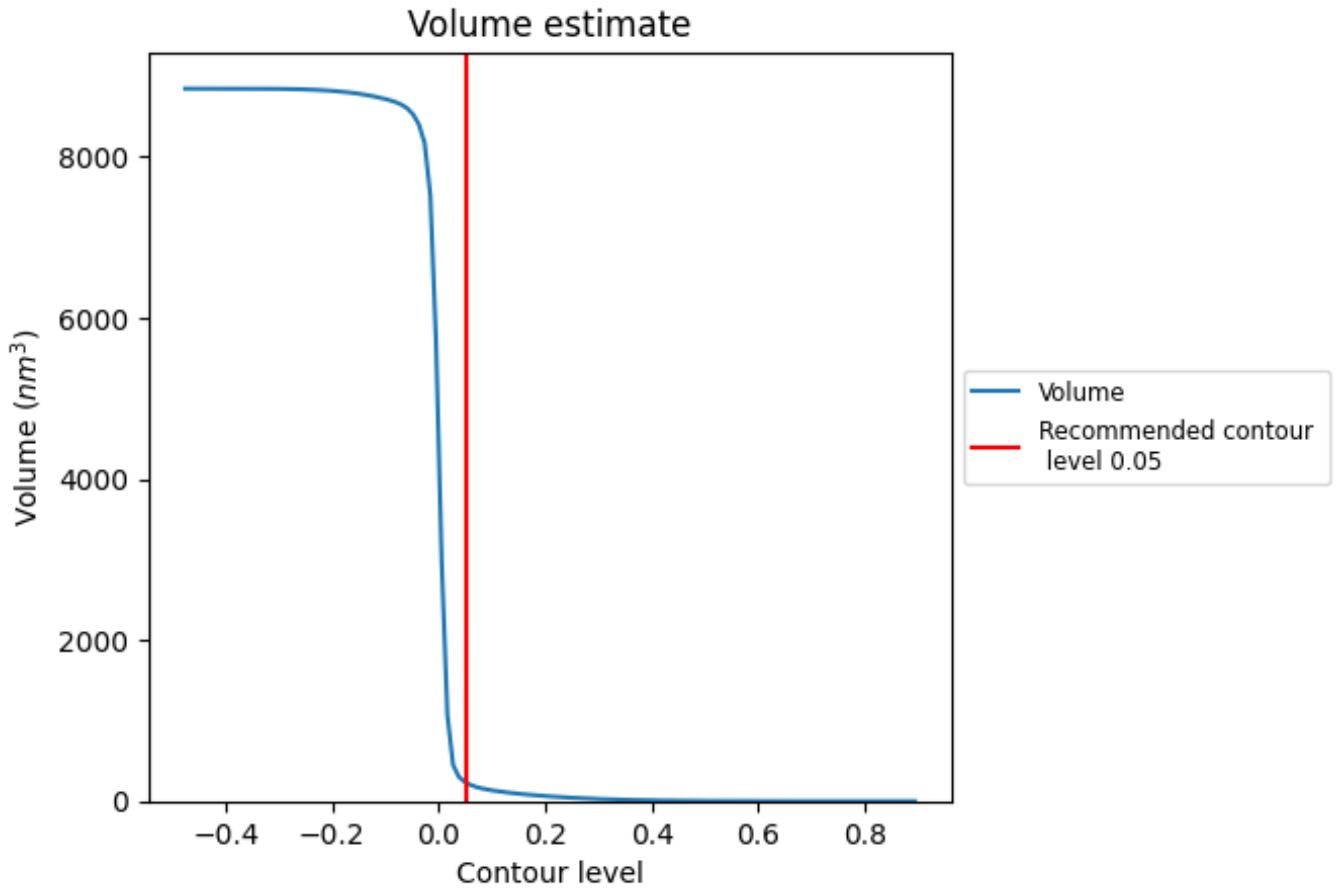
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate



The volume at the recommended contour level is 236 nm^3; this corresponds to an approximate mass of 213 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

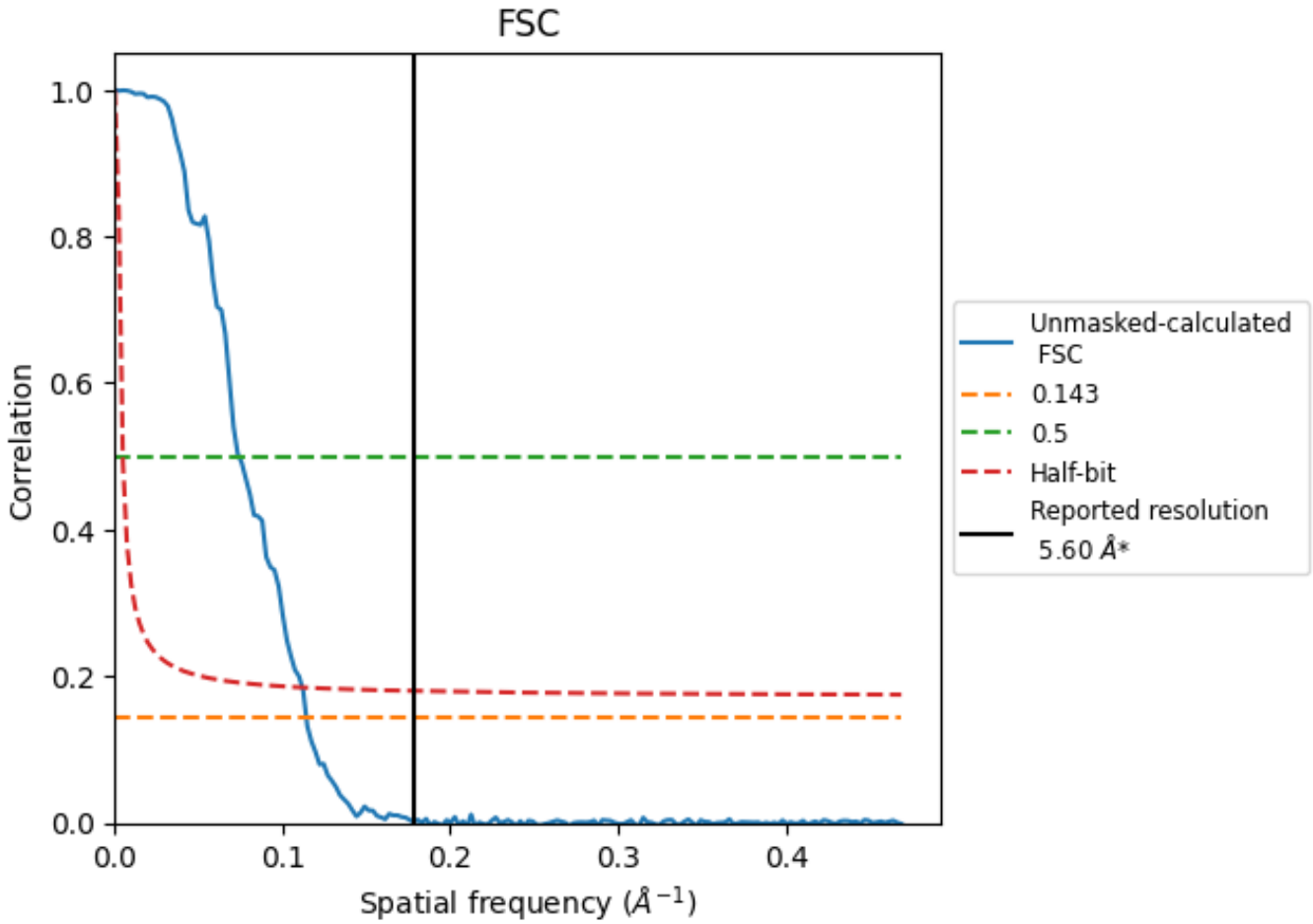
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

8.2 Resolution estimates (i)

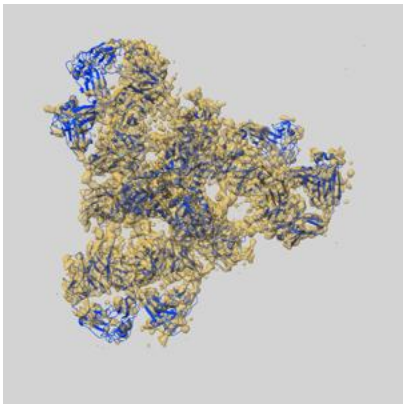
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.76	13.53	8.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.76 differs from the reported value 5.6 by more than 10 %

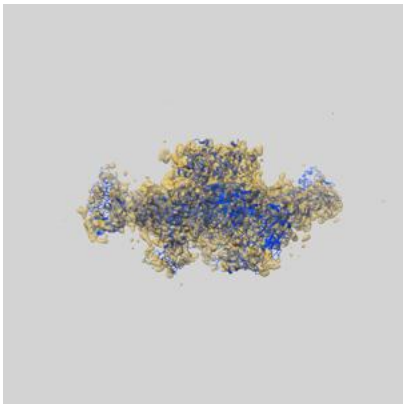
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23518 and PDB model 7LU9. Per-residue inclusion information can be found in section 3 on page 11.

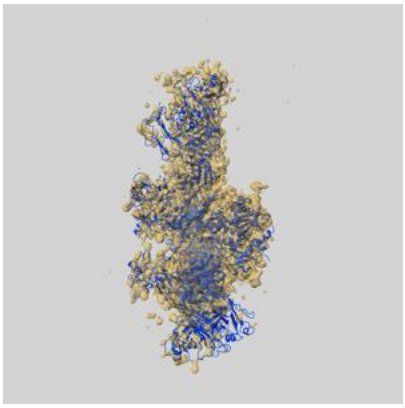
9.1 Map-model overlay



X



Y



Z

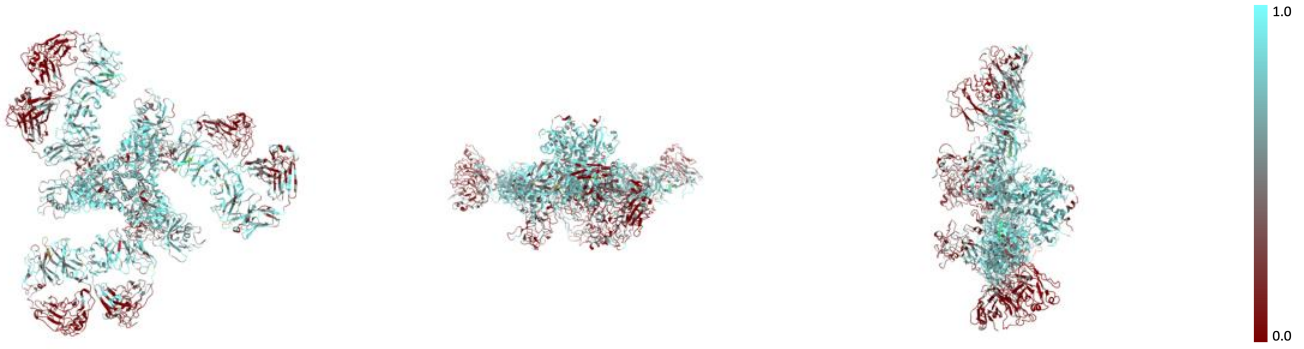
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

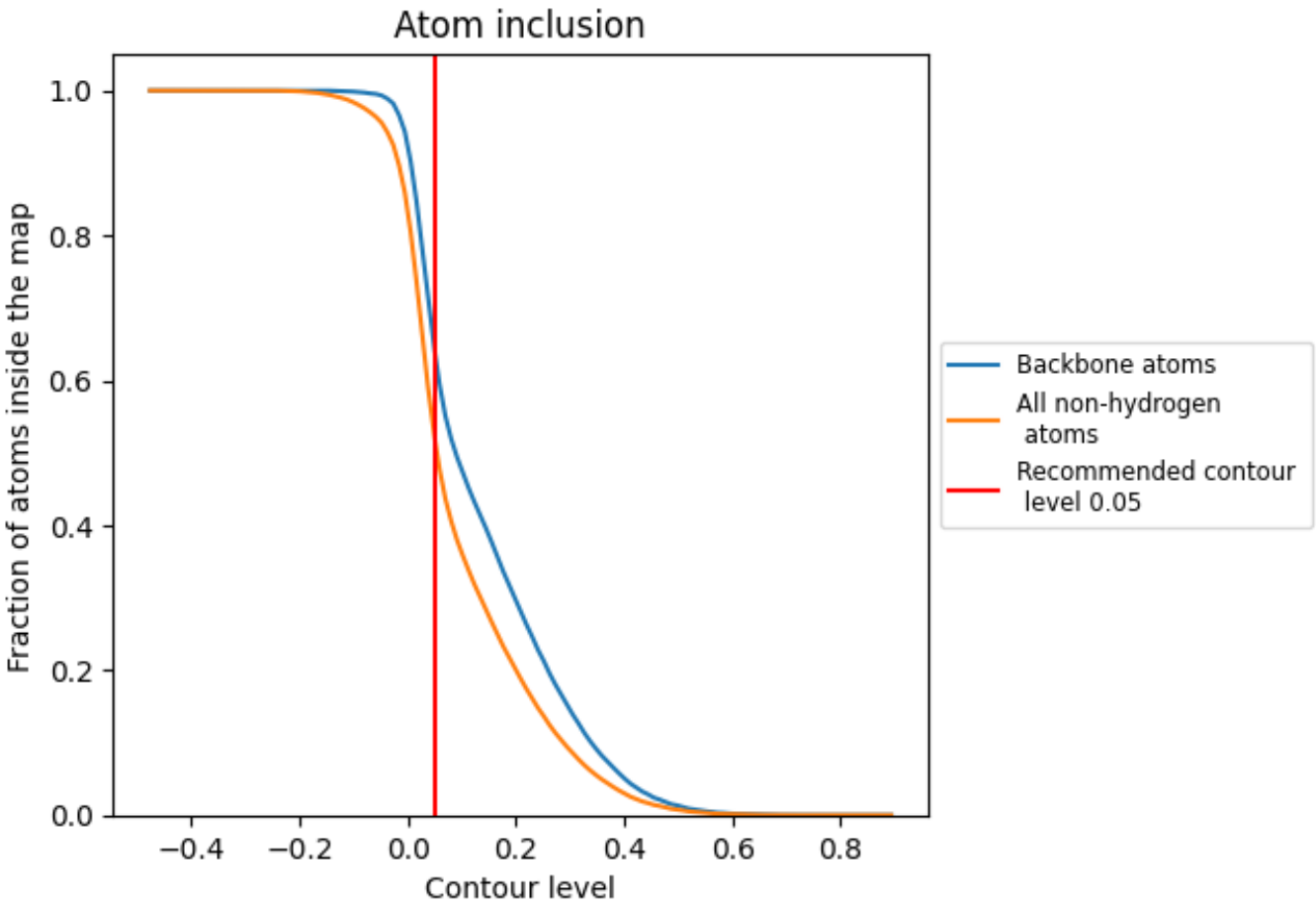
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5203	0.2200
A	0.5385	0.3720
B	0.8197	0.3510
C	0.9333	0.4290
D	0.5472	0.3430
E	0.4103	0.3500
F	0.6557	0.2750
G	0.2143	0.1990
H	0.5385	0.2830
I	0.9508	0.3500
J	0.9200	0.3850
K	0.6604	0.2620
L	0.5641	0.3450
M	0.5902	0.2430
N	0.2143	0.1380
O	0.6923	0.3100
P	0.8852	0.3750
Q	0.9333	0.4120
R	0.6038	0.2810
S	0.4103	0.2340
T	0.3607	0.2520
U	0.2500	0.2540
a	0.6952	0.2890
b	0.7234	0.2930
c	0.7056	0.2650
d	0.5472	0.2400
e	0.5427	0.2380
f	0.4901	0.2230
g	0.4197	0.2150
h	0.5381	0.2370
i	0.4403	0.1770
j	0.3539	0.1440
k	0.5079	0.1840
l	0.5857	0.2440
m	0.4807	0.1870

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Chain	Atom inclusion	Q-score
n	0.3433	0.1270
o	0.4987	0.1800
p	0.5955	0.2420
q	0.5000	0.2190
r	0.4384	0.1840