Full wwPDB EM Validation Report ⓘ

Aug 21, 2023 – 08:17 PM JST

PDB ID	:	7WM4
EMDB ID	:	EMD-32599
Title	:	Cryo-EM structure of tetrameric TLR3 in complex with dsRNA (90 bp)
Authors	:	Sakaniwa, K.; Ohto, U.; Shimizu, T.
Deposited on	:	2022-01-14
Resolution	:	3.20 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:

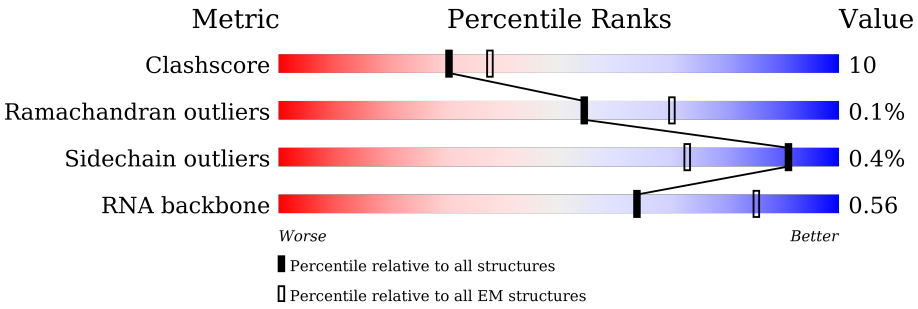
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C	680	73% 24% .
1	D	680	73% 25% .
1	E	680	72% 25% .
1	F	680	. 70% 28% .
2	A	81	51% 36% 14%
3	B	81	42% 44% 14%
4	G	3	33% 67% 33%

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Mol	Chain	Length	Quality of chain
4	K	3	33% 67%
4	L	3	100%
4	M	3	100%
4	Q	3	33% 100%
4	R	3	67% 33%
4	S	3	100%
4	U	3	100%
4	Y	3	100%
4	Z	3	100%
4	a	3	100%
4	e	3	33% 100%
4	f	3	100%
4	g	3	100%
5	H	2	50% 50%
5	I	2	100%
5	J	2	50% 50%
5	N	2	100%
5	O	2	50% 50%
5	P	2	100%
5	T	2	50% 50%
5	V	2	100%
5	W	2	100%
5	X	2	100%
5	b	2	100%
5	c	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	d	2	100%
5	h	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25848 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	661	Total 5310	C 3392	N 905	O 999	S 14	0	0
1	D	668	Total 5360	C 3422	N 914	O 1010	S 14	0	0
1	E	661	Total 5310	C 3392	N 905	O 999	S 14	0	0
1	F	668	Total 5360	C 3422	N 914	O 1010	S 14	0	0

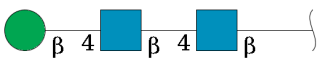
- Molecule 2 is a RNA chain called RNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	81	Total 1702	C 770	N 285	O 566	P 81	0	0

- Molecule 3 is a RNA chain called RNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	81	Total 1700	C 769	N 282	O 568	P 81	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	3	Total 39	C 22	N 2	O 15	0	0
4	K	3	Total 39	C 22	N 2	O 15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	3	Total	C	N	O	0	0
			39	22	2	15		
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		
4	U	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	Z	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		
4	e	3	Total	C	N	O	0	0
			39	22	2	15		
4	f	3	Total	C	N	O	0	0
			39	22	2	15		
4	g	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		

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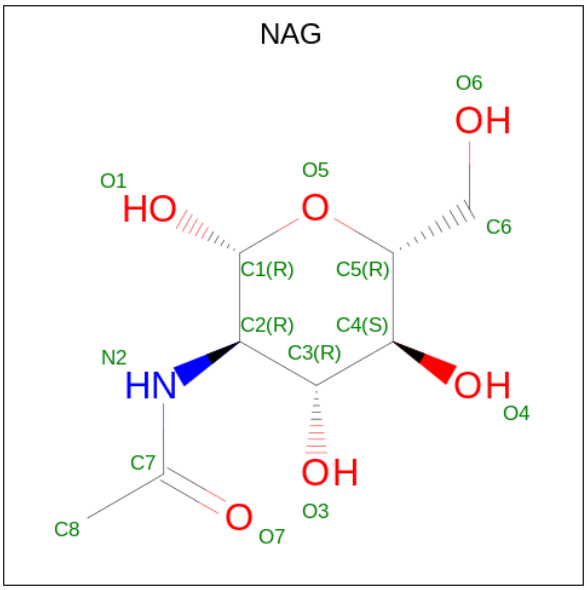
Mol	Chain	Residues	Atoms	AltConf	Trace
5	P	2	Total C N O 28 16 2 10	0	0
5	T	2	Total C N O 28 16 2 10	0	0
5	V	2	Total C N O 28 16 2 10	0	0
5	W	2	Total C N O 28 16 2 10	0	0
5	X	2	Total C N O 28 16 2 10	0	0
5	b	2	Total C N O 28 16 2 10	0	0
5	c	2	Total C N O 28 16 2 10	0	0
5	d	2	Total C N O 28 16 2 10	0	0
5	h	2	Total C N O 28 16 2 10	0	0

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



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

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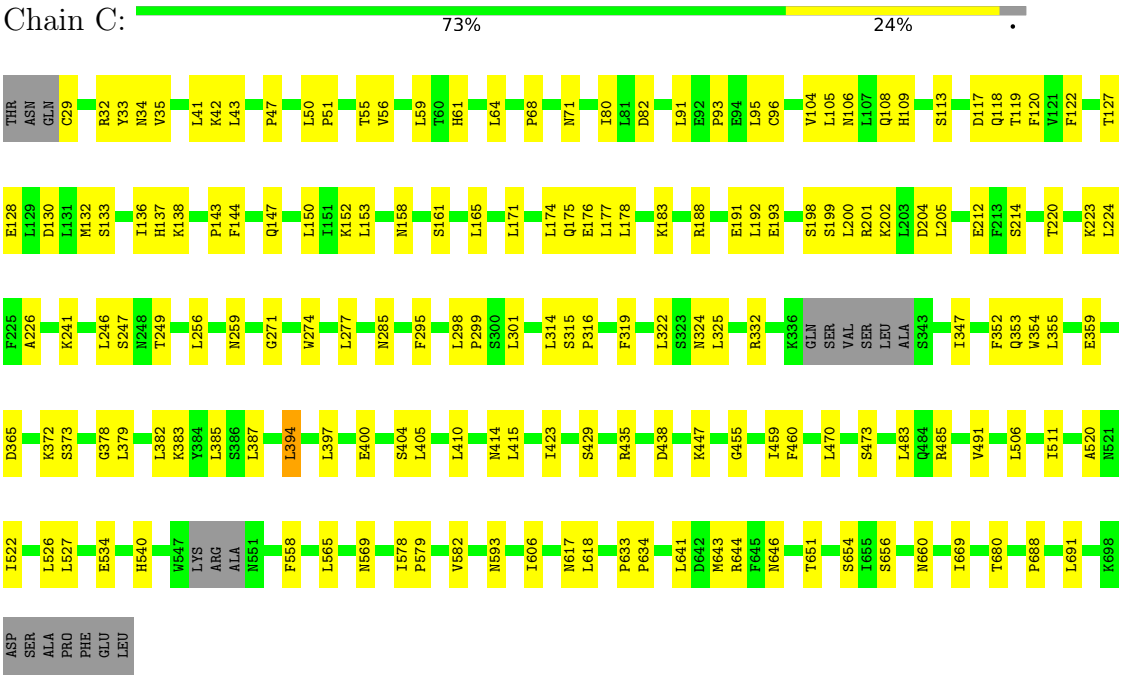
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6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

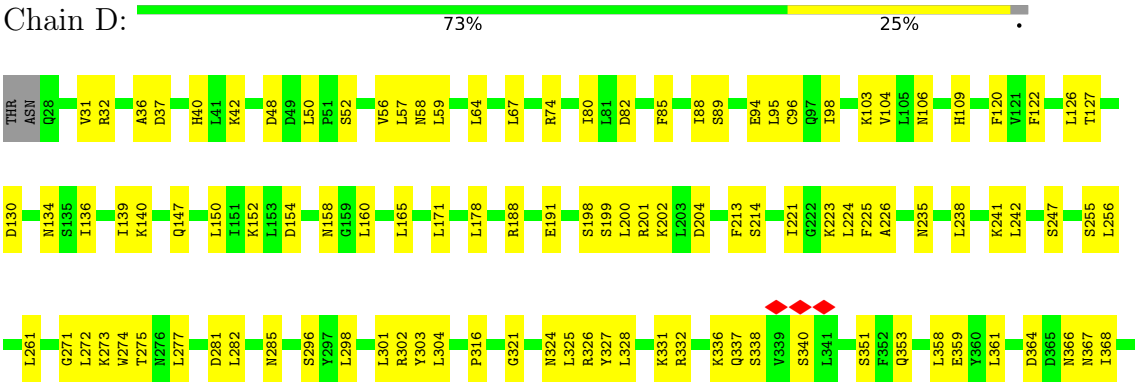
• Molecule 1: Toll-like receptor 3

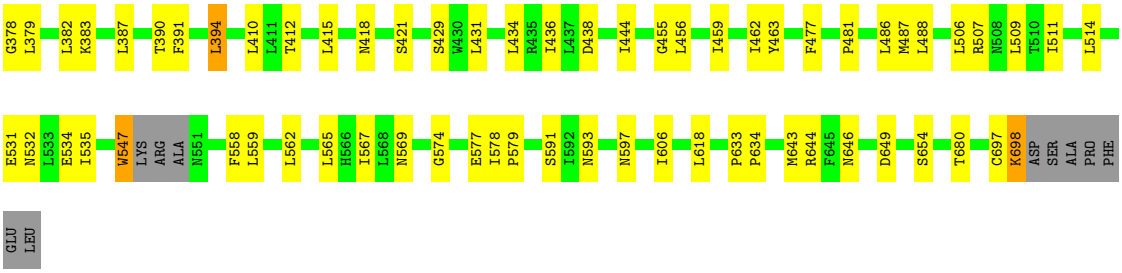
Chain C:



• Molecule 1: Toll-like receptor 3

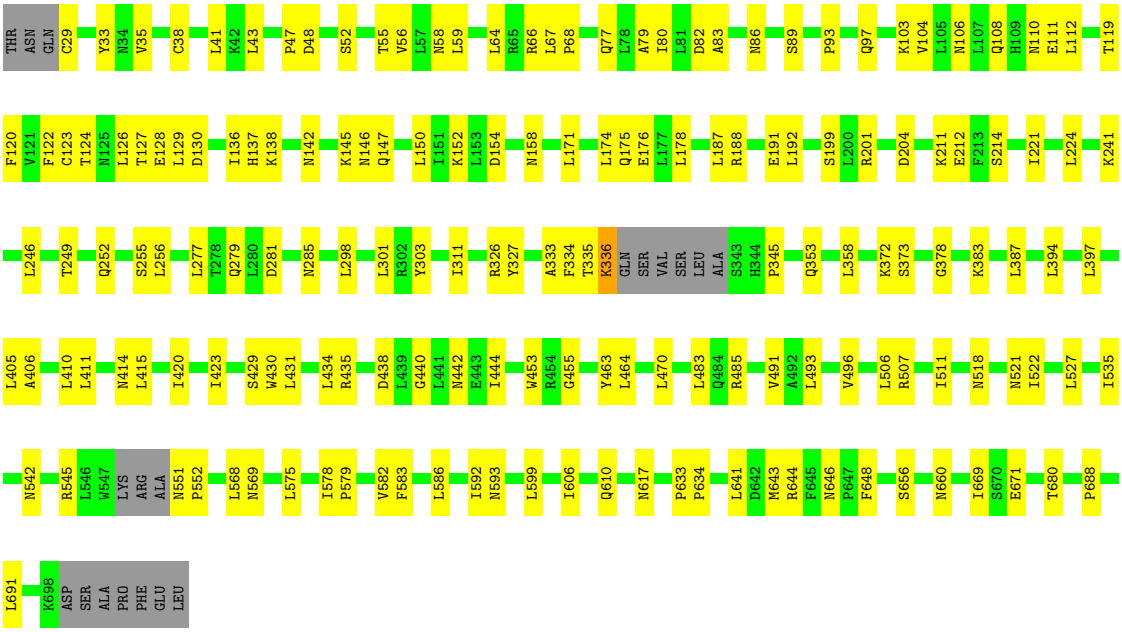
Chain D:





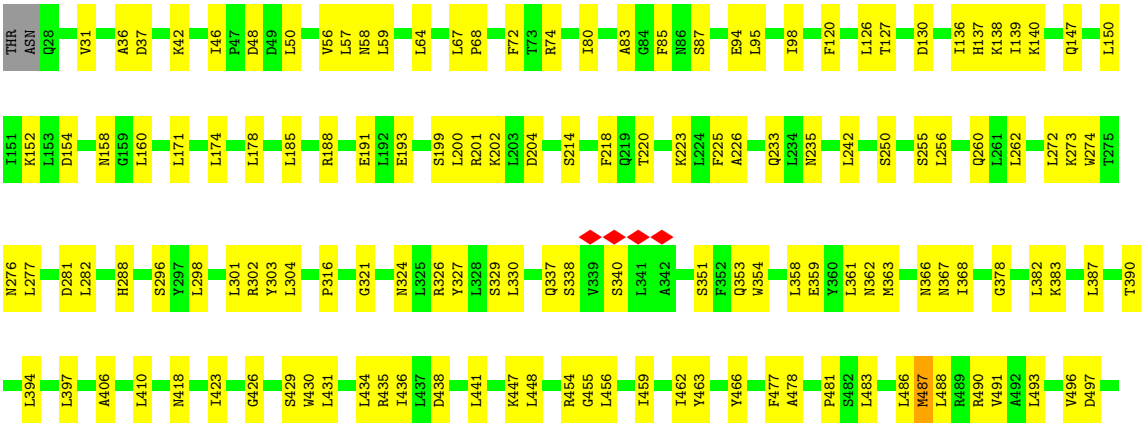
• Molecule 1: Toll-like receptor 3

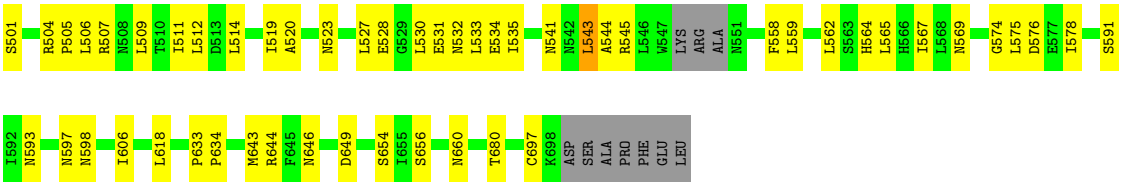
Chain E:



• Molecule 1: Toll-like receptor 3

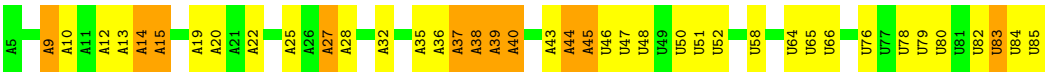
Chain F:





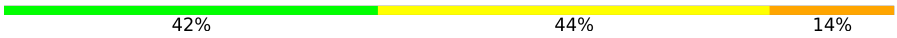
• Molecule 2: RNA (81-MER)

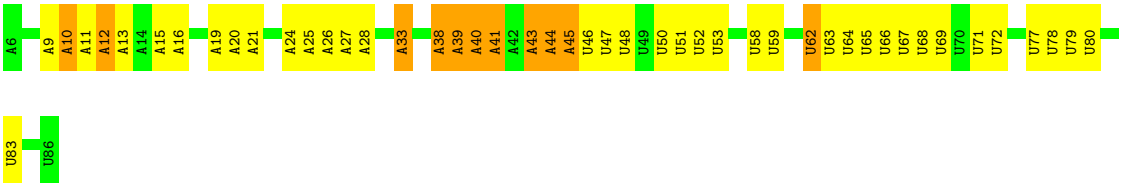
Chain A:



• Molecule 3: RNA (81-MER)

Chain B:



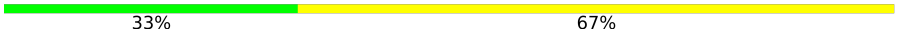


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

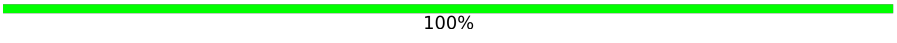
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



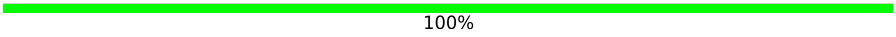
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



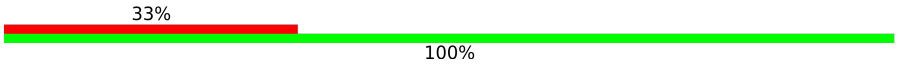
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

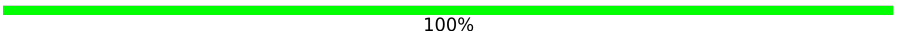
Chain S:

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

Chain U:

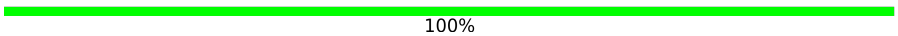
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

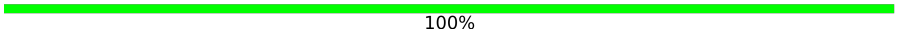


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

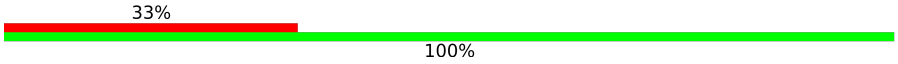
Chain Z:



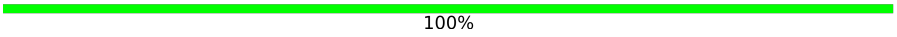
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

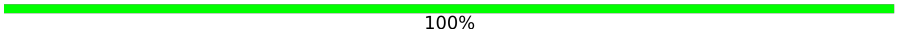
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

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

Chain f: 

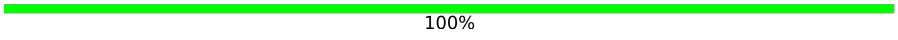
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 

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

Chain H: 

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

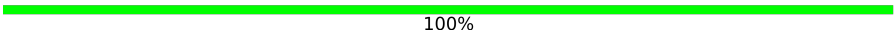
Chain I: 

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

Chain J:

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

Chain N:

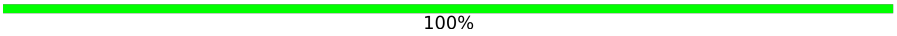


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:

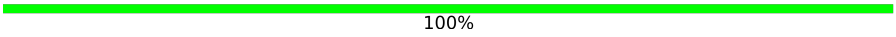


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

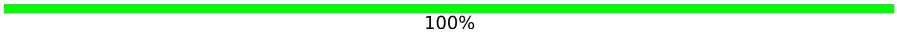
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

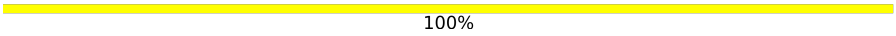


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

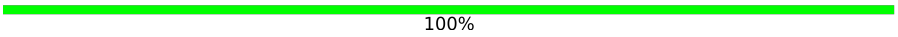
Chain W:



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

Chain X: 

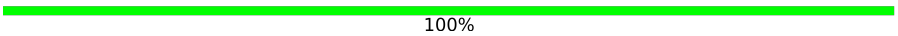
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

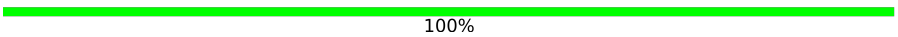
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

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

Chain d: 

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

Chain h: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	274002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.446	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	315.84, 315.84, 315.84	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.128, 1.128, 1.128	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

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	C	0.24	0/5421	0.48	1/7360 (0.0%)
1	D	0.24	0/5472	0.47	1/7431 (0.0%)
1	E	0.24	0/5421	0.48	0/7360
1	F	0.24	0/5472	0.48	1/7431 (0.0%)
2	A	0.20	0/1904	0.83	0/2955
3	B	0.21	0/1901	0.85	0/2950
All	All	0.24	0/25591	0.56	3/35487 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	394	LEU	CA-CB-CG	5.59	128.16	115.30
1	F	543	LEU	CA-CB-CG	5.20	127.27	115.30
1	D	394	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5310	0	5314	110	0
1	D	5360	0	5366	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5310	0	5313	105	0
1	F	5360	0	5365	115	0
2	A	1702	0	852	20	0
3	B	1700	0	851	43	0
4	G	39	0	34	1	0
4	K	39	0	34	2	0
4	L	39	0	34	0	0
4	M	39	0	34	0	0
4	Q	39	0	34	0	0
4	R	39	0	34	1	0
4	S	39	0	34	0	0
4	U	39	0	34	0	0
4	Y	39	0	34	0	0
4	Z	39	0	34	0	0
4	a	39	0	34	0	0
4	e	39	0	34	0	0
4	f	39	0	34	0	0
4	g	39	0	34	0	0
5	H	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	2	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	X	28	0	25	1	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	h	28	0	25	0	0
6	C	28	0	26	1	0
6	D	56	0	50	0	0
6	E	28	0	23	0	0
6	F	56	0	52	2	0
All	All	25848	0	24038	488	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 10.

All (488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:58:U:H3	3:B:33:A:H61	1.19	0.88
1:E:335:THR:HG22	1:E:336:LYS:H	1.42	0.84
2:A:44:A:HO2'	2:A:45:A:H8	1.34	0.75
1:C:298:LEU:HB3	1:C:301:LEU:HD23	1.68	0.75
1:E:298:LEU:HB3	1:E:301:LEU:HD23	1.69	0.74
1:C:68:PRO:HG3	6:C:801:NAG:H82	1.69	0.74
1:F:501:SER:HB3	1:F:504:ARG:HE	1.54	0.73
1:D:296:SER:HA	1:D:321:GLY:HA3	1.71	0.73
2:A:80:U:O4	3:B:11:A:N1	2.22	0.73
1:F:296:SER:HA	1:F:321:GLY:HA3	1.71	0.72
1:C:618:LEU:HB2	1:C:643:MET:HG2	1.70	0.72
1:C:50:LEU:HD12	1:C:51:PRO:HD2	1.71	0.72
1:E:124:THR:HG22	1:E:146:ASN:HB3	1.72	0.72
1:F:330:LEU:HB2	1:F:363:MET:HE1	1.72	0.71
1:F:530:LEU:HB3	1:F:533:LEU:HD23	1.72	0.70
1:C:256:LEU:O	1:C:285:ASN:ND2	2.25	0.69
1:E:171:LEU:HD13	1:E:174:LEU:HD22	1.74	0.69
1:F:337:GLN:HE21	1:F:367:ASN:HB3	1.57	0.69
1:F:618:LEU:HB2	1:F:643:MET:HG2	1.75	0.68
1:E:521:ASN:HB3	1:E:545:ARG:HH22	1.59	0.68
2:A:27:A:H61	3:B:64:U:H3	1.39	0.68
1:E:256:LEU:O	1:E:285:ASN:ND2	2.27	0.67
1:E:59:LEU:HB2	1:E:83:ALA:HA	1.78	0.66
1:E:279:GLN:HG2	1:E:303:TYR:HB2	1.77	0.66
1:F:562:LEU:HB3	1:F:565:LEU:HD23	1.78	0.66
1:F:504:ARG:NH1	1:F:528:GLU:O	2.27	0.66
1:F:429:SER:HA	1:F:455:GLY:HA3	1.78	0.66
1:E:199:SER:OG	1:E:201:ARG:NH2	2.30	0.65
1:D:358:LEU:HD21	1:D:361:LEU:HD13	1.79	0.65
1:D:506:LEU:HB3	1:D:509:LEU:HD23	1.78	0.64
1:D:547:TRP:CD1	1:D:579:PRO:HD2	2.32	0.64
1:E:414:ASN:HA	1:E:438:ASP:HB2	1.79	0.64
1:D:85:PHE:HB3	3:B:11:A:H5'	1.79	0.64
1:D:438:ASP:HA	1:D:463:TYR:HB2	1.79	0.64
1:C:414:ASN:HA	1:C:438:ASP:HB2	1.78	0.64
1:E:518:ASN:OD1	1:E:542:ASN:ND2	2.30	0.64
1:C:176:GLU:HG3	1:C:202:LYS:HB3	1.80	0.64
1:D:547:TRP:CD1	1:D:578:ILE:HG22	2.33	0.64
1:C:201:ARG:NH2	5:H:1:NAG:O7	2.31	0.63
1:E:52:SER:O	1:E:77:GLN:NE2	2.31	0.63
1:C:43:LEU:HD21	1:C:47:PRO:HD3	1.81	0.63
1:E:93:PRO:HG3	1:E:119:THR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:SER:OG	1:D:271:GLY:O	2.14	0.63
1:E:397:LEU:HD11	1:E:420:ILE:HD12	1.81	0.63
1:C:82:ASP:OD1	1:C:106:ASN:ND2	2.32	0.62
1:F:438:ASP:HA	1:F:463:TYR:HB2	1.81	0.62
1:D:507:ARG:HH12	1:D:531:GLU:HB3	1.64	0.62
1:C:379:LEU:HD13	1:C:382:LEU:HD12	1.79	0.62
1:D:429:SER:HA	1:D:455:GLY:HA3	1.82	0.62
1:D:562:LEU:HB3	1:D:565:LEU:HD23	1.81	0.62
1:E:97:GLN:HB2	1:E:122:PHE:HE2	1.64	0.62
1:C:93:PRO:HG3	1:C:119:THR:HA	1.81	0.61
1:D:82:ASP:OD1	1:D:106:ASN:ND2	2.31	0.61
1:D:578:ILE:HD12	1:D:606:ILE:HG12	1.81	0.61
1:F:353:GLN:HA	1:F:378:GLY:HA3	1.81	0.61
1:C:171:LEU:HD13	1:C:174:LEU:HD22	1.82	0.61
1:C:314:LEU:HB2	1:C:347:ILE:HG22	1.83	0.61
1:D:412:THR:HA	1:D:436:ILE:HB	1.80	0.61
1:C:429:SER:HA	1:C:455:GLY:HA3	1.81	0.61
1:D:36:ALA:HB3	1:D:57:LEU:HA	1.83	0.61
1:E:89:SER:HA	1:E:111:GLU:HB2	1.82	0.61
1:E:104:VAL:HA	1:E:128:GLU:HB3	1.81	0.60
1:C:224:LEU:HD21	1:C:249:THR:HB	1.84	0.60
1:E:178:LEU:HA	1:E:204:ASP:HB3	1.84	0.60
1:D:547:TRP:CD1	1:D:578:ILE:HA	2.37	0.59
1:D:547:TRP:HD1	1:D:578:ILE:HA	1.66	0.59
1:F:447:LYS:NZ	1:F:448:LEU:O	2.34	0.59
1:E:58:ASN:HA	1:E:82:ASP:HB3	1.84	0.59
1:F:68:PRO:HG3	6:F:801:NAG:H82	1.84	0.59
1:C:299:PRO:O	1:C:324:ASN:ND2	2.35	0.59
1:C:578:ILE:HD12	1:C:606:ILE:HG12	1.85	0.59
1:E:405:LEU:HB2	1:E:431:LEU:HD11	1.85	0.59
1:C:68:PRO:HB2	1:C:71:ASN:HB2	1.85	0.58
1:F:171:LEU:HB3	1:F:174:LEU:HD22	1.84	0.58
1:C:113:SER:OG	3:B:50:U:O2'	2.21	0.58
1:C:322:LEU:HB3	1:C:325:LEU:HD23	1.84	0.58
1:E:586:LEU:HB2	1:E:610:GLN:HE22	1.68	0.58
1:D:481:PRO:HA	1:D:506:LEU:HD13	1.85	0.58
1:D:618:LEU:HB2	1:D:643:MET:HG2	1.84	0.58
1:D:126:LEU:HG	1:D:150:LEU:HD13	1.85	0.58
1:F:202:LYS:HA	1:F:226:ALA:HB3	1.86	0.58
1:F:394:LEU:HD21	1:F:397:LEU:HG	1.86	0.58
1:F:497:ASP:O	1:F:523:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:ILE:HD12	1:E:606:ILE:HG12	1.85	0.58
1:D:383:LYS:HA	1:D:410:LEU:HA	1.86	0.58
1:E:142:ASN:HB3	1:E:145:LYS:HE3	1.85	0.58
1:E:429:SER:HA	1:E:455:GLY:HA3	1.86	0.57
1:C:120:PHE:HB3	1:C:147:GLN:HE22	1.68	0.57
1:F:276:ASN:HB3	6:F:803:NAG:C7	2.35	0.56
3:B:10:A:H2'	3:B:11:A:H8	1.70	0.56
1:F:188:ARG:HA	1:F:214:SER:HB3	1.88	0.56
1:F:303:TYR:HD2	1:F:327:TYR:HB3	1.69	0.56
1:C:153:LEU:HD23	1:C:177:LEU:HD13	1.87	0.56
1:C:171:LEU:O	1:C:198:SER:OG	2.18	0.56
1:C:59:LEU:HD13	1:C:64:LEU:HD21	1.86	0.56
1:C:405:LEU:HD22	1:C:410:LEU:HD11	1.86	0.56
1:E:123:CYS:O	1:E:147:GLN:NE2	2.39	0.56
1:E:593:ASN:HA	1:E:617:ASN:HB3	1.87	0.56
1:D:85:PHE:HA	1:D:109:HIS:HB2	1.86	0.56
1:F:574:GLY:N	1:F:597:ASN:OD1	2.38	0.56
1:F:130:ASP:HA	1:F:154:ASP:HB3	1.86	0.56
1:C:104:VAL:HA	1:C:128:GLU:HB3	1.88	0.56
1:F:120:PHE:HB3	1:F:147:GLN:HE22	1.71	0.56
1:F:359:GLU:HA	1:F:382:LEU:HA	1.87	0.56
1:D:353:GLN:HA	1:D:378:GLY:HA3	1.88	0.55
1:D:547:TRP:HH2	1:D:558:PHE:HB3	1.71	0.55
1:E:126:LEU:HD21	1:E:129:LEU:HB2	1.88	0.55
1:D:188:ARG:HA	1:D:214:SER:HB3	1.88	0.55
1:C:152:LYS:HA	1:C:176:GLU:HB2	1.88	0.55
1:F:36:ALA:HB3	1:F:57:LEU:HA	1.86	0.55
1:F:136:ILE:H	1:F:158:ASN:HB3	1.70	0.55
1:C:644:ARG:O	1:C:646:ASN:ND2	2.39	0.55
1:E:579:PRO:HG2	1:E:582:VAL:HG11	1.87	0.55
1:F:441:LEU:H	1:F:466:TYR:HB2	1.71	0.55
1:E:335:THR:HG22	1:E:336:LYS:N	2.17	0.55
1:E:97:GLN:HB2	1:E:122:PHE:CE2	2.41	0.55
1:F:534:GLU:HA	1:F:565:LEU:HA	1.88	0.55
1:E:64:LEU:HD22	1:E:86:ASN:HD21	1.72	0.54
1:F:383:LYS:HA	1:F:410:LEU:HA	1.89	0.54
1:F:478:ALA:HA	1:F:505:PRO:HG3	1.88	0.54
1:C:246:LEU:O	1:C:249:THR:OG1	2.20	0.54
1:E:136:ILE:H	1:E:158:ASN:HB3	1.72	0.54
1:C:579:PRO:HG2	1:C:582:VAL:HG11	1.89	0.54
1:E:353:GLN:HA	1:E:378:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD23	1:C:394:LEU:O	2.07	0.54
1:D:534:GLU:HA	1:D:565:LEU:HA	1.88	0.54
1:F:200:LEU:N	1:F:223:LYS:O	2.40	0.54
1:D:569:ASN:OD1	1:D:593:ASN:ND2	2.41	0.54
1:F:67:LEU:HB3	1:F:95:LEU:HD21	1.89	0.54
1:D:255:SER:HA	1:D:281:ASP:HB3	1.89	0.53
1:C:178:LEU:HA	1:C:204:ASP:HB3	1.90	0.53
1:C:353:GLN:HA	1:C:378:GLY:HA3	1.90	0.53
1:F:324:ASN:OD1	1:F:326:ARG:NH1	2.42	0.53
1:D:332:ARG:HH21	1:D:336:LYS:HE3	1.73	0.53
1:E:154:ASP:HA	1:E:178:LEU:HB2	1.90	0.53
1:D:574:GLY:N	1:D:597:ASN:OD1	2.41	0.53
1:E:127:THR:HA	1:E:150:LEU:HA	1.90	0.53
1:F:42:LYS:HE3	2:A:12:A:H5'	1.91	0.53
1:F:493:LEU:HD11	1:F:519:ILE:HG22	1.91	0.53
1:D:387:LEU:O	1:D:418:ASN:ND2	2.32	0.53
1:C:680:THR:HG21	1:D:680:THR:HG21	1.91	0.53
1:F:126:LEU:HG	1:F:150:LEU:HD13	1.91	0.53
1:C:332:ARG:NH1	1:C:365:ASP:OD1	2.42	0.53
1:D:316:PRO:HA	1:D:351:SER:HA	1.91	0.53
1:F:59:LEU:HD13	1:F:64:LEU:HD21	1.90	0.53
1:D:301:LEU:HD21	1:D:304:LEU:HB2	1.91	0.53
1:D:324:ASN:OD1	1:D:326:ARG:NH1	2.41	0.53
1:E:431:LEU:HB3	1:E:434:LEU:HG	1.91	0.53
1:E:583:PHE:O	1:E:610:GLN:NE2	2.42	0.53
1:F:366:ASN:HB2	1:F:390:THR:HG23	1.90	0.52
1:C:540:HIS:ND1	3:B:28:A:OP1	2.32	0.52
1:D:277:LEU:HD12	1:D:298:LEU:HD22	1.92	0.52
1:F:255:SER:HA	1:F:281:ASP:HB3	1.91	0.52
1:F:507:ARG:O	1:F:532:ASN:ND2	2.35	0.52
1:D:644:ARG:O	1:D:646:ASN:ND2	2.42	0.52
1:D:120:PHE:HB3	1:D:147:GLN:HE22	1.75	0.52
1:E:55:THR:O	1:E:79:ALA:N	2.42	0.52
1:F:139:ILE:HD12	1:F:160:LEU:HD11	1.91	0.52
1:D:394:LEU:O	1:D:394:LEU:HD23	2.10	0.52
1:E:58:ASN:ND2	1:E:82:ASP:OD2	2.43	0.52
1:E:66:ARG:HH12	1:E:68:PRO:HA	1.74	0.52
1:E:680:THR:HG21	1:F:680:THR:HG21	1.92	0.52
1:E:246:LEU:O	1:E:249:THR:OG1	2.22	0.52
1:F:37:ASP:HA	1:F:58:ASN:HB3	1.92	0.52
1:C:372:LYS:HG3	1:C:373:SER:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:HA	1:C:214:SER:HB3	1.92	0.51
1:E:56:VAL:HG22	1:E:80:ILE:HG12	1.92	0.51
1:D:547:TRP:HD1	1:D:578:ILE:HG22	1.74	0.51
1:D:59:LEU:HD13	1:D:64:LEU:HD21	1.92	0.51
1:F:488:LEU:HB2	1:F:514:LEU:HD23	1.93	0.51
1:C:400:GLU:HG2	4:K:1:NAG:H82	1.93	0.51
1:F:188:ARG:HB2	1:F:191:GLU:HG2	1.92	0.51
1:F:316:PRO:HA	1:F:351:SER:HA	1.93	0.51
1:C:522:ILE:HG23	1:C:558:PHE:HZ	1.75	0.51
1:D:379:LEU:HD13	1:D:382:LEU:HD22	1.92	0.51
1:E:147:GLN:HB3	1:E:150:LEU:HD22	1.92	0.51
1:F:567:ILE:HG22	1:F:591:SER:HB3	1.93	0.51
2:A:37:A:O2'	2:A:38:A:OP1	2.26	0.51
1:C:397:LEU:HB2	1:C:423:ILE:HG22	1.93	0.50
1:D:136:ILE:H	1:D:158:ASN:HB3	1.76	0.50
1:F:338:SER:O	1:F:340:SER:N	2.44	0.50
1:D:200:LEU:N	1:D:223:LYS:O	2.44	0.50
3:B:43:A:O2'	3:B:44:A:OP1	2.24	0.50
1:D:37:ASP:HA	1:D:58:ASN:HB3	1.94	0.50
1:D:547:TRP:HB3	1:D:577:GLU:O	2.11	0.50
1:C:188:ARG:HB2	1:C:191:GLU:HG2	1.92	0.50
1:E:188:ARG:HB2	1:E:191:GLU:HG2	1.92	0.50
1:F:644:ARG:O	1:F:646:ASN:ND2	2.45	0.50
3:B:38:A:H2'	3:B:39:A:C8	2.46	0.50
1:D:511:ILE:HG12	1:D:535:ILE:HD13	1.94	0.50
1:E:493:LEU:HD13	1:E:496:VAL:HG11	1.94	0.50
1:D:80:ILE:HG22	1:D:103:LYS:HB2	1.93	0.50
1:E:485:ARG:HG2	1:E:511:ILE:HD12	1.93	0.50
1:F:435:ARG:HB2	1:F:436:ILE:HD12	1.94	0.50
1:C:485:ARG:HG2	1:C:511:ILE:HD12	1.94	0.49
1:C:593:ASN:HA	1:C:617:ASN:HB3	1.92	0.49
1:D:338:SER:O	1:D:340:SER:N	2.44	0.49
1:D:431:LEU:HD12	1:D:434:LEU:HB2	1.94	0.49
1:F:201:ARG:HA	1:F:225:PHE:HB2	1.94	0.49
3:B:47:U:H2'	3:B:48:U:C6	2.47	0.49
1:D:507:ARG:O	1:D:532:ASN:ND2	2.36	0.49
1:E:438:ASP:HA	1:E:463:TYR:HB3	1.94	0.49
1:F:262:LEU:O	1:F:288:HIS:N	2.40	0.49
1:C:387:LEU:HB2	1:C:415:LEU:HD23	1.95	0.49
1:C:394:LEU:HD21	1:C:397:LEU:HD21	1.95	0.49
1:E:470:LEU:HD12	1:E:491:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:644:ARG:O	1:E:646:ASN:ND2	2.45	0.49
3:B:10:A:H2'	3:B:11:A:C8	2.47	0.49
1:D:139:ILE:HD12	1:D:160:LEU:HD11	1.95	0.49
1:F:493:LEU:HD13	1:F:496:VAL:HG21	1.95	0.49
1:F:519:ILE:HG12	1:F:541:ASN:HB3	1.95	0.49
1:C:470:LEU:HD12	1:C:491:VAL:HB	1.94	0.48
1:E:453:TRP:HZ2	1:E:464:LEU:HD11	1.77	0.48
2:A:40:A:H61	3:B:51:U:H3	1.60	0.48
1:D:303:TYR:HD2	1:D:327:TYR:HB3	1.78	0.48
1:C:105:LEU:N	1:C:128:GLU:O	2.41	0.48
1:C:199:SER:HA	1:C:223:LYS:HB2	1.94	0.48
1:F:48:ASP:HB2	1:F:74:ARG:HD3	1.95	0.48
1:E:80:ILE:HG22	1:E:103:LYS:HB2	1.93	0.48
1:F:488:LEU:HD12	1:F:491:VAL:HG21	1.94	0.48
1:D:547:TRP:CG	1:D:579:PRO:HD2	2.49	0.48
1:F:178:LEU:HA	1:F:204:ASP:HB3	1.95	0.48
1:F:520:ALA:O	1:F:545:ARG:NH2	2.47	0.48
1:C:373:SER:O	1:C:404:SER:OG	2.30	0.48
1:D:130:ASP:HA	1:D:154:ASP:HB3	1.96	0.48
1:E:43:LEU:HD11	1:E:47:PRO:HD3	1.95	0.48
1:F:127:THR:HA	1:F:150:LEU:HA	1.96	0.48
1:D:558:PHE:CD2	1:D:559:LEU:HG	2.48	0.48
1:E:80:ILE:HB	1:E:104:VAL:HB	1.96	0.48
1:F:85:PHE:HB3	2:A:10:A:H5'	1.96	0.48
1:C:109:HIS:HA	1:C:133:SER:HB2	1.96	0.47
1:C:247:SER:OG	1:C:271:GLY:O	2.25	0.47
1:D:59:LEU:N	1:D:82:ASP:O	2.46	0.47
1:F:301:LEU:HD21	1:F:304:LEU:HB2	1.96	0.47
3:B:65:U:H2'	3:B:66:U:H6	1.79	0.47
1:E:496:VAL:HG23	1:E:522:ILE:HD13	1.96	0.47
1:F:578:ILE:HD12	1:F:606:ILE:HG21	1.96	0.47
1:F:302:ARG:NH1	1:F:303:TYR:OH	2.47	0.47
1:F:358:LEU:HD21	1:F:361:LEU:HD13	1.96	0.47
3:B:12:A:H2'	3:B:13:A:H8	1.80	0.47
1:D:387:LEU:HB2	1:D:415:LEU:HD23	1.97	0.47
1:C:522:ILE:HG12	1:C:526:LEU:HD22	1.95	0.47
1:E:643:MET:HG3	1:E:648:PHE:HZ	1.79	0.47
1:C:200:LEU:N	1:C:223:LYS:O	2.40	0.47
1:D:40:HIS:ND1	3:B:12:A:OP1	2.48	0.47
1:D:331:LYS:HG3	1:D:364:ASP:HB2	1.97	0.47
2:A:51:U:H2'	2:A:52:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:HB2	1:D:191:GLU:HG2	1.97	0.47
1:E:106:ASN:HA	1:E:130:ASP:HB3	1.96	0.47
1:F:59:LEU:HB2	1:F:83:ALA:HA	1.95	0.47
1:F:298:LEU:HD13	1:F:301:LEU:HD13	1.96	0.47
2:A:37:A:H2'	2:A:38:A:C8	2.49	0.47
1:F:543:LEU:O	1:F:543:LEU:HD23	2.15	0.46
1:D:649:ASP:O	1:D:654:SER:OG	2.28	0.46
1:E:252:GLN:HA	1:E:277:LEU:HA	1.97	0.46
1:C:522:ILE:HG23	1:C:558:PHE:CZ	2.50	0.46
1:D:302:ARG:NH1	1:D:303:TYR:OH	2.48	0.46
1:F:558:PHE:CD2	1:F:559:LEU:HG	2.50	0.46
1:C:447:LYS:HE3	1:C:473:SER:HB3	1.96	0.46
1:D:48:ASP:N	1:D:48:ASP:OD1	2.48	0.46
1:E:211:LYS:HA	1:E:211:LYS:HD3	1.82	0.46
3:B:19:A:H2'	3:B:20:A:H8	1.81	0.46
1:C:33:TYR:O	1:C:35:VAL:N	2.48	0.46
1:E:335:THR:O	1:E:336:LYS:C	2.53	0.46
1:E:394:LEU:HD23	1:E:394:LEU:O	2.16	0.46
1:F:462:ILE:HG12	1:F:483:LEU:HD11	1.98	0.46
1:F:656:SER:O	1:F:660:ASN:ND2	2.49	0.46
3:B:52:U:H2'	3:B:53:U:C6	2.51	0.46
1:C:108:GLN:HB2	1:C:132:MET:HB3	1.98	0.46
1:C:202:LYS:HA	1:C:226:ALA:HB3	1.97	0.46
1:F:48:ASP:N	1:F:48:ASP:OD1	2.48	0.46
1:C:80:ILE:HB	1:C:104:VAL:HB	1.97	0.46
1:C:161:SER:HB2	1:C:183:LYS:HZ2	1.81	0.46
1:C:316:PRO:O	1:C:354:TRP:NE1	2.35	0.46
1:D:89:SER:HB3	2:A:83:U:H4'	1.98	0.46
1:C:569:ASN:OD1	1:C:593:ASN:ND2	2.49	0.45
1:C:319:PHE:HD2	1:C:355:LEU:HD21	1.81	0.45
1:D:456:LEU:HD12	1:D:459:ILE:HD13	1.97	0.45
1:E:33:TYR:O	1:E:35:VAL:N	2.48	0.45
1:F:233:GLN:HB2	1:F:260:GLN:HE22	1.82	0.45
1:C:295:PHE:HB3	1:C:322:LEU:HD21	1.99	0.45
1:D:42:LYS:HD2	3:B:12:A:H4'	1.98	0.45
1:F:218:PHE:HE2	1:F:242:LEU:HD11	1.82	0.45
1:D:462:ILE:HB	1:D:486:LEU:HD12	1.98	0.45
1:E:575:LEU:HG	1:E:599:LEU:HD21	1.97	0.45
1:F:481:PRO:HA	1:F:506:LEU:HD13	1.98	0.45
1:F:544:ALA:HA	1:F:575:LEU:HD13	1.99	0.45
1:D:488:LEU:HB2	1:D:514:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:GLU:HA	1:E:241:LYS:HZ1	1.82	0.45
3:B:68:U:H2'	3:B:69:U:H6	1.81	0.45
1:C:56:VAL:HG22	1:C:80:ILE:HG12	1.98	0.45
1:C:315:SER:HB2	5:J:1:NAG:H3	1.99	0.45
1:E:110:ASN:HB3	1:E:112:LEU:HD23	1.98	0.45
1:E:440:GLY:O	1:E:442:ASN:ND2	2.50	0.45
1:C:688:PRO:HG2	1:C:691:LEU:HD12	1.98	0.45
1:E:188:ARG:HA	1:E:214:SER:HB3	1.99	0.45
1:D:178:LEU:HA	1:D:204:ASP:HB3	1.98	0.45
1:C:316:PRO:HG2	5:J:1:NAG:H5	1.99	0.45
1:D:201:ARG:HA	1:D:225:PHE:HB2	1.99	0.45
3:B:62:U:H2'	3:B:63:U:C6	2.52	0.45
1:F:387:LEU:O	1:F:418:ASN:ND2	2.34	0.44
1:F:426:GLY:HA2	1:F:454:ARG:HB3	2.00	0.44
1:D:67:LEU:HB3	1:D:95:LEU:HD21	1.99	0.44
1:D:256:LEU:HB2	1:D:282:LEU:HD23	1.97	0.44
1:F:250:SER:HA	1:F:276:ASN:HD21	1.81	0.44
1:F:649:ASP:O	1:F:654:SER:OG	2.24	0.44
3:B:52:U:H2'	3:B:53:U:H6	1.82	0.44
1:E:483:LEU:HB2	1:E:506:LEU:HD11	2.00	0.44
1:F:185:LEU:HD23	1:F:185:LEU:H	1.82	0.44
1:C:117:ASP:HA	1:C:143:PRO:HA	2.00	0.44
1:F:67:LEU:HD22	1:F:72:PHE:HZ	1.83	0.44
1:F:137:HIS:HD2	1:F:138:LYS:HG2	1.83	0.44
1:F:511:ILE:HG12	1:F:535:ILE:HD13	1.99	0.44
1:C:96:CYS:HB3	1:C:122:PHE:HB2	1.99	0.44
1:C:352:PHE:HB3	1:C:379:LEU:HD21	1.99	0.44
1:D:421:SER:HA	1:D:444:ILE:HA	2.00	0.44
1:F:193:GLU:HA	1:F:220:THR:HB	1.99	0.44
1:F:256:LEU:HB2	1:F:282:LEU:HD23	1.99	0.44
1:C:191:GLU:HG3	1:C:192:LEU:HD12	2.00	0.44
1:C:520:ALA:HB1	2:A:66:U:H4'	1.99	0.44
1:E:411:LEU:HG	1:E:435:ARG:HG3	2.00	0.44
1:F:50:LEU:HA	1:F:74:ARG:HH21	1.83	0.44
1:C:34:ASN:OD1	1:C:55:THR:OG1	2.35	0.44
1:C:383:LYS:HA	1:C:410:LEU:HA	1.99	0.44
1:D:221:ILE:HG21	1:D:224:LEU:HB2	2.00	0.44
1:F:431:LEU:HD12	1:F:434:LEU:HB2	1.99	0.44
1:F:487:MET:SD	1:F:487:MET:N	2.91	0.44
1:F:656:SER:OG	1:F:697:CYS:SG	2.71	0.44
2:A:14:A:O2'	2:A:15:A:OP1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:HB2	1:D:74:ARG:HD3	1.99	0.44
3:B:27:A:H2'	3:B:28:A:H8	1.81	0.44
3:B:58:U:H2'	3:B:59:U:H6	1.83	0.44
1:C:435:ARG:HA	1:C:459:ILE:HA	2.00	0.43
1:E:397:LEU:HB2	1:E:423:ILE:HG22	1.98	0.43
1:E:406:ALA:HB2	1:E:430:TRP:HB3	2.00	0.43
1:F:273:LYS:HG2	1:F:274:TRP:CE3	2.53	0.43
1:F:366:ASN:HB3	1:F:368:ILE:HD12	1.99	0.43
1:F:406:ALA:HA	1:F:430:TRP:HB3	2.00	0.43
1:D:235:ASN:HB2	1:D:238:LEU:HB2	2.00	0.43
1:D:298:LEU:HD13	1:D:301:LEU:HD13	2.00	0.43
1:F:46:ILE:HD11	1:F:64:LEU:HG	1.99	0.43
1:C:641:LEU:HB3	1:C:669:ILE:HG12	2.00	0.43
1:E:38:CYS:H	1:E:58:ASN:HB3	1.84	0.43
1:E:656:SER:O	1:E:660:ASN:ND2	2.51	0.43
3:B:67:U:H2'	3:B:68:U:H6	1.81	0.43
1:D:199:SER:HA	1:D:223:LYS:HB2	2.00	0.43
1:E:108:GLN:O	1:E:110:ASN:ND2	2.51	0.43
1:E:192:LEU:HB3	1:E:221:ILE:HD11	2.00	0.43
1:C:526:LEU:O	1:C:527:LEU:HG	2.18	0.43
1:D:67:LEU:HG	1:D:88:ILE:HD13	2.00	0.43
1:D:359:GLU:HA	1:D:382:LEU:HA	1.99	0.43
1:E:303:TYR:HD1	1:E:327:TYR:HB3	1.83	0.43
5:X:1:NAG:H62	5:X:2:NAG:HN2	1.83	0.43
1:D:366:ASN:HB2	1:D:390:THR:HG23	2.00	0.43
2:A:39:A:H2'	2:A:40:A:C8	2.54	0.43
1:D:50:LEU:HA	1:D:74:ARG:HH21	1.83	0.43
1:E:255:SER:HA	1:E:281:ASP:HB3	2.00	0.43
1:C:259:ASN:N	1:C:285:ASN:OD1	2.52	0.43
1:C:382:LEU:HD21	1:C:385:LEU:HB2	2.01	0.43
1:E:568:LEU:HB3	1:E:592:ILE:HD13	2.01	0.43
2:A:14:A:H2'	2:A:15:A:C8	2.54	0.43
3:B:40:A:H2'	3:B:41:A:C8	2.54	0.43
1:C:193:GLU:HA	1:C:220:THR:HB	2.01	0.43
1:C:483:LEU:HB2	1:C:506:LEU:HD11	2.01	0.43
1:C:656:SER:O	1:C:660:ASN:ND2	2.51	0.43
1:D:139:ILE:HG21	1:D:165:LEU:HD12	2.00	0.43
3:B:62:U:H2'	3:B:63:U:H6	1.84	0.43
1:D:567:ILE:HG22	1:D:591:SER:HB3	2.01	0.43
1:E:224:LEU:H	1:E:224:LEU:HD23	1.84	0.43
1:C:144:PHE:HD2	1:C:165:LEU:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ILE:HD11	1:C:526:LEU:HB2	2.01	0.42
1:D:272:LEU:HD13	1:D:275:THR:HG21	2.00	0.42
1:E:372:LYS:HG3	1:E:373:SER:H	1.83	0.42
1:C:61:HIS:HA	2:A:45:A:OP1	2.20	0.42
1:C:144:PHE:CD2	1:C:165:LEU:HD21	2.54	0.42
1:D:134:ASN:N	1:D:158:ASN:OD1	2.42	0.42
3:B:43:A:H2'	3:B:44:A:C8	2.54	0.42
1:C:127:THR:HA	1:C:150:LEU:HA	2.01	0.42
1:D:241:LYS:HE2	1:D:241:LYS:HB3	1.90	0.42
1:F:483:LEU:HD23	1:F:506:LEU:HD11	2.01	0.42
3:B:64:U:H2'	3:B:65:U:H6	1.84	0.42
1:C:359:GLU:HA	1:C:382:LEU:HA	2.02	0.42
1:D:368:ILE:O	1:D:391:PHE:HA	2.20	0.42
1:D:547:TRP:CH2	1:D:558:PHE:HB3	2.52	0.42
1:F:363:MET:HB2	1:F:387:LEU:HD23	2.01	0.42
1:F:569:ASN:OD1	1:F:593:ASN:ND2	2.52	0.42
3:B:38:A:H2'	3:B:39:A:H8	1.83	0.42
1:D:633:PRO:N	1:D:634:PRO:HD2	2.35	0.42
1:E:93:PRO:HB2	1:E:122:PHE:CZ	2.54	0.42
1:E:522:ILE:HD12	1:E:522:ILE:HA	1.90	0.42
1:C:435:ARG:O	1:C:460:PHE:N	2.36	0.42
1:D:127:THR:HA	1:D:150:LEU:HA	2.00	0.42
1:D:438:ASP:OD2	4:R:1:NAG:N2	2.43	0.42
1:D:477:PHE:HB3	1:D:506:LEU:HD21	2.01	0.42
3:B:38:A:O2'	3:B:39:A:OP1	2.28	0.42
1:C:175:GLN:HB3	1:C:201:ARG:HB3	2.00	0.42
1:C:651:THR:OG1	1:C:654:SER:OG	2.29	0.42
1:E:175:GLN:O	1:E:201:ARG:N	2.52	0.42
1:E:511:ILE:HG23	1:E:535:ILE:HB	2.00	0.42
1:E:633:PRO:N	1:E:634:PRO:HD2	2.35	0.42
1:F:199:SER:HA	1:F:223:LYS:HB2	2.02	0.42
1:C:224:LEU:H	1:C:224:LEU:HD23	1.85	0.42
1:E:551:ASN:HB2	1:E:552:PRO:HD3	2.02	0.42
1:E:688:PRO:HG2	1:E:691:LEU:HD12	2.02	0.42
1:F:466:TYR:HD1	1:F:490:ARG:HH11	1.67	0.42
1:F:477:PHE:HB3	1:F:506:LEU:HD21	2.01	0.42
1:F:506:LEU:HB3	1:F:509:LEU:HD23	2.02	0.42
1:C:137:HIS:ND1	1:C:138:LYS:HE3	2.35	0.42
1:D:697:CYS:O	1:D:698:LYS:HG3	2.20	0.42
2:A:51:U:H2'	2:A:52:U:H6	1.84	0.42
3:B:63:U:H2'	3:B:64:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:VAL:HG22	1:D:80:ILE:HG12	2.02	0.42
1:D:171:LEU:O	1:D:198:SER:OG	2.31	0.42
1:E:569:ASN:OD1	1:E:593:ASN:ND2	2.53	0.42
3:B:65:U:H2'	3:B:66:U:C6	2.54	0.42
1:D:94:GLU:O	1:D:98:ILE:HG12	2.20	0.41
1:D:213:PHE:CG	1:D:242:LEU:HD13	2.55	0.41
1:D:511:ILE:HG12	1:D:535:ILE:HB	2.02	0.41
1:F:94:GLU:O	1:F:98:ILE:HG12	2.20	0.41
1:F:329:SER:HA	1:F:362:ASN:HB3	2.02	0.41
4:K:1:NAG:H61	4:K:2:NAG:N2	2.35	0.41
1:C:29:CYS:N	1:C:41:LEU:HD21	2.34	0.41
1:D:366:ASN:HB3	1:D:368:ILE:HD12	2.01	0.41
1:E:29:CYS:N	1:E:41:LEU:HD21	2.35	0.41
1:E:383:LYS:HA	1:E:410:LEU:HA	2.02	0.41
3:B:44:A:C2'	3:B:45:A:H5'	2.50	0.41
3:B:47:U:H2'	3:B:48:U:H6	1.84	0.41
1:C:117:ASP:OD1	1:C:118:GLN:N	2.53	0.41
1:C:633:PRO:N	1:C:634:PRO:HD2	2.35	0.41
1:E:187:LEU:HD23	1:E:192:LEU:HD11	2.02	0.41
1:E:641:LEU:HB3	1:E:669:ILE:HG12	2.02	0.41
1:E:644:ARG:NH1	1:E:671:GLU:OE1	2.52	0.41
1:F:456:LEU:HD12	1:F:459:ILE:HD13	2.02	0.41
2:A:50:U:H3	3:B:41:A:H61	1.69	0.41
3:B:12:A:H2'	3:B:13:A:C8	2.55	0.41
1:C:212:GLU:HA	1:C:241:LYS:HZ1	1.85	0.41
1:E:48:ASP:OD1	1:E:48:ASP:N	2.53	0.41
3:B:63:U:H2'	3:B:64:U:C6	2.55	0.41
3:B:71:U:H2'	3:B:72:U:H6	1.85	0.41
1:C:277:LEU:HD23	1:C:277:LEU:HA	1.94	0.41
1:D:32:ARG:HD3	1:D:32:ARG:HA	1.91	0.41
1:E:152:LYS:HA	1:E:176:GLU:HB2	2.02	0.41
1:E:485:ARG:HG2	1:E:511:ILE:HB	2.02	0.41
1:F:316:PRO:O	1:F:354:TRP:NE1	2.37	0.41
1:E:527:LEU:HD23	1:E:527:LEU:O	2.20	0.41
1:F:531:GLU:O	1:F:564:HIS:HB2	2.21	0.41
1:C:136:ILE:H	1:C:158:ASN:HB3	1.85	0.41
1:D:273:LYS:HG2	1:D:274:TRP:CE3	2.54	0.41
1:D:337:GLN:H	1:D:367:ASN:HD22	1.69	0.41
3:B:19:A:H2'	3:B:20:A:C8	2.56	0.41
1:C:32:ARG:HG3	1:C:35:VAL:HG23	2.02	0.41
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:HB	1:D:104:VAL:HB	2.03	0.41
1:D:534:GLU:HB2	1:D:535:ILE:HD12	2.03	0.41
1:F:512:LEU:HD23	1:F:527:LEU:HD11	2.02	0.41
1:C:42:LYS:HD3	1:C:42:LYS:HA	1.88	0.41
1:C:106:ASN:HA	1:C:130:ASP:HB3	2.03	0.41
1:C:534:GLU:HA	1:C:565:LEU:HA	2.03	0.41
1:D:202:LYS:HA	1:D:226:ALA:HB3	2.02	0.41
1:D:261:LEU:HB2	1:D:285:ASN:HB3	2.02	0.41
1:E:311:ILE:HD12	1:E:333:ALA:HB1	2.03	0.41
1:E:326:ARG:HA	1:E:358:LEU:HA	2.03	0.41
1:E:334:PHE:HD1	1:E:345:PRO:HB2	1.86	0.41
1:F:56:VAL:HG22	1:F:80:ILE:HG12	2.03	0.41
1:F:87:SER:OG	2:A:9:A:N3	2.52	0.41
1:F:633:PRO:N	1:F:634:PRO:HD2	2.35	0.41
3:B:24:A:H2'	3:B:25:A:H8	1.86	0.41
3:B:68:U:H2'	3:B:69:U:C6	2.55	0.41
1:C:485:ARG:HG2	1:C:511:ILE:HB	2.03	0.41
1:D:50:LEU:O	1:D:52:SER:N	2.52	0.41
1:E:67:LEU:HD23	1:E:67:LEU:HA	1.92	0.41
1:E:137:HIS:ND1	1:E:138:LYS:HE3	2.36	0.41
1:E:387:LEU:HB2	1:E:415:LEU:HD23	2.03	0.41
1:F:486:LEU:HD12	1:F:486:LEU:HA	1.94	0.41
3:B:27:A:H2'	3:B:28:A:C8	2.56	0.41
1:F:235:ASN:ND2	1:F:260:GLN:HE21	2.19	0.40
1:F:272:LEU:HD12	1:F:277:LEU:HD11	2.02	0.40
1:F:507:ARG:HH21	1:F:530:LEU:HD22	1.87	0.40
2:A:64:U:H2'	2:A:65:U:H6	1.86	0.40
1:D:96:CYS:HB3	1:D:122:PHE:HB2	2.03	0.40
1:F:576:ASP:HA	1:F:598:ASN:O	2.21	0.40
1:C:274:TRP:NE1	4:G:1:NAG:O6	2.55	0.40
1:C:91:LEU:HD11	1:C:95:LEU:HD22	2.04	0.40
1:E:420:ILE:HG22	1:E:444:ILE:HG12	2.03	0.40
1:F:397:LEU:HB2	1:F:423:ILE:HG22	2.03	0.40
3:B:50:U:H2'	3:B:51:U:H6	1.86	0.40
1:D:325:LEU:HD21	1:D:328:LEU:HD13	2.03	0.40
1:E:120:PHE:HB3	1:E:147:GLN:HE22	1.87	0.40

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	C	655/680 (96%)	625 (95%)	30 (5%)	0	100	100
1	D	664/680 (98%)	630 (95%)	33 (5%)	1 (0%)	47	79
1	E	655/680 (96%)	625 (95%)	30 (5%)	0	100	100
1	F	664/680 (98%)	628 (95%)	35 (5%)	1 (0%)	47	79
All	All	2638/2720 (97%)	2508 (95%)	128 (5%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	31	VAL
1	F	31	VAL

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	C	619/635 (98%)	619 (100%)	0	100	100
1	D	625/635 (98%)	620 (99%)	5 (1%)	81	93
1	E	619/635 (98%)	617 (100%)	2 (0%)	92	96
1	F	625/635 (98%)	622 (100%)	3 (0%)	88	95
All	All	2488/2540 (98%)	2478 (100%)	10 (0%)	91	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	140	LYS
1	D	152	LYS
1	D	487	MET
1	D	547	TRP
1	D	698	LYS
1	E	336	LYS
1	E	507	ARG
1	F	140	LYS
1	F	152	LYS
1	F	487	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	569	ASN
1	C	593	ASN
1	D	110	ASN
1	D	569	ASN
1	D	593	ASN
1	E	542	ASN
1	E	569	ASN
1	E	593	ASN
1	E	610	GLN
1	F	110	ASN
1	F	260	GLN
1	F	337	GLN
1	F	569	ASN
1	F	593	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	80/81 (98%)	30 (37%)	3 (3%)
3	B	80/81 (98%)	20 (25%)	5 (6%)
All	All	160/162 (98%)	50 (31%)	8 (5%)

All (50) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	A
2	A	13	A

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Mol	Chain	Res	Type
2	A	14	A
2	A	15	A
2	A	19	A
2	A	20	A
2	A	22	A
2	A	25	A
2	A	27	A
2	A	28	A
2	A	32	A
2	A	35	A
2	A	36	A
2	A	37	A
2	A	38	A
2	A	39	A
2	A	40	A
2	A	43	A
2	A	44	A
2	A	45	A
2	A	46	U
2	A	47	U
2	A	48	U
2	A	76	U
2	A	78	U
2	A	79	U
2	A	82	U
2	A	83	U
2	A	84	U
2	A	85	U
3	B	9	A
3	B	10	A
3	B	12	A
3	B	16	A
3	B	21	A
3	B	26	A
3	B	33	A
3	B	39	A
3	B	40	A
3	B	41	A
3	B	43	A
3	B	44	A
3	B	45	A
3	B	46	U

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Mol	Chain	Res	Type
3	B	62	U
3	B	77	U
3	B	78	U
3	B	79	U
3	B	80	U
3	B	83	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	14	A
2	A	37	A
2	A	39	A
3	B	15	A
3	B	38	A
3	B	40	A
3	B	43	A
3	B	77	U

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

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

5.5 Carbohydrates (i)

70 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.44	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.77	0
5	NAG	H	1	1,5	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	H	2	5	14,14,15	0.26	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	I	1	1,5	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	I	2	5	14,14,15	0.60	0	17,19,21	0.42	0
5	NAG	J	1	1,5	14,14,15	0.24	0	17,19,21	0.38	0
5	NAG	J	2	5	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	K	1	1,4	14,14,15	0.48	0	17,19,21	0.36	0
4	NAG	K	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	BMA	K	3	4	11,11,12	0.88	0	15,15,17	0.90	0
4	NAG	L	1	1,4	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.55	0
4	BMA	L	3	4	11,11,12	0.61	0	15,15,17	0.69	0
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.40	0
4	BMA	M	3	4	11,11,12	0.59	0	15,15,17	0.77	0
5	NAG	N	1	1,5	14,14,15	0.18	0	17,19,21	0.40	0
5	NAG	N	2	5	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	O	1	1,5	14,14,15	0.42	0	17,19,21	0.68	1 (5%)
5	NAG	O	2	5	14,14,15	0.27	0	17,19,21	0.38	0
5	NAG	P	1	1,5	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	Q	1	1,4	14,14,15	0.19	0	17,19,21	0.39	0
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	BMA	Q	3	4	11,11,12	0.63	0	15,15,17	0.69	0
4	NAG	R	1	1,4	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.50	0
4	BMA	R	3	4	11,11,12	0.60	0	15,15,17	0.72	0
4	NAG	S	1	1,4	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	BMA	S	3	4	11,11,12	0.59	0	15,15,17	0.75	0
5	NAG	T	1	1,5	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
5	NAG	T	2	5	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	U	1	1,4	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	U	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	BMA	U	3	4	11,11,12	0.60	0	15,15,17	0.74	0
5	NAG	V	1	1,5	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	W	1	1,5	14,14,15	0.28	0	17,19,21	0.54	0
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	X	1	1,5	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	X	2	5	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	Y	1	1,4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	Y	2	4	14,14,15	0.20	0	17,19,21	0.46	0
4	BMA	Y	3	4	11,11,12	0.55	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	Z	1	1,4	14,14,15	0.16	0	17,19,21	0.43	0
4	NAG	Z	2	4	14,14,15	0.24	0	17,19,21	0.57	0
4	BMA	Z	3	4	11,11,12	0.61	0	15,15,17	0.69	0
4	NAG	a	1	1,4	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	a	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	BMA	a	3	4	11,11,12	0.57	0	15,15,17	0.77	0
5	NAG	b	1	1,5	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	b	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	c	1	1,5	14,14,15	0.63	1 (7%)	17,19,21	0.63	1 (5%)
5	NAG	c	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	d	1	1,5	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	d	2	5	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	e	1	1,4	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	e	2	4	14,14,15	0.25	0	17,19,21	0.45	0
4	BMA	e	3	4	11,11,12	0.66	0	15,15,17	0.69	0
4	NAG	f	1	1,4	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	f	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	BMA	f	3	4	11,11,12	0.61	0	15,15,17	0.72	0
4	NAG	g	1	1,4	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	g	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	BMA	g	3	4	11,11,12	0.59	0	15,15,17	0.75	0
5	NAG	h	1	1,5	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	h	2	5	14,14,15	0.24	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	1	NAG	C1-C2	2.02	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	1	NAG	C1-O5-C5	2.95	116.19	112.19
5	O	1	NAG	C1-O5-C5	2.17	115.14	112.19
5	c	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	b	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	b	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	Z	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
4	e	3	BMA	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
4	g	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Y	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6

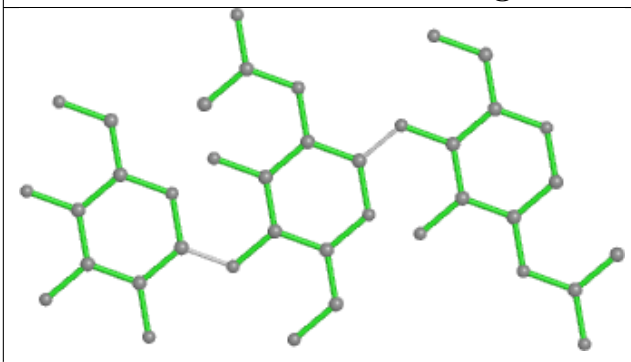
There are no ring outliers.

8 monomers are involved in 8 short contacts:

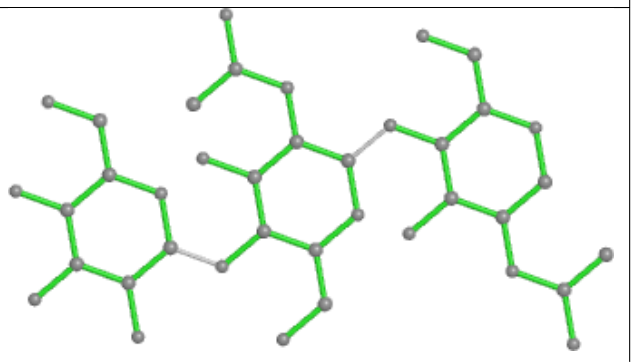
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	1	NAG	1	0
4	K	2	NAG	1	0
5	X	1	NAG	1	0
5	H	1	NAG	1	0
5	J	1	NAG	2	0
4	K	1	NAG	2	0
5	X	2	NAG	1	0
4	G	1	NAG	1	0

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

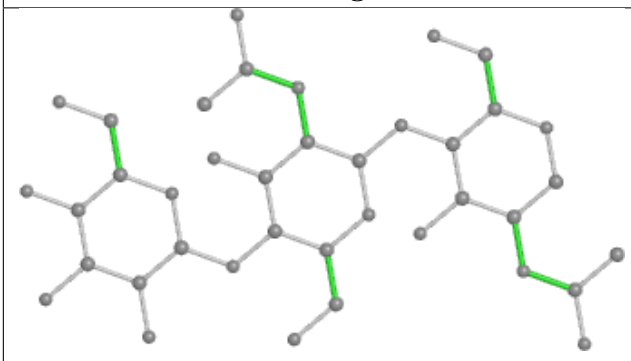
Oligosaccharide Chain G



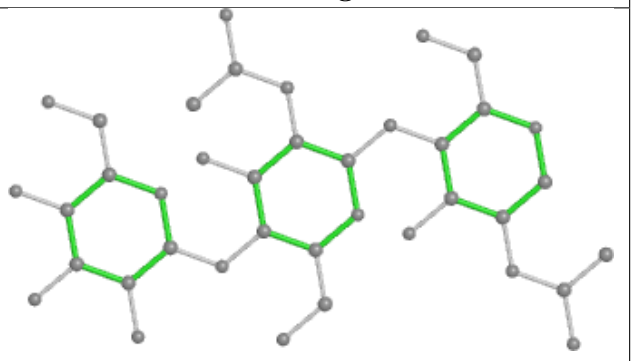
Bond lengths



Bond angles

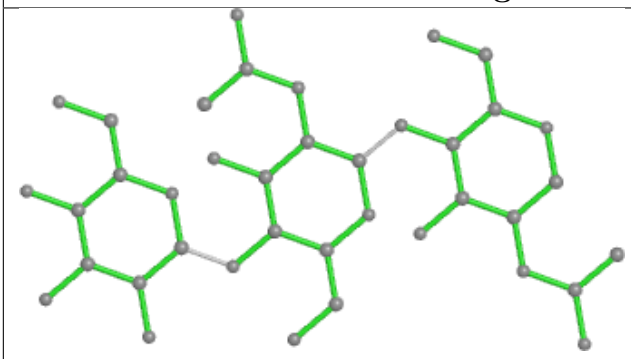


Torsions

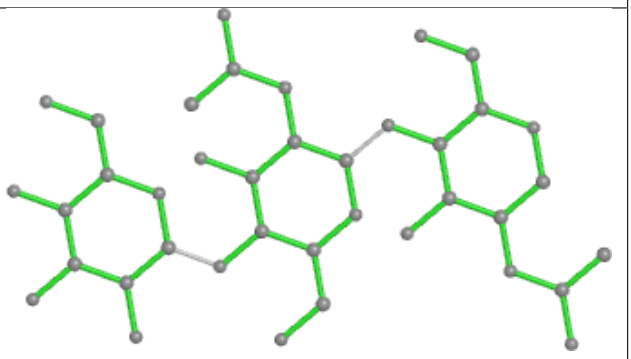


Rings

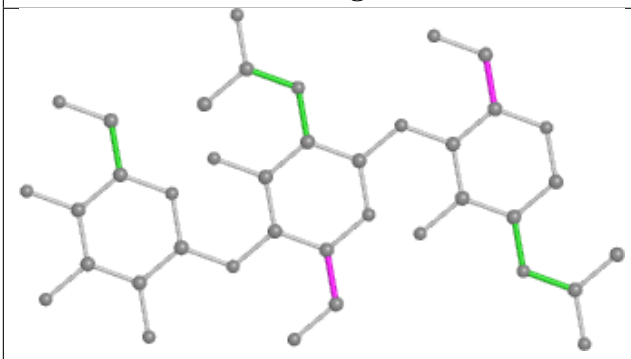
Oligosaccharide Chain K



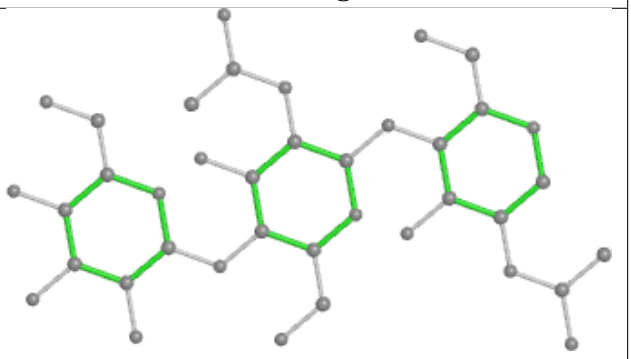
Bond lengths



Bond angles

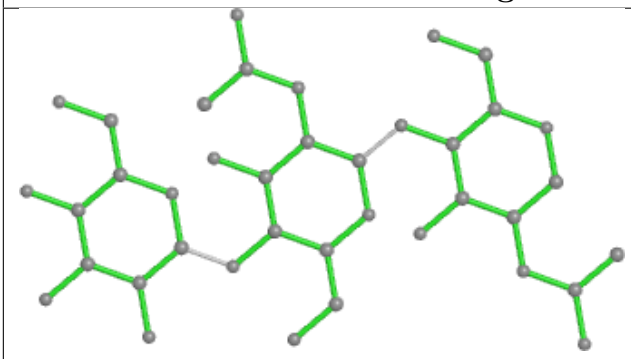


Torsions

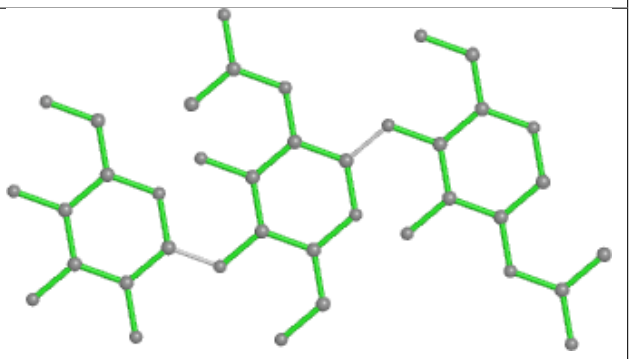


Rings

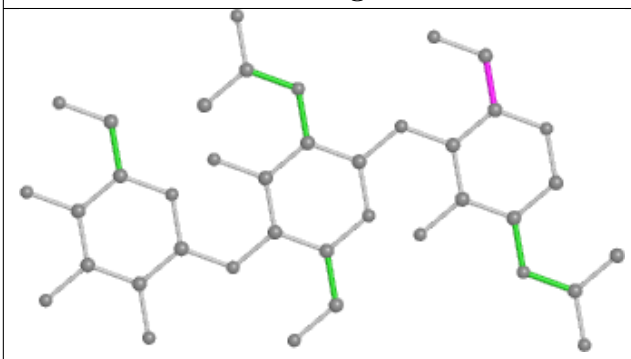
Oligosaccharide Chain L



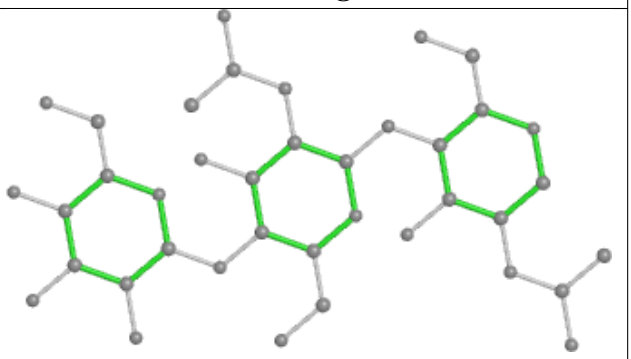
Bond lengths



Bond angles

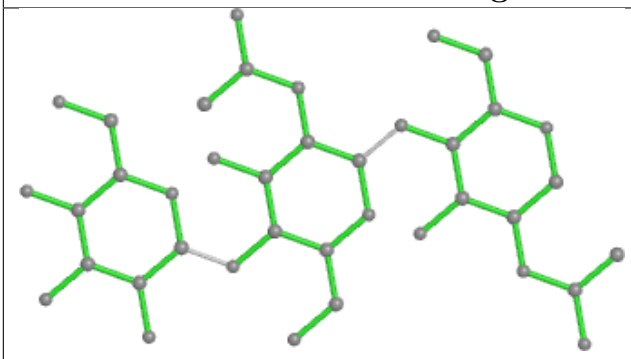


Torsions

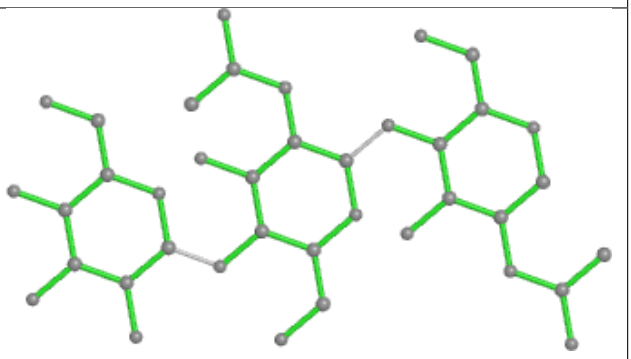


Rings

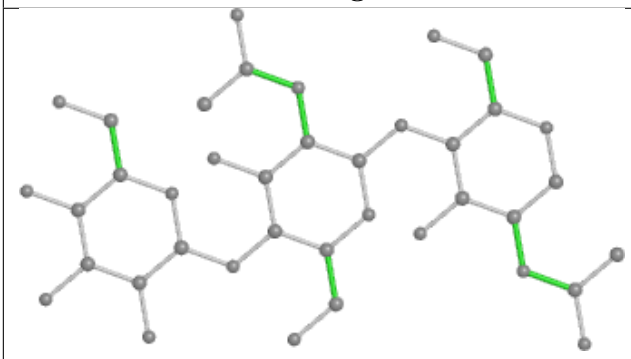
Oligosaccharide Chain M



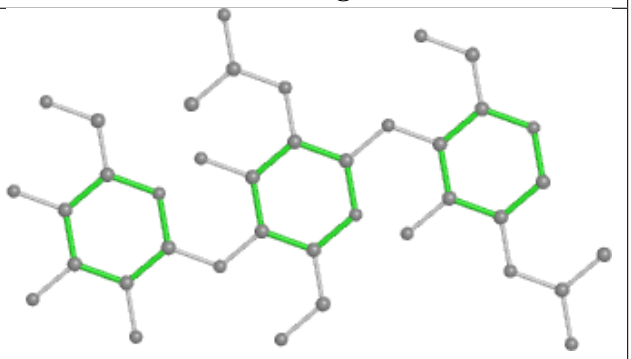
Bond lengths



Bond angles

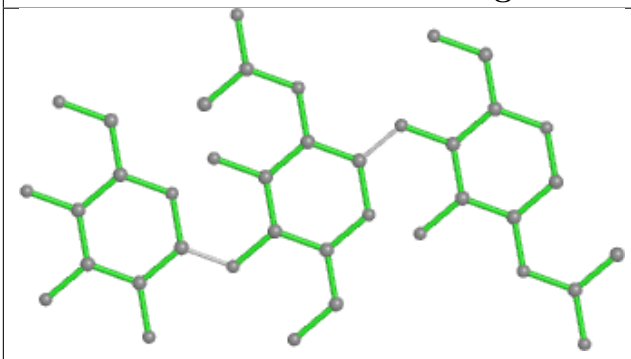


Torsions

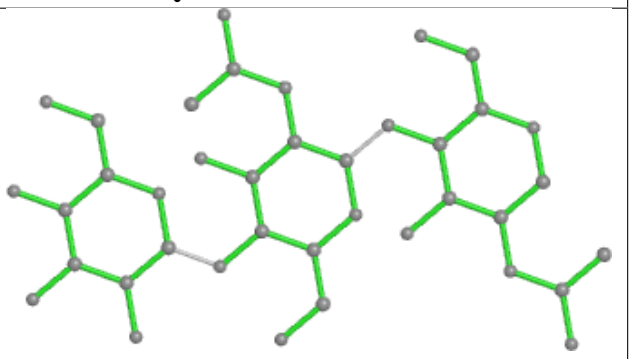


Rings

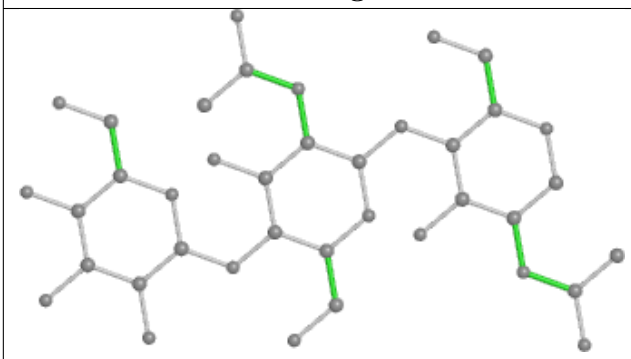
Oligosaccharide Chain Q



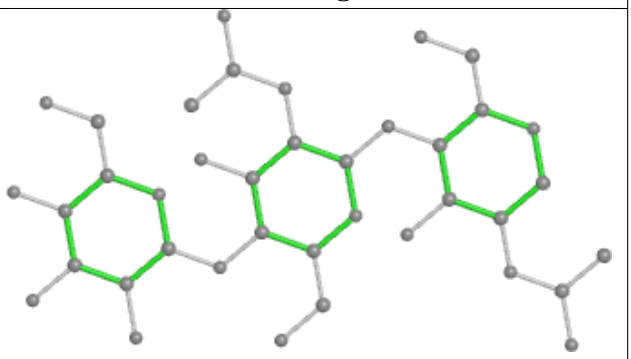
Bond lengths



Bond angles

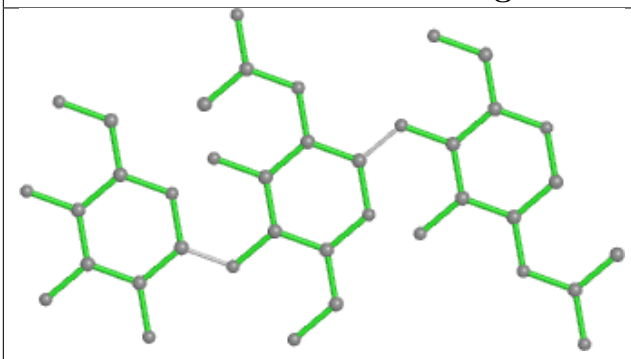


Torsions

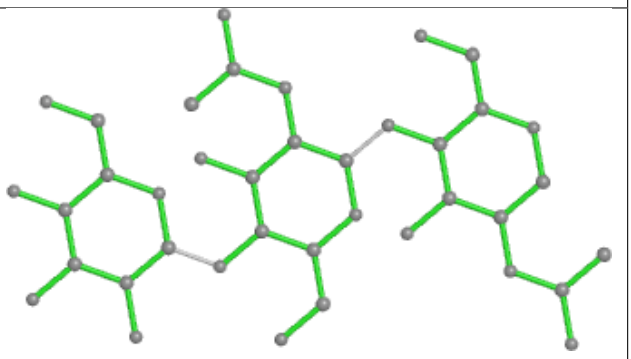


Rings

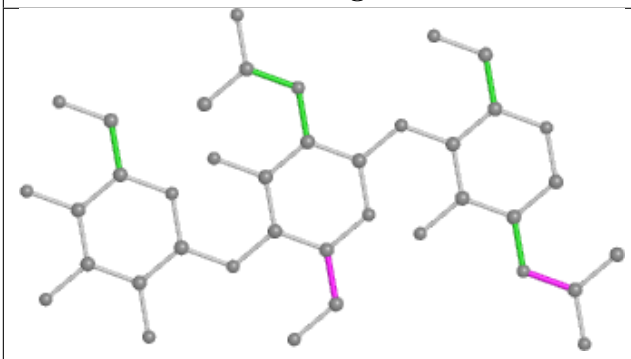
Oligosaccharide Chain R



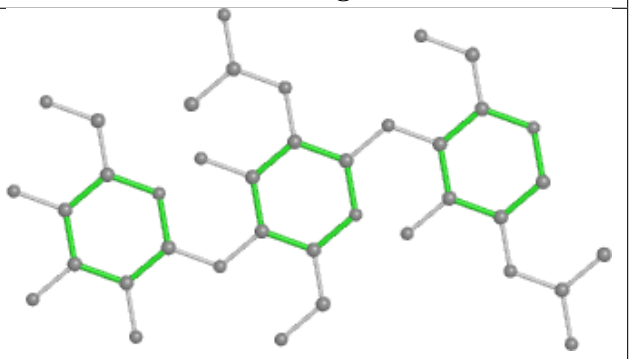
Bond lengths



Bond angles

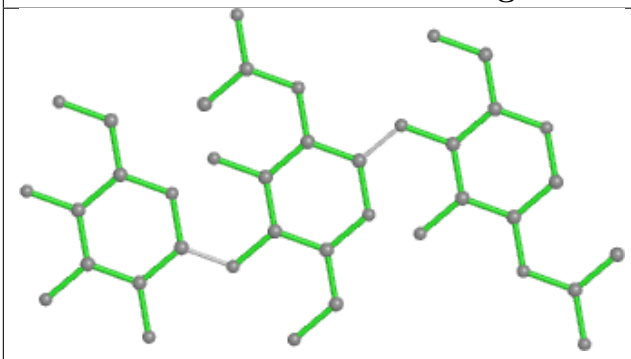


Torsions

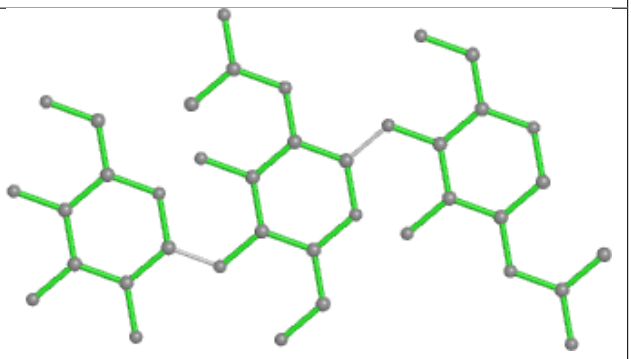


Rings

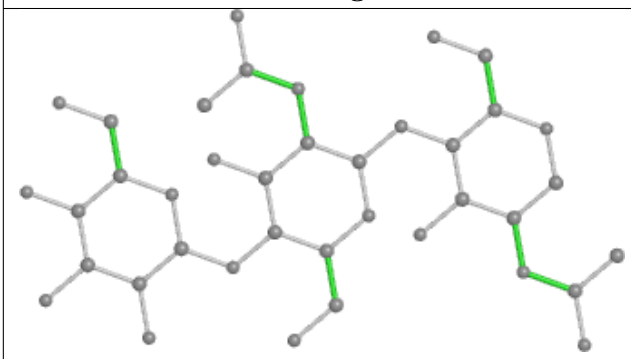
Oligosaccharide Chain S



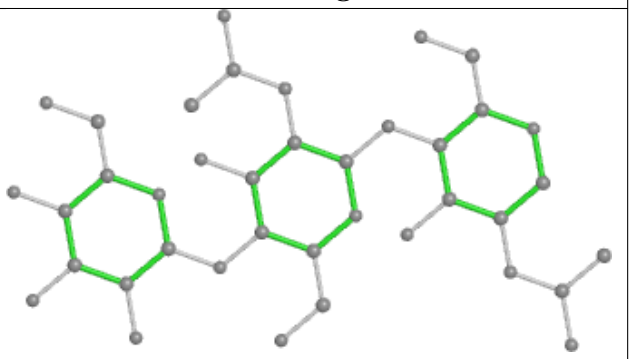
Bond lengths



Bond angles

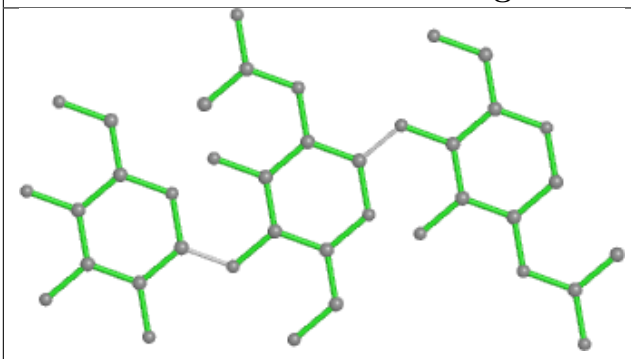


Torsions

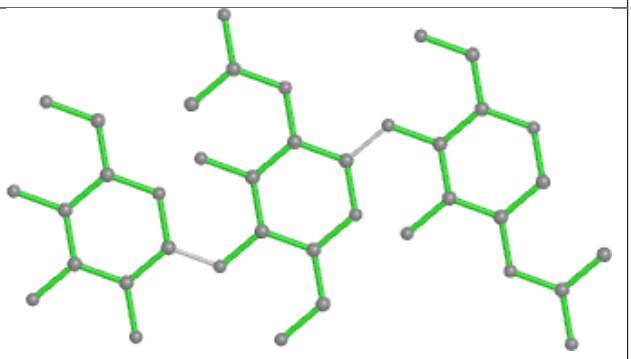


Rings

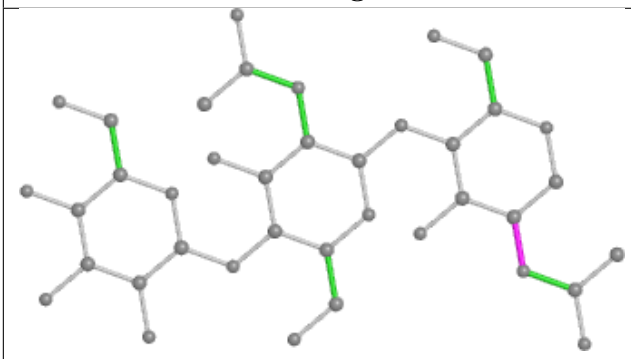
Oligosaccharide Chain U



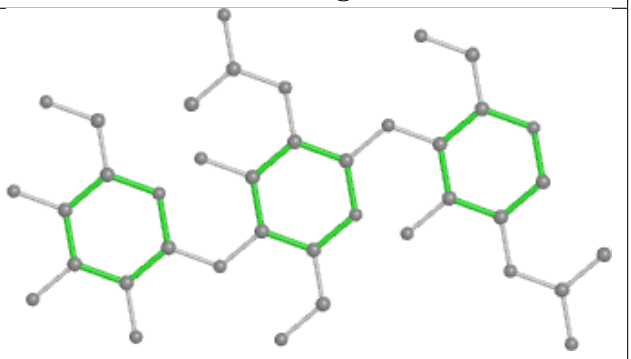
Bond lengths



Bond angles

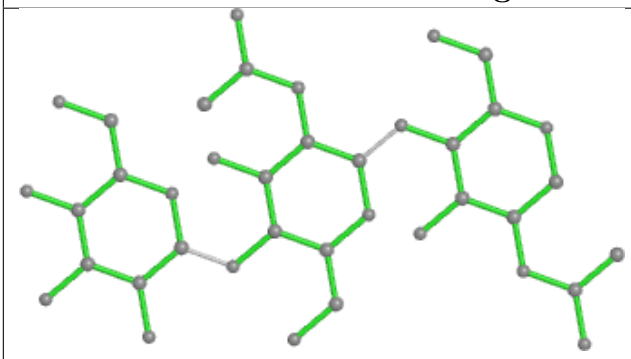


Torsions

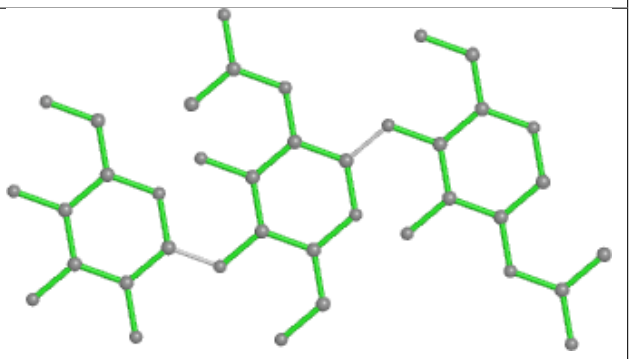


Rings

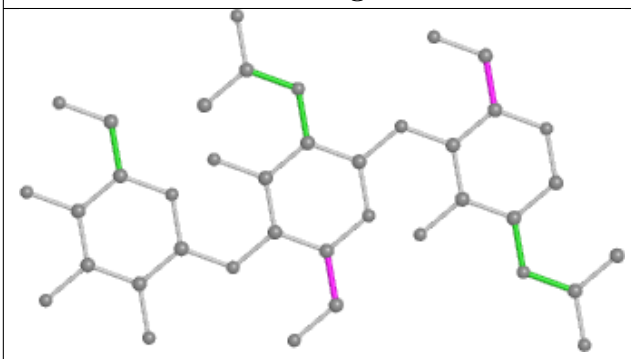
Oligosaccharide Chain Y



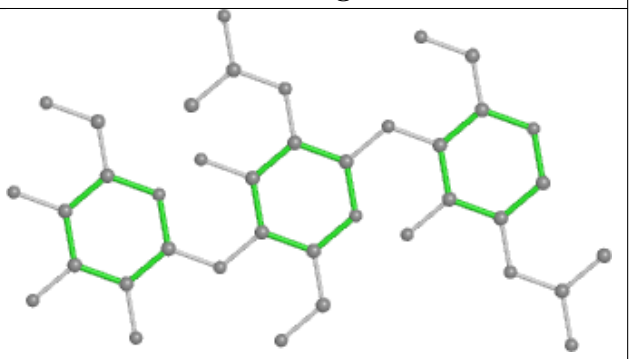
Bond lengths



Bond angles

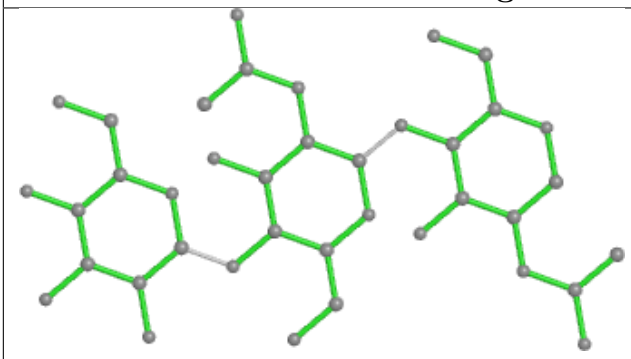


Torsions

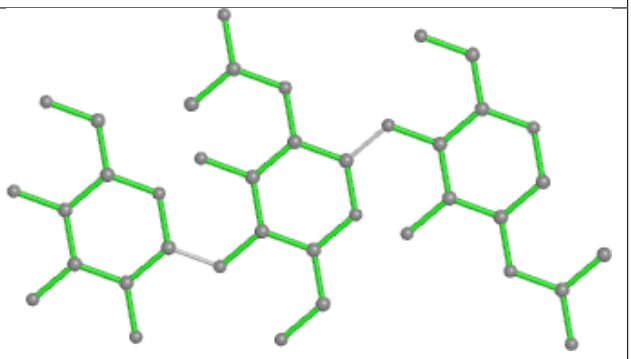


Rings

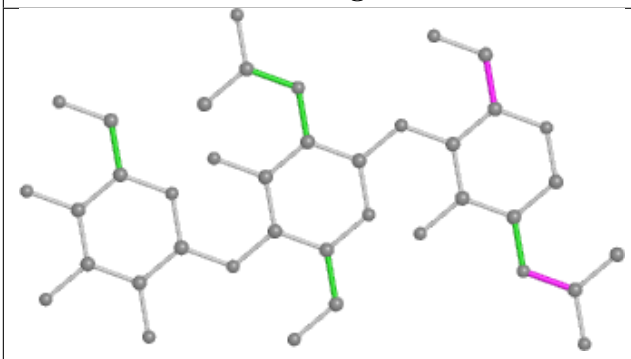
Oligosaccharide Chain Z



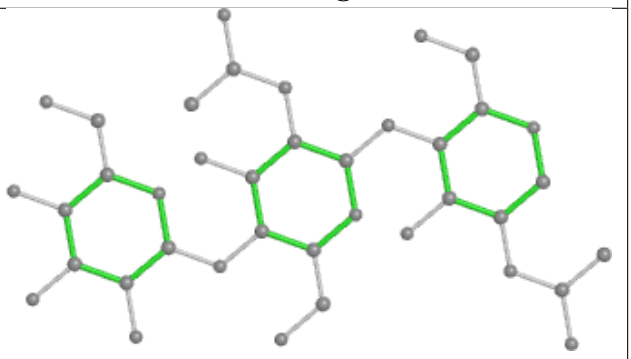
Bond lengths



Bond angles

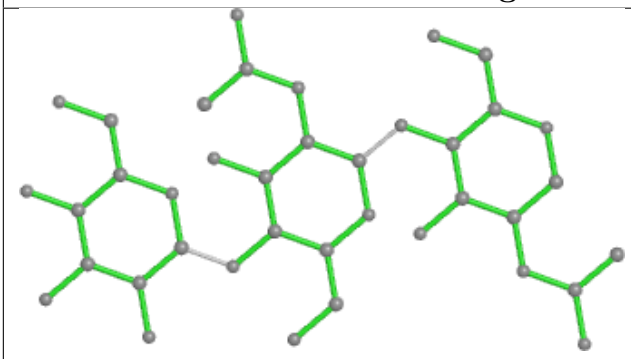


Torsions



Rings

Oligosaccharide Chain a



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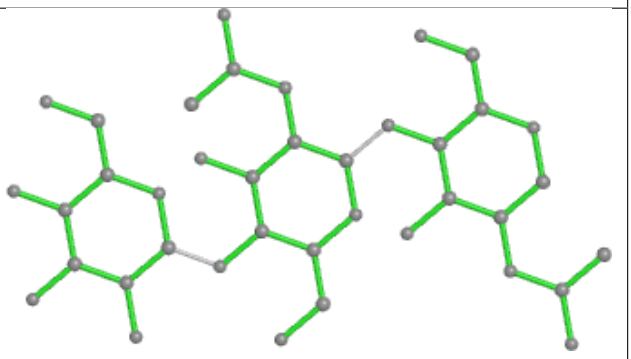
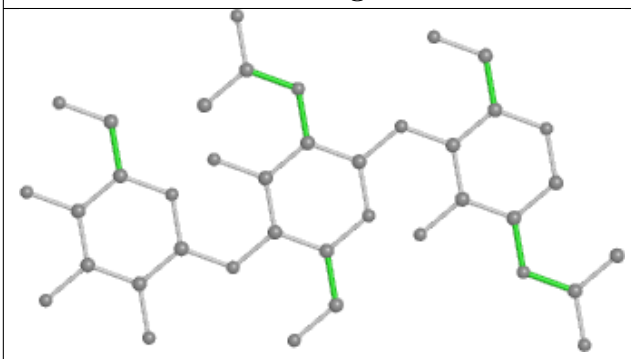
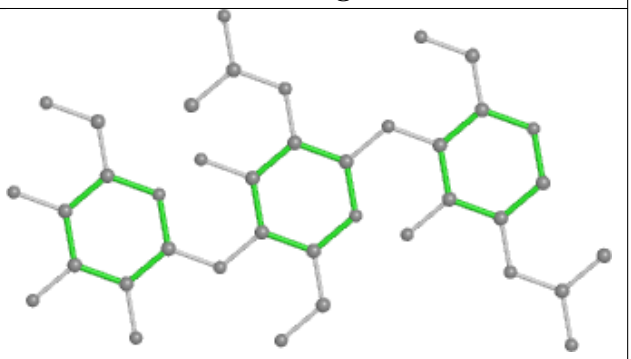


Bond angles

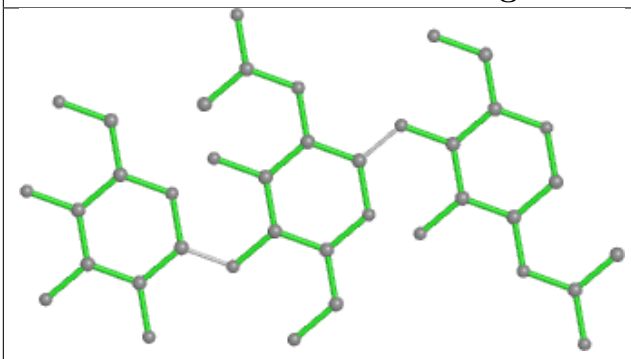


Torsions



Rings

Oligosaccharide Chain e



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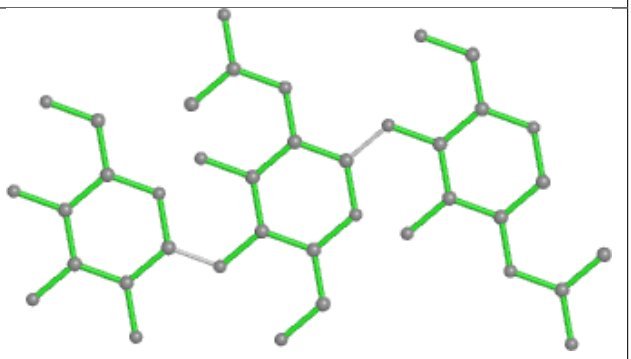
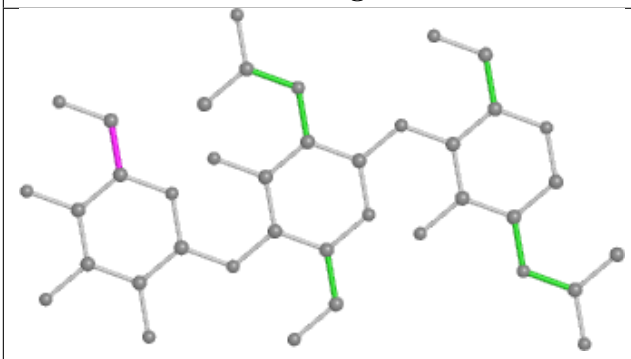


Bond angles



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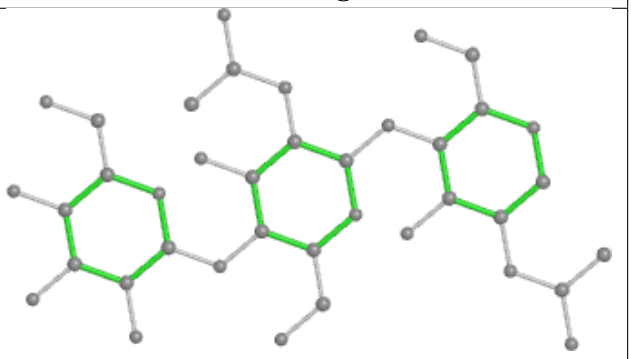
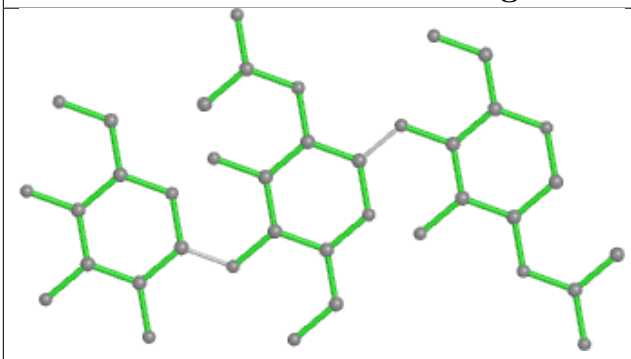


Rings

Oligosaccharide Chain f



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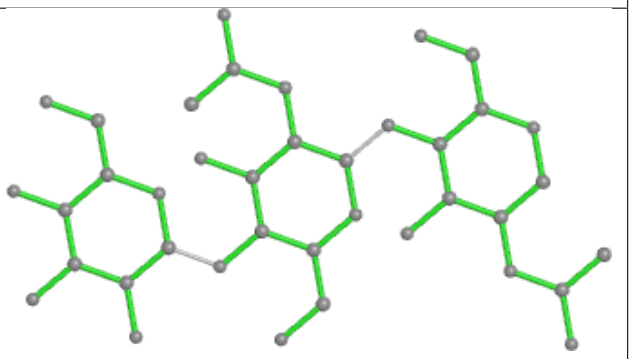
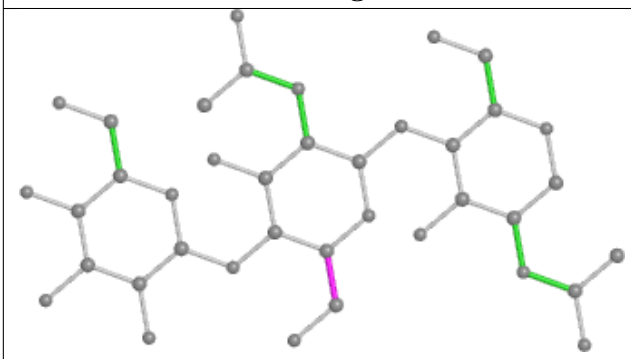


Bond angles



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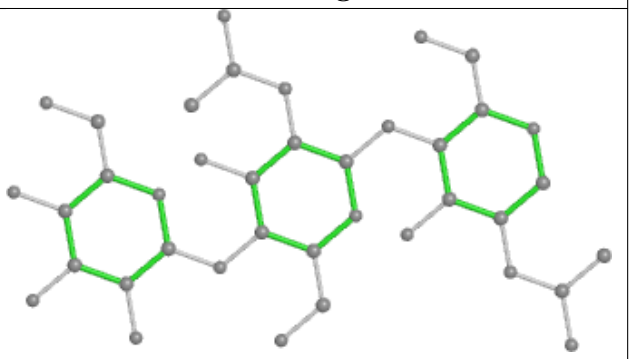
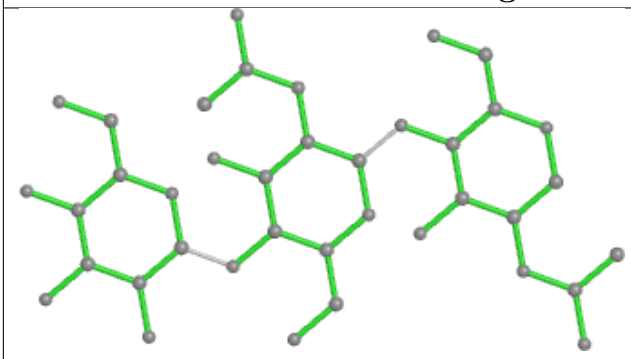


Rings

Oligosaccharide Chain g



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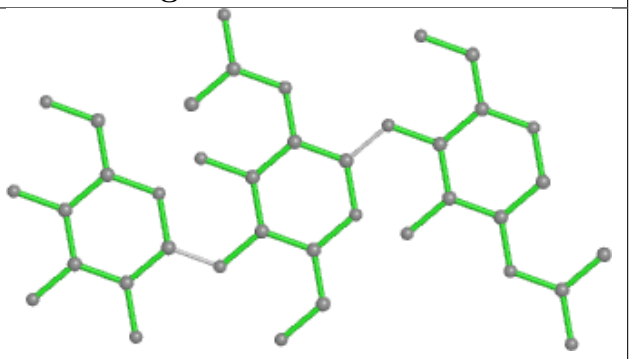
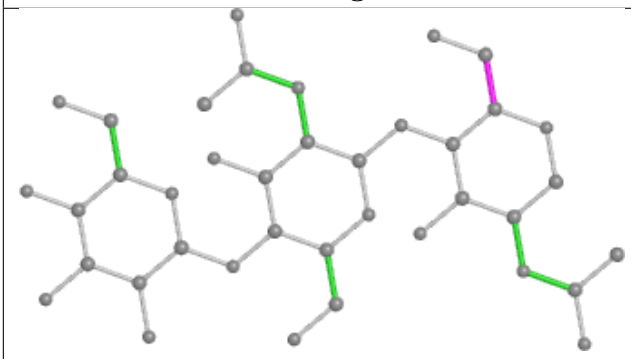


Bond angles



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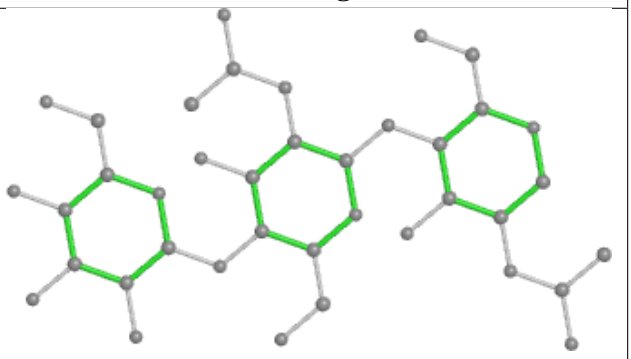
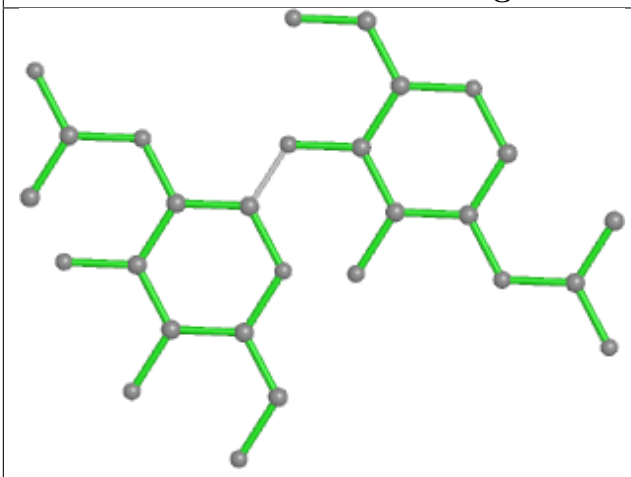


Rings

Oligosaccharide Chain H



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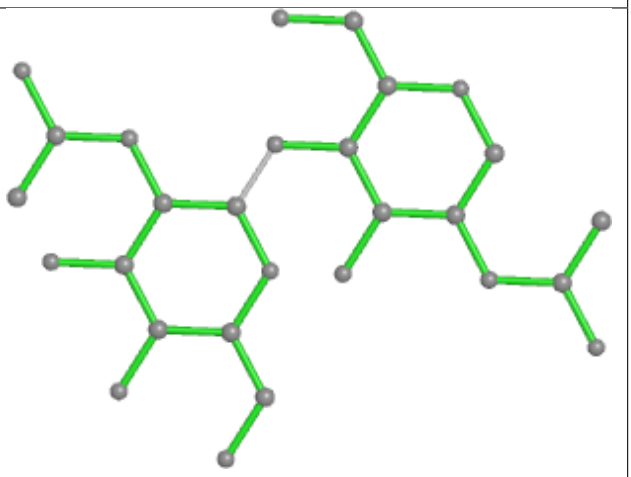
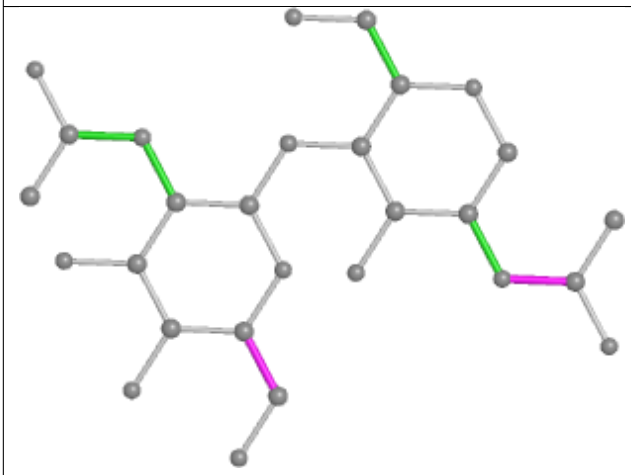


Bond angles



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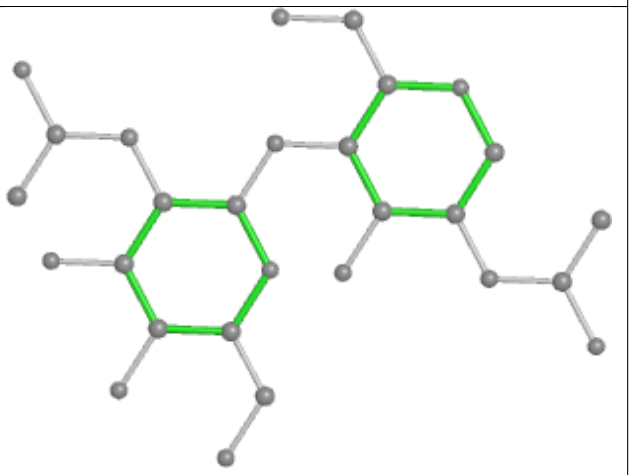
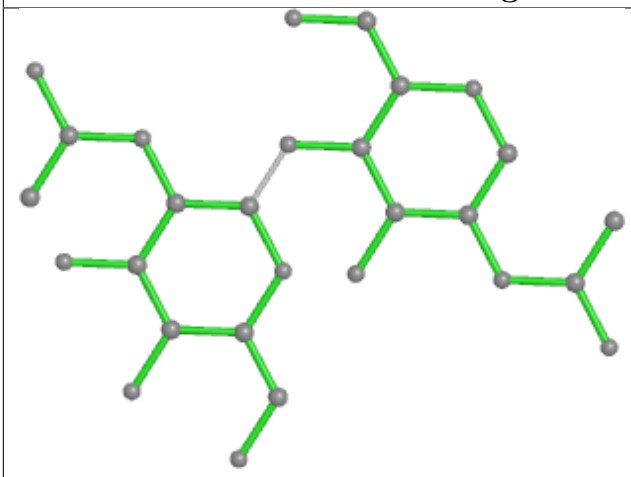


Rings

Oligosaccharide Chain I



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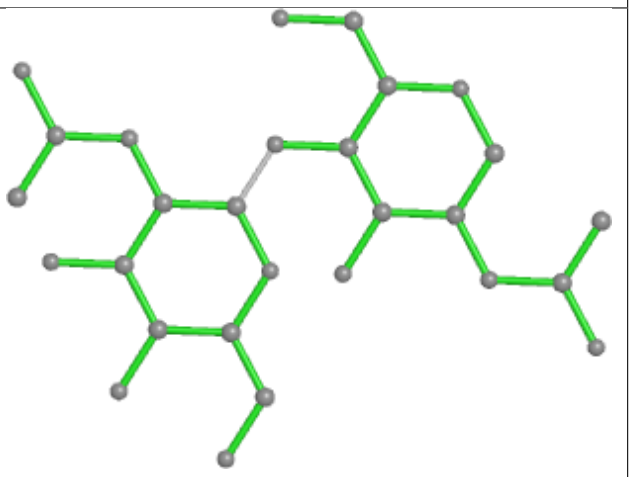
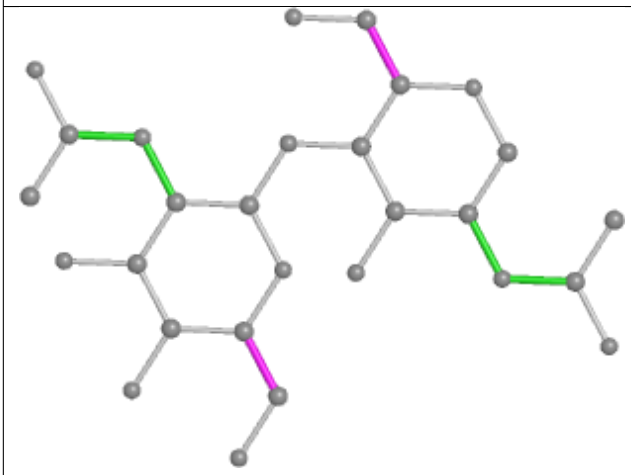


Bond angles



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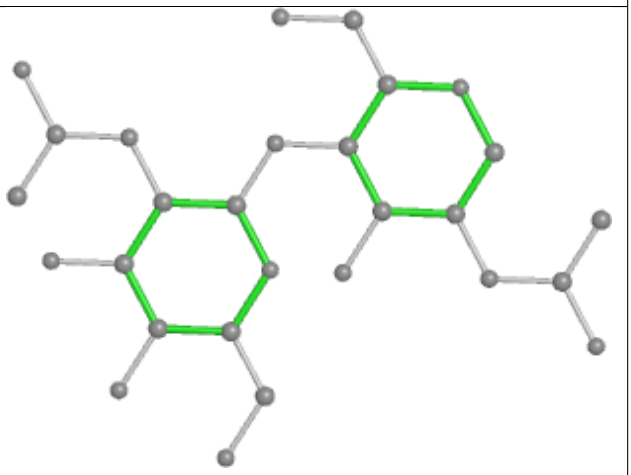
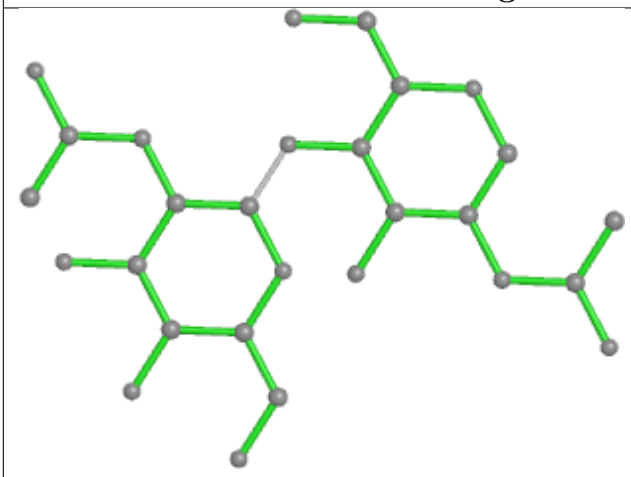


Rings

Oligosaccharide Chain J



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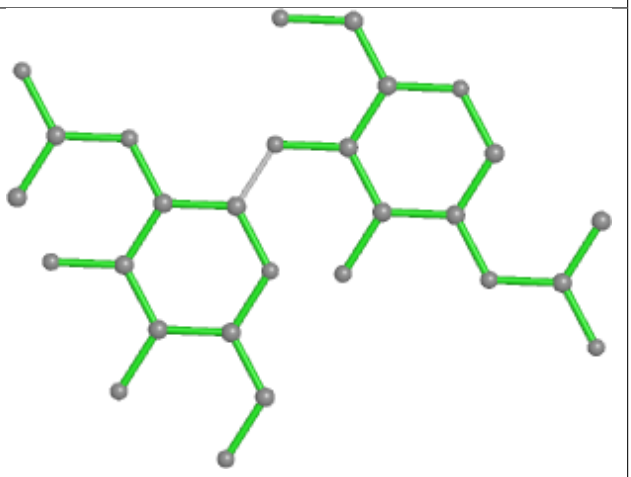
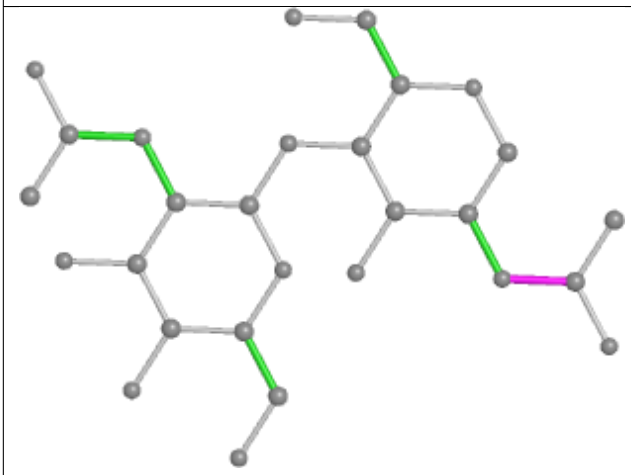


Bond angles



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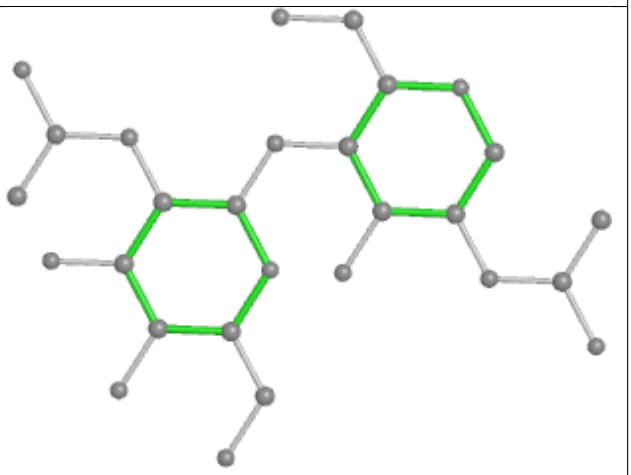
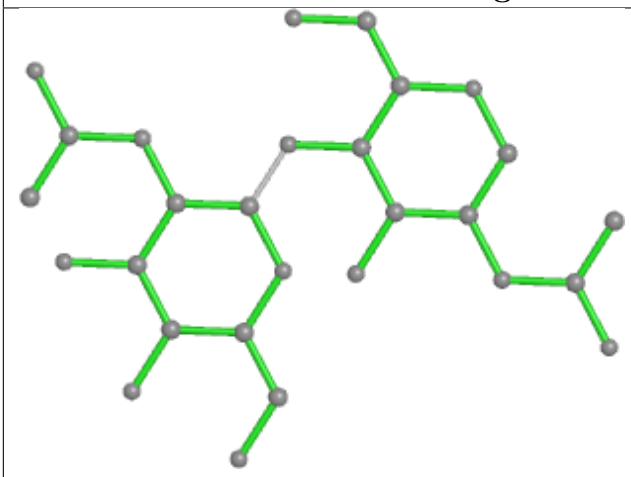


Rings

Oligosaccharide Chain N



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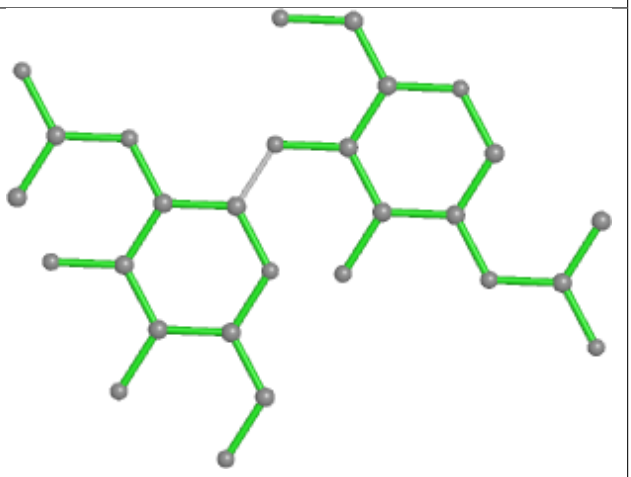
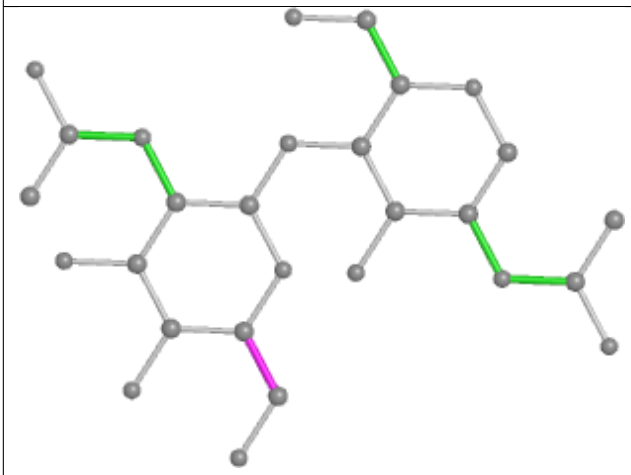


Bond angles



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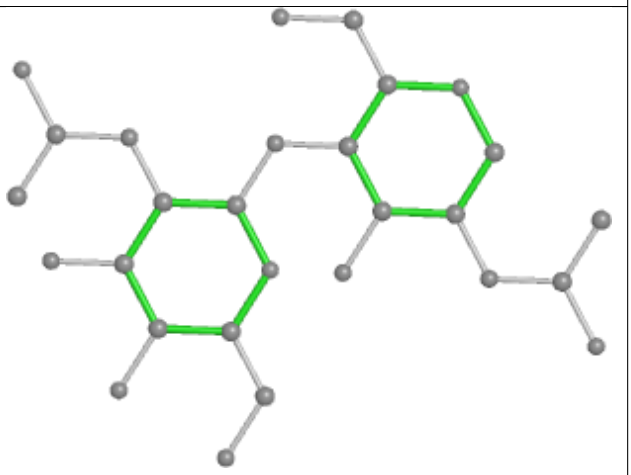
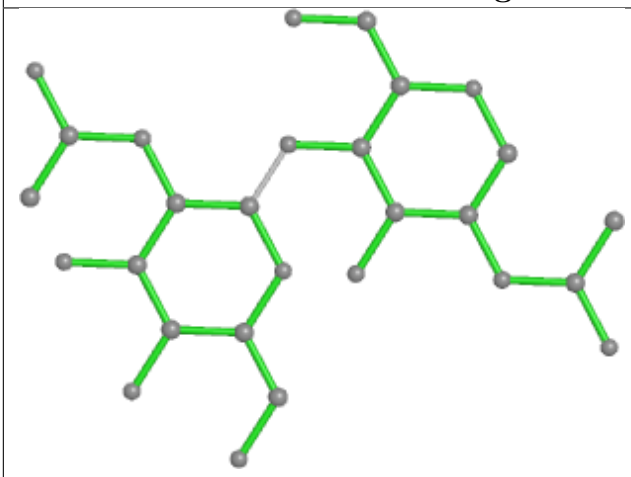


Rings

Oligosaccharide Chain O



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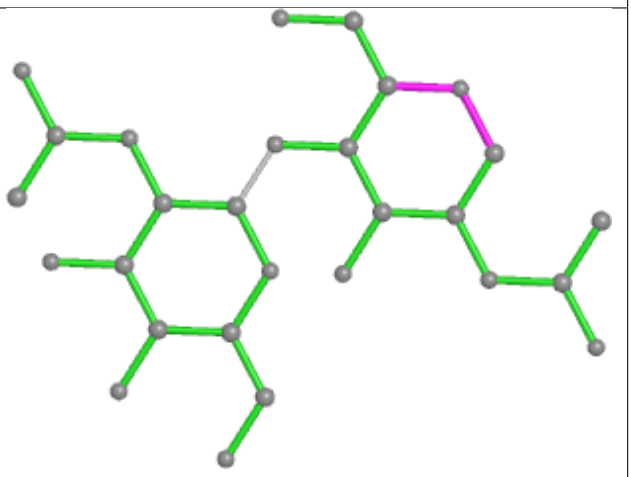
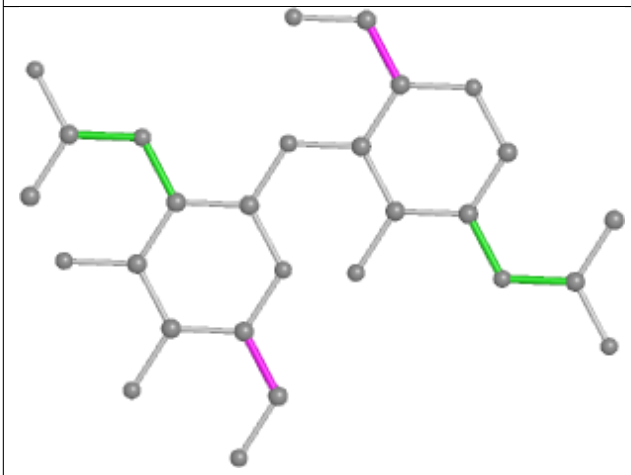


Bond angles



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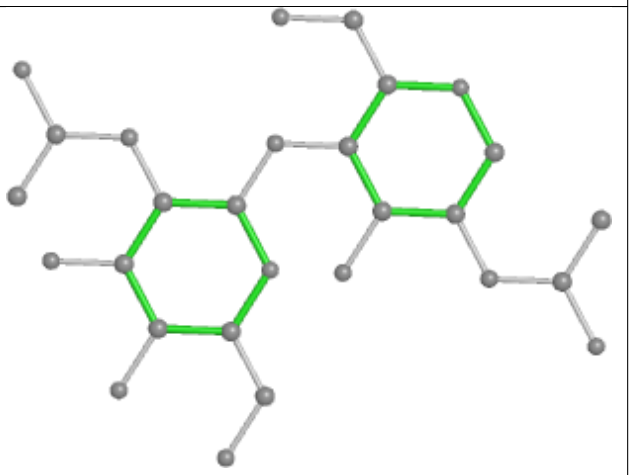
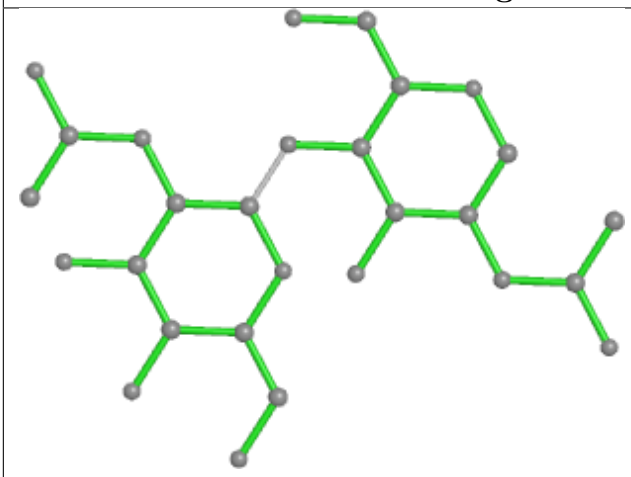


Rings

Oligosaccharide Chain P



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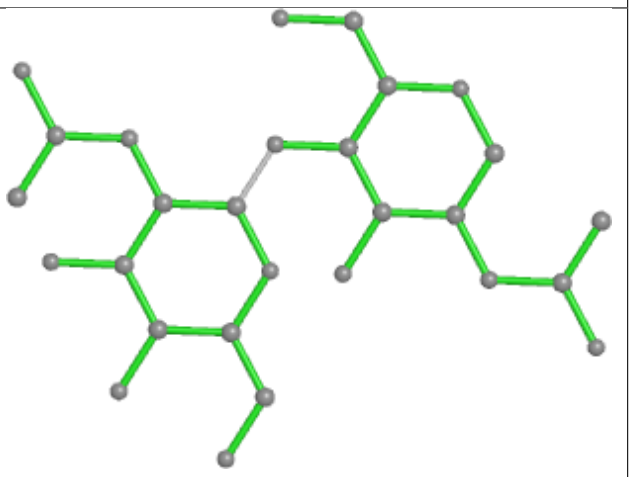
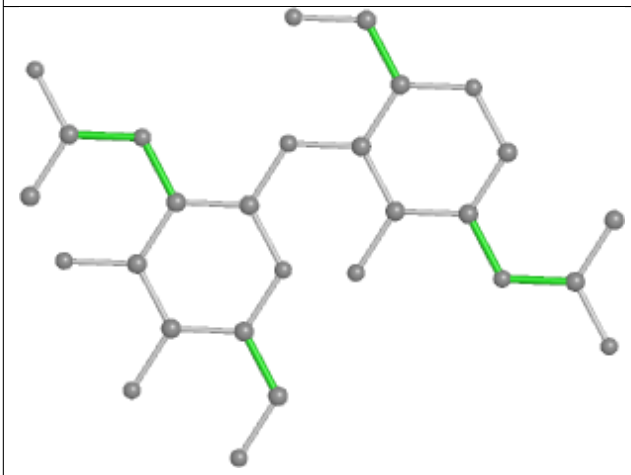
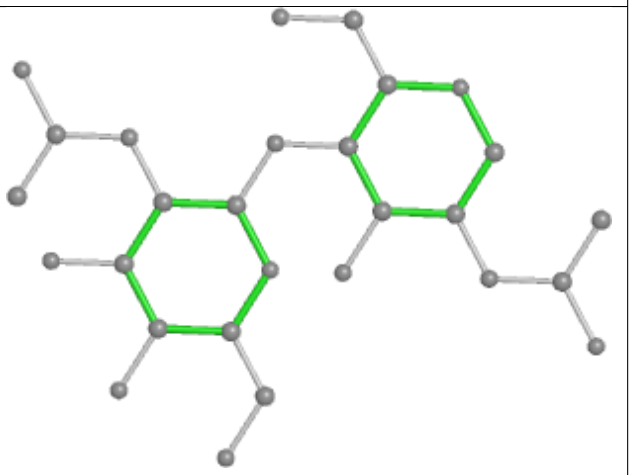


Bond angles

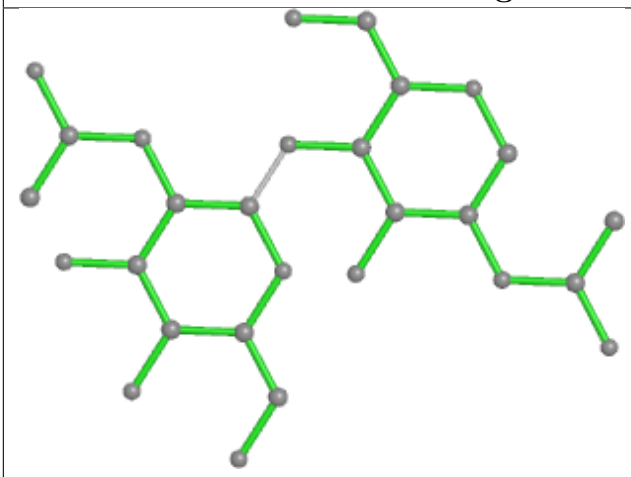


Torsions



Rings

Oligosaccharide Chain T



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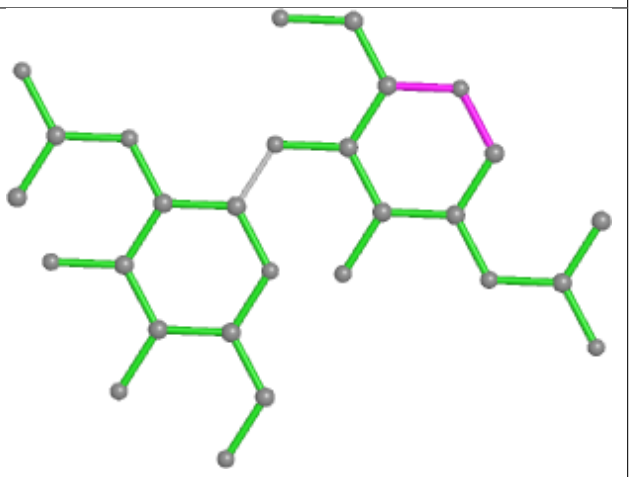
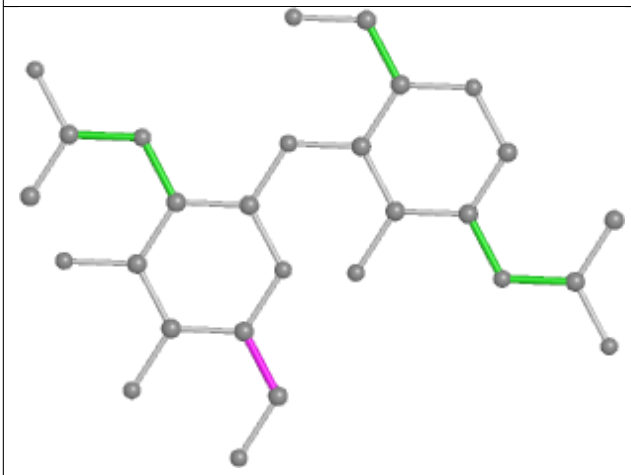
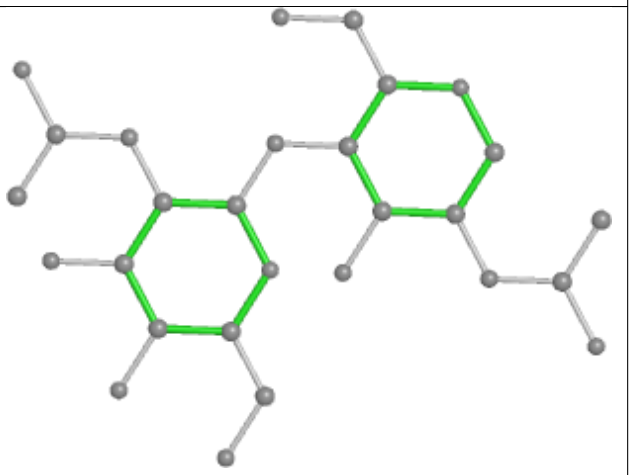


Bond angles

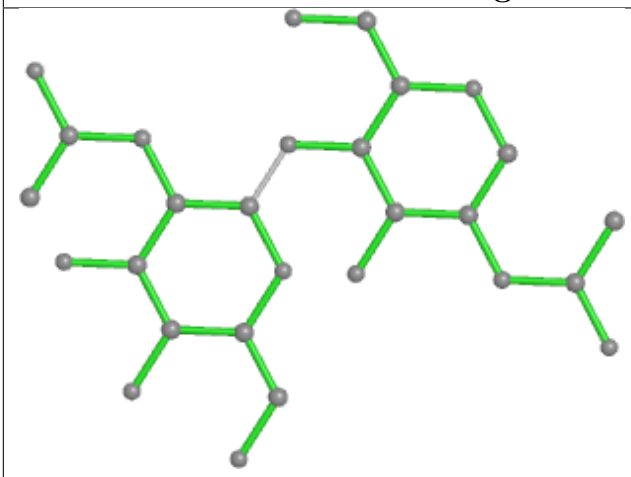


Torsions



Rings

Oligosaccharide Chain V



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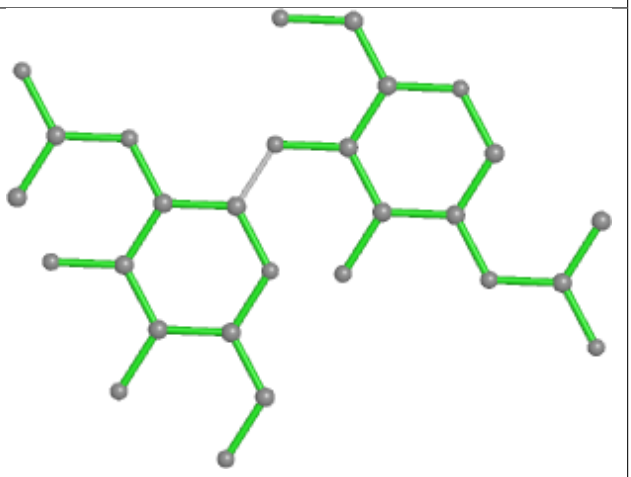
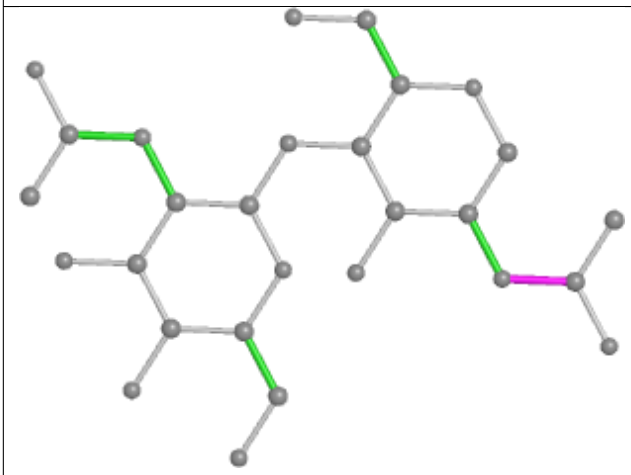


Bond angles



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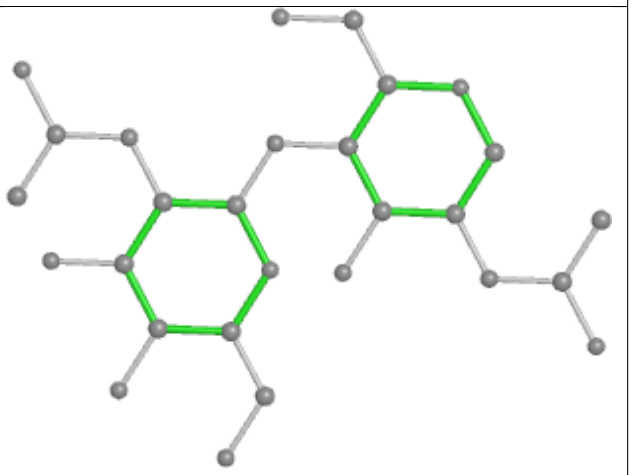
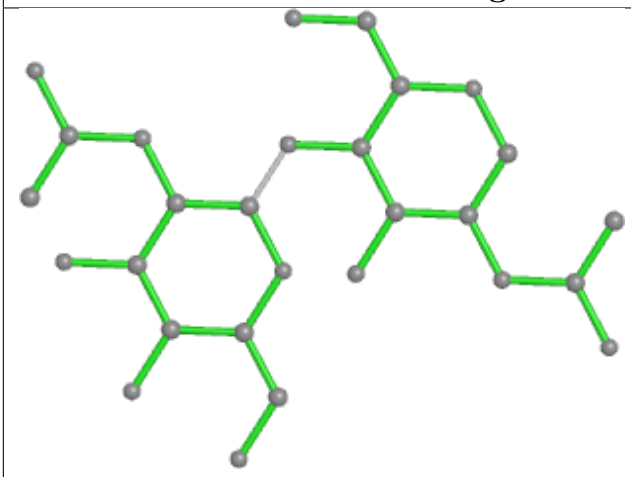


Rings

Oligosaccharide Chain W



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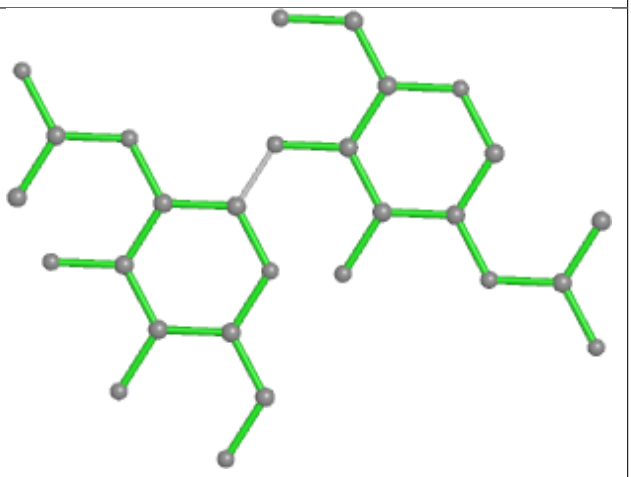
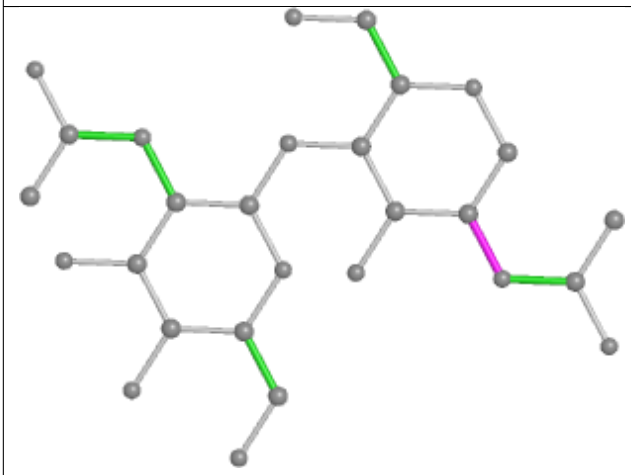
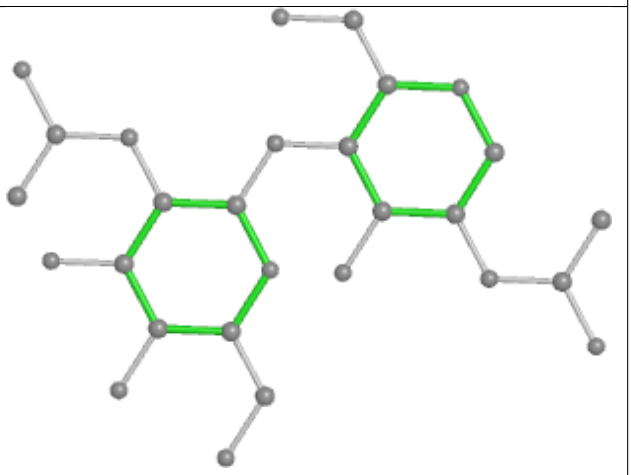


Bond angles

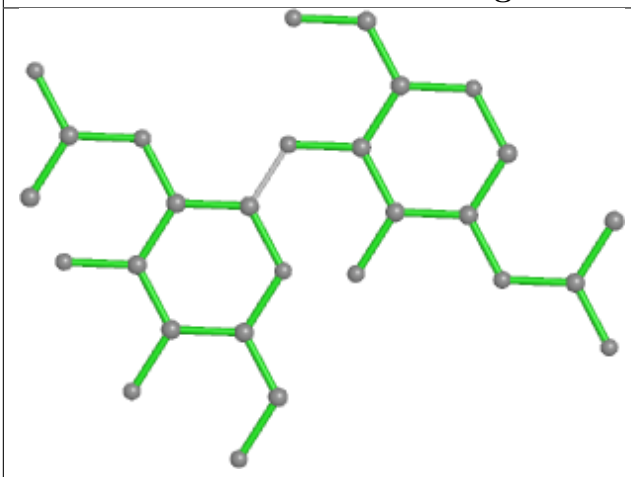


Torsions

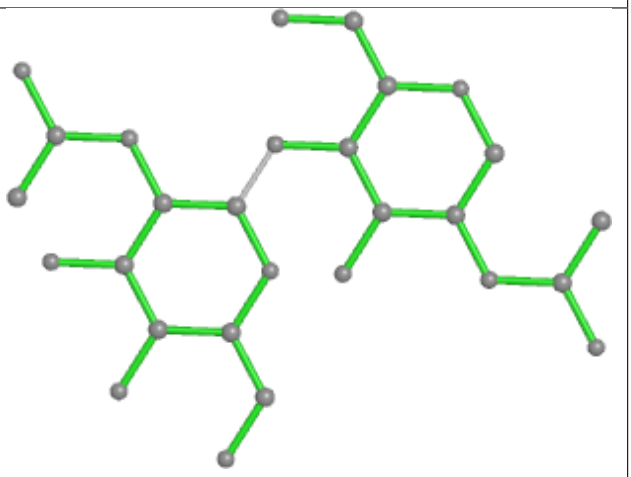


Rings

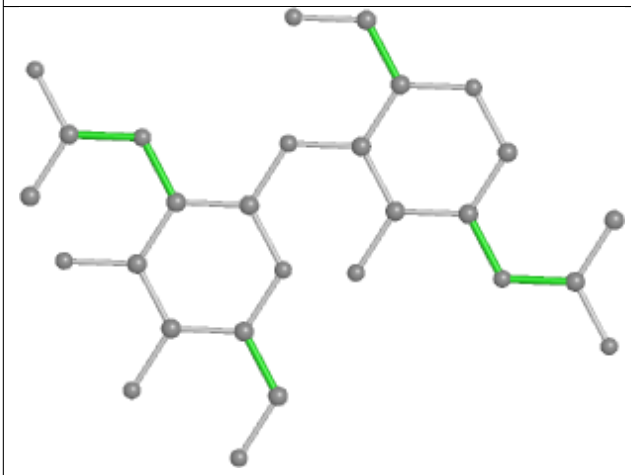
Oligosaccharide Chain X



Bond lengths



Bond angles



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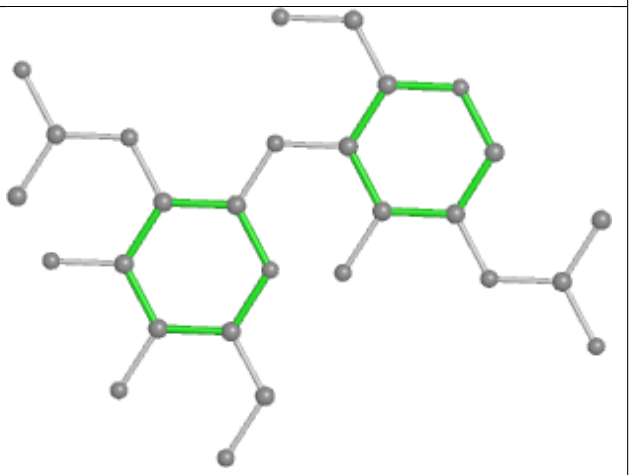
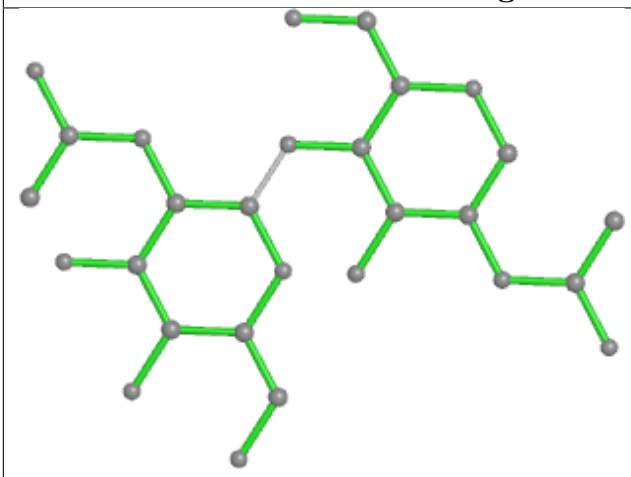
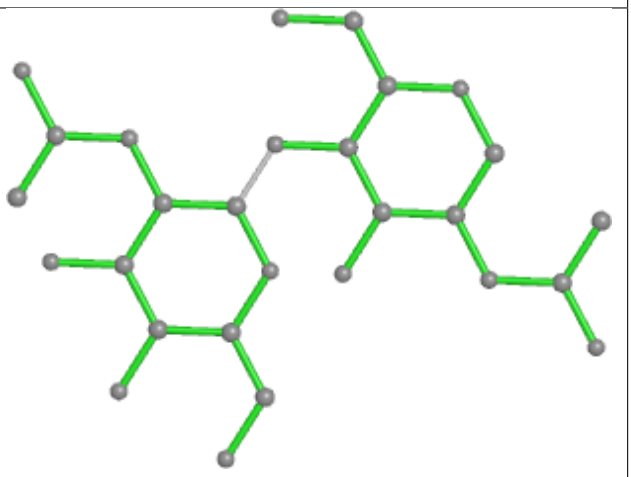


Rings

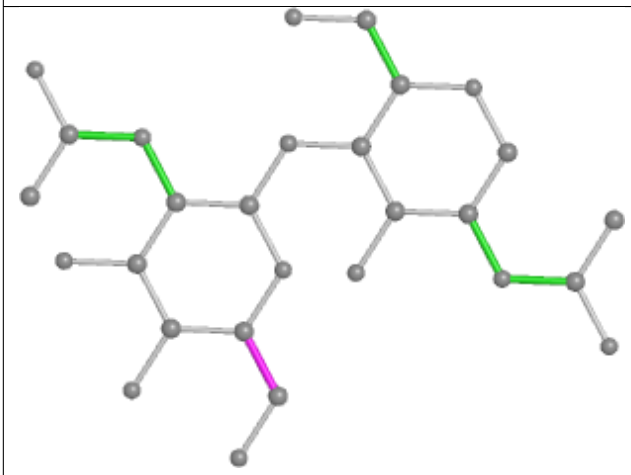
Oligosaccharide Chain b



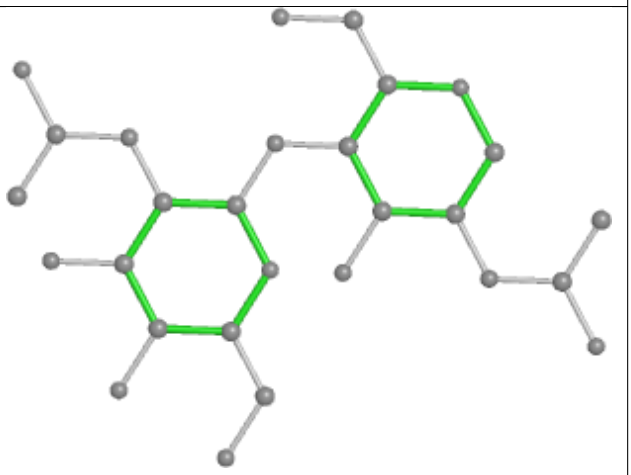
Bond lengths



Bond angles

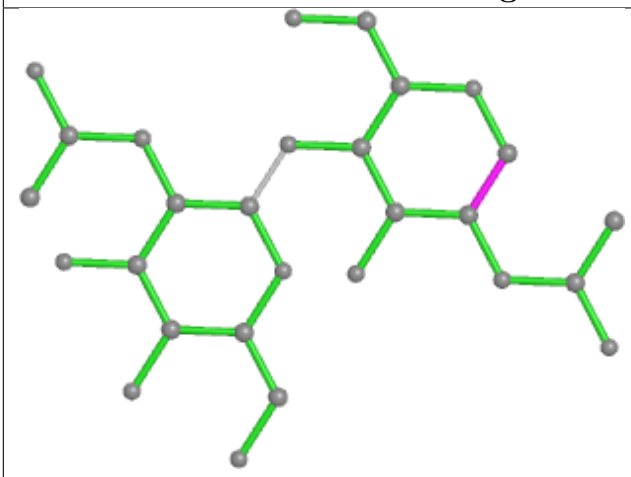


Torsions

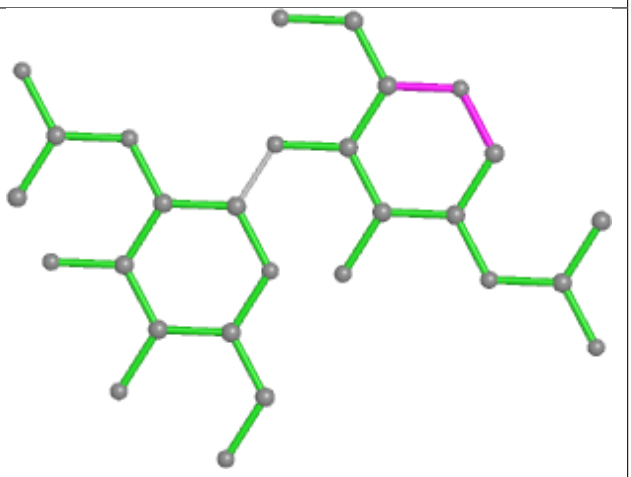


Rings

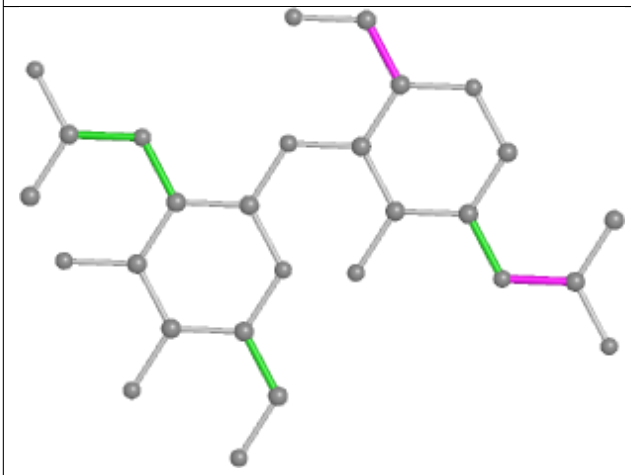
Oligosaccharide Chain c



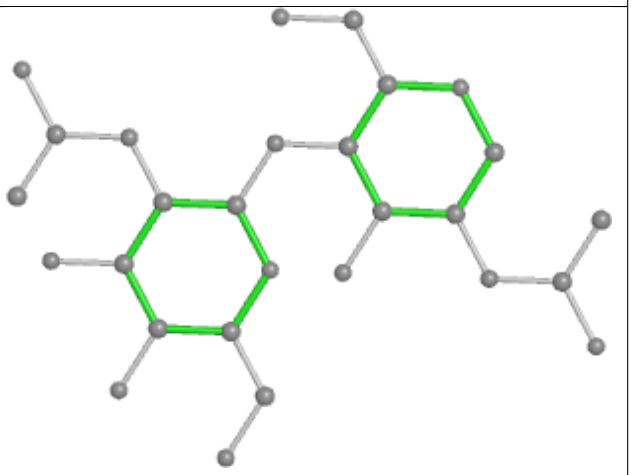
Bond lengths



Bond angles

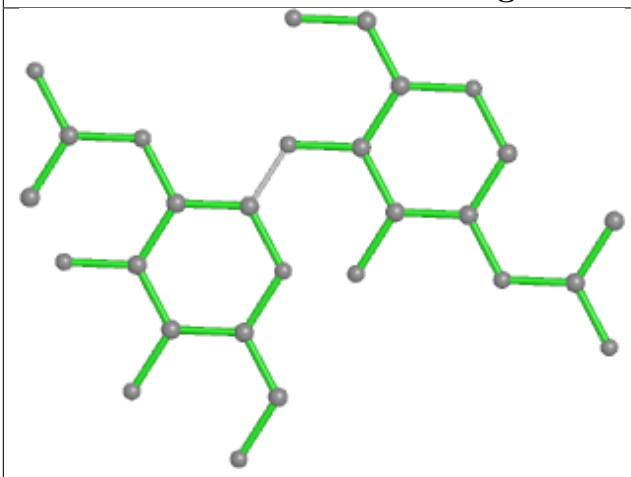


Torsions

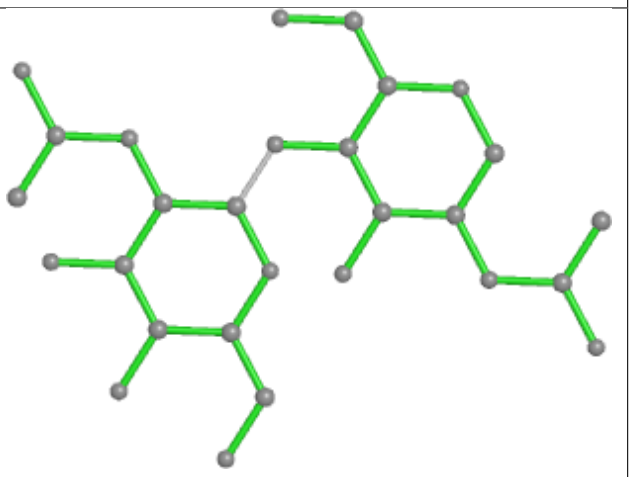


Rings

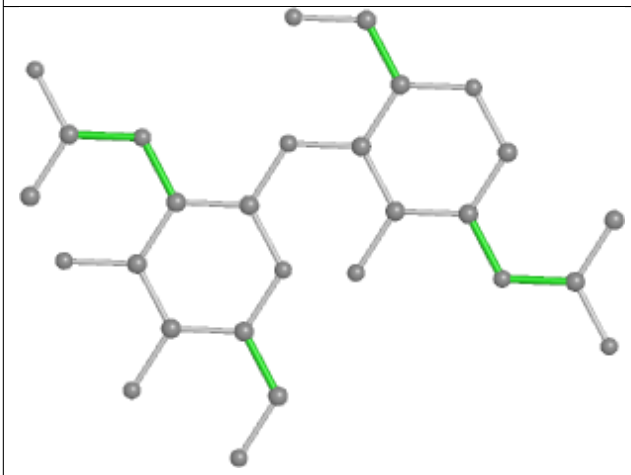
Oligosaccharide Chain d



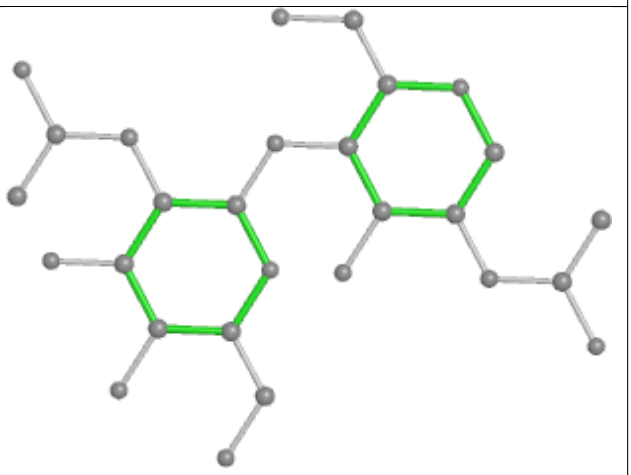
Bond lengths



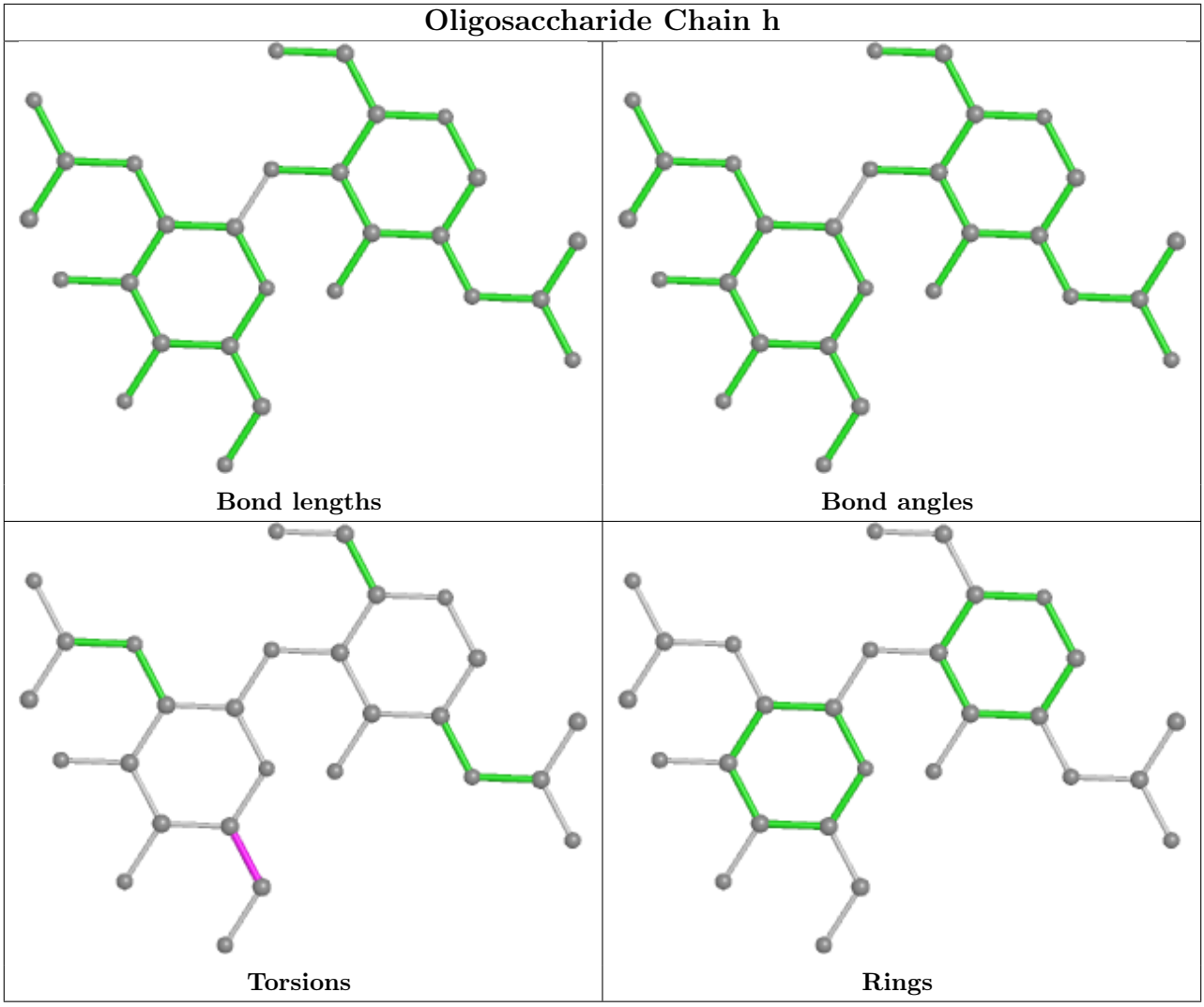
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	D	802	1	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	D	801	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	C	802	1	14,14,15	0.22	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	D	803	1	14,14,15	0.72	1 (7%)	17,19,21	1.55	3 (17%)
6	NAG	F	803	1	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
6	NAG	F	801	1	14,14,15	0.30	0	17,19,21	0.44	0
6	NAG	E	802	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	E	801	1	14,14,15	0.19	0	17,19,21	0.55	0
6	NAG	C	801	1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	F	802	1	14,14,15	0.29	0	17,19,21	0.37	0
6	NAG	D	804	1	14,14,15	0.41	0	17,19,21	0.44	0
6	NAG	F	804	1	14,14,15	0.36	0	17,19,21	0.43	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
6	NAG	D	802	1	-	4/6/23/26	0/1/1/1
6	NAG	D	801	1	-	0/6/23/26	0/1/1/1
6	NAG	C	802	1	-	2/6/23/26	0/1/1/1
6	NAG	D	803	1	-	1/6/23/26	0/1/1/1
6	NAG	F	803	1	-	1/6/23/26	0/1/1/1
6	NAG	F	801	1	-	0/6/23/26	0/1/1/1
6	NAG	E	802	1	-	0/6/23/26	0/1/1/1
6	NAG	E	801	1	-	2/6/23/26	0/1/1/1
6	NAG	C	801	1	-	2/6/23/26	0/1/1/1
6	NAG	F	802	1	-	4/6/23/26	0/1/1/1
6	NAG	D	804	1	-	0/6/23/26	0/1/1/1
6	NAG	F	804	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	803	NAG	C1-C2	2.11	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	803	NAG	C1-O5-C5	4.77	118.66	112.19
6	D	803	NAG	C2-N2-C7	2.42	126.35	122.90
6	F	803	NAG	C1-O5-C5	2.42	115.47	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	803	NAG	C1-C2-N2	2.13	114.12	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	802	NAG	O5-C5-C6-O6
6	D	802	NAG	O5-C5-C6-O6
6	F	802	NAG	C4-C5-C6-O6
6	D	802	NAG	C4-C5-C6-O6
6	D	802	NAG	C8-C7-N2-C2
6	D	802	NAG	O7-C7-N2-C2
6	F	802	NAG	C8-C7-N2-C2
6	F	802	NAG	O7-C7-N2-C2
6	C	801	NAG	O5-C5-C6-O6
6	C	801	NAG	C4-C5-C6-O6
6	C	802	NAG	O5-C5-C6-O6
6	D	803	NAG	C1-C2-N2-C7
6	F	803	NAG	C3-C2-N2-C7
6	E	801	NAG	C3-C2-N2-C7
6	C	802	NAG	C4-C5-C6-O6
6	E	801	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	803	NAG	1	0
6	F	801	NAG	1	0
6	C	801	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

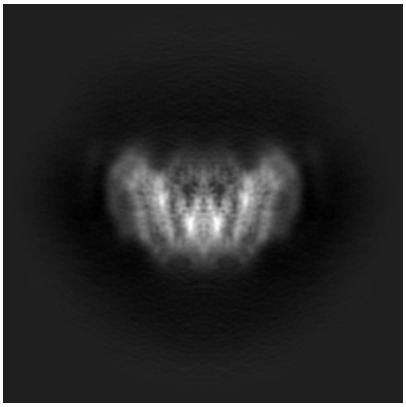
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32599. These allow visual inspection of the internal detail of the map and identification of artifacts.

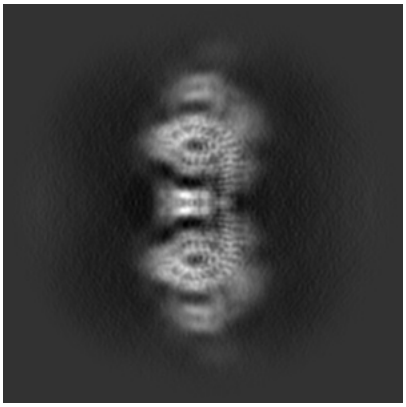
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

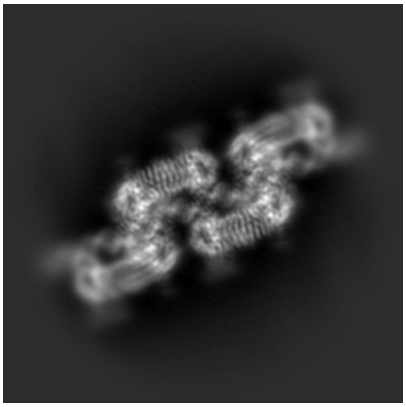
6.1.1 Primary map



X



Y

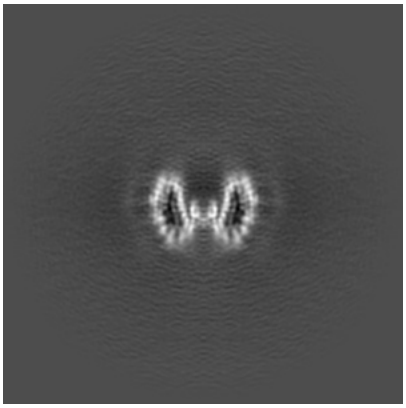


Z

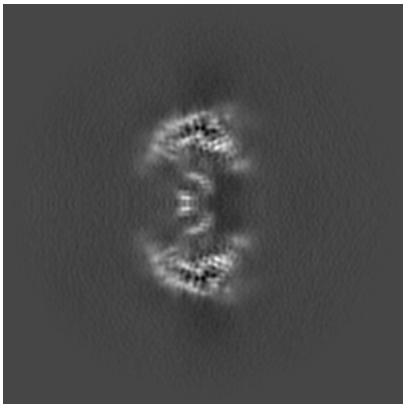
The images above show the map projected in three orthogonal directions.

6.2 Central slices

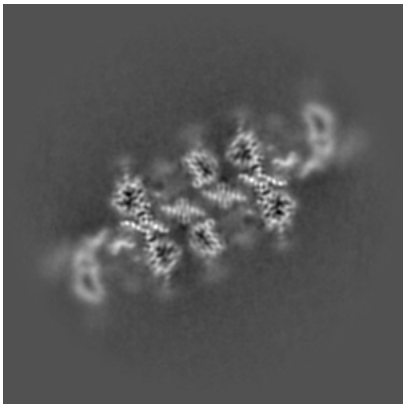
6.2.1 Primary map



X Index: 140



Y Index: 140

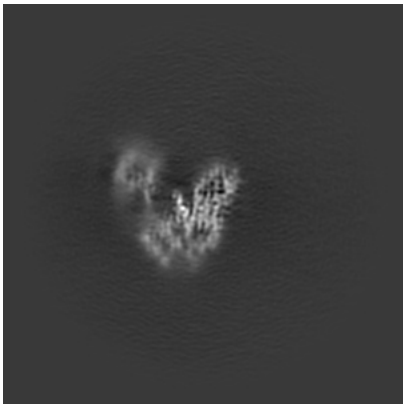


Z Index: 140

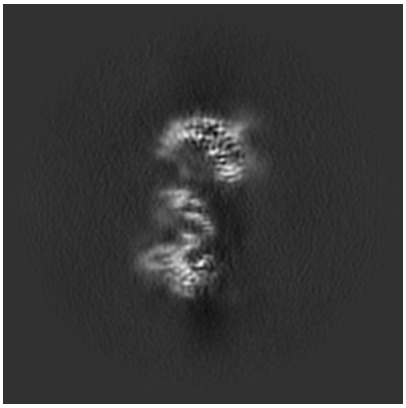
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

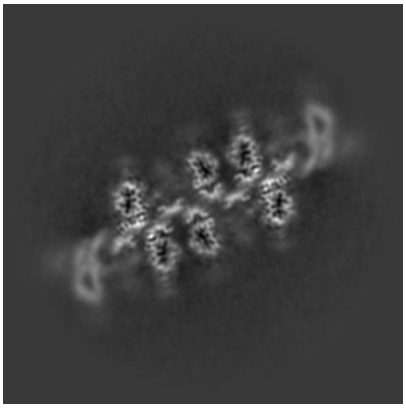
6.3.1 Primary map



X Index: 94



Y Index: 131

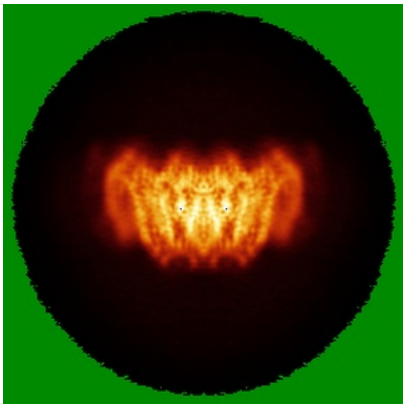


Z Index: 136

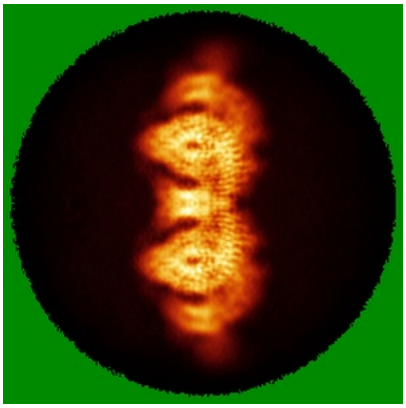
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

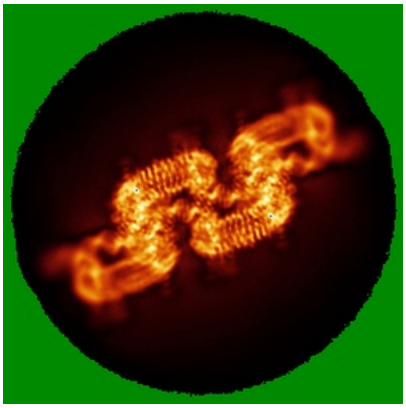
6.4.1 Primary map



X



Y

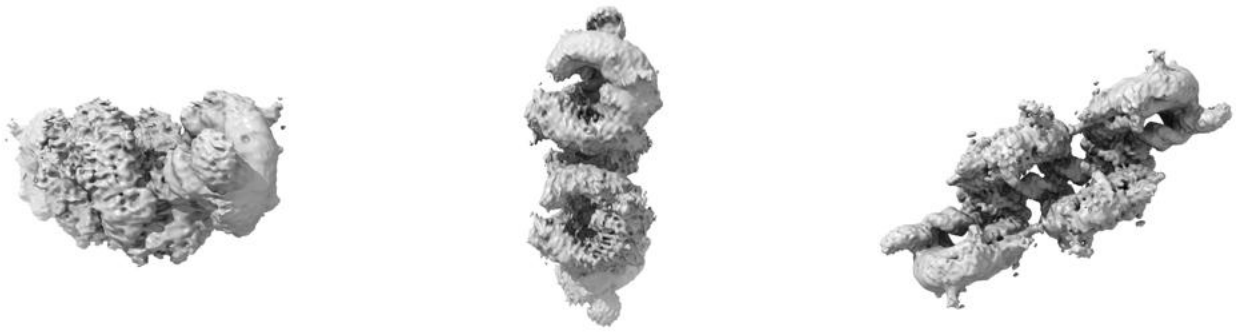


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 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.

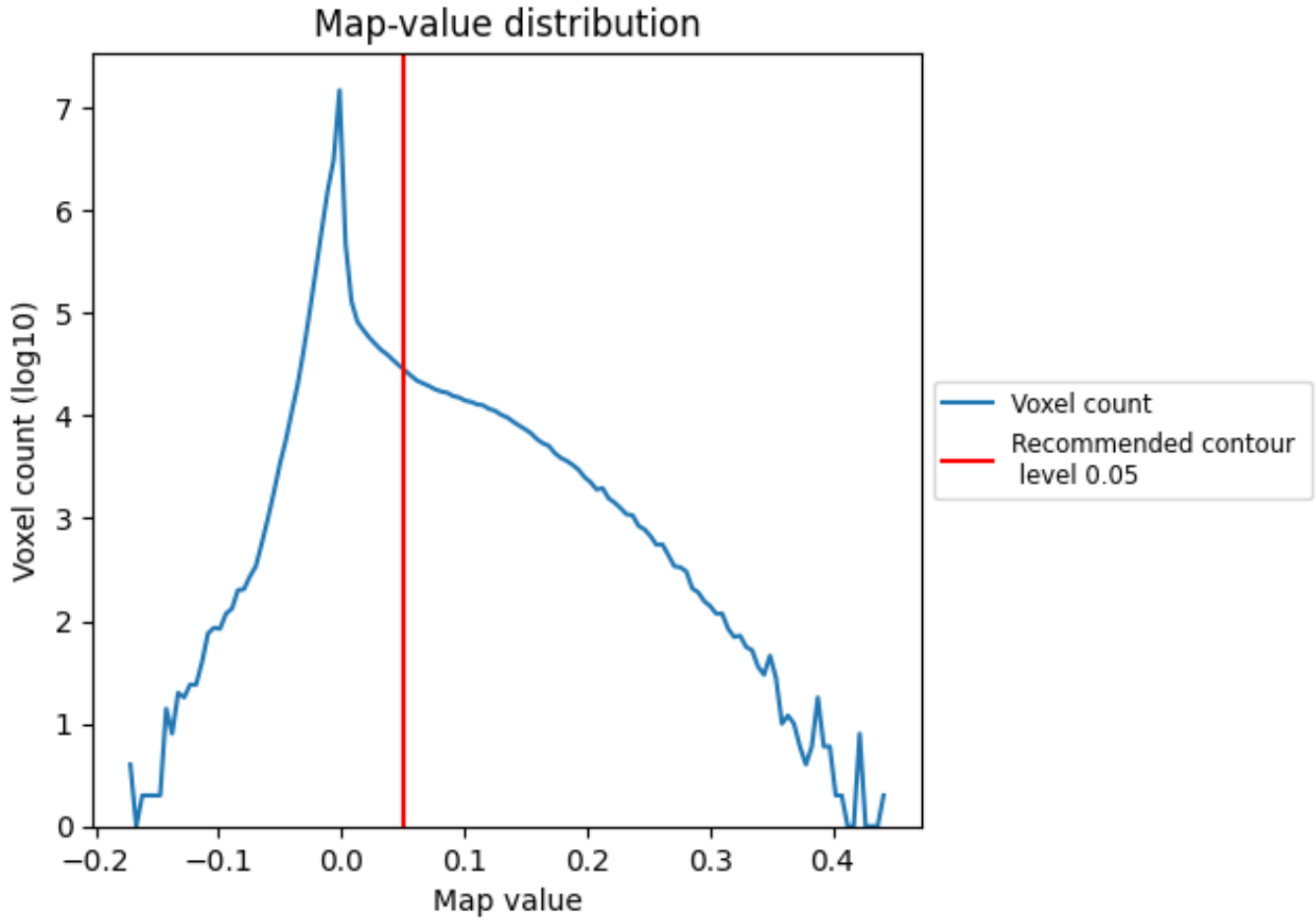
6.6 Mask visualisation (i)

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

7 Map analysis

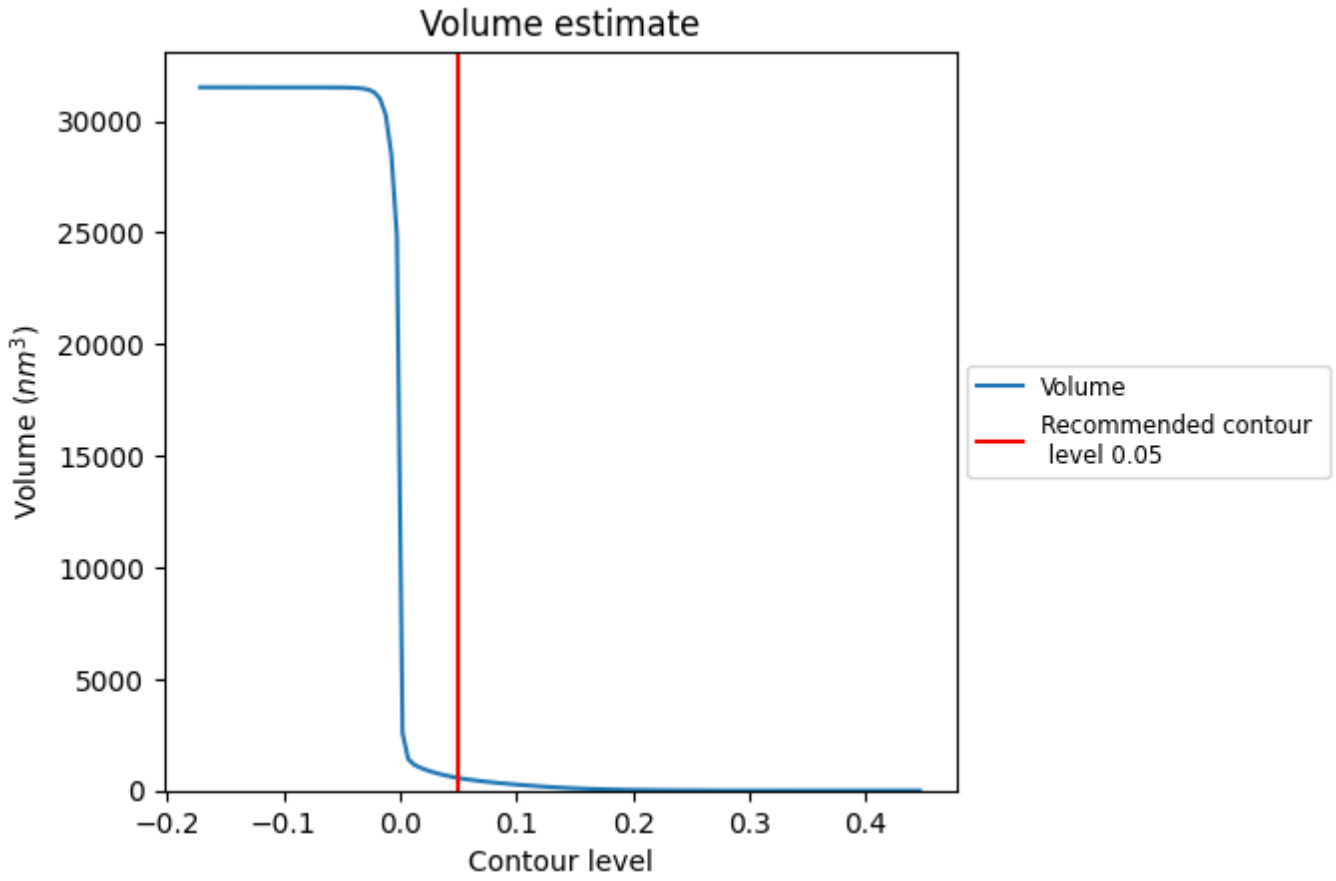
This section contains the results of statistical analysis of the map.

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.

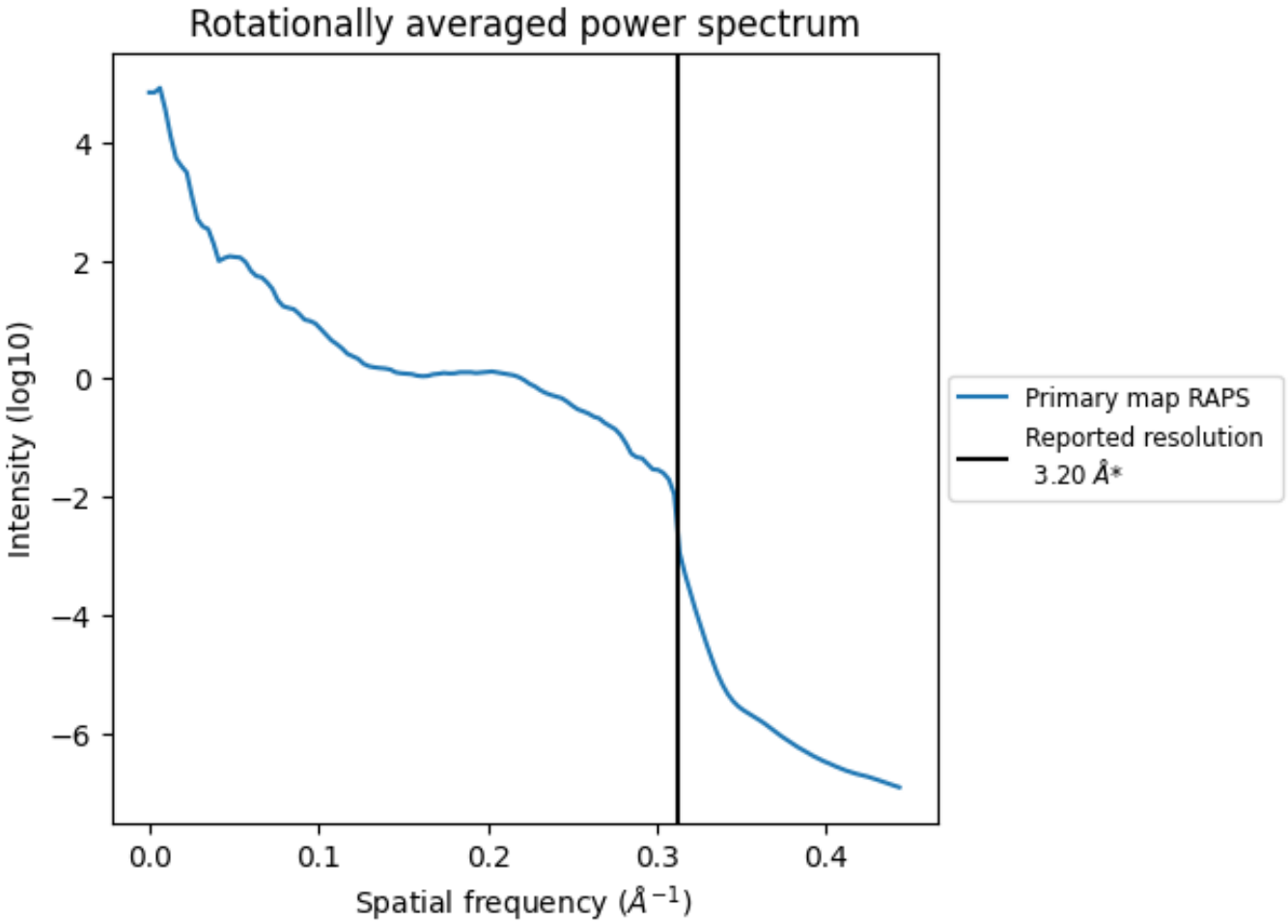
7.2 Volume estimate



The volume at the recommended contour level is 564 nm^3; this corresponds to an approximate mass of 509 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

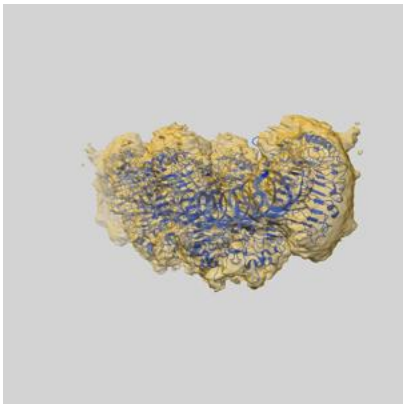
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

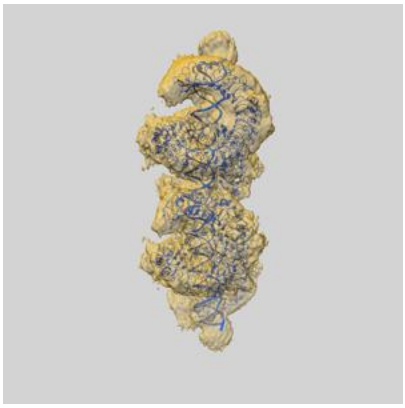
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32599 and PDB model 7WM4. Per-residue inclusion information can be found in section 3 on page 9.

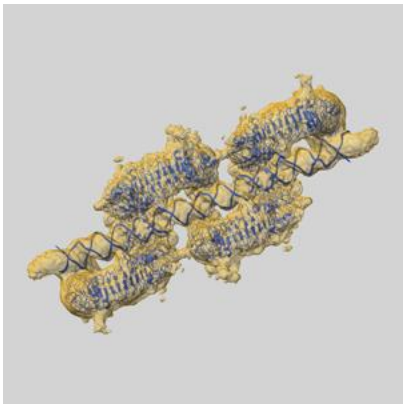
9.1 Map-model overlay



X



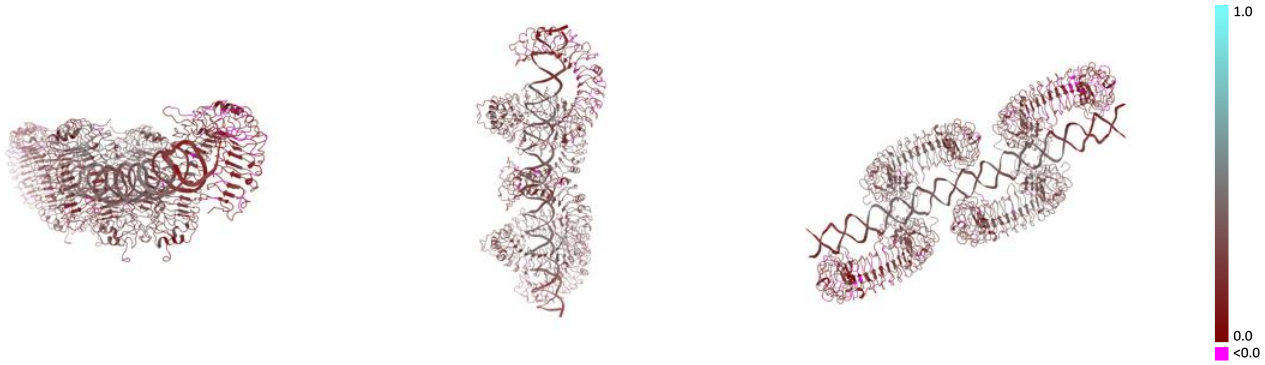
Y



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.

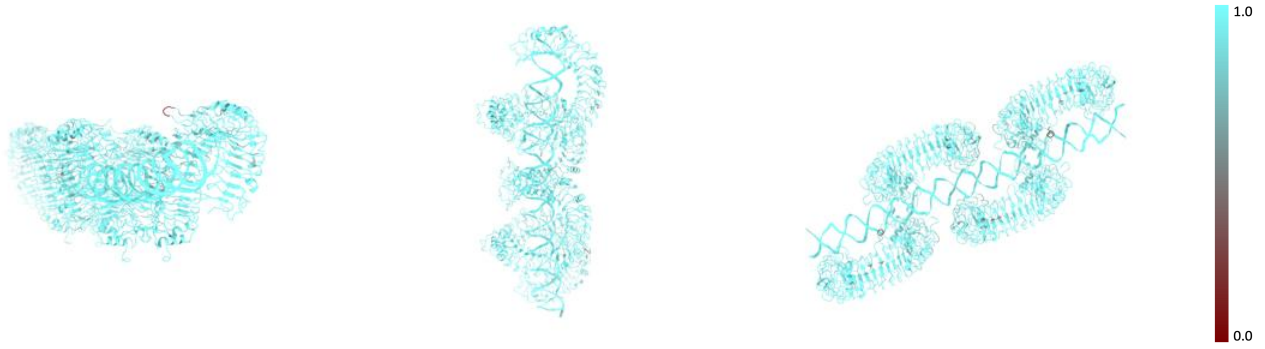
9.2 Q-score mapped to coordinate model (i)



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.

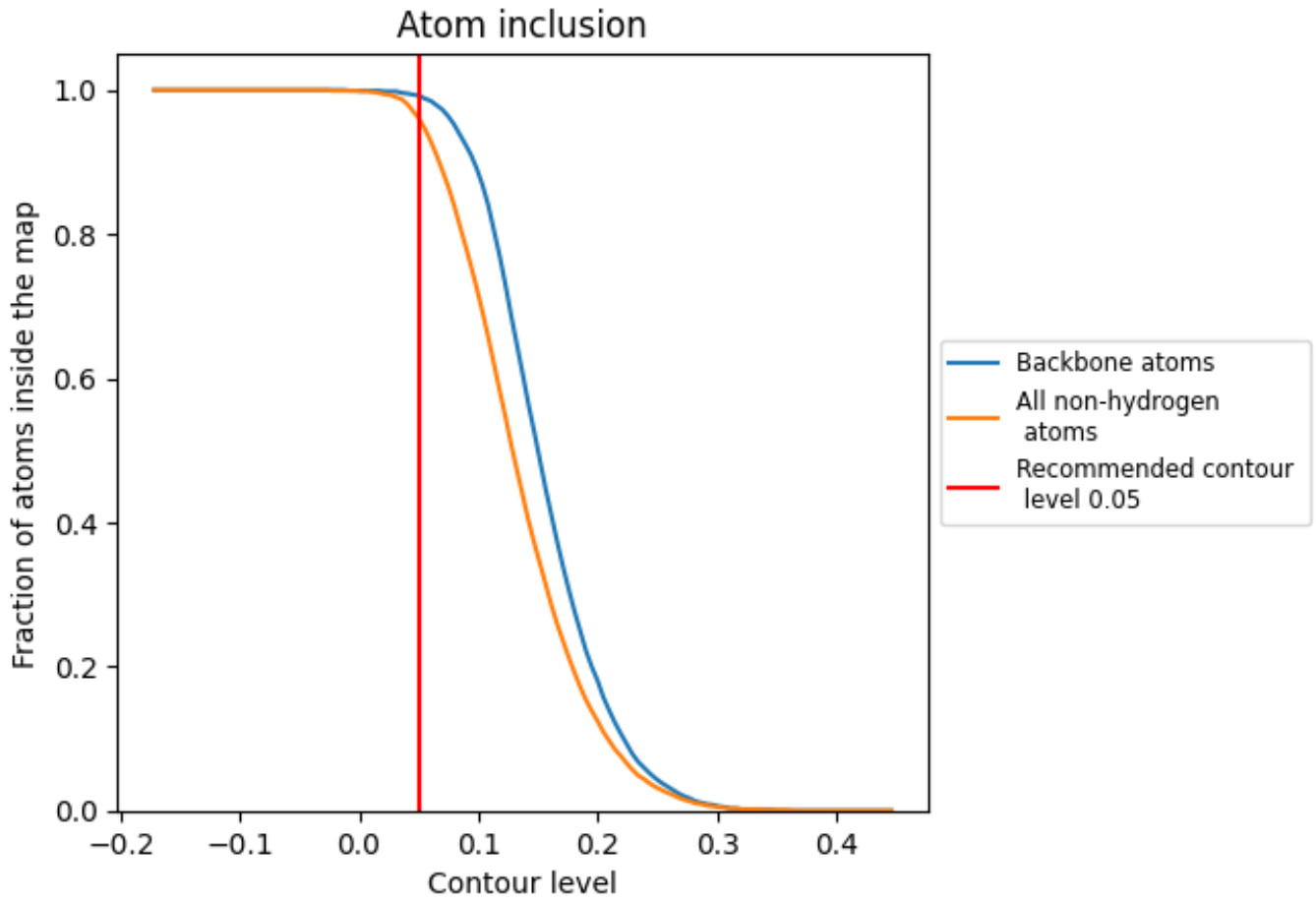
9.3 Atom inclusion mapped to coordinate model (i)



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, 99% of all backbone atoms, 96% 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	0.9610	0.2560
A	0.9850	0.3000
B	0.9820	0.3010
C	0.9680	0.3070
D	0.9570	0.2000
E	0.9640	0.2890
F	0.9550	0.1940
G	0.6670	0.1950
H	1.0000	0.3270
I	0.9290	0.2790
J	1.0000	0.0760
K	0.9740	0.3220
L	0.8970	0.4260
M	0.9740	0.3920
N	0.7860	0.3460
O	0.7860	0.1960
P	1.0000	0.3090
Q	0.6150	0.2950
R	0.9740	0.3830
S	0.9230	0.3350
T	0.7860	0.3940
U	0.7180	0.2800
V	0.9290	0.2540
W	0.7500	0.2300
X	1.0000	0.1520
Y	0.9740	0.2930
Z	0.8970	0.4240
a	0.9490	0.4030
b	0.7860	0.3310
c	0.9290	0.2540
d	1.0000	0.3260
e	0.6150	0.3100
f	0.9740	0.3890
g	0.8720	0.3500
h	0.7860	0.4020