wwPDB EM Validation Summary Report ⓘ

Jul 1, 2024 – 10:28 am BST

PDB ID	:	8OZP
EMDB ID	:	EMD-17317
Title	:	In situ subtomogram average of Prototype Foamy Virus Env pentamer of trimers
Authors	:	Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on	:	2023-05-09
Resolution	:	11.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

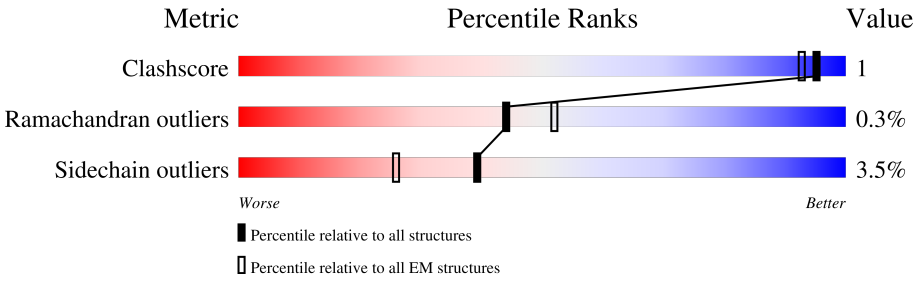
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 11.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	988	6% 94%
1	B	988	37% 58%
1	C	988	36% 5% 58%
1	D	988	37% 59%
1	E	988	5% 94%
1	F	988	99%
1	G	988	35% 5% 59%
1	H	988	37% 59%

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Mol	Chain	Length	Quality of chain
1	I	988	6% 94%
1	L	988	37% 59%
2	M	2	50% 100%
2	N	2	50% 100%
2	O	2	100%
2	Y	2	50% 100%
2	Z	2	50% 100%
2	a	2	50% 100%
2	b	2	100%
2	c	2	100%
2	d	2	50% 100%
3	S	3	67% 100%
3	T	3	67% 100%
3	U	3	100% 100%
4	V	6	17% 100%
4	W	6	17% 17% 83%
4	X	6	17% 100%
5	P	4	75% 100%
5	Q	4	50% 25% 75%
5	R	4	75% 100%
6	e	8	50% 25% 75%
6	f	8	50% 100%
6	g	8	38% 100%
7	h	6	67% 100%
7	i	6	83% 17% 83%

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Mol	Chain	Length	Quality of chain
7	j	6	67% 100%

2 Entry composition

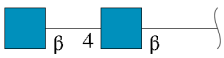
There are 10 unique types of molecules in this entry. The entry contains 22752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	58	Total C N O S 466 309 76 77 4	0	0
1	B	411	Total C N O S 3380 2164 561 636 19	0	0
1	D	405	Total C N O S 3190 2054 536 586 14	0	0
1	F	11	Total C N O S 94 61 18 14 1	0	0
1	H	405	Total C N O S 3190 2054 536 586 14	0	0
1	L	405	Total C N O S 3190 2054 536 586 14	0	0
1	E	58	Total C N O S 466 309 76 77 4	0	0
1	I	58	Total C N O S 466 309 76 77 4	0	0
1	C	411	Total C N O S 3380 2164 561 636 19	0	0
1	G	405	Total C N O S 3328 2133 549 628 18	0	0

- Molecule 2 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
2	M	2	Total C N O 28 16 2 10	0	0
2	a	2	Total C N O 28 16 2 10	0	0

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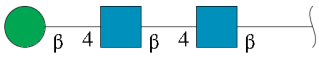
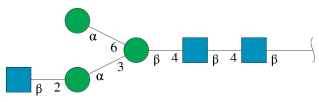
Mol	Chain	Residues	Atoms	AltConf	Trace
2	b	2	Total C N O 28 16 2 10	0	0
2	c	2	Total C N O 28 16 2 10	0	0
2	d	2	Total C N O 28 16 2 10	0	0
2	N	2	Total C N O 28 16 2 10	0	0
2	O	2	Total C N O 28 16 2 10	0	0
2	Y	2	Total C N O 28 16 2 10	0	0
2	Z	2	Total C N O 28 16 2 10	0	0

- Molecule 3 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
3	U	3	Total C N O 39 22 2 15	0	0
3	S	3	Total C N O 39 22 2 15	0	0
3	T	3	Total C N O 39 22 2 15	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
4	X	6	Total C N O 75 42 3 30	0	0

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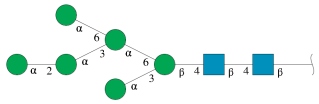
Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	6	Total	C	N	O	0	0
			75	42	3	30		
4	W	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

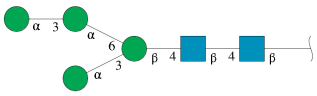
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		

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



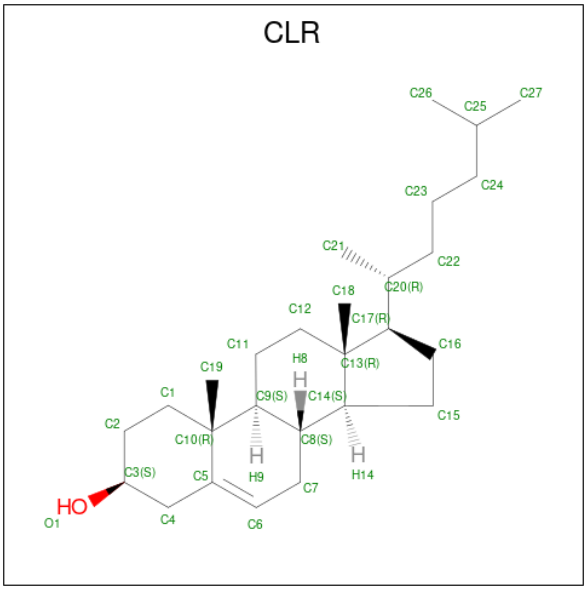
Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	g	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



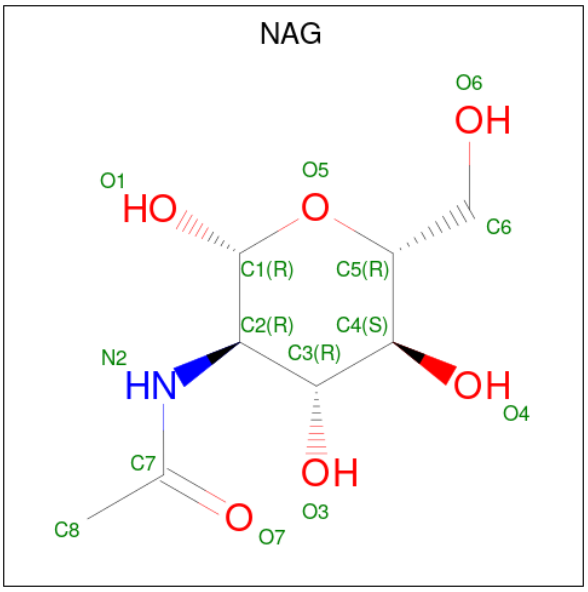
Mol	Chain	Residues	Atoms	AltConf	Trace
7	h	6	Total C N O 72 40 2 30	0	0
7	i	6	Total C N O 72 40 2 30	0	0
7	j	6	Total C N O 72 40 2 30	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



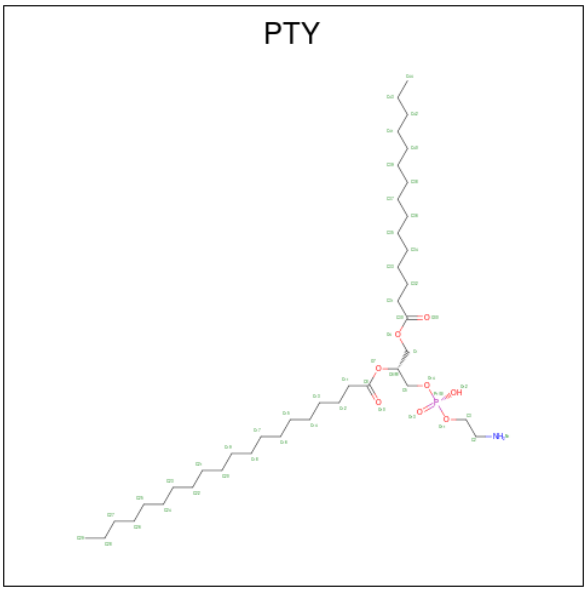
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C O 28 27 1	0
8	D	1	Total C O 28 27 1	0
8	L	1	Total C O 28 27 1	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0
9	G	1	Total C N O 14 8 1 5	0

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



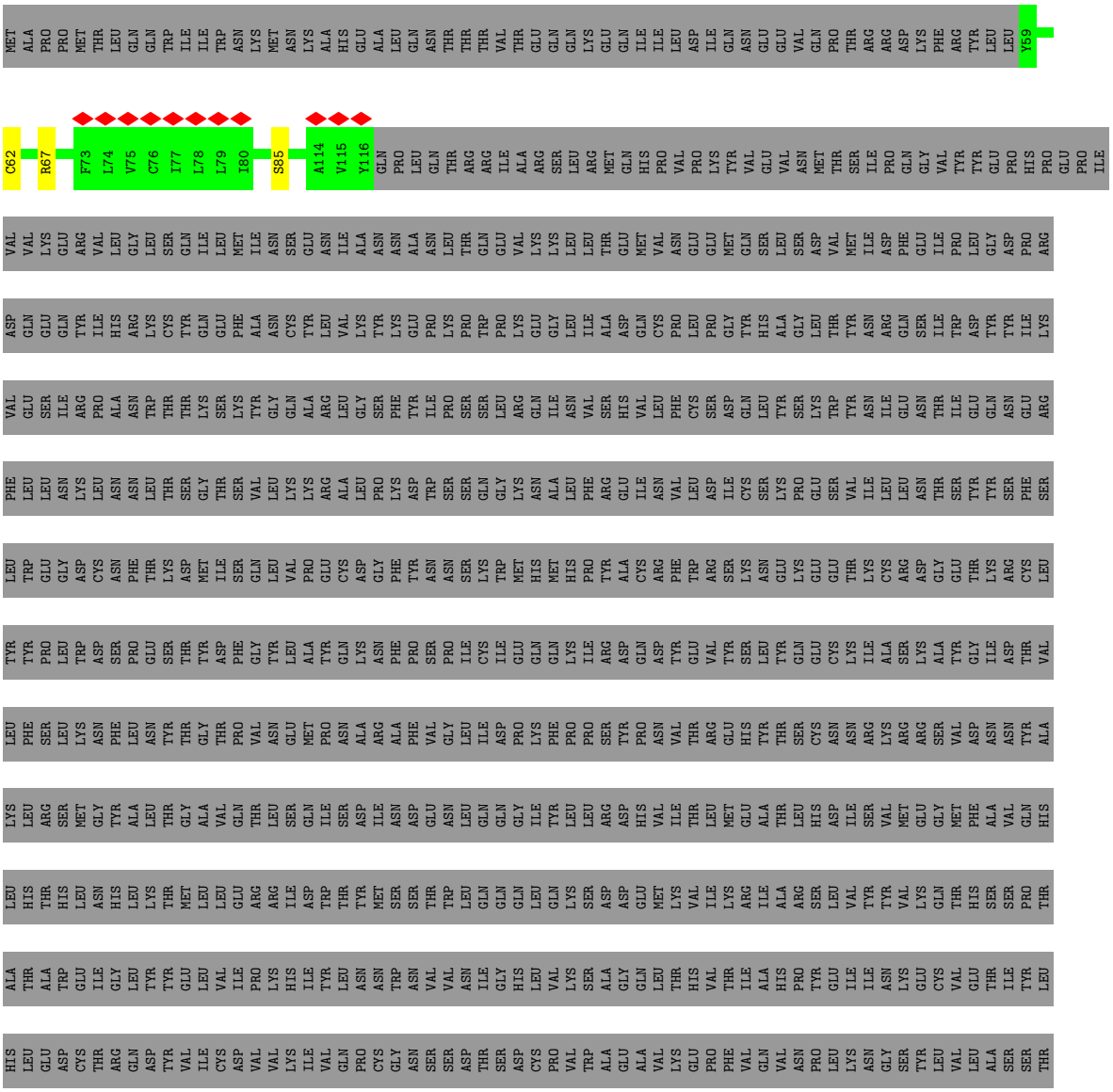
Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

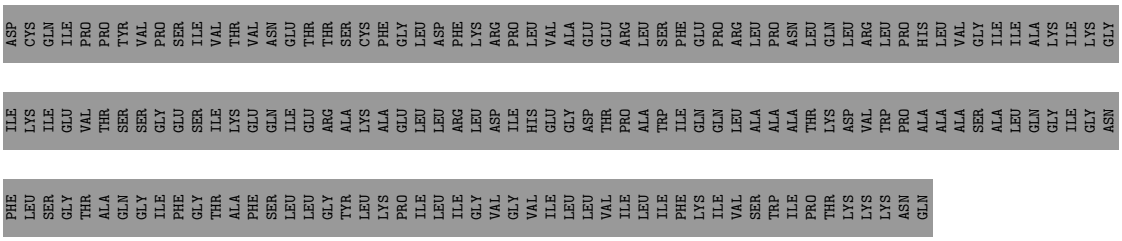
3 Residue-property plots (i)

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: Envelope glycoprotein

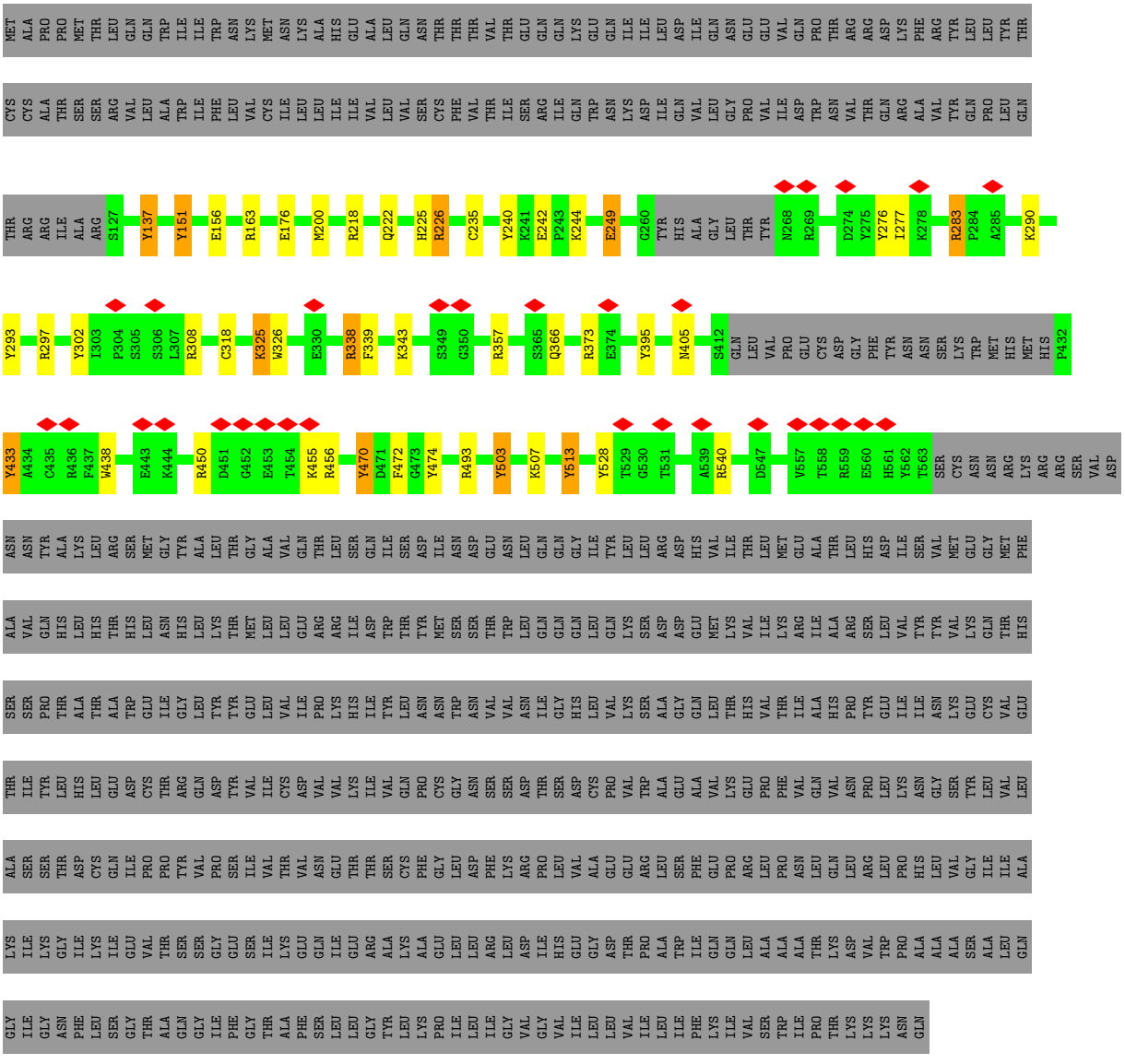
Chain A: 6% 94%





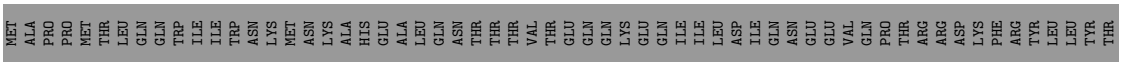
• Molecule 1: Envelope glycoprotein

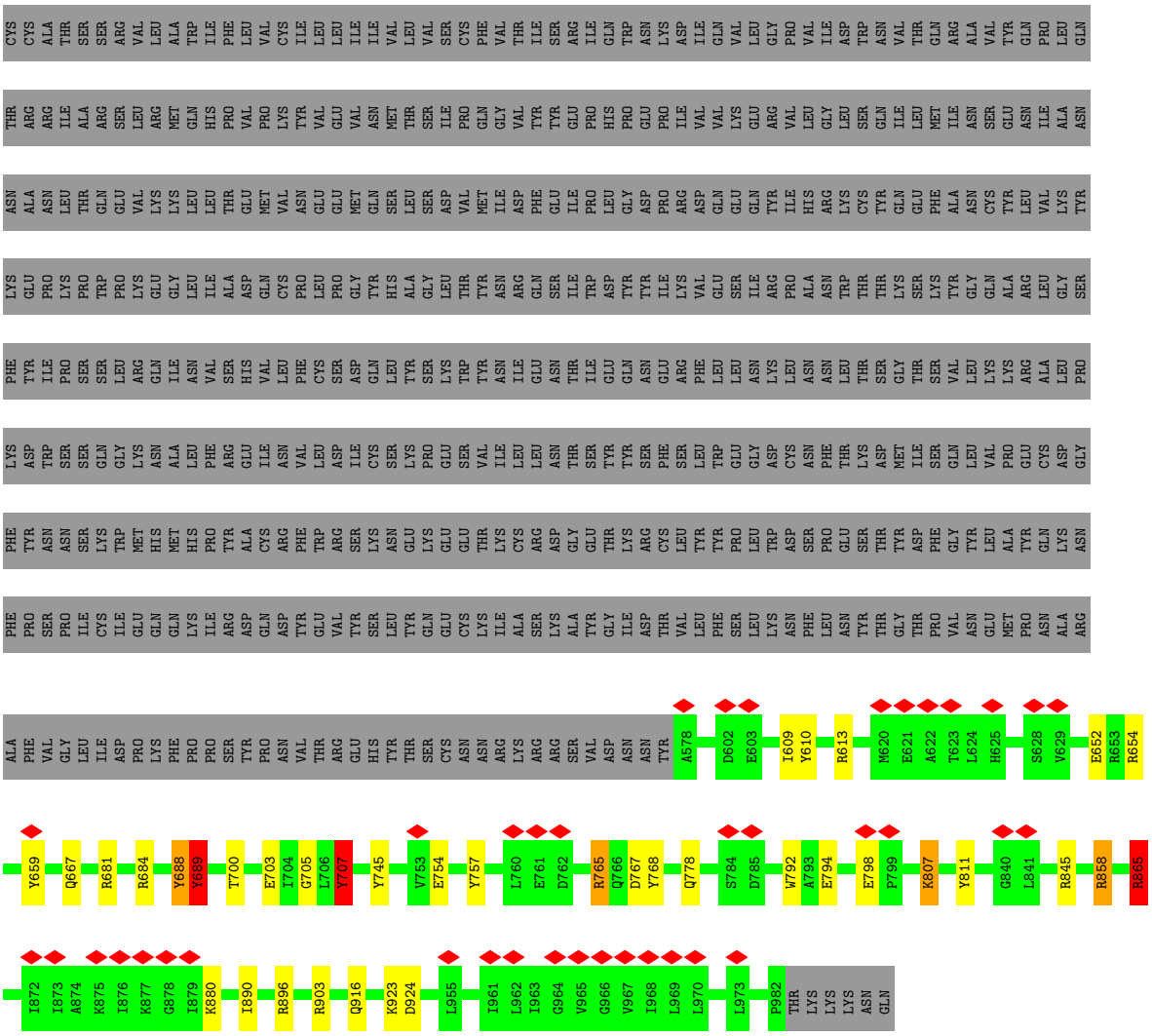
Chain B:



• Molecule 1: Envelope glycoprotein

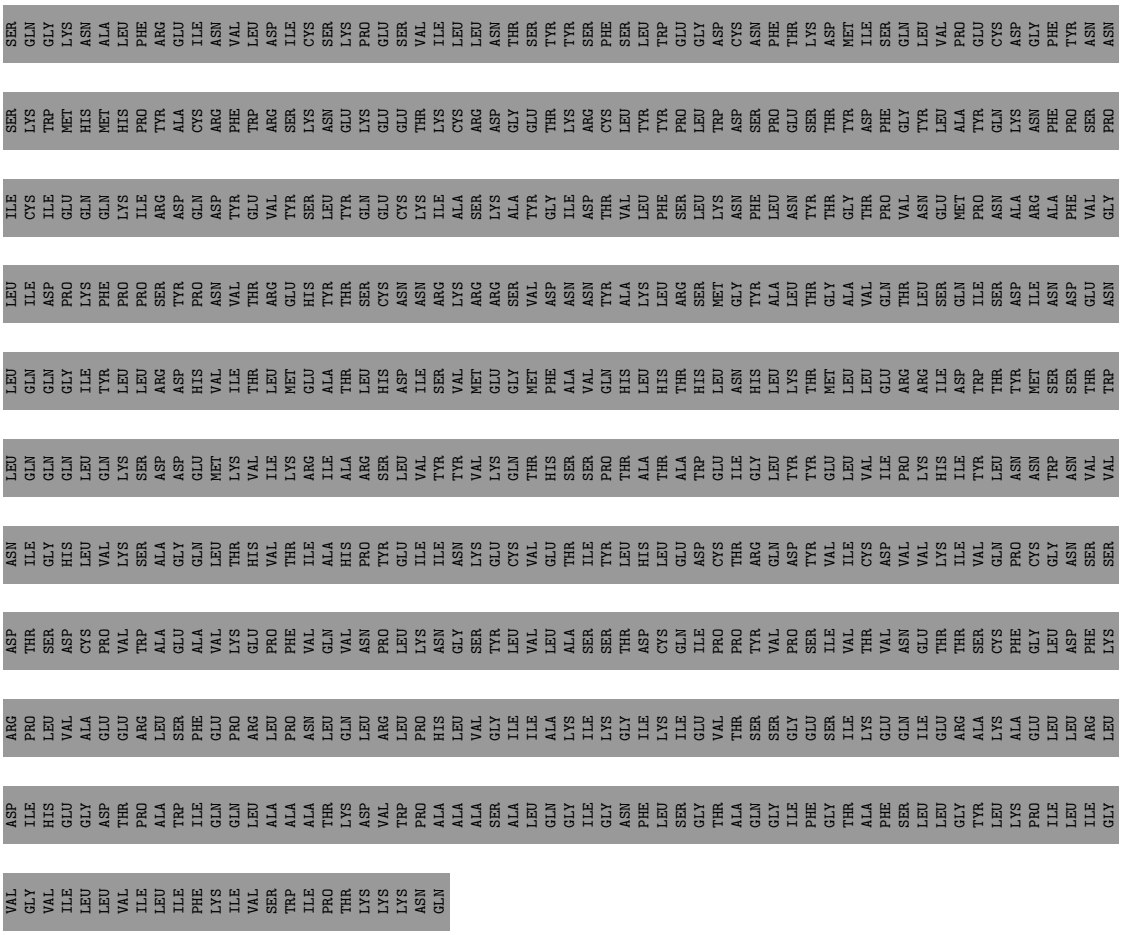
Chain D:





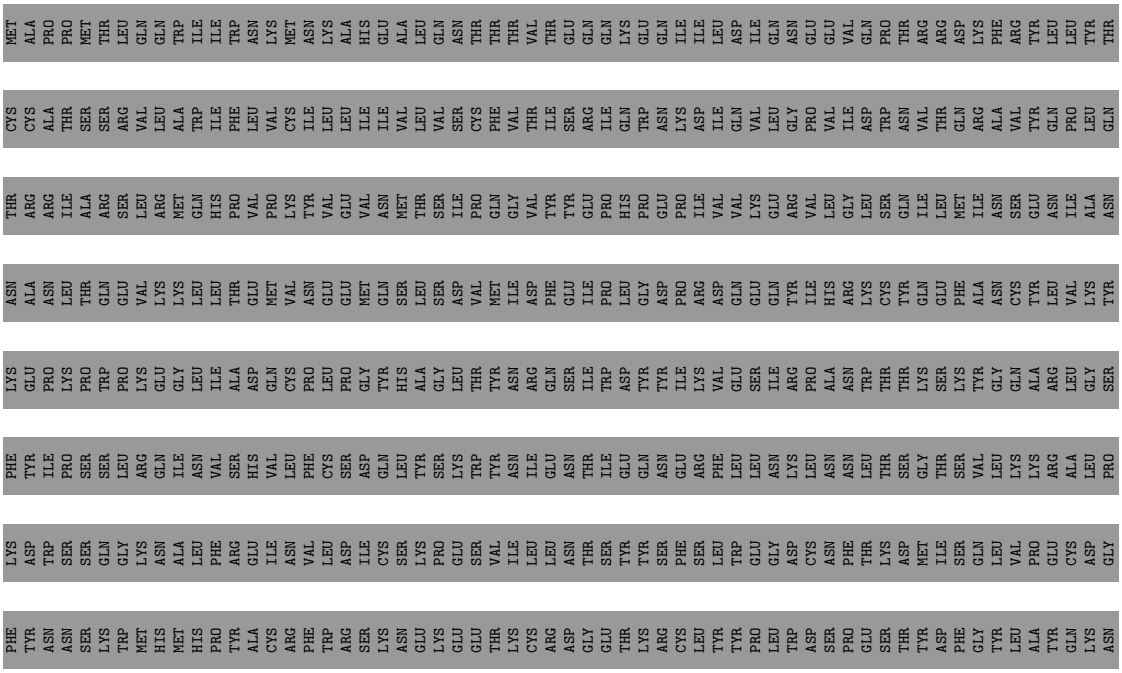
• Molecule 1: Envelope glycoprotein

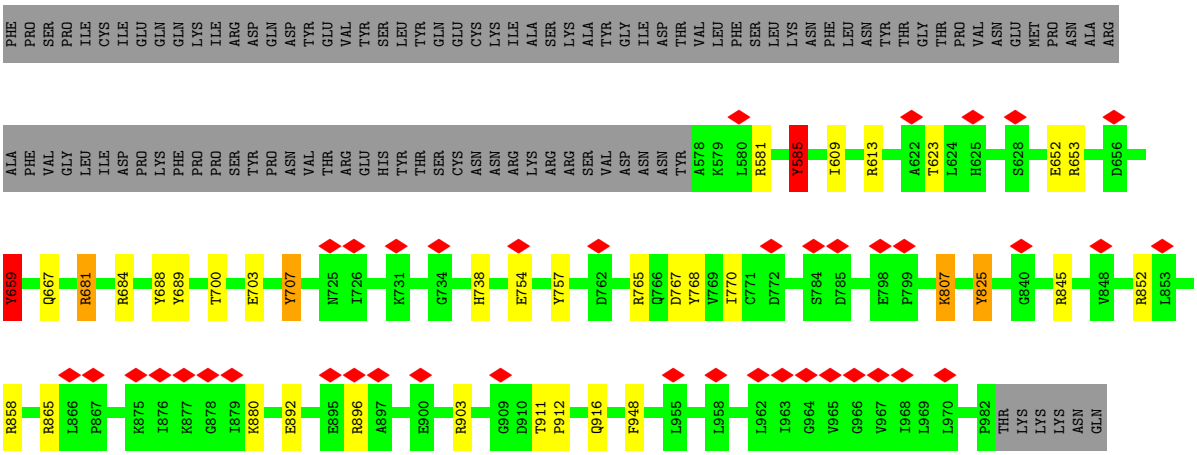
Chain F: 99%



• Molecule 1: Envelope glycoprotein

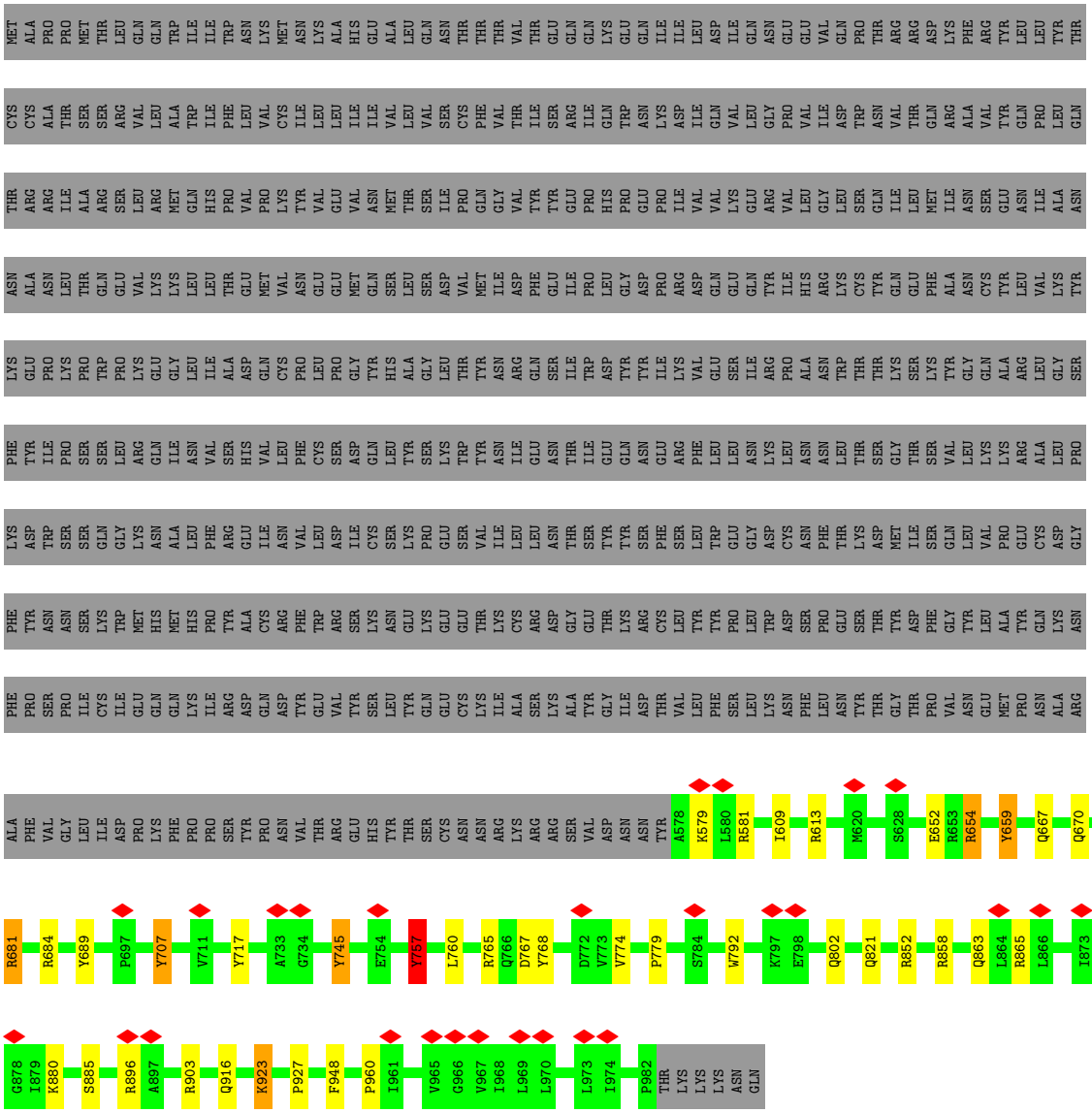
Chain H:





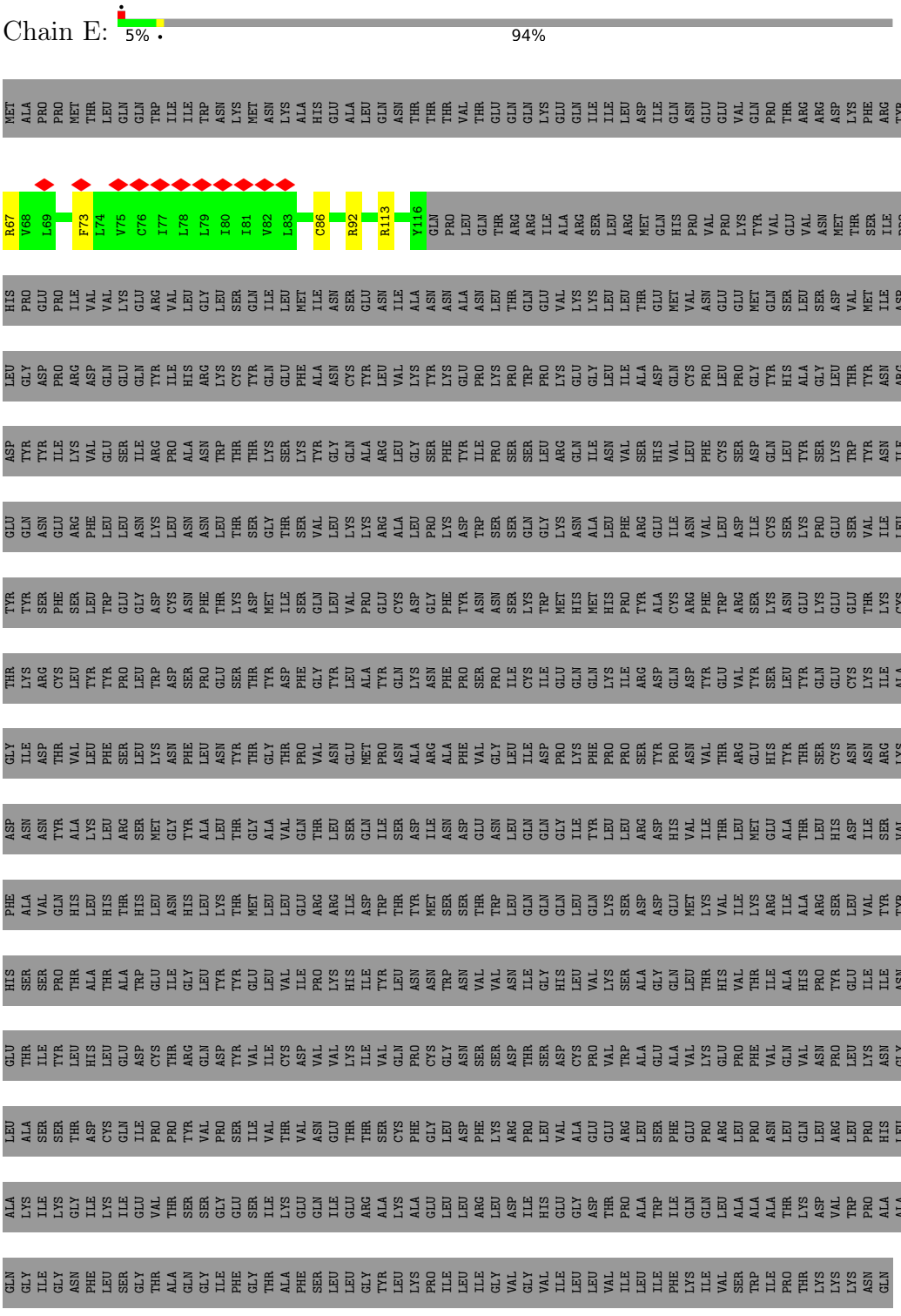
• Molecule 1: Envelope glycoprotein

Chain L:



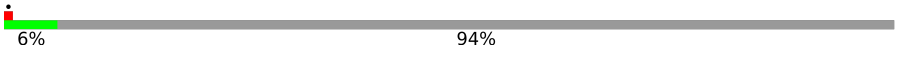
• Molecule 1: Envelope glycoprotein

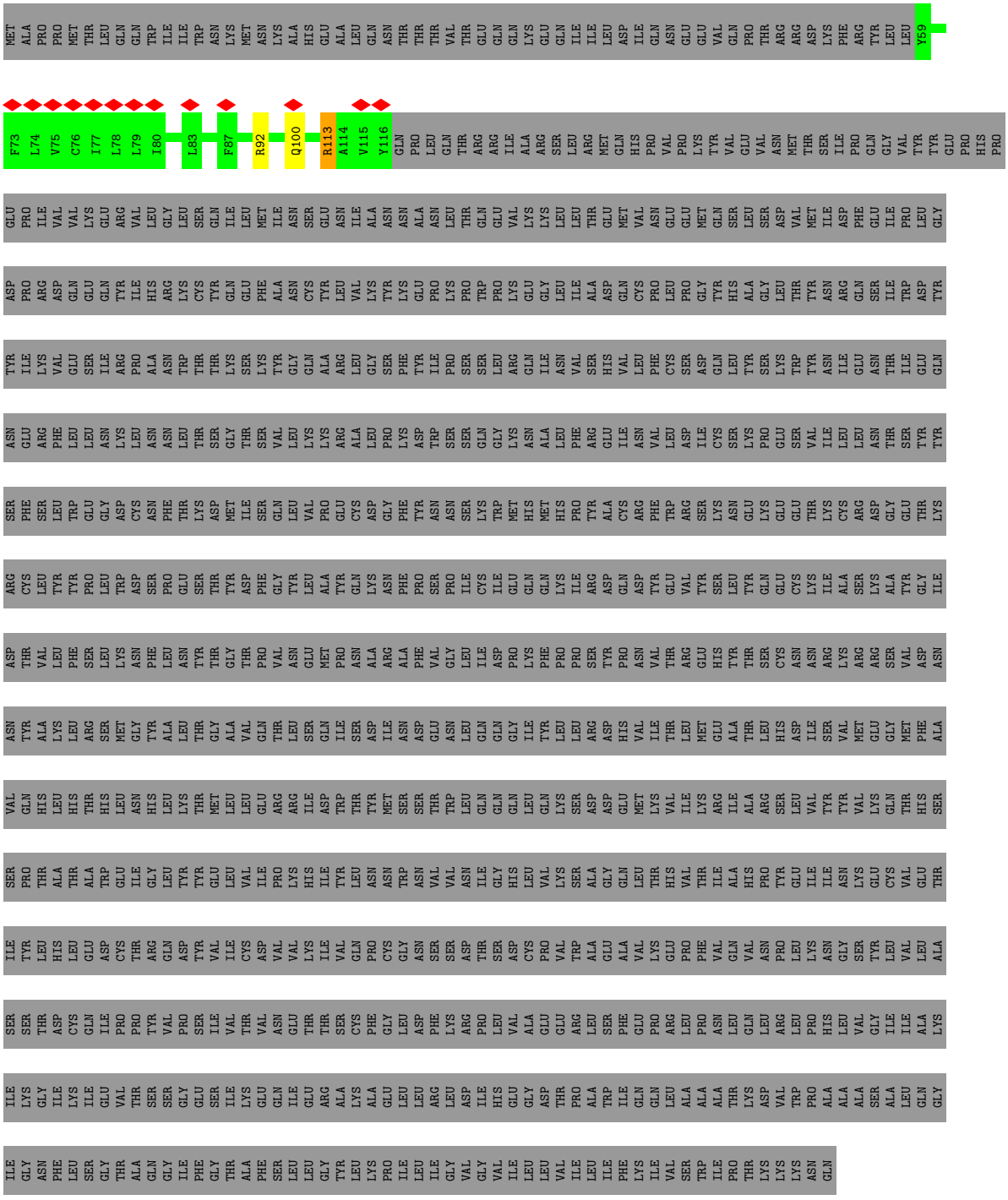
Chain E:

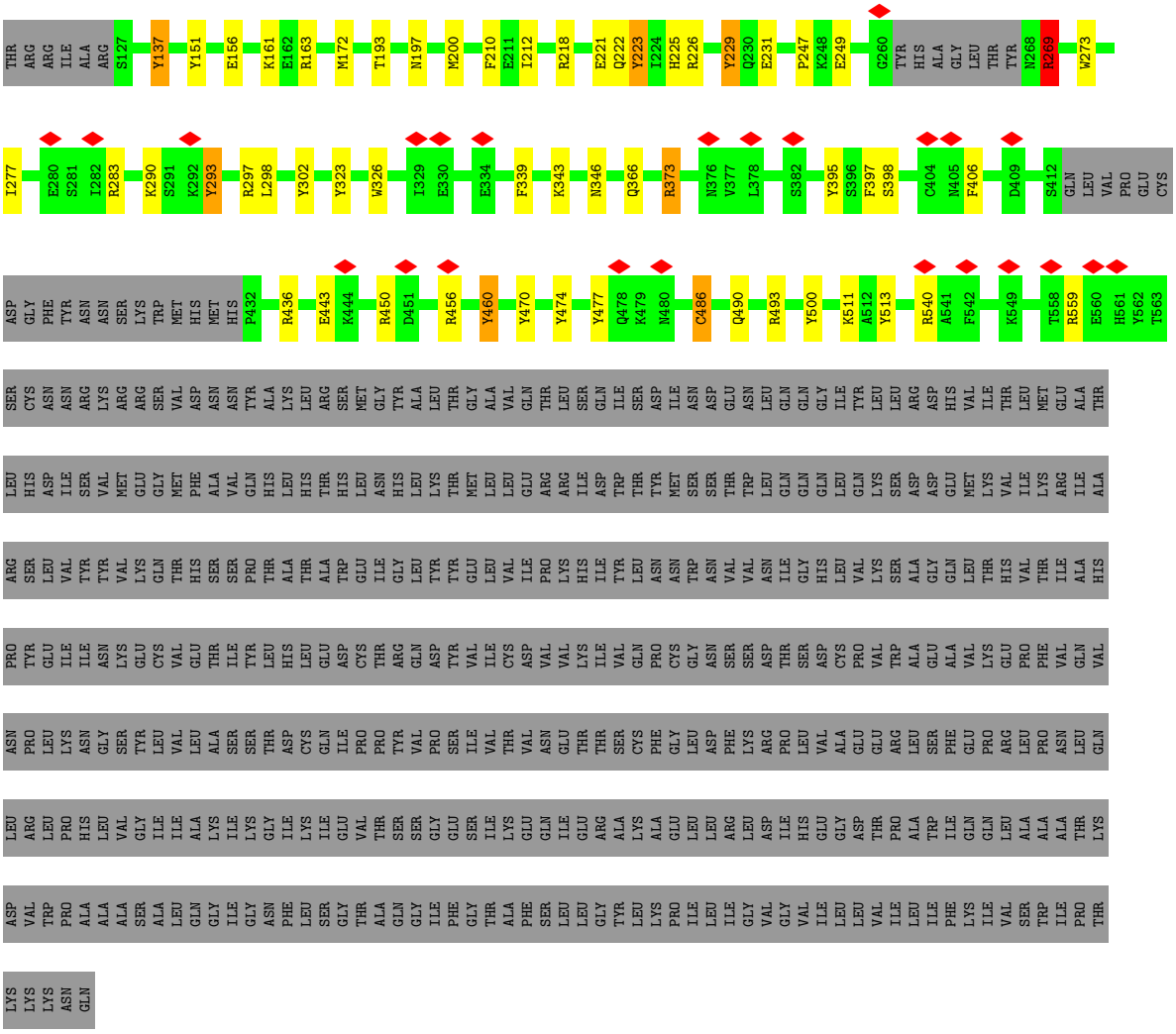


• Molecule 1: Envelope glycoprotein

Chain I:

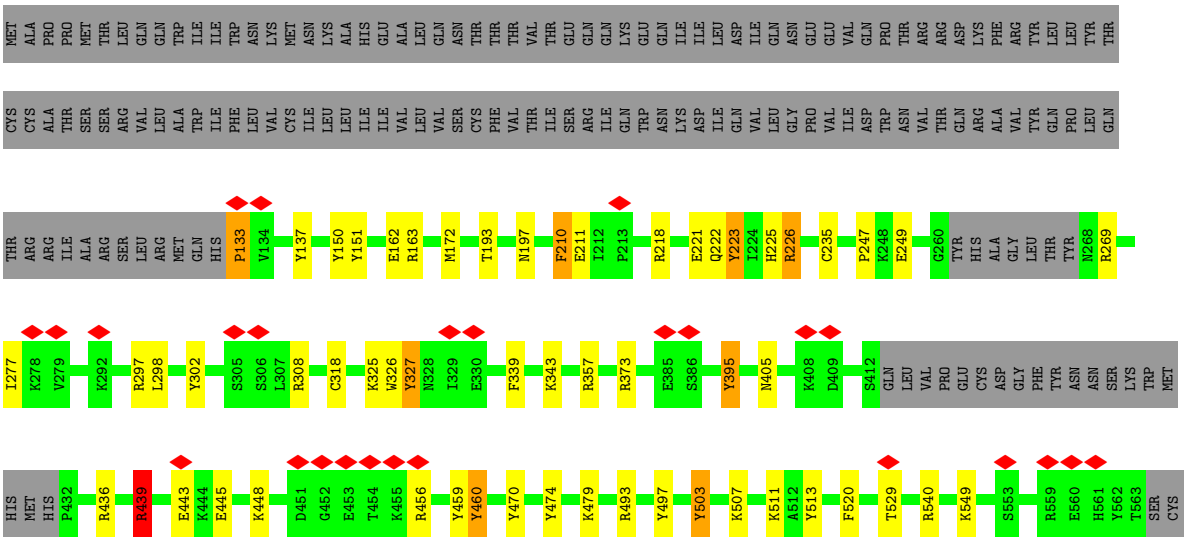



MET ALA PRO PRO MET THR LEU GLN GLN TRP ILE ILE TRP ASN LYS MET ASN LYS ALA HIS GLU ALA LEU GLN ASN THR THR VAL THR GLU GLN GLN LYS GLU GLN ILE ILE LEU ASP ILE GLN ASN GLU GLU VAL GLN PRO THR ARG ARG ASP LYS PHE ARG TYR LEU LEU Y59
F73 L74 V75 C76 I77 L78 L79 I80 L83 F87 R92 Q100 R113 A114 V115 Y116 GLN PRO LEU GLN THR ARG ARG ILE ALA ARG SER LEU ARG THR GLU MET GLN HIS PRO VAL PRO LYS TYR VAL GLU VAL ASN MET THR SER ILE PRO GLN GLY VAL TYR TYR GLU PRO HIS PRO
GLU PRO ILE VAL VAL LYS GLU ARG VAL LEU GLY LEU SER GLN ILE LEU MET ILE ASN SER GLU ASN ILE ALA ASN ASN ALA ASN LEU THR GLN GLU VAL LYS LYS LEU LEU THR GLU MET VAL ASN GLU GLU MET GLN SER LEU SER ASP VAL MET ILE ASP PHE GLU ILE PRO LEU GLY
ASP PRO ARG ASP GLN GLU GLN TYR ILE HIS ARG LYS CYS TYR GLN GLU PHE ALA ASN CYS TYR LEU VAL LYS TYR LYS GLU PRO LYS GLU GLY LEU ILE ALA ASP GLN CYS PRO LEU PRO GLY TYR HIS ALA GLY LEU THR TYR ASN ARG GLN SER ILE TRP ASP TYR
TYR ILE LYS VAL GLU SER ILE ARG PRO ALA ASN TRP THR THR LYS SER LYS TYR GLY GLN ALA ARG LEU GLY SER PHE TYR ILE PRO SER SER LEU ARG GLN ILE ASN VAL SER HIS VAL LEU PHE CYS SER ASP GLN LEU TYR SER LYS TRP TYR ASN ILE GLU ASN THR ILE GLU GLN
ASN GLU ARG PHE LEU LEU ASN LYS LEU ASN ASN LEU THR SER GLY THR SER VAL LEU LYS LYS ARG ALA LEU PRO LYS ASP TRP SER SER GLN GLY LYS ASN ALA LEU PHE ARG GLU ILE ASN VAL LEU ASP ILE CYS SER LYS PRO GLU SER VAL ILE LEU LEU ASN THR SER TYR TYR
SER PHE SER LEU TRP GLU GLY ASP CYS ASN PHE THR LYS ASP MET ILE SER GLN LEU VAL PRO GLU CYS ASP GLY PHE TYR ASN ASN SER LYS TRP MET HIS MET HIS PRO TYR ALA CYS ARG PHE TRP ARG SER LYS ASN GLU LYS GLU GLU THR LYS CYS ARG ASP GLY GLU THR LYS
ARG CYS LEU TYR TYR PRO LEU TRP ASP SER PRO GLU SER THR TYR ASP PHE GLY TYR LEU ALA LEU TYR ASP GLN LYS ASN PHE PRO SER PRO ILE CYS ILE GLU GLN GLN LYS ILE ARG ASP GLN ASP TYR GLU VAL TYR SER LEU TYR GLN GLU CYS LYS ILE ALA SER LYS ALA TYR GLY ILE
ASP THR VAL LEU PHE SER LEU LYS ASN PHE LEU ASN TYR THR GLY THR PRO VAL ASN GLU MET PRO ASN ALA ARG ALA PHE VAL GLY LEU ILE ASP PRO LYS PHE PRO PRO SER TYR PRO ASN VAL THR ARG GLU HIS TYR THR SER CYS ASN ASN ARG LYS ARG ARG SER VAL ASP ASN
ASN TYR ALA LYS LEU ARG SER MET GLY TYR ALA LEU THR GLY ALA VAL GLN THR LEU SER GLN ILE SER ASP ILE ASN ASP GLU ASN LEU GLN GLN GLN GLY ILE TYR LEU LEU ARG ASP HIS VAL ILE THR LEU MET GLU ALA THR LEU HIS ASP ILE SER VAL MET GLU GLY MET PHE ALA
VAL GLN HIS LEU HIS HIS LEU ASN HIS LEU LYS THR MET LEU LEU GLU GLU ARG ARG ILE ASP TRP THR TYR MET SER SER THR TRP LEU GLN GLN GLN LEU GLN LYS SER ASP ASP GLU MET LYS VAL ILE LEU LYS ARG ILE ALA ARG SER LEU VAL TYR TYR VAL LYS GLN THR HIS SER
SER PRO THR ALA THR TRP GLU ILE GLY LEU TYR TYR GLU GLU LEU VAL ILE PRO LYS HIS ILE TYR LEU ASN TRP ASN VAL VAL ASN ILE GLY HIS LEU GLU VAL LYS SER ALA GLY GLN LEU THR HIS VAL THR ILE ALA HIS PRO TYR GLU ILE ILE ASN LYS GLU CYS VAL GLU THR
ILE TYR LEU HIS LEU GLU ASP CYS THR ARG GLN ASP TYR VAL ILE CYS ASP VAL VAL LYS ILE VAL GLN PRO CYS GLY ASN SER SER ASP THR SER ASP CYS PRO VAL TRP ALA GLU ALA VAL LYS GLU PRO PHE VAL GLN VAL ASN PRO LEU LYS ASN GLY SER TYR LEU VAL LEU ALA
SER SER THR ASP CYS GLN ILE PRO PRO TYR VAL PRO SER ILE VAL THR VAL ASN GLU THR THR SER CYS PHE GLY LEU ASP PHE LYS ARG PRO LEU VAL ALA GLU GLU GLU ARG LEU SER PHE GLU PRO ARG LEU PRO ASN LEU GLN LEU ARG PRO HIS LEU VAL GLY ILE ILE ALA LYS
ILE LYS GLY ILE LYS ILE GLU VAL THR SER GLY GLU SER ILE LYS GLU GLN ILE GLU GLU ARG ALA LYS ALA GLU LEU LEU ARG LEU ASP ILE HIS GLU GLY ASP THR PRO ALA TRP ILE GLN GLN LEU ALA ALA THR LYS ASP VAL TRP PRO ALA ALA ALA SER ALA LEU GLN GLY
ILE GLY ASN PHE LEU SER GLY THR ALA PHE SER LEU LEU GLY TYR LEU LYS PRO ILE LEU ILE GLY VAL GLY VAL ILE LEU LEU VAL ILE ILE LEU ILE PHE LYS ILE VAL SER TRP ILE PRO THR LYS LYS LYS ASN GLN
• Molecule 1: Envelope glycoprotein
Chain C: 36% 5% 58%
MET ALA PRO PRO MET THR LEU GLN GLN TRP ILE ILE TRP ASN LYS MET ASN LYS ALA HIS GLU ALA LEU GLN ASN THR THR VAL THR GLU GLN GLN LYS GLU GLN ILE ILE LEU ASP ILE GLN ASN GLU GLU VAL GLN PRO THR ARG ARG ASP LYS PHE ARG TYR LEU LEU THR
CYS CYS ALA THR SER SER ARG VAL LEU ALA TRP ILE PHE LEU VAL CYS ILE LEU LEU ILE ILE VAL ALA LEU VAL SER CYS PHE VAL THR ILE SER ARG ILE GLN TRP ASN LYS ASP ILE GLN VAL LEU GLY PRO VAL ILE ASP TRP ASN VAL THR GLN ARG ALA VAL TYR GLN PRO LEU GLN



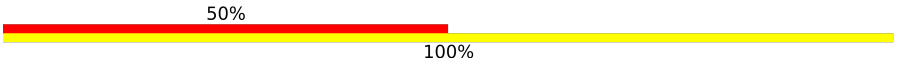
• Molecule 1: Envelope glycoprotein

Chain G:



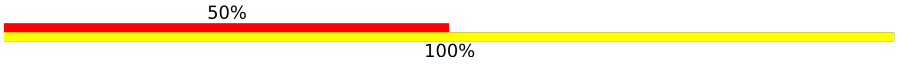
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



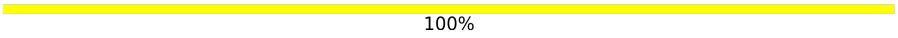
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



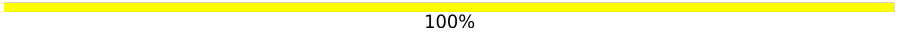
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



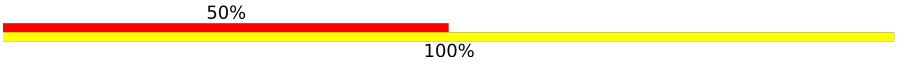
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



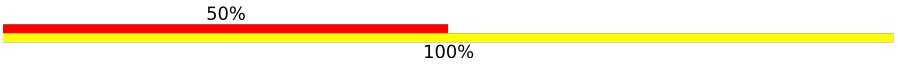
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



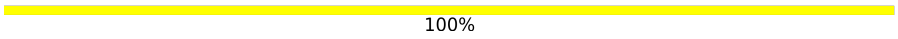
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



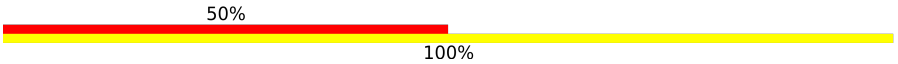
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



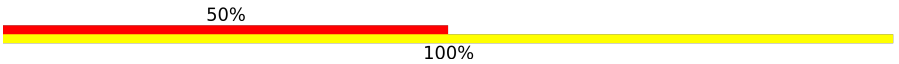
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



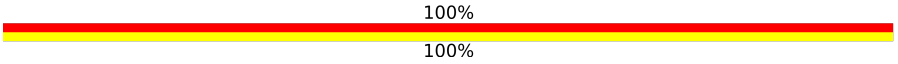
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain U:

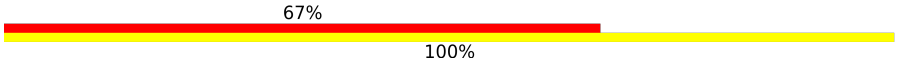


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

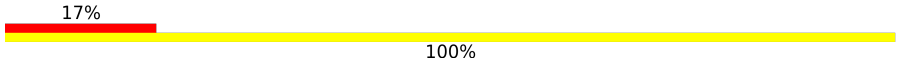
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



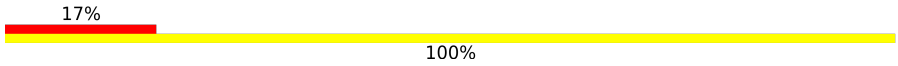
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



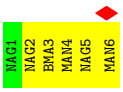
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



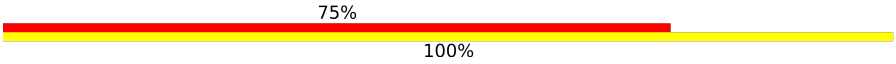
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

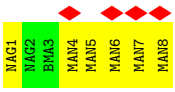
Chain P:

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

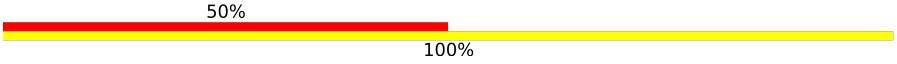
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

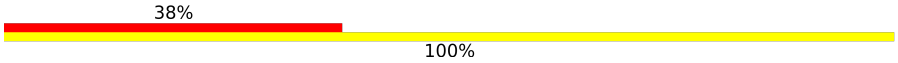
Chain f:



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1

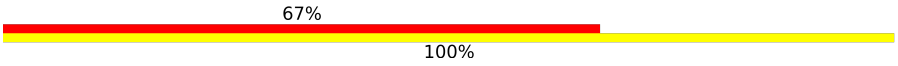
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain g:



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam
ido-2-deoxy-beta-D-glucopyranose

Chain h:



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam
ido-2-deoxy-beta-D-glucopyranose

Chain i:

• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam
ido-2-deoxy-beta-D-glucopyranose

Chain j:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of subtomograms used	2220	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	107.42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.064	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.76, 2.76, 2.76	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.69	0/476	1.02	0/653
1	B	0.72	0/3469	1.11	22/4705 (0.5%)
1	C	0.71	0/3469	1.13	25/4705 (0.5%)
1	D	0.64	0/3260	1.08	17/4441 (0.4%)
1	E	0.68	0/476	1.13	4/653 (0.6%)
1	F	0.77	0/97	1.19	1/130 (0.8%)
1	G	0.72	0/3416	1.16	32/4634 (0.7%)
1	H	0.64	0/3260	1.08	16/4441 (0.4%)
1	I	0.70	0/476	1.09	2/653 (0.3%)
1	L	0.64	0/3260	1.10	18/4441 (0.4%)
All	All	0.68	0/21659	1.11	137/29456 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	10
1	C	0	11
1	D	0	11
1	E	0	1
1	G	0	9
1	H	0	10
1	I	0	1
1	L	0	5
All	All	0	58

There are no bond length outliers.

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	745	TYR	CB-CG-CD1	-12.05	113.77	121.00
1	B	513	TYR	CB-CG-CD2	-9.86	115.08	121.00
1	C	373	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	G	395	TYR	CB-CG-CD2	-9.70	115.18	121.00
1	G	223	TYR	CB-CG-CD2	-9.51	115.30	121.00

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	TYR	Sidechain
1	B	225	HIS	Sidechain
1	B	283	ARG	Sidechain
1	B	293	TYR	Sidechain
1	B	338	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	466	0	488	1	0
1	B	3380	0	3293	7	0
1	C	3380	0	3293	9	0
1	D	3190	0	3242	9	0
1	E	466	0	488	0	0
1	F	94	0	97	1	0
1	G	3328	0	3241	9	0
1	H	3190	0	3242	9	0
1	I	466	0	488	0	0
1	L	3190	0	3242	7	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	28	0	25	0	0
3	S	39	0	34	0	0
3	T	39	0	34	0	0
3	U	39	0	34	0	0
4	V	75	0	64	0	0
4	W	75	0	64	0	0
4	X	75	0	64	0	0
5	P	50	0	43	0	0
5	Q	50	0	43	0	0
5	R	50	0	43	0	0
6	e	94	0	79	0	0
6	f	94	0	79	0	0
6	g	94	0	79	0	0
7	h	72	0	61	0	0
7	i	72	0	61	0	0
7	j	72	0	61	0	0
8	A	28	0	46	1	0
8	D	28	0	46	3	0
8	L	28	0	46	0	0
9	B	42	0	39	0	0
9	C	42	0	39	0	0
9	G	42	0	39	0	0
10	D	50	0	79	0	0
10	H	50	0	79	0	0
10	L	50	0	79	0	0
All	All	22752	0	22674	46	0

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

The worst 5 of 46 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:TRP:CG	1:B:343:LYS:HE3	2.31	0.65
1:G:326:TRP:CG	1:G:343:LYS:HE3	2.33	0.65
8:D:1100:CLR:H192	1:L:960:PRO:HB3	1.79	0.64
1:C:277:ILE:HG21	1:C:298:LEU:HD12	1.87	0.55
1:D:865:ARG:HE	1:D:890:ILE:HD11	1.75	0.52

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	56/988 (6%)	54 (96%)	2 (4%)	0	100	100
1	B	405/988 (41%)	382 (94%)	22 (5%)	1 (0%)	47	81
1	C	405/988 (41%)	379 (94%)	24 (6%)	2 (0%)	29	69
1	D	403/988 (41%)	387 (96%)	15 (4%)	1 (0%)	47	81
1	E	56/988 (6%)	54 (96%)	2 (4%)	0	100	100
1	F	9/988 (1%)	9 (100%)	0	0	100	100
1	G	399/988 (40%)	374 (94%)	23 (6%)	2 (0%)	29	69
1	H	403/988 (41%)	387 (96%)	15 (4%)	1 (0%)	47	81
1	I	56/988 (6%)	53 (95%)	3 (5%)	0	100	100
1	L	403/988 (41%)	386 (96%)	16 (4%)	1 (0%)	47	81
All	All	2595/9880 (26%)	2465 (95%)	122 (5%)	8 (0%)	44	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	470	TYR
1	G	470	TYR
1	B	470	TYR
1	L	767	ASP
1	H	767	ASP

5.3.2 Protein sidechains

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	A	54/899 (6%)	52 (96%)	2 (4%)	34	58
1	B	382/899 (42%)	366 (96%)	16 (4%)	30	54
1	C	382/899 (42%)	365 (96%)	17 (4%)	27	52
1	D	356/899 (40%)	345 (97%)	11 (3%)	40	62
1	E	54/899 (6%)	54 (100%)	0	100	100
1	F	11/899 (1%)	11 (100%)	0	100	100
1	G	376/899 (42%)	360 (96%)	16 (4%)	29	53
1	H	356/899 (40%)	347 (98%)	9 (2%)	47	68
1	I	54/899 (6%)	53 (98%)	1 (2%)	57	75
1	L	356/899 (40%)	344 (97%)	12 (3%)	37	60
All	All	2381/8990 (26%)	2297 (96%)	84 (4%)	39	59

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	231	GLU
1	G	211	GLU
1	C	269	ARG
1	C	486	CYS
1	G	249	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	225	HIS
1	D	934	GLN
1	L	670	GLN
1	C	489	GLN
1	G	495	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

99 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	$\#\|Z\| > 2$
2	NAG	M	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	1.27	2 (11%)
2	NAG	M	2	2	14,14,15	1.36	2 (14%)	17,19,21	0.77	0
2	NAG	N	1	1,2	14,14,15	1.24	2 (14%)	17,19,21	0.85	0
2	NAG	N	2	2	14,14,15	1.21	1 (7%)	17,19,21	0.72	0
2	NAG	O	1	1,2	14,14,15	1.08	0	17,19,21	1.26	2 (11%)
2	NAG	O	2	2	14,14,15	1.09	1 (7%)	17,19,21	0.87	0
5	NAG	P	1	1,5	14,14,15	1.11	1 (7%)	17,19,21	1.16	1 (5%)
5	NAG	P	2	5	14,14,15	1.40	4 (28%)	17,19,21	1.01	2 (11%)
5	BMA	P	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.10	1 (6%)
5	MAN	P	4	5	11,11,12	1.33	2 (18%)	15,15,17	1.03	1 (6%)
5	NAG	Q	1	1,5	14,14,15	1.01	0	17,19,21	0.71	0
5	NAG	Q	2	5	14,14,15	1.17	1 (7%)	17,19,21	1.10	2 (11%)
5	BMA	Q	3	5	11,11,12	1.16	1 (9%)	15,15,17	0.98	1 (6%)
5	MAN	Q	4	5	11,11,12	1.37	2 (18%)	15,15,17	1.15	2 (13%)
5	NAG	R	1	1,5	14,14,15	1.14	2 (14%)	17,19,21	0.90	0
5	NAG	R	2	5	14,14,15	1.55	4 (28%)	17,19,21	0.85	1 (5%)
5	BMA	R	3	5	11,11,12	1.19	1 (9%)	15,15,17	1.11	0
5	MAN	R	4	5	11,11,12	1.28	2 (18%)	15,15,17	0.87	1 (6%)
3	NAG	S	1	1,3	14,14,15	1.20	1 (7%)	17,19,21	1.50	2 (11%)
3	NAG	S	2	3	14,14,15	1.19	1 (7%)	17,19,21	0.70	0
3	BMA	S	3	3	11,11,12	1.15	2 (18%)	15,15,17	1.05	1 (6%)
3	NAG	T	1	1,3	14,14,15	1.09	0	17,19,21	1.47	3 (17%)
3	NAG	T	2	3	14,14,15	1.29	2 (14%)	17,19,21	0.91	0
3	BMA	T	3	3	11,11,12	1.32	2 (18%)	15,15,17	0.87	0
3	NAG	U	1	1,3	14,14,15	1.28	3 (21%)	17,19,21	0.93	1 (5%)
3	NAG	U	2	3	14,14,15	1.17	2 (14%)	17,19,21	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	U	3	3	11,11,12	1.36	2 (18%)	15,15,17	0.78	0
4	NAG	V	1	1,4	14,14,15	1.25	4 (28%)	17,19,21	0.86	0
4	NAG	V	2	4	14,14,15	0.99	1 (7%)	17,19,21	1.00	1 (5%)
4	BMA	V	3	4	11,11,12	1.20	1 (9%)	15,15,17	0.79	0
4	MAN	V	4	4	11,11,12	1.51	3 (27%)	15,15,17	1.42	2 (13%)
4	NAG	V	5	4	14,14,15	0.87	0	17,19,21	1.26	2 (11%)
4	MAN	V	6	4	11,11,12	1.47	2 (18%)	15,15,17	1.23	1 (6%)
4	NAG	W	1	1,4	14,14,15	1.04	0	17,19,21	1.11	0
4	NAG	W	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.02	1 (5%)
4	BMA	W	3	4	11,11,12	1.10	1 (9%)	15,15,17	0.91	0
4	MAN	W	4	4	11,11,12	1.47	3 (27%)	15,15,17	1.23	2 (13%)
4	NAG	W	5	4	14,14,15	0.84	1 (7%)	17,19,21	1.21	2 (11%)
4	MAN	W	6	4	11,11,12	1.40	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	X	1	1,4	14,14,15	1.29	3 (21%)	17,19,21	1.00	1 (5%)
4	NAG	X	2	4	14,14,15	1.06	1 (7%)	17,19,21	1.16	2 (11%)
4	BMA	X	3	4	11,11,12	1.17	1 (9%)	15,15,17	1.04	1 (6%)
4	MAN	X	4	4	11,11,12	1.59	3 (27%)	15,15,17	1.31	2 (13%)
4	NAG	X	5	4	14,14,15	0.86	1 (7%)	17,19,21	1.18	2 (11%)
4	MAN	X	6	4	11,11,12	1.40	2 (18%)	15,15,17	1.05	1 (6%)
2	NAG	Y	1	1,2	14,14,15	1.06	2 (14%)	17,19,21	0.78	1 (5%)
2	NAG	Y	2	2	14,14,15	1.19	2 (14%)	17,19,21	1.18	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.15	2 (14%)	17,19,21	0.93	1 (5%)
2	NAG	Z	2	2	14,14,15	1.22	2 (14%)	17,19,21	0.88	0
2	NAG	a	1	1,2	14,14,15	1.43	3 (21%)	17,19,21	0.73	0
2	NAG	a	2	2	14,14,15	1.05	1 (7%)	17,19,21	0.97	2 (11%)
2	NAG	b	1	1,2	14,14,15	0.99	1 (7%)	17,19,21	1.98	6 (35%)
2	NAG	b	2	2	14,14,15	1.30	3 (21%)	17,19,21	1.64	3 (17%)
2	NAG	c	1	1,2	14,14,15	1.26	2 (14%)	17,19,21	1.27	3 (17%)
2	NAG	c	2	2	14,14,15	1.27	1 (7%)	17,19,21	1.21	1 (5%)
2	NAG	d	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	1.76	5 (29%)
2	NAG	d	2	2	14,14,15	1.20	1 (7%)	17,19,21	1.38	2 (11%)
6	NAG	e	1	1,6	14,14,15	1.25	2 (14%)	17,19,21	1.41	2 (11%)
6	NAG	e	2	6	14,14,15	1.01	0	17,19,21	0.79	0
6	BMA	e	3	6	11,11,12	1.09	0	15,15,17	0.91	0
6	MAN	e	4	6	11,11,12	1.30	1 (9%)	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	e	5	6	11,11,12	1.18	2 (18%)	15,15,17	1.72	5 (33%)
6	MAN	e	6	6	11,11,12	1.18	2 (18%)	15,15,17	1.20	1 (6%)
6	MAN	e	7	6	11,11,12	1.34	2 (18%)	15,15,17	0.71	0
6	MAN	e	8	6	11,11,12	1.29	1 (9%)	15,15,17	0.75	0
6	NAG	f	1	1,6	14,14,15	1.27	2 (14%)	17,19,21	1.16	2 (11%)
6	NAG	f	2	6	14,14,15	1.09	1 (7%)	17,19,21	0.89	1 (5%)
6	BMA	f	3	6	11,11,12	1.20	1 (9%)	15,15,17	0.66	0
6	MAN	f	4	6	11,11,12	1.18	1 (9%)	15,15,17	0.99	1 (6%)
6	MAN	f	5	6	11,11,12	1.25	2 (18%)	15,15,17	1.33	2 (13%)
6	MAN	f	6	6	11,11,12	1.32	2 (18%)	15,15,17	0.94	1 (6%)
6	MAN	f	7	6	11,11,12	1.28	1 (9%)	15,15,17	0.81	0
6	MAN	f	8	6	11,11,12	1.21	1 (9%)	15,15,17	0.84	1 (6%)
6	NAG	g	1	1,6	14,14,15	1.11	1 (7%)	17,19,21	1.21	2 (11%)
6	NAG	g	2	6	14,14,15	1.26	3 (21%)	17,19,21	0.83	0
6	BMA	g	3	6	11,11,12	1.12	1 (9%)	15,15,17	1.00	1 (6%)
6	MAN	g	4	6	11,11,12	1.27	1 (9%)	15,15,17	0.93	1 (6%)
6	MAN	g	5	6	11,11,12	1.18	2 (18%)	15,15,17	1.38	4 (26%)
6	MAN	g	6	6	11,11,12	1.19	1 (9%)	15,15,17	0.91	1 (6%)
6	MAN	g	7	6	11,11,12	1.28	2 (18%)	15,15,17	0.88	1 (6%)
6	MAN	g	8	6	11,11,12	1.15	1 (9%)	15,15,17	0.81	1 (6%)
7	NAG	h	1	1,7	14,14,15	0.99	0	17,19,21	1.30	2 (11%)
7	NAG	h	2	7	14,14,15	0.97	1 (7%)	17,19,21	1.02	1 (5%)
7	BMA	h	3	7	11,11,12	1.24	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	h	4	7	11,11,12	1.23	1 (9%)	15,15,17	0.85	1 (6%)
7	MAN	h	5	7	11,11,12	1.37	2 (18%)	15,15,17	1.16	1 (6%)
7	MAN	h	6	7	11,11,12	1.33	2 (18%)	15,15,17	0.81	1 (6%)
7	NAG	i	1	1,7	14,14,15	1.03	0	17,19,21	0.82	0
7	NAG	i	2	7	14,14,15	1.24	2 (14%)	17,19,21	0.84	1 (5%)
7	BMA	i	3	7	11,11,12	1.42	2 (18%)	15,15,17	1.21	1 (6%)
7	MAN	i	4	7	11,11,12	1.30	3 (27%)	15,15,17	1.17	1 (6%)
7	MAN	i	5	7	11,11,12	1.40	2 (18%)	15,15,17	1.25	2 (13%)
7	MAN	i	6	7	11,11,12	1.36	2 (18%)	15,15,17	0.51	0
7	NAG	j	1	1,7	14,14,15	1.06	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	j	2	7	14,14,15	1.27	2 (14%)	17,19,21	0.92	0
7	BMA	j	3	7	11,11,12	1.37	2 (18%)	15,15,17	1.54	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	j	4	7	11,11,12	1.20	2 (18%)	15,15,17	1.27	1 (6%)
7	MAN	j	5	7	11,11,12	1.39	2 (18%)	15,15,17	1.29	1 (6%)
7	MAN	j	6	7	11,11,12	1.33	2 (18%)	15,15,17	1.05	1 (6%)

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
2	NAG	M	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	1/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	0/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	V	4	4	-	1/2/19/22	0/1/1/1
4	NAG	V	5	4	-	1/6/23/26	0/1/1/1
4	MAN	V	6	4	-	1/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	MAN	W	4	4	-	1/2/19/22	0/1/1/1
4	NAG	W	5	4	-	2/6/23/26	0/1/1/1
4	MAN	W	6	4	-	1/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
4	MAN	X	4	4	-	1/2/19/22	0/1/1/1
4	NAG	X	5	4	-	2/6/23/26	0/1/1/1
4	MAN	X	6	4	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	1/6/23/26	0/1/1/1
2	NAG	b	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	3/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	1/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	3/6/23/26	0/1/1/1
6	NAG	e	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
6	MAN	e	5	6	-	0/2/19/22	0/1/1/1
6	MAN	e	6	6	-	0/2/19/22	0/1/1/1
6	MAN	e	7	6	-	0/2/19/22	0/1/1/1
6	MAN	e	8	6	-	0/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	0/6/23/26	0/1/1/1
6	BMA	f	3	6	-	0/2/19/22	0/1/1/1
6	MAN	f	4	6	-	0/2/19/22	0/1/1/1
6	MAN	f	5	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	f	6	6	-	2/2/19/22	0/1/1/1
6	MAN	f	7	6	-	0/2/19/22	0/1/1/1
6	MAN	f	8	6	-	1/2/19/22	0/1/1/1
6	NAG	g	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	0/2/19/22	0/1/1/1
6	MAN	g	4	6	-	0/2/19/22	0/1/1/1
6	MAN	g	5	6	-	0/2/19/22	0/1/1/1
6	MAN	g	6	6	-	0/2/19/22	0/1/1/1
6	MAN	g	7	6	-	0/2/19/22	0/1/1/1
6	MAN	g	8	6	-	1/2/19/22	0/1/1/1
7	NAG	h	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	0/6/23/26	0/1/1/1
7	BMA	h	3	7	-	0/2/19/22	0/1/1/1
7	MAN	h	4	7	-	1/2/19/22	0/1/1/1
7	MAN	h	5	7	-	0/2/19/22	0/1/1/1
7	MAN	h	6	7	-	0/2/19/22	0/1/1/1
7	NAG	i	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	0/2/19/22	0/1/1/1
7	MAN	i	4	7	-	1/2/19/22	0/1/1/1
7	MAN	i	5	7	-	0/2/19/22	0/1/1/1
7	MAN	i	6	7	-	1/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	MAN	j	4	7	-	1/2/19/22	0/1/1/1
7	MAN	j	5	7	-	0/2/19/22	0/1/1/1
7	MAN	j	6	7	-	0/2/19/22	0/1/1/1

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	j	5	MAN	O5-C5	3.17	1.49	1.43
4	V	6	MAN	O5-C5	3.17	1.49	1.43
7	i	5	MAN	O5-C5	3.15	1.49	1.43
7	h	5	MAN	O5-C5	3.14	1.49	1.43
4	X	4	MAN	O5-C1	3.11	1.48	1.43

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	1	NAG	C2-N2-C7	4.65	129.53	122.90
3	S	1	NAG	C2-N2-C7	4.57	129.41	122.90
7	j	3	BMA	C1-O5-C5	4.52	118.32	112.19
7	j	4	MAN	C1-O5-C5	4.42	118.18	112.19
2	d	1	NAG	O5-C5-C6	-4.22	100.58	107.20

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

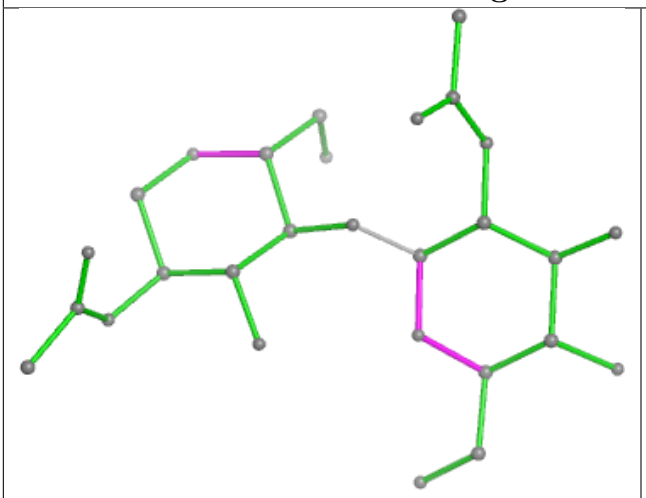
Mol	Chain	Res	Type	Atoms
2	b	2	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C4-C5-C6-O6

There are no ring outliers.

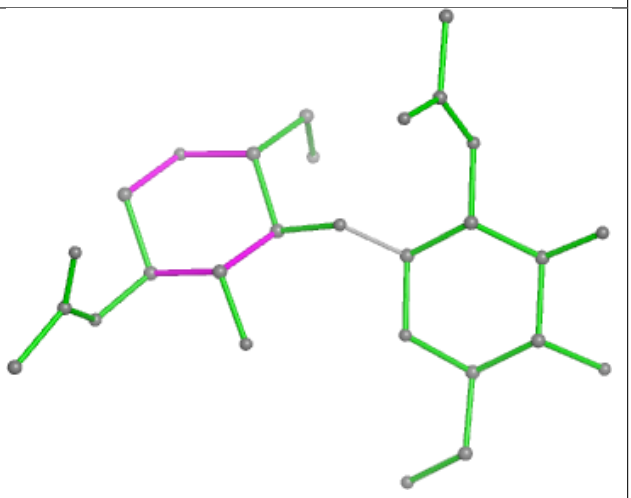
No monomer is involved in short contacts.

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

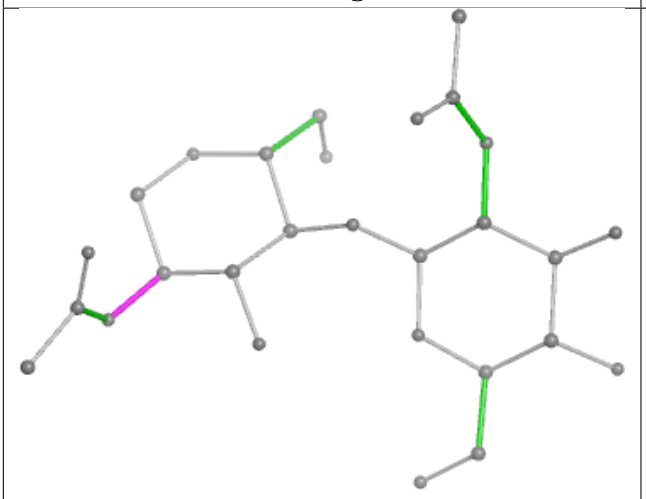
Oligosaccharide Chain M



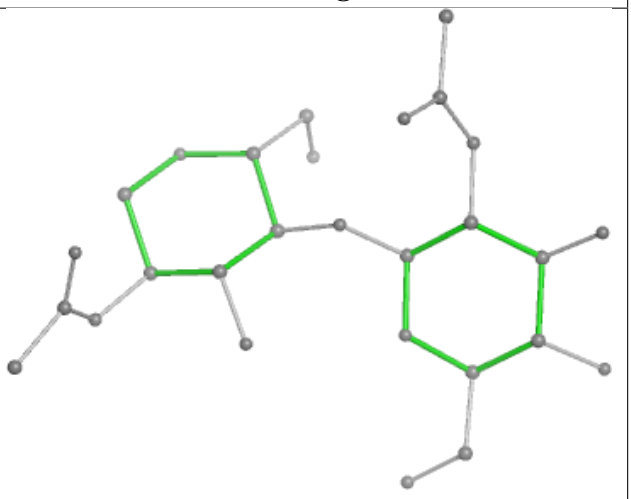
Bond lengths



Bond angles

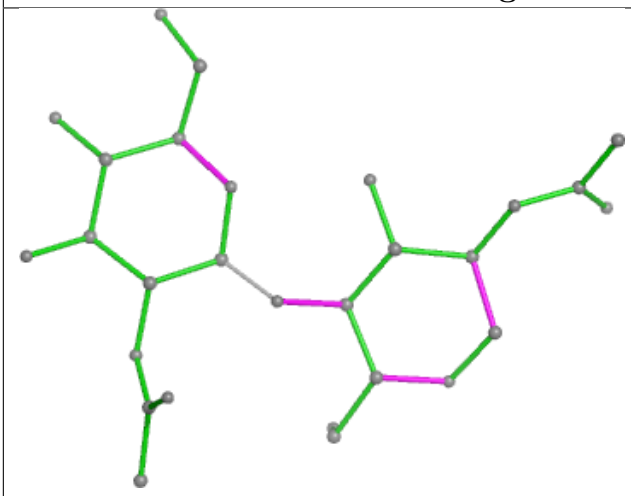


Torsions

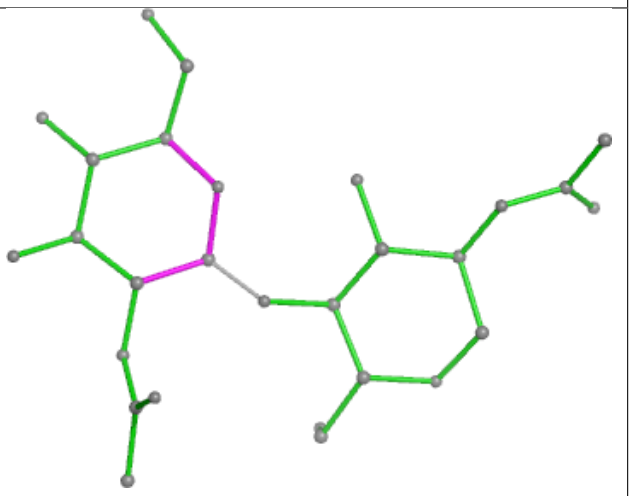


Rings

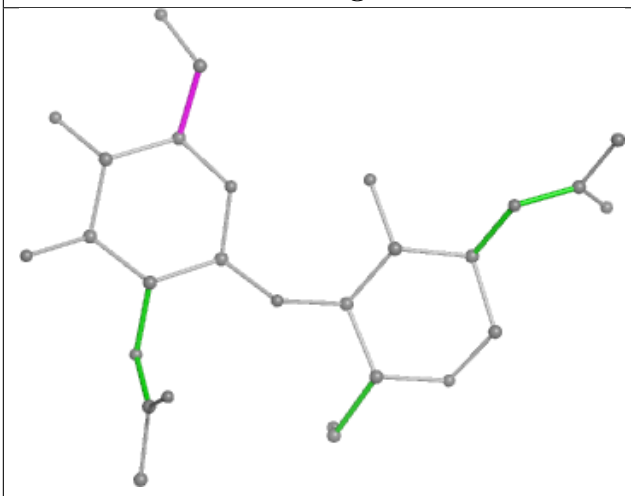
Oligosaccharide Chain a



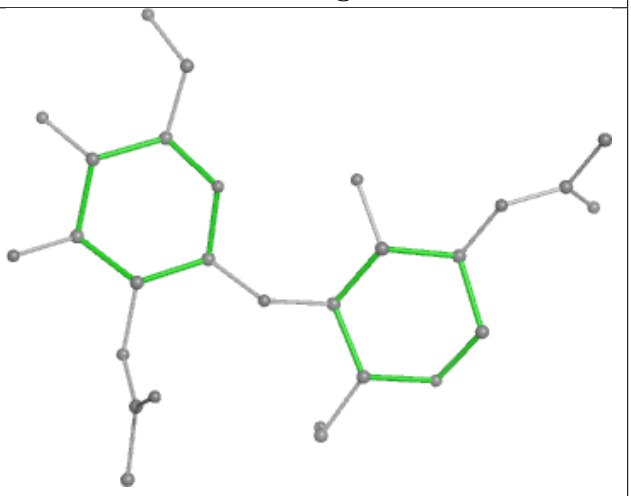
Bond lengths



Bond angles

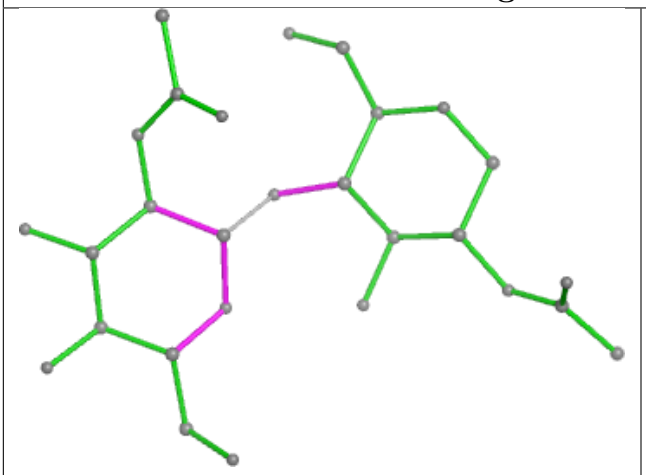


Torsions

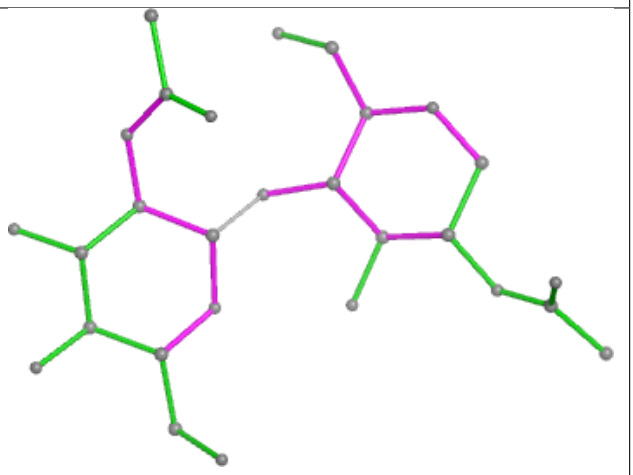


Rings

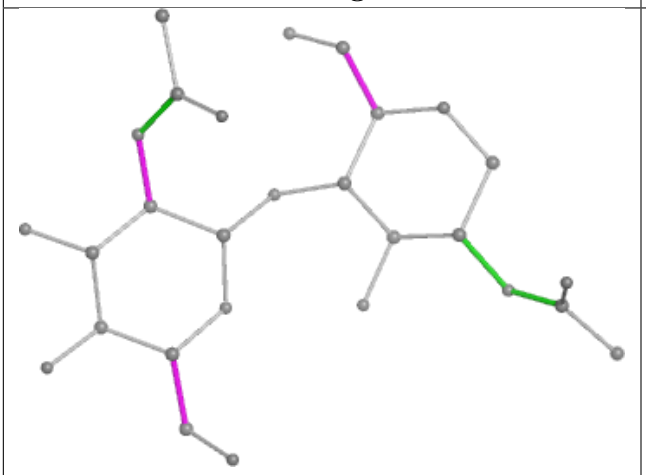
Oligosaccharide Chain b



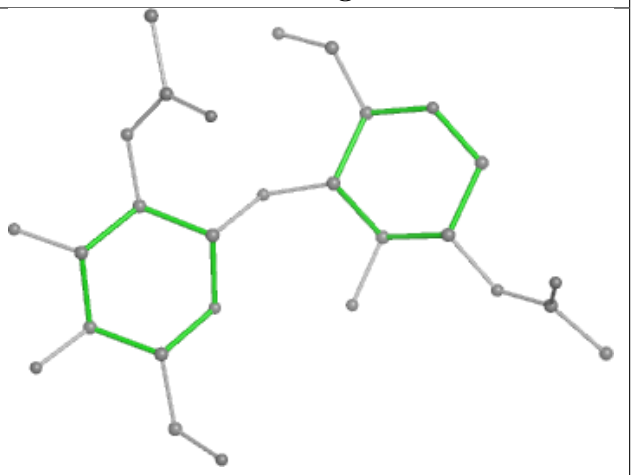
Bond lengths



Bond angles

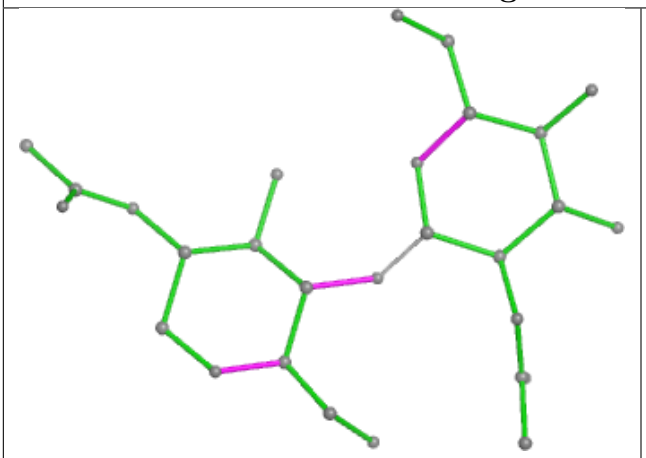


Torsions

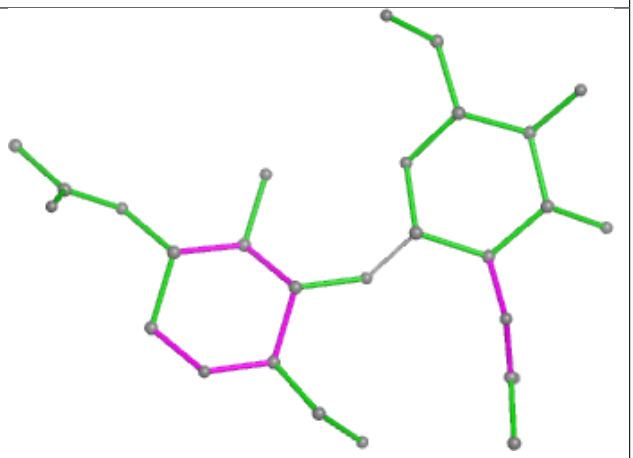


Rings

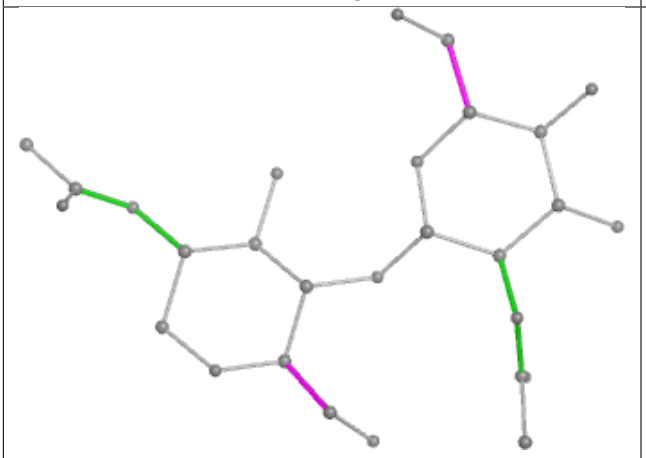
Oligosaccharide Chain c



Bond lengths



Bond angles



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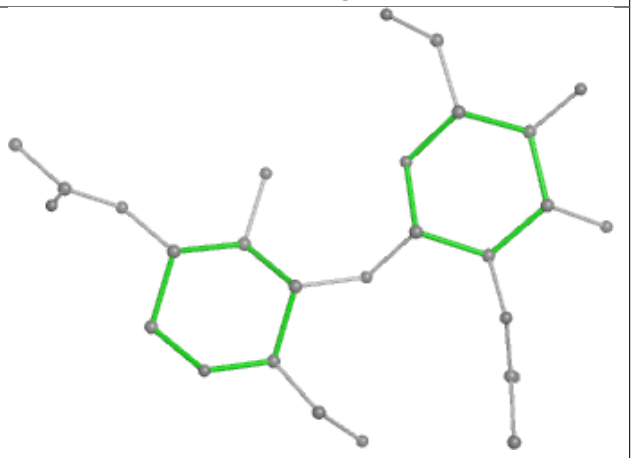
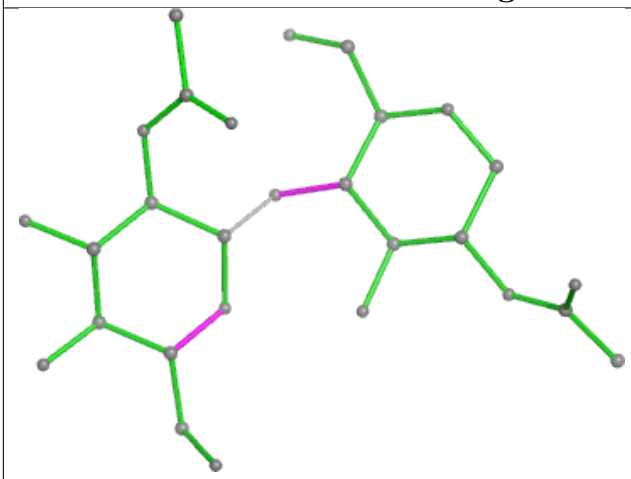
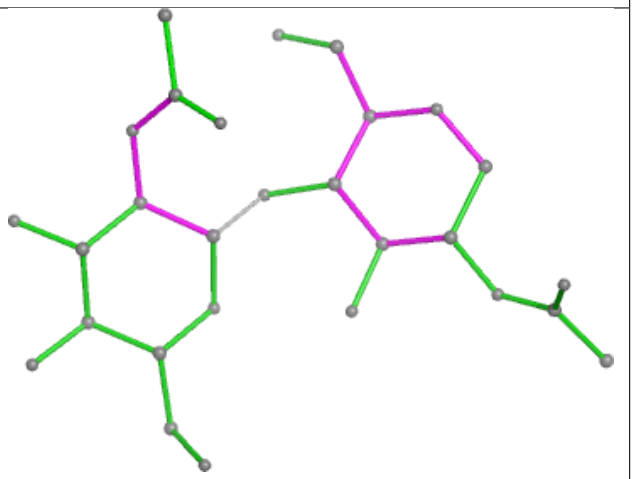


Rings

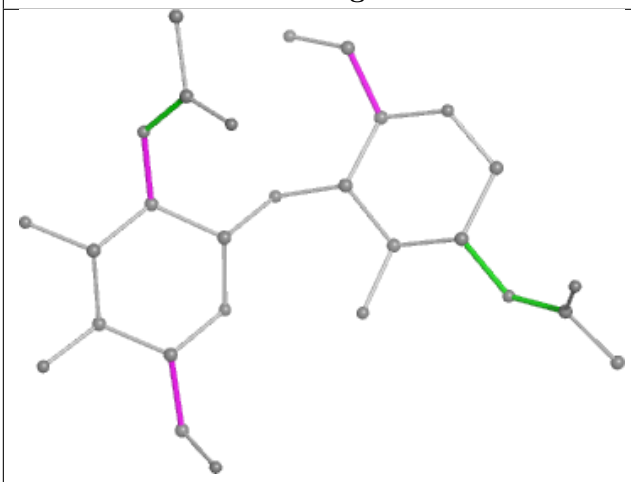
Oligosaccharide Chain d



Bond lengths



Bond angles



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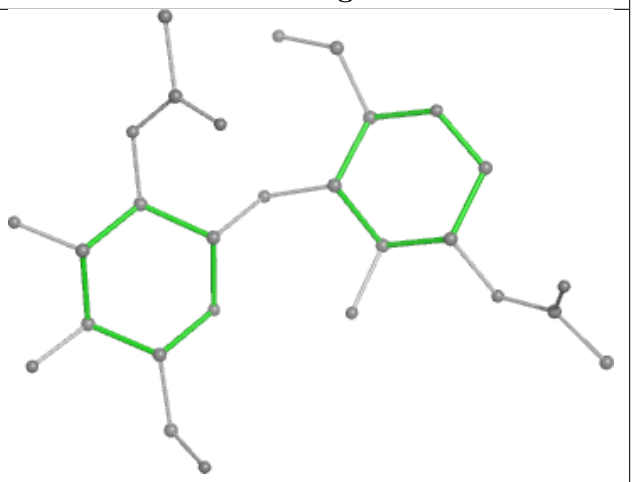
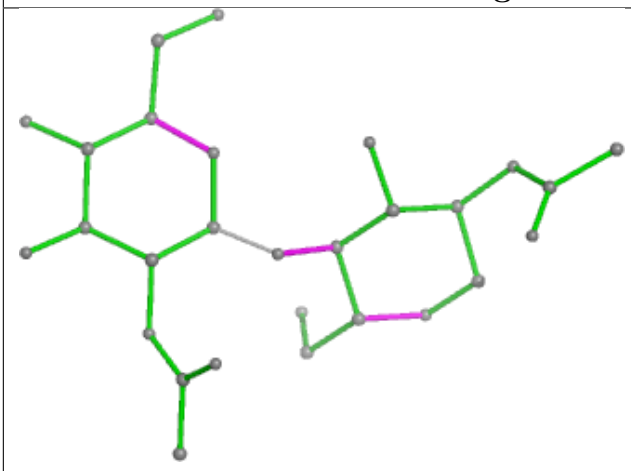


Rings

Oligosaccharide Chain N



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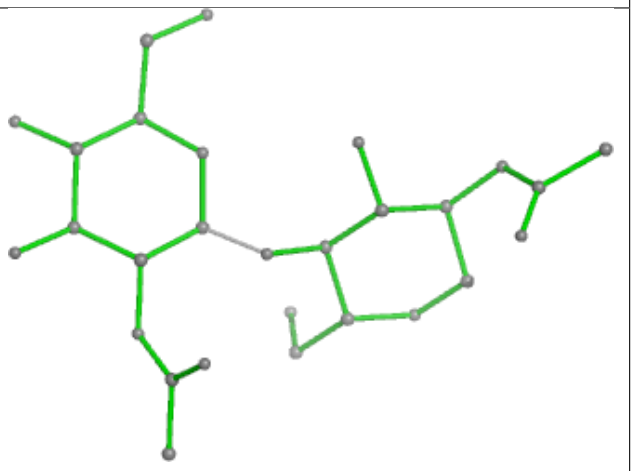
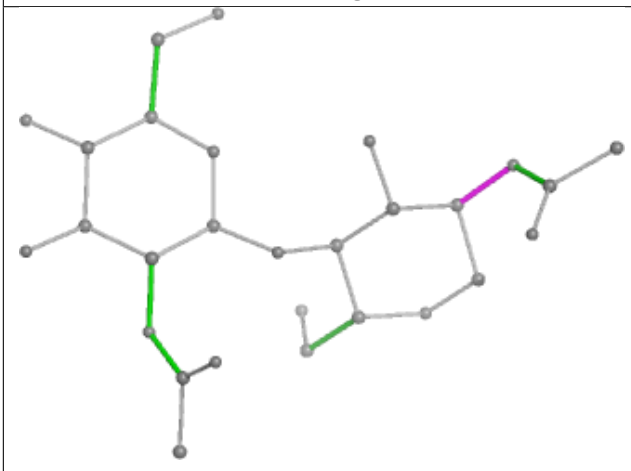


Bond angles



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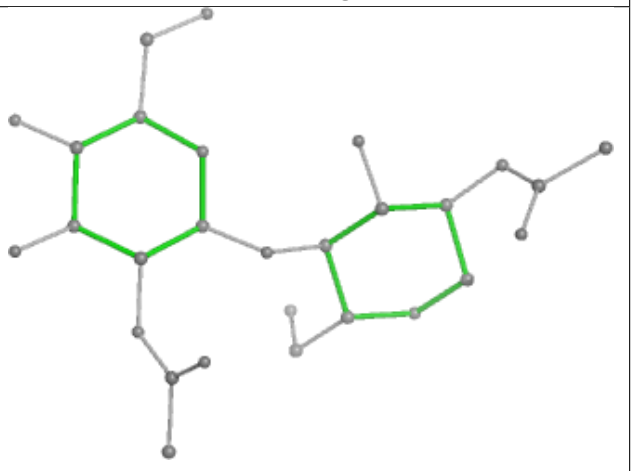
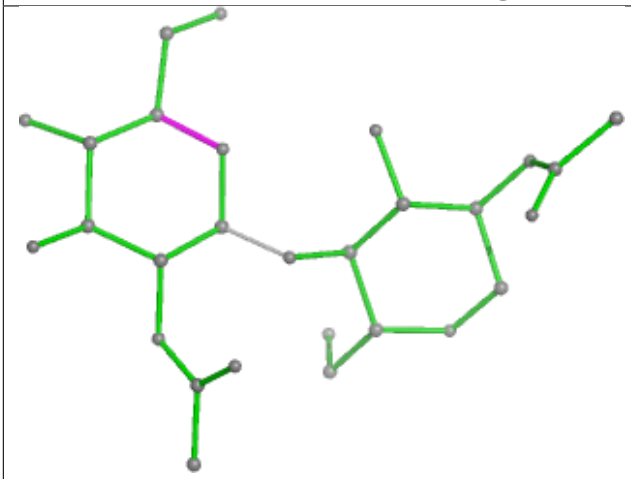
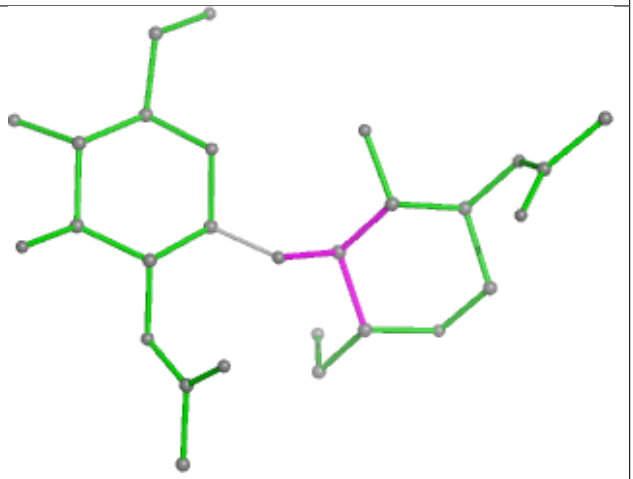


Rings

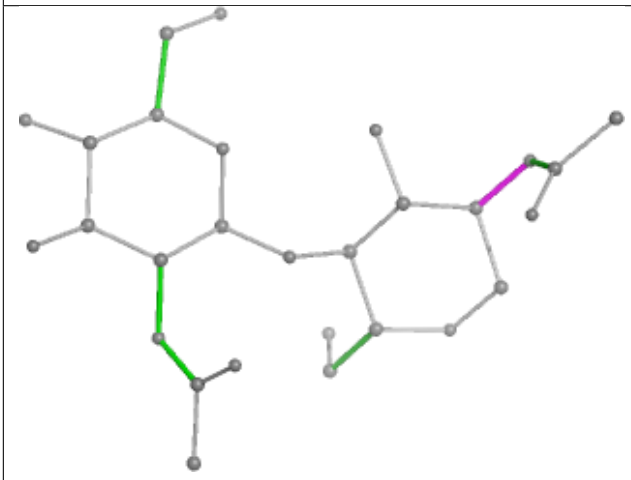
Oligosaccharide Chain O



Bond lengths



Bond angles



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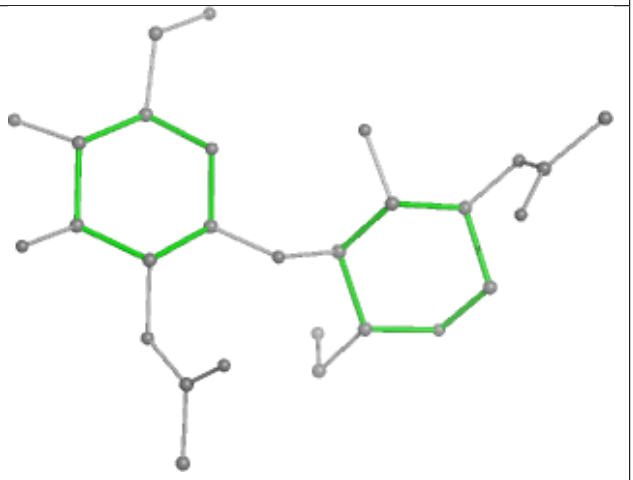
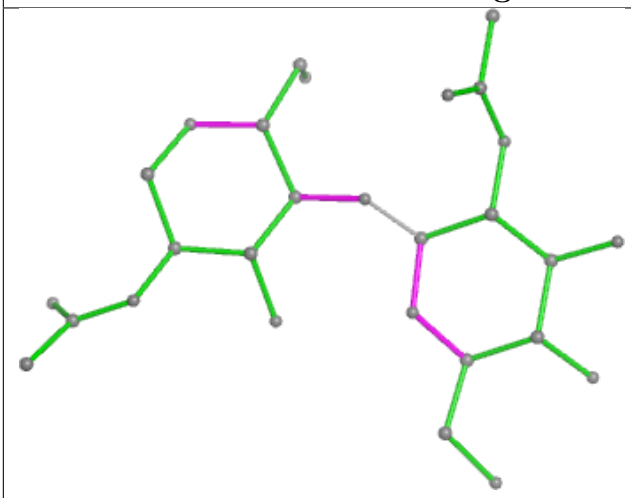


Rings

Oligosaccharide Chain Y



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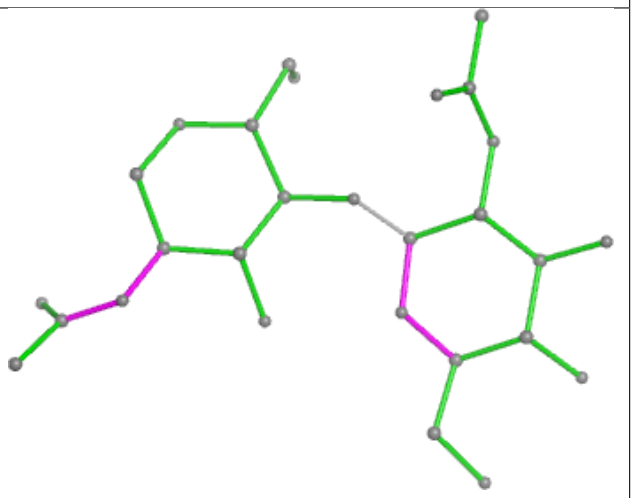
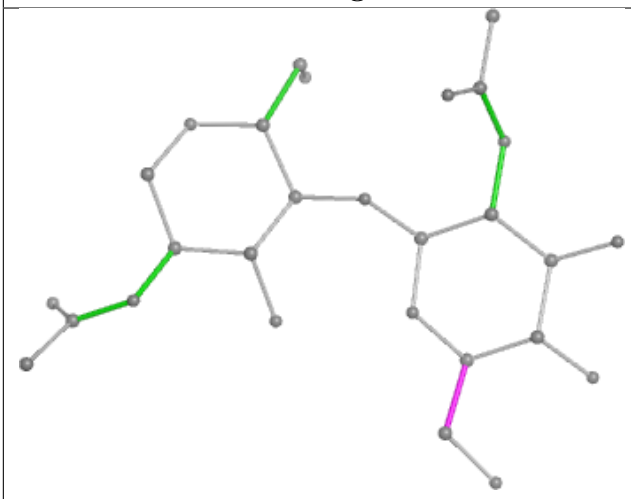


Bond angles



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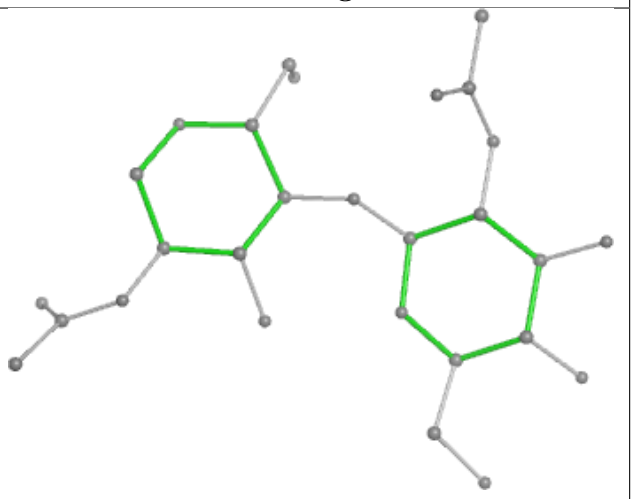
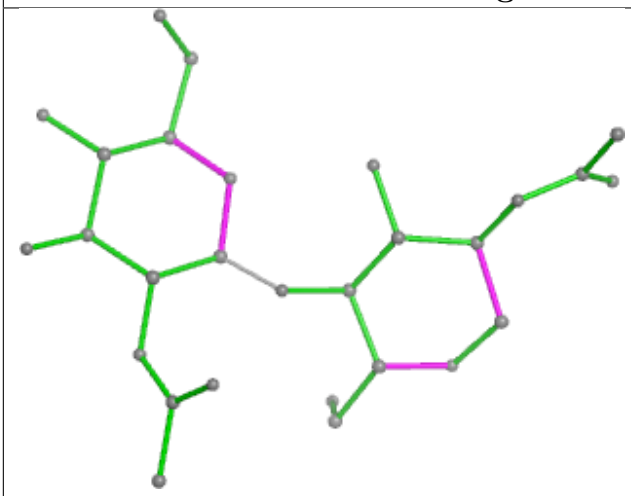
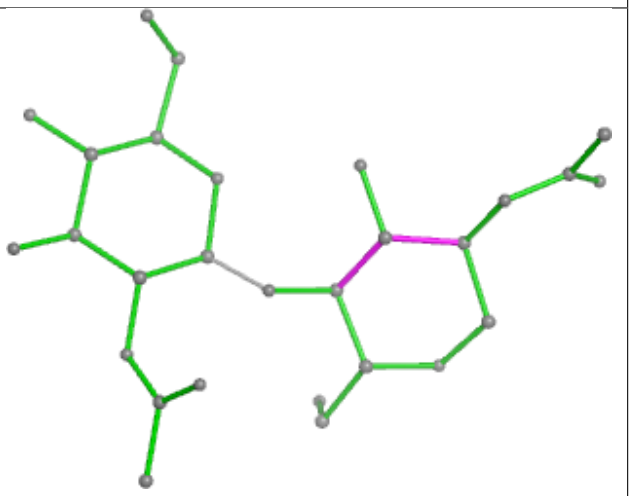


Rings

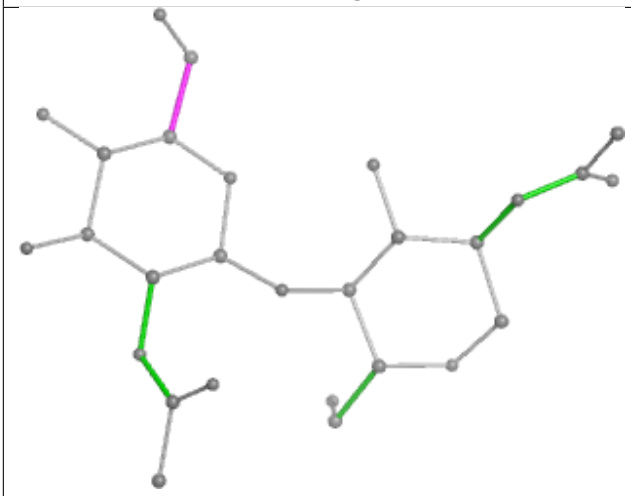
Oligosaccharide Chain Z



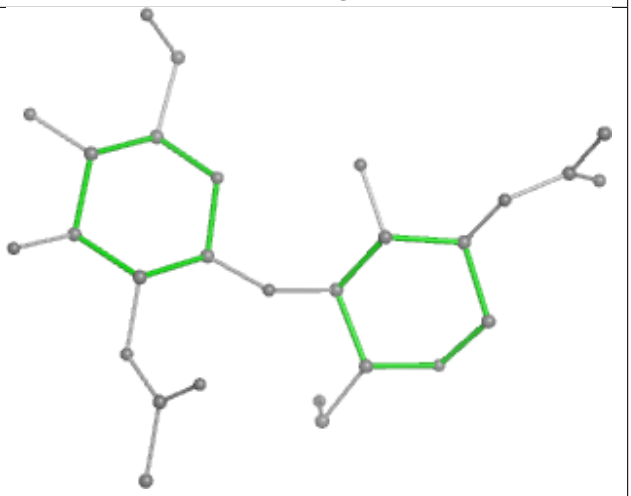
Bond lengths



Bond angles

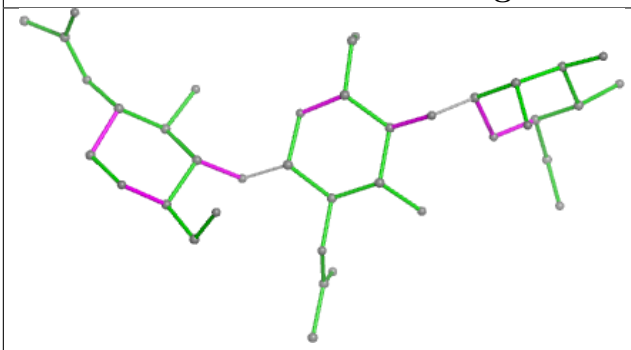


Torsions

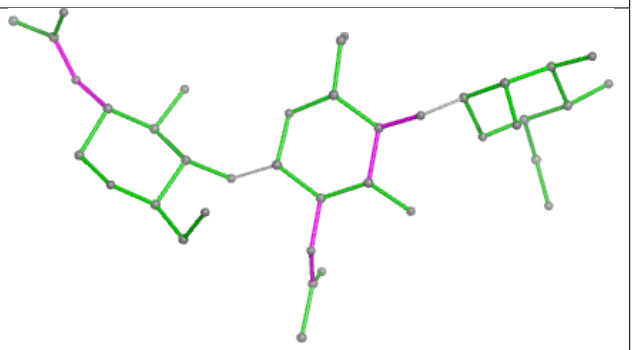


Rings

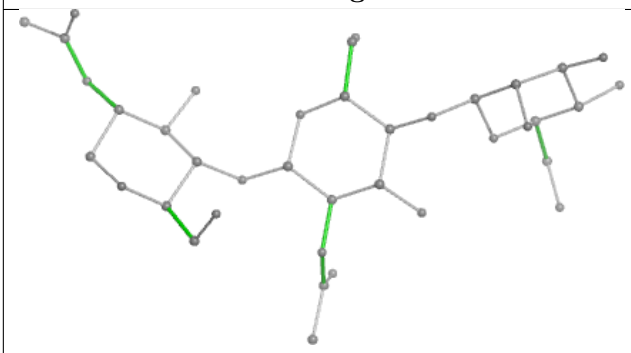
Oligosaccharide Chain U



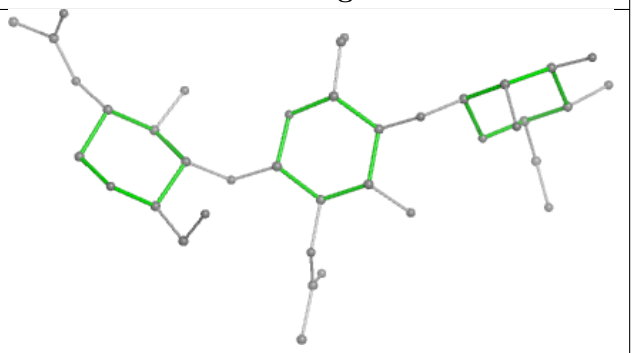
Bond lengths



Bond angles

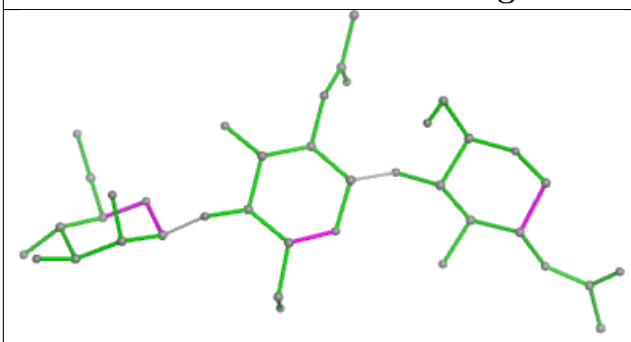


Torsions

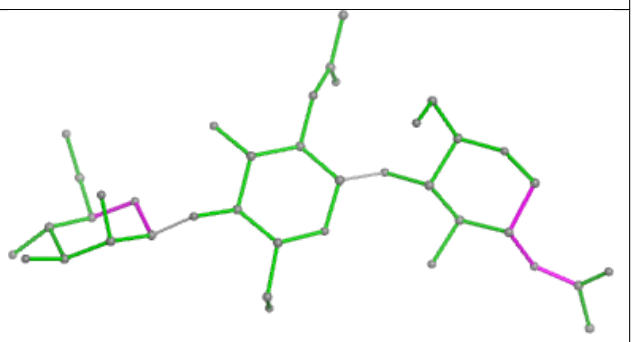


Rings

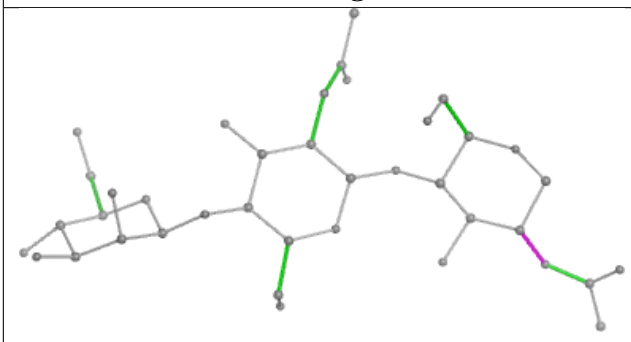
Oligosaccharide Chain S



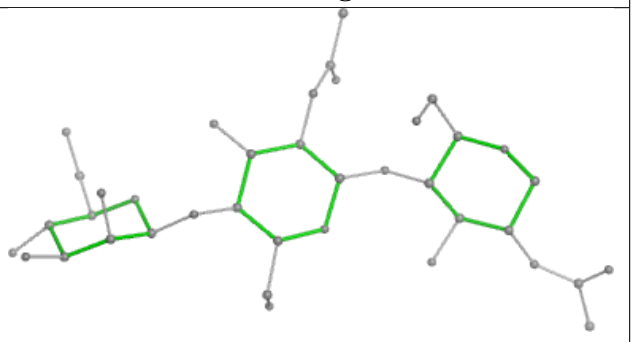
Bond lengths



Bond angles

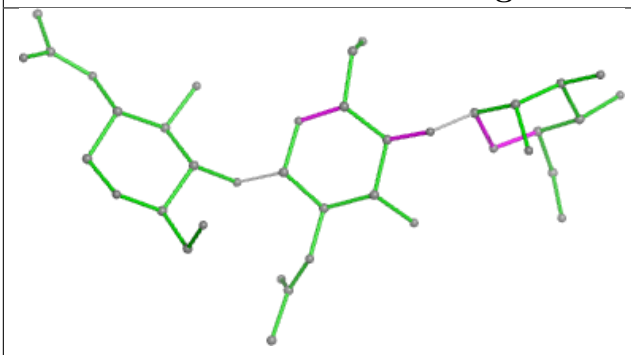


Torsions

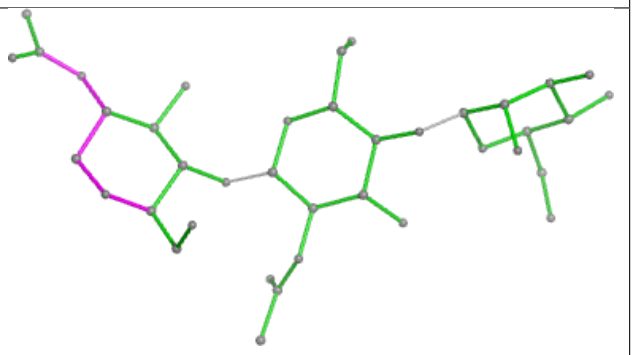


Rings

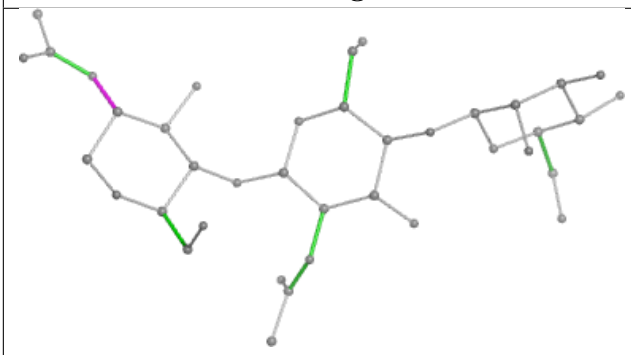
Oligosaccharide Chain T



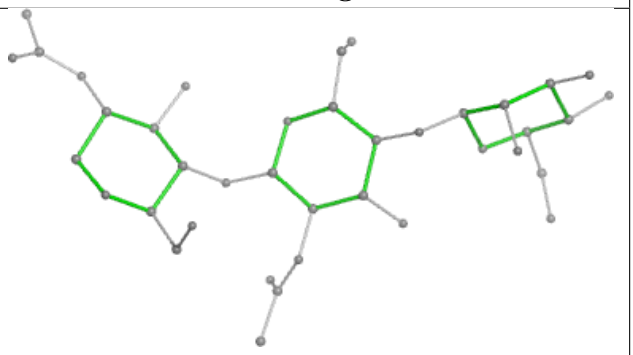
Bond lengths



Bond angles

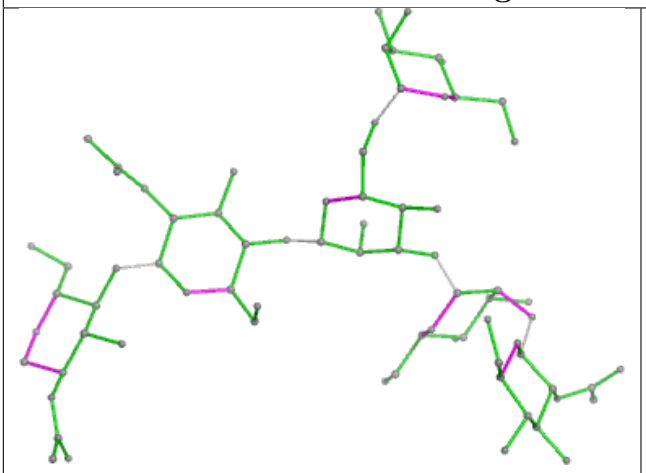


Torsions

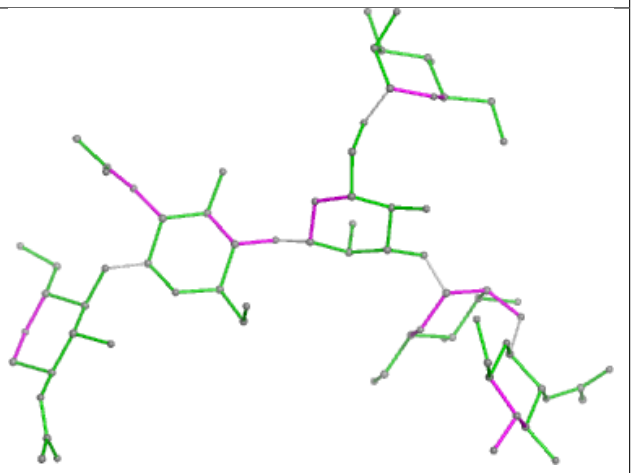


Rings

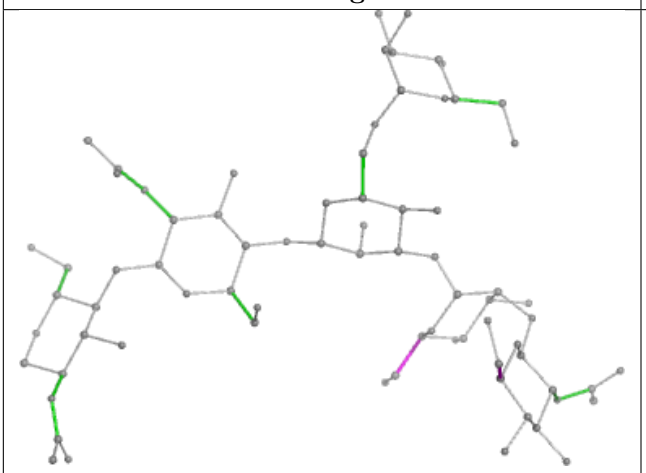
Oligosaccharide Chain X



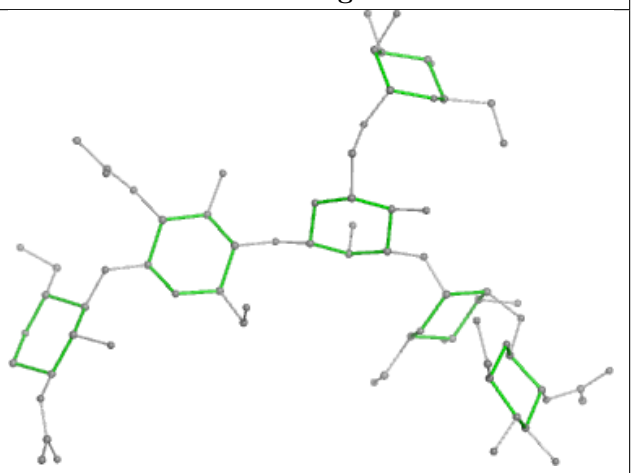
Bond lengths



Bond angles

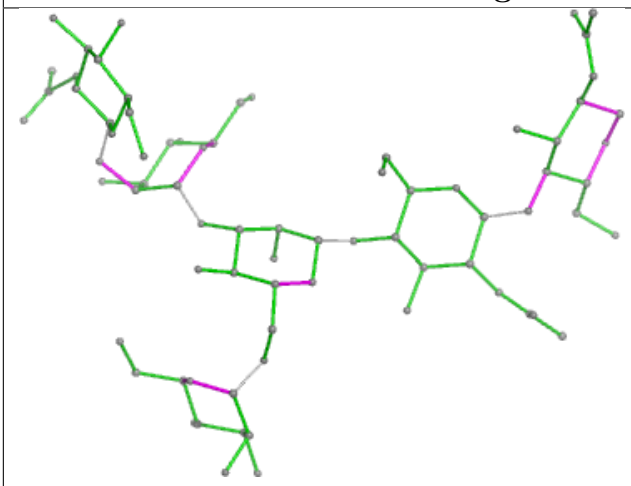


Torsions

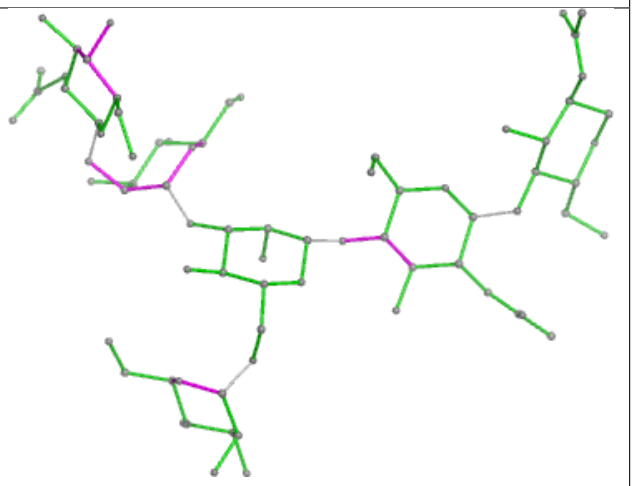


Rings

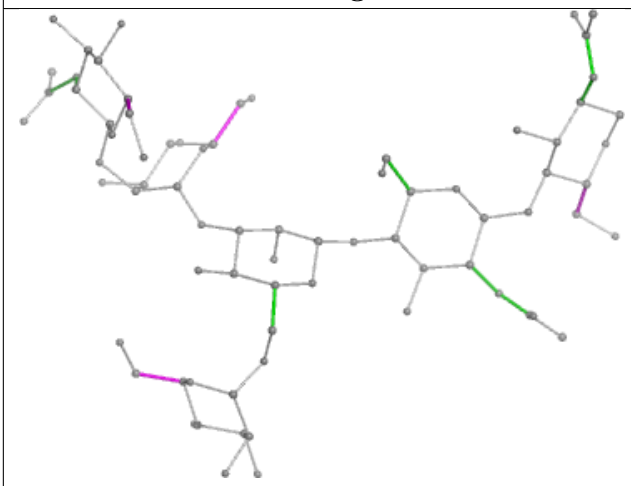
Oligosaccharide Chain V



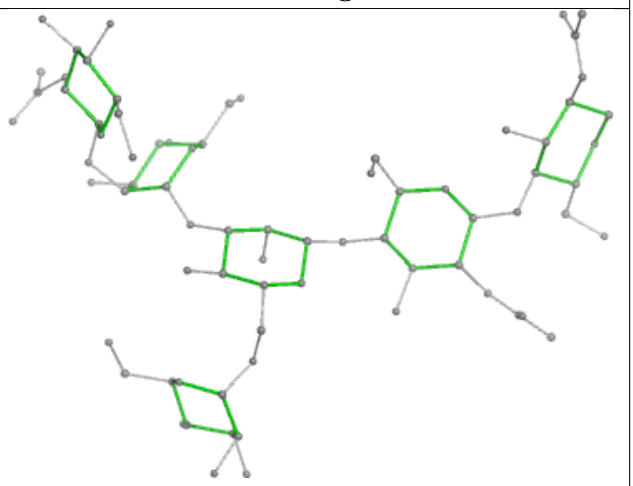
Bond lengths



Bond angles

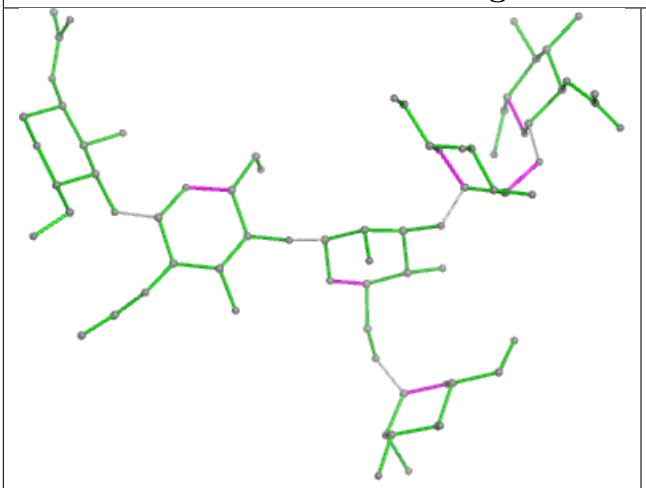


Torsions

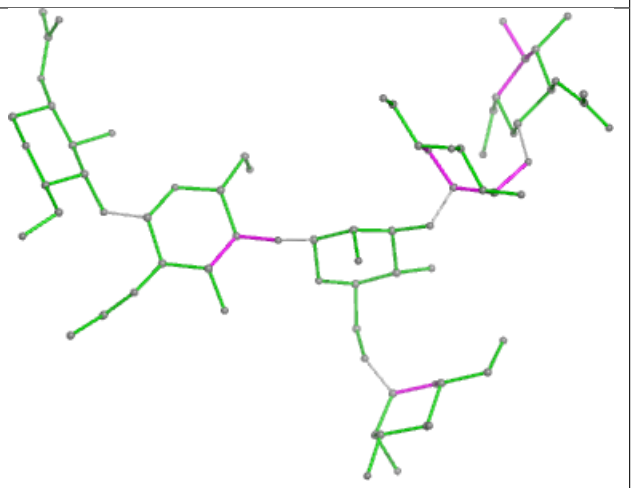


Rings

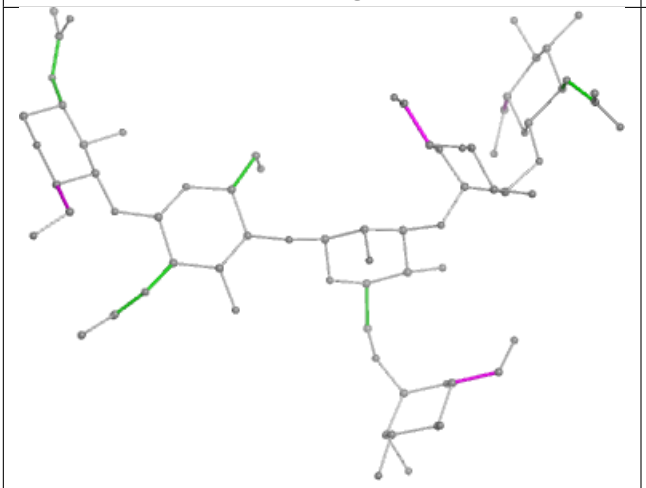
Oligosaccharide Chain W



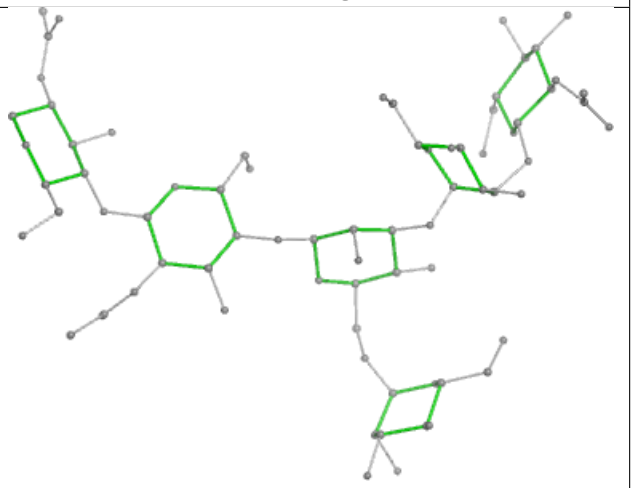
Bond lengths



Bond angles

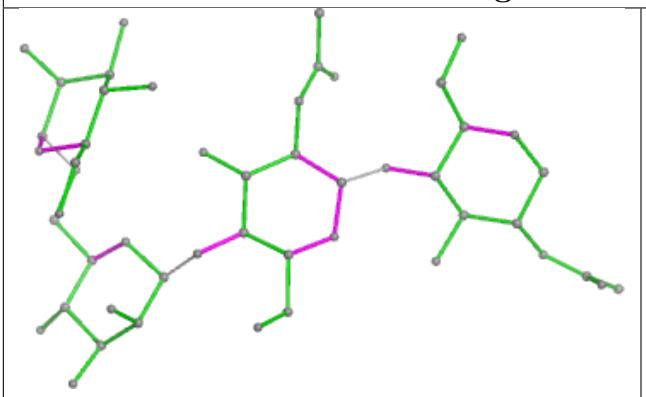


Torsions

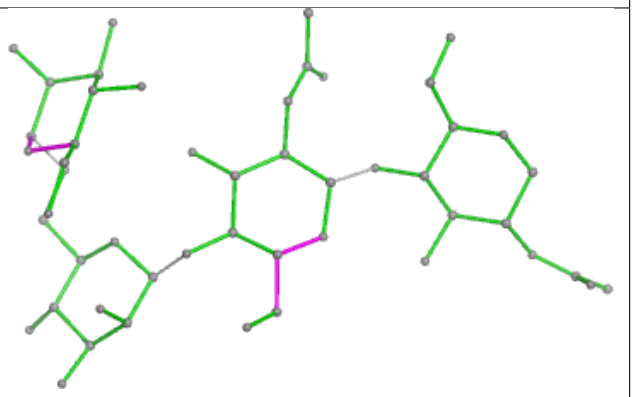


Rings

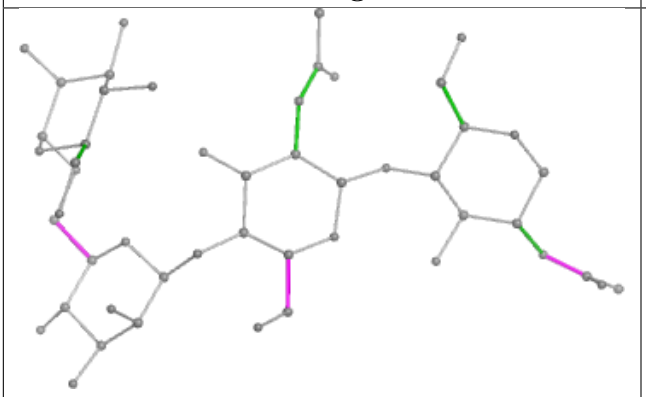
Oligosaccharide Chain R



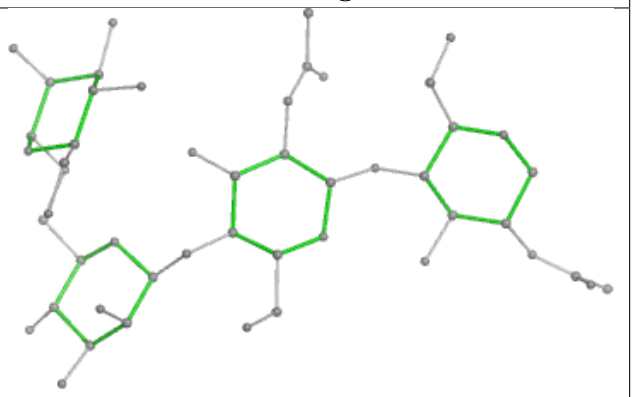
Bond lengths



Bond angles

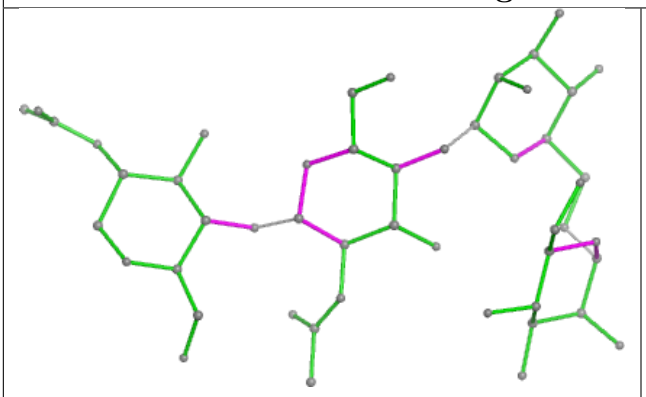


Torsions

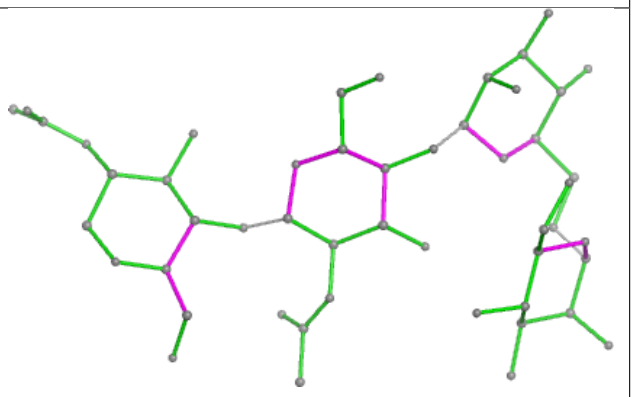


Rings

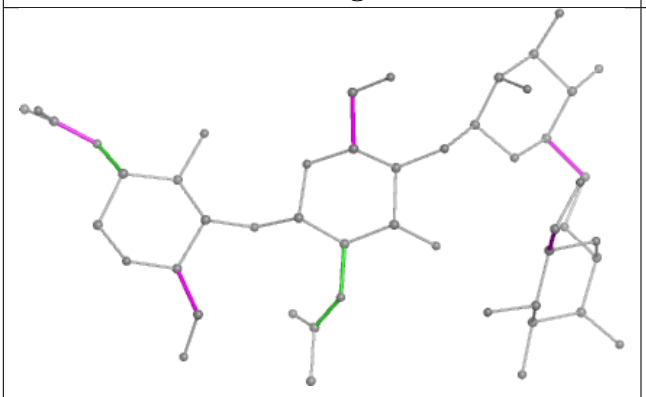
Oligosaccharide Chain P



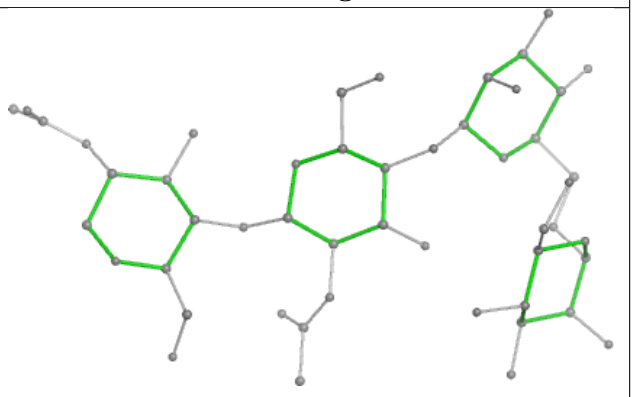
Bond lengths



Bond angles

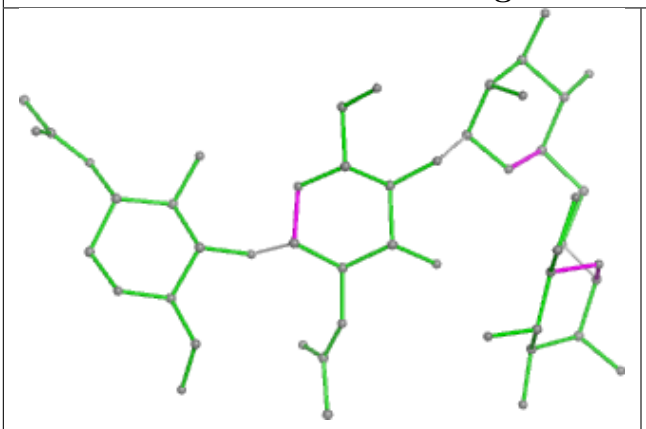


Torsions

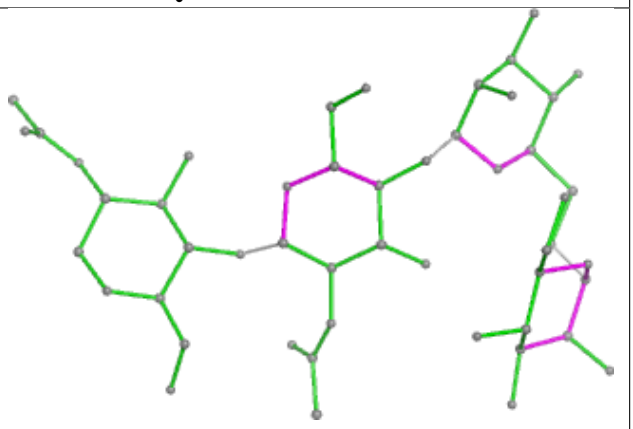


Rings

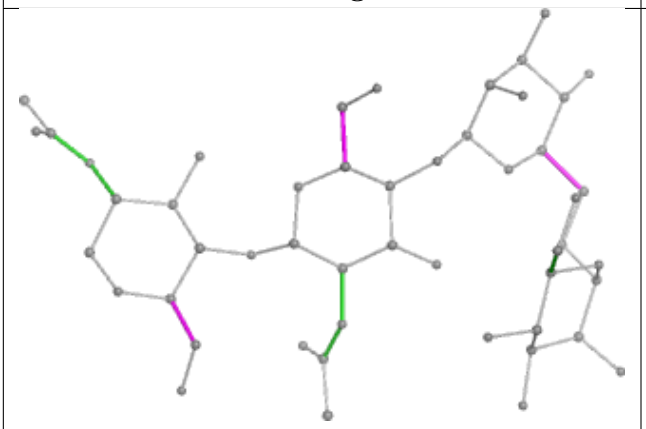
Oligosaccharide Chain Q



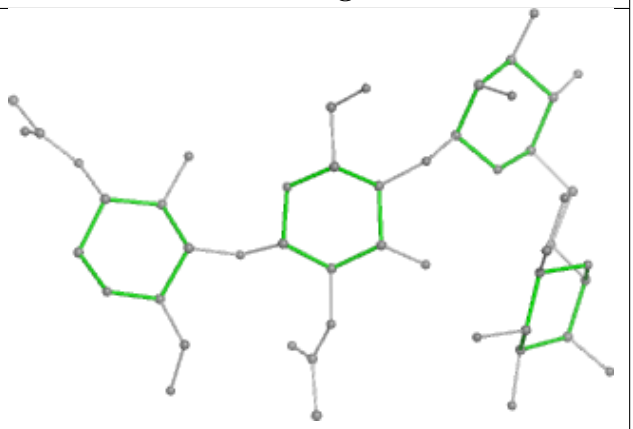
Bond lengths



Bond angles

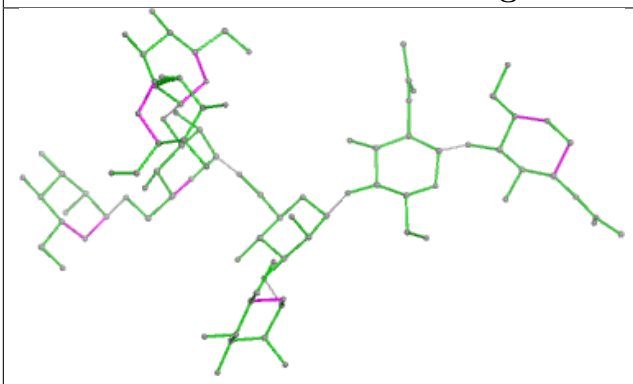


Torsions

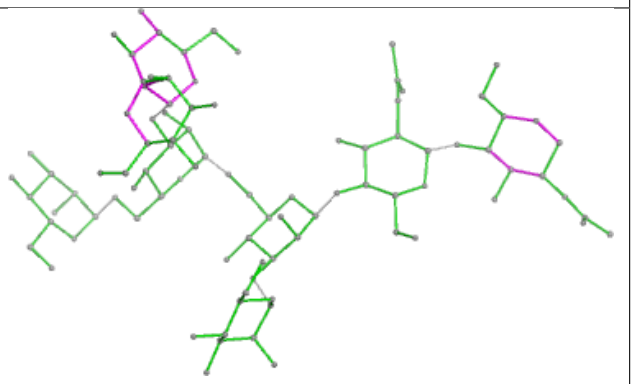


Rings

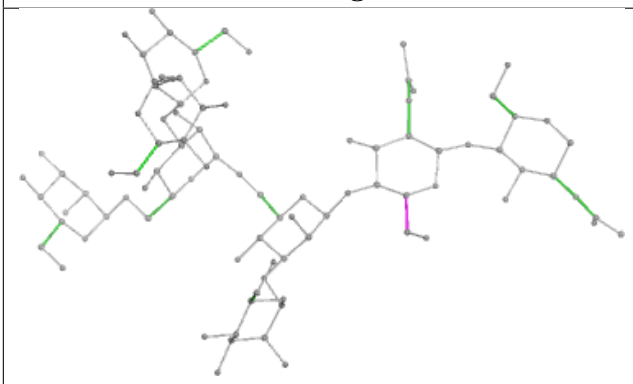
Oligosaccharide Chain e



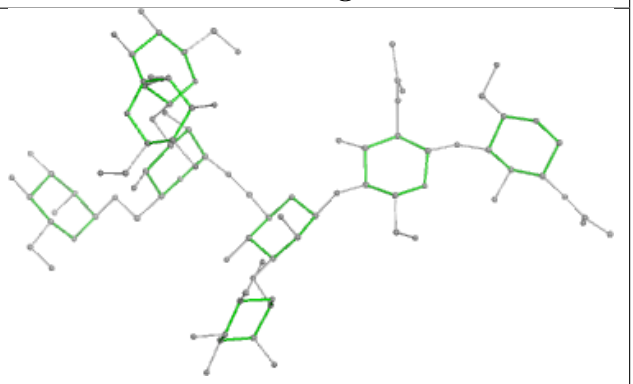
Bond lengths



Bond angles

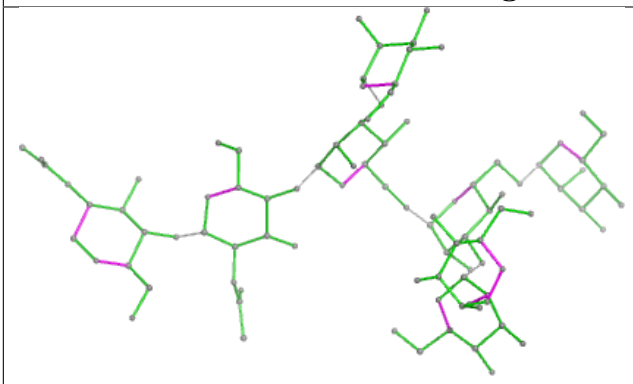


Torsions

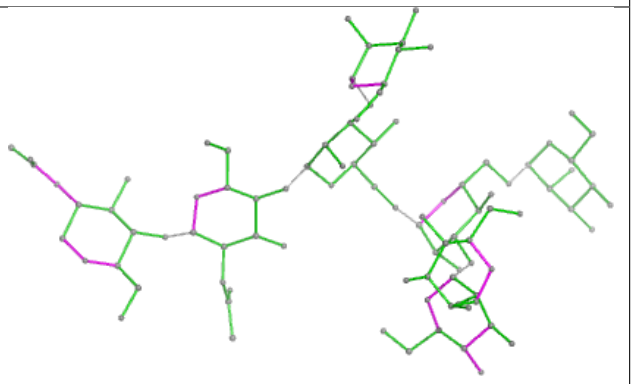


Rings

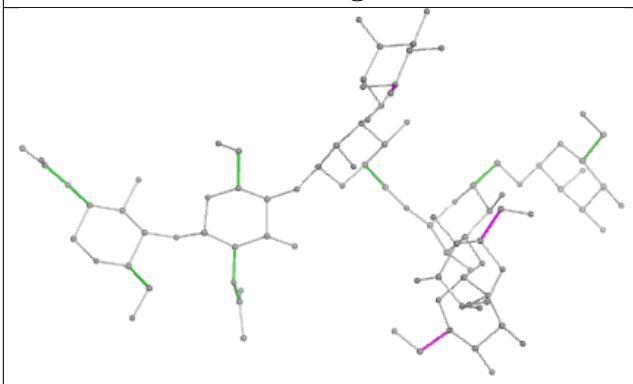
Oligosaccharide Chain f



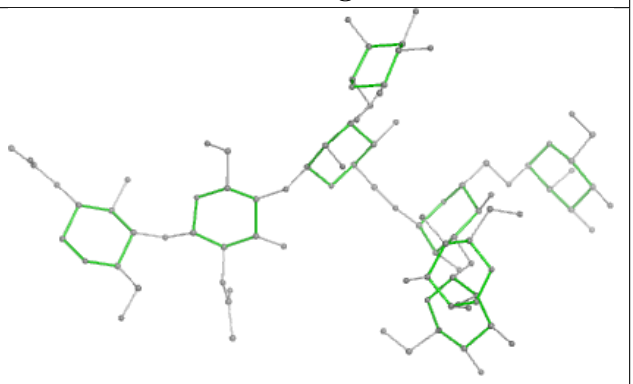
Bond lengths



Bond angles

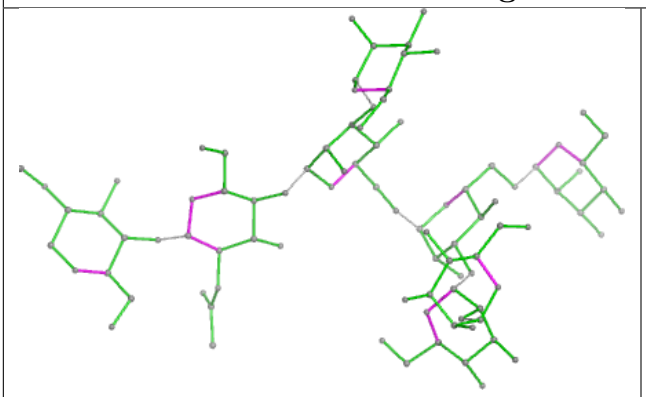


Torsions

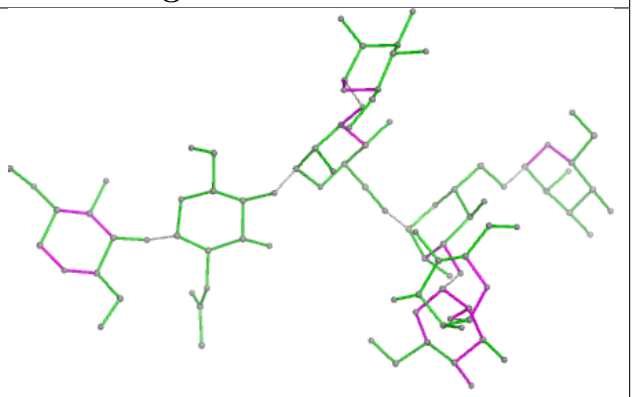


Rings

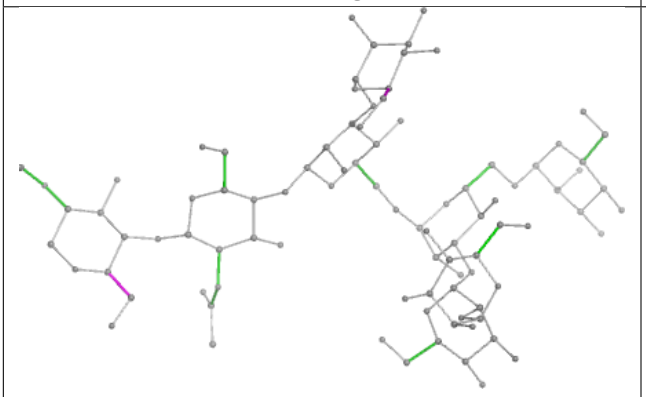
Oligosaccharide Chain g



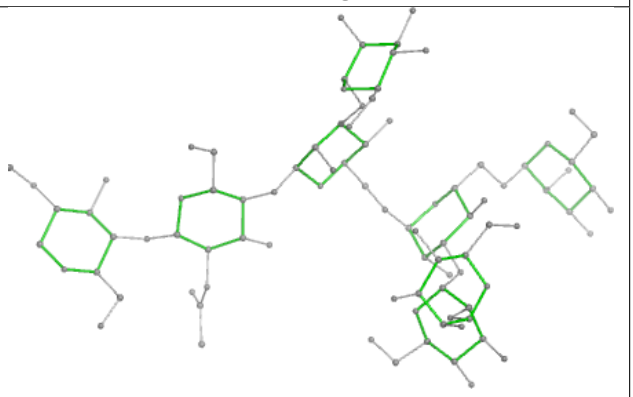
Bond lengths



Bond angles

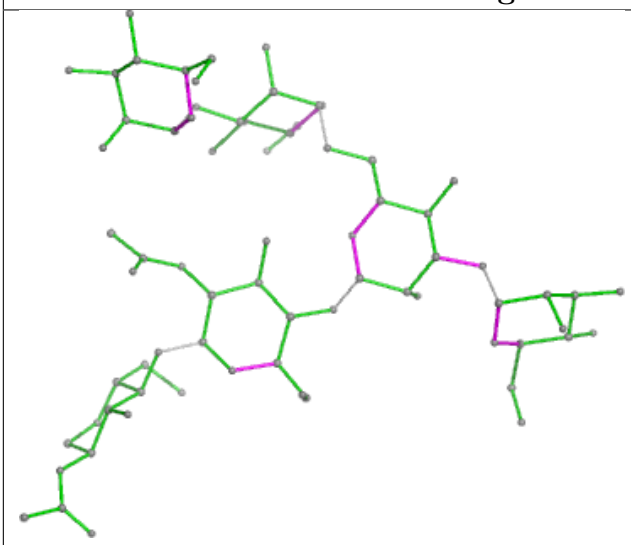


Torsions

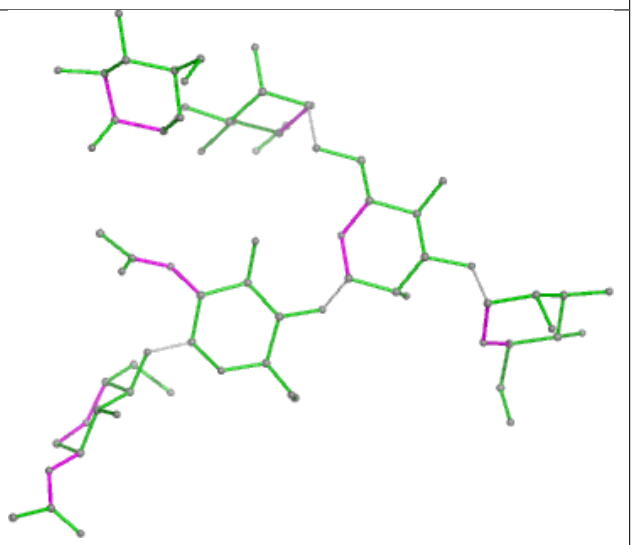


Rings

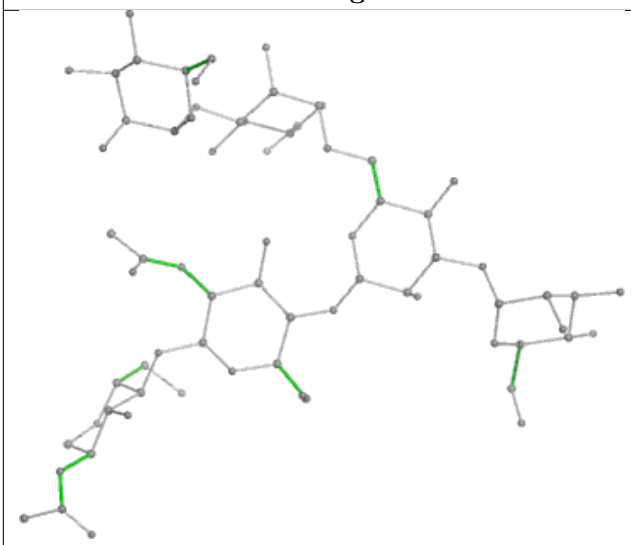
Oligosaccharide Chain h



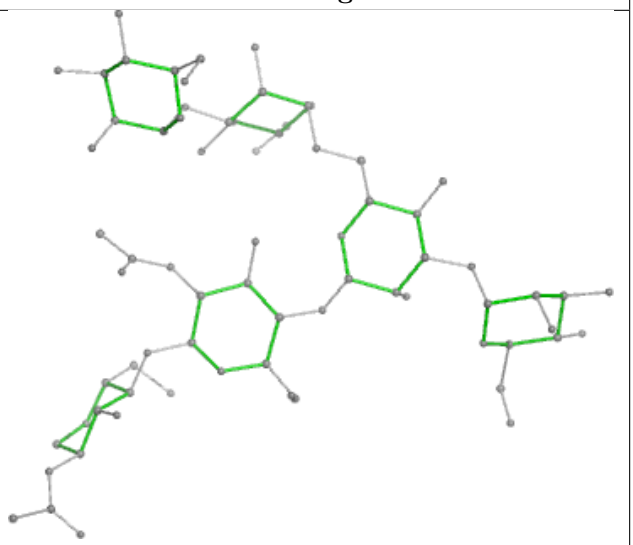
Bond lengths



Bond angles

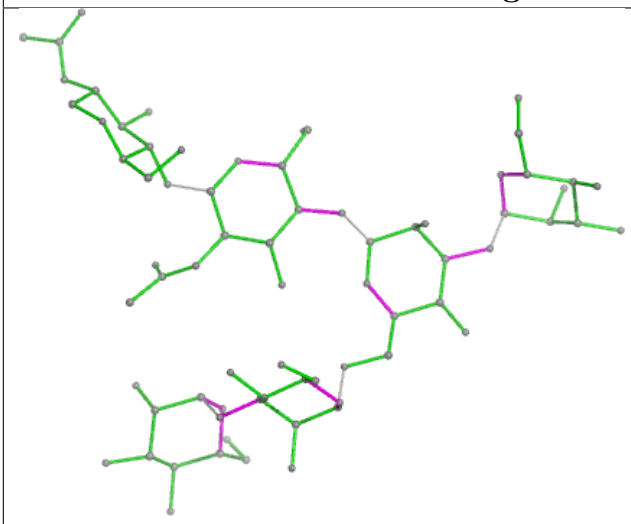


Torsions

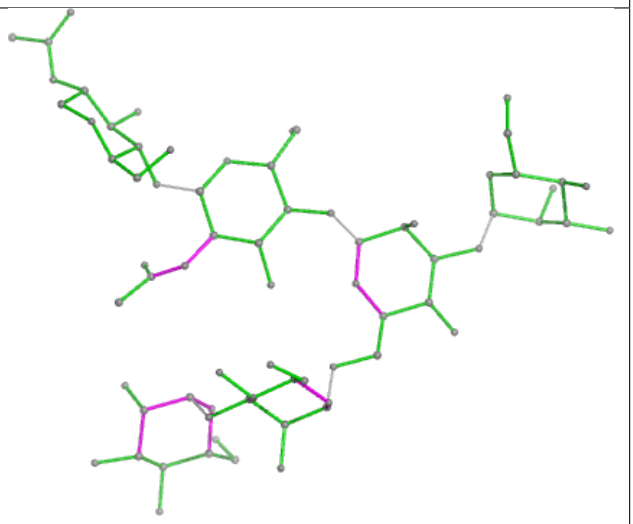


Rings

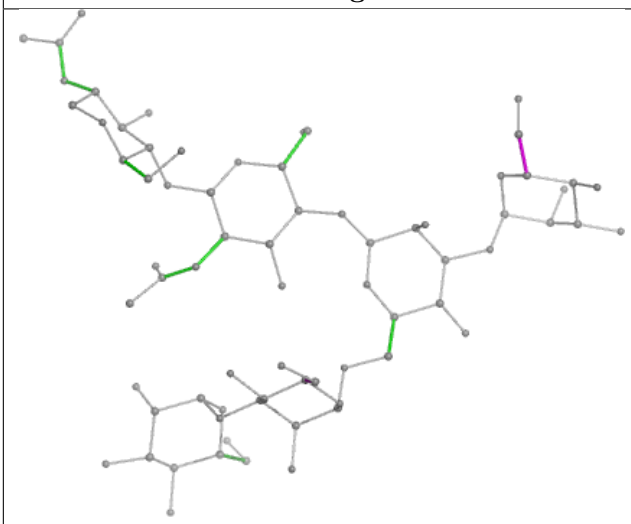
Oligosaccharide Chain i



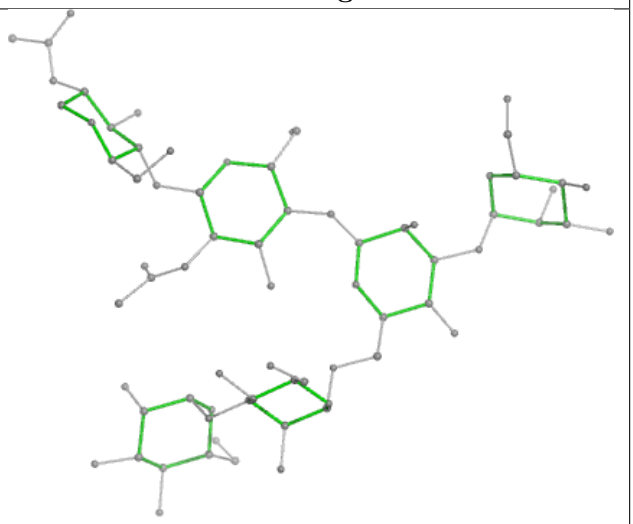
Bond lengths



Bond angles

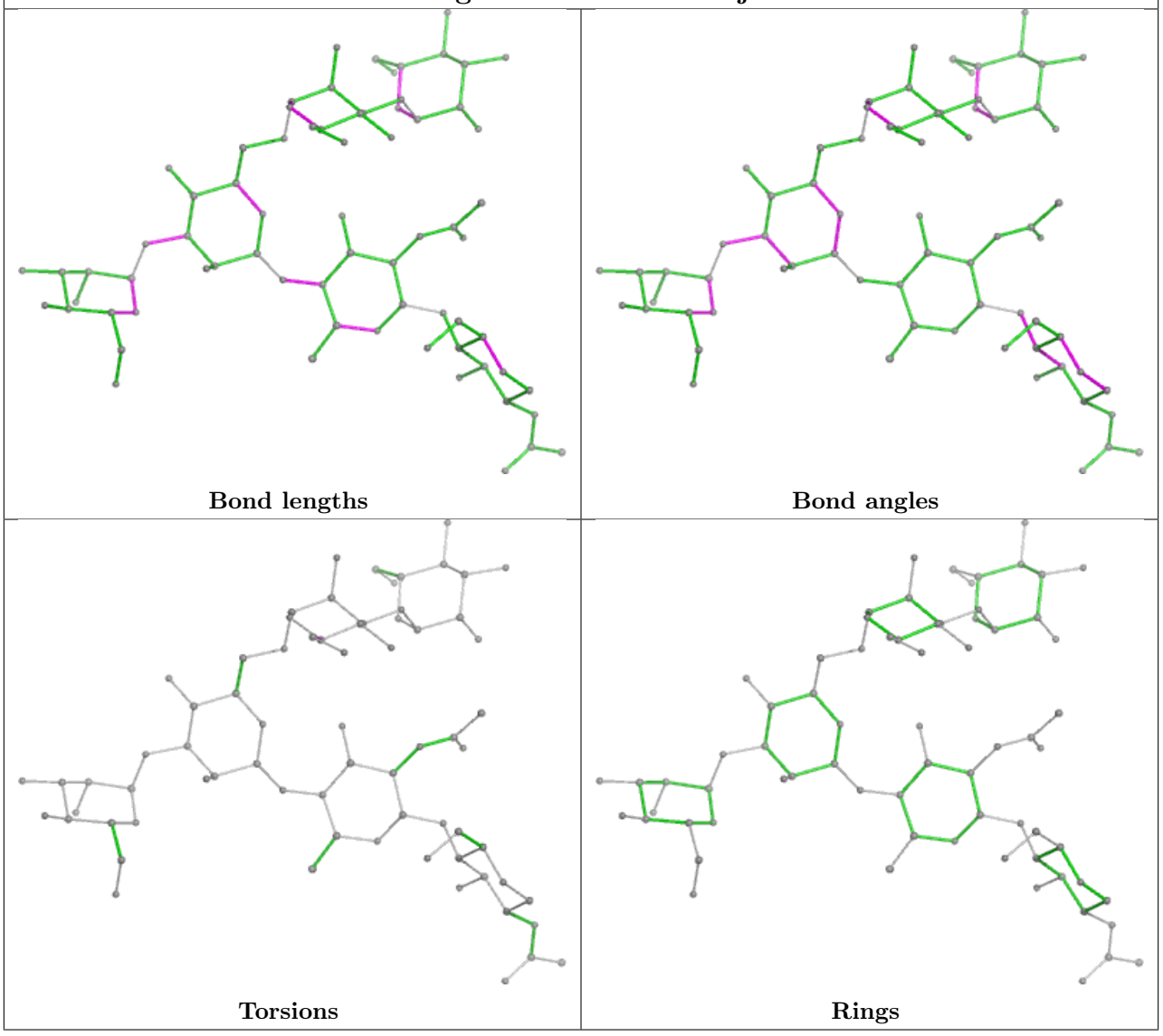


Torsions



Rings

Oligosaccharide Chain j



5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
10	PTY	D	1101	-	49,49,49	0.74	0	52,54,54	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CLR	L	1100	-	31,31,31	1.00	2 (6%)	48,48,48	0.96	4 (8%)
9	NAG	B	1001	1	14,14,15	1.41	3 (21%)	17,19,21	1.04	1 (5%)
9	NAG	C	1002	1	14,14,15	1.16	2 (14%)	17,19,21	0.96	1 (5%)
8	CLR	D	1100	-	31,31,31	1.04	1 (3%)	48,48,48	0.95	3 (6%)
9	NAG	G	1002	1	14,14,15	1.20	2 (14%)	17,19,21	0.84	0
9	NAG	B	1002	1	14,14,15	1.22	2 (14%)	17,19,21	0.71	0
9	NAG	C	1001	1	14,14,15	1.27	2 (14%)	17,19,21	0.83	0
9	NAG	G	1001	1	14,14,15	1.48	3 (21%)	17,19,21	0.97	1 (5%)
9	NAG	B	1003	1	14,14,15	1.21	2 (14%)	17,19,21	1.14	1 (5%)
10	PTY	L	1101	-	49,49,49	0.79	0	52,54,54	0.62	0
8	CLR	A	1100	-	31,31,31	0.93	0	48,48,48	1.04	5 (10%)
9	NAG	G	1003	1	14,14,15	1.06	1 (7%)	17,19,21	0.99	1 (5%)
9	NAG	C	1003	1	14,14,15	1.14	2 (14%)	17,19,21	0.86	0
10	PTY	H	1101	-	49,49,49	0.67	0	52,54,54	0.45	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
10	PTY	D	1101	-	-	13/53/53/53	-
8	CLR	L	1100	-	-	1/10/68/68	0/4/4/4
9	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1002	1	-	1/6/23/26	0/1/1/1
8	CLR	D	1100	-	-	0/10/68/68	0/4/4/4
9	NAG	G	1002	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	G	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1003	1	-	1/6/23/26	0/1/1/1
10	PTY	L	1101	-	-	8/53/53/53	-
8	CLR	A	1100	-	-	2/10/68/68	0/4/4/4
9	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1003	1	-	1/6/23/26	0/1/1/1
10	PTY	H	1101	-	-	7/53/53/53	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	NAG	O5-C5	2.80	1.49	1.43
9	G	1001	NAG	O5-C5	2.71	1.48	1.43
9	G	1001	NAG	C1-C2	2.66	1.56	1.52
9	B	1001	NAG	O5-C1	2.63	1.47	1.43
8	D	1100	CLR	C11-C9	2.63	1.58	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1001	NAG	C1-O5-C5	3.33	116.70	112.19
9	B	1003	NAG	C1-C2-N2	3.01	115.64	110.49
9	G	1001	NAG	C1-O5-C5	2.83	116.03	112.19
9	G	1003	NAG	C1-C2-N2	2.75	115.18	110.49
8	A	1100	CLR	C1-C2-C3	2.65	113.87	110.47

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	1101	PTY	C2-C3-O11-P1
10	D	1101	PTY	C6-C5-O14-P1
10	H	1101	PTY	C6-C5-O14-P1
10	L	1101	PTY	N1-C2-C3-O11
10	L	1101	PTY	C6-C5-O14-P1

There are no ring outliers.

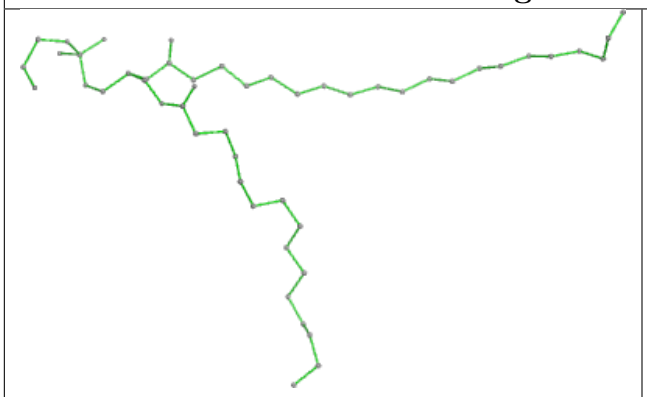
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1100	CLR	3	0
8	A	1100	CLR	1	0

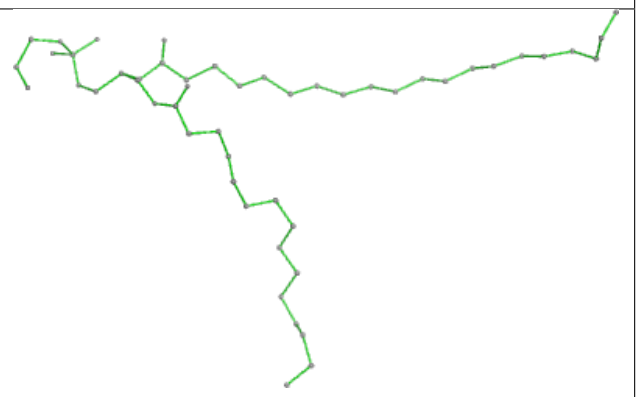
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

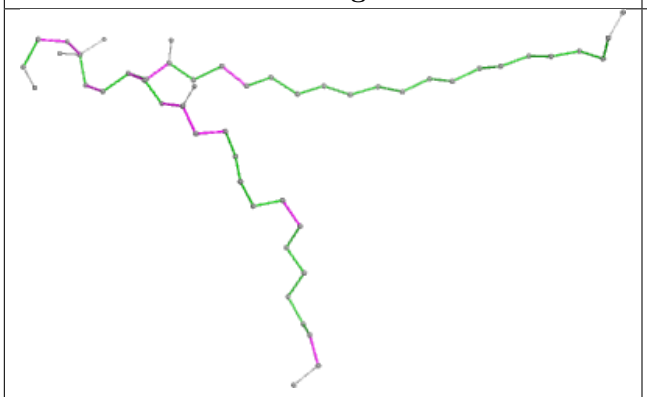
Ligand PTY D 1101



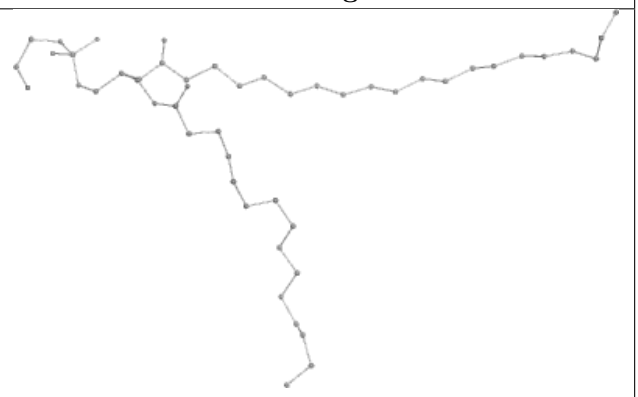
Bond lengths



Bond angles

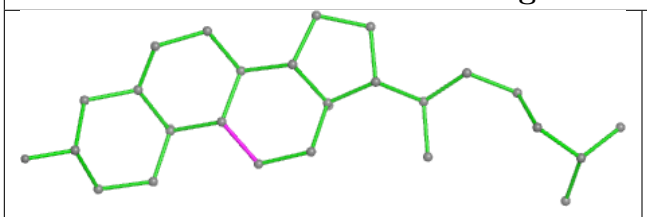


Torsions

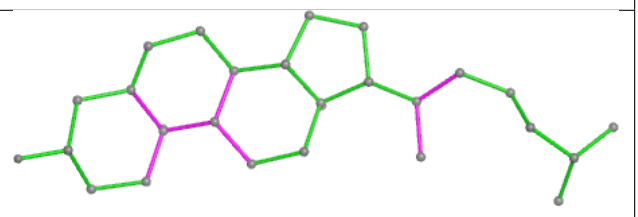


Rings

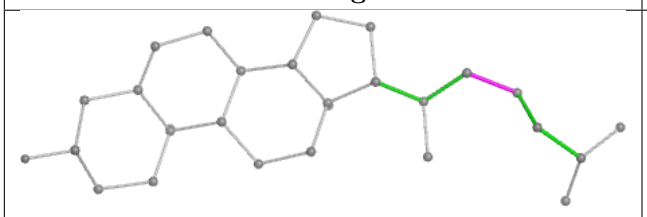
Ligand CLR L 1100



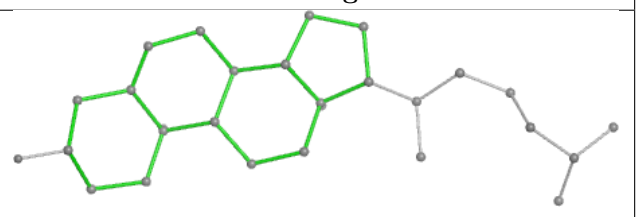
Bond lengths



Bond angles

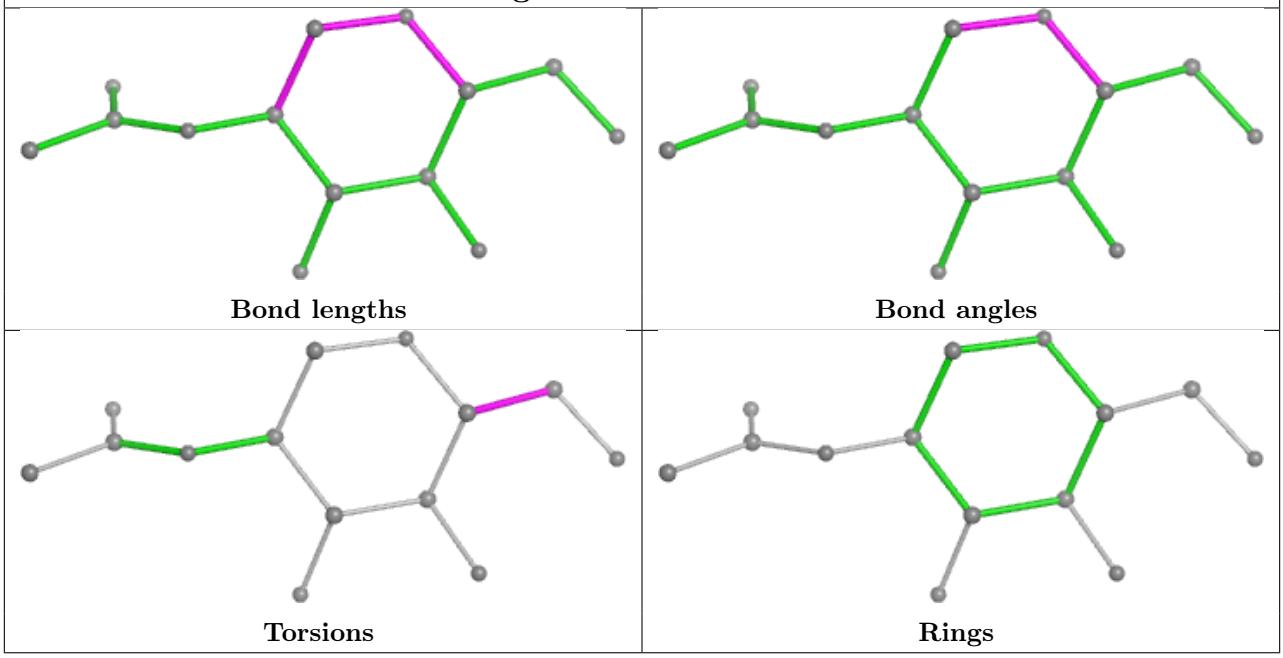


Torsions

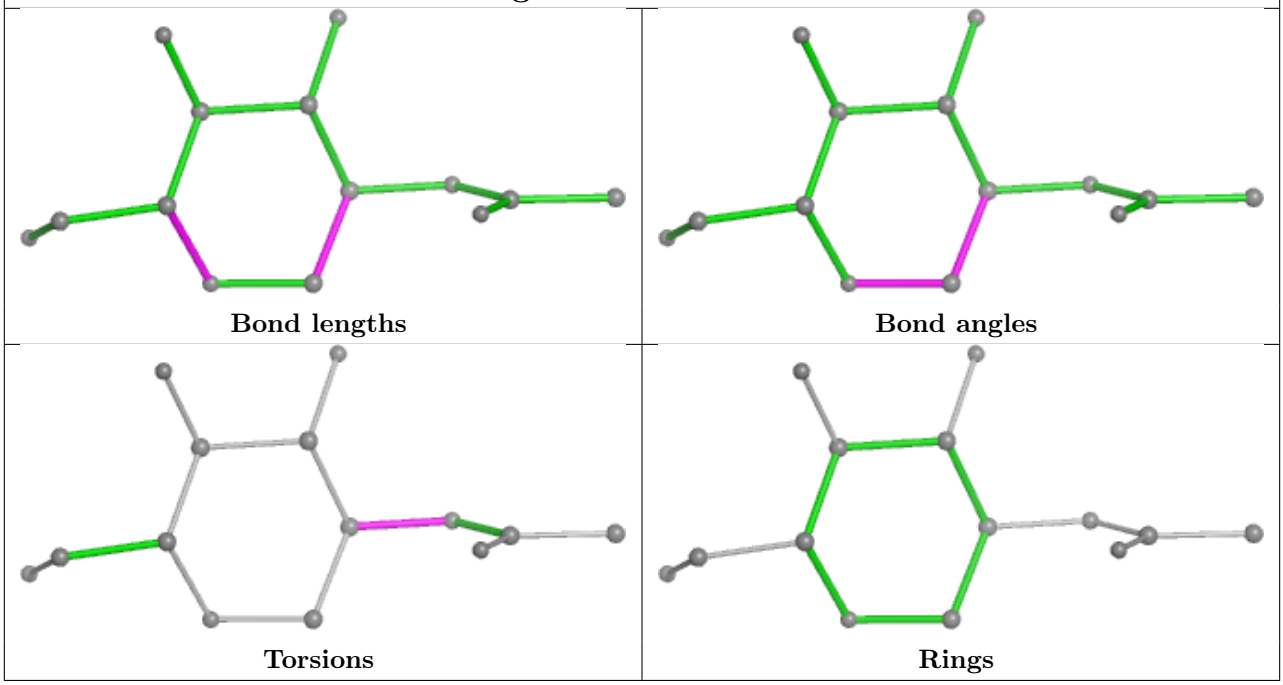


Rings

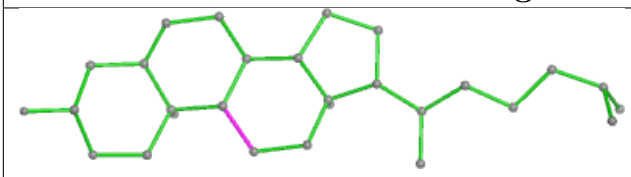
Ligand NAG B 1001



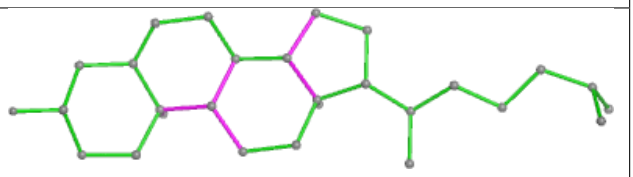
Ligand NAG C 1002



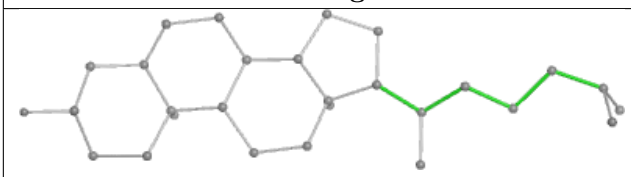
Ligand CLR D 1100



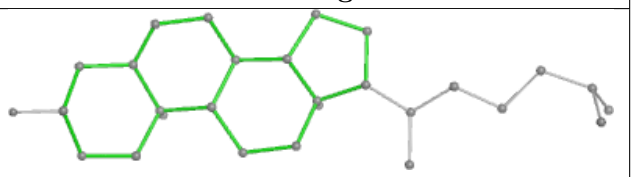
Bond lengths



Bond angles

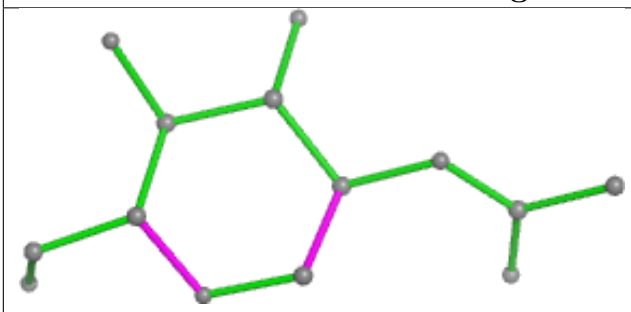


Torsions

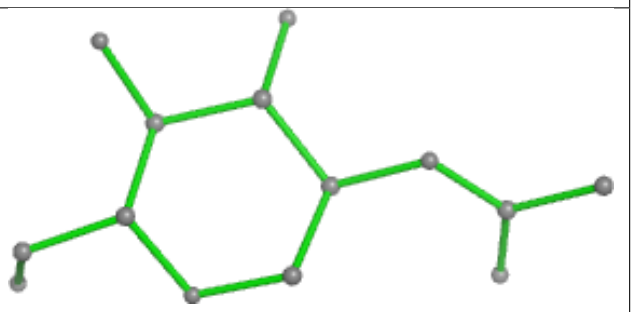


Rings

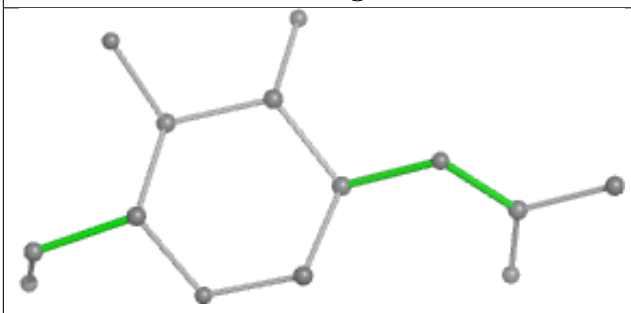
Ligand NAG G 1002



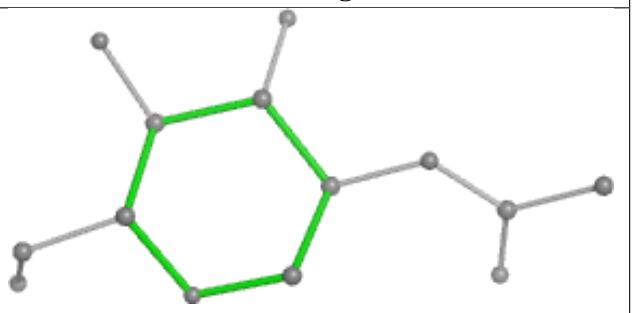
Bond lengths



Bond angles

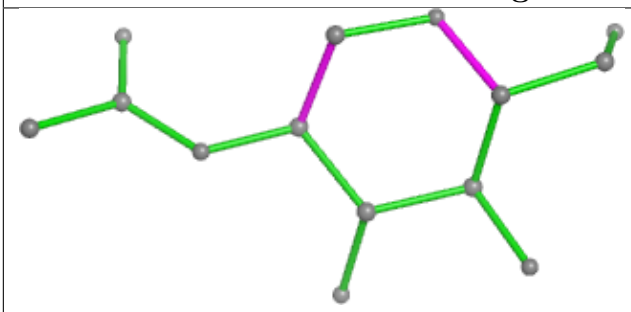


Torsions

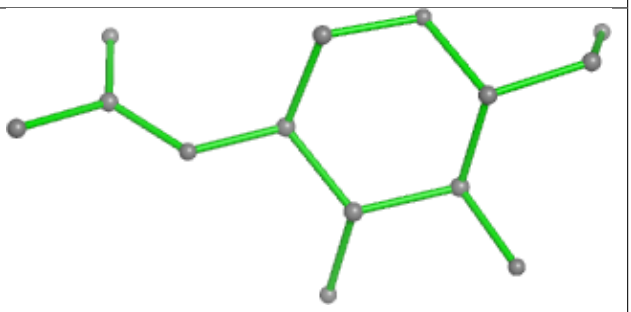


Rings

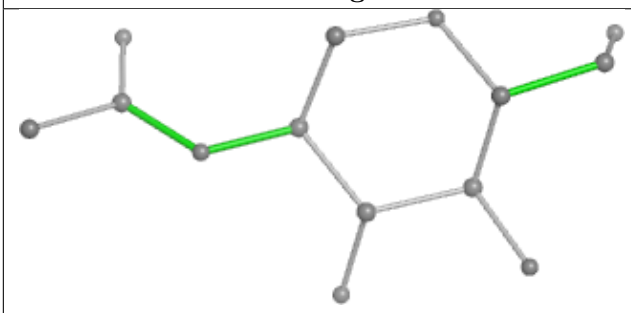
Ligand NAG B 1002



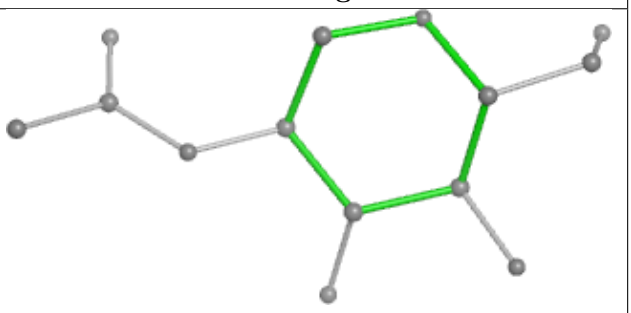
Bond lengths



Bond angles

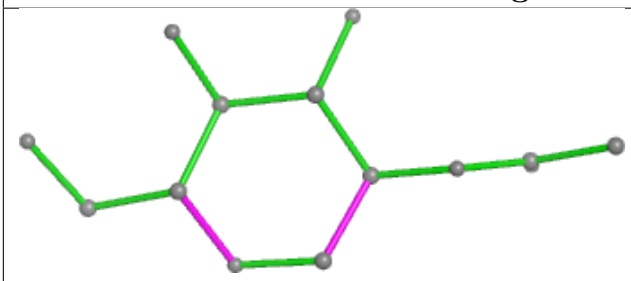


Torsions

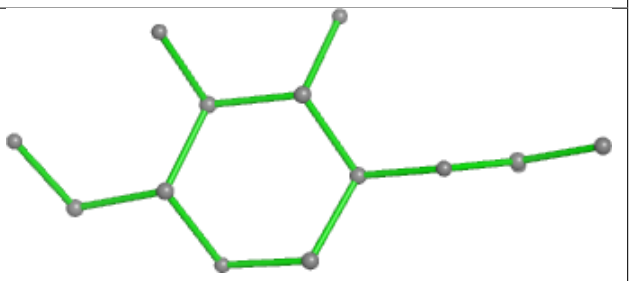


Rings

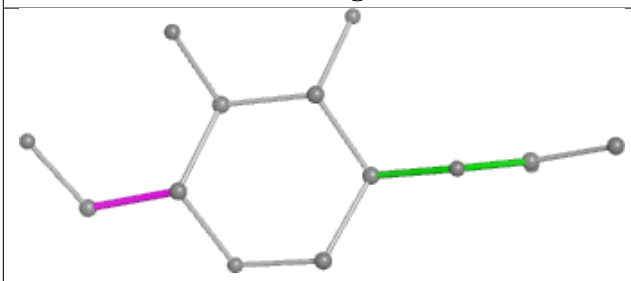
Ligand NAG C 1001



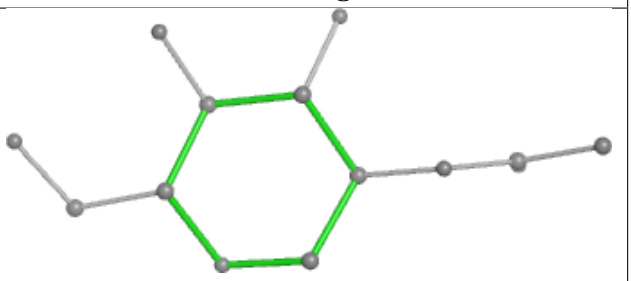
Bond lengths



Bond angles

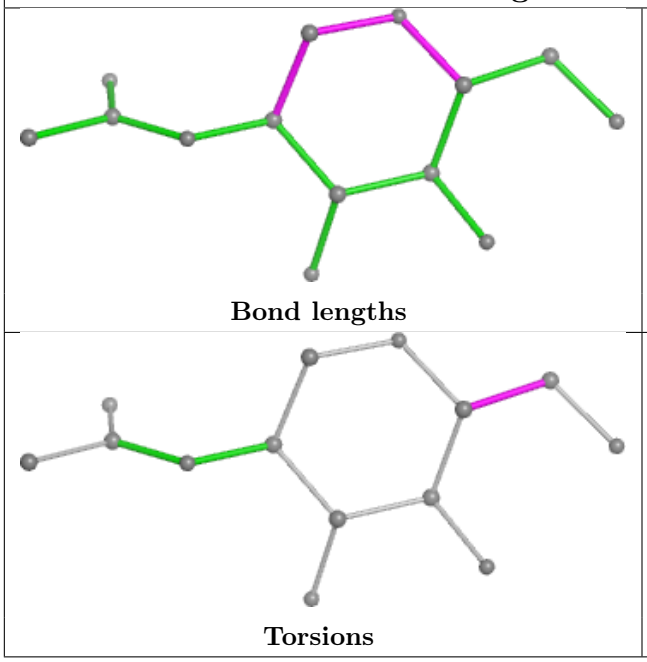


Torsions

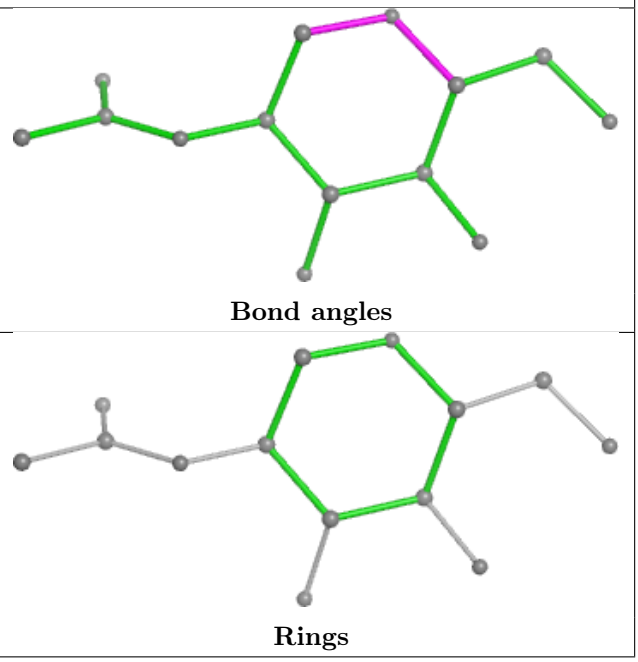


Rings

Ligand NAG G 1001



Bond lengths

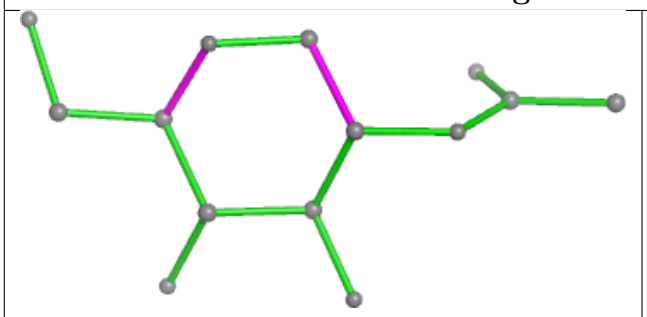


Bond angles

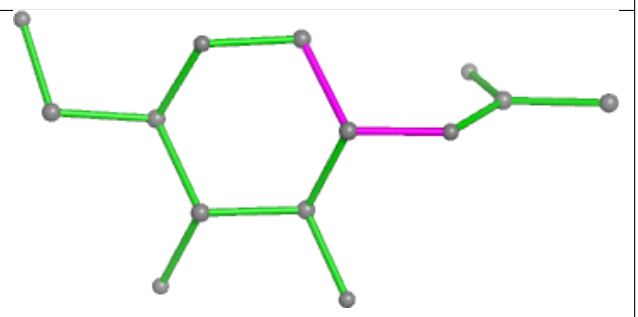
Torsions

Rings

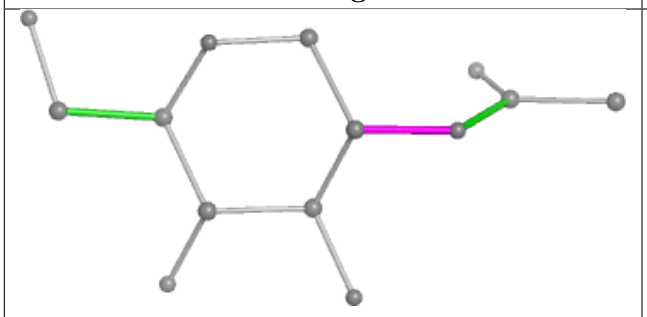
Ligand NAG B 1003



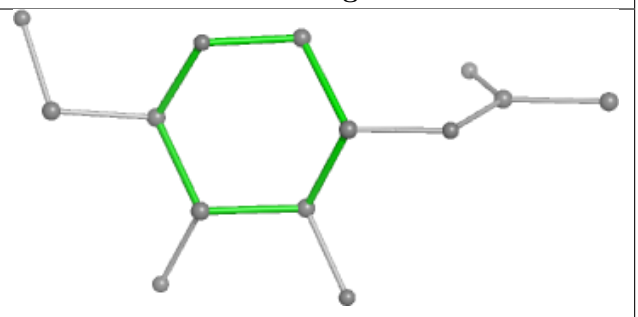
Bond lengths



Bond angles

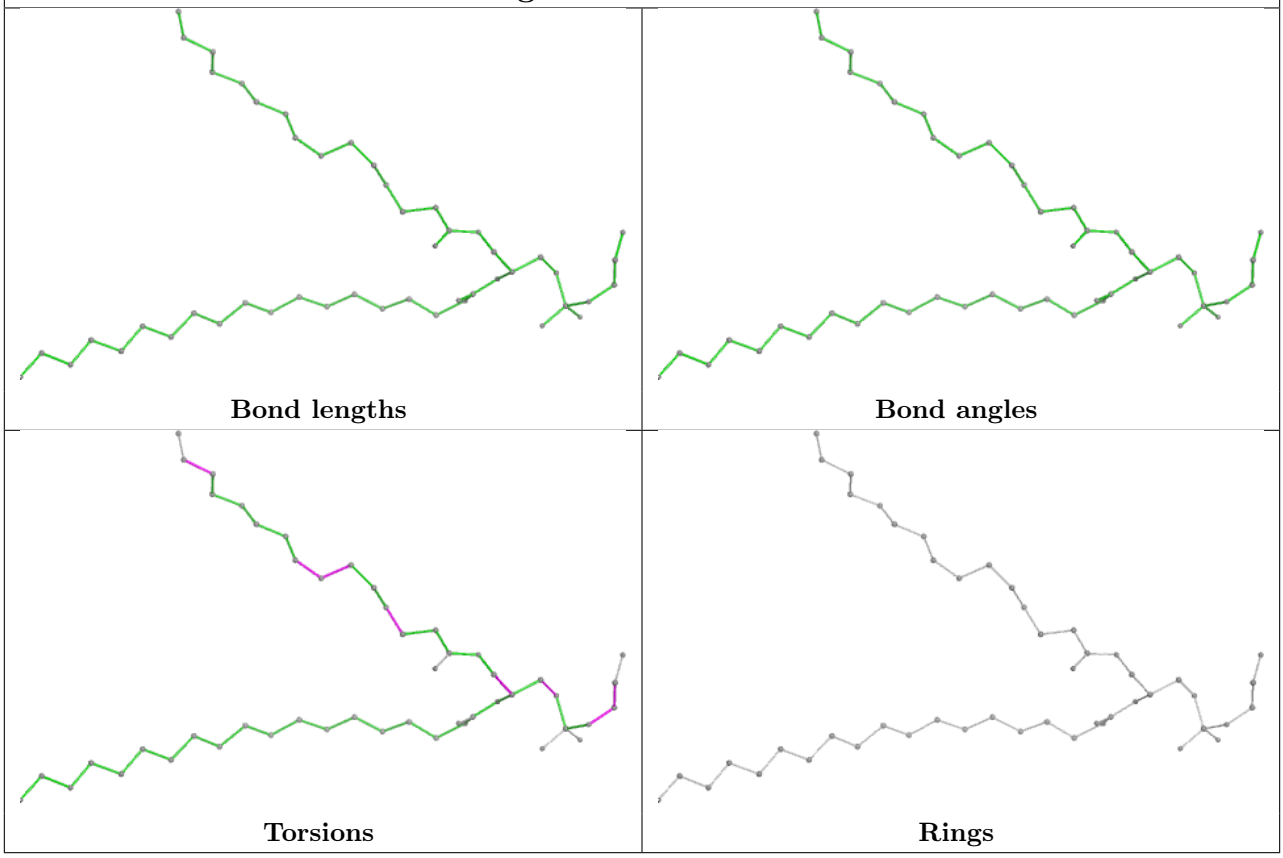


Torsions

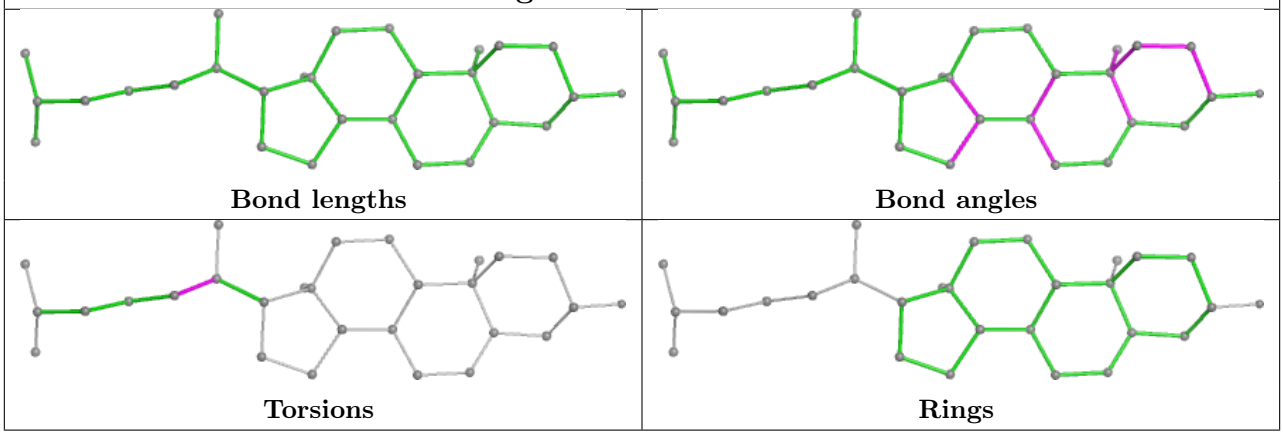


Rings

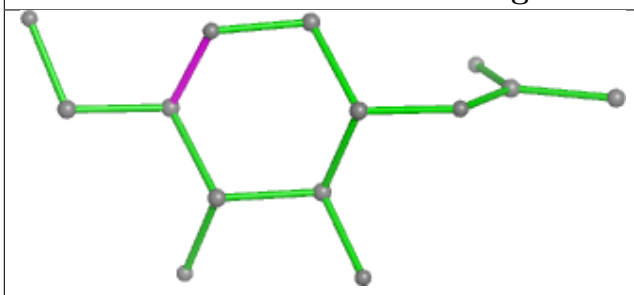
Ligand PTY L 1101



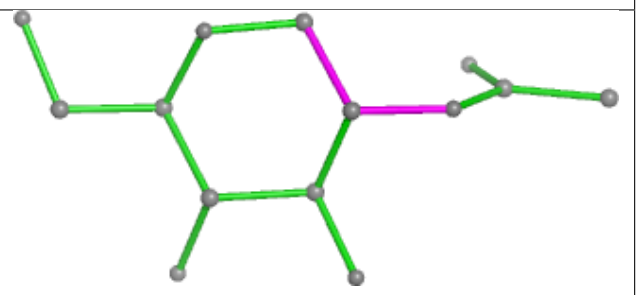
Ligand CLR A 1100



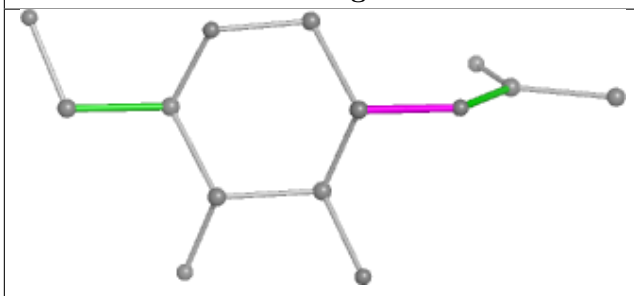
Ligand NAG G 1003



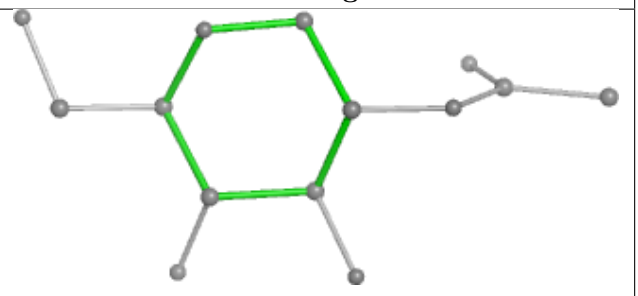
Bond lengths



Bond angles

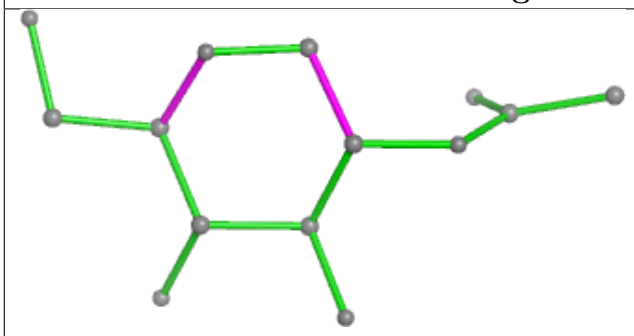


Torsions

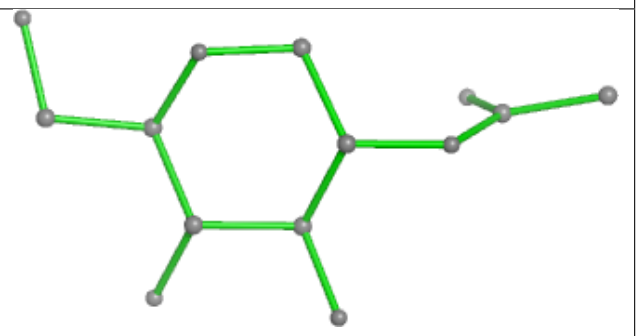


Rings

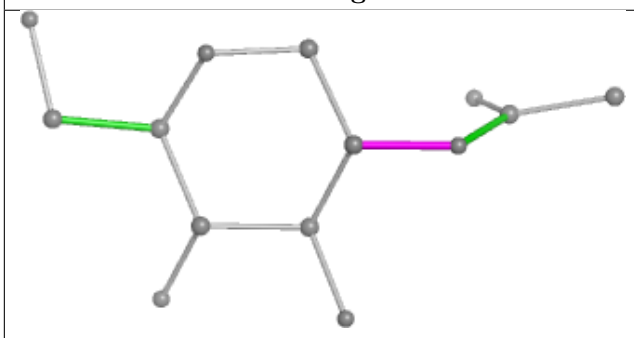
Ligand NAG C 1003



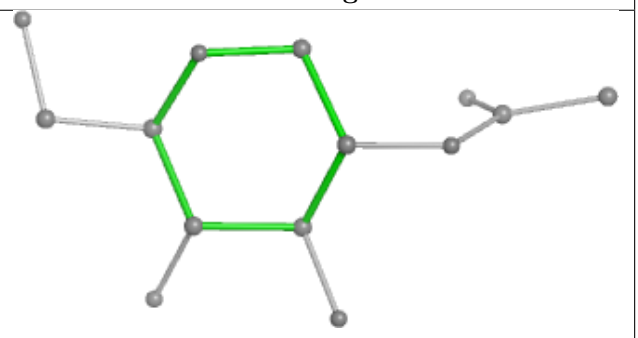
Bond lengths



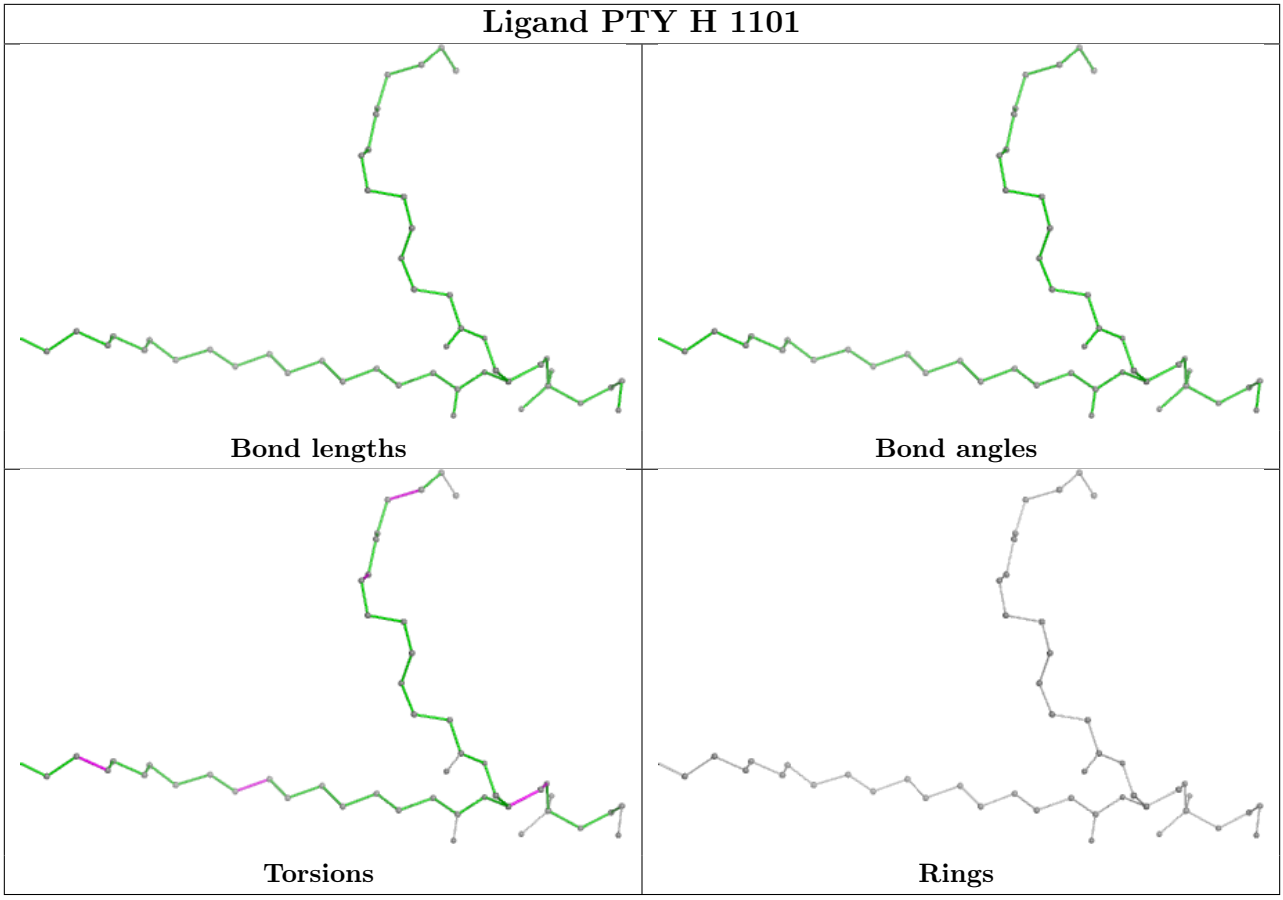
Bond angles



Torsions



Rings



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.

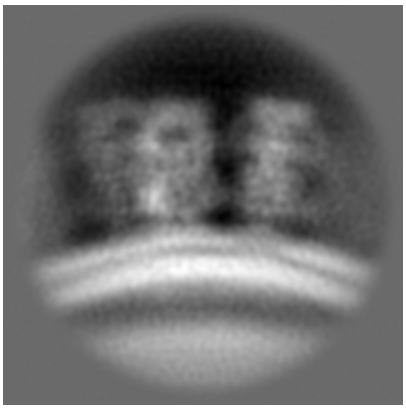
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17317. These allow visual inspection of the internal detail of the map and identification of artifacts.

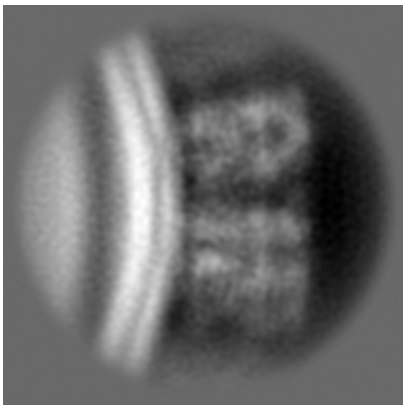
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

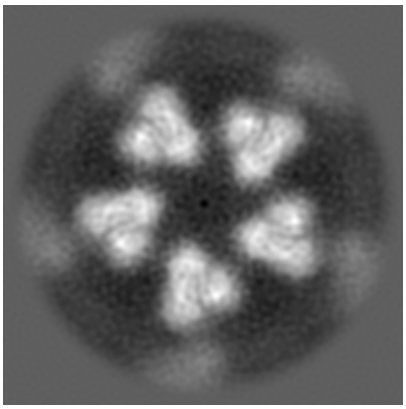
6.1.1 Primary map



X

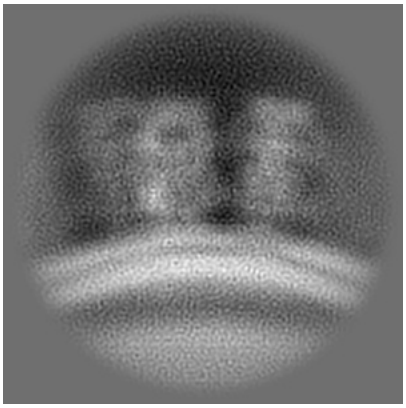


Y

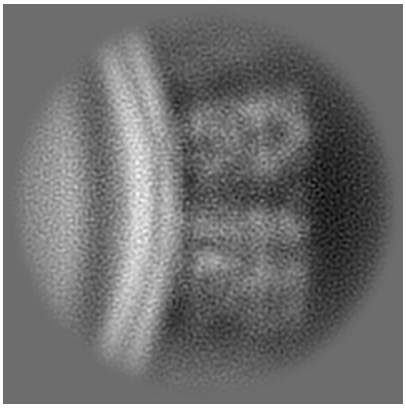


Z

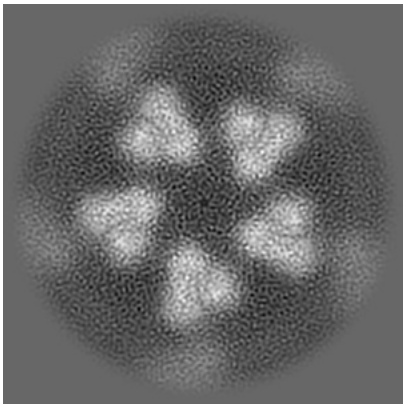
6.1.2 Raw map



X



Y

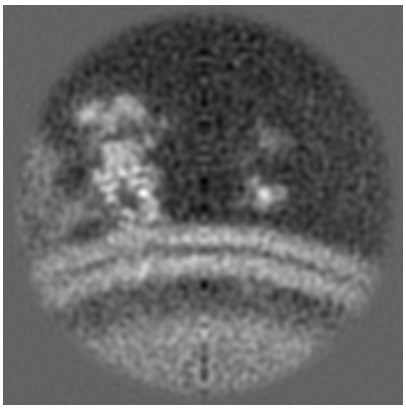


Z

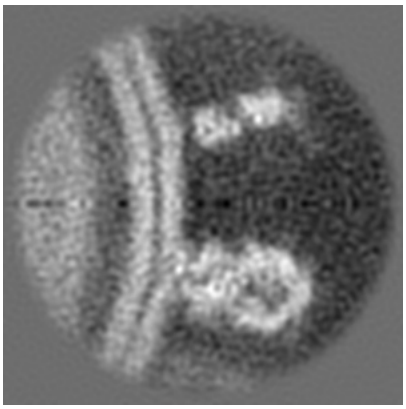
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

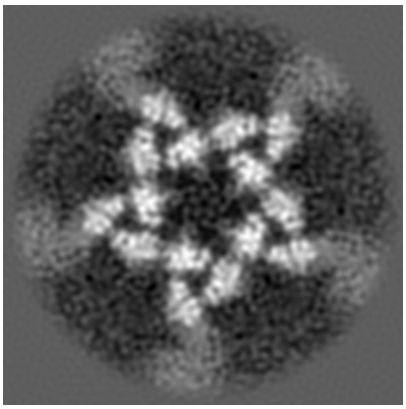
6.2.1 Primary map



X Index: 80

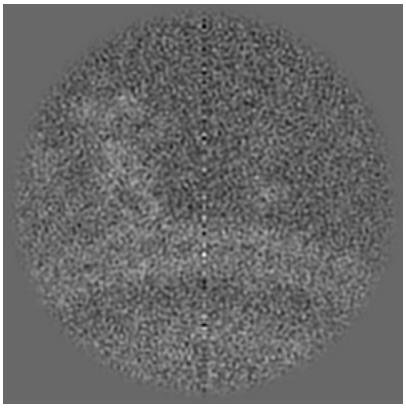


Y Index: 80

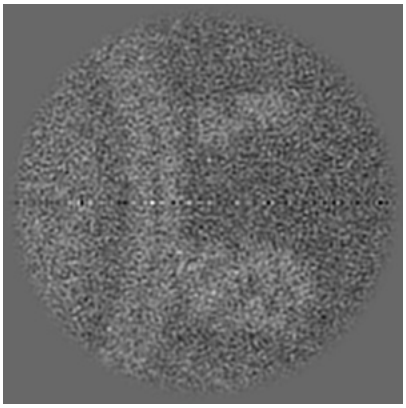


Z Index: 80

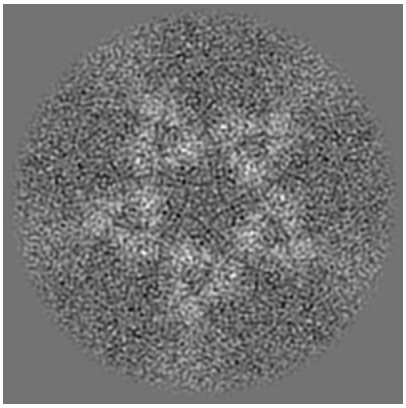
6.2.2 Raw map



X Index: 80



Y Index: 80

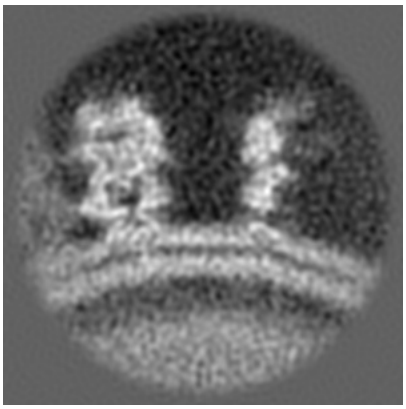


Z Index: 80

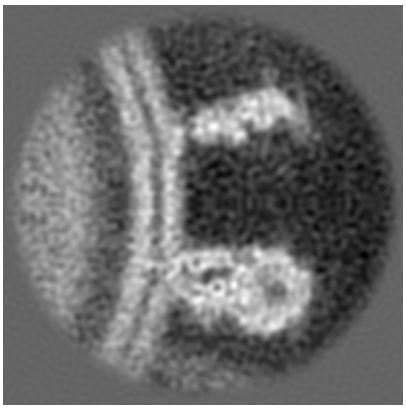
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

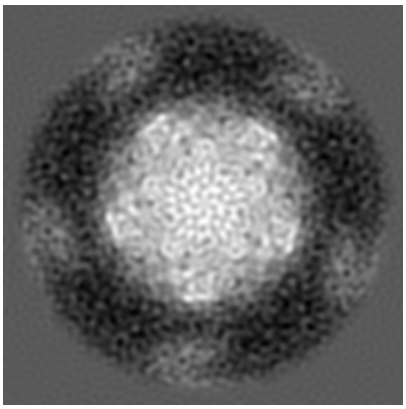
6.3.1 Primary map



X Index: 74

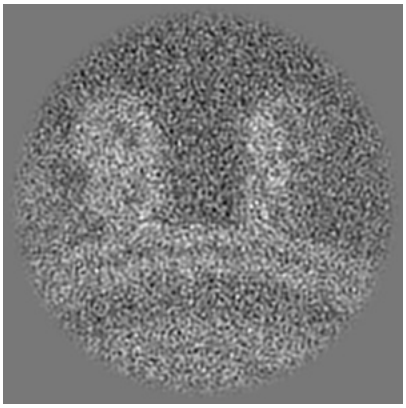


Y Index: 78

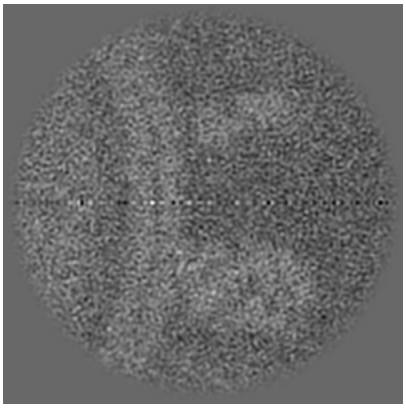


Z Index: 66

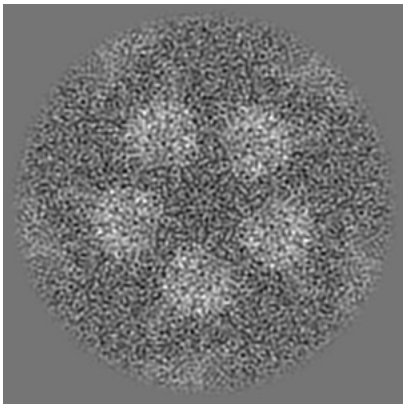
6.3.2 Raw map



X Index: 72



Y Index: 80

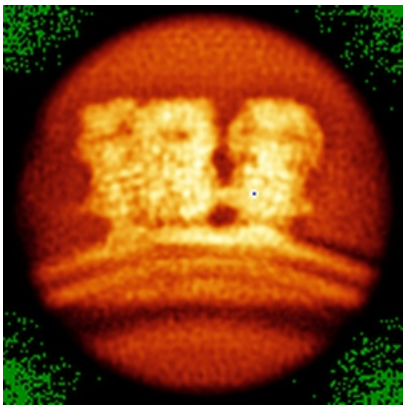


Z Index: 91

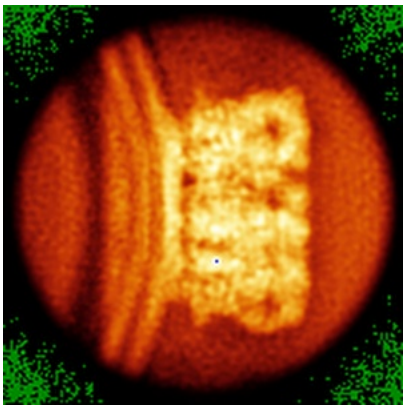
The images above show the largest variance slices of the map in three orthogonal directions.

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

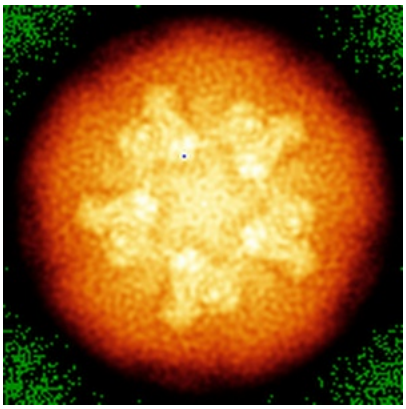
6.4.1 Primary map



X

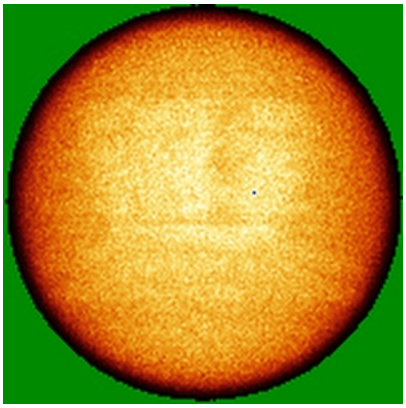


Y

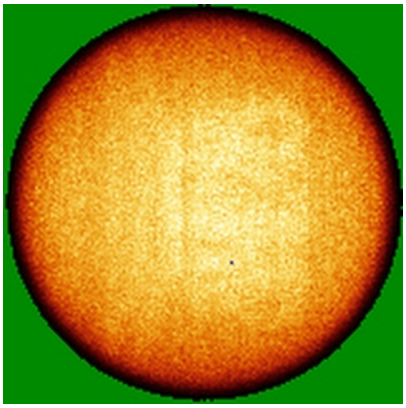


Z

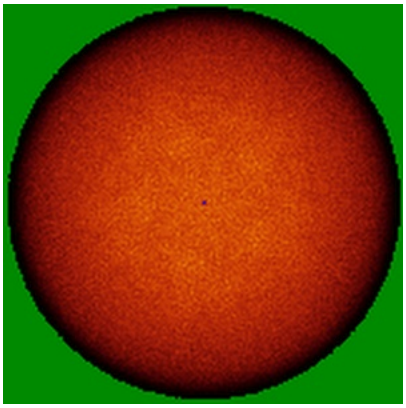
6.4.2 Raw map



X



Y

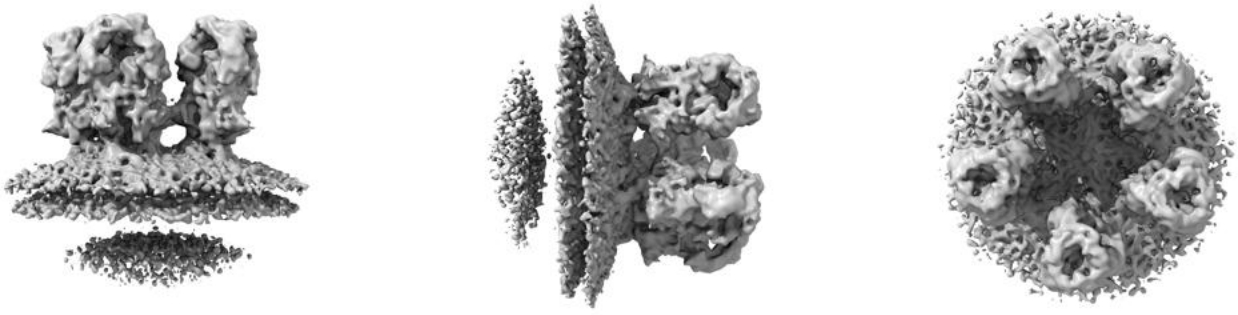


Z

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 0.064. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

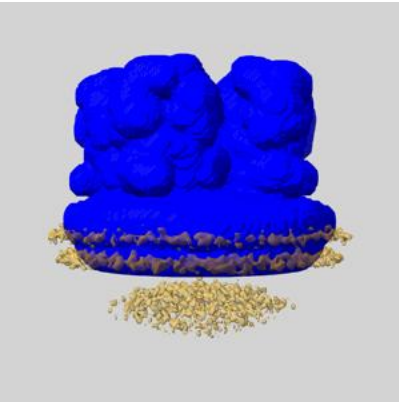
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

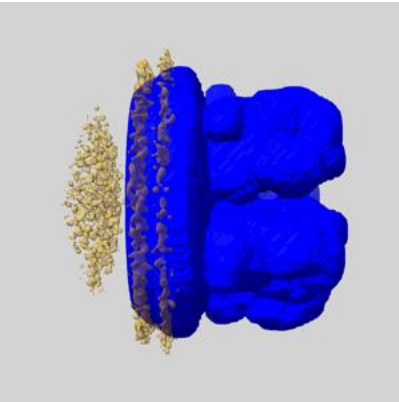
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

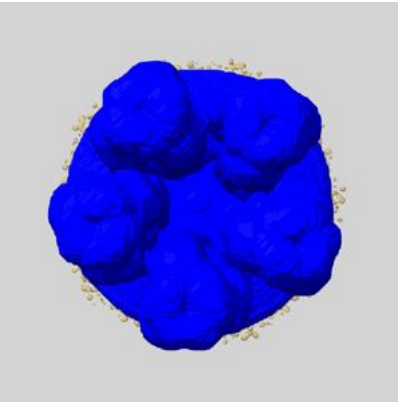
6.6.1 emd_17317_msk_1.map (i)



X



Y

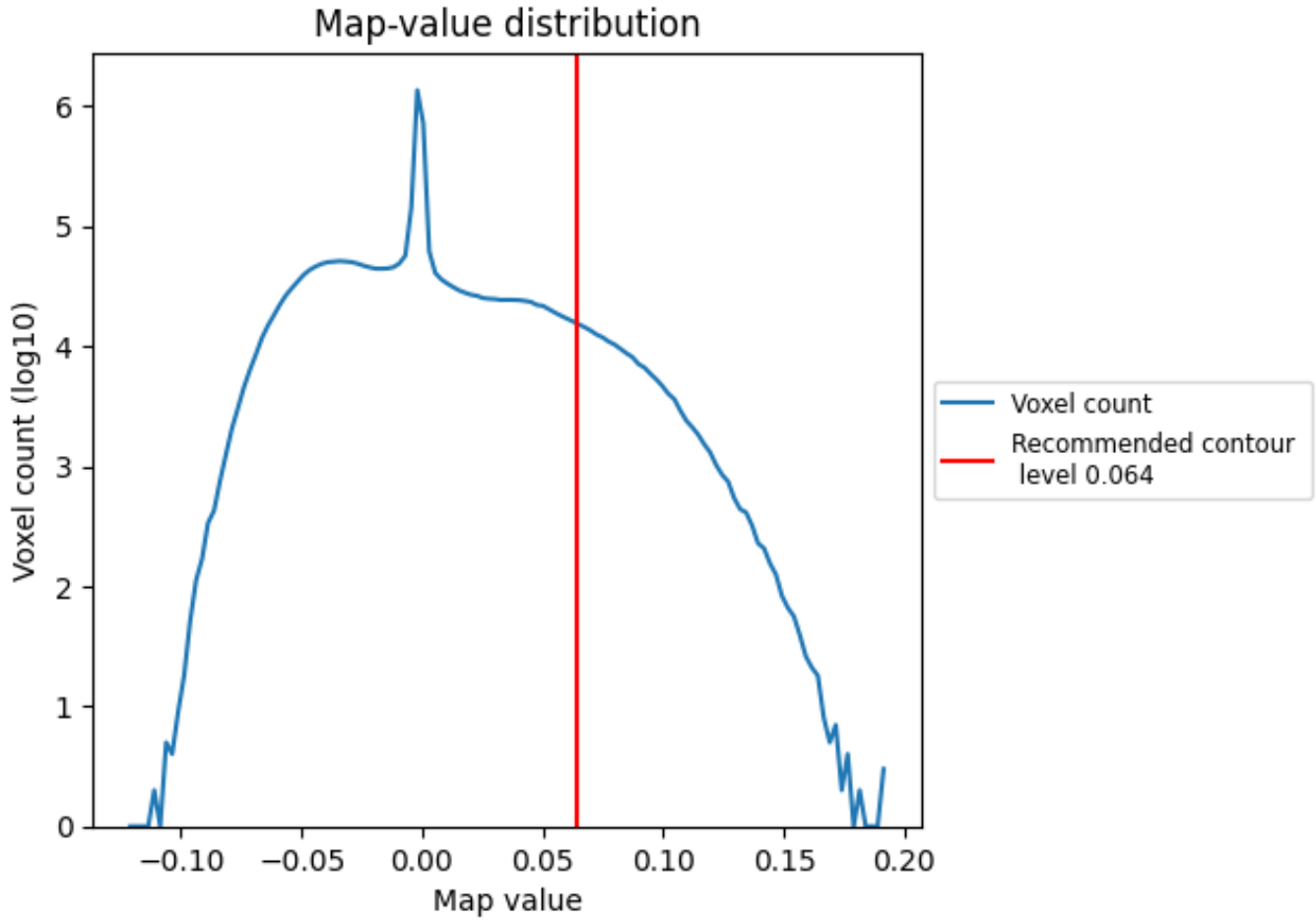


Z

7 Map analysis

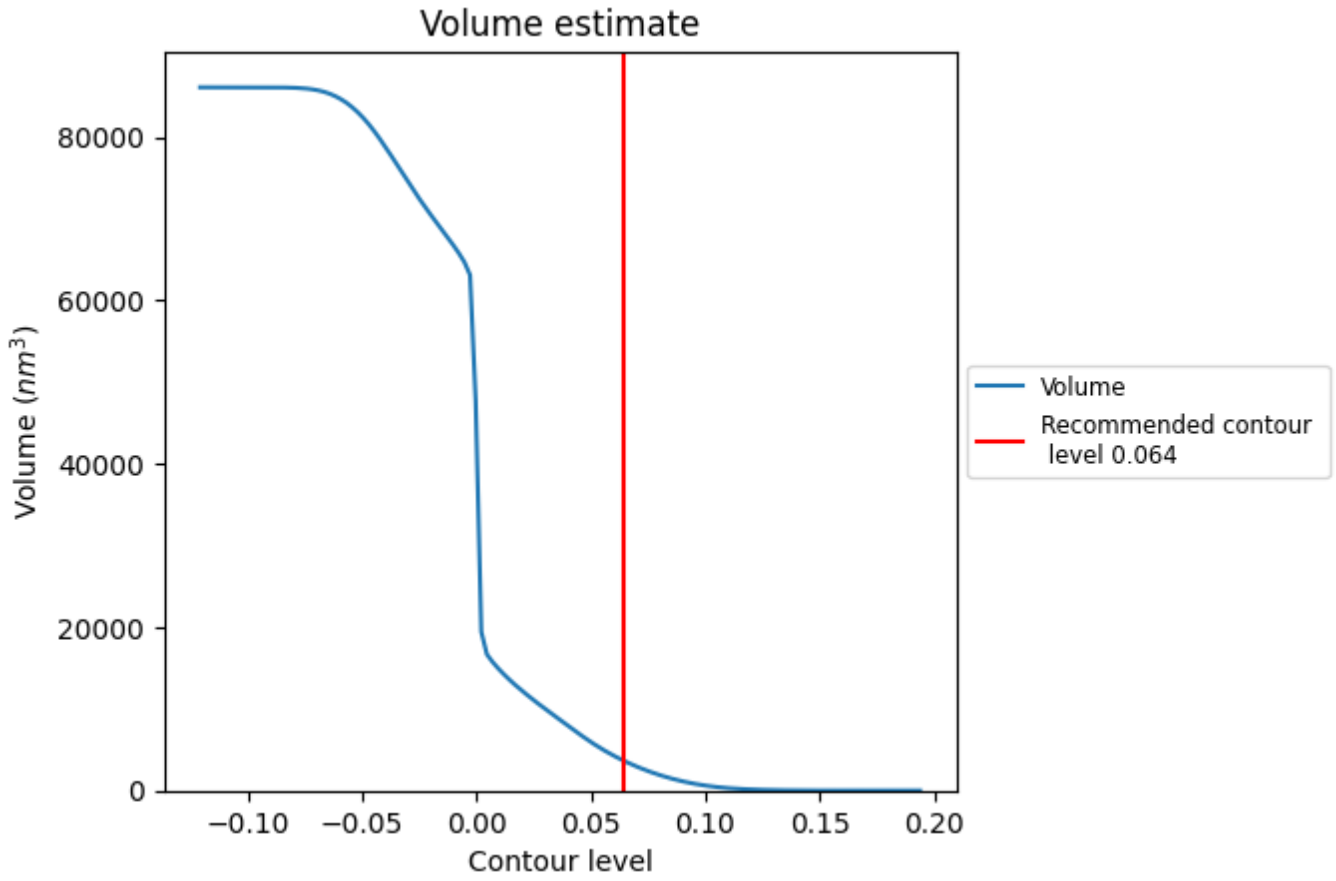
This section contains the results of statistical analysis of the map.

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.

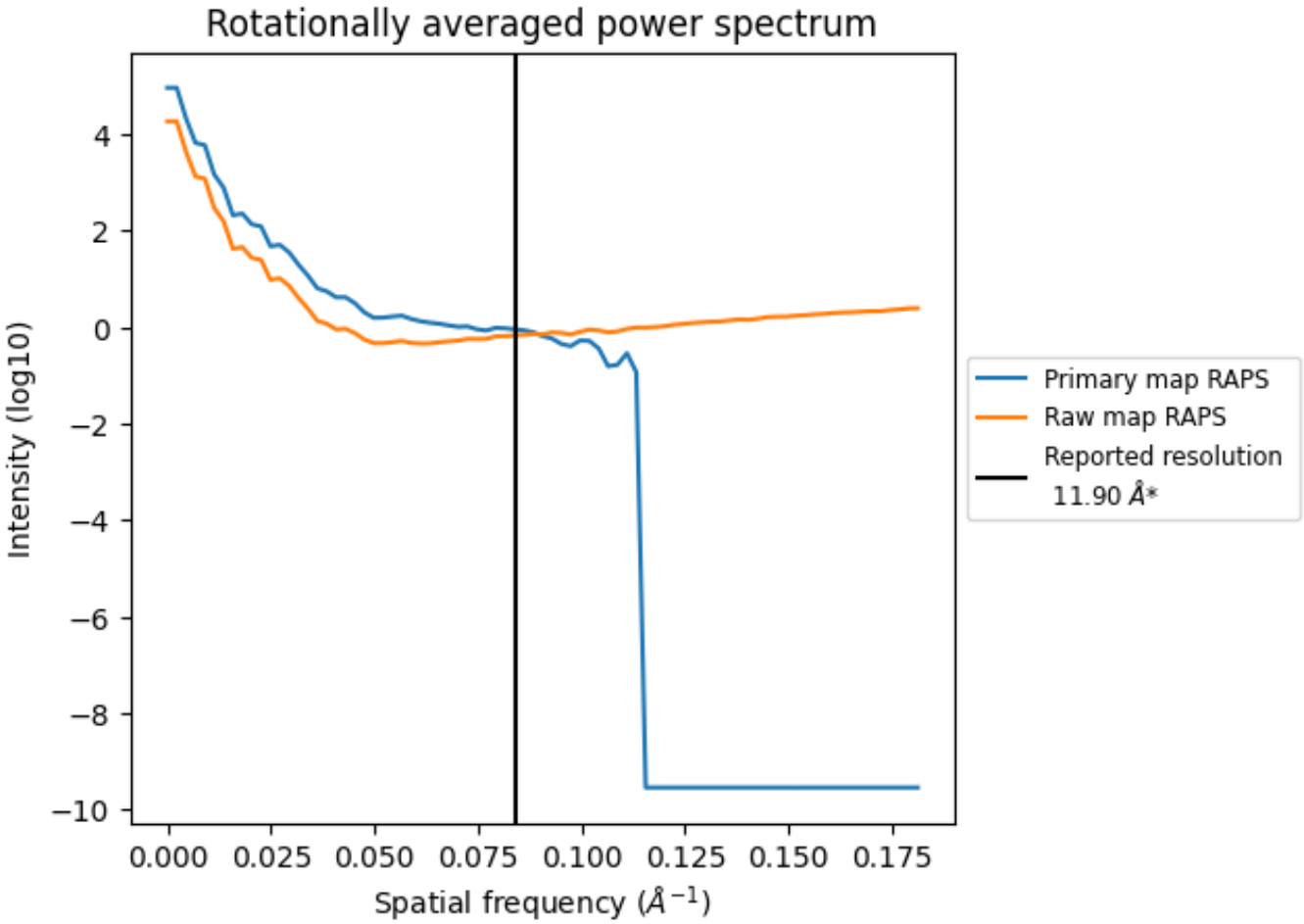
7.2 Volume estimate (i)



The volume at the recommended contour level is 3695 nm^3; this corresponds to an approximate mass of 3337 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)

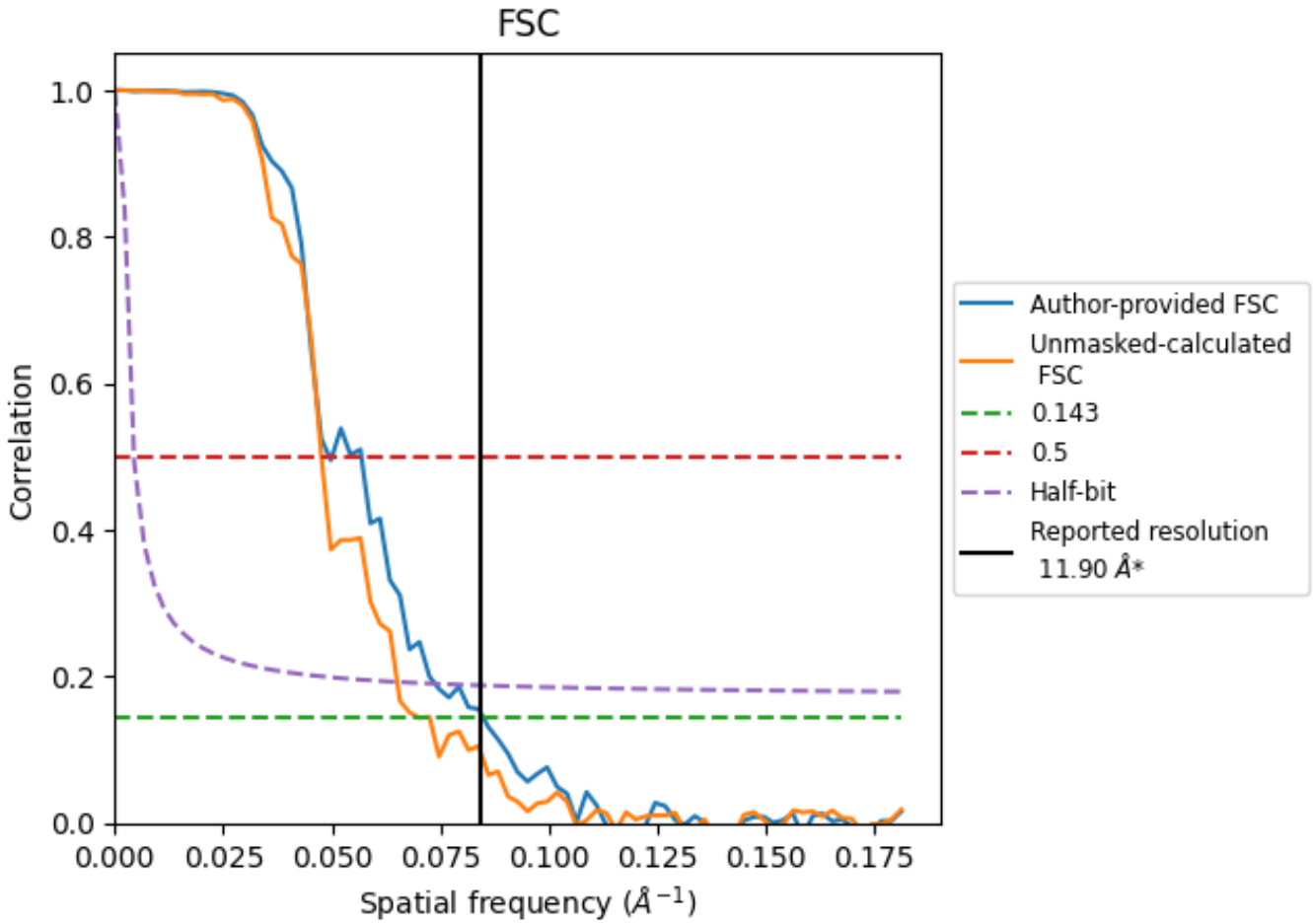


*Reported resolution corresponds to spatial frequency of 0.084 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.084 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.90	-	-
Author-provided FSC curve	11.78	20.24	13.53
Unmasked-calculated*	14.25	21.01	15.36

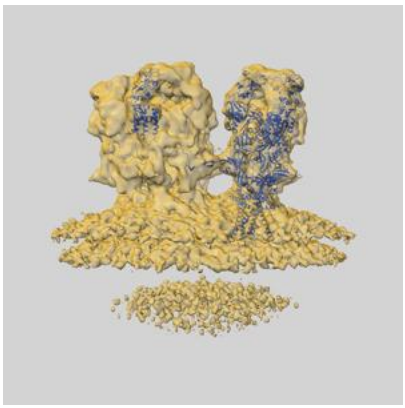
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.25 differs from the reported value 11.9 by more than 10 %

9 Map-model fit

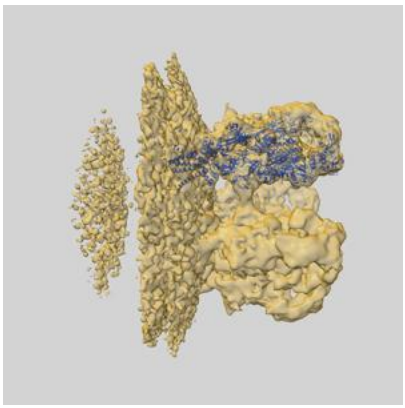
This section contains information regarding the fit between EMDB map EMD-17317 and PDB model 8OZP. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

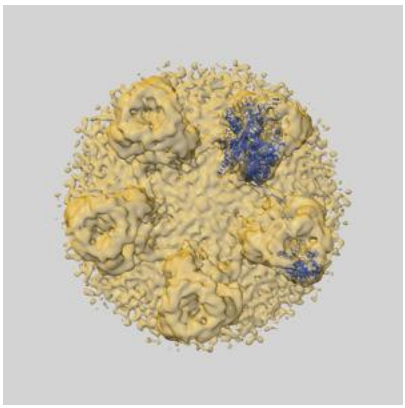
9.1.1 Map-model overlay



X

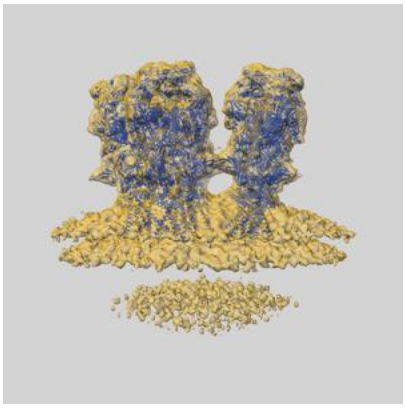


Y

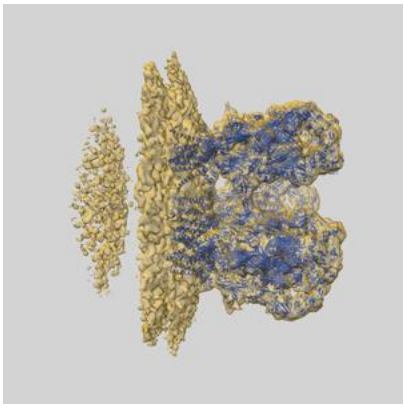


Z

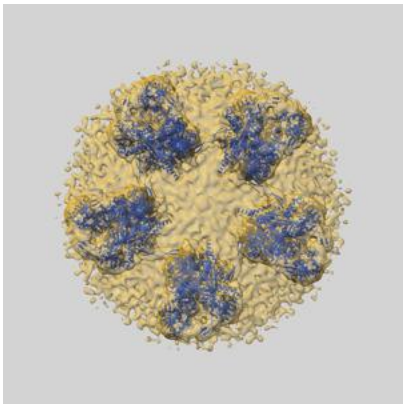
9.1.2 Map-model assembly overlay



X



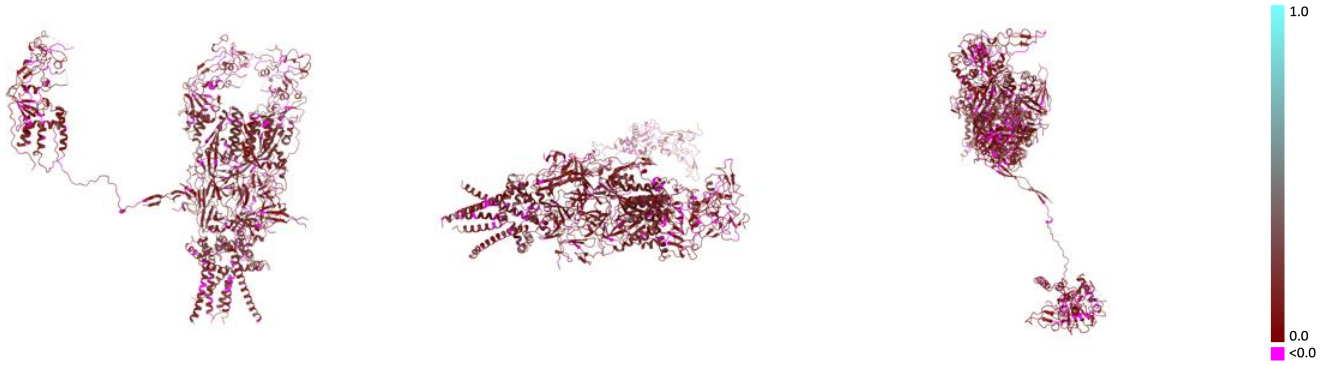
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.064 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

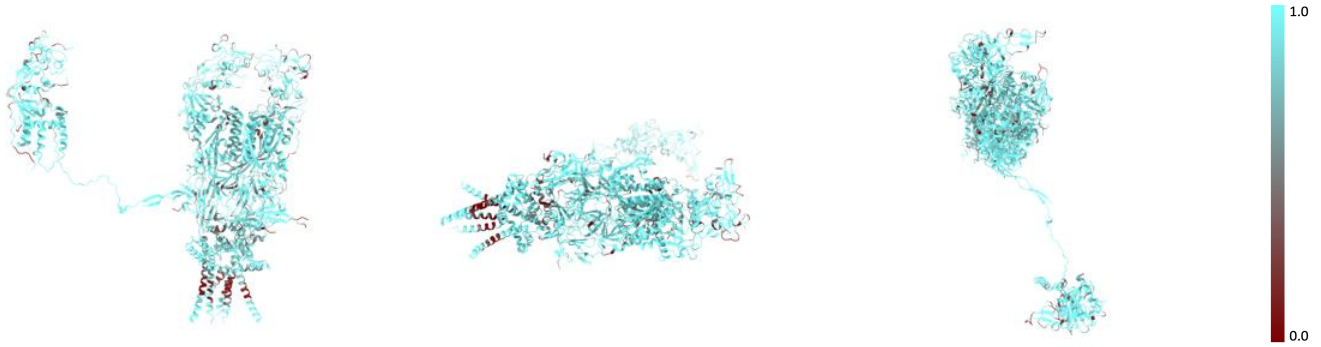
9.2 Q-score mapped to coordinate model



X Y Z

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

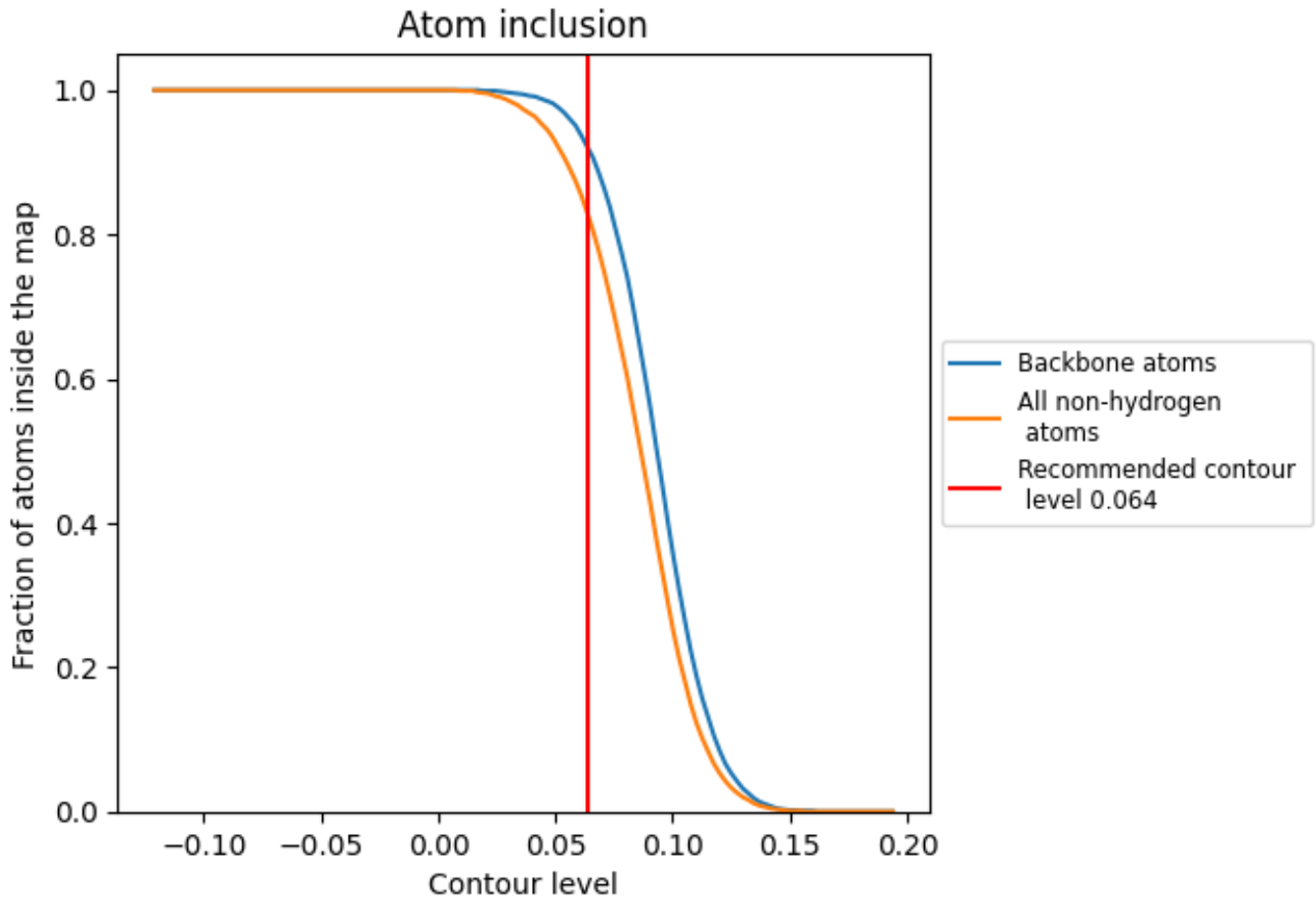
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.064).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.1150
A	0.7270	0.1210
B	0.8600	0.1000
C	0.8680	0.1160
D	0.8400	0.1270
E	0.7800	0.1330
F	0.6590	0.1300
G	0.8530	0.1030
H	0.8470	0.1210
I	0.7320	0.1070
L	0.8660	0.1250
M	0.2140	0.0540
N	0.4290	0.0990
O	0.7860	0.1960
P	0.2600	0.2070
Q	0.4200	0.2220
R	0.2400	0.1400
S	0.2050	0.1320
T	0.1790	0.1570
U	0.1030	0.0430
V	0.6670	0.0710
W	0.6530	0.1100
X	0.6270	0.0640
Y	0.3570	0.1410
Z	0.3570	0.2380
a	0.2500	0.2150
b	0.7140	0.1340
c	0.7500	0.0890
d	0.6430	0.0720
e	0.5750	0.0600
f	0.5110	0.0270
g	0.6700	0.0920
h	0.3890	0.1060
i	0.2220	0.1020
j	0.3330	0.1170