Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 03:27 PM EST

PDB ID	:	6CV0
EMDB ID	:	EMD-7631
Title	:	Cryo-electron microscopy structure of infectious bronchitis coronavirus spike protein
Authors	:	Shang, J.; Zheng, Y.; Yang, Y.; Liu, C.; Geng, Q.; Luo, C.; Zhang, W.; Li, F.
Deposited on	:	2018-03-27
Resolution	:	3.93 Å(reported)

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

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

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

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

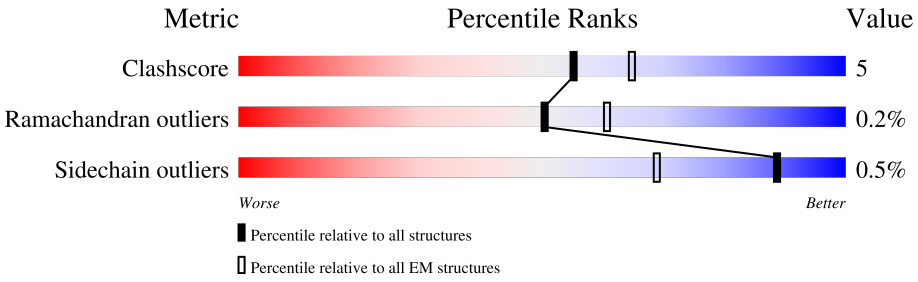
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.93 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	1105	16% 78% 11% 10%
1	B	1105	16% 79% 11% 10%
1	C	1105	17% 78% 11% 10%
2	D	2	50% 50%
2	E	2	50% 100%
2	F	2	100%
2	G	2	100% 50% 50%
2	J	2	50% 50% 50%

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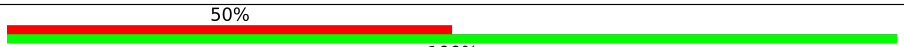
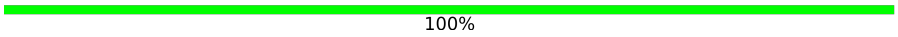
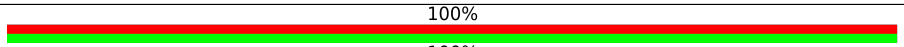
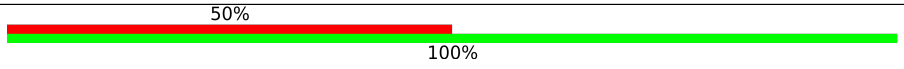
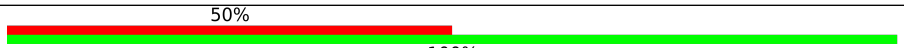
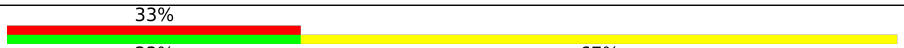
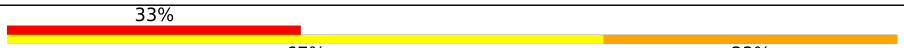
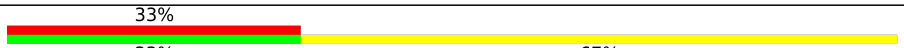
Mol	Chain	Length	Quality of chain
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	X	2	
3	H	3	
3	I	3	
3	O	3	
3	P	3	
3	V	3	
3	W	3	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24192 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	993	Total	C	N	O	S	0	0
			7658	4856	1291	1469	42		
1	B	993	Total	C	N	O	S	0	0
			7658	4856	1291	1469	42		
1	C	993	Total	C	N	O	S	0	0
			7658	4856	1291	1469	42		

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	LEU	LEU	conflict	UNP F4MIW6
A	823	HIS	ASP	conflict	UNP F4MIW6
A	829	ASN	SER	conflict	UNP F4MIW6
A	849	LEU	VAL	conflict	UNP F4MIW6
A	1077	VAL	-	insertion	UNP F4MIW6
A	1078	ASP	-	insertion	UNP F4MIW6
A	1079	ILE	-	insertion	UNP F4MIW6
A	1080	LYS	-	insertion	UNP F4MIW6
A	1081	GLN	LEU	expression tag	UNP F4MIW6
A	1082	ILE	ILE	expression tag	UNP F4MIW6
A	1083	GLU	-	insertion	UNP F4MIW6
A	1084	ASP	ASP	expression tag	UNP F4MIW6
A	1085	LYS	-	insertion	UNP F4MIW6
A	1086	ILE	-	insertion	UNP F4MIW6
A	1087	GLU	LEU	expression tag	UNP F4MIW6
A	1088	GLU	GLU	expression tag	UNP F4MIW6
A	1089	ILE	LYS	expression tag	UNP F4MIW6
A	1090	LEU	LEU	expression tag	UNP F4MIW6
A	1091	SER	-	expression tag	UNP F4MIW6
A	1092	LYS	-	expression tag	UNP F4MIW6
A	1093	ILE	-	expression tag	UNP F4MIW6
A	1094	TYR	-	expression tag	UNP F4MIW6
A	1095	HIS	-	expression tag	UNP F4MIW6
A	1096	ILE	-	expression tag	UNP F4MIW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1097	GLU	-	expression tag	UNP F4MIW6
A	1098	ASN	-	expression tag	UNP F4MIW6
A	1099	GLU	-	expression tag	UNP F4MIW6
A	1100	ILE	-	expression tag	UNP F4MIW6
A	1101	ALA	-	expression tag	UNP F4MIW6
A	1102	ARG	-	expression tag	UNP F4MIW6
A	1103	ILE	-	expression tag	UNP F4MIW6
A	1104	LYS	-	expression tag	UNP F4MIW6
A	1105	LYS	-	expression tag	UNP F4MIW6
A	1106	LEU	-	expression tag	UNP F4MIW6
A	1107	ILE	-	expression tag	UNP F4MIW6
A	1108	GLY	-	expression tag	UNP F4MIW6
A	1109	GLU	-	expression tag	UNP F4MIW6
A	1110	ILE	-	expression tag	UNP F4MIW6
A	1111	GLY	-	expression tag	UNP F4MIW6
A	1112	GLY	-	expression tag	UNP F4MIW6
A	1113	GLY	-	expression tag	UNP F4MIW6
A	1114	GLY	-	expression tag	UNP F4MIW6
A	1115	SER	-	expression tag	UNP F4MIW6
A	1116	HIS	-	expression tag	UNP F4MIW6
A	1117	HIS	-	expression tag	UNP F4MIW6
A	1118	HIS	-	expression tag	UNP F4MIW6
A	1119	HIS	-	expression tag	UNP F4MIW6
A	1120	HIS	-	expression tag	UNP F4MIW6
A	1121	HIS	-	expression tag	UNP F4MIW6
A	1122	HIS	-	expression tag	UNP F4MIW6
A	1123	HIS	-	expression tag	UNP F4MIW6
B	126	LEU	LEU	conflict	UNP F4MIW6
B	823	HIS	ASP	conflict	UNP F4MIW6
B	829	ASN	SER	conflict	UNP F4MIW6
B	849	LEU	VAL	conflict	UNP F4MIW6
B	1077	VAL	-	insertion	UNP F4MIW6
B	1078	ASP	-	insertion	UNP F4MIW6
B	1079	ILE	-	insertion	UNP F4MIW6
B	1080	LYS	-	insertion	UNP F4MIW6
B	1081	GLN	LEU	expression tag	UNP F4MIW6
B	1082	ILE	ILE	expression tag	UNP F4MIW6
B	1083	GLU	-	insertion	UNP F4MIW6
B	1084	ASP	ASP	expression tag	UNP F4MIW6
B	1085	LYS	-	insertion	UNP F4MIW6
B	1086	ILE	-	insertion	UNP F4MIW6
B	1087	GLU	LEU	expression tag	UNP F4MIW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1088	GLU	GLU	expression tag	UNP F4MIW6
B	1089	ILE	LYS	expression tag	UNP F4MIW6
B	1090	LEU	LEU	expression tag	UNP F4MIW6
B	1091	SER	-	expression tag	UNP F4MIW6
B	1092	LYS	-	expression tag	UNP F4MIW6
B	1093	ILE	-	expression tag	UNP F4MIW6
B	1094	TYR	-	expression tag	UNP F4MIW6
B	1095	HIS	-	expression tag	UNP F4MIW6
B	1096	ILE	-	expression tag	UNP F4MIW6
B	1097	GLU	-	expression tag	UNP F4MIW6
B	1098	ASN	-	expression tag	UNP F4MIW6
B	1099	GLU	-	expression tag	UNP F4MIW6
B	1100	ILE	-	expression tag	UNP F4MIW6
B	1101	ALA	-	expression tag	UNP F4MIW6
B	1102	ARG	-	expression tag	UNP F4MIW6
B	1103	ILE	-	expression tag	UNP F4MIW6
B	1104	LYS	-	expression tag	UNP F4MIW6
B	1105	LYS	-	expression tag	UNP F4MIW6
B	1106	LEU	-	expression tag	UNP F4MIW6
B	1107	ILE	-	expression tag	UNP F4MIW6
B	1108	GLY	-	expression tag	UNP F4MIW6
B	1109	GLU	-	expression tag	UNP F4MIW6
B	1110	ILE	-	expression tag	UNP F4MIW6
B	1111	GLY	-	expression tag	UNP F4MIW6
B	1112	GLY	-	expression tag	UNP F4MIW6
B	1113	GLY	-	expression tag	UNP F4MIW6
B	1114	GLY	-	expression tag	UNP F4MIW6
B	1115	SER	-	expression tag	UNP F4MIW6
B	1116	HIS	-	expression tag	UNP F4MIW6
B	1117	HIS	-	expression tag	UNP F4MIW6
B	1118	HIS	-	expression tag	UNP F4MIW6
B	1119	HIS	-	expression tag	UNP F4MIW6
B	1120	HIS	-	expression tag	UNP F4MIW6
B	1121	HIS	-	expression tag	UNP F4MIW6
B	1122	HIS	-	expression tag	UNP F4MIW6
B	1123	HIS	-	expression tag	UNP F4MIW6
C	126	LEU	LEU	conflict	UNP F4MIW6
C	823	HIS	ASP	conflict	UNP F4MIW6
C	829	ASN	SER	conflict	UNP F4MIW6
C	849	LEU	VAL	conflict	UNP F4MIW6
C	1077	VAL	-	insertion	UNP F4MIW6
C	1078	ASP	-	insertion	UNP F4MIW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1079	ILE	-	insertion	UNP F4MIW6
C	1080	LYS	-	insertion	UNP F4MIW6
C	1081	GLN	LEU	expression tag	UNP F4MIW6
C	1082	ILE	ILE	expression tag	UNP F4MIW6
C	1083	GLU	-	insertion	UNP F4MIW6
C	1084	ASP	ASP	expression tag	UNP F4MIW6
C	1085	LYS	-	insertion	UNP F4MIW6
C	1086	ILE	-	insertion	UNP F4MIW6
C	1087	GLU	LEU	expression tag	UNP F4MIW6
C	1088	GLU	GLU	expression tag	UNP F4MIW6
C	1089	ILE	LYS	expression tag	UNP F4MIW6
C	1090	LEU	LEU	expression tag	UNP F4MIW6
C	1091	SER	-	expression tag	UNP F4MIW6
C	1092	LYS	-	expression tag	UNP F4MIW6
C	1093	ILE	-	expression tag	UNP F4MIW6
C	1094	TYR	-	expression tag	UNP F4MIW6
C	1095	HIS	-	expression tag	UNP F4MIW6
C	1096	ILE	-	expression tag	UNP F4MIW6
C	1097	GLU	-	expression tag	UNP F4MIW6
C	1098	ASN	-	expression tag	UNP F4MIW6
C	1099	GLU	-	expression tag	UNP F4MIW6
C	1100	ILE	-	expression tag	UNP F4MIW6
C	1101	ALA	-	expression tag	UNP F4MIW6
C	1102	ARG	-	expression tag	UNP F4MIW6
C	1103	ILE	-	expression tag	UNP F4MIW6
C	1104	LYS	-	expression tag	UNP F4MIW6
C	1105	LYS	-	expression tag	UNP F4MIW6
C	1106	LEU	-	expression tag	UNP F4MIW6
C	1107	ILE	-	expression tag	UNP F4MIW6
C	1108	GLY	-	expression tag	UNP F4MIW6
C	1109	GLU	-	expression tag	UNP F4MIW6
C	1110	ILE	-	expression tag	UNP F4MIW6
C	1111	GLY	-	expression tag	UNP F4MIW6
C	1112	GLY	-	expression tag	UNP F4MIW6
C	1113	GLY	-	expression tag	UNP F4MIW6
C	1114	GLY	-	expression tag	UNP F4MIW6
C	1115	SER	-	expression tag	UNP F4MIW6
C	1116	HIS	-	expression tag	UNP F4MIW6
C	1117	HIS	-	expression tag	UNP F4MIW6
C	1118	HIS	-	expression tag	UNP F4MIW6
C	1119	HIS	-	expression tag	UNP F4MIW6
C	1120	HIS	-	expression tag	UNP F4MIW6

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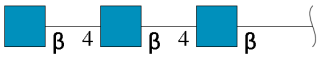
Chain	Residue	Modelled	Actual	Comment	Reference
C	1121	HIS	-	expression tag	UNP F4MIW6
C	1122	HIS	-	expression tag	UNP F4MIW6
C	1123	HIS	-	expression tag	UNP F4MIW6

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

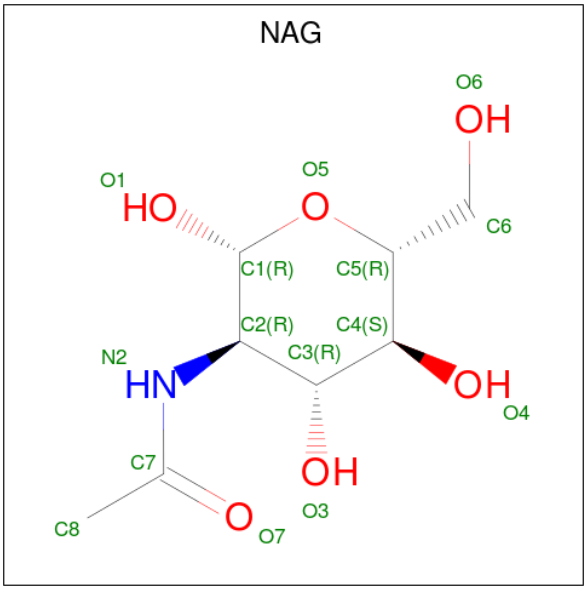
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	H	3	Total	C	N	O	0	0
			42	24	3	15		
3	I	3	Total	C	N	O	0	0
			42	24	3	15		
3	O	3	Total	C	N	O	0	0
			42	24	3	15		
3	P	3	Total	C	N	O	0	0
			42	24	3	15		
3	V	3	Total	C	N	O	0	0
			42	24	3	15		
3	W	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	

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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	A	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0

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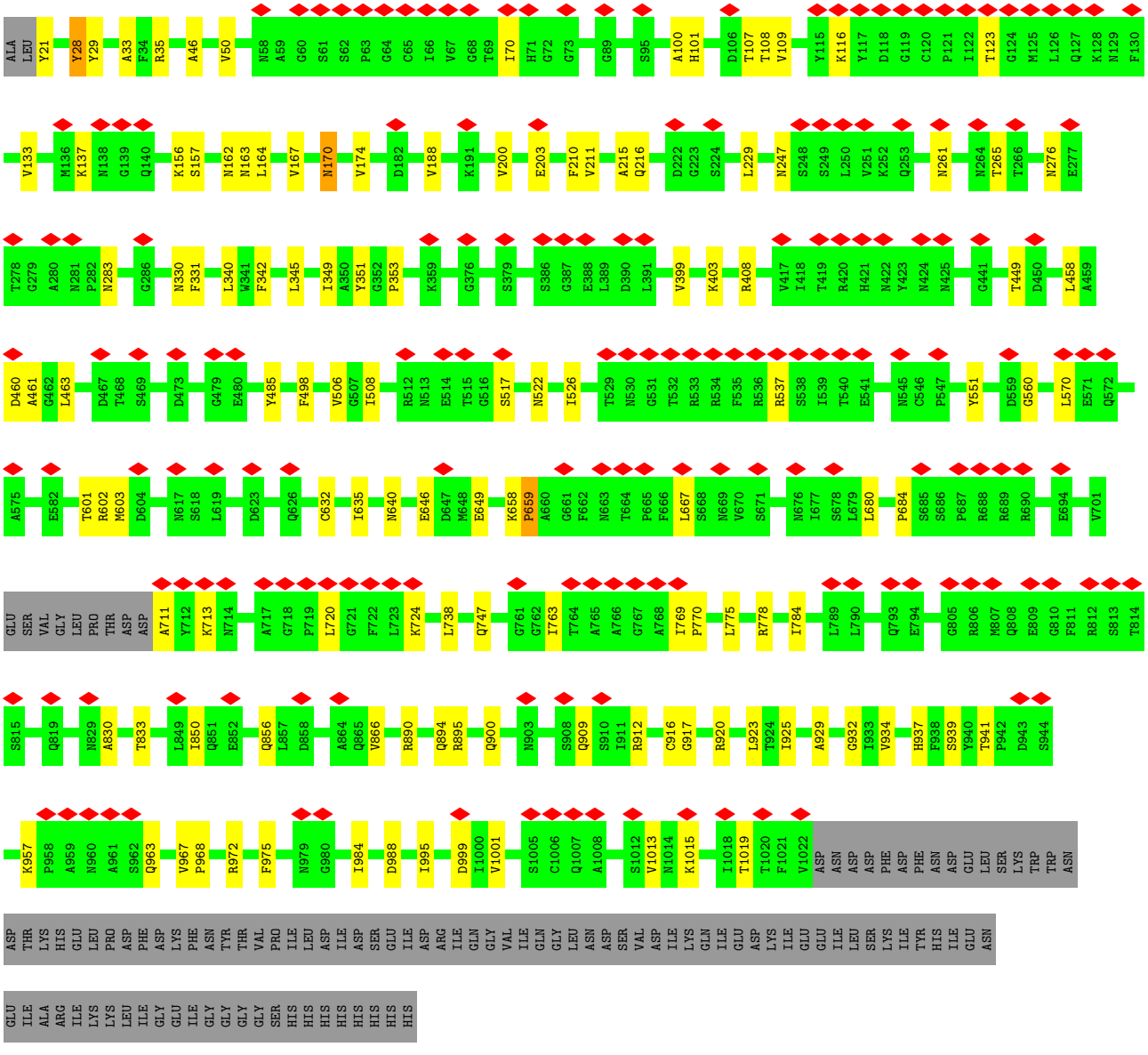
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	B	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0
4	C	1	Total 182	C 104	N 13	O 65	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

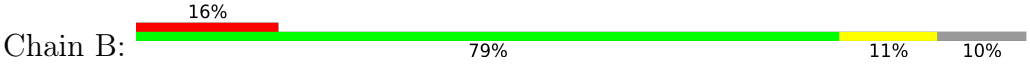
- Molecule 1: Spike glycoprotein

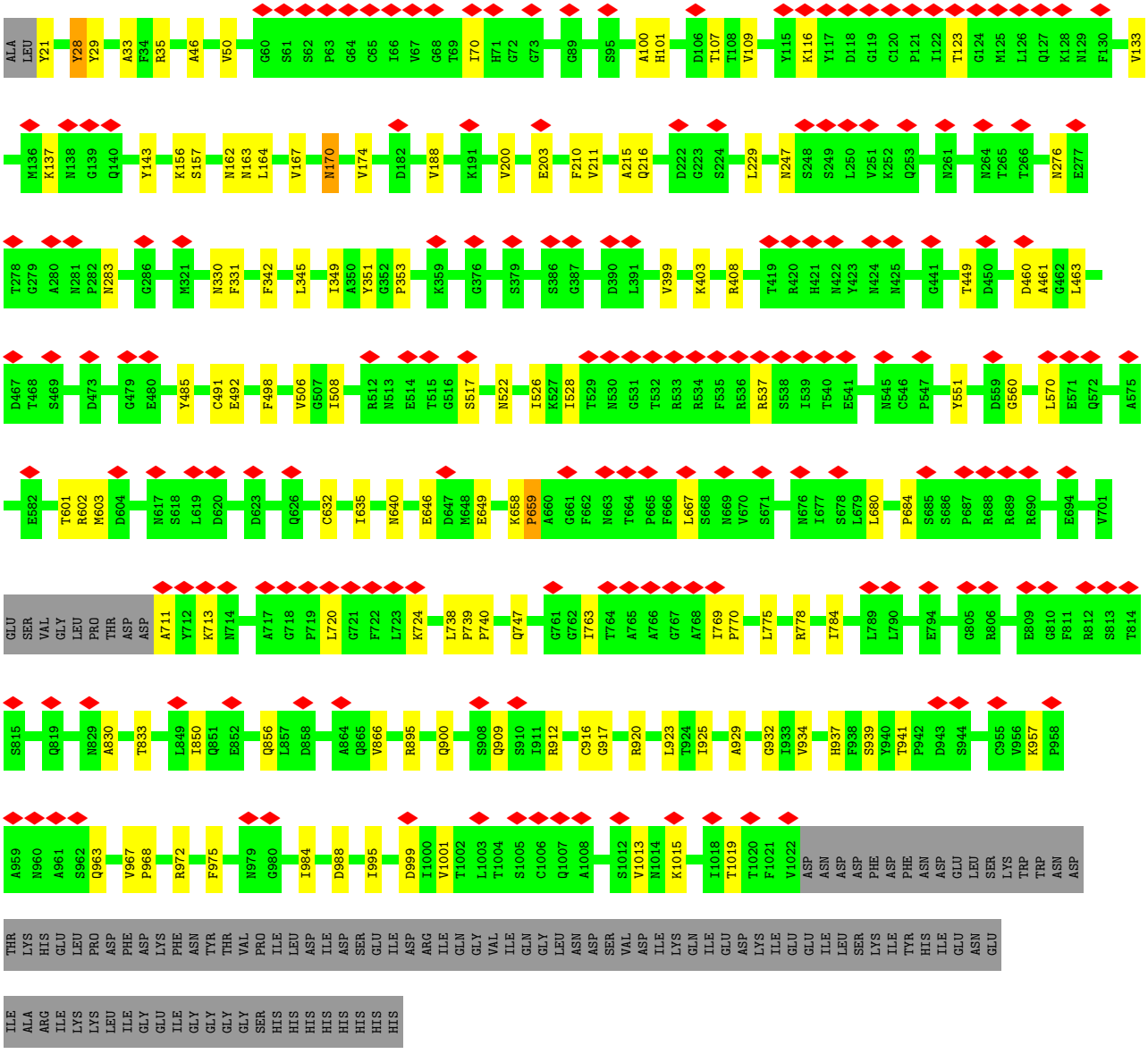
Chain A: 



• Molecule 1: Spike glycoprotein

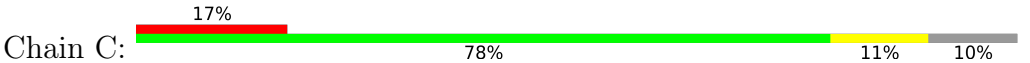
Chain B:

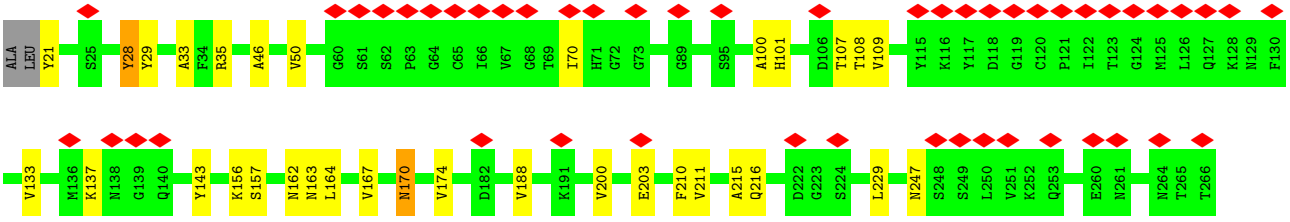


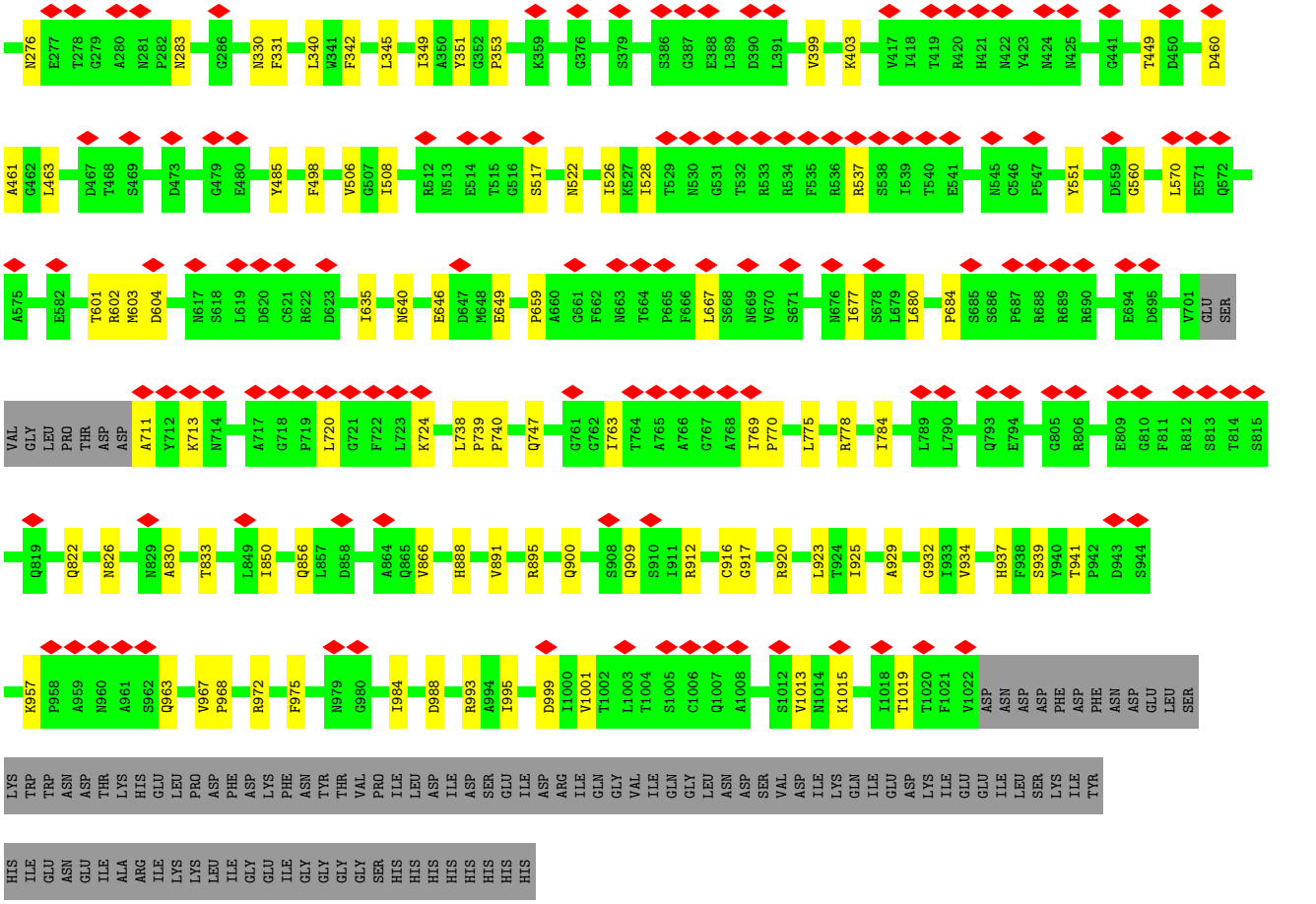


• Molecule 1: Spike glycoprotein

Chain C:





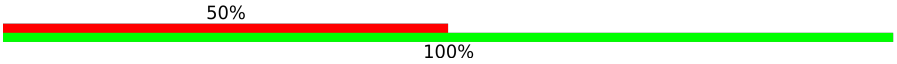


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

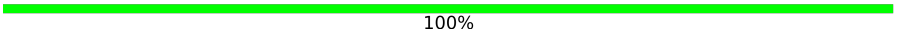
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



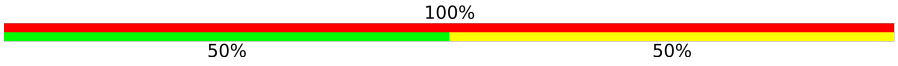
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:



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

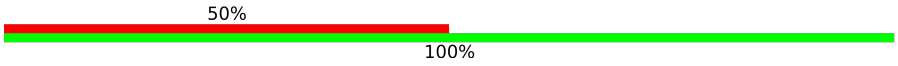
Chain J:

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

Chain K:

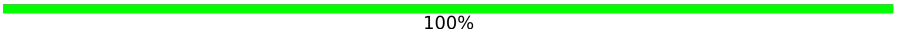
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• 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 N:

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

Chain Q:

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

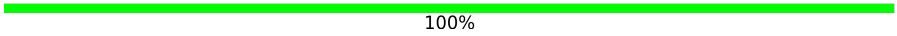
Chain R:

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

Chain S:

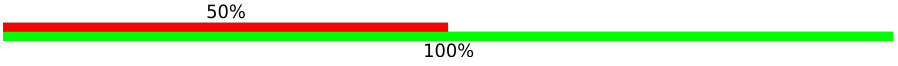
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:



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

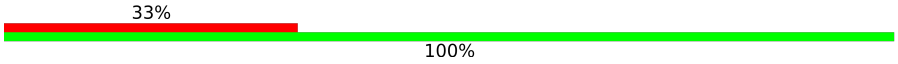
Chain X:

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

Chain H:

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

Chain I:

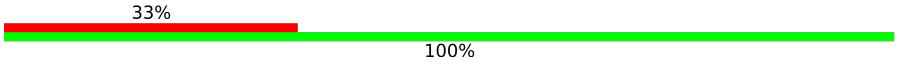


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:

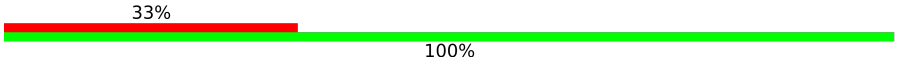


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

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

Chain W:




NAG1
NAG2
NAG3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	102471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	5.366	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0454	Depositor
Map size (Å)	330.47998, 330.47998, 330.47998	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/7823	0.63	0/10639
1	B	0.35	0/7823	0.63	0/10639
1	C	0.35	0/7823	0.63	0/10639
All	All	0.35	0/23469	0.63	0/31917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7658	0	7444	89	0
1	B	7658	0	7445	92	0
1	C	7658	0	7444	91	0
2	D	28	0	25	3	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	2	0
2	L	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	3	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	X	28	0	25	1	0
3	H	42	0	37	0	0
3	I	42	0	37	0	0
3	O	42	0	37	1	0
3	P	42	0	37	0	0
3	V	42	0	37	0	0
3	W	42	0	37	0	0
4	A	182	0	169	0	0
4	B	182	0	169	0	0
4	C	182	0	169	0	0
All	All	24192	0	23437	250	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 5.

All (250) 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:C:28:TYR:HD2	1:C:29:TYR:N	1.27	1.33
1:A:28:TYR:HD2	1:A:29:TYR:N	1.29	1.30
1:B:28:TYR:HD2	1:B:29:TYR:N	1.28	1.29
1:A:763:ILE:HG21	1:A:769:ILE:HD12	1.20	1.15
1:B:763:ILE:HG21	1:B:769:ILE:CD1	1.79	1.13
1:C:763:ILE:HG21	1:C:769:ILE:CD1	1.78	1.12
1:B:763:ILE:CG2	1:B:769:ILE:HD12	1.90	1.02
1:C:763:ILE:CG2	1:C:769:ILE:HD12	1.90	1.00
1:C:763:ILE:HG21	1:C:769:ILE:HD12	0.98	0.97
1:A:763:ILE:HG21	1:A:769:ILE:CD1	1.94	0.96
1:B:763:ILE:HG21	1:B:769:ILE:HD12	0.98	0.95
1:A:28:TYR:CD2	1:A:29:TYR:N	2.15	0.89
1:B:21:TYR:HB2	1:B:28:TYR:HB2	1.58	0.85
1:B:763:ILE:CG2	1:B:769:ILE:CD1	2.53	0.85
1:C:21:TYR:HB2	1:C:28:TYR:HB2	1.58	0.85
1:C:28:TYR:CD2	1:C:29:TYR:N	2.15	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TYR:HB2	1:A:28:TYR:HB2	1.58	0.84
1:B:28:TYR:CD2	1:B:29:TYR:N	2.15	0.83
1:C:763:ILE:CG2	1:C:769:ILE:CD1	2.53	0.81
1:A:769:ILE:HG22	2:R:1:NAG:C8	2.13	0.79
1:A:763:ILE:CG2	1:A:769:ILE:HD12	2.09	0.78
1:C:163:ASN:O	1:C:164:LEU:HB2	1.83	0.76
1:B:769:ILE:HG22	2:D:1:NAG:C8	2.20	0.71
1:A:763:ILE:CG2	1:A:769:ILE:CD1	2.69	0.68
1:A:21:TYR:CD2	1:A:28:TYR:HB3	2.30	0.67
1:C:769:ILE:HG22	2:K:1:NAG:C8	2.25	0.66
1:C:21:TYR:CD2	1:C:28:TYR:HB3	2.31	0.66
1:B:21:TYR:CD2	1:B:28:TYR:HB3	2.30	0.65
1:C:763:ILE:HB	1:C:769:ILE:HD11	1.79	0.65
1:A:769:ILE:HG22	2:R:1:NAG:H83	1.79	0.64
1:B:763:ILE:HB	1:B:769:ILE:HD11	1.80	0.64
1:B:912:ARG:HH22	1:C:900:GLN:HE21	1.44	0.64
1:A:461:ALA:HB3	1:B:35:ARG:HH22	1.64	0.63
1:A:35:ARG:HH22	1:C:461:ALA:HB3	1.64	0.62
1:B:349:ILE:HG22	1:B:399:VAL:HG12	1.83	0.61
1:A:900:GLN:HE21	1:C:912:ARG:HH22	1.49	0.60
1:C:349:ILE:HG22	1:C:399:VAL:HG12	1.83	0.60
1:A:912:ARG:HH22	1:B:900:GLN:HE21	1.49	0.60
1:B:461:ALA:HB3	1:C:35:ARG:HH22	1.66	0.60
1:C:70:ILE:O	1:C:101:HIS:NE2	2.35	0.59
1:A:349:ILE:HG22	1:A:399:VAL:HG12	1.83	0.59
1:B:769:ILE:HG22	2:D:1:NAG:H83	1.84	0.59
1:A:70:ILE:O	1:A:101:HIS:NE2	2.35	0.59
1:B:70:ILE:O	1:B:101:HIS:NE2	2.35	0.59
1:C:283:ASN:HD21	1:C:353:PRO:HD3	1.68	0.59
1:C:649:GLU:OE2	1:C:895:ARG:NH2	2.36	0.59
1:B:649:GLU:OE2	1:B:895:ARG:NH2	2.36	0.58
1:C:601:THR:HG22	1:C:932:GLY:HA2	1.85	0.58
1:B:920:ARG:NH1	1:B:988:ASP:OD2	2.36	0.58
1:A:283:ASN:HD21	1:A:353:PRO:HD3	1.68	0.58
1:B:283:ASN:HD21	1:B:353:PRO:HD3	1.68	0.58
1:B:601:THR:HG22	1:B:932:GLY:HA2	1.85	0.58
1:C:769:ILE:HG22	2:K:1:NAG:H83	1.84	0.58
1:A:920:ARG:NH1	1:A:988:ASP:OD2	2.36	0.58
1:A:649:GLU:OE2	1:A:895:ARG:NH2	2.36	0.57
1:A:601:THR:HG22	1:A:932:GLY:HA2	1.85	0.57
1:C:920:ARG:NH1	1:C:988:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PHE:HB3	1:C:215:ALA:HA	1.89	0.54
1:B:763:ILE:CB	1:B:769:ILE:HD11	2.38	0.54
1:C:763:ILE:CB	1:C:769:ILE:HD11	2.37	0.53
1:B:210:PHE:HB3	1:B:215:ALA:HA	1.89	0.53
1:A:229:LEU:HB2	1:A:498:PHE:HZ	1.74	0.53
1:B:769:ILE:N	1:B:770:PRO:HD3	2.24	0.53
1:C:769:ILE:N	1:C:770:PRO:HD3	2.24	0.53
1:A:33:ALA:HB1	1:C:463:LEU:HD23	1.91	0.53
1:A:210:PHE:HB3	1:A:215:ALA:HA	1.90	0.52
1:B:463:LEU:HD23	1:C:33:ALA:HB1	1.91	0.52
1:B:50:VAL:HG23	1:B:200:VAL:HG23	1.91	0.52
1:B:229:LEU:HB2	1:B:498:PHE:HZ	1.74	0.52
1:C:229:LEU:HB2	1:C:498:PHE:HZ	1.74	0.52
1:A:108:THR:HG21	2:J:1:NAG:H62	1.91	0.52
1:B:917:GLY:O	1:B:939:SER:OG	2.28	0.52
1:C:211:VAL:H	1:C:216:GLN:HE22	1.58	0.52
1:A:769:ILE:N	1:A:770:PRO:HD3	2.24	0.52
1:A:917:GLY:O	1:A:939:SER:OG	2.28	0.52
1:C:763:ILE:CG2	1:C:769:ILE:HD11	2.39	0.52
1:B:21:TYR:CD2	1:B:28:TYR:CB	2.93	0.52
1:C:50:VAL:HG23	1:C:200:VAL:HG23	1.91	0.52
1:A:21:TYR:CD2	1:A:28:TYR:CB	2.93	0.52
1:A:50:VAL:HG23	1:A:200:VAL:HG23	1.91	0.52
1:A:463:LEU:HD23	1:B:33:ALA:HB1	1.92	0.51
1:C:917:GLY:O	1:C:939:SER:OG	2.28	0.51
1:A:211:VAL:H	1:A:216:GLN:HE22	1.58	0.51
1:C:108:THR:HG21	2:X:1:NAG:H62	1.91	0.51
1:B:211:VAL:H	1:B:216:GLN:HE22	1.58	0.51
1:B:972:ARG:NH2	1:B:999:ASP:OD1	2.44	0.51
1:A:460:ASP:OD1	1:A:460:ASP:N	2.45	0.50
1:A:972:ARG:NH2	1:A:999:ASP:OD1	2.44	0.50
1:C:21:TYR:CD2	1:C:28:TYR:CB	2.94	0.50
1:A:156:LYS:HB2	1:A:170:ASN:HD22	1.77	0.50
1:B:460:ASP:OD1	1:B:460:ASP:N	2.45	0.50
1:B:156:LYS:HB2	1:B:170:ASN:HD22	1.77	0.50
1:C:156:LYS:HB2	1:C:170:ASN:HD22	1.77	0.50
1:C:602:ARG:HH22	1:C:747:GLN:HB2	1.77	0.50
1:C:972:ARG:NH2	1:C:999:ASP:OD1	2.44	0.50
1:B:763:ILE:CG2	1:B:769:ILE:HD11	2.38	0.49
1:C:508:ILE:HB	1:C:526:ILE:HD11	1.95	0.49
1:B:713:LYS:NZ	1:B:724:LYS:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LYS:NZ	1:C:724:LYS:O	2.46	0.49
1:A:508:ILE:HB	1:A:526:ILE:HD11	1.95	0.48
1:A:602:ARG:HH22	1:A:747:GLN:HB2	1.77	0.48
1:B:508:ILE:HB	1:B:526:ILE:HD11	1.95	0.48
1:A:713:LYS:NZ	1:A:724:LYS:O	2.46	0.48
1:C:720:LEU:HD22	1:C:724:LYS:HD3	1.95	0.48
1:C:276:ASN:OD1	1:C:351:TYR:OH	2.26	0.48
1:C:916:CYS:HB2	1:C:937:HIS:CE1	2.48	0.48
1:B:107:THR:HG22	1:B:137:LYS:HG2	1.96	0.48
1:B:830:ALA:HA	1:B:833:THR:HG22	1.95	0.48
1:A:769:ILE:CG2	2:R:1:NAG:H83	2.41	0.48
1:C:157:SER:H	1:C:170:ASN:HB3	1.79	0.48
1:A:916:CYS:HB2	1:A:937:HIS:CE1	2.48	0.48
1:B:551:TYR:HE1	1:C:738:LEU:HD22	1.79	0.48
1:C:107:THR:HG22	1:C:137:LYS:HG2	1.96	0.48
1:C:602:ARG:HH12	1:C:747:GLN:HG3	1.79	0.48
1:B:602:ARG:HH22	1:B:747:GLN:HB2	1.77	0.48
1:A:157:SER:H	1:A:170:ASN:HB3	1.79	0.47
1:B:602:ARG:HH12	1:B:747:GLN:HG3	1.79	0.47
1:B:916:CYS:HB2	1:B:937:HIS:CE1	2.48	0.47
1:A:602:ARG:HH12	1:A:747:GLN:HG3	1.79	0.47
1:A:720:LEU:HD22	1:A:724:LYS:HD3	1.95	0.47
1:A:968:PRO:HD3	1:A:975:PHE:HE1	1.80	0.47
1:B:667:LEU:HD13	1:B:684:PRO:HG3	1.96	0.47
1:B:720:LEU:HD22	1:B:724:LYS:HD3	1.95	0.47
1:C:830:ALA:HA	1:C:833:THR:HG22	1.96	0.47
1:A:107:THR:HG22	1:A:137:LYS:HG2	1.96	0.47
1:A:667:LEU:HD13	1:A:684:PRO:HG3	1.96	0.47
1:A:830:ALA:HA	1:A:833:THR:HG22	1.96	0.47
1:B:157:SER:H	1:B:170:ASN:HB3	1.79	0.47
1:B:850:ILE:HD11	1:B:866:VAL:HG13	1.97	0.47
1:C:667:LEU:HD13	1:C:684:PRO:HG3	1.96	0.47
1:C:968:PRO:HD3	1:C:975:PHE:HE1	1.80	0.47
1:A:778:ARG:HH11	1:A:909:GLN:HB2	1.80	0.47
1:C:460:ASP:N	1:C:460:ASP:OD1	2.45	0.47
1:A:850:ILE:HD11	1:A:866:VAL:HG13	1.97	0.46
1:A:957:LYS:HB3	1:A:963:GLN:HE22	1.81	0.46
1:B:769:ILE:CG2	2:D:1:NAG:H83	2.45	0.46
1:A:738:LEU:HD22	1:C:551:TYR:HE1	1.80	0.46
1:B:408:ARG:NH1	1:C:143:TYR:OH	2.49	0.46
1:B:778:ARG:HH11	1:B:909:GLN:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ILE:HB	1:A:769:ILE:HD11	1.98	0.46
1:B:968:PRO:HD3	1:B:975:PHE:HE1	1.80	0.46
1:C:778:ARG:HH11	1:C:909:GLN:HB2	1.80	0.46
1:C:850:ILE:HD11	1:C:866:VAL:HG13	1.97	0.46
1:B:957:LYS:HB3	1:B:963:GLN:HE22	1.80	0.45
1:C:763:ILE:CB	1:C:769:ILE:CD1	2.95	0.45
1:A:331:PHE:HE1	1:A:403:LYS:HD3	1.82	0.45
1:A:522:ASN:ND2	1:B:711:ALA:O	2.50	0.45
1:B:331:PHE:HE1	1:B:403:LYS:HD3	1.82	0.45
1:B:601:THR:HG23	1:B:602:ARG:HG3	1.98	0.45
1:A:163:ASN:O	1:A:164:LEU:CB	2.63	0.45
1:A:763:ILE:CG2	1:A:769:ILE:HD11	2.46	0.45
1:C:957:LYS:HB3	1:C:963:GLN:HE22	1.80	0.45
1:A:247:ASN:N	1:A:247:ASN:OD1	2.50	0.45
1:A:601:THR:HG23	1:A:602:ARG:HG3	1.98	0.45
1:B:1013:VAL:HG12	1:B:1015:LYS:H	1.82	0.45
1:C:603:MET:HE2	1:C:646:GLU:HG3	1.99	0.45
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.85	0.45
1:C:528:ILE:H	1:C:528:ILE:HG13	1.62	0.44
1:C:601:THR:HG23	1:C:602:ARG:HG3	1.98	0.44
1:B:163:ASN:O	1:B:164:LEU:CB	2.62	0.44
1:B:247:ASN:OD1	1:B:247:ASN:N	2.50	0.44
1:C:331:PHE:HE1	1:C:403:LYS:HD3	1.82	0.44
1:B:276:ASN:OD1	1:B:351:TYR:OH	2.26	0.44
1:A:775:LEU:HD23	1:A:923:LEU:HD13	2.00	0.44
1:A:1013:VAL:HG12	1:A:1015:LYS:H	1.82	0.44
1:C:247:ASN:OD1	1:C:247:ASN:N	2.50	0.44
1:A:856:GLN:HG2	1:C:340:LEU:HD11	1.98	0.44
1:B:929:ALA:HB2	1:B:934:VAL:HG23	2.00	0.44
1:C:929:ALA:HB2	1:C:934:VAL:HG23	2.00	0.44
1:B:763:ILE:CB	1:B:769:ILE:CD1	2.96	0.43
1:B:995:ILE:O	1:B:1019:THR:OG1	2.36	0.43
1:C:133:VAL:HG11	1:C:174:VAL:HB	2.00	0.43
1:C:1013:VAL:HG12	1:C:1015:LYS:H	1.82	0.43
1:A:330:ASN:ND2	1:B:856:GLN:OE1	2.50	0.43
1:B:46:ALA:HA	1:B:203:GLU:HA	2.00	0.43
1:C:109:VAL:HG11	1:C:167:VAL:HG11	2.01	0.43
1:A:133:VAL:HG11	1:A:174:VAL:HB	2.01	0.43
1:A:603:MET:HE2	1:A:646:GLU:HG3	2.00	0.43
1:B:603:MET:HE2	1:B:646:GLU:HG3	2.01	0.43
1:A:711:ALA:O	1:C:522:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG11	1:B:174:VAL:HB	2.00	0.43
1:C:506:VAL:HG13	1:C:560:GLY:HA2	2.00	0.43
1:A:929:ALA:HB2	1:A:934:VAL:HG23	2.00	0.43
1:B:570:LEU:HD12	1:B:941:THR:HG21	2.01	0.43
1:B:775:LEU:HD23	1:B:923:LEU:HD13	2.00	0.43
1:C:995:ILE:O	1:C:1019:THR:OG1	2.36	0.43
1:A:517:SER:O	1:A:537:ARG:NH1	2.52	0.43
1:B:739:PRO:HA	1:B:740:PRO:HD3	1.92	0.43
1:A:109:VAL:HG11	1:A:167:VAL:HG11	2.00	0.43
1:C:517:SER:O	1:C:537:ARG:NH1	2.52	0.43
1:B:517:SER:O	1:B:537:ARG:NH1	2.52	0.43
1:A:46:ALA:HA	1:A:203:GLU:HA	2.00	0.42
1:A:995:ILE:O	1:A:1019:THR:OG1	2.36	0.42
1:A:551:TYR:HE1	1:B:738:LEU:HD22	1.84	0.42
1:B:528:ILE:H	1:B:528:ILE:HG13	1.62	0.42
1:C:775:LEU:HD23	1:C:923:LEU:HD13	2.00	0.42
1:B:522:ASN:ND2	1:C:711:ALA:O	2.52	0.42
1:C:604:ASP:OD1	1:C:604:ASP:N	2.52	0.42
1:B:109:VAL:HG11	1:B:167:VAL:HG11	2.00	0.42
1:B:506:VAL:HG13	1:B:560:GLY:HA2	2.00	0.42
1:A:570:LEU:HD12	1:A:941:THR:HG21	2.01	0.42
1:C:46:ALA:HA	1:C:203:GLU:HA	2.00	0.42
1:C:570:LEU:HD12	1:C:941:THR:HG21	2.01	0.42
1:A:506:VAL:HG13	1:A:560:GLY:HA2	2.00	0.42
1:A:680:LEU:HD21	1:A:925:ILE:HG21	2.01	0.42
1:B:658:LYS:HA	1:B:659:PRO:HD3	1.93	0.42
1:C:449:THR:HB	1:C:485:TYR:H	1.85	0.42
1:C:680:LEU:HD21	1:C:925:ILE:HG21	2.02	0.42
1:A:342:PHE:HD2	1:A:345:LEU:HD22	1.85	0.41
1:A:408:ARG:NH1	1:B:143:TYR:OH	2.53	0.41
1:B:967:VAL:HB	1:B:1001:VAL:HB	2.02	0.41
1:A:449:THR:HB	1:A:485:TYR:H	1.85	0.41
1:B:449:THR:HB	1:B:485:TYR:H	1.85	0.41
1:C:635:ILE:HA	1:C:635:ILE:HD12	1.84	0.41
1:A:163:ASN:O	1:A:164:LEU:HB3	2.21	0.41
1:A:856:GLN:OE1	1:C:330:ASN:ND2	2.53	0.41
1:C:163:ASN:O	1:C:164:LEU:CB	2.60	0.41
1:C:967:VAL:HB	1:C:1001:VAL:HB	2.02	0.41
1:C:342:PHE:HD2	1:C:345:LEU:HD22	1.86	0.41
1:C:822:GLN:NE2	1:C:826:ASN:OD1	2.48	0.41
1:A:100:ALA:HB2	1:A:188:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:OD1	1:A:351:TYR:OH	2.26	0.41
1:A:890:ARG:HH12	1:A:894:GLN:HE21	1.68	0.41
1:B:116:LYS:HD2	1:B:123:THR:HA	2.03	0.41
1:B:975:PHE:HB3	1:B:984:ILE:HG22	2.03	0.41
1:C:975:PHE:HB3	1:C:984:ILE:HG22	2.03	0.41
1:C:677:ILE:H	1:C:677:ILE:HG13	1.69	0.41
1:C:739:PRO:HA	1:C:740:PRO:HD3	1.92	0.41
1:A:632:CYS:HA	1:A:635:ILE:HG22	2.03	0.41
1:A:658:LYS:HA	1:A:659:PRO:HD3	1.92	0.41
1:B:100:ALA:HB2	1:B:188:VAL:HG13	2.03	0.41
1:C:100:ALA:HA	1:C:188:VAL:HA	2.03	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.96	0.41
1:A:975:PHE:HB3	1:A:984:ILE:HG22	2.03	0.41
1:B:163:ASN:O	1:B:164:LEU:HB3	2.20	0.41
1:B:330:ASN:ND2	1:C:856:GLN:OE1	2.53	0.41
1:B:342:PHE:HD2	1:B:345:LEU:HD22	1.86	0.41
1:B:680:LEU:HD21	1:B:925:ILE:HG21	2.02	0.41
1:B:1001:VAL:HG22	1:C:993:ARG:HH12	1.86	0.41
1:A:116:LYS:HD2	1:A:123:THR:HA	2.03	0.40
1:A:261:ASN:HB3	1:A:265:THR:HG21	2.04	0.40
1:B:100:ALA:HA	1:B:188:VAL:HA	2.03	0.40
1:B:632:CYS:HA	1:B:635:ILE:HG22	2.03	0.40
3:O:1:NAG:H61	3:O:2:NAG:N2	2.36	0.40
1:A:635:ILE:HA	1:A:635:ILE:HD12	1.84	0.40
1:B:491:CYS:SG	1:B:492:GLU:N	2.93	0.40
1:C:100:ALA:HB2	1:C:188:VAL:HG13	2.03	0.40
1:C:888:HIS:HA	1:C:891:VAL:HG12	2.04	0.40
1:A:340:LEU:HD11	1:B:856:GLN:HG2	2.03	0.40
1:A:967:VAL:HB	1:A:1001:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	989/1105 (90%)	857 (87%)	130 (13%)	2 (0%)	47 79
1	B	989/1105 (90%)	854 (86%)	133 (13%)	2 (0%)	47 79
1	C	989/1105 (90%)	855 (86%)	132 (13%)	2 (0%)	47 79
All	All	2967/3315 (90%)	2566 (86%)	395 (13%)	6 (0%)	50 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	B	170	ASN
1	C	170	ASN
1	A	659	PRO
1	B	659	PRO
1	C	659	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	849/953 (89%)	845 (100%)	4 (0%)	88 93
1	B	849/953 (89%)	845 (100%)	4 (0%)	88 93
1	C	849/953 (89%)	845 (100%)	4 (0%)	88 93
All	All	2547/2859 (89%)	2535 (100%)	12 (0%)	89 93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	TYR
1	A	162	ASN
1	A	640	ASN
1	A	784	ILE
1	B	28	TYR
1	B	162	ASN
1	B	640	ASN

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Mol	Chain	Res	Type
1	B	784	ILE
1	C	28	TYR
1	C	162	ASN
1	C	640	ASN
1	C	784	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	43	HIS
1	A	162	ASN
1	A	216	GLN
1	A	410	GLN
1	A	888	HIS
1	A	894	GLN
1	A	900	GLN
1	A	963	GLN
1	B	41	HIS
1	B	43	HIS
1	B	162	ASN
1	B	216	GLN
1	B	410	GLN
1	B	888	HIS
1	B	894	GLN
1	B	900	GLN
1	B	963	GLN
1	C	41	HIS
1	C	43	HIS
1	C	162	ASN
1	C	170	ASN
1	C	216	GLN
1	C	410	GLN
1	C	888	HIS
1	C	894	GLN
1	C	900	GLN
1	C	963	GLN

5.3.3 RNA

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)

48 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	D	1	2,1	14,14,15	0.22	0	17,19,21	0.66	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.62	0
2	NAG	E	1	2,1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	F	1	2,1	14,14,15	0.22	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	G	1	2,1	14,14,15	0.31	0	17,19,21	0.69	0
2	NAG	G	2	2	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.45	0	17,19,21	0.90	1 (5%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	0.62	0
3	NAG	H	3	3	14,14,15	0.45	0	17,19,21	0.68	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	I	3	3	14,14,15	0.34	0	17,19,21	0.60	0
2	NAG	J	1	2,1	14,14,15	0.37	0	17,19,21	0.40	0
2	NAG	J	2	2	14,14,15	0.37	0	17,19,21	0.51	0
2	NAG	K	1	2,1	14,14,15	0.27	0	17,19,21	0.66	0
2	NAG	K	2	2	14,14,15	0.34	0	17,19,21	0.62	0
2	NAG	L	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	L	2	2	14,14,15	0.36	0	17,19,21	0.59	0
2	NAG	M	1	2,1	14,14,15	0.23	0	17,19,21	0.57	0
2	NAG	M	2	2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	N	1	2,1	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	N	2	2	14,14,15	0.39	0	17,19,21	0.59	0
3	NAG	O	1	3,1	14,14,15	0.43	0	17,19,21	0.90	1 (5%)
3	NAG	O	2	3	14,14,15	0.41	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	O	3	3	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
3	NAG	P	1	3,1	14,14,15	0.35	0	17,19,21	0.59	0
3	NAG	P	2	3	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	P	3	3	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	Q	1	2,1	14,14,15	0.23	0	17,19,21	0.62	0
2	NAG	Q	2	2	14,14,15	0.35	0	17,19,21	0.51	0
2	NAG	R	1	2,1	14,14,15	0.26	0	17,19,21	0.56	0
2	NAG	R	2	2	14,14,15	0.35	0	17,19,21	0.61	0
2	NAG	S	1	2,1	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	S	2	2	14,14,15	0.33	0	17,19,21	0.60	1 (5%)
2	NAG	T	1	2,1	14,14,15	0.22	0	17,19,21	0.59	0
2	NAG	T	2	2	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	U	1	2,1	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	U	2	2	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	V	1	3,1	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
3	NAG	V	2	3	14,14,15	0.39	0	17,19,21	0.62	0
3	NAG	V	3	3	14,14,15	0.43	0	17,19,21	0.66	1 (5%)
3	NAG	W	1	3,1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	W	2	3	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	W	3	3	14,14,15	0.33	0	17,19,21	0.61	0
2	NAG	X	1	2,1	14,14,15	0.31	0	17,19,21	0.44	0
2	NAG	X	2	2	14,14,15	0.30	0	17,19,21	0.54	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
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	3	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	3	3	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	3	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	3	3	-	3/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	T	2	2	-	3/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	U	2	2	-	4/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	3	3	-	3/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	W	3	3	-	4/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	2.77	115.95	112.19
3	O	1	NAG	C1-O5-C5	2.77	115.95	112.19
3	V	1	NAG	C1-O5-C5	2.69	115.84	112.19
2	G	2	NAG	C1-O5-C5	2.27	115.27	112.19
3	H	3	NAG	C1-O5-C5	2.14	115.09	112.19
3	O	3	NAG	C1-O5-C5	2.10	115.04	112.19
3	V	3	NAG	C1-O5-C5	2.07	114.99	112.19
2	S	2	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	3	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	O	3	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	W	3	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
3	W	3	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	R	1	NAG	C8-C7-N2-C2
2	R	1	NAG	O7-C7-N2-C2
2	R	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	R	2	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	H	3	NAG	C8-C7-N2-C2
3	H	3	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	I	3	NAG	C8-C7-N2-C2
3	I	3	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	O	3	NAG	C8-C7-N2-C2
3	O	3	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	P	3	NAG	C8-C7-N2-C2
3	P	3	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	V	2	NAG	C8-C7-N2-C2
3	V	2	NAG	O7-C7-N2-C2
3	V	3	NAG	C8-C7-N2-C2
3	V	3	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	W	3	NAG	C8-C7-N2-C2
3	W	3	NAG	O7-C7-N2-C2
2	Q	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	I	3	NAG	O5-C5-C6-O6
3	H	3	NAG	C4-C5-C6-O6
3	I	3	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	P	3	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	H	3	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	V	3	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

There are no ring outliers.

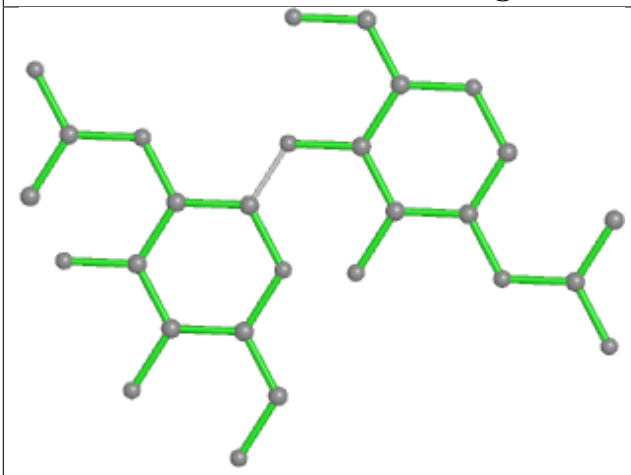
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1	NAG	1	0
2	R	1	NAG	3	0
2	J	1	NAG	1	0
2	K	1	NAG	2	0
3	O	1	NAG	1	0
3	O	2	NAG	1	0
2	D	1	NAG	3	0

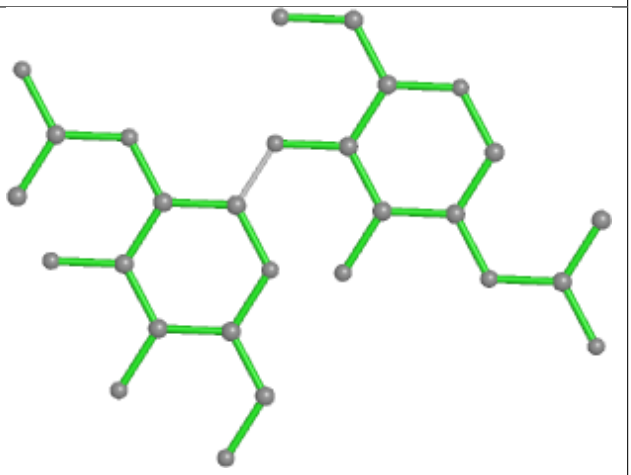
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

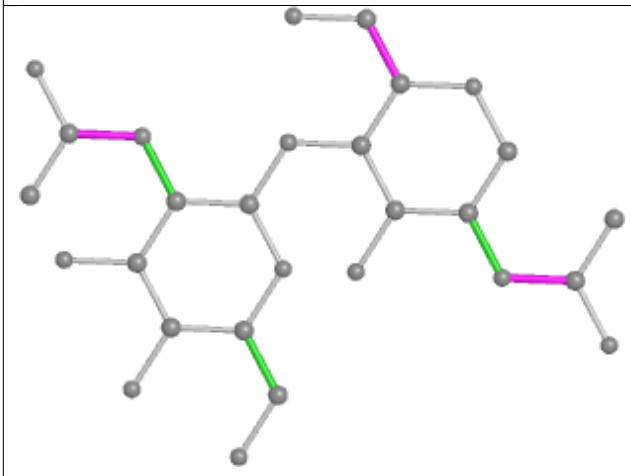
Oligosaccharide Chain D



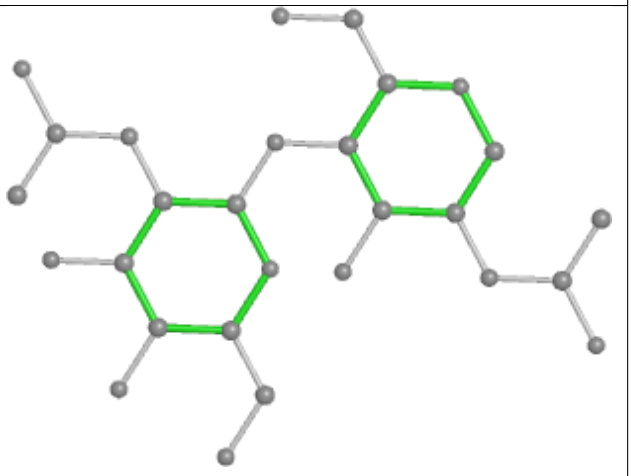
Bond lengths



Bond angles

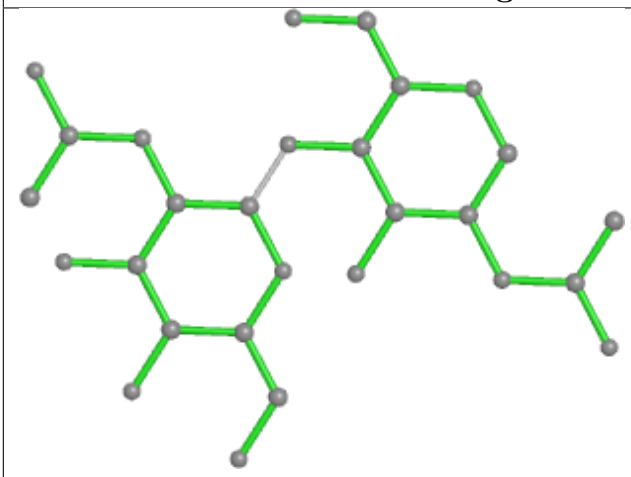


Torsions

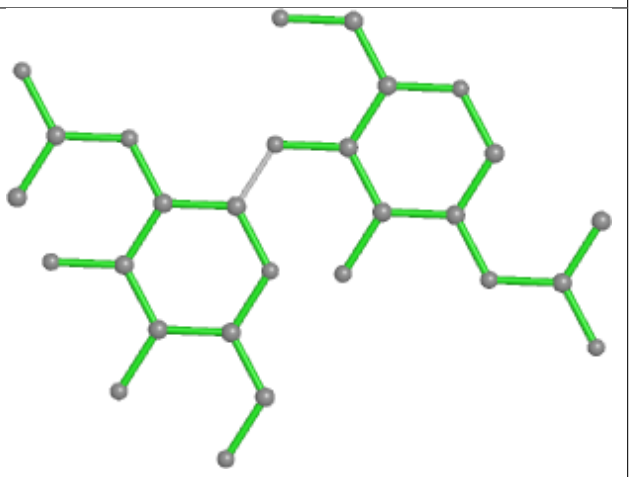


Rings

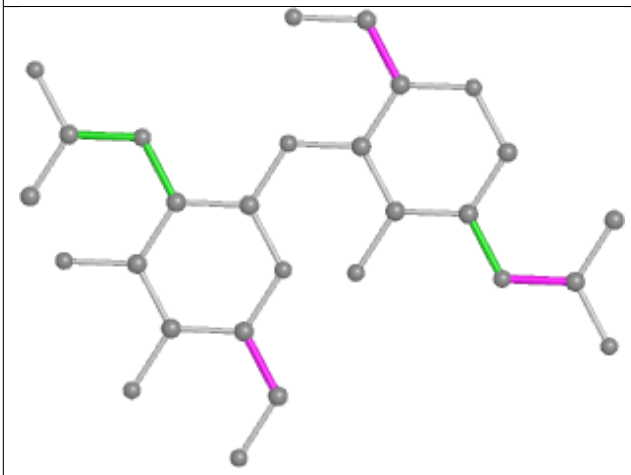
Oligosaccharide Chain E



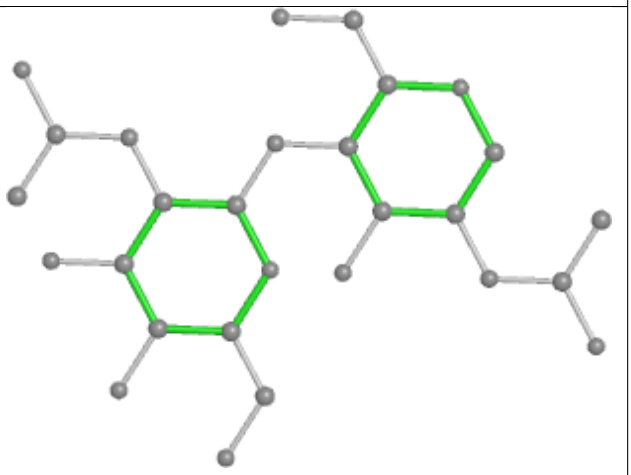
Bond lengths



Bond angles

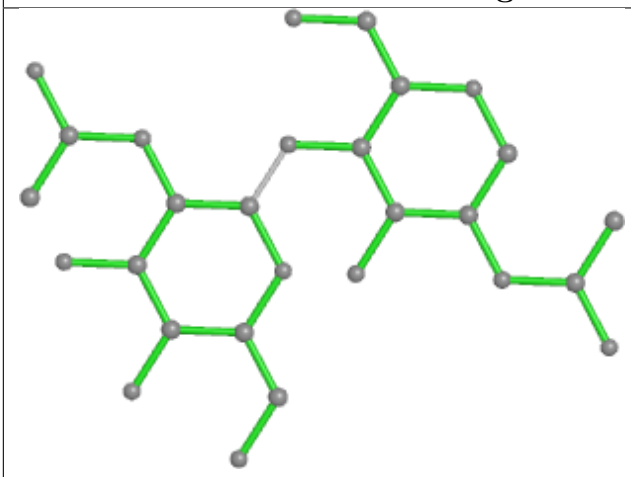


Torsions

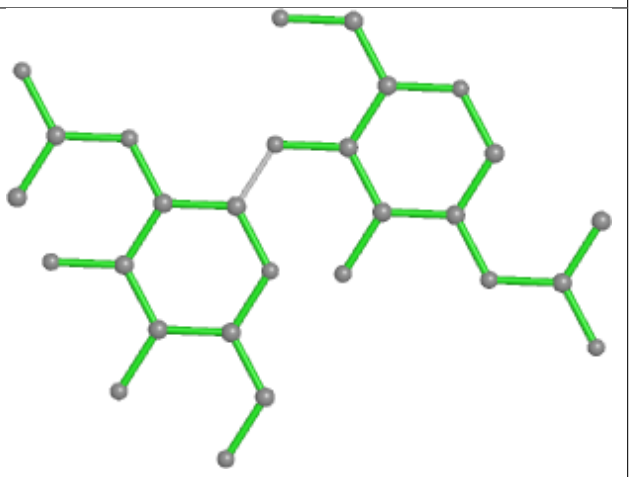


Rings

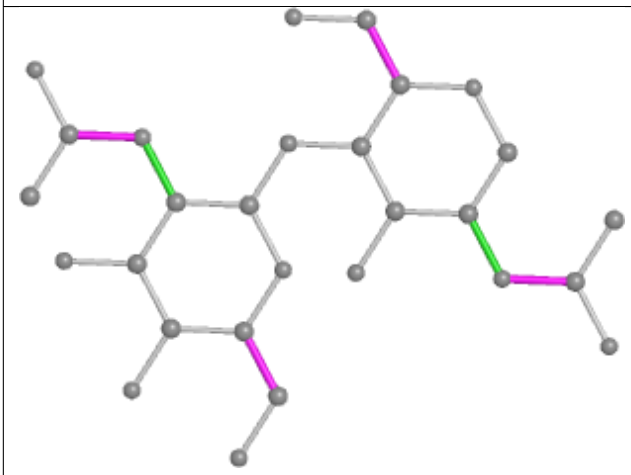
Oligosaccharide Chain F



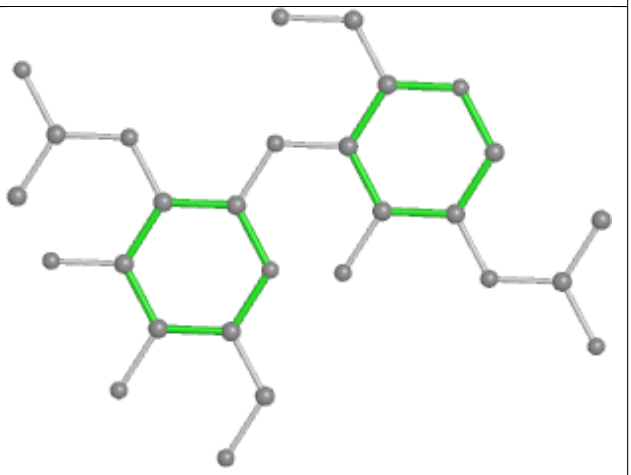
Bond lengths



Bond angles

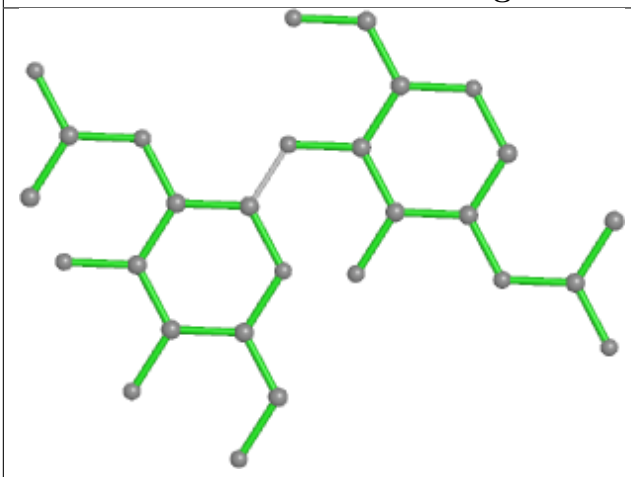


Torsions

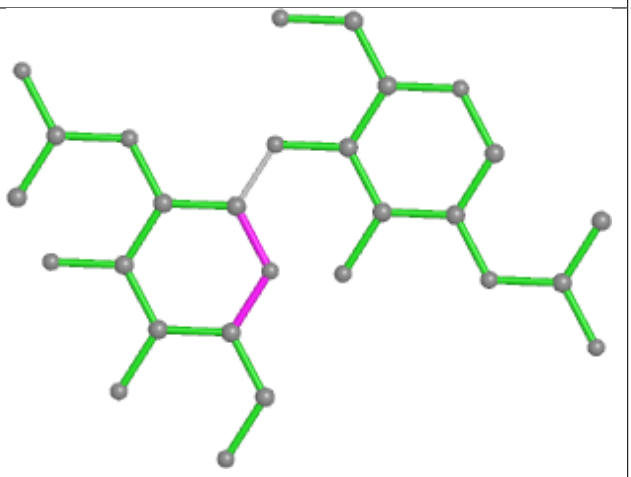


Rings

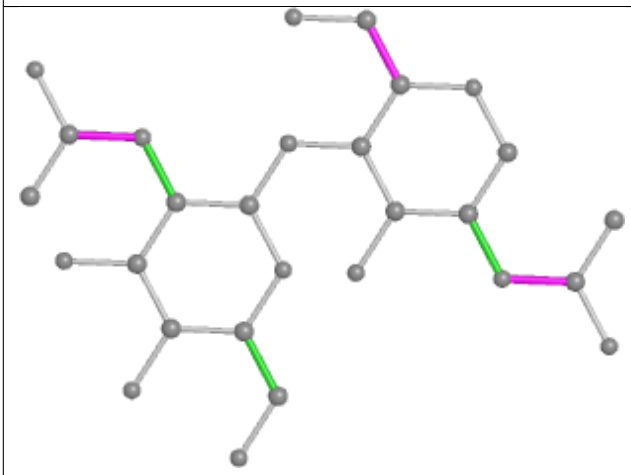
Oligosaccharide Chain G



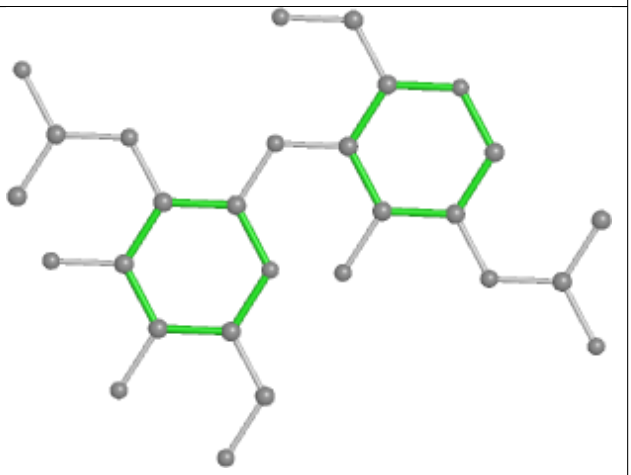
Bond lengths



Bond angles

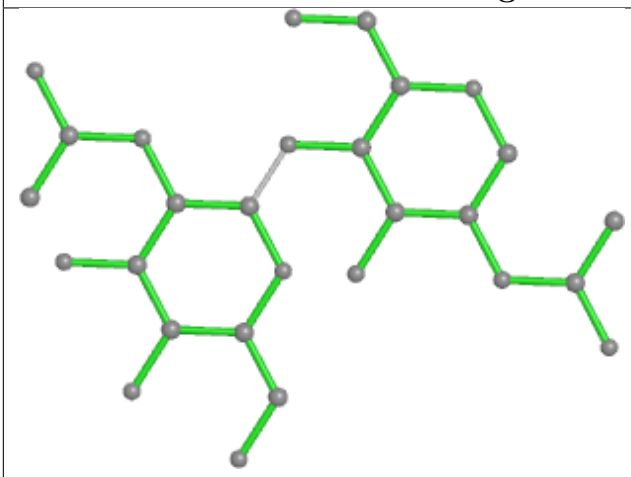


Torsions

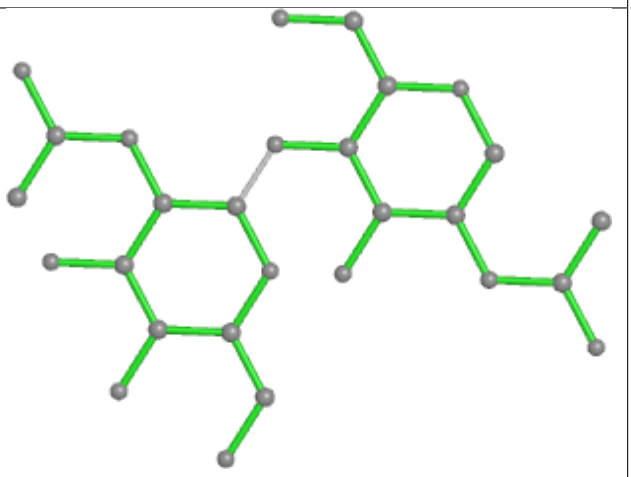


Rings

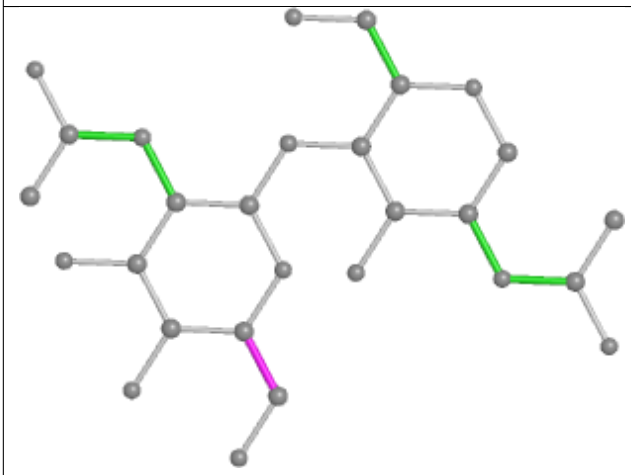
Oligosaccharide Chain J



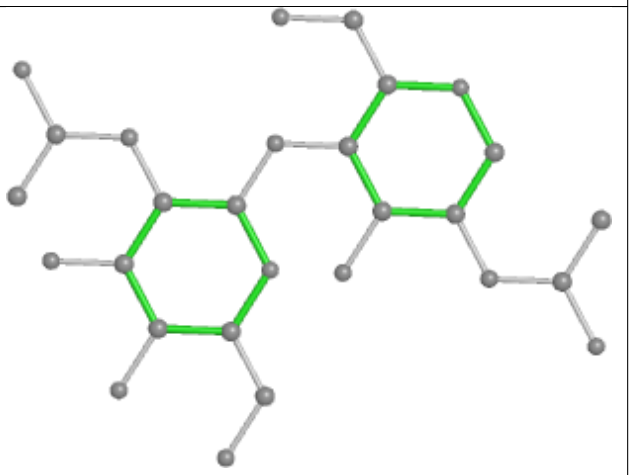
Bond lengths



Bond angles

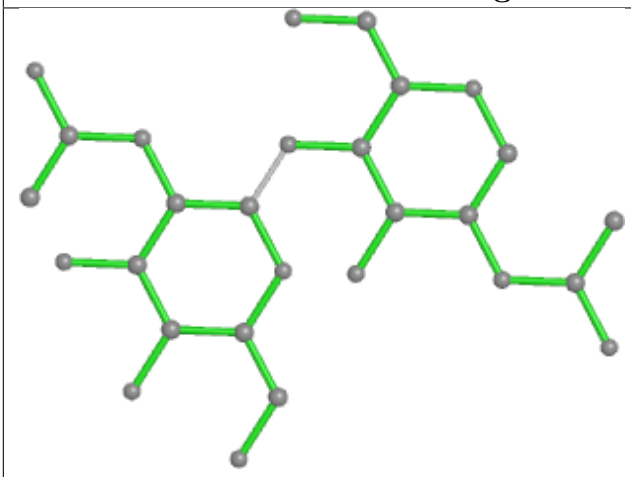


Torsions

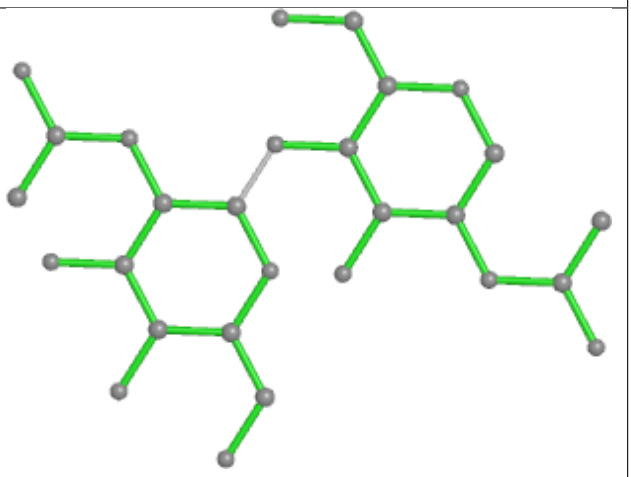


Rings

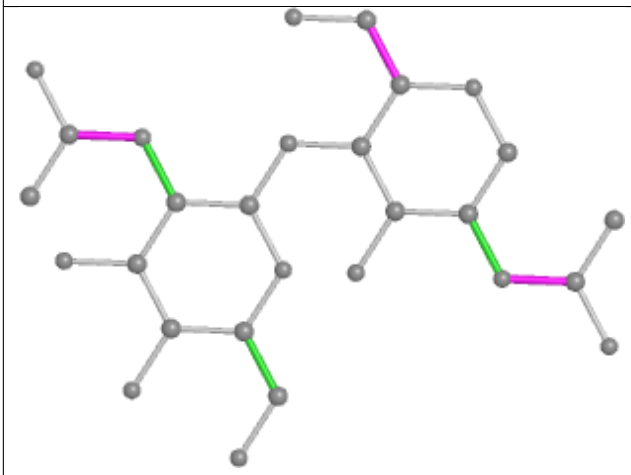
Oligosaccharide Chain K



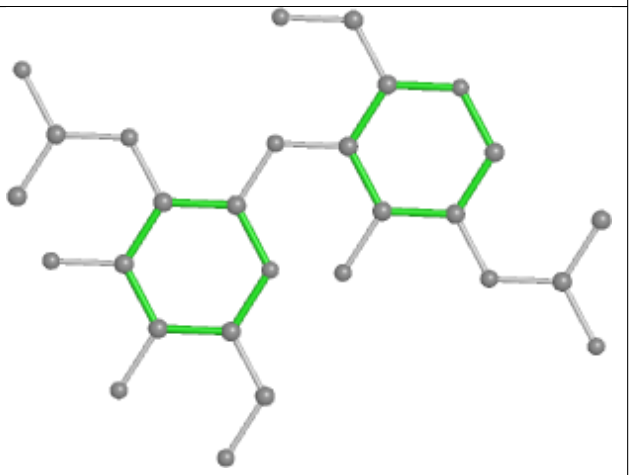
Bond lengths



Bond angles

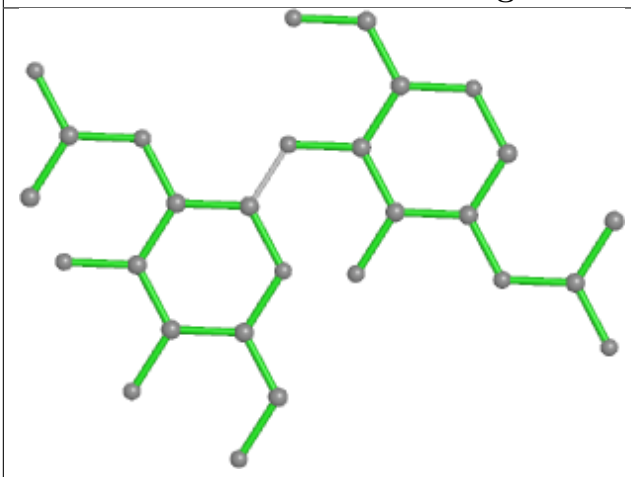


Torsions

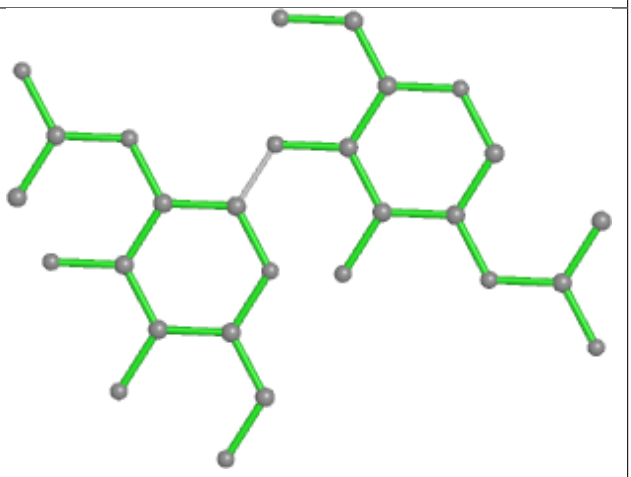


Rings

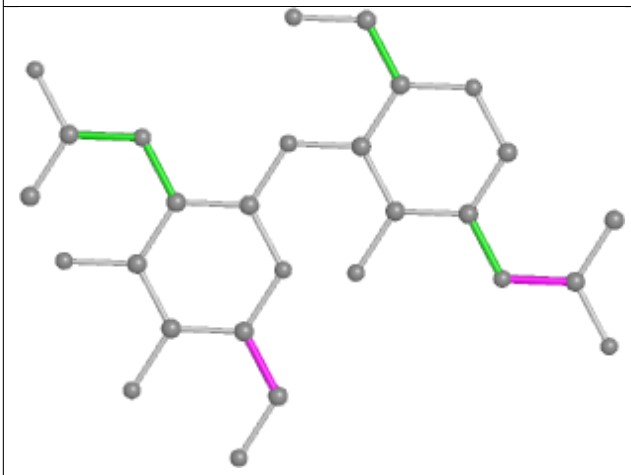
Oligosaccharide Chain L



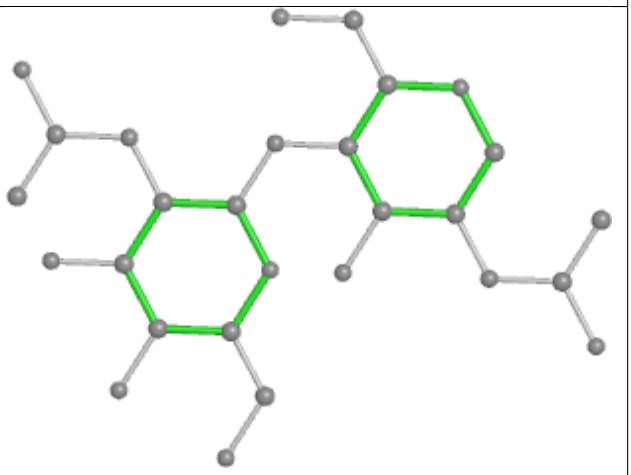
Bond lengths



Bond angles

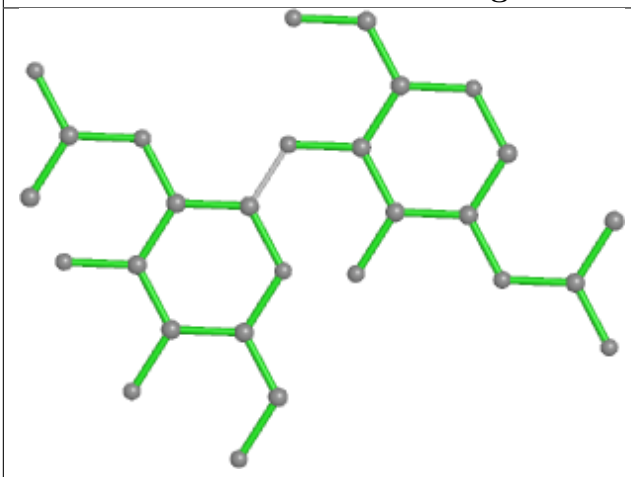


Torsions



Rings

Oligosaccharide Chain M



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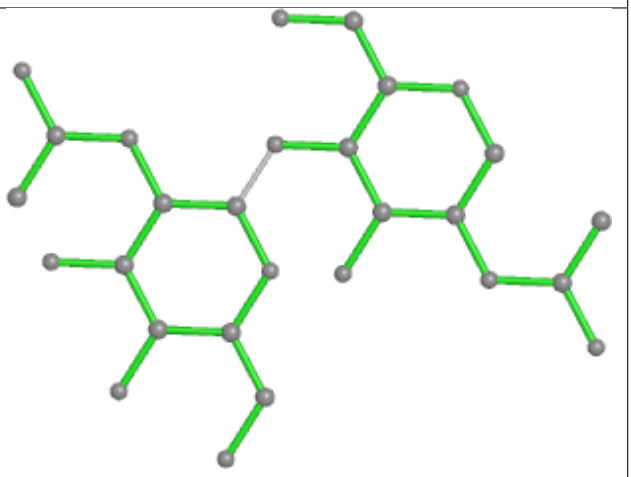
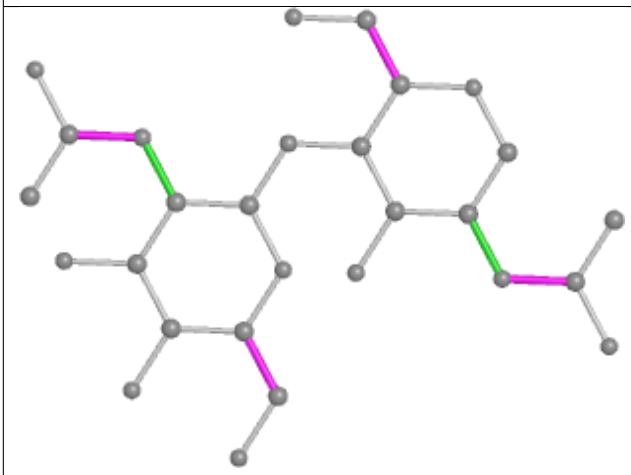


Bond angles



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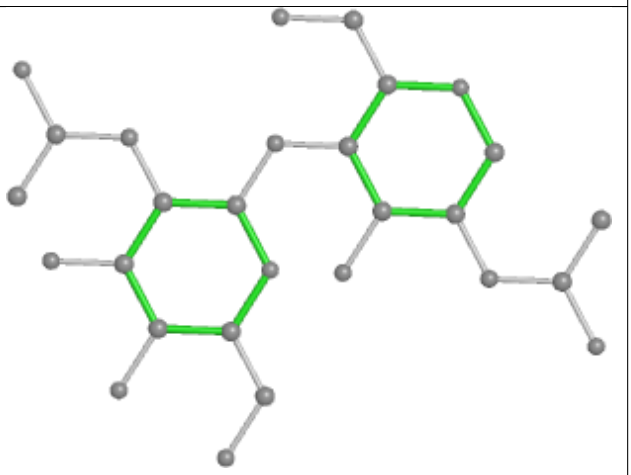
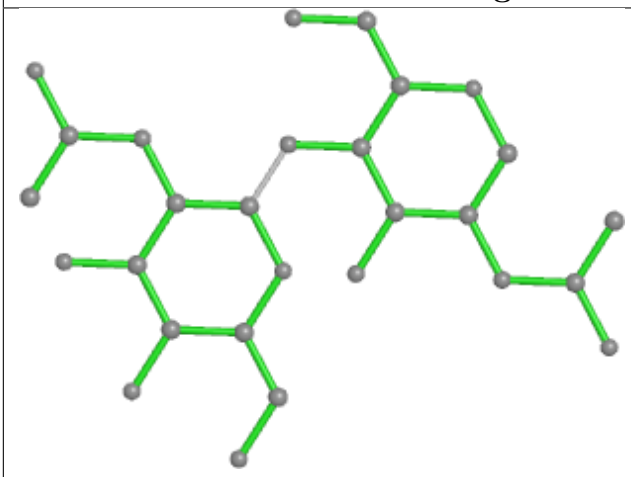


Rings

Oligosaccharide Chain N



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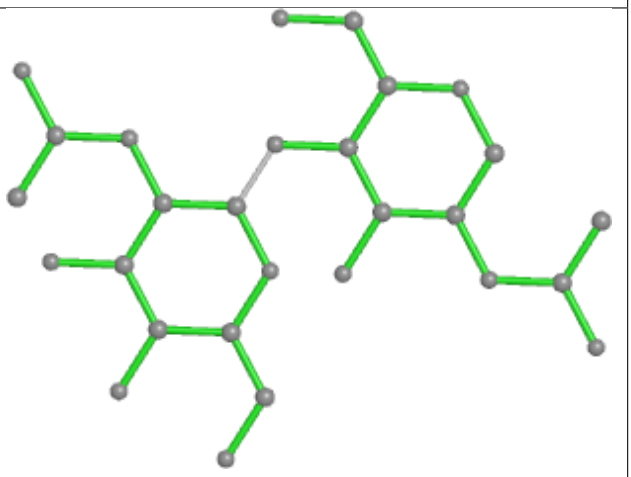
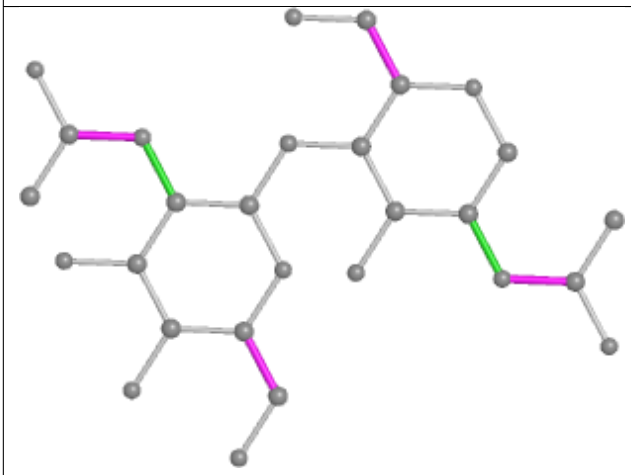
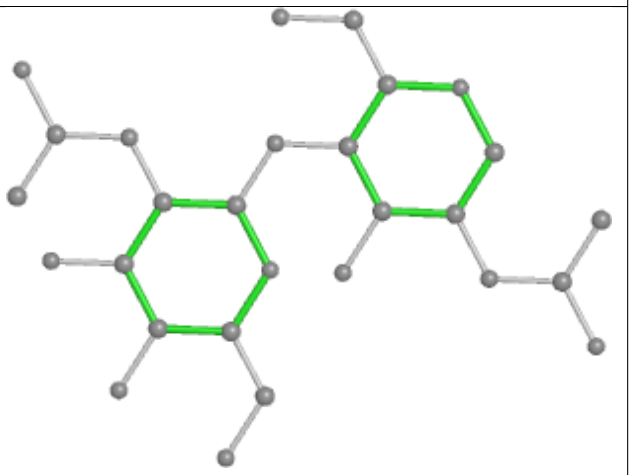


Bond angles

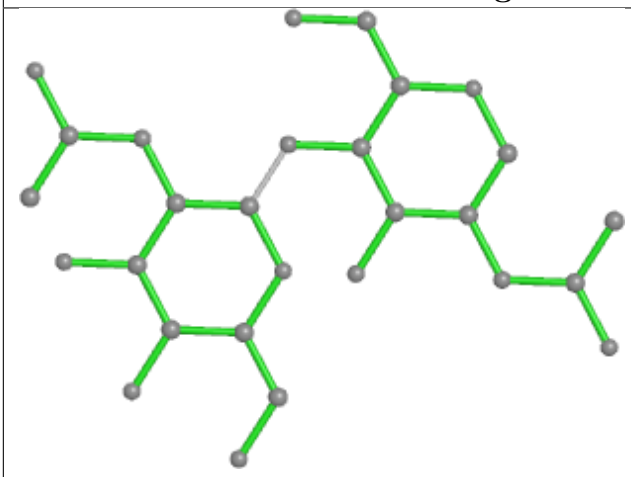


Torsions



Rings

Oligosaccharide Chain Q



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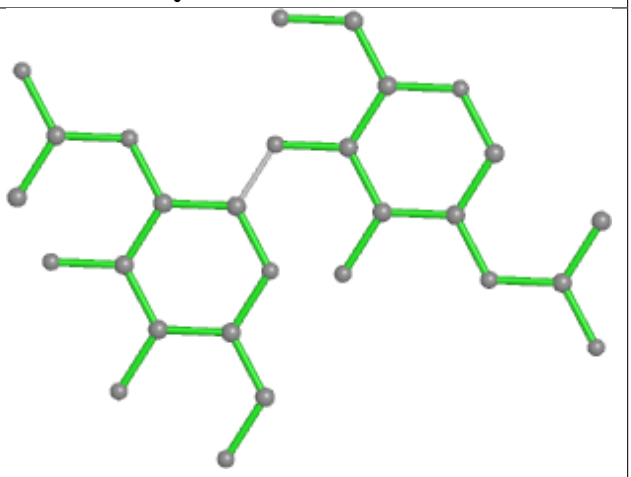
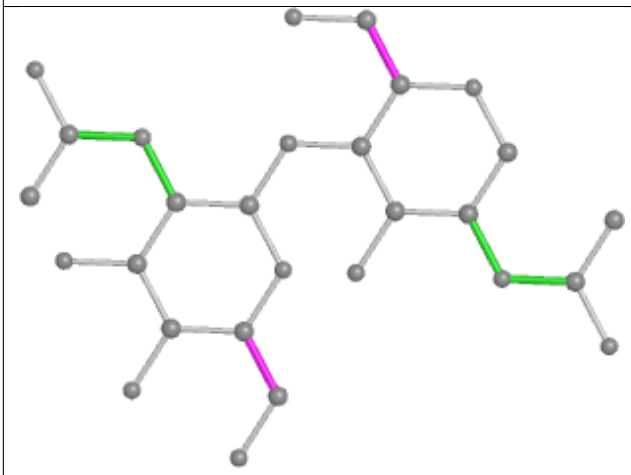


Bond angles



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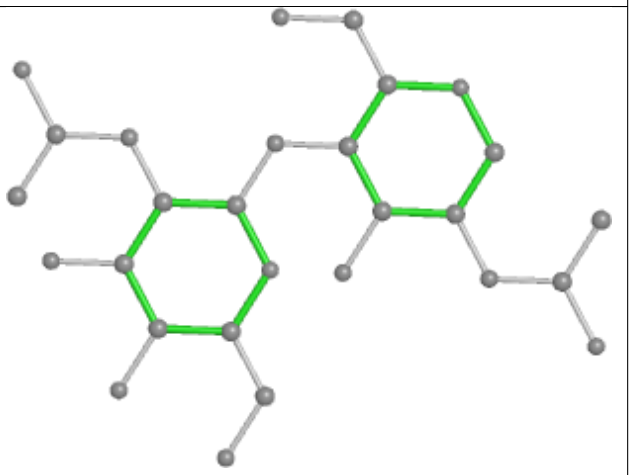
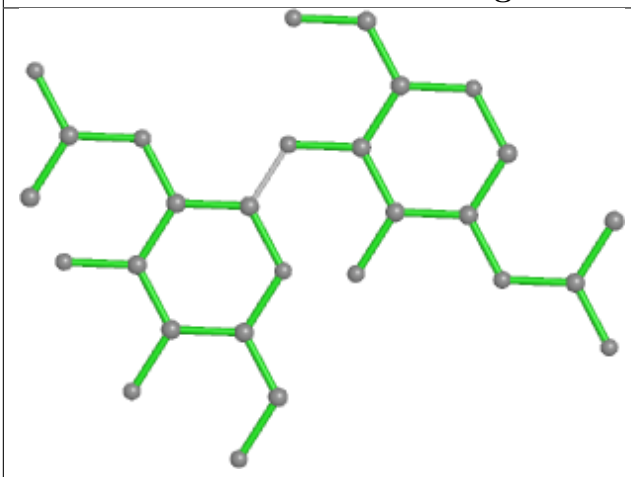


Rings

Oligosaccharide Chain R



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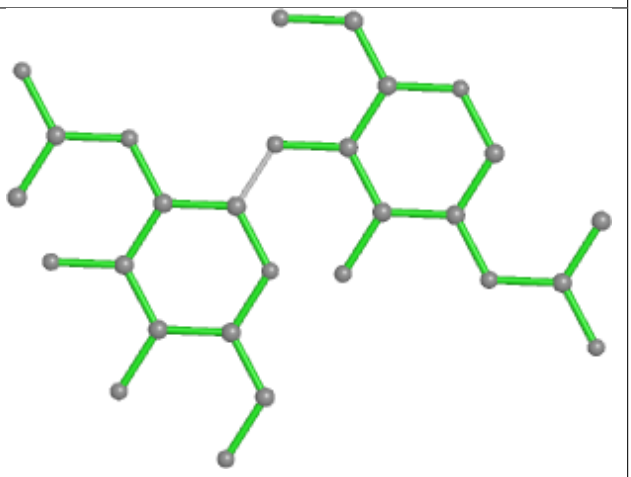
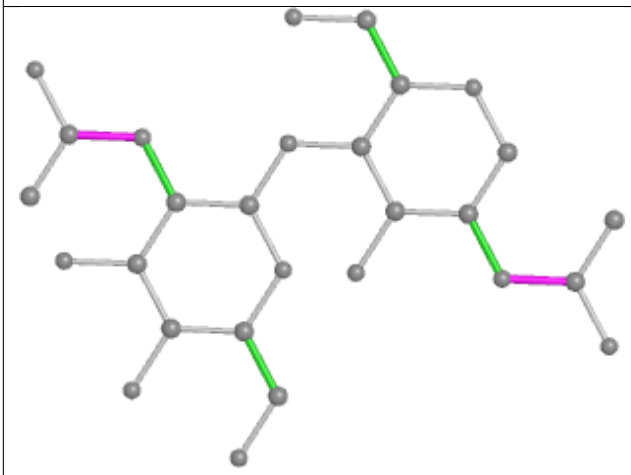


Bond angles



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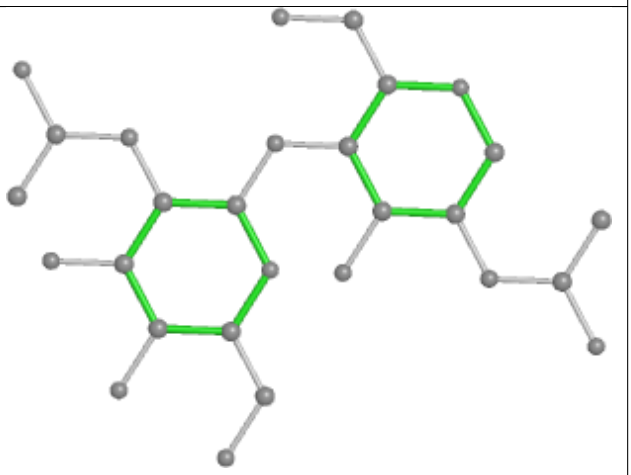
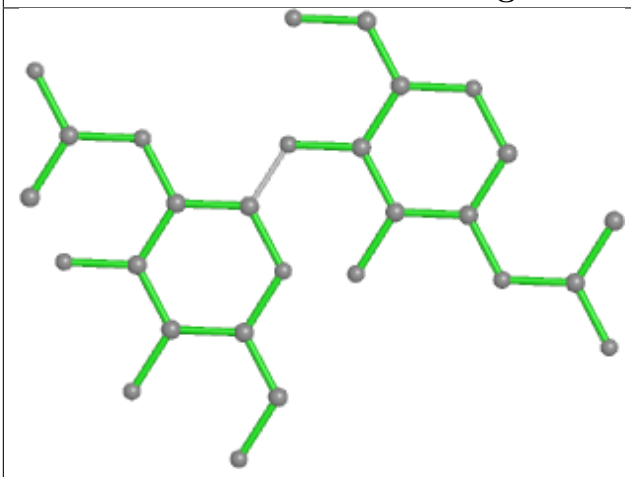


Rings

Oligosaccharide Chain S



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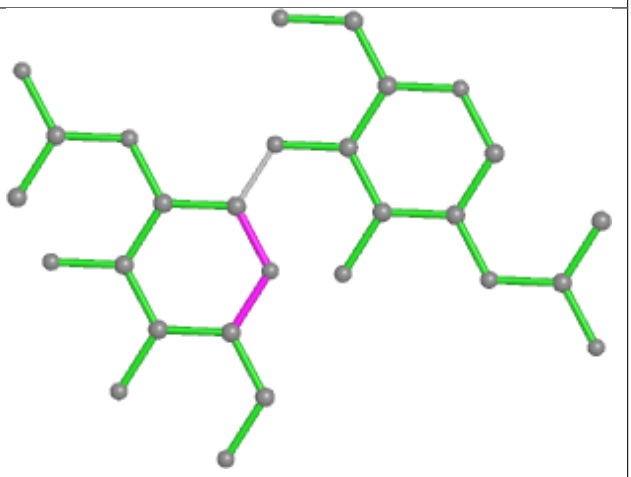
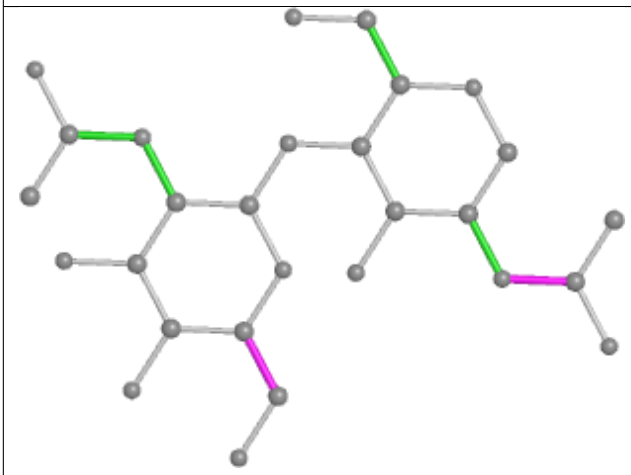


Bond angles



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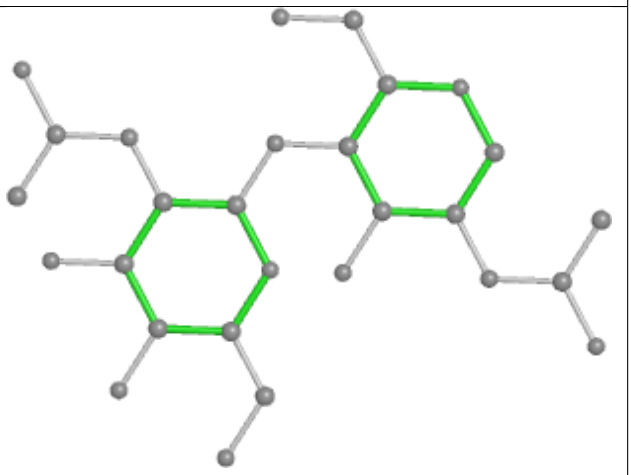
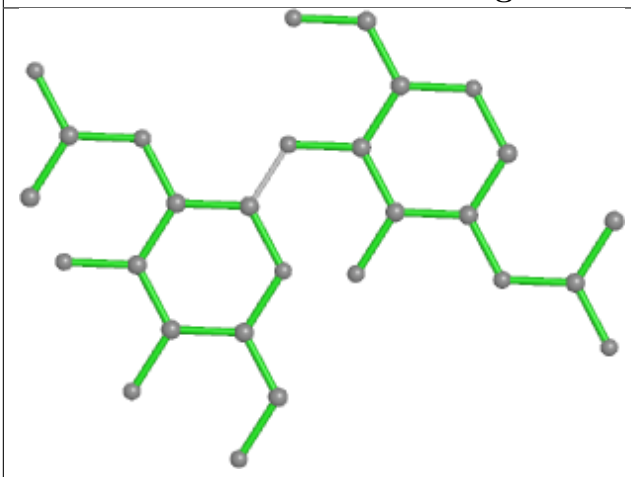


Rings

Oligosaccharide Chain T



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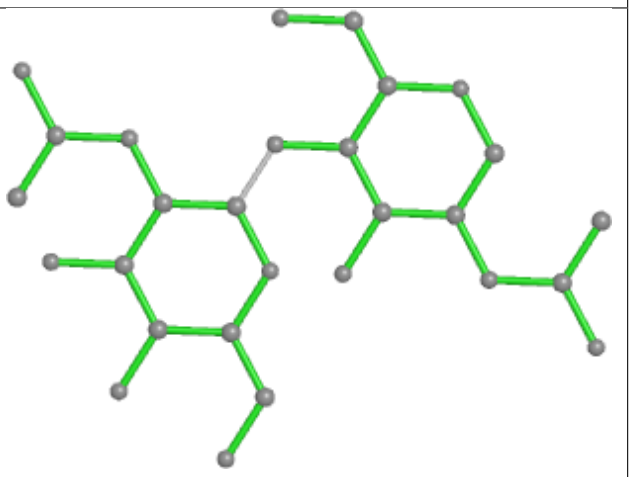
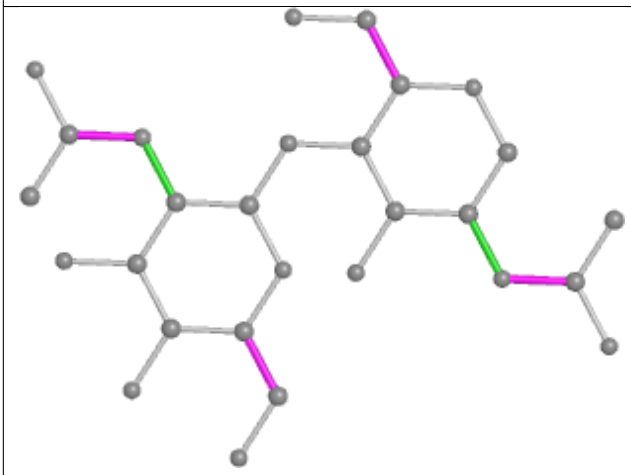


Bond angles



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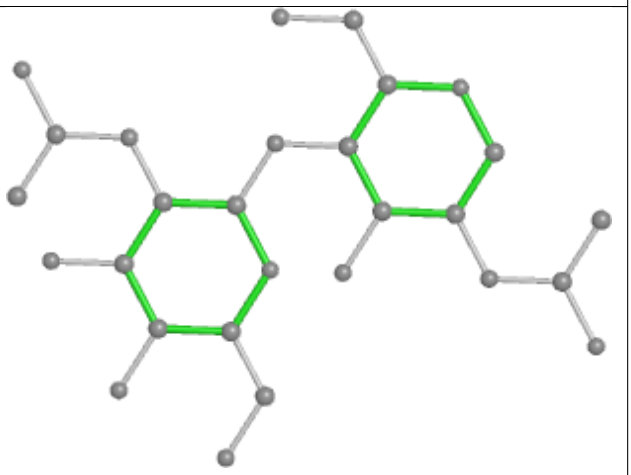
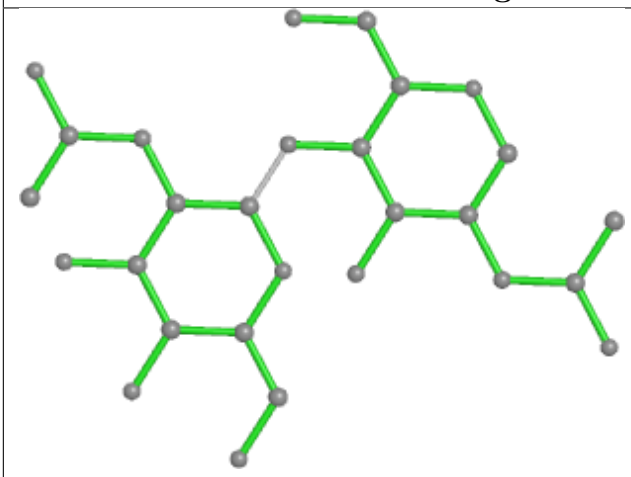


Rings

Oligosaccharide Chain U



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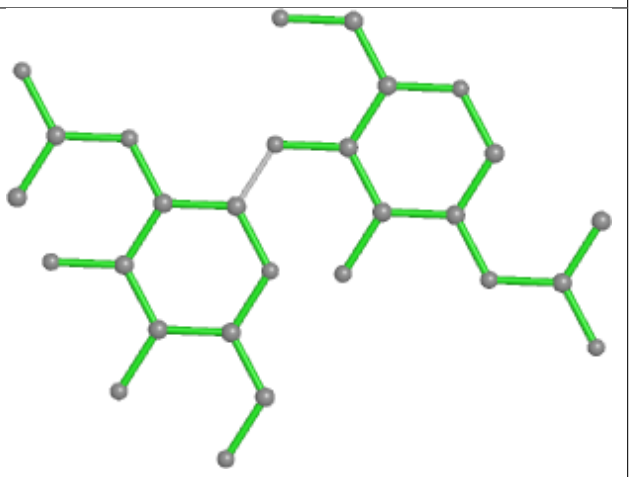
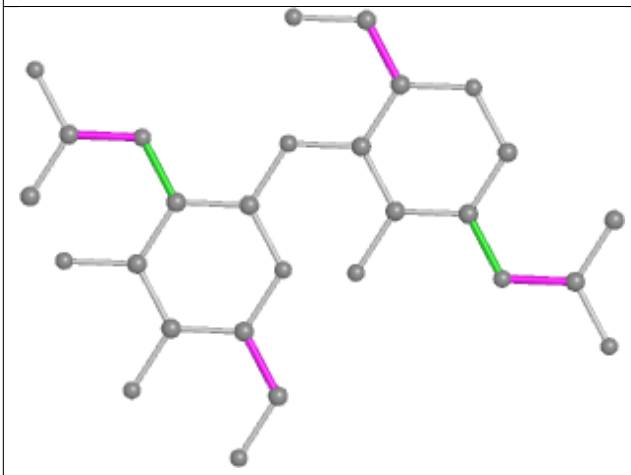


Bond angles



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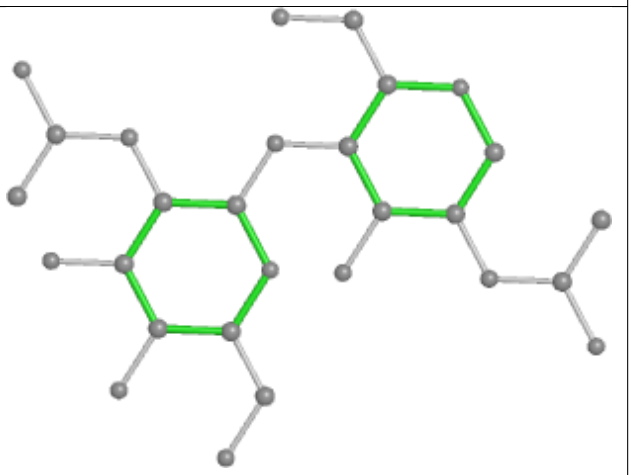
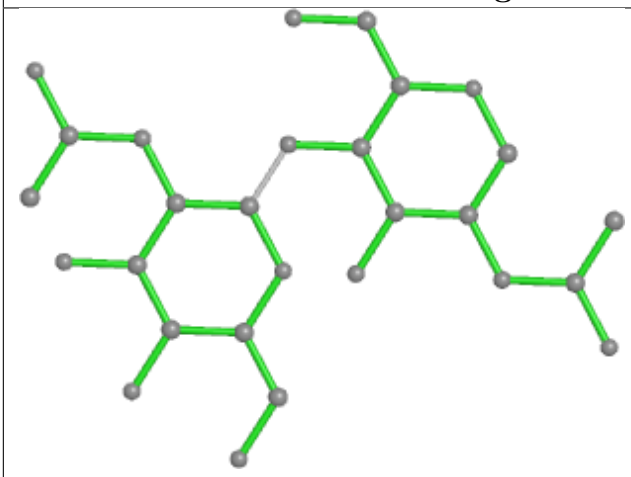


Rings

Oligosaccharide Chain X



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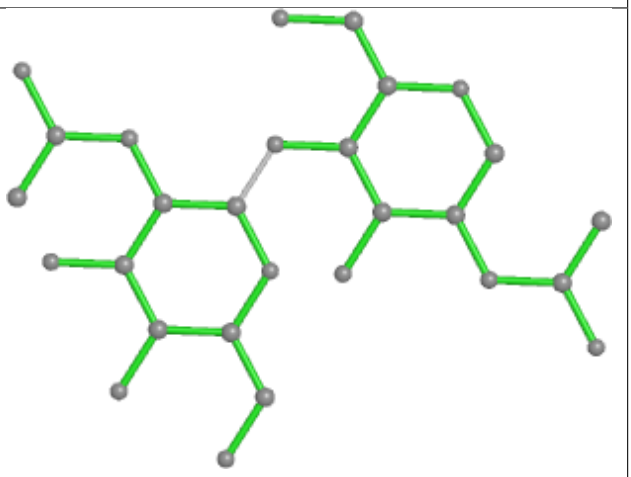
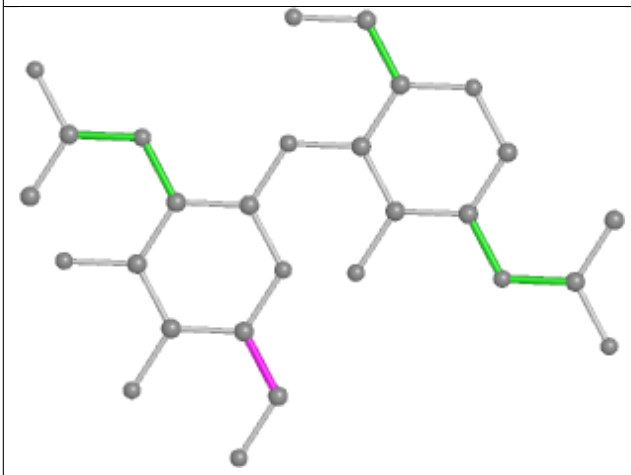


Bond angles



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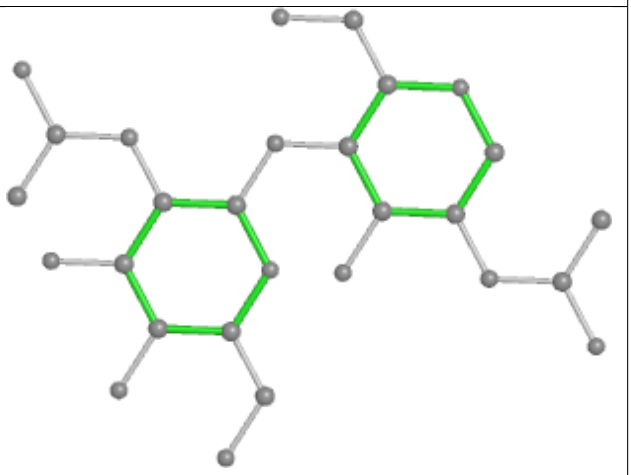
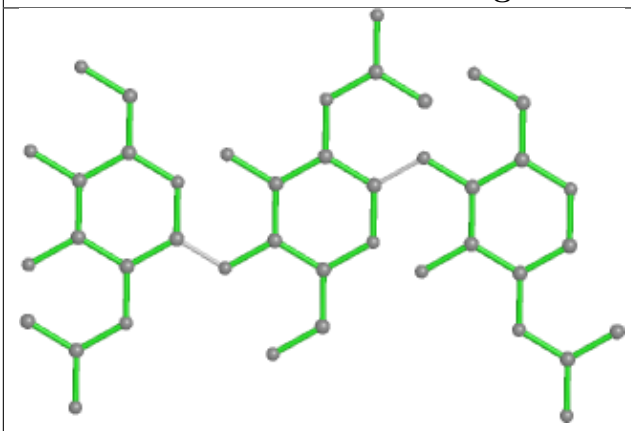


Rings

Oligosaccharide Chain H



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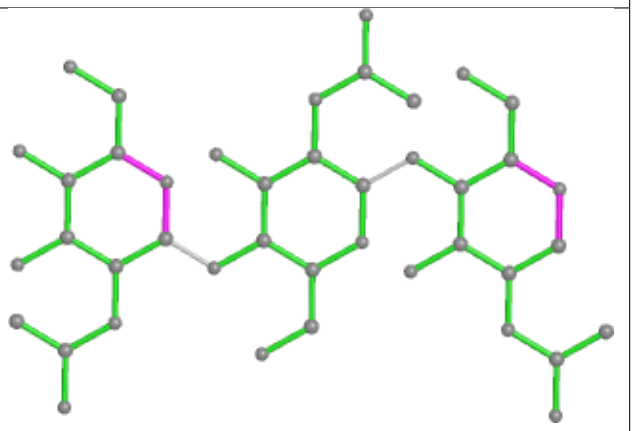
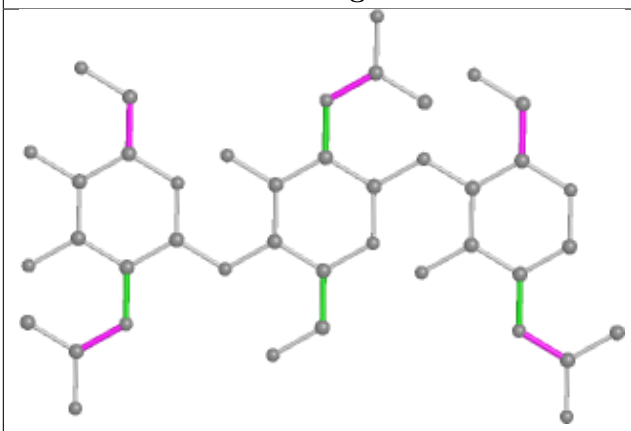
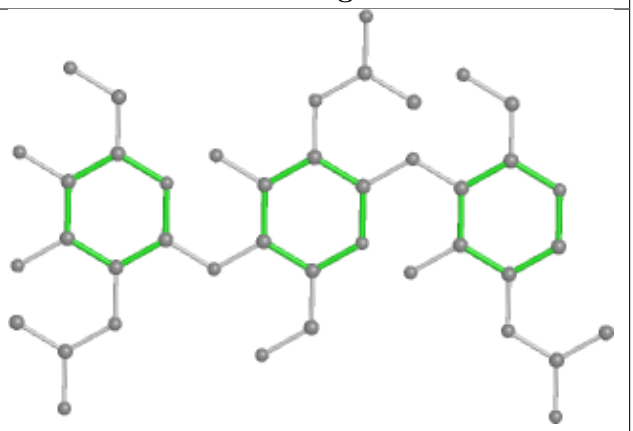


Bond angles

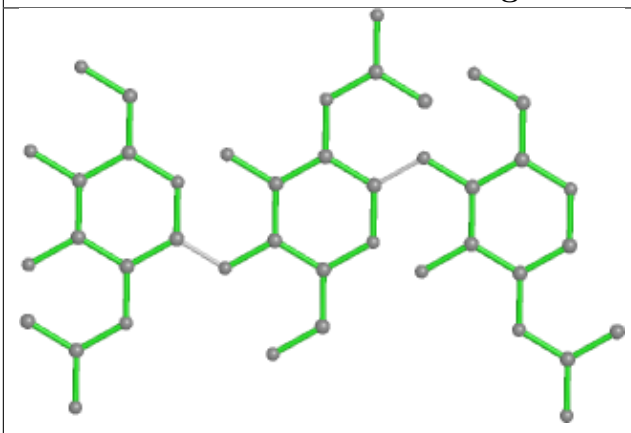


Torsions



Rings

Oligosaccharide Chain I



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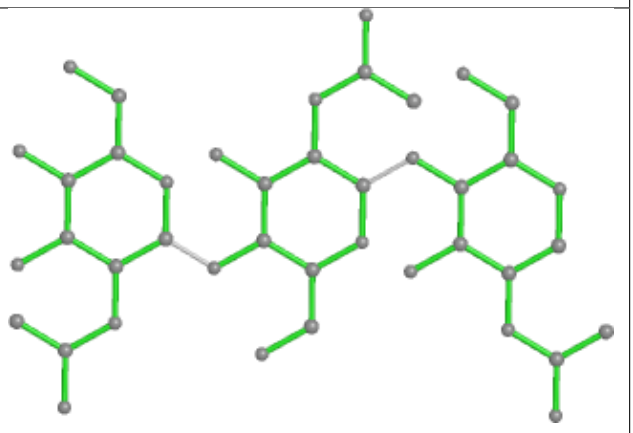
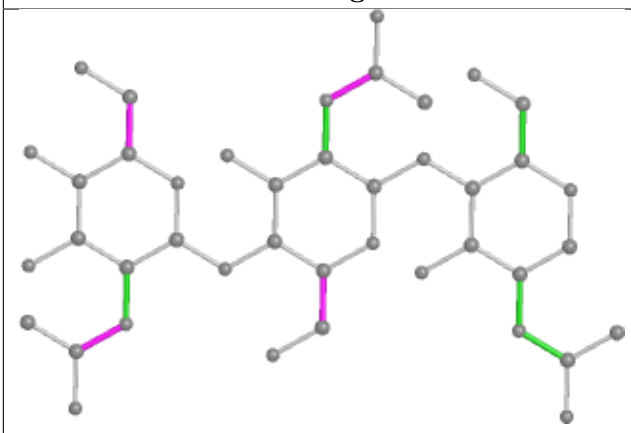


Bond angles



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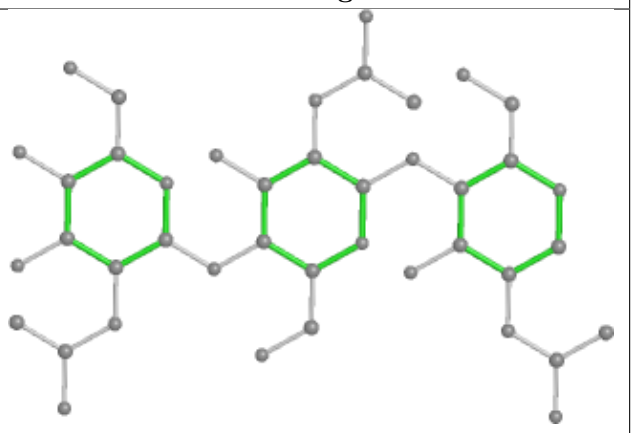
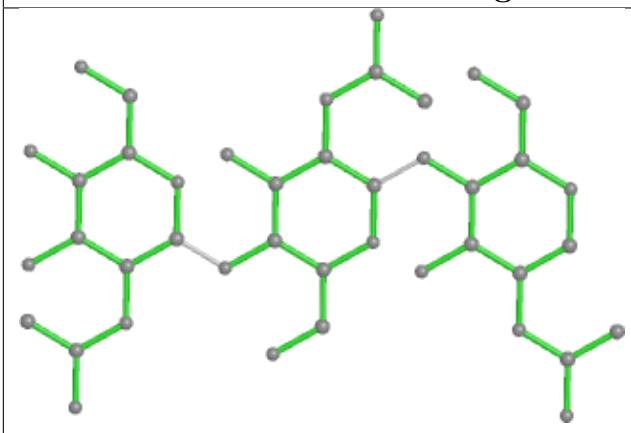


Rings

Oligosaccharide Chain O



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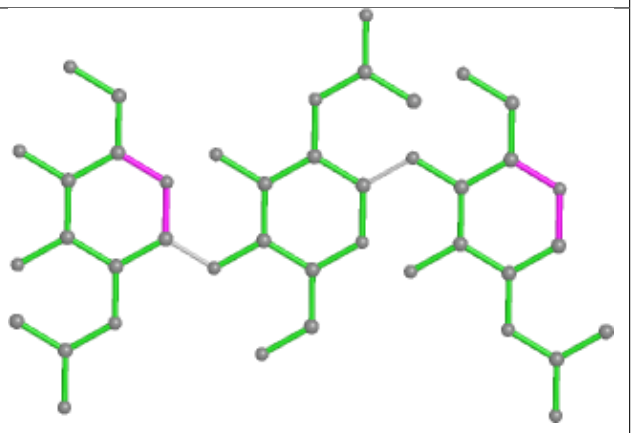
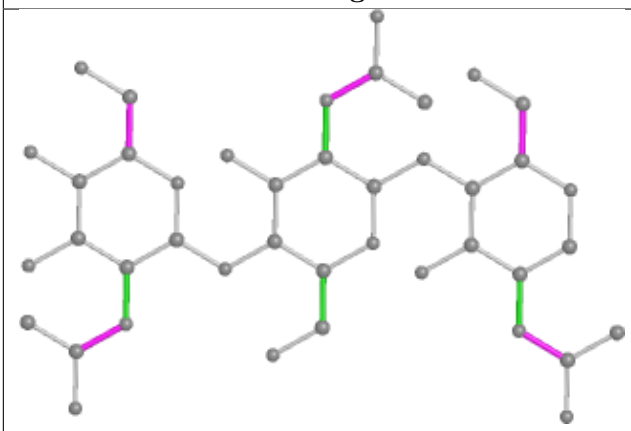
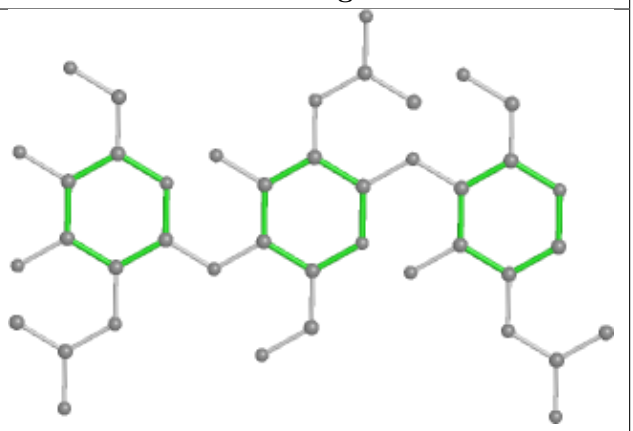


Bond angles

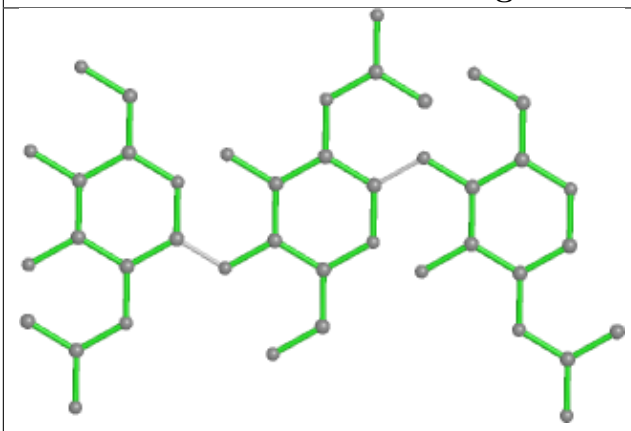


Torsions

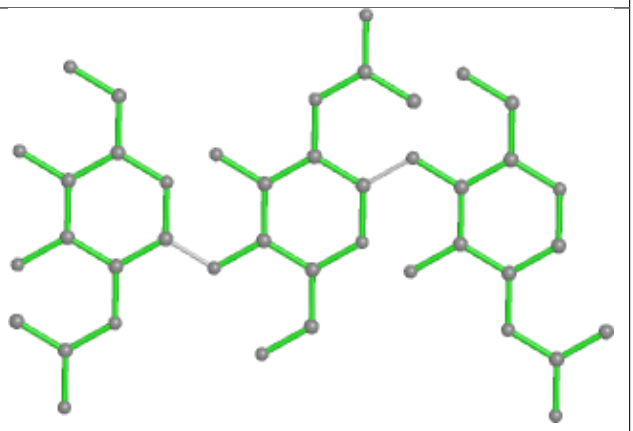


Rings

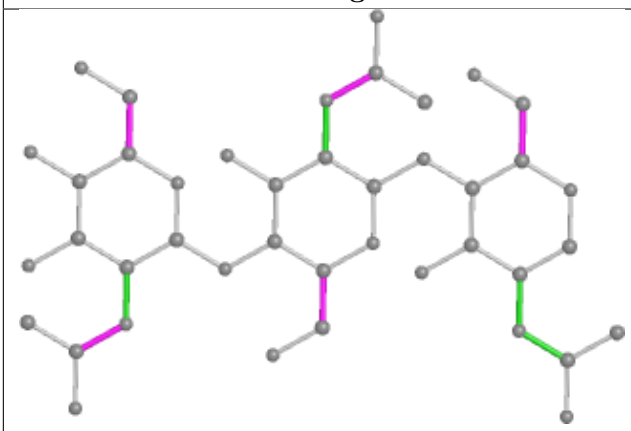
Oligosaccharide Chain P



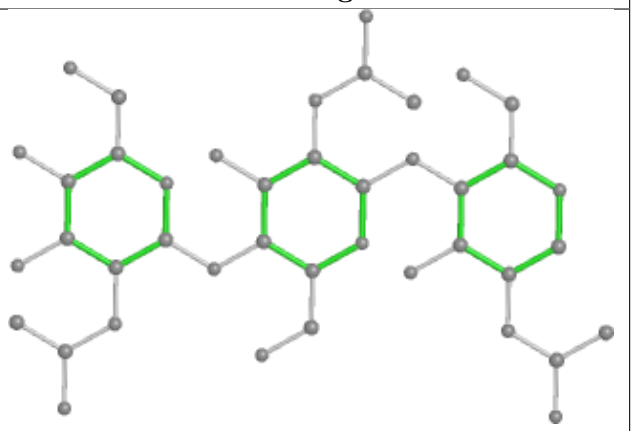
Bond lengths



Bond angles

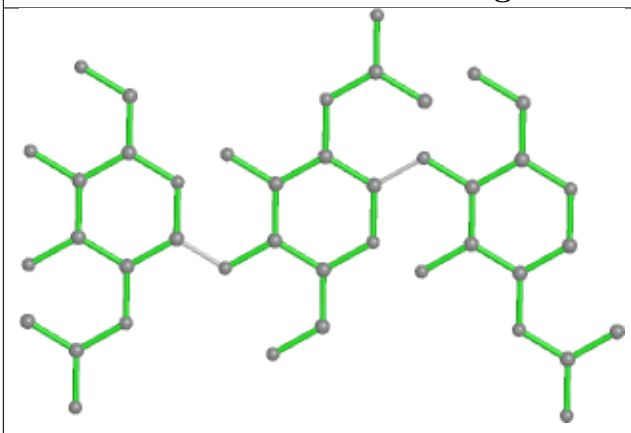


Torsions

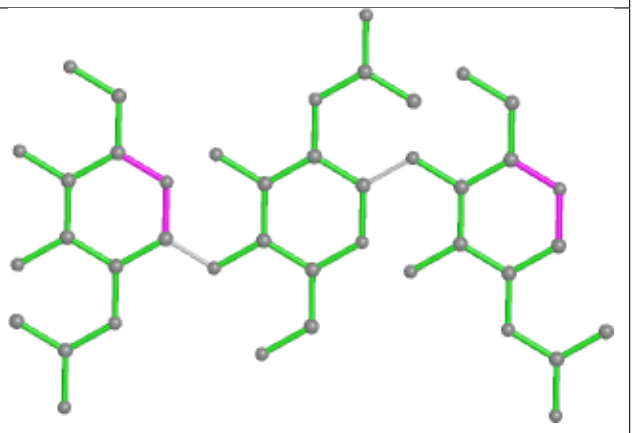


Rings

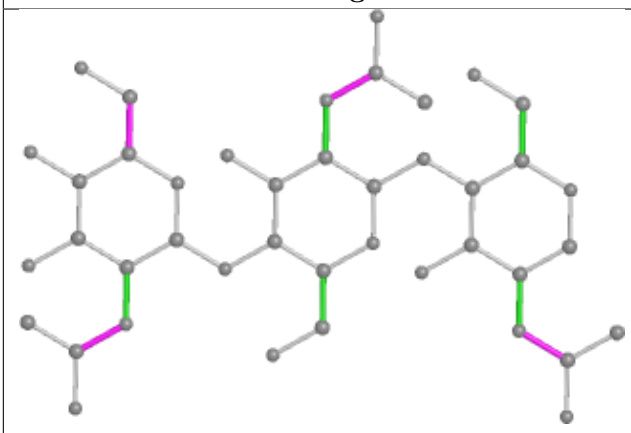
Oligosaccharide Chain V



Bond lengths



Bond angles



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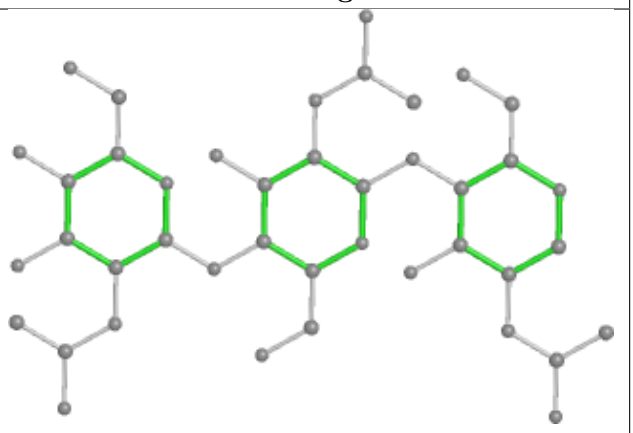
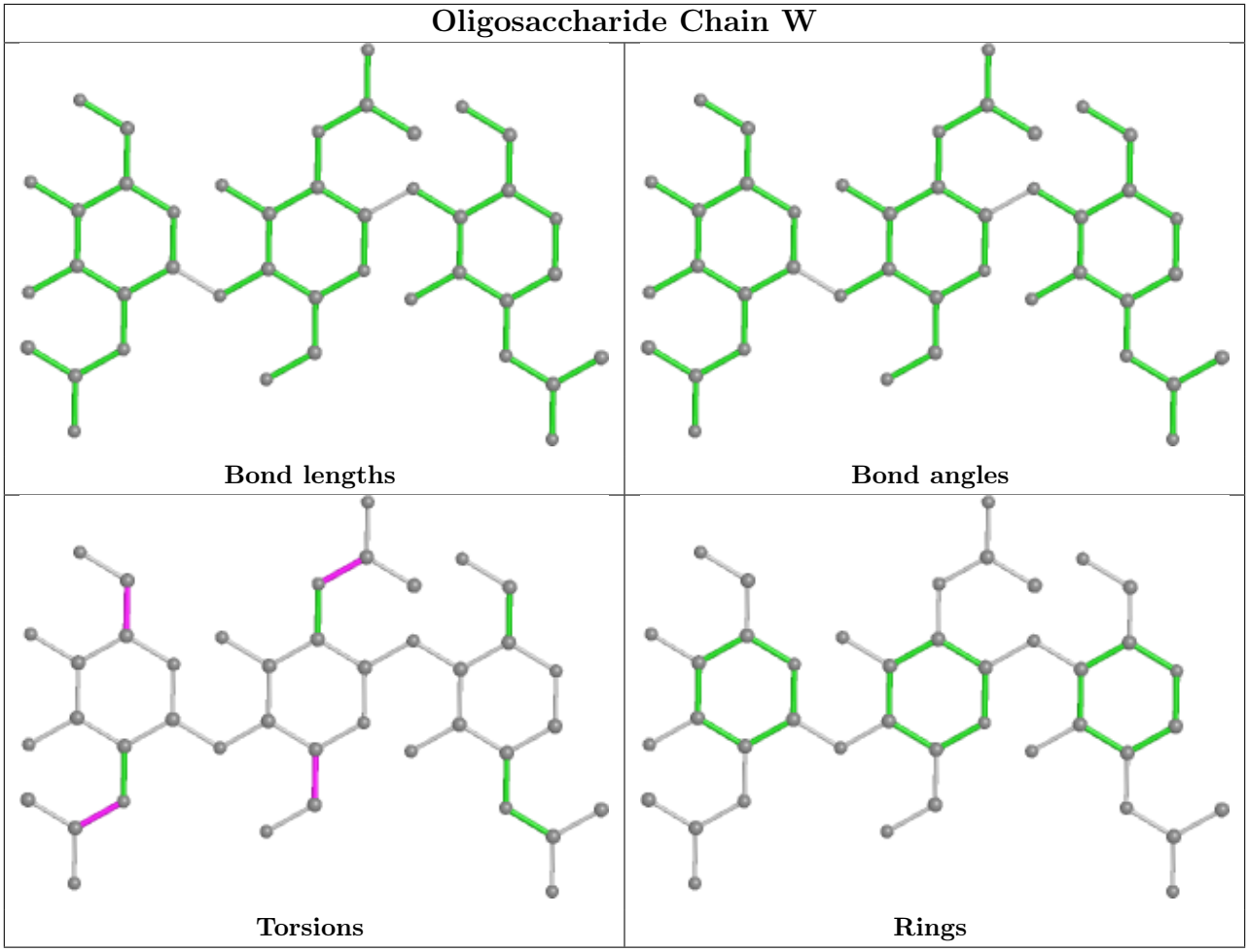


Rings



5.6 Ligand geometry (i)

39 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	$\#\|Z\| > 2$
4	NAG	C	1226	1	14,14,15	0.42	0	17,19,21	0.63	0
4	NAG	B	1218	1	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	A	1218	1	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	C	1229	1	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	B	1226	1	14,14,15	0.40	0	17,19,21	0.57	0
4	NAG	A	1212	1	14,14,15	0.31	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1217	1	14,14,15	0.37	0	17,19,21	0.70	1 (5%)
4	NAG	B	1213	1	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	C	1218	1	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	B	1229	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	C	1219	1	14,14,15	0.31	0	17,19,21	0.63	0
4	NAG	B	1203	1	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	A	1204	1	14,14,15	0.40	0	17,19,21	0.61	0
4	NAG	C	1212	1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	C	1204	1	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	A	1213	1	14,14,15	0.60	0	17,19,21	0.67	1 (5%)
4	NAG	A	1226	1	14,14,15	0.41	0	17,19,21	0.57	0
4	NAG	A	1217	1	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
4	NAG	B	1216	1	14,14,15	0.45	0	17,19,21	0.54	0
4	NAG	C	1213	1	14,14,15	0.46	0	17,19,21	0.47	0
4	NAG	B	1212	1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	C	1203	1	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	C	1207	1	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	B	1201	1	14,14,15	0.33	0	17,19,21	0.59	0
4	NAG	A	1201	1	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	B	1219	1	14,14,15	0.27	0	17,19,21	0.64	0
4	NAG	B	1202	1	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	A	1216	1	14,14,15	0.47	0	17,19,21	0.51	0
4	NAG	B	1204	1	14,14,15	0.40	0	17,19,21	0.61	0
4	NAG	A	1219	1	14,14,15	0.36	0	17,19,21	0.61	0
4	NAG	C	1201	1	14,14,15	0.32	0	17,19,21	0.60	0
4	NAG	B	1207	1	14,14,15	0.25	0	17,19,21	0.57	0
4	NAG	B	1217	1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
4	NAG	A	1207	1	14,14,15	0.26	0	17,19,21	0.56	0
4	NAG	C	1202	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	A	1229	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	A	1202	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	C	1216	1	14,14,15	0.51	0	17,19,21	0.59	0
4	NAG	A	1203	1	14,14,15	0.21	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1226	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1218	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1218	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1229	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1226	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1212	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1217	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1213	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1218	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1229	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1219	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1203	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1212	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1204	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1213	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1226	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1217	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1216	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1213	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1212	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1207	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1219	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1202	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1216	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1204	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1219	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1207	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1217	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1207	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1229	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1202	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1216	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1217	NAG	C1-O5-C5	2.41	115.46	112.19
4	A	1217	NAG	C1-O5-C5	2.36	115.39	112.19
4	C	1217	NAG	C1-O5-C5	2.33	115.35	112.19
4	A	1213	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1207	NAG	O5-C5-C6-O6
4	B	1226	NAG	O5-C5-C6-O6
4	A	1201	NAG	C4-C5-C6-O6
4	A	1203	NAG	C4-C5-C6-O6
4	A	1217	NAG	C4-C5-C6-O6
4	B	1201	NAG	C4-C5-C6-O6
4	B	1212	NAG	C4-C5-C6-O6
4	B	1217	NAG	C4-C5-C6-O6
4	C	1201	NAG	C4-C5-C6-O6
4	C	1203	NAG	O5-C5-C6-O6
4	A	1212	NAG	C4-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6
4	C	1204	NAG	O5-C5-C6-O6
4	C	1226	NAG	O5-C5-C6-O6
4	B	1203	NAG	C4-C5-C6-O6
4	B	1226	NAG	C4-C5-C6-O6
4	C	1217	NAG	C4-C5-C6-O6
4	A	1226	NAG	O5-C5-C6-O6
4	A	1219	NAG	O5-C5-C6-O6
4	A	1229	NAG	O5-C5-C6-O6
4	A	1226	NAG	C4-C5-C6-O6
4	C	1216	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1229	NAG	C4-C5-C6-O6
4	C	1203	NAG	C4-C5-C6-O6
4	A	1201	NAG	O5-C5-C6-O6
4	A	1203	NAG	O5-C5-C6-O6
4	A	1207	NAG	O5-C5-C6-O6
4	A	1212	NAG	O5-C5-C6-O6
4	B	1201	NAG	O5-C5-C6-O6
4	B	1212	NAG	O5-C5-C6-O6
4	C	1201	NAG	O5-C5-C6-O6
4	C	1229	NAG	O5-C5-C6-O6
4	A	1217	NAG	O5-C5-C6-O6
4	A	1207	NAG	C4-C5-C6-O6
4	B	1207	NAG	C4-C5-C6-O6
4	A	1201	NAG	C8-C7-N2-C2
4	A	1201	NAG	O7-C7-N2-C2
4	A	1202	NAG	C8-C7-N2-C2
4	A	1202	NAG	O7-C7-N2-C2
4	A	1203	NAG	C8-C7-N2-C2
4	A	1203	NAG	O7-C7-N2-C2
4	A	1204	NAG	C8-C7-N2-C2
4	A	1204	NAG	O7-C7-N2-C2
4	A	1207	NAG	C8-C7-N2-C2
4	A	1207	NAG	O7-C7-N2-C2
4	A	1212	NAG	C8-C7-N2-C2
4	A	1212	NAG	O7-C7-N2-C2
4	A	1213	NAG	C8-C7-N2-C2
4	A	1213	NAG	O7-C7-N2-C2
4	A	1216	NAG	C8-C7-N2-C2
4	A	1216	NAG	O7-C7-N2-C2
4	A	1217	NAG	C8-C7-N2-C2
4	A	1217	NAG	O7-C7-N2-C2
4	A	1218	NAG	C8-C7-N2-C2
4	A	1218	NAG	O7-C7-N2-C2
4	A	1219	NAG	C8-C7-N2-C2
4	A	1219	NAG	O7-C7-N2-C2
4	A	1226	NAG	C8-C7-N2-C2
4	A	1226	NAG	O7-C7-N2-C2
4	A	1229	NAG	C8-C7-N2-C2
4	A	1229	NAG	O7-C7-N2-C2
4	B	1201	NAG	C8-C7-N2-C2
4	B	1201	NAG	O7-C7-N2-C2
4	B	1202	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1202	NAG	O7-C7-N2-C2
4	B	1203	NAG	C8-C7-N2-C2
4	B	1203	NAG	O7-C7-N2-C2
4	B	1204	NAG	C8-C7-N2-C2
4	B	1204	NAG	O7-C7-N2-C2
4	B	1207	NAG	C8-C7-N2-C2
4	B	1207	NAG	O7-C7-N2-C2
4	B	1212	NAG	C8-C7-N2-C2
4	B	1212	NAG	O7-C7-N2-C2
4	B	1213	NAG	C8-C7-N2-C2
4	B	1213	NAG	O7-C7-N2-C2
4	B	1216	NAG	C8-C7-N2-C2
4	B	1216	NAG	O7-C7-N2-C2
4	B	1217	NAG	C8-C7-N2-C2
4	B	1217	NAG	O7-C7-N2-C2
4	B	1218	NAG	C8-C7-N2-C2
4	B	1218	NAG	O7-C7-N2-C2
4	B	1219	NAG	C8-C7-N2-C2
4	B	1219	NAG	O7-C7-N2-C2
4	B	1226	NAG	C8-C7-N2-C2
4	B	1226	NAG	O7-C7-N2-C2
4	B	1229	NAG	C8-C7-N2-C2
4	B	1229	NAG	O7-C7-N2-C2
4	C	1201	NAG	C8-C7-N2-C2
4	C	1201	NAG	O7-C7-N2-C2
4	C	1202	NAG	C8-C7-N2-C2
4	C	1202	NAG	O7-C7-N2-C2
4	C	1203	NAG	C8-C7-N2-C2
4	C	1203	NAG	O7-C7-N2-C2
4	C	1204	NAG	C8-C7-N2-C2
4	C	1204	NAG	O7-C7-N2-C2
4	C	1207	NAG	C8-C7-N2-C2
4	C	1207	NAG	O7-C7-N2-C2
4	C	1212	NAG	C8-C7-N2-C2
4	C	1212	NAG	O7-C7-N2-C2
4	C	1213	NAG	C8-C7-N2-C2
4	C	1213	NAG	O7-C7-N2-C2
4	C	1216	NAG	C8-C7-N2-C2
4	C	1216	NAG	O7-C7-N2-C2
4	C	1217	NAG	C8-C7-N2-C2
4	C	1217	NAG	O7-C7-N2-C2
4	C	1218	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	1218	NAG	O7-C7-N2-C2
4	C	1219	NAG	C8-C7-N2-C2
4	C	1219	NAG	O7-C7-N2-C2
4	C	1226	NAG	C8-C7-N2-C2
4	C	1226	NAG	O7-C7-N2-C2
4	C	1229	NAG	C8-C7-N2-C2
4	C	1229	NAG	O7-C7-N2-C2
4	B	1217	NAG	O5-C5-C6-O6
4	B	1216	NAG	O5-C5-C6-O6
4	C	1216	NAG	C4-C5-C6-O6
4	B	1204	NAG	O5-C5-C6-O6
4	A	1204	NAG	C4-C5-C6-O6
4	C	1204	NAG	C4-C5-C6-O6
4	C	1226	NAG	C4-C5-C6-O6
4	B	1203	NAG	O5-C5-C6-O6
4	C	1217	NAG	O5-C5-C6-O6
4	C	1202	NAG	C4-C5-C6-O6
4	B	1219	NAG	O5-C5-C6-O6
4	B	1229	NAG	O5-C5-C6-O6
4	A	1202	NAG	O5-C5-C6-O6
4	C	1207	NAG	O5-C5-C6-O6
4	B	1213	NAG	O5-C5-C6-O6
4	B	1216	NAG	C4-C5-C6-O6
4	C	1202	NAG	O5-C5-C6-O6
4	C	1213	NAG	O5-C5-C6-O6
4	A	1216	NAG	O5-C5-C6-O6
4	A	1213	NAG	O5-C5-C6-O6
4	B	1202	NAG	O5-C5-C6-O6
4	A	1219	NAG	C4-C5-C6-O6
4	A	1229	NAG	C4-C5-C6-O6
4	B	1219	NAG	C4-C5-C6-O6
4	C	1229	NAG	C4-C5-C6-O6
4	B	1204	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

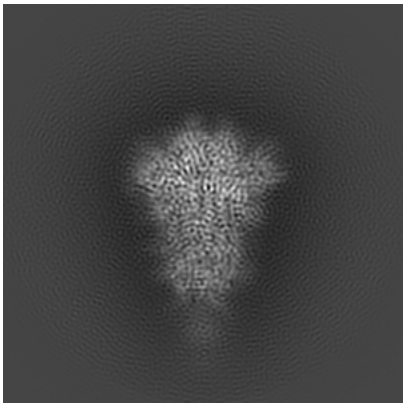
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7631. These allow visual inspection of the internal detail of the map and identification of artifacts.

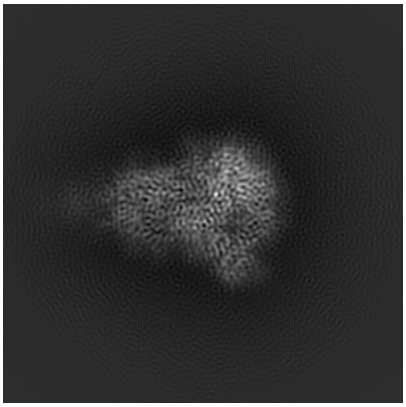
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

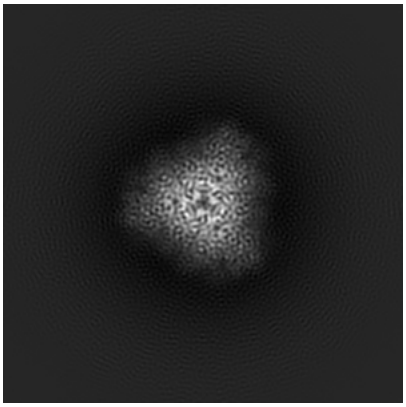
6.1.1 Primary map



X



Y

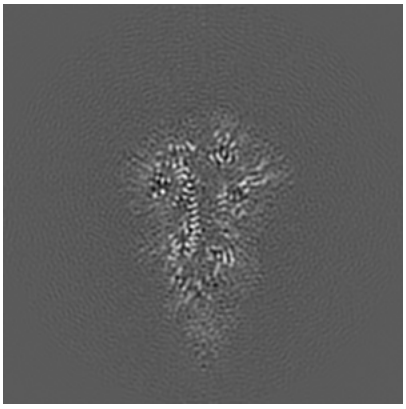


Z

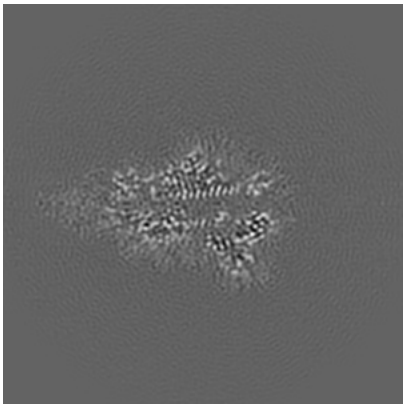
The images above show the map projected in three orthogonal directions.

6.2 Central slices

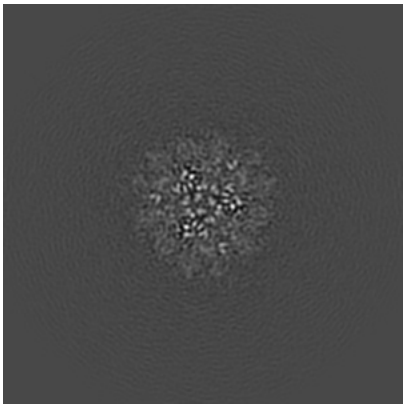
6.2.1 Primary map



X Index: 162



Y Index: 162

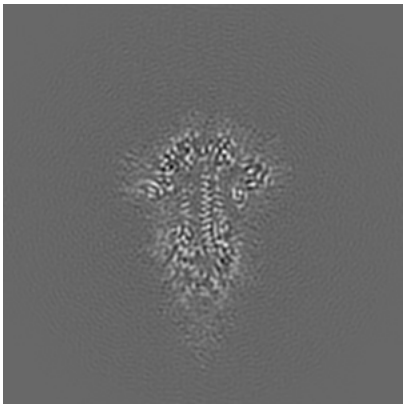


Z Index: 162

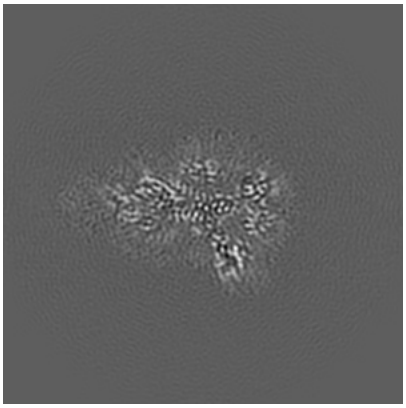
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

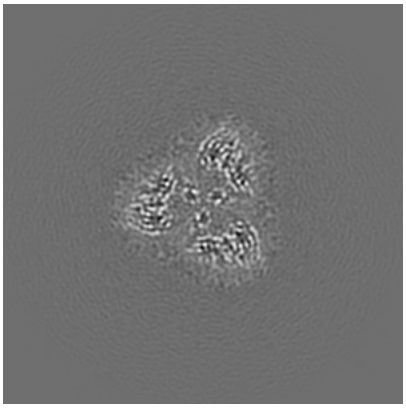
6.3.1 Primary map



X Index: 170



Y Index: 150

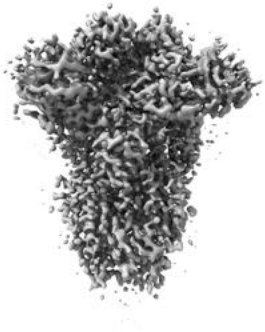


Z Index: 180

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0454. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

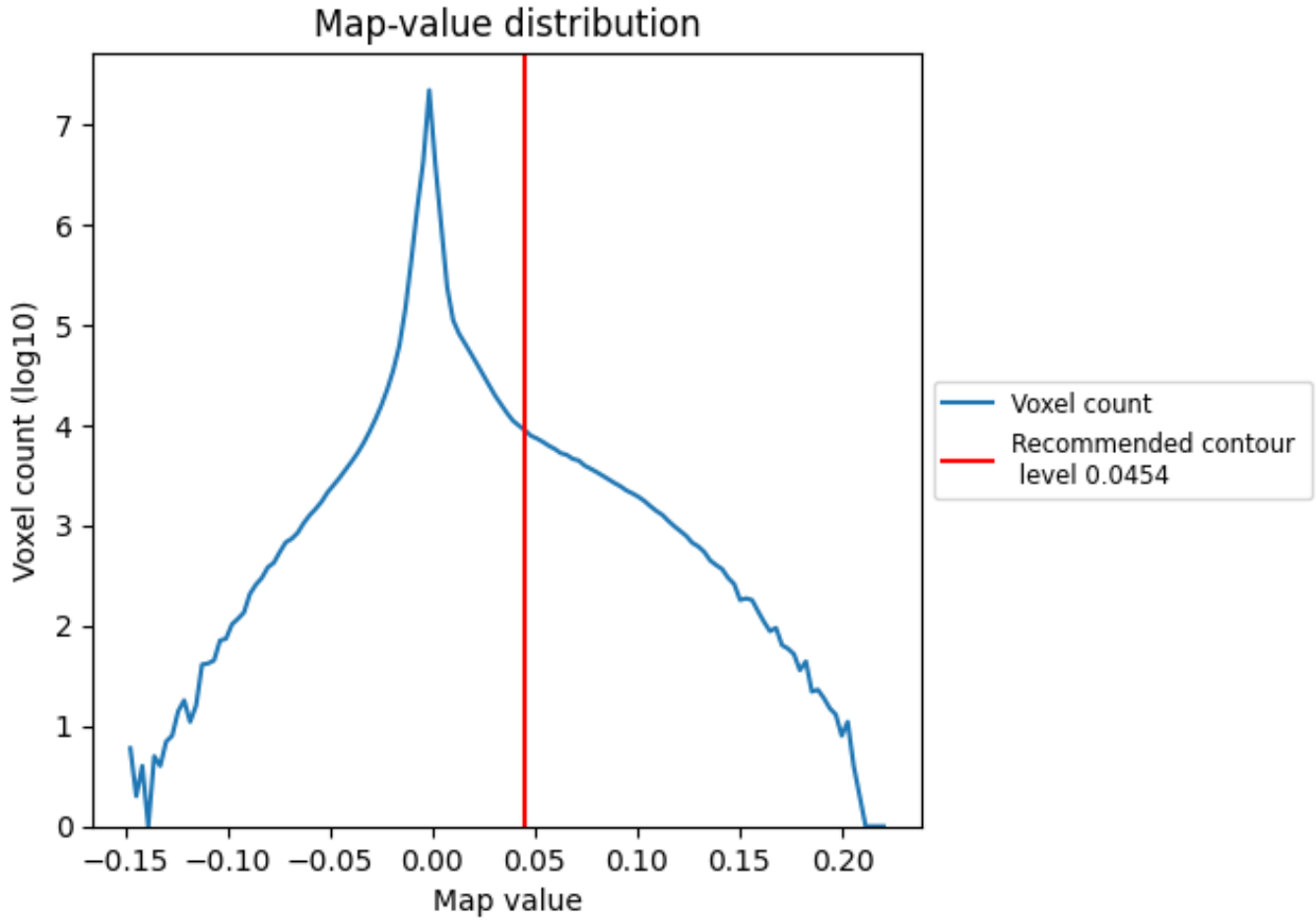
6.5 Mask visualisation (i)

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

7 Map analysis

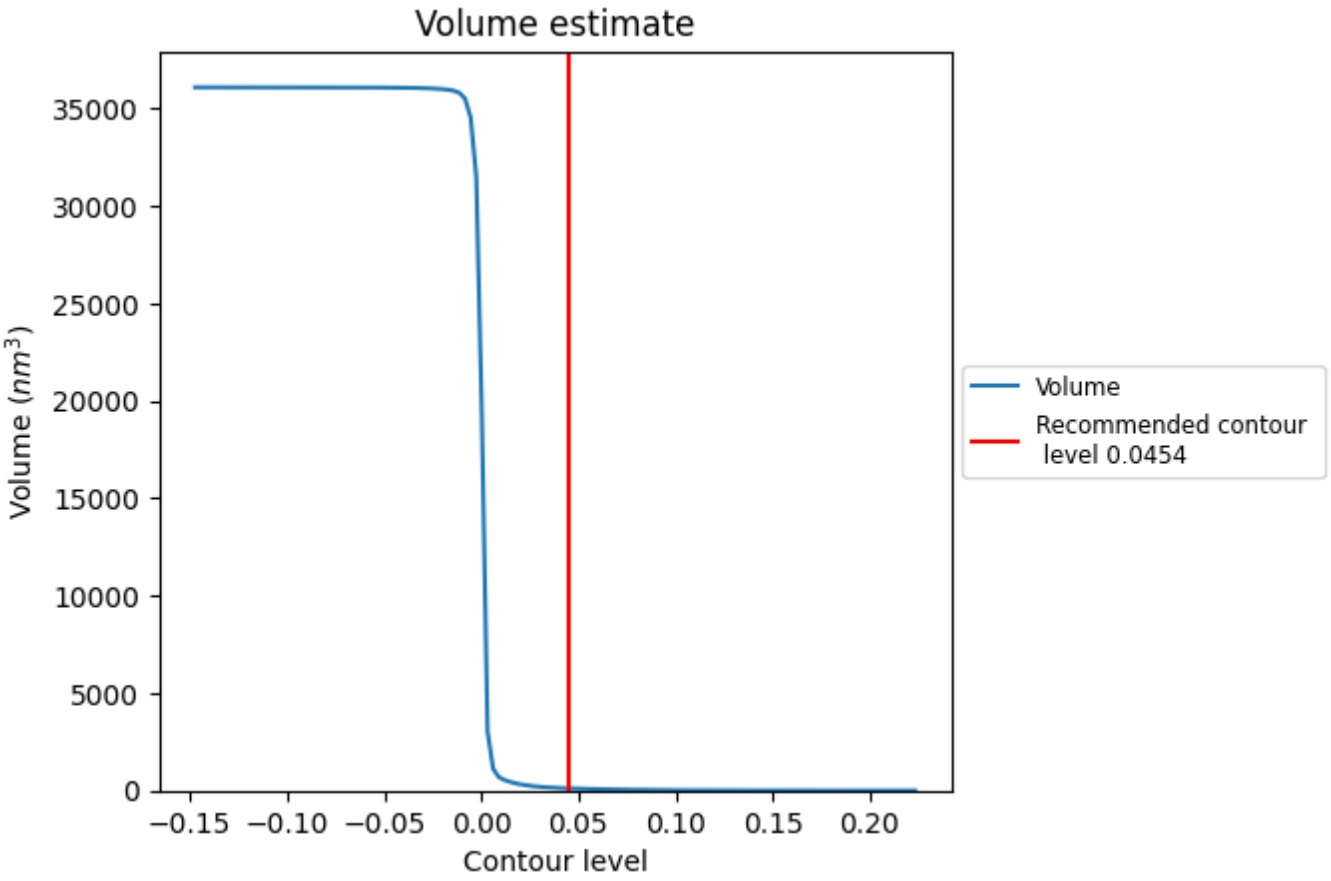
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

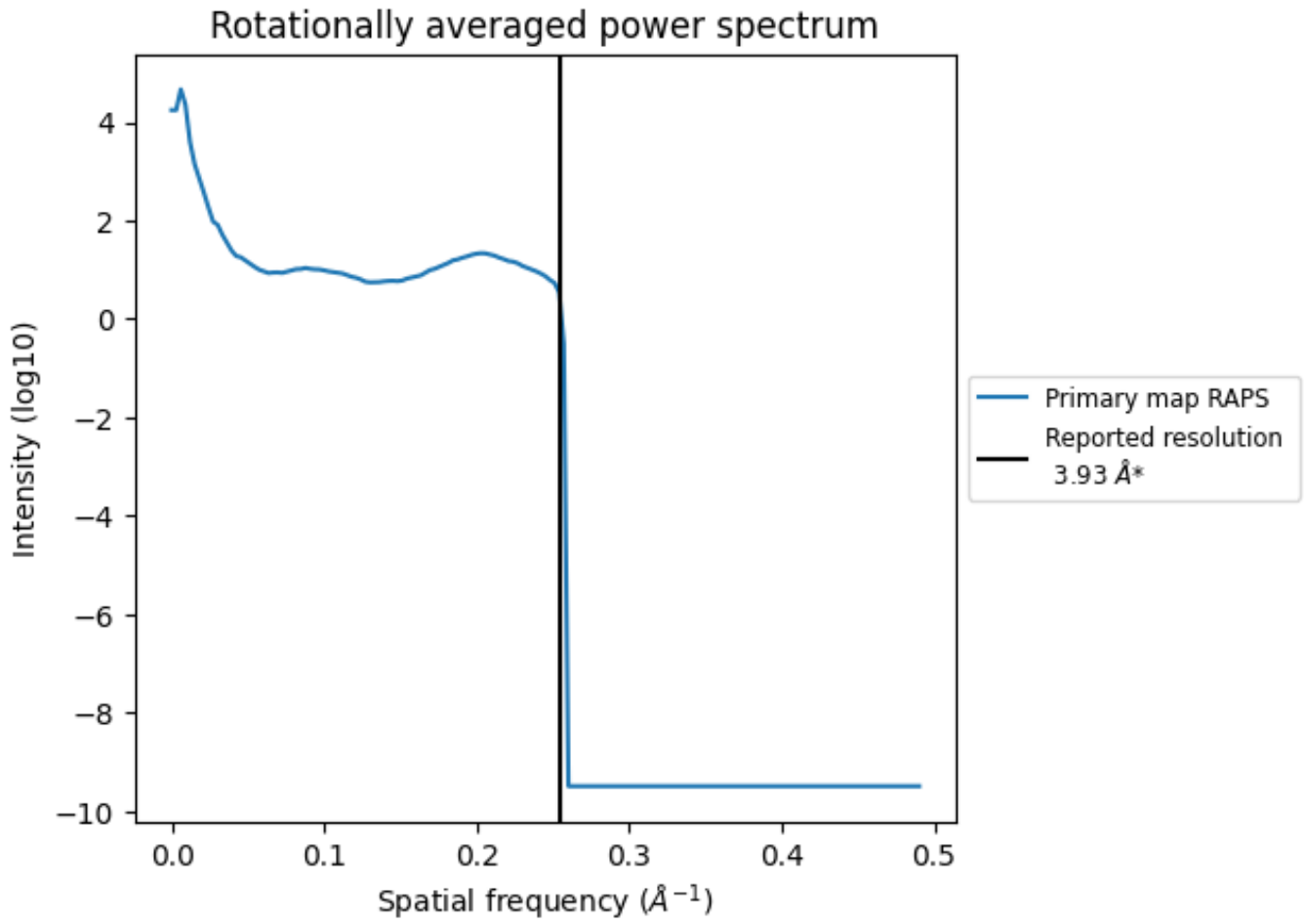
7.2 Volume estimate



The volume at the recommended contour level is 111 nm^3; this corresponds to an approximate mass of 100 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 0.254 Å^{-1}

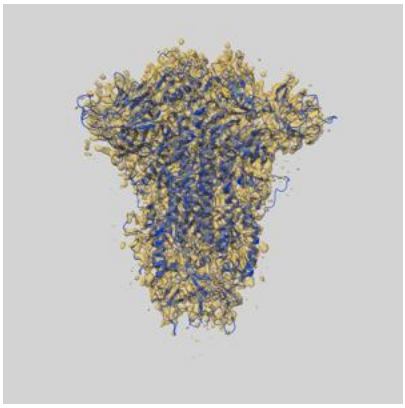
8 Fourier-Shell correlation

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

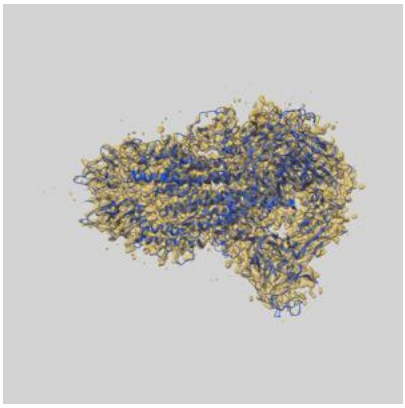
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7631 and PDB model 6CV0. Per-residue inclusion information can be found in section 3 on page 12.

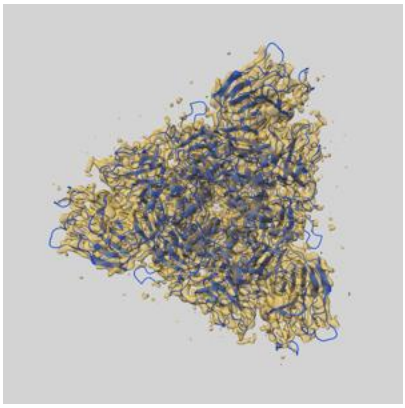
9.1 Map-model overlay



X



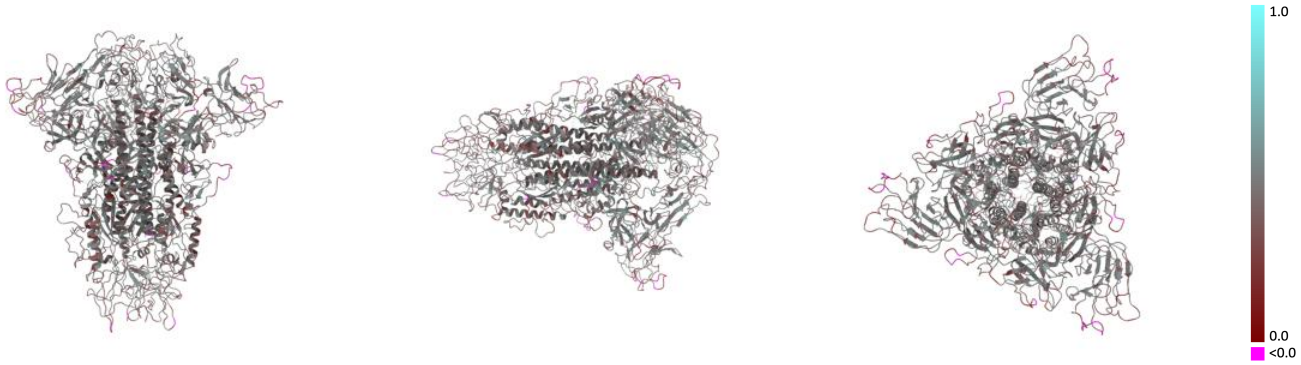
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0454 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

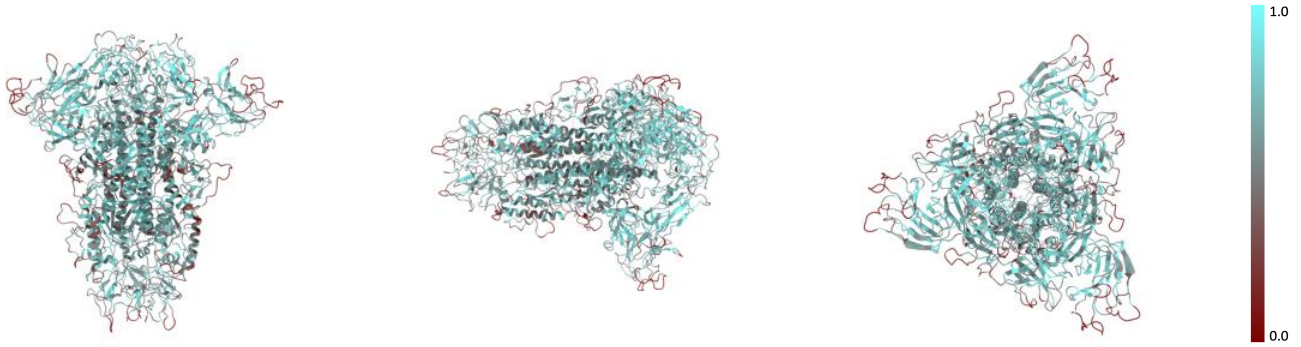
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

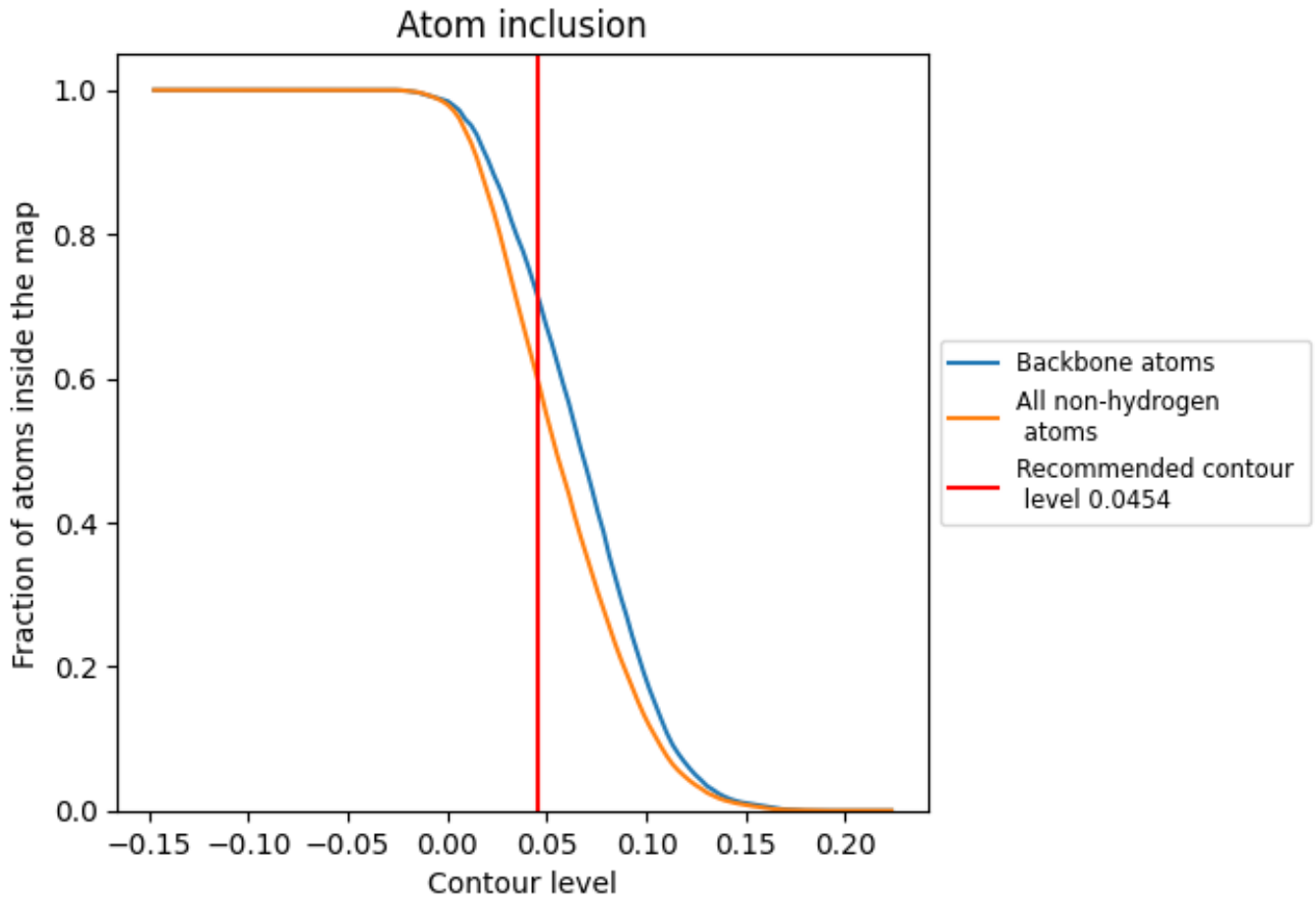
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0454).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 60% 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 (0.0454) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.4200
A	0.6035	0.4210
B	0.6031	0.4200
C	0.6030	0.4210
D	0.5714	0.4340
E	0.4286	0.3500
F	0.5357	0.4860
G	0.2857	0.3580
H	0.4286	0.4070
I	0.4286	0.3710
J	0.2500	0.3700
K	0.6071	0.4320
L	0.3929	0.3610
M	0.6071	0.4550
N	0.2143	0.2200
O	0.4286	0.4010
P	0.4524	0.4050
Q	0.2500	0.4290
R	0.5357	0.4340
S	0.3929	0.3690
T	0.5714	0.4560
U	0.2500	0.2300
V	0.4286	0.3970
W	0.4524	0.3870
X	0.2500	0.3990