wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 01:24 pm GMT

PDB ID	:	7AKJ
EMDB ID	:	EMD-11813
Title	:	Structure of the SARS-CoV spike glycoprotein in complex with the 47D11 neutralizing antibody Fab fragment
Authors	:	Fedry, J.; Hurdiss, D.L.; Wang, C.; Li, W.; Obal, G.; Drulyte, I.; Howes, S.C.; van Kuppeveld, F.J.M.; Foerster, F.; Bosch, B.J.
Deposited on	:	2020-10-01
Resolution	:	3.80 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 (i) symbol.

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

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

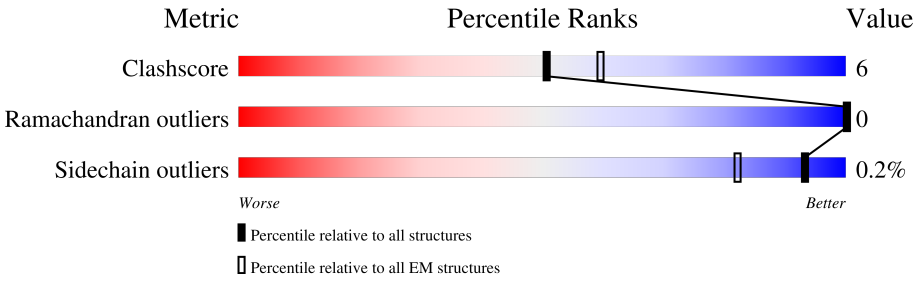
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.80 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	1193	78% 12% 9%
1	B	1193	79% 12% 9%
1	C	1193	79% 12% 9%
2	E	121	17% 83% 17%
2	G	121	19% 81% 18%
2	H	121	17% 81% 18%
3	D	106	8% 91% 9%
3	F	106	8% 91% 9%

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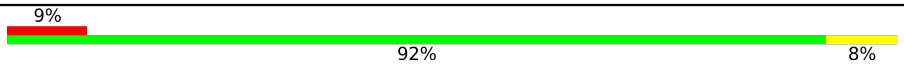
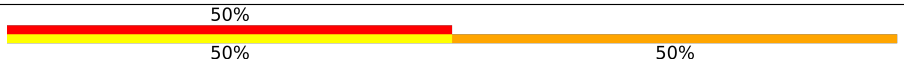
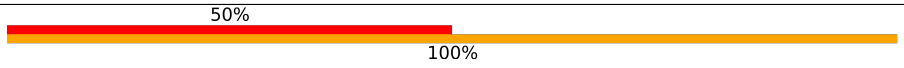
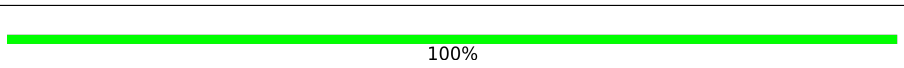
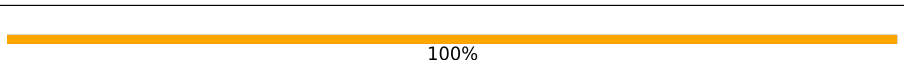
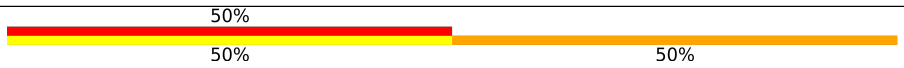
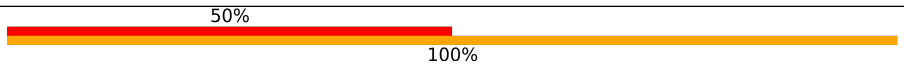
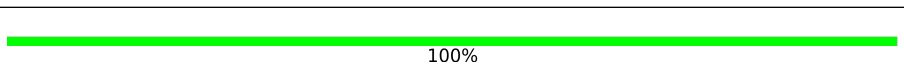
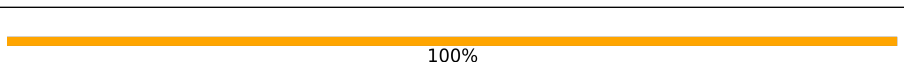
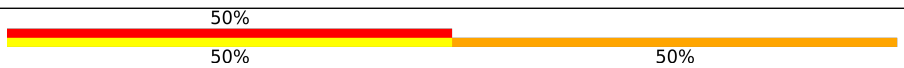
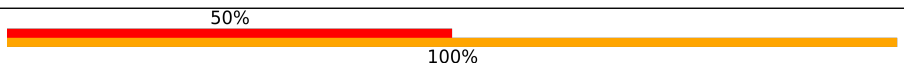
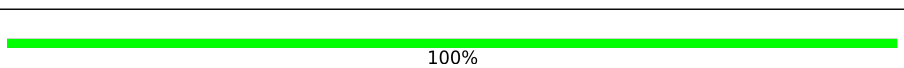
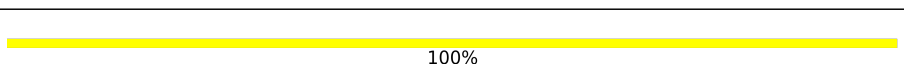
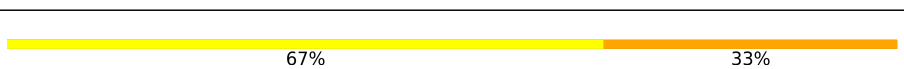
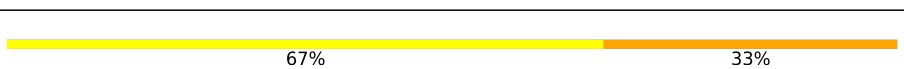
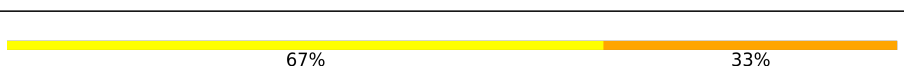
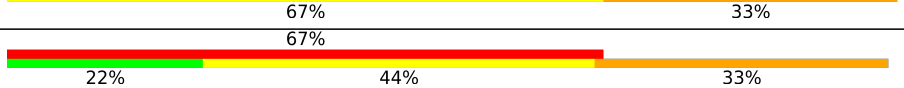
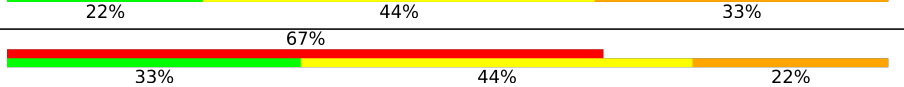
Mol	Chain	Length	Quality of chain
3	L	106	
4	I	2	
4	K	2	
4	M	2	
4	O	2	
4	P	2	
4	R	2	
4	S	2	
4	U	2	
4	V	2	
4	X	2	
4	Y	2	
4	a	2	
5	J	3	
5	Q	3	
5	W	3	
6	N	9	
6	T	9	
6	Z	9	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31812 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	C	1084	Total	C	N	O	S	0	0
			8459	5402	1398	1613	46		
1	B	1084	Total	C	N	O	S	0	0
			8459	5402	1398	1613	46		
1	A	1084	Total	C	N	O	S	0	0
			8459	5402	1398	1613	46		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	968	PRO	LYS	conflict	UNP Q5DIC5
C	969	PRO	VAL	conflict	UNP Q5DIC5
C	1161	LEU	-	expression tag	UNP Q5DIC5
C	1162	ILE	-	expression tag	UNP Q5DIC5
C	1163	LYS	-	expression tag	UNP Q5DIC5
C	1164	GLY	-	expression tag	UNP Q5DIC5
C	1165	SER	-	expression tag	UNP Q5DIC5
C	1166	GLY	-	expression tag	UNP Q5DIC5
C	1167	TYR	-	expression tag	UNP Q5DIC5
C	1168	ILE	-	expression tag	UNP Q5DIC5
C	1169	PRO	-	expression tag	UNP Q5DIC5
C	1170	GLU	-	expression tag	UNP Q5DIC5
C	1171	ALA	-	expression tag	UNP Q5DIC5
C	1172	PRO	-	expression tag	UNP Q5DIC5
C	1173	ARG	-	expression tag	UNP Q5DIC5
C	1174	ASP	-	expression tag	UNP Q5DIC5
C	1175	GLY	-	expression tag	UNP Q5DIC5
C	1176	GLN	-	expression tag	UNP Q5DIC5
C	1177	ALA	-	expression tag	UNP Q5DIC5
C	1178	TYR	-	expression tag	UNP Q5DIC5
C	1179	VAL	-	expression tag	UNP Q5DIC5
C	1180	ARG	-	expression tag	UNP Q5DIC5
C	1181	LYS	-	expression tag	UNP Q5DIC5
C	1182	ASP	-	expression tag	UNP Q5DIC5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1183	GLY	-	expression tag	UNP Q5DIC5
C	1184	GLU	-	expression tag	UNP Q5DIC5
C	1185	TRP	-	expression tag	UNP Q5DIC5
C	1186	VAL	-	expression tag	UNP Q5DIC5
C	1187	LEU	-	expression tag	UNP Q5DIC5
C	1188	LEU	-	expression tag	UNP Q5DIC5
C	1189	SER	-	expression tag	UNP Q5DIC5
C	1190	THR	-	expression tag	UNP Q5DIC5
C	1191	PHE	-	expression tag	UNP Q5DIC5
C	1192	LEU	-	expression tag	UNP Q5DIC5
C	1193	ILE	-	expression tag	UNP Q5DIC5
C	1194	LYS	-	expression tag	UNP Q5DIC5
C	1195	LEU	-	expression tag	UNP Q5DIC5
C	1196	VAL	-	expression tag	UNP Q5DIC5
C	1197	PRO	-	expression tag	UNP Q5DIC5
C	1198	ARG	-	expression tag	UNP Q5DIC5
C	1199	GLY	-	expression tag	UNP Q5DIC5
C	1200	SER	-	expression tag	UNP Q5DIC5
C	1201	LEU	-	expression tag	UNP Q5DIC5
C	1202	GLU	-	expression tag	UNP Q5DIC5
C	1203	TRP	-	expression tag	UNP Q5DIC5
C	1204	SER	-	expression tag	UNP Q5DIC5
C	1205	HIS	-	expression tag	UNP Q5DIC5
C	1206	PRO	-	expression tag	UNP Q5DIC5
C	1207	GLN	-	expression tag	UNP Q5DIC5
C	1208	PHE	-	expression tag	UNP Q5DIC5
C	1209	GLU	-	expression tag	UNP Q5DIC5
C	1210	LYS	-	expression tag	UNP Q5DIC5
B	968	PRO	LYS	conflict	UNP Q5DIC5
B	969	PRO	VAL	conflict	UNP Q5DIC5
B	1161	LEU	-	expression tag	UNP Q5DIC5
B	1162	ILE	-	expression tag	UNP Q5DIC5
B	1163	LYS	-	expression tag	UNP Q5DIC5
B	1164	GLY	-	expression tag	UNP Q5DIC5
B	1165	SER	-	expression tag	UNP Q5DIC5
B	1166	GLY	-	expression tag	UNP Q5DIC5
B	1167	TYR	-	expression tag	UNP Q5DIC5
B	1168	ILE	-	expression tag	UNP Q5DIC5
B	1169	PRO	-	expression tag	UNP Q5DIC5
B	1170	GLU	-	expression tag	UNP Q5DIC5
B	1171	ALA	-	expression tag	UNP Q5DIC5
B	1172	PRO	-	expression tag	UNP Q5DIC5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1173	ARG	-	expression tag	UNP Q5DIC5
B	1174	ASP	-	expression tag	UNP Q5DIC5
B	1175	GLY	-	expression tag	UNP Q5DIC5
B	1176	GLN	-	expression tag	UNP Q5DIC5
B	1177	ALA	-	expression tag	UNP Q5DIC5
B	1178	TYR	-	expression tag	UNP Q5DIC5
B	1179	VAL	-	expression tag	UNP Q5DIC5
B	1180	ARG	-	expression tag	UNP Q5DIC5
B	1181	LYS	-	expression tag	UNP Q5DIC5
B	1182	ASP	-	expression tag	UNP Q5DIC5
B	1183	GLY	-	expression tag	UNP Q5DIC5
B	1184	GLU	-	expression tag	UNP Q5DIC5
B	1185	TRP	-	expression tag	UNP Q5DIC5
B	1186	VAL	-	expression tag	UNP Q5DIC5
B	1187	LEU	-	expression tag	UNP Q5DIC5
B	1188	LEU	-	expression tag	UNP Q5DIC5
B	1189	SER	-	expression tag	UNP Q5DIC5
B	1190	THR	-	expression tag	UNP Q5DIC5
B	1191	PHE	-	expression tag	UNP Q5DIC5
B	1192	LEU	-	expression tag	UNP Q5DIC5
B	1193	ILE	-	expression tag	UNP Q5DIC5
B	1194	LYS	-	expression tag	UNP Q5DIC5
B	1195	LEU	-	expression tag	UNP Q5DIC5
B	1196	VAL	-	expression tag	UNP Q5DIC5
B	1197	PRO	-	expression tag	UNP Q5DIC5
B	1198	ARG	-	expression tag	UNP Q5DIC5
B	1199	GLY	-	expression tag	UNP Q5DIC5
B	1200	SER	-	expression tag	UNP Q5DIC5
B	1201	LEU	-	expression tag	UNP Q5DIC5
B	1202	GLU	-	expression tag	UNP Q5DIC5
B	1203	TRP	-	expression tag	UNP Q5DIC5
B	1204	SER	-	expression tag	UNP Q5DIC5
B	1205	HIS	-	expression tag	UNP Q5DIC5
B	1206	PRO	-	expression tag	UNP Q5DIC5
B	1207	GLN	-	expression tag	UNP Q5DIC5
B	1208	PHE	-	expression tag	UNP Q5DIC5
B	1209	GLU	-	expression tag	UNP Q5DIC5
B	1210	LYS	-	expression tag	UNP Q5DIC5
A	968	PRO	LYS	conflict	UNP Q5DIC5
A	969	PRO	VAL	conflict	UNP Q5DIC5
A	1161	LEU	-	expression tag	UNP Q5DIC5
A	1162	ILE	-	expression tag	UNP Q5DIC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1163	LYS	-	expression tag	UNP Q5DIC5
A	1164	GLY	-	expression tag	UNP Q5DIC5
A	1165	SER	-	expression tag	UNP Q5DIC5
A	1166	GLY	-	expression tag	UNP Q5DIC5
A	1167	TYR	-	expression tag	UNP Q5DIC5
A	1168	ILE	-	expression tag	UNP Q5DIC5
A	1169	PRO	-	expression tag	UNP Q5DIC5
A	1170	GLU	-	expression tag	UNP Q5DIC5
A	1171	ALA	-	expression tag	UNP Q5DIC5
A	1172	PRO	-	expression tag	UNP Q5DIC5
A	1173	ARG	-	expression tag	UNP Q5DIC5
A	1174	ASP	-	expression tag	UNP Q5DIC5
A	1175	GLY	-	expression tag	UNP Q5DIC5
A	1176	GLN	-	expression tag	UNP Q5DIC5
A	1177	ALA	-	expression tag	UNP Q5DIC5
A	1178	TYR	-	expression tag	UNP Q5DIC5
A	1179	VAL	-	expression tag	UNP Q5DIC5
A	1180	ARG	-	expression tag	UNP Q5DIC5
A	1181	LYS	-	expression tag	UNP Q5DIC5
A	1182	ASP	-	expression tag	UNP Q5DIC5
A	1183	GLY	-	expression tag	UNP Q5DIC5
A	1184	GLU	-	expression tag	UNP Q5DIC5
A	1185	TRP	-	expression tag	UNP Q5DIC5
A	1186	VAL	-	expression tag	UNP Q5DIC5
A	1187	LEU	-	expression tag	UNP Q5DIC5
A	1188	LEU	-	expression tag	UNP Q5DIC5
A	1189	SER	-	expression tag	UNP Q5DIC5
A	1190	THR	-	expression tag	UNP Q5DIC5
A	1191	PHE	-	expression tag	UNP Q5DIC5
A	1192	LEU	-	expression tag	UNP Q5DIC5
A	1193	ILE	-	expression tag	UNP Q5DIC5
A	1194	LYS	-	expression tag	UNP Q5DIC5
A	1195	LEU	-	expression tag	UNP Q5DIC5
A	1196	VAL	-	expression tag	UNP Q5DIC5
A	1197	PRO	-	expression tag	UNP Q5DIC5
A	1198	ARG	-	expression tag	UNP Q5DIC5
A	1199	GLY	-	expression tag	UNP Q5DIC5
A	1200	SER	-	expression tag	UNP Q5DIC5
A	1201	LEU	-	expression tag	UNP Q5DIC5
A	1202	GLU	-	expression tag	UNP Q5DIC5
A	1203	TRP	-	expression tag	UNP Q5DIC5
A	1204	SER	-	expression tag	UNP Q5DIC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1205	HIS	-	expression tag	UNP Q5DIC5
A	1206	PRO	-	expression tag	UNP Q5DIC5
A	1207	GLN	-	expression tag	UNP Q5DIC5
A	1208	PHE	-	expression tag	UNP Q5DIC5
A	1209	GLU	-	expression tag	UNP Q5DIC5
A	1210	LYS	-	expression tag	UNP Q5DIC5

- Molecule 2 is a protein called 47D11 neutralizing antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	120	Total	C	N	O	S	0	0
			925	593	152	177	3		
2	E	120	Total	C	N	O	S	0	0
			925	593	152	177	3		
2	H	120	Total	C	N	O	S	0	0
			925	593	152	177	3		

- Molecule 3 is a protein called 47D11 neutralizing antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	106	Total	C	N	O	S	0	0
			798	502	135	158	3		
3	D	106	Total	C	N	O	S	0	0
			798	502	135	158	3		
3	L	106	Total	C	N	O	S	0	0
			798	502	135	158	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		

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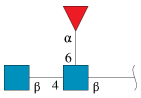
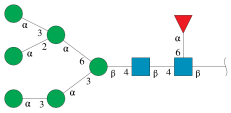
Mol	Chain	Residues	Atoms				AltConf	Trace
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		

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



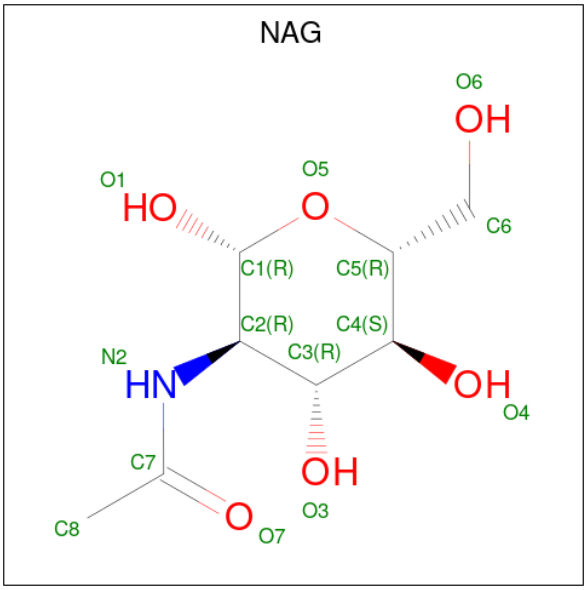
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			38	22	2	14		
5	Q	3	Total	C	N	O	0	0
			38	22	2	14		
5	W	3	Total	C	N	O	0	0
			38	22	2	14		

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



Mol	Chain	Residues	Atoms	AltConf	Trace
6	N	9	Total C N O 104 58 2 44	0	0
6	T	9	Total C N O 104 58 2 44	0	0
6	Z	9	Total C N O 104 58 2 44	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0
7	C	1	Total C N O 168 96 12 60	0

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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 168	C 96	N 12	O 60	0
7	C	1	Total 168	C 96	N 12	O 60	0
7	C	1	Total 168	C 96	N 12	O 60	0
7	C	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	B	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0

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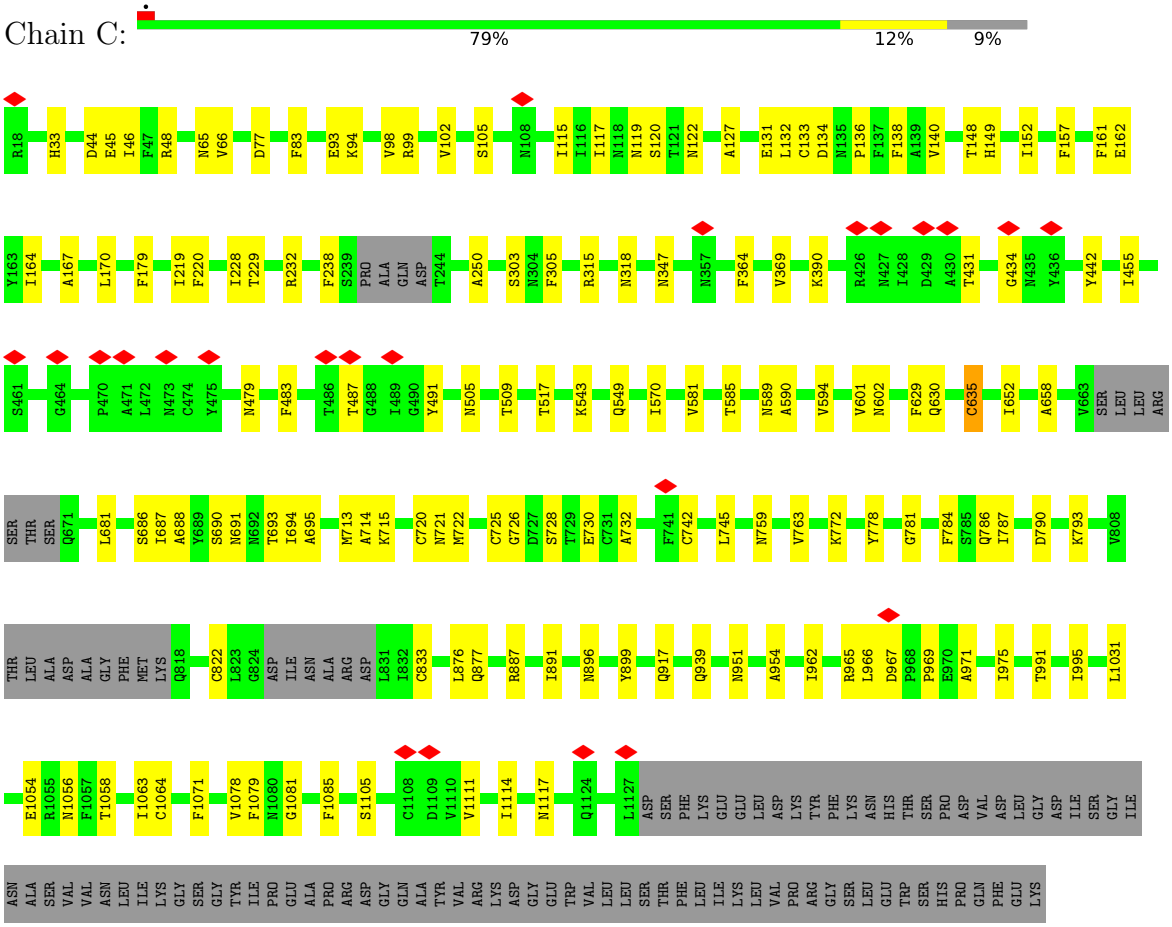
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0
7	A	1	Total 168	C 96	N 12	O 60	0

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.

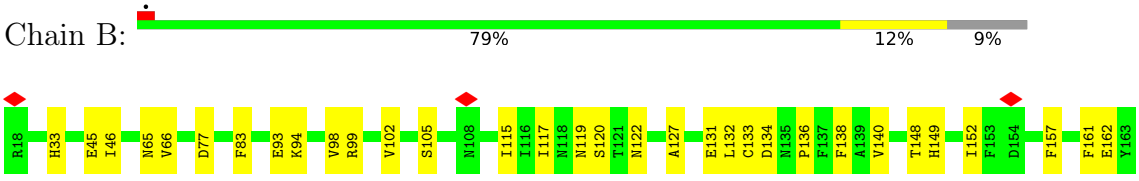
- Molecule 1: Spike glycoprotein

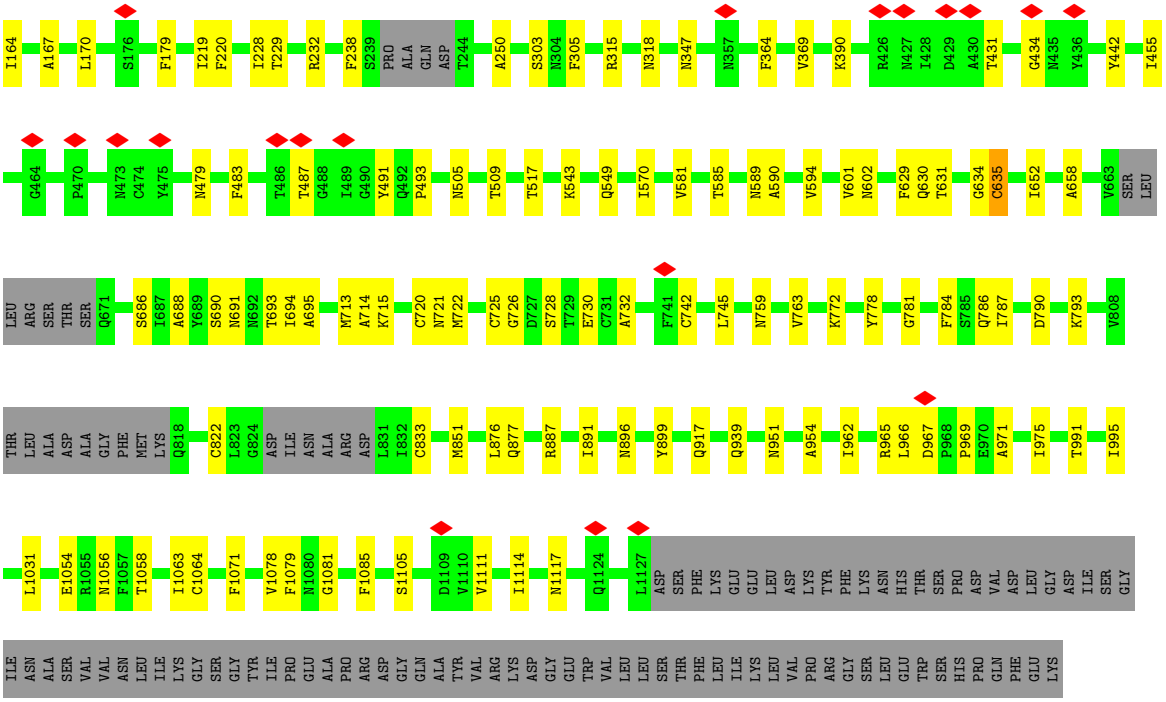
Chain C:



- Molecule 1: Spike glycoprotein

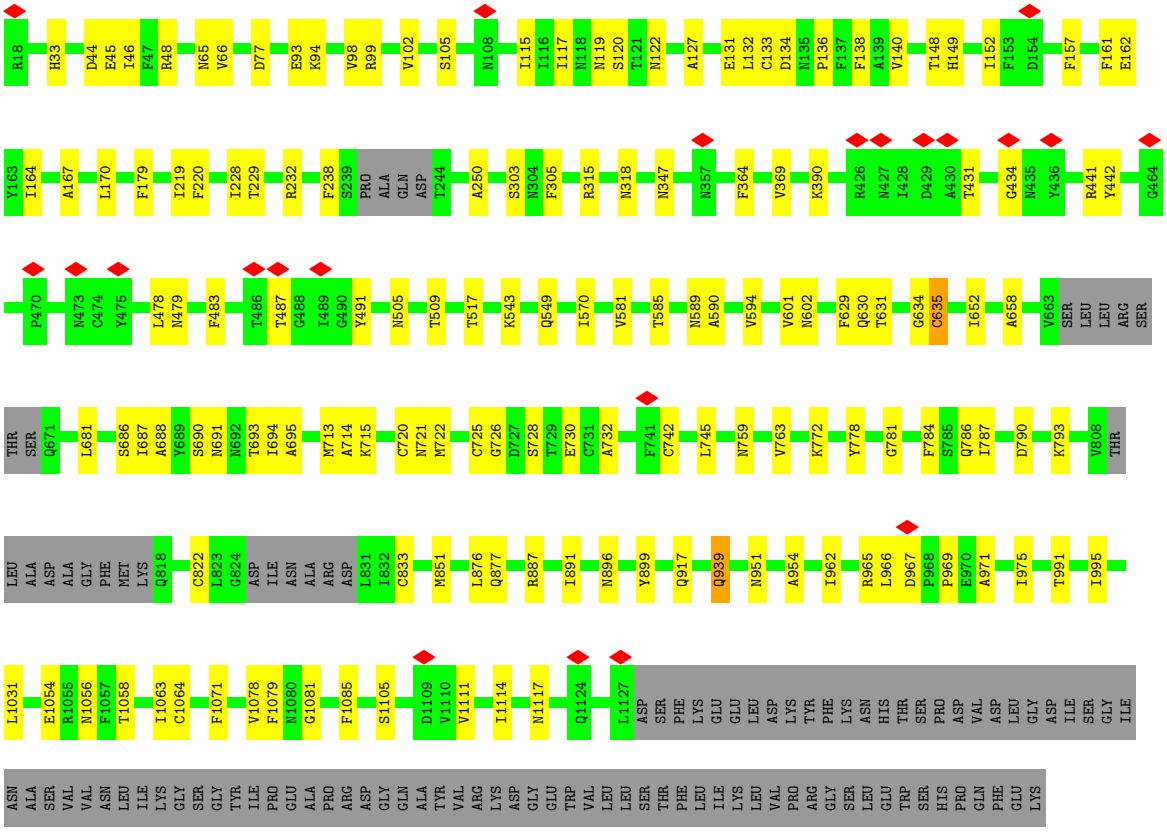
Chain B:





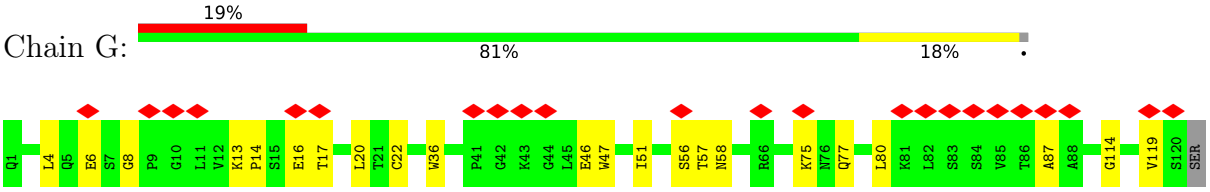
• Molecule 1: Spike glycoprotein

Chain A:



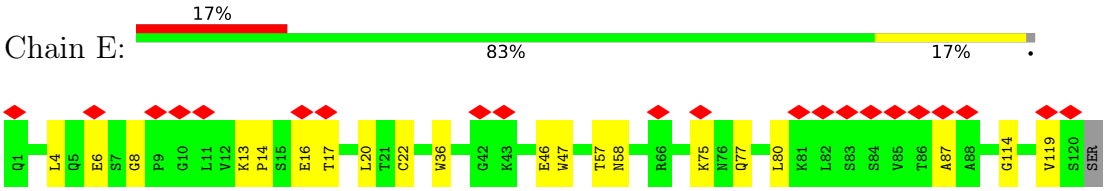
• Molecule 2: 47D11 neutralizing antibody heavy chain

Chain G:



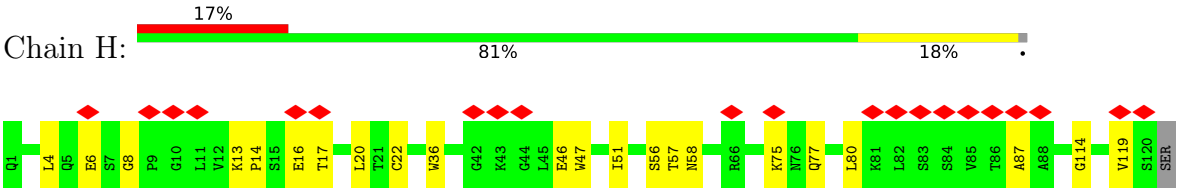
• Molecule 2: 47D11 neutralizing antibody heavy chain

Chain E:



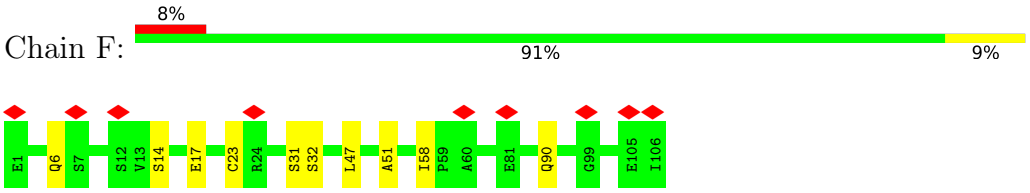
• Molecule 2: 47D11 neutralizing antibody heavy chain

Chain H:



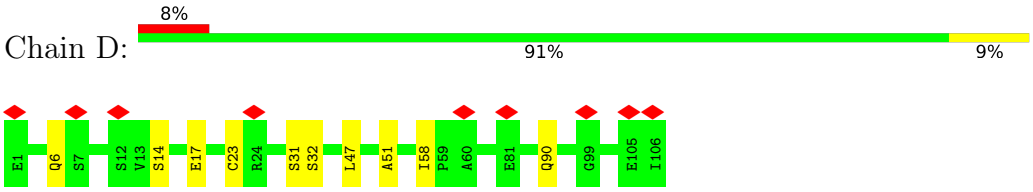
• Molecule 3: 47D11 neutralizing antibody light chain

Chain F:



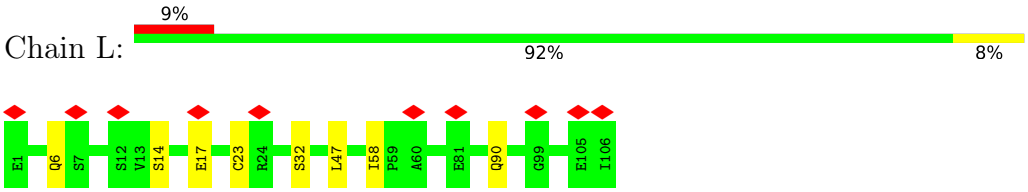
• Molecule 3: 47D11 neutralizing antibody light chain

Chain D:



• Molecule 3: 47D11 neutralizing antibody light chain

Chain L:

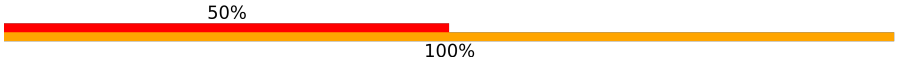


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

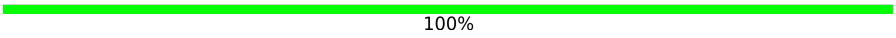
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain M:



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

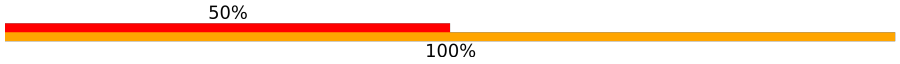
Chain O:

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

Chain P:

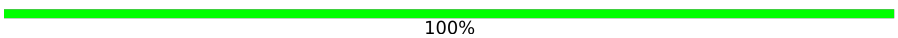
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain S:



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

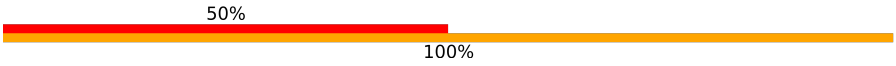
Chain U:

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

Chain V:

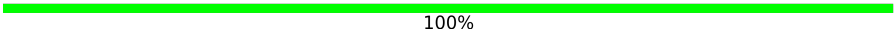
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



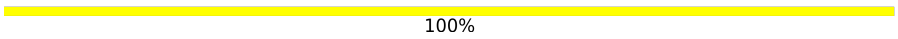
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



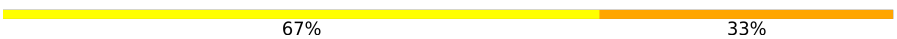
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain N:

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

Chain T:

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

Chain Z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	260941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.29	0/8662	0.53	2/11792 (0.0%)
1	B	0.29	0/8662	0.53	2/11792 (0.0%)
1	C	0.29	0/8662	0.53	2/11792 (0.0%)
2	E	0.25	0/951	0.49	0/1297
2	G	0.25	0/951	0.50	0/1297
2	H	0.25	0/951	0.50	0/1297
3	D	0.28	0/817	0.55	0/1112
3	F	0.27	0/817	0.55	0/1112
3	L	0.28	0/817	0.55	0/1112
All	All	0.28	0/31290	0.53	6/42603 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	635	CYS	CA-CB-SG	6.75	126.14	114.00
1	A	635	CYS	CA-CB-SG	6.74	126.14	114.00
1	C	635	CYS	CA-CB-SG	6.74	126.13	114.00
1	B	720	CYS	CA-CB-SG	6.26	125.27	114.00
1	A	720	CYS	CA-CB-SG	6.25	125.25	114.00

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	8459	0	8194	105	0
1	B	8459	0	8194	103	0
1	C	8459	0	8194	102	0
2	E	925	0	905	14	0
2	G	925	0	905	15	0
2	H	925	0	905	15	0
3	D	798	0	776	5	0
3	F	798	0	776	5	0
3	L	798	0	776	4	0
4	I	28	0	25	1	0
4	K	28	0	25	1	0
4	M	28	0	25	0	0
4	O	28	0	25	2	0
4	P	28	0	25	1	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	U	28	0	25	2	0
4	V	28	0	25	1	0
4	X	28	0	25	1	0
4	Y	28	0	25	0	0
4	a	28	0	25	0	0
5	J	38	0	34	3	0
5	Q	38	0	34	3	0
5	W	38	0	34	3	0
6	N	104	0	88	3	0
6	T	104	0	88	3	0
6	Z	104	0	88	2	0
7	A	168	0	156	10	0
7	B	168	0	156	10	0
7	C	168	0	156	10	0
All	All	31812	0	30759	365	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 6.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:LYS:HE3	2:G:14:PRO:HD2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:CYS:HB3	1:C:833:CYS:HA	1.49	0.92
1:B:822:CYS:HB3	1:B:833:CYS:HA	1.49	0.92
1:A:822:CYS:HB3	1:A:833:CYS:HA	1.49	0.91
2:H:13:LYS:HE3	2:H:14:PRO:HD2	1.50	0.91

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	1074/1193 (90%)	1042 (97%)	32 (3%)	0	100	100
1	B	1074/1193 (90%)	1043 (97%)	31 (3%)	0	100	100
1	C	1074/1193 (90%)	1043 (97%)	31 (3%)	0	100	100
2	E	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
2	G	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
2	H	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
3	D	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
3	F	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
3	L	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
All	All	3888/4260 (91%)	3776 (97%)	112 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	941/1035 (91%)	939 (100%)	2 (0%)	93 97
1	B	941/1035 (91%)	939 (100%)	2 (0%)	93 97
1	C	941/1035 (91%)	939 (100%)	2 (0%)	93 97
2	E	104/105 (99%)	104 (100%)	0	100 100
2	G	104/105 (99%)	104 (100%)	0	100 100
2	H	104/105 (99%)	104 (100%)	0	100 100
3	D	87/87 (100%)	87 (100%)	0	100 100
3	F	87/87 (100%)	87 (100%)	0	100 100
3	L	87/87 (100%)	87 (100%)	0	100 100
All	All	3396/3681 (92%)	3390 (100%)	6 (0%)	93 97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	939	GLN
1	A	364	PHE
1	A	939	GLN
1	C	939	GLN
1	C	364	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	I	1	1,4	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	J	1	5,1	14,14,15	1.13	1 (7%)	17,19,21	1.07	0
5	NAG	J	2	5	14,14,15	0.45	0	17,19,21	0.47	0
5	FUC	J	3	5	10,10,11	0.84	1 (10%)	14,14,16	0.80	0
4	NAG	K	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
4	NAG	M	1	1,4	14,14,15	0.39	0	17,19,21	0.65	0
4	NAG	M	2	4	14,14,15	0.48	0	17,19,21	0.51	0
6	NAG	N	1	6,1	14,14,15	0.38	0	17,19,21	0.49	0
6	NAG	N	2	6	14,14,15	0.33	0	17,19,21	0.53	0
6	BMA	N	3	6	11,11,12	0.60	0	15,15,17	0.74	0
6	MAN	N	4	6	11,11,12	1.61	3 (27%)	15,15,17	1.21	1 (6%)
6	MAN	N	5	6	11,11,12	2.05	3 (27%)	15,15,17	3.01	7 (46%)
6	MAN	N	6	6	11,11,12	1.10	1 (9%)	15,15,17	0.83	0
6	MAN	N	7	6	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
6	MAN	N	8	6	11,11,12	1.06	1 (9%)	15,15,17	1.32	3 (20%)
6	FUC	N	9	6	10,10,11	0.80	1 (10%)	14,14,16	1.32	3 (21%)
4	NAG	O	1	1,4	14,14,15	0.58	1 (7%)	17,19,21	0.49	0
4	NAG	O	2	4	14,14,15	0.46	0	17,19,21	1.27	2 (11%)
4	NAG	P	1	1,4	14,14,15	0.32	0	17,19,21	0.68	1 (5%)
4	NAG	P	2	4	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	Q	1	5,1	14,14,15	1.14	1 (7%)	17,19,21	1.08	0
5	NAG	Q	2	5	14,14,15	0.46	0	17,19,21	0.48	0
5	FUC	Q	3	5	10,10,11	0.85	1 (10%)	14,14,16	0.79	0
4	NAG	R	1	1,4	14,14,15	0.84	1 (7%)	17,19,21	0.50	0
4	NAG	R	2	4	14,14,15	0.56	0	17,19,21	0.72	1 (5%)
4	NAG	S	1	1,4	14,14,15	0.39	0	17,19,21	0.64	0
4	NAG	S	2	4	14,14,15	0.48	0	17,19,21	0.50	0
6	NAG	T	1	6,1	14,14,15	0.37	0	17,19,21	0.50	0
6	NAG	T	2	6	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	T	3	6	11,11,12	0.62	0	15,15,17	0.75	0
6	MAN	T	4	6	11,11,12	1.60	3 (27%)	15,15,17	1.22	1 (6%)
6	MAN	T	5	6	11,11,12	2.04	3 (27%)	15,15,17	3.01	7 (46%)
6	MAN	T	6	6	11,11,12	1.11	1 (9%)	15,15,17	0.83	0
6	MAN	T	7	6	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
6	MAN	T	8	6	11,11,12	1.05	1 (9%)	15,15,17	1.32	3 (20%)
6	FUC	T	9	6	10,10,11	0.80	1 (10%)	14,14,16	1.32	3 (21%)
4	NAG	U	1	1,4	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
4	NAG	U	2	4	14,14,15	0.46	0	17,19,21	1.27	2 (11%)
4	NAG	V	1	1,4	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
4	NAG	V	2	4	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	W	1	5,1	14,14,15	1.13	1 (7%)	17,19,21	1.08	0
5	NAG	W	2	5	14,14,15	0.45	0	17,19,21	0.48	0
5	FUC	W	3	5	10,10,11	0.84	1 (10%)	14,14,16	0.80	0
4	NAG	X	1	1,4	14,14,15	0.84	1 (7%)	17,19,21	0.50	0
4	NAG	X	2	4	14,14,15	0.57	0	17,19,21	0.71	1 (5%)
4	NAG	Y	1	1,4	14,14,15	0.38	0	17,19,21	0.64	0
4	NAG	Y	2	4	14,14,15	0.47	0	17,19,21	0.51	0
6	NAG	Z	1	6,1	14,14,15	0.38	0	17,19,21	0.50	0
6	NAG	Z	2	6	14,14,15	0.32	0	17,19,21	0.52	0
6	BMA	Z	3	6	11,11,12	0.60	0	15,15,17	0.74	0
6	MAN	Z	4	6	11,11,12	1.60	3 (27%)	15,15,17	1.21	1 (6%)
6	MAN	Z	5	6	11,11,12	2.05	3 (27%)	15,15,17	3.02	7 (46%)
6	MAN	Z	6	6	11,11,12	1.10	1 (9%)	15,15,17	0.82	0
6	MAN	Z	7	6	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
6	MAN	Z	8	6	11,11,12	1.05	1 (9%)	15,15,17	1.32	3 (20%)
6	FUC	Z	9	6	10,10,11	0.81	1 (10%)	14,14,16	1.32	3 (21%)
4	NAG	a	1	1,4	14,14,15	0.58	1 (7%)	17,19,21	0.50	0
4	NAG	a	2	4	14,14,15	0.46	0	17,19,21	1.27	2 (11%)

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	I	1	1,4	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	T	8	6	-	2/2/19/22	0/1/1/1
6	FUC	T	9	6	-	-	0/1/1/1
4	NAG	U	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	U	2	4	-	5/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	FUC	W	3	5	-	-	0/1/1/1
4	NAG	X	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	3/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	3/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	1/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	6	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	7	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	8	6	-	2/2/19/22	0/1/1/1
6	FUC	Z	9	6	-	-	0/1/1/1
4	NAG	a	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	a	2	4	-	5/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	5	MAN	C1-C2	4.90	1.63	1.52
6	Z	5	MAN	C1-C2	4.89	1.63	1.52
6	T	5	MAN	C1-C2	4.87	1.63	1.52
5	Q	1	NAG	O5-C1	-4.11	1.37	1.43
5	J	1	NAG	O5-C1	-4.10	1.37	1.43

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	5	MAN	C1-O5-C5	7.75	122.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	5	MAN	C1-O5-C5	7.74	122.68	112.19
6	T	5	MAN	C1-O5-C5	7.74	122.67	112.19
6	Z	5	MAN	O5-C5-C6	4.43	114.14	107.20
6	Z	5	MAN	C1-C2-C3	4.41	115.09	109.67

There are no chirality outliers.

5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6

There are no ring outliers.

32 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	2	NAG	1	0
4	V	1	NAG	1	0
4	U	2	NAG	2	0
6	T	3	BMA	1	0
4	X	2	NAG	1	0
4	I	1	NAG	1	0
6	T	4	MAN	2	0
4	O	1	NAG	1	0
6	T	5	MAN	2	0
6	N	3	BMA	1	0
4	V	2	NAG	1	0
5	Q	1	NAG	2	0
4	O	2	NAG	2	0
4	I	2	NAG	1	0
5	J	1	NAG	2	0
5	J	2	NAG	3	0
4	K	1	NAG	1	0
4	K	2	NAG	1	0
4	R	2	NAG	1	0
6	Z	4	MAN	2	0
4	X	1	NAG	1	0
6	T	6	MAN	1	0

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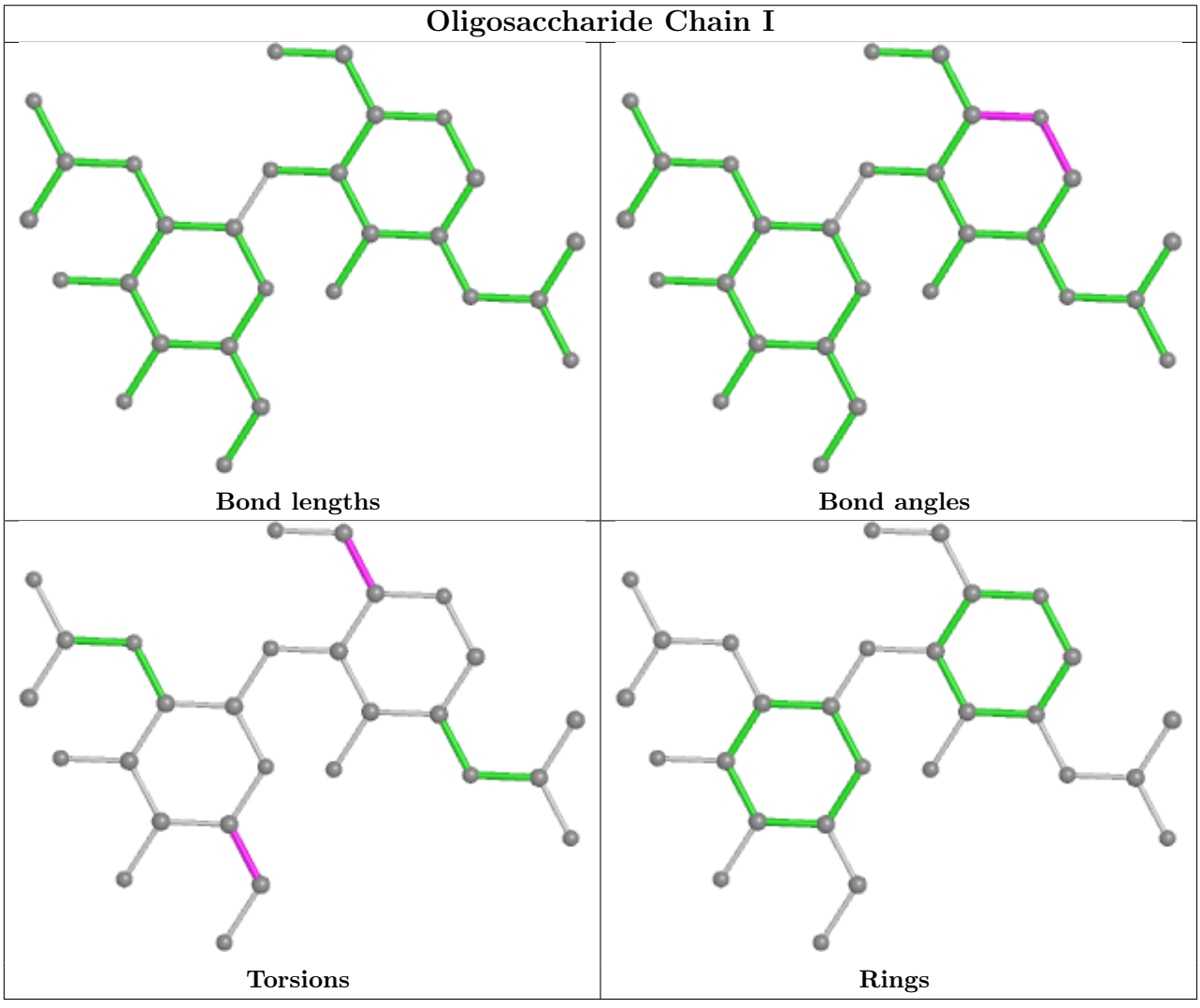
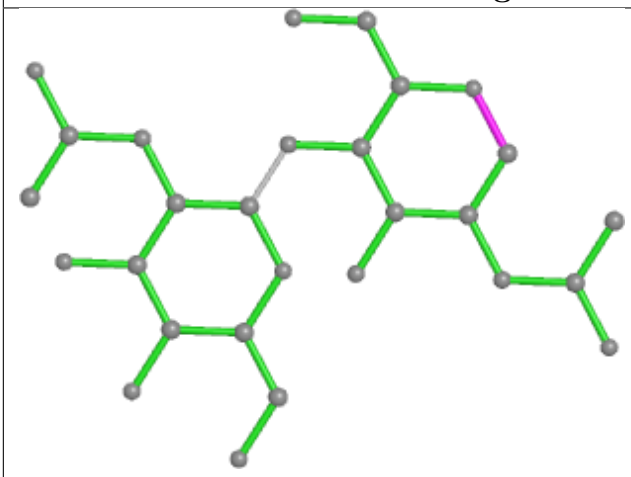
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	1	NAG	2	0
6	Z	5	MAN	2	0
5	W	2	NAG	3	0
5	Q	2	NAG	3	0
6	N	4	MAN	2	0
6	N	5	MAN	2	0
4	P	1	NAG	1	0
6	N	6	MAN	1	0
4	R	1	NAG	1	0
4	U	1	NAG	1	0

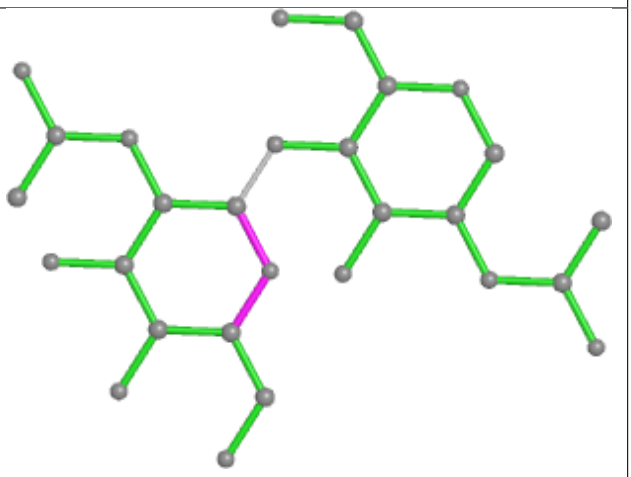
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



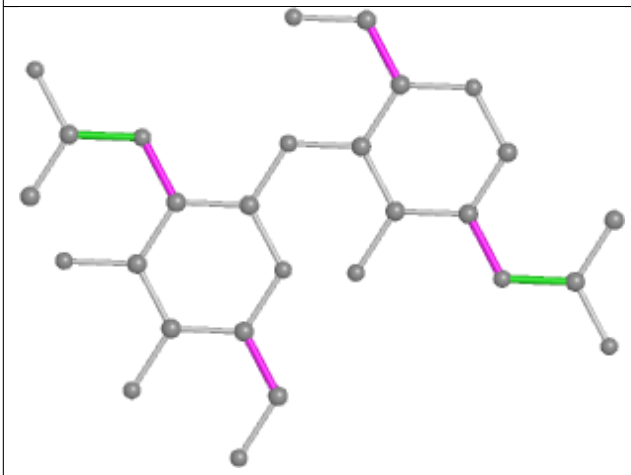
Oligosaccharide Chain K



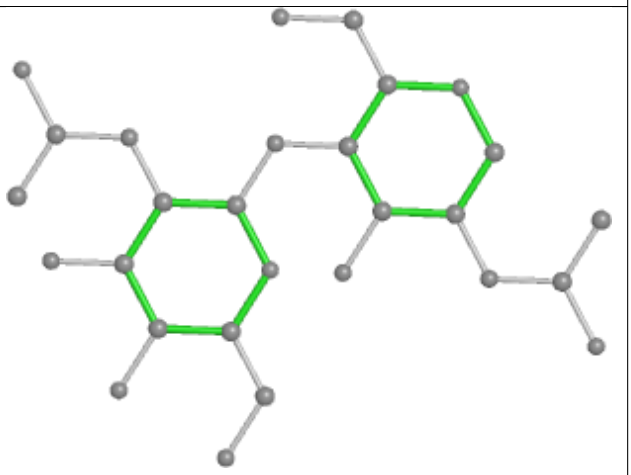
Bond lengths



Bond angles

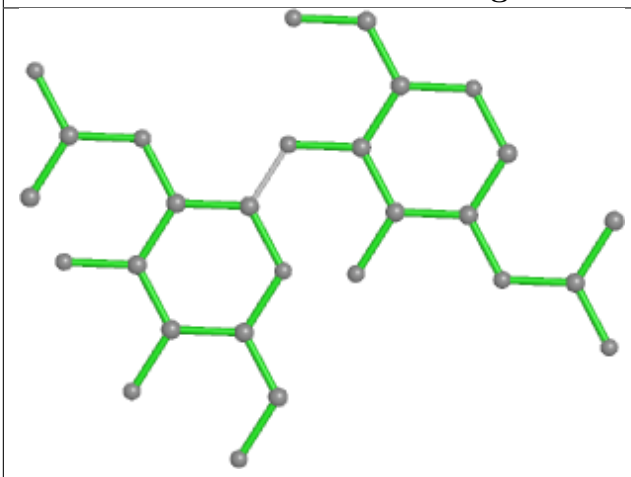


Torsions

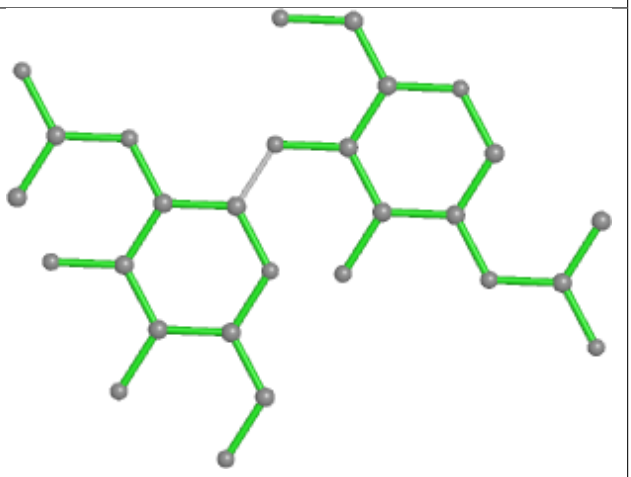


Rings

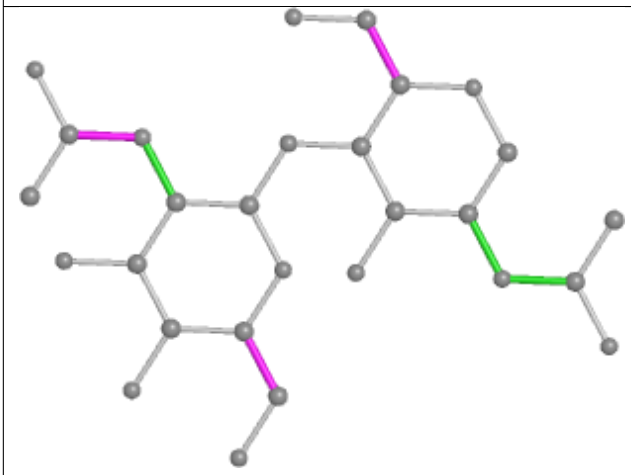
Oligosaccharide Chain M



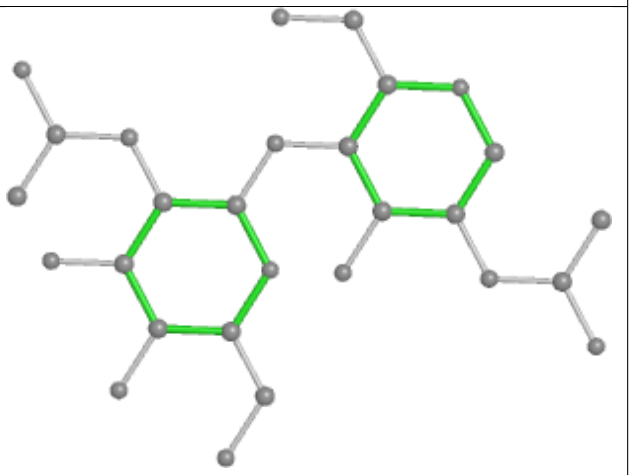
Bond lengths



Bond angles

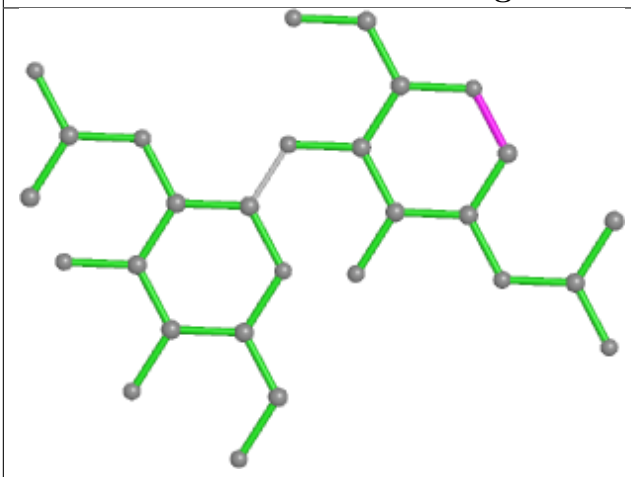


Torsions

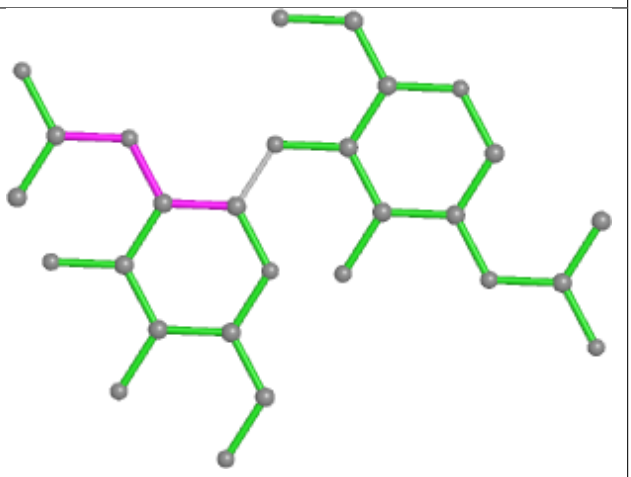


Rings

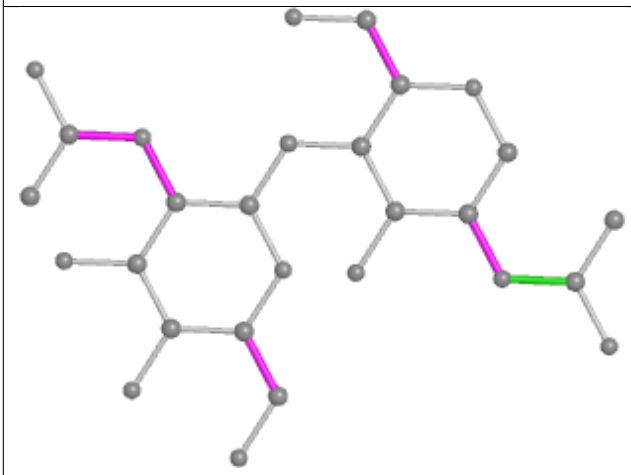
Oligosaccharide Chain O



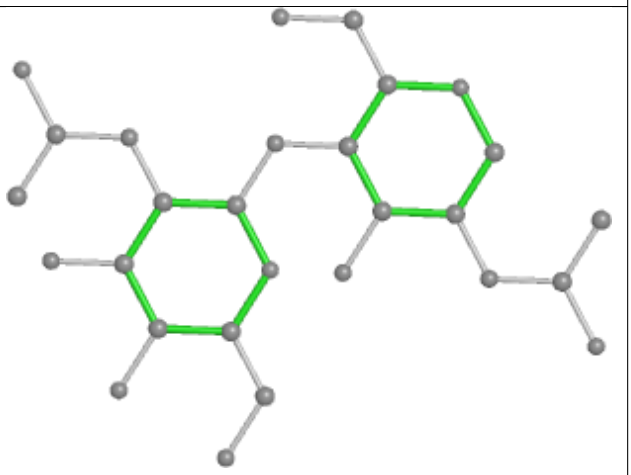
Bond lengths



Bond angles

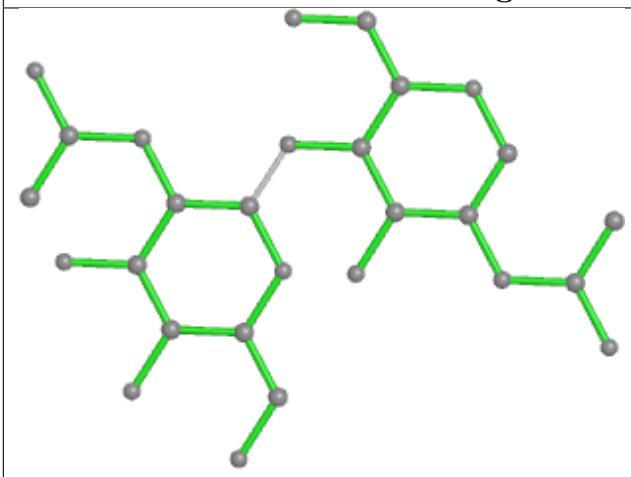


Torsions

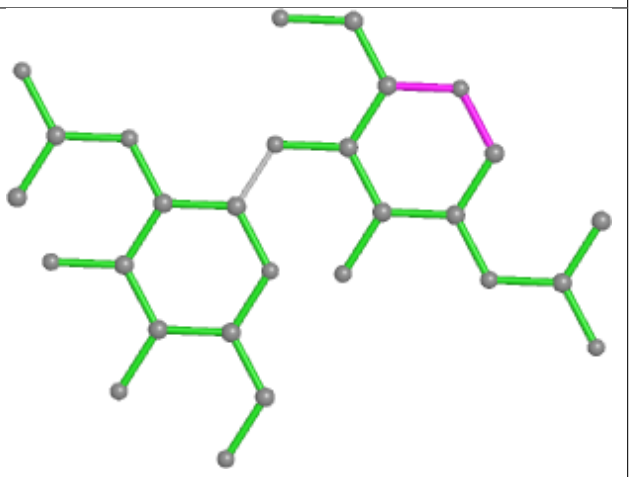


Rings

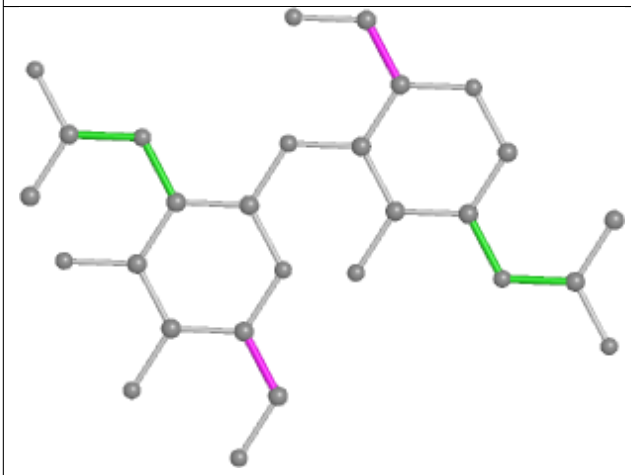
Oligosaccharide Chain P



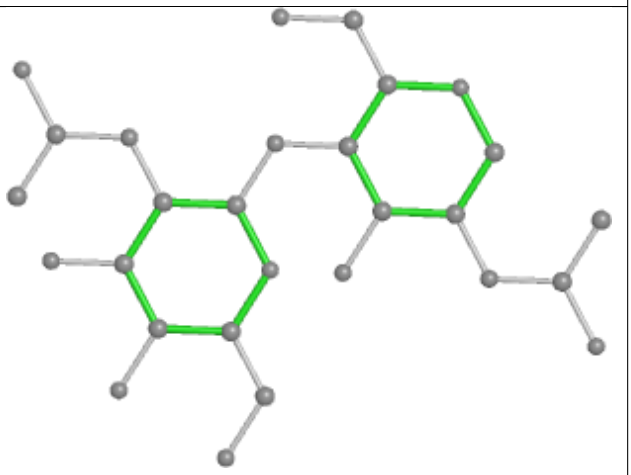
Bond lengths



Bond angles

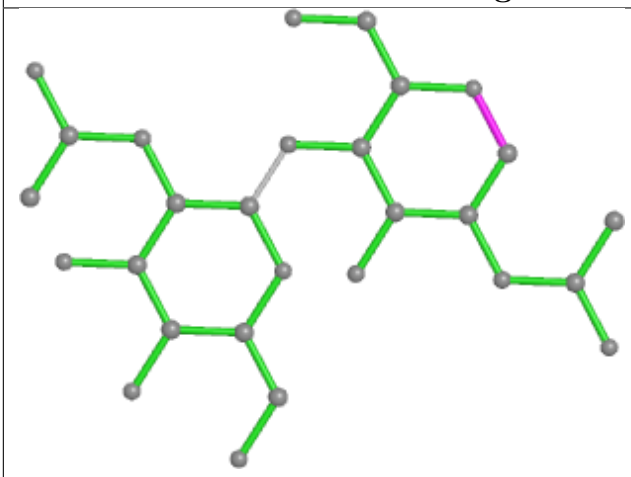


Torsions



Rings

Oligosaccharide Chain R



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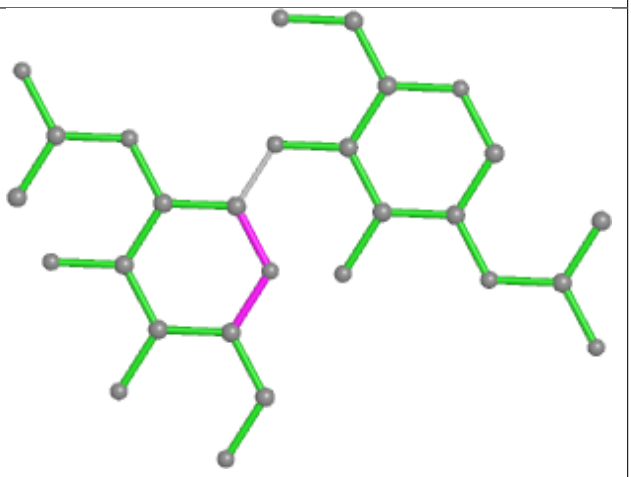
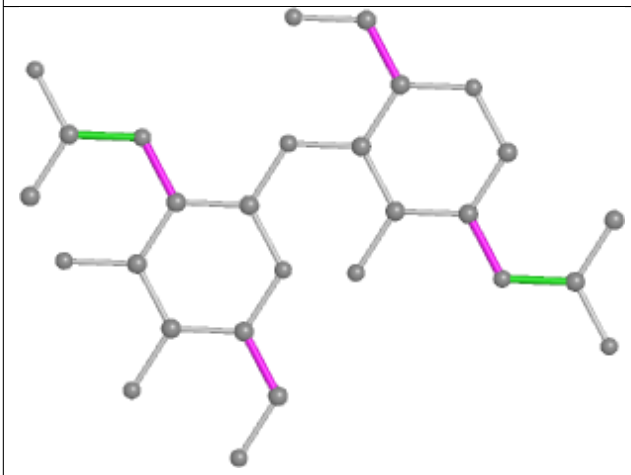


Bond angles



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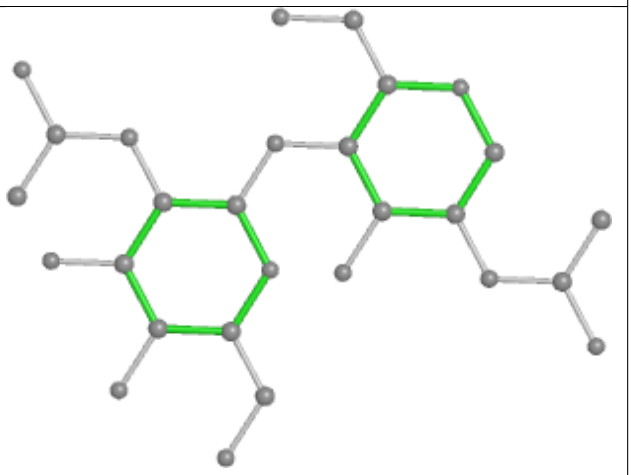
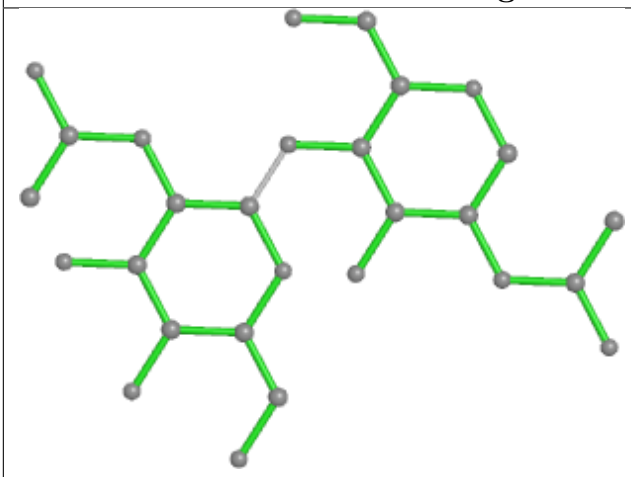


Rings

Oligosaccharide Chain S



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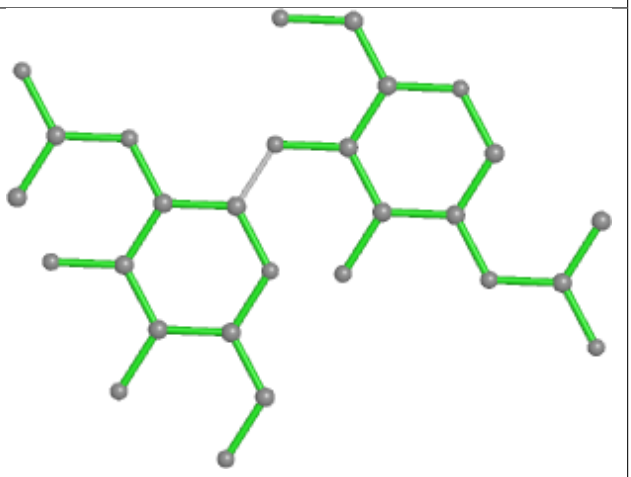
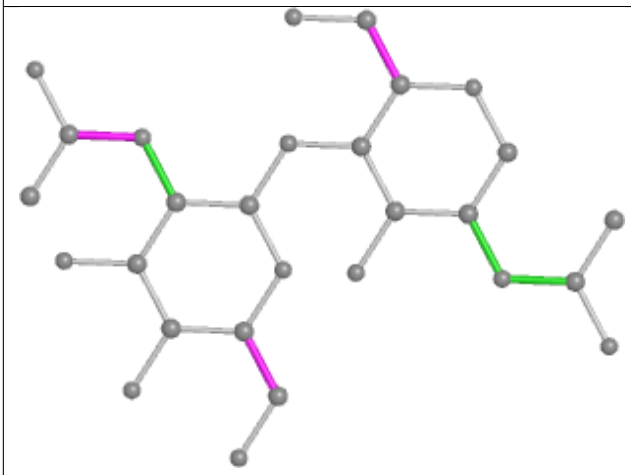


Bond angles



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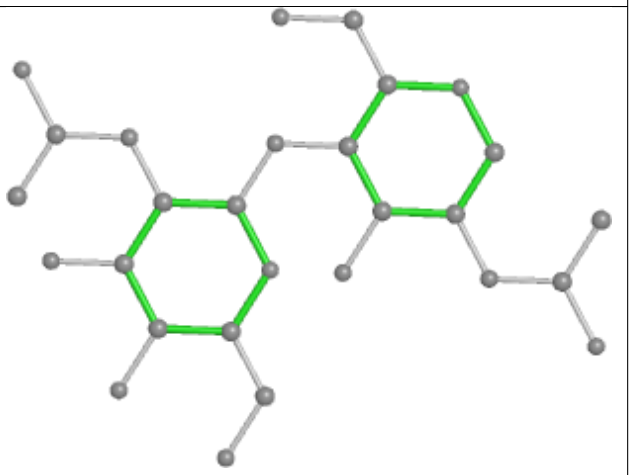
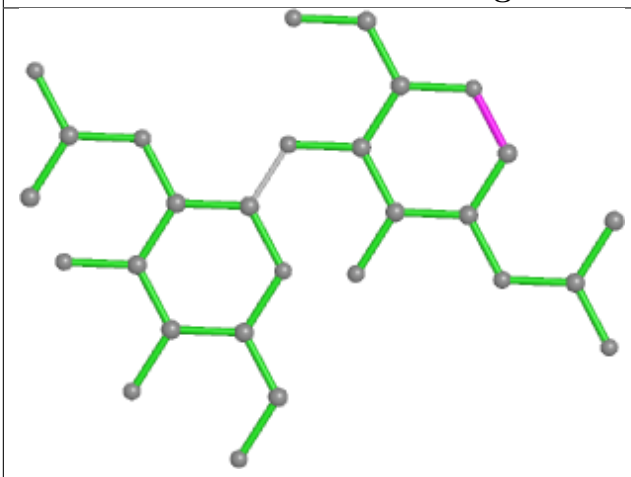
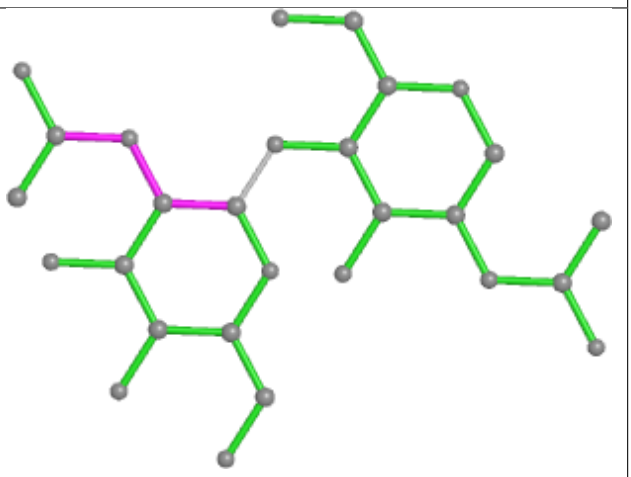


Rings

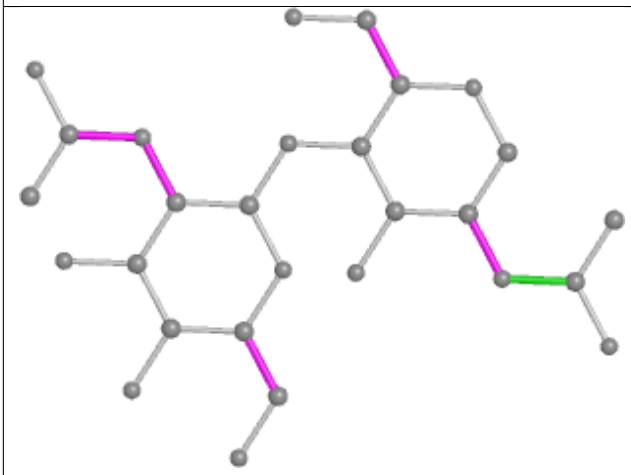
Oligosaccharide Chain U



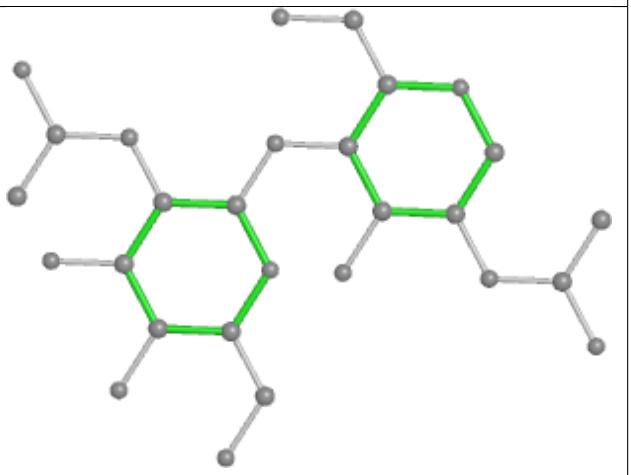
Bond lengths



Bond angles

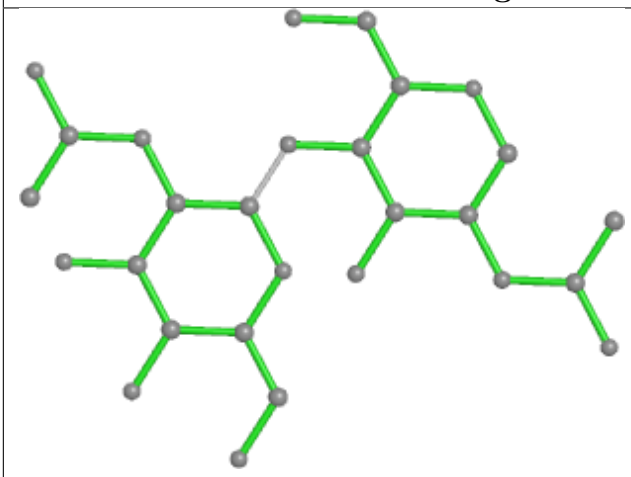


Torsions

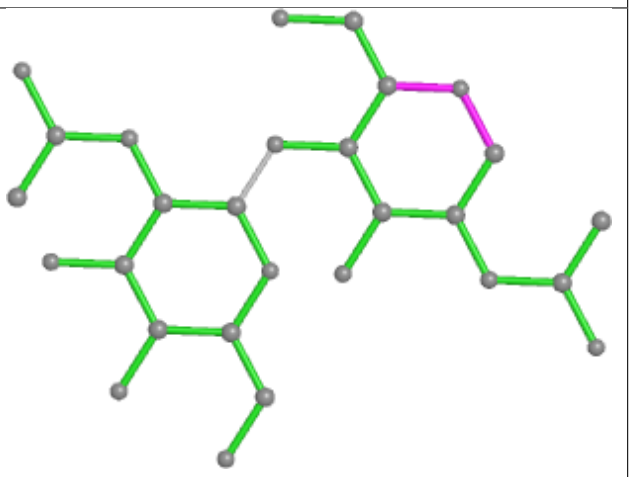


Rings

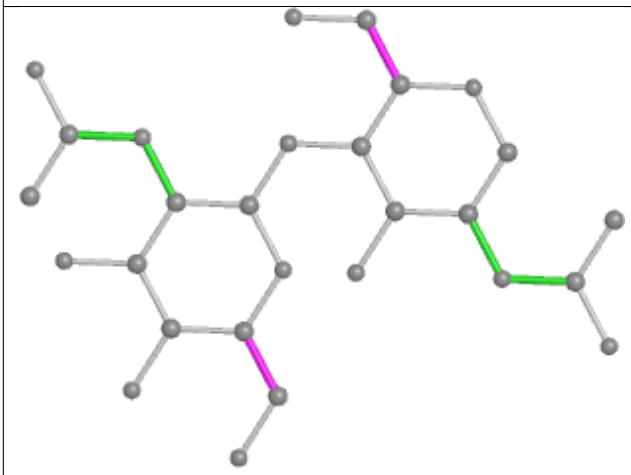
Oligosaccharide Chain V



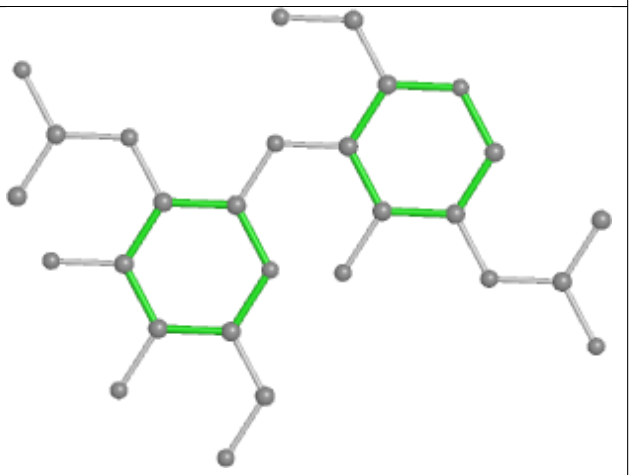
Bond lengths



Bond angles

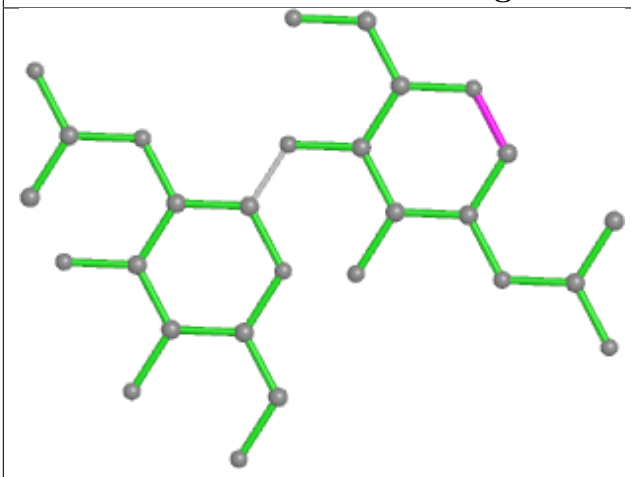


Torsions

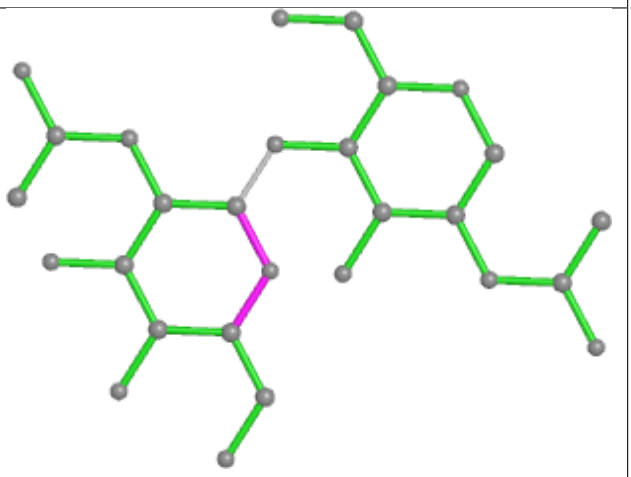


Rings

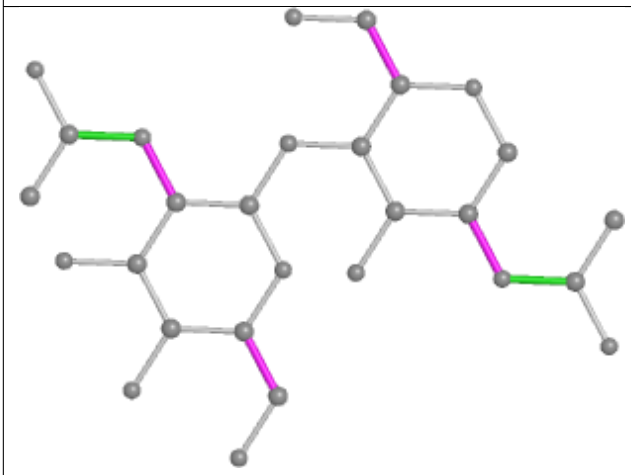
Oligosaccharide Chain X



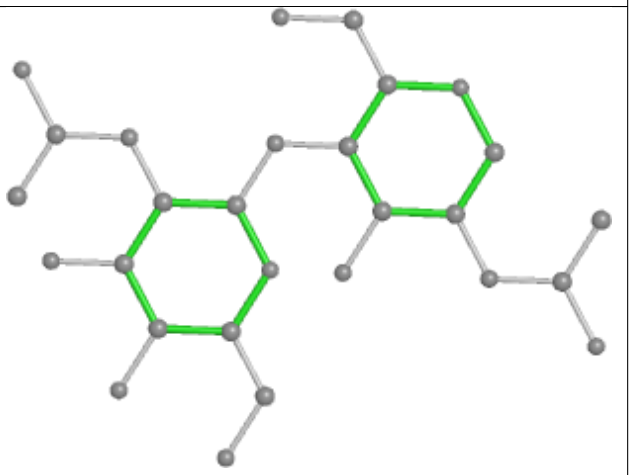
Bond lengths



Bond angles

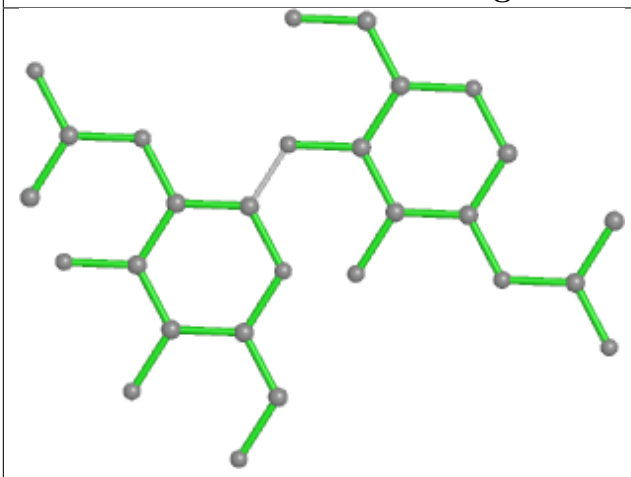


Torsions

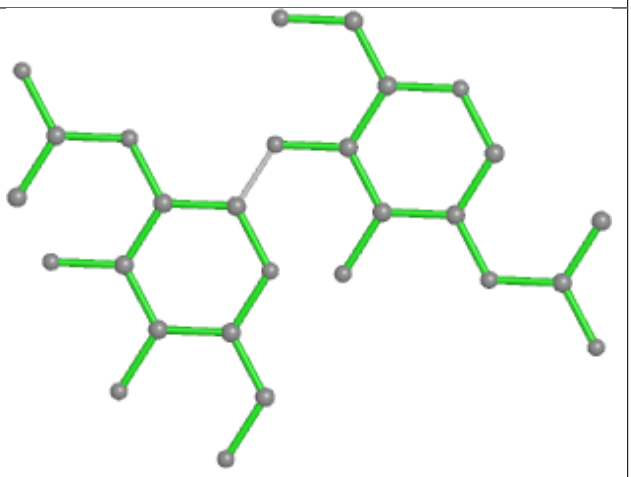


Rings

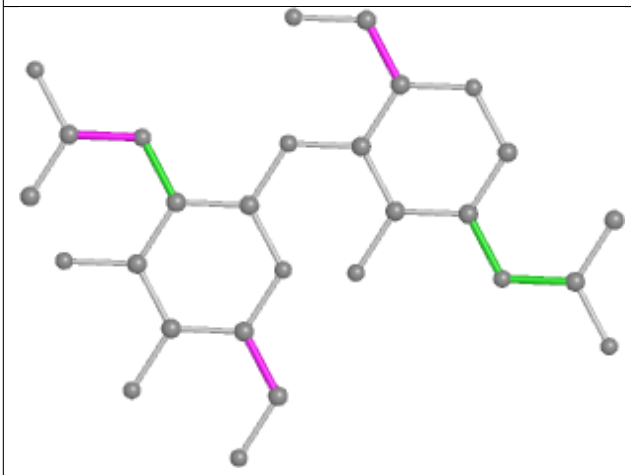
Oligosaccharide Chain Y



Bond lengths



Bond angles



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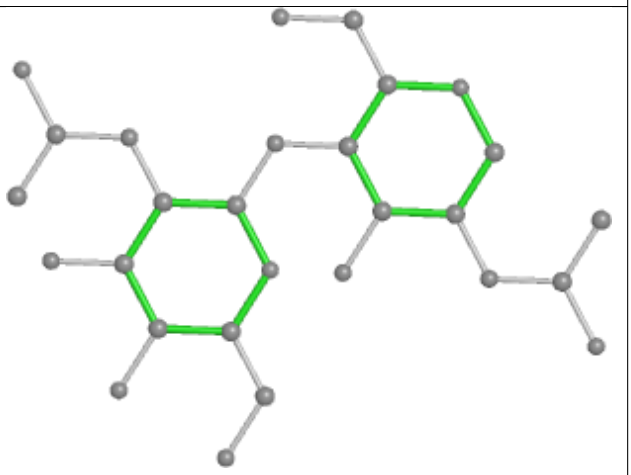
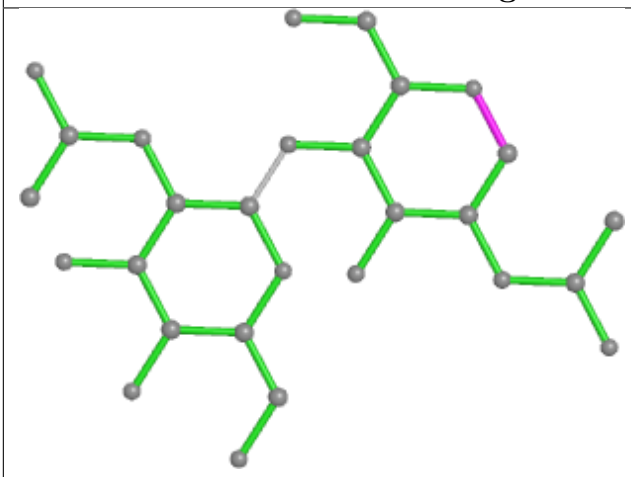
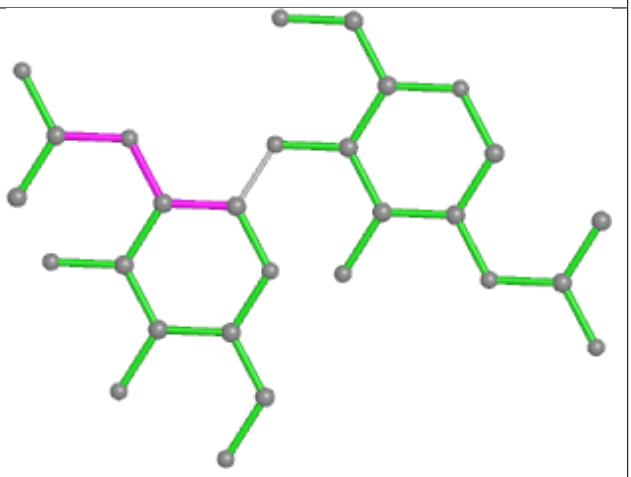


Rings

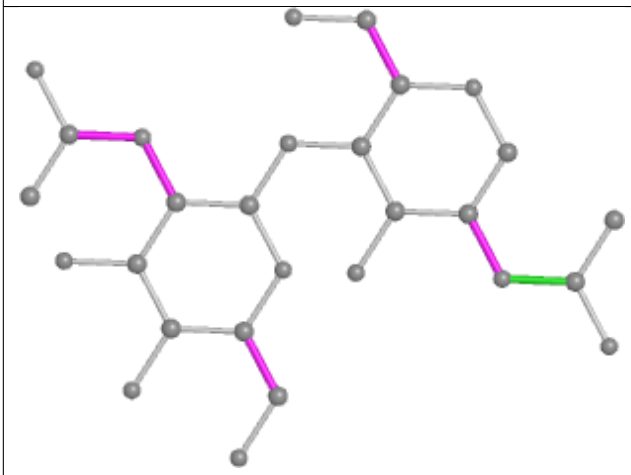
Oligosaccharide Chain a



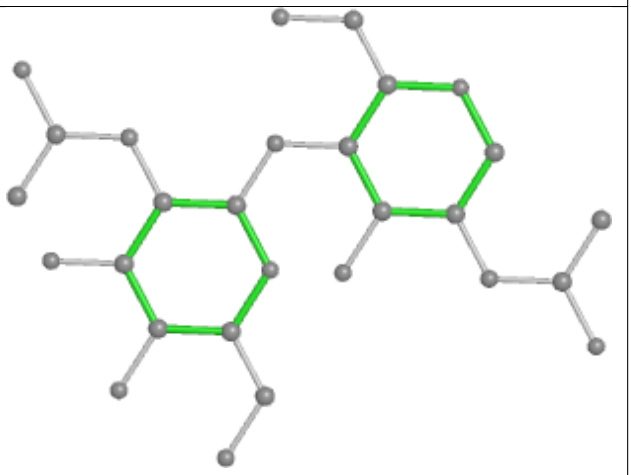
Bond lengths



Bond angles

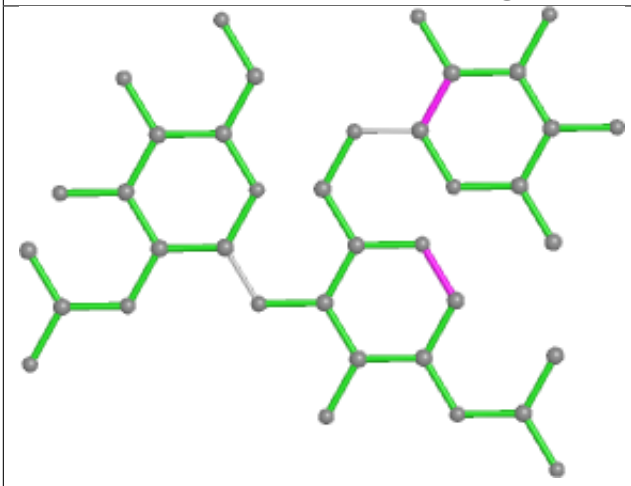


Torsions

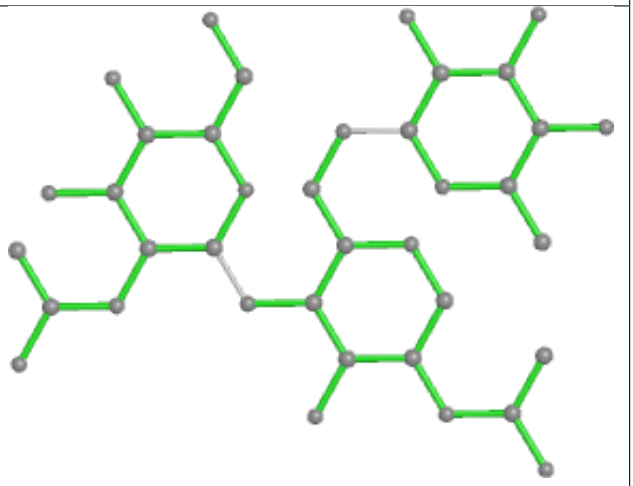


Rings

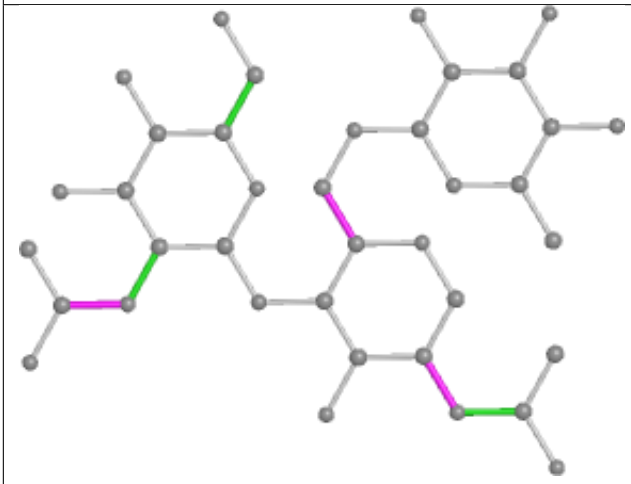
Oligosaccharide Chain J



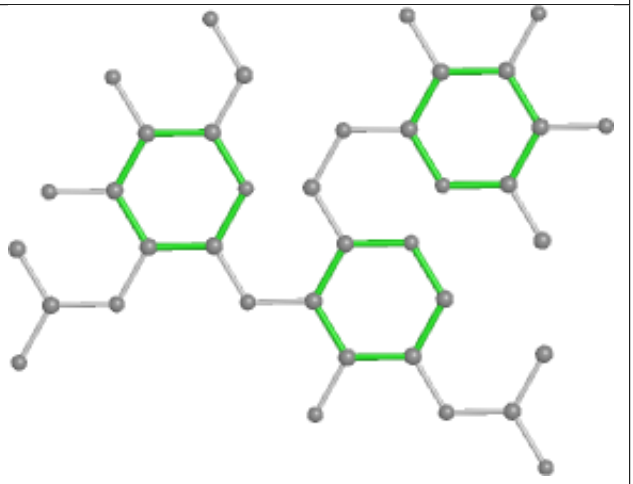
Bond lengths



Bond angles

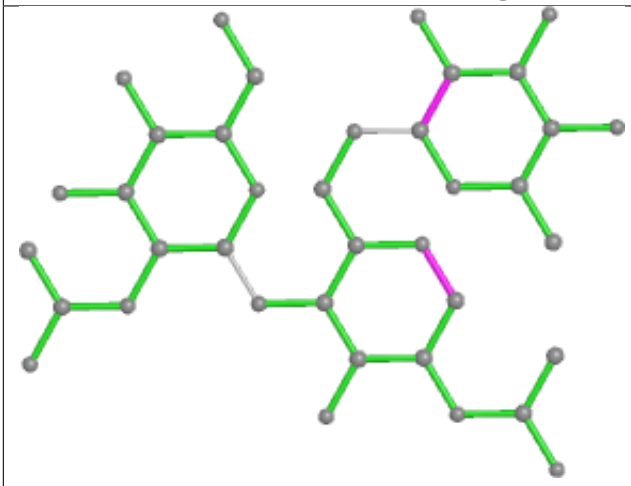


Torsions

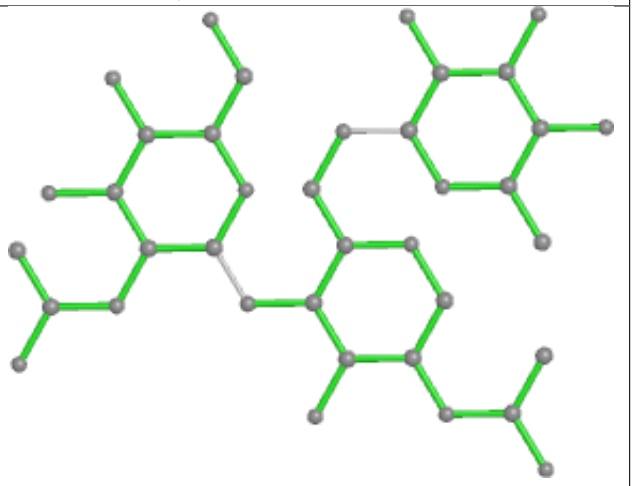


Rings

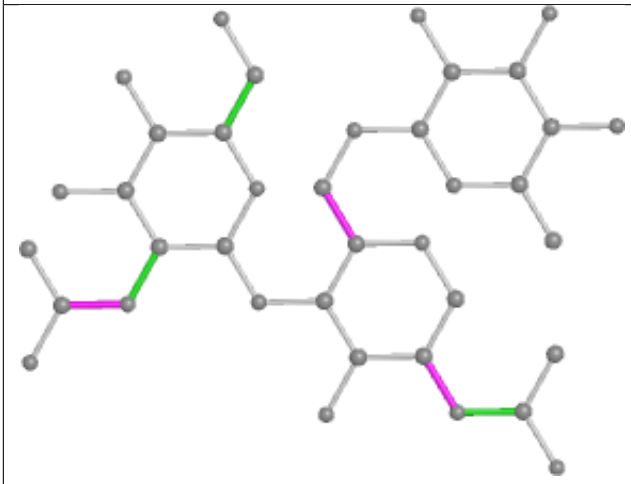
Oligosaccharide Chain Q



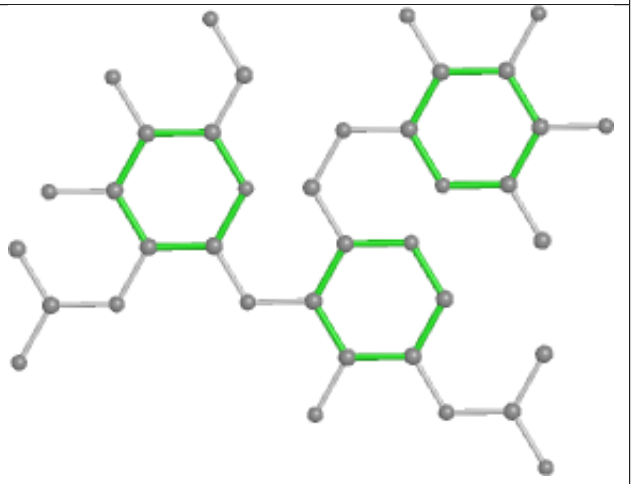
Bond lengths



Bond angles

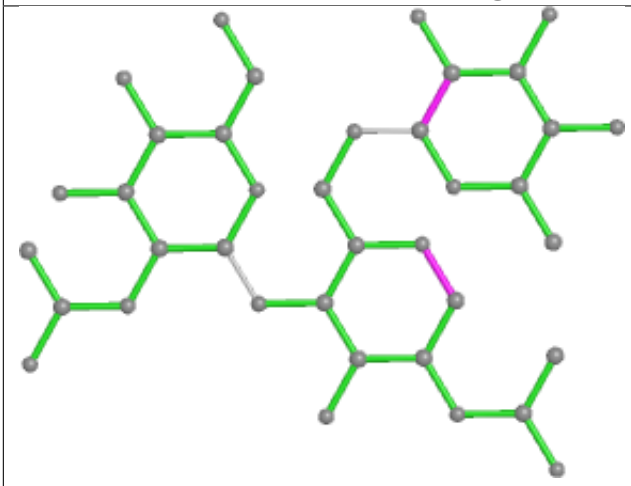


Torsions

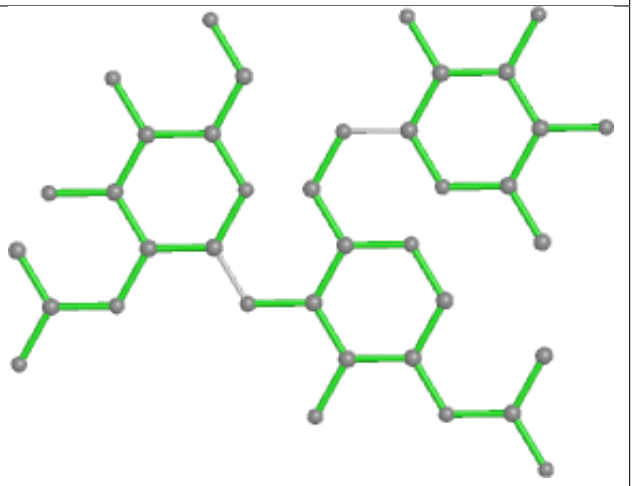


Rings

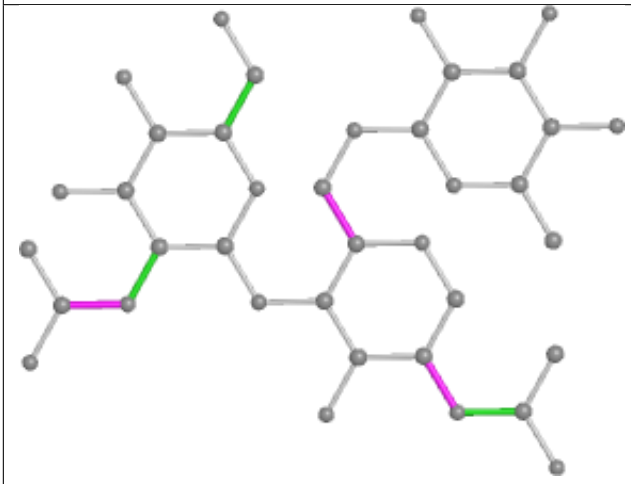
Oligosaccharide Chain W



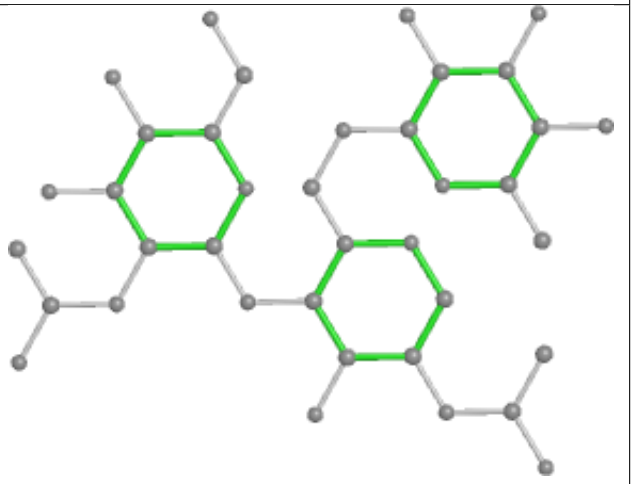
Bond lengths



Bond angles

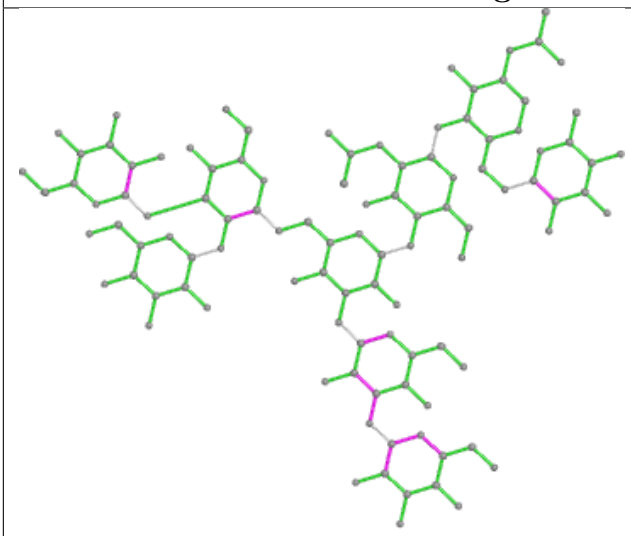


Torsions

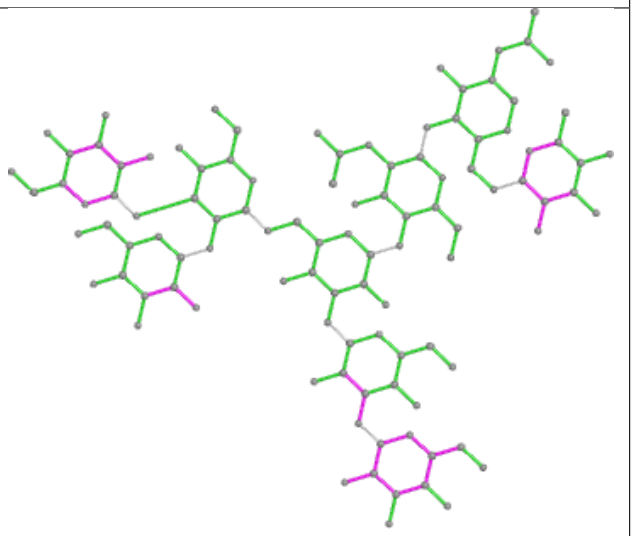


Rings

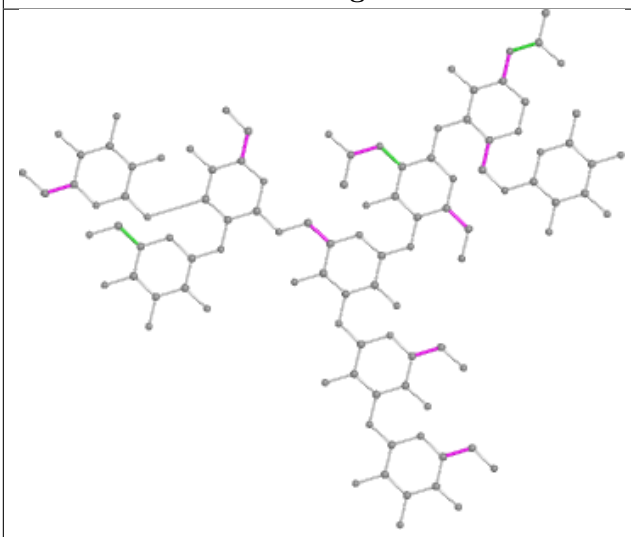
Oligosaccharide Chain N



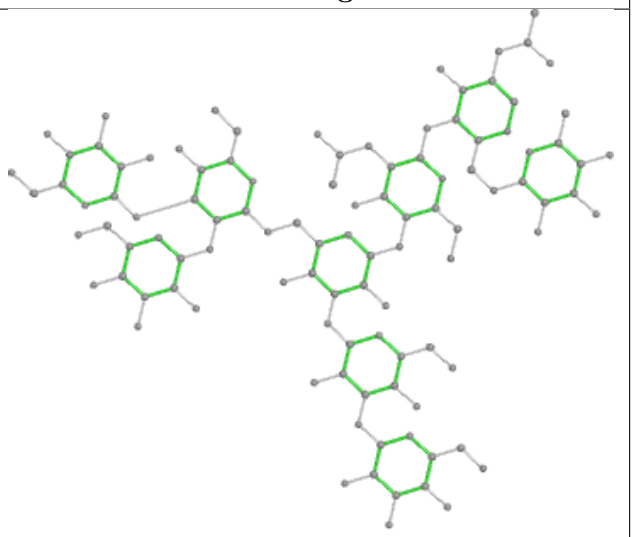
Bond lengths



Bond angles

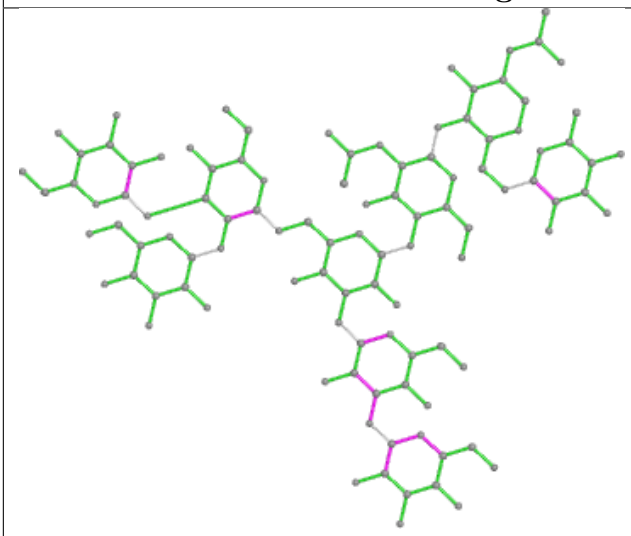


Torsions

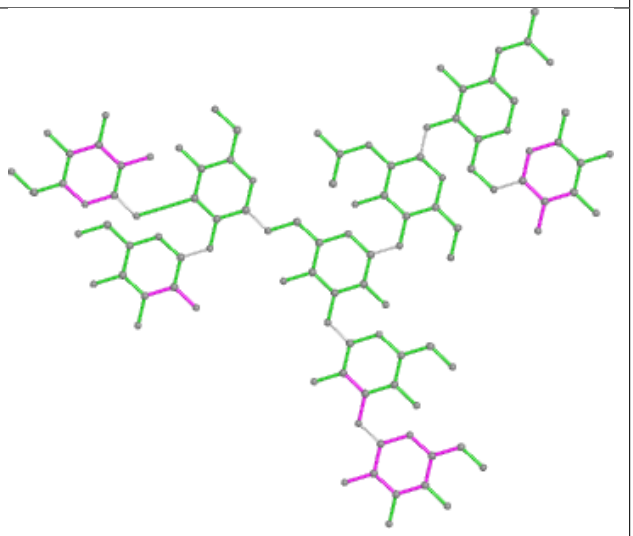


Rings

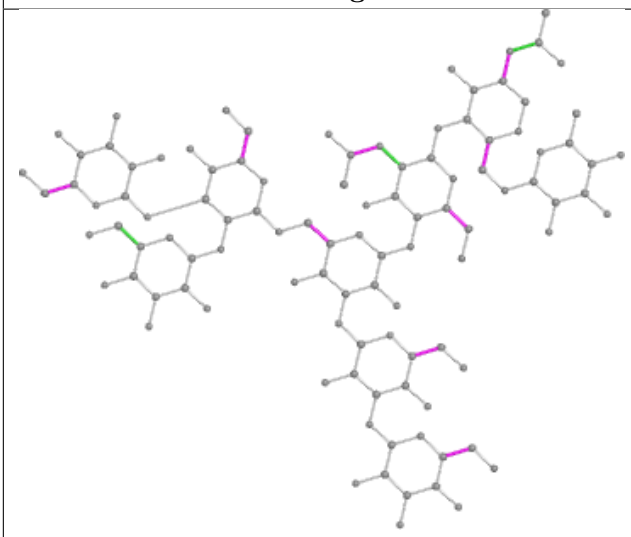
Oligosaccharide Chain T



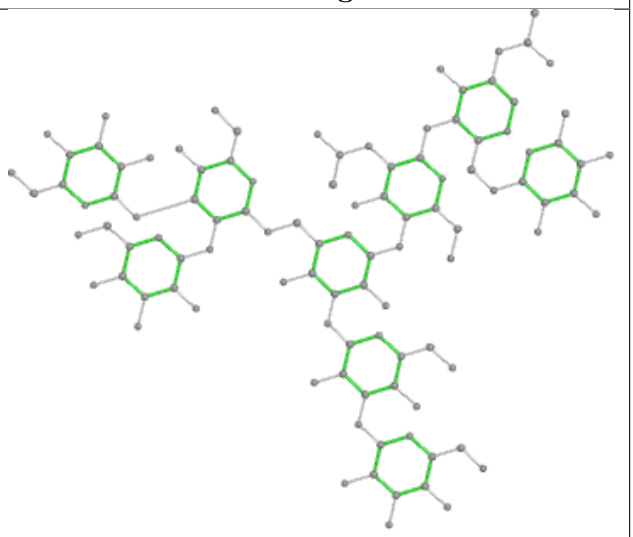
Bond lengths



Bond angles

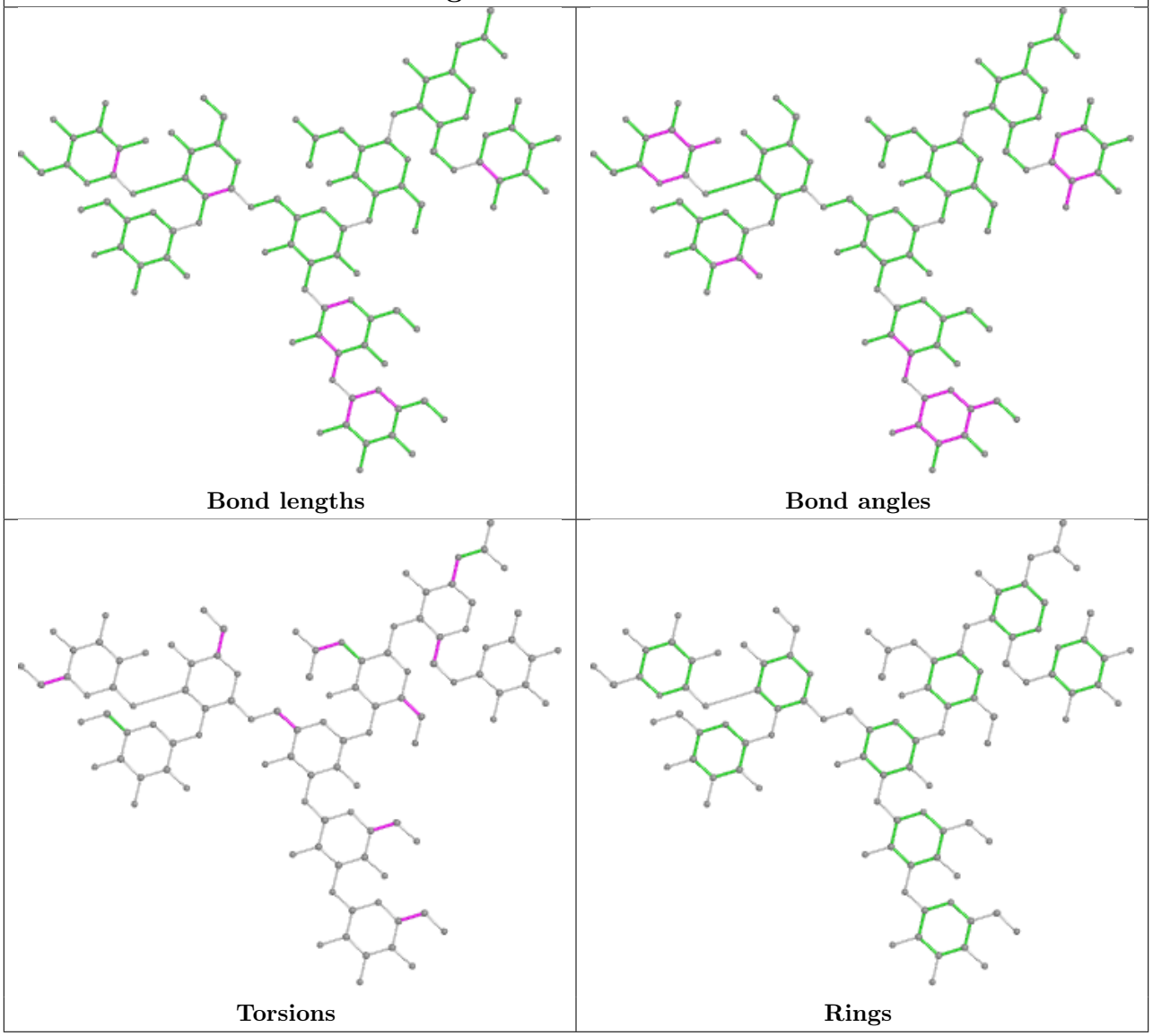


Torsions



Rings

Oligosaccharide Chain Z



5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
7	NAG	B	1311	1	14,14,15	0.45	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	1309	1	14,14,15	0.48	0	17,19,21	0.55	0
7	NAG	C	1311	1	14,14,15	0.46	0	17,19,21	0.52	0
7	NAG	B	1312	1	14,14,15	0.51	0	17,19,21	0.63	0
7	NAG	B	1303	1	14,14,15	0.69	0	17,19,21	0.65	0
7	NAG	B	1307	-	14,14,15	0.30	0	17,19,21	0.51	0
7	NAG	C	1306	-	14,14,15	1.10	1 (7%)	17,19,21	0.72	0
7	NAG	A	1307	-	14,14,15	0.31	0	17,19,21	0.50	0
7	NAG	C	1310	1	14,14,15	0.58	0	17,19,21	0.50	0
7	NAG	A	1311	1	14,14,15	0.44	0	17,19,21	0.52	0
7	NAG	C	1305	1	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
7	NAG	A	1308	1	14,14,15	0.77	1 (7%)	17,19,21	1.42	3 (17%)
7	NAG	C	1302	-	14,14,15	0.34	0	17,19,21	0.59	0
7	NAG	B	1306	-	14,14,15	1.11	1 (7%)	17,19,21	0.72	0
7	NAG	C	1304	1	14,14,15	0.55	0	17,19,21	0.62	0
7	NAG	B	1308	1	14,14,15	0.77	1 (7%)	17,19,21	1.42	3 (17%)
7	NAG	A	1312	1	14,14,15	0.51	0	17,19,21	0.63	0
7	NAG	B	1301	1	14,14,15	0.58	1 (7%)	17,19,21	0.53	0
7	NAG	A	1301	1	14,14,15	0.58	1 (7%)	17,19,21	0.54	0
7	NAG	C	1301	1	14,14,15	0.59	1 (7%)	17,19,21	0.54	0
7	NAG	A	1306	-	14,14,15	1.09	1 (7%)	17,19,21	0.73	0
7	NAG	A	1309	1	14,14,15	0.49	0	17,19,21	0.55	0
7	NAG	A	1302	-	14,14,15	0.35	0	17,19,21	0.58	0
7	NAG	B	1309	1	14,14,15	0.50	0	17,19,21	0.54	0
7	NAG	C	1312	1	14,14,15	0.51	0	17,19,21	0.63	0
7	NAG	A	1305	1	14,14,15	0.49	0	17,19,21	1.35	2 (11%)
7	NAG	B	1305	1	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
7	NAG	A	1304	1	14,14,15	0.55	0	17,19,21	0.61	0
7	NAG	B	1304	1	14,14,15	0.55	0	17,19,21	0.61	0
7	NAG	C	1308	1	14,14,15	0.77	1 (7%)	17,19,21	1.42	3 (17%)
7	NAG	B	1310	1	14,14,15	0.57	0	17,19,21	0.51	0
7	NAG	C	1303	1	14,14,15	0.69	0	17,19,21	0.64	0
7	NAG	A	1303	1	14,14,15	0.68	0	17,19,21	0.65	0
7	NAG	C	1307	-	14,14,15	0.29	0	17,19,21	0.50	0
7	NAG	A	1310	1	14,14,15	0.58	0	17,19,21	0.50	0
7	NAG	B	1302	-	14,14,15	0.33	0	17,19,21	0.59	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
7	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1312	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1307	-	-	4/6/23/26	0/1/1/1
7	NAG	C	1306	-	-	1/6/23/26	0/1/1/1
7	NAG	A	1307	-	-	4/6/23/26	0/1/1/1
7	NAG	C	1310	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1302	-	-	3/6/23/26	0/1/1/1
7	NAG	B	1306	-	-	1/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1312	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1306	-	-	1/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1302	-	-	3/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1312	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1307	-	-	4/6/23/26	0/1/1/1
7	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1302	-	-	3/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1306	NAG	O5-C1	-4.05	1.37	1.43
7	C	1306	NAG	O5-C1	-4.04	1.37	1.43
7	A	1306	NAG	O5-C1	-3.99	1.37	1.43
7	A	1308	NAG	O5-C1	-2.44	1.39	1.43
7	C	1308	NAG	O5-C1	-2.44	1.39	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1308	NAG	C2-N2-C7	4.54	129.37	122.90
7	B	1308	NAG	C2-N2-C7	4.48	129.28	122.90
7	A	1308	NAG	C2-N2-C7	4.48	129.28	122.90
7	C	1305	NAG	C2-N2-C7	4.27	128.98	122.90
7	A	1305	NAG	C2-N2-C7	4.26	128.97	122.90

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1304	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	A	1304	NAG	O5-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	B	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

24 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1311	NAG	1	0
7	C	1311	NAG	1	0
7	B	1303	NAG	2	0
7	B	1307	NAG	1	0
7	A	1307	NAG	1	0
7	C	1310	NAG	1	0
7	A	1311	NAG	1	0
7	C	1305	NAG	1	0
7	A	1308	NAG	2	0
7	C	1304	NAG	1	0
7	B	1308	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1301	NAG	1	0
7	A	1301	NAG	1	0
7	C	1301	NAG	1	0
7	A	1305	NAG	1	0
7	B	1305	NAG	1	0
7	A	1304	NAG	1	0
7	B	1304	NAG	1	0
7	C	1308	NAG	2	0
7	B	1310	NAG	1	0
7	C	1303	NAG	2	0
7	A	1303	NAG	2	0
7	C	1307	NAG	1	0
7	A	1310	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

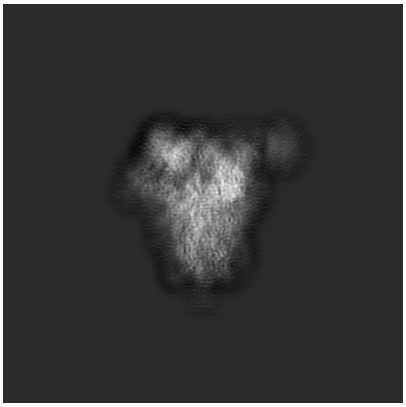
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11813. These allow visual inspection of the internal detail of the map and identification of artifacts.

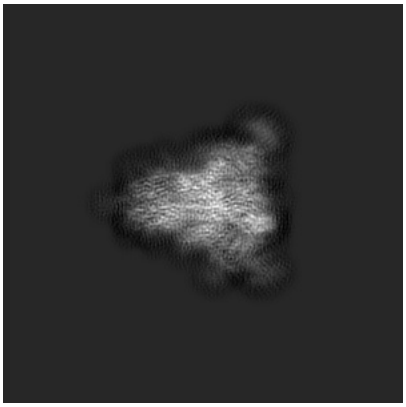
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

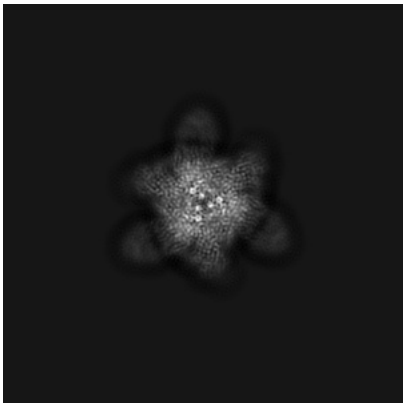
6.1.1 Primary map



X



Y

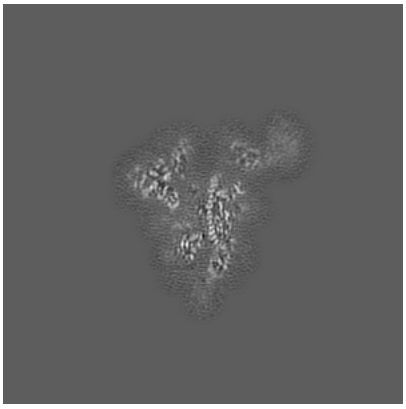


Z

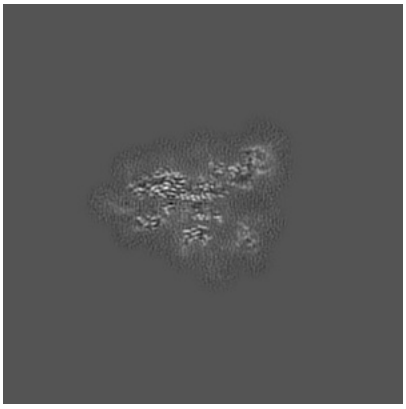
The images above show the map projected in three orthogonal directions.

6.2 Central slices

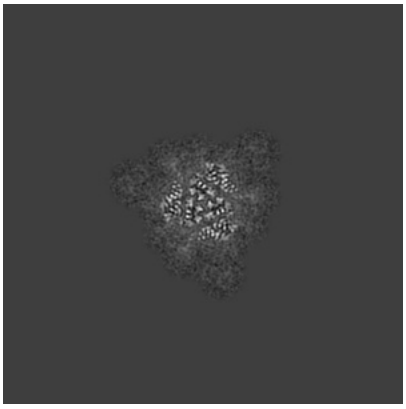
6.2.1 Primary map



X Index: 200



Y Index: 200

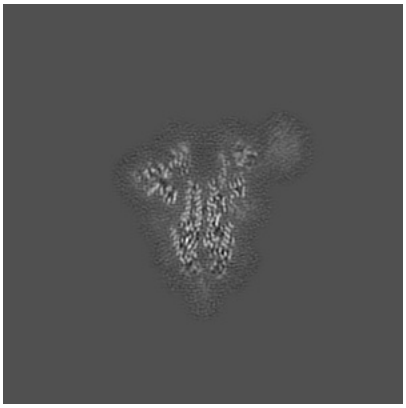


Z Index: 200

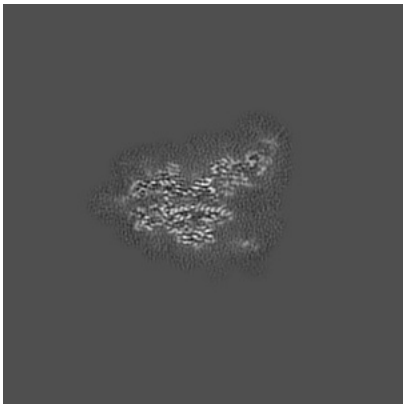
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

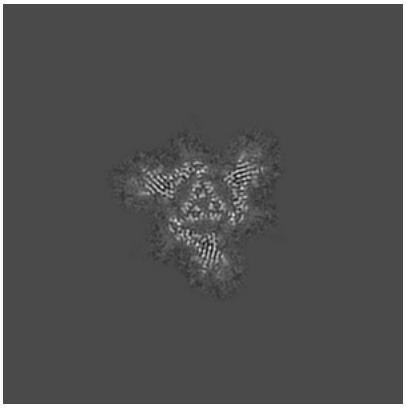
6.3.1 Primary map



X Index: 196



Y Index: 193



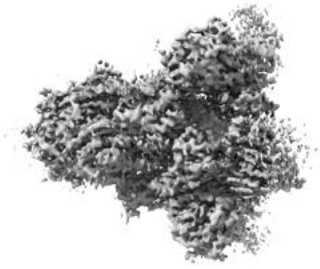
Z Index: 217

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

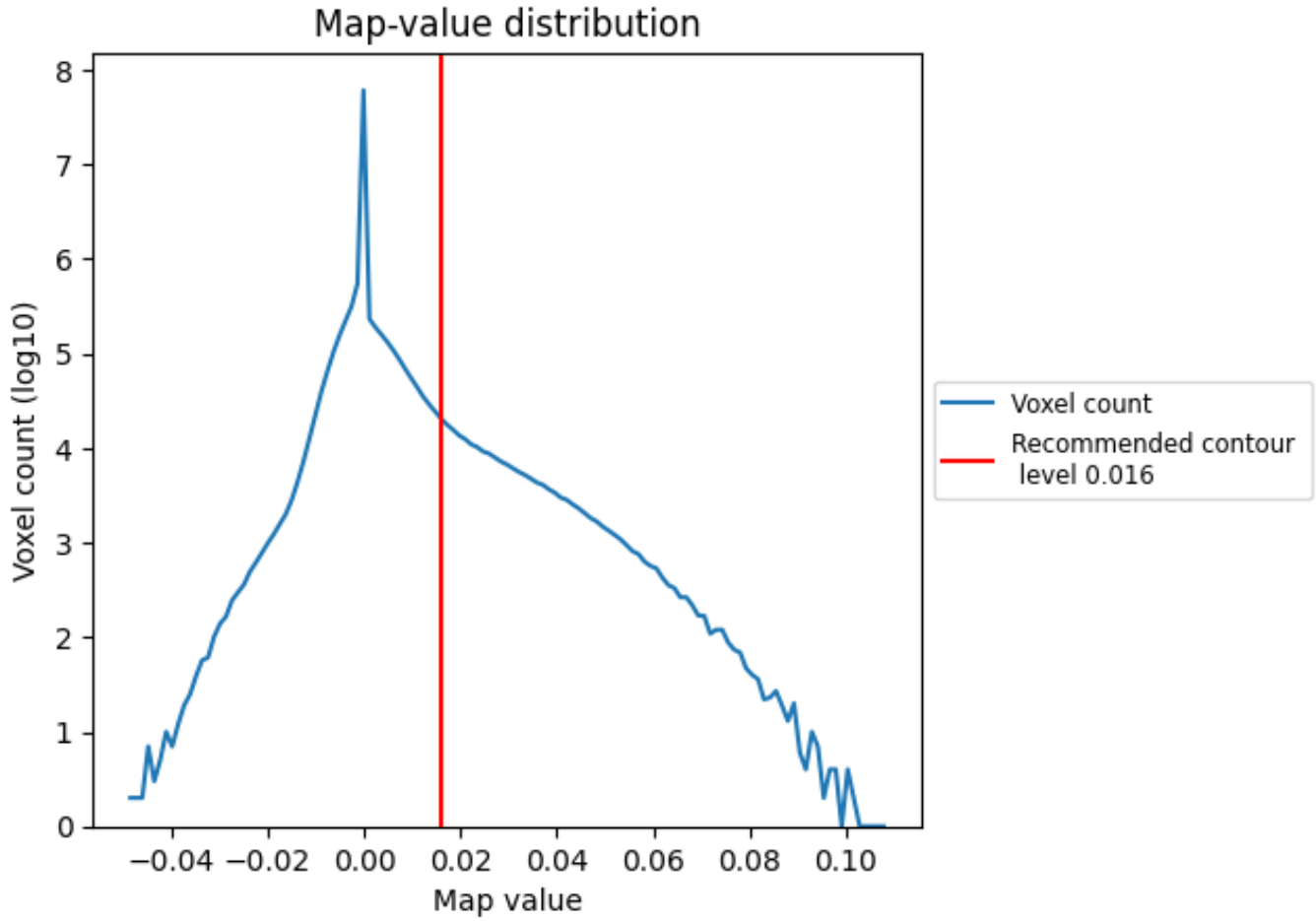
6.5 Mask visualisation (i)

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

7 Map analysis

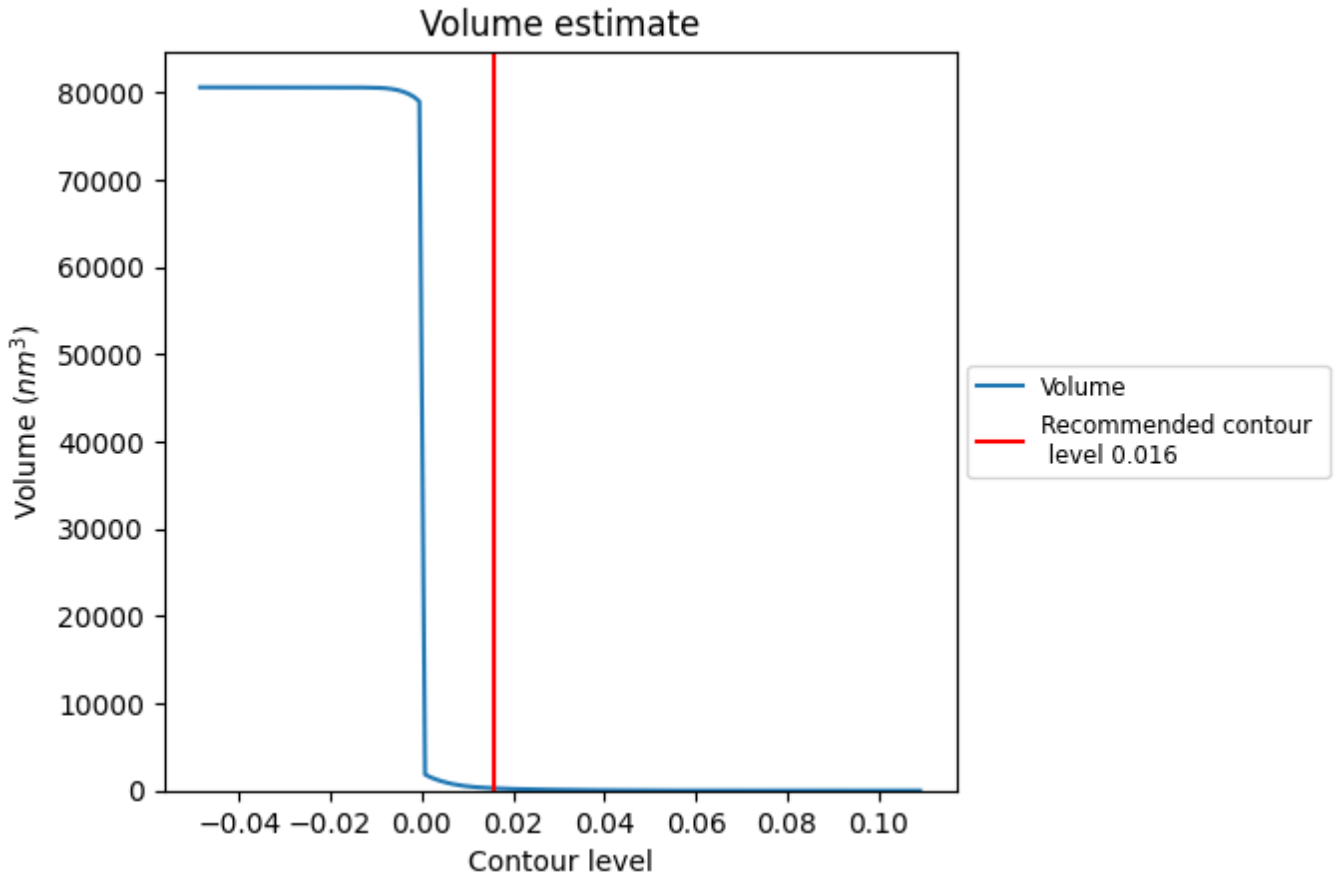
This section contains the results of statistical analysis of the map.

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.

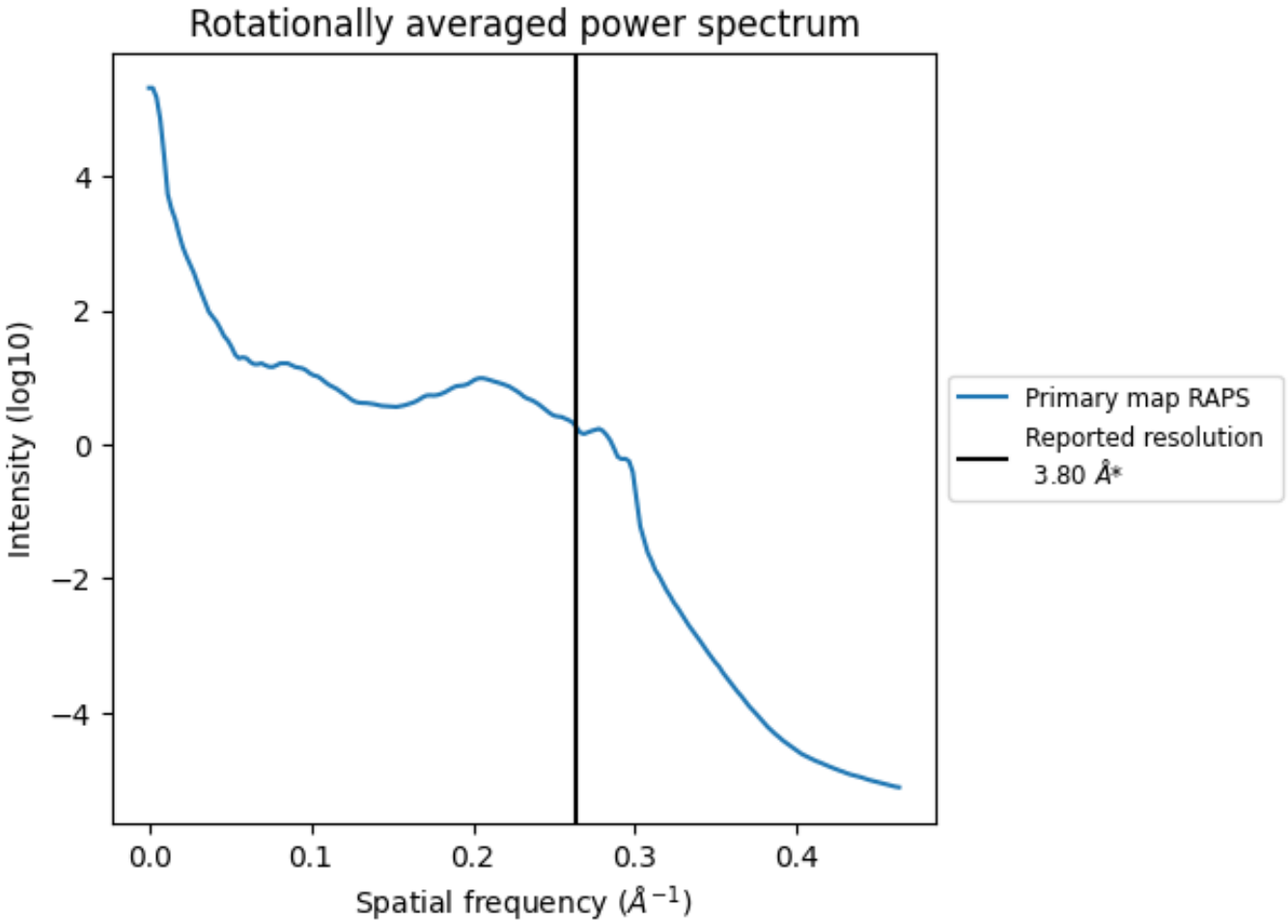
7.2 Volume estimate (i)



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 236 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)

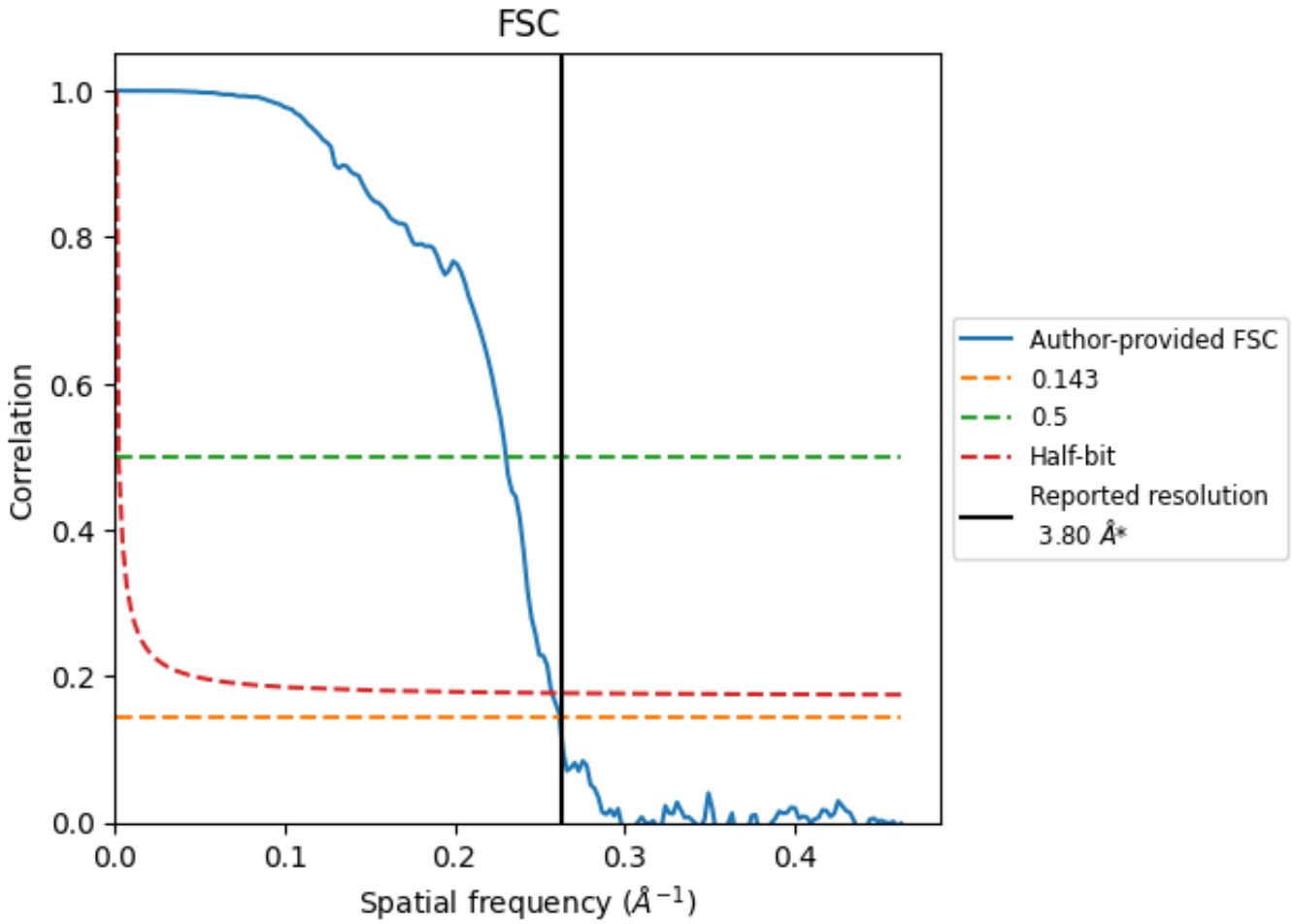


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

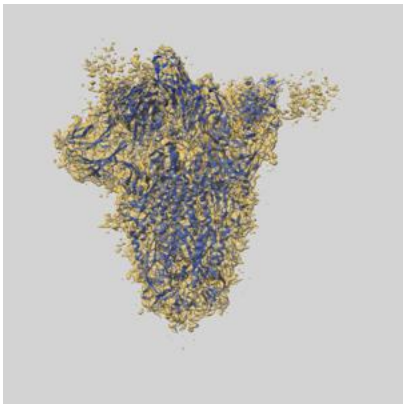
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.34	3.89
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

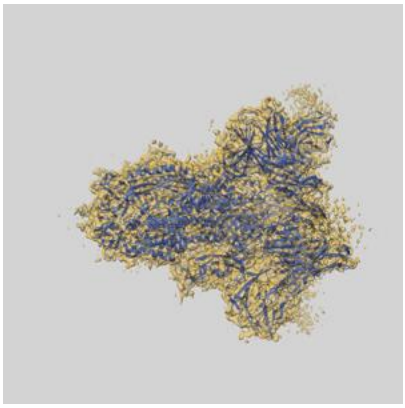
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11813 and PDB model 7AKJ. Per-residue inclusion information can be found in section 3 on page 13.

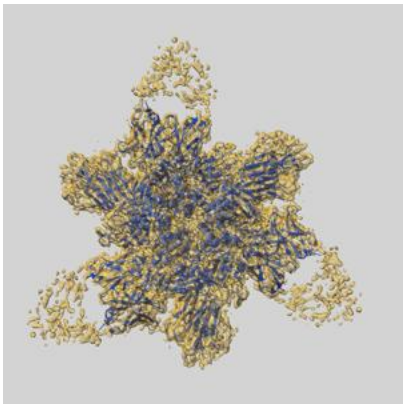
9.1 Map-model overlay



X



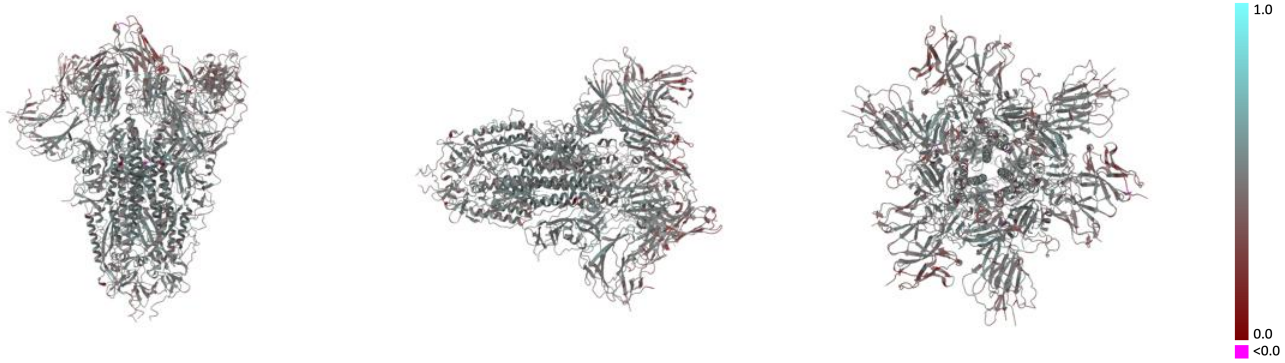
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

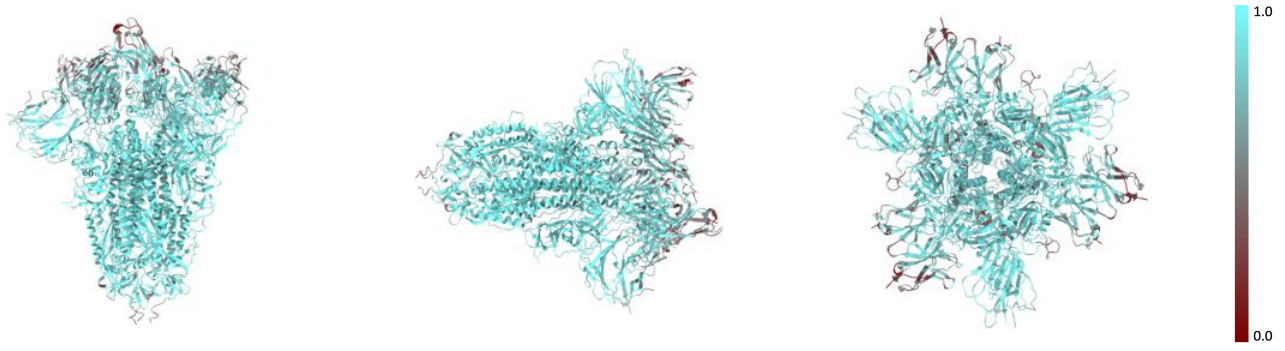
9.2 Q-score mapped to coordinate model (i)



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.

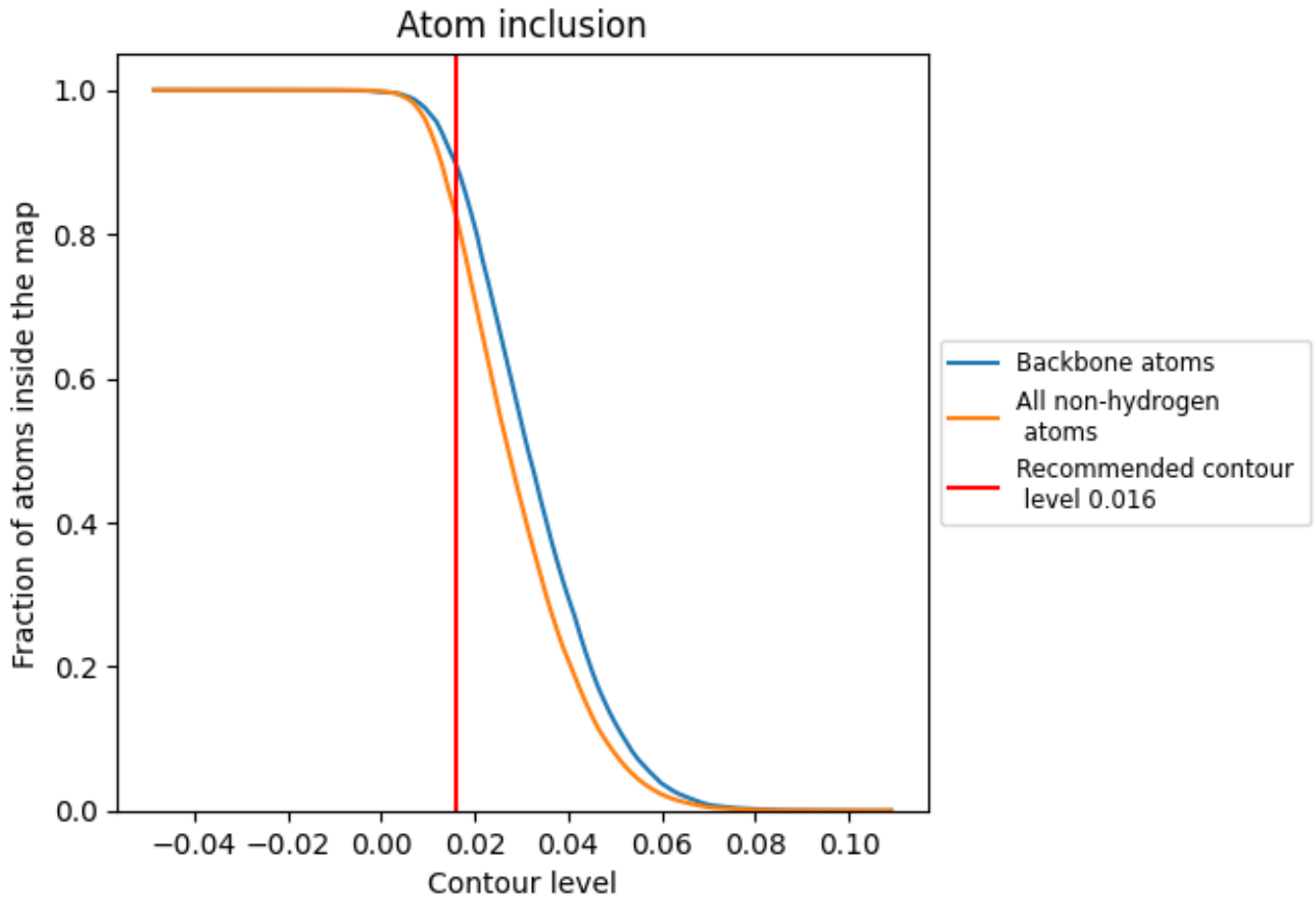
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 90% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8258	0.4640
A	0.8647	0.4730
B	0.8630	0.4740
C	0.8623	0.4740
D	0.7286	0.4520
E	0.6553	0.4170
F	0.7273	0.4510
G	0.6520	0.4210
H	0.6619	0.4200
I	0.5000	0.3880
J	0.6053	0.2990
K	0.5000	0.2650
L	0.7183	0.4500
M	0.6071	0.3370
N	0.3077	0.3480
O	0.8214	0.4250
P	0.5000	0.3900
Q	0.6053	0.3020
R	0.5000	0.2600
S	0.6071	0.3240
T	0.2981	0.3560
U	0.8214	0.4300
V	0.5357	0.3870
W	0.6053	0.2980
X	0.5000	0.2850
Y	0.6071	0.3380
Z	0.3077	0.3580
a	0.8214	0.4260