wwPDB EM Validation Summary Report (i)

Sep 30, 2021 – 11:22 pm BST

PDB ID	:	7OAN
EMDB ID	:	EMD-12777
Title	:	Nanobody C5 bound to Spike
Authors	:	Naismith, J.H.; Weckener, M.
Deposited on	:	2021-04-19
Resolution	:	3.00 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 following versions of software and data (see references (i)) were used in the production of this report:

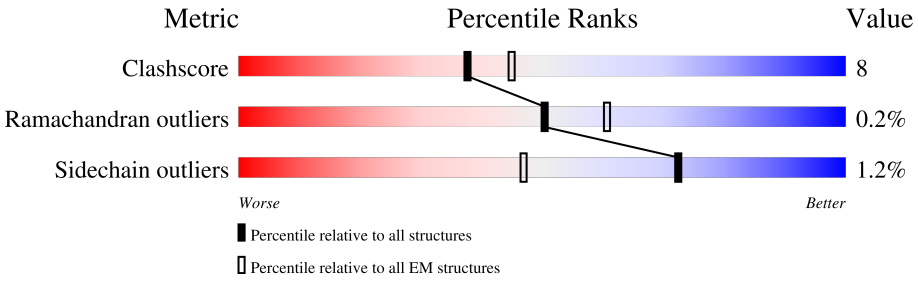
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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	1260	69% 14% 17%
1	B	1260	70% 13% 17%
1	C	1260	70% 13% 17%
2	F	129	40% 55% 38% 6%
2	G	129	39% 55% 38% 6%
2	H	129	40% 55% 38% 6%
3	D	2	50% 100%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	50% 50%
3	K	2	100%
3	L	2	50% 100%
3	M	2	100%
3	N	2	100%
3	O	2	50% 50%
3	P	2	100%
3	Q	2	50% 100%
3	R	2	100%
3	S	2	100%
3	T	2	50% 50%
3	U	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28203 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	1049	Total	C	N	O	S	0	0
			8192	5227	1366	1561	38		
1	B	1049	Total	C	N	O	S	0	0
			8192	5227	1366	1561	38		
1	C	1049	Total	C	N	O	S	0	0
			8192	5227	1366	1561	38		

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	ASN	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	ILE	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	ALA	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	LYS	-	expression tag	UNP P0DTC2
A	1249	ILE	-	expression tag	UNP P0DTC2
A	1250	GLU	-	expression tag	UNP P0DTC2
A	1251	TRP	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	GLU	-	expression tag	UNP P0DTC2
A	1254	LYS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	ASN	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	ILE	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	ALA	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	LYS	-	expression tag	UNP P0DTC2
B	1249	ILE	-	expression tag	UNP P0DTC2
B	1250	GLU	-	expression tag	UNP P0DTC2
B	1251	TRP	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	GLU	-	expression tag	UNP P0DTC2
B	1254	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	ASN	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	ILE	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	ALA	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	LYS	-	expression tag	UNP P0DTC2
C	1249	ILE	-	expression tag	UNP P0DTC2
C	1250	GLU	-	expression tag	UNP P0DTC2
C	1251	TRP	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	GLU	-	expression tag	UNP P0DTC2
C	1254	LYS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called immunoglobulin mu heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	121	Total	C	N	O	S	0	0
			901	559	158	178	6		
2	G	121	Total	C	N	O	S	0	0
			901	559	158	178	6		
2	H	121	Total	C	N	O	S	0	0
			901	559	158	178	6		

- Molecule 3 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
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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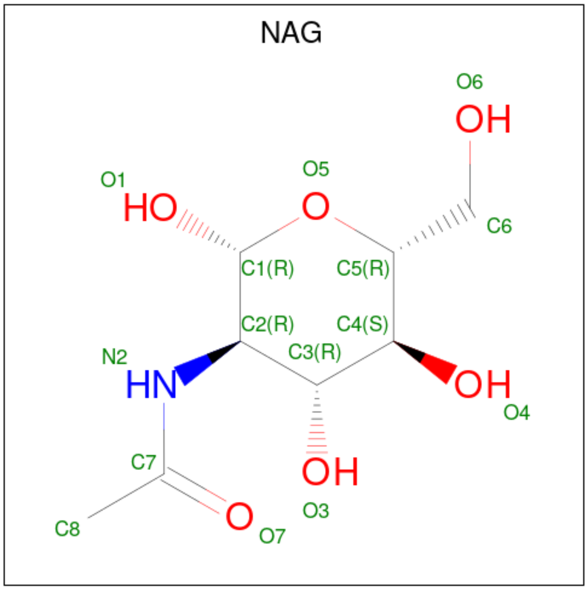
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		

- 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 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0

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

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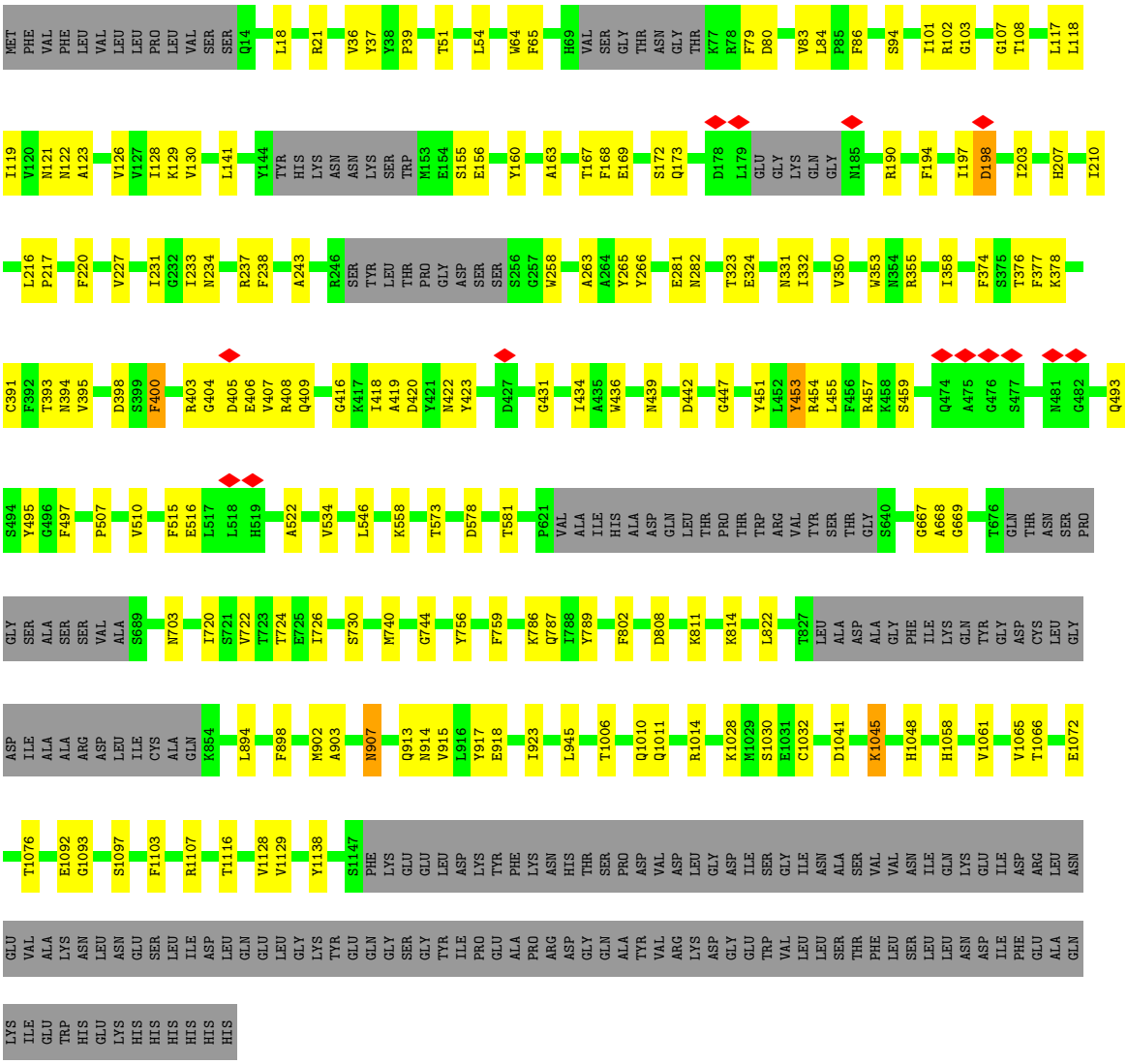
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			168	96	12	60	

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.

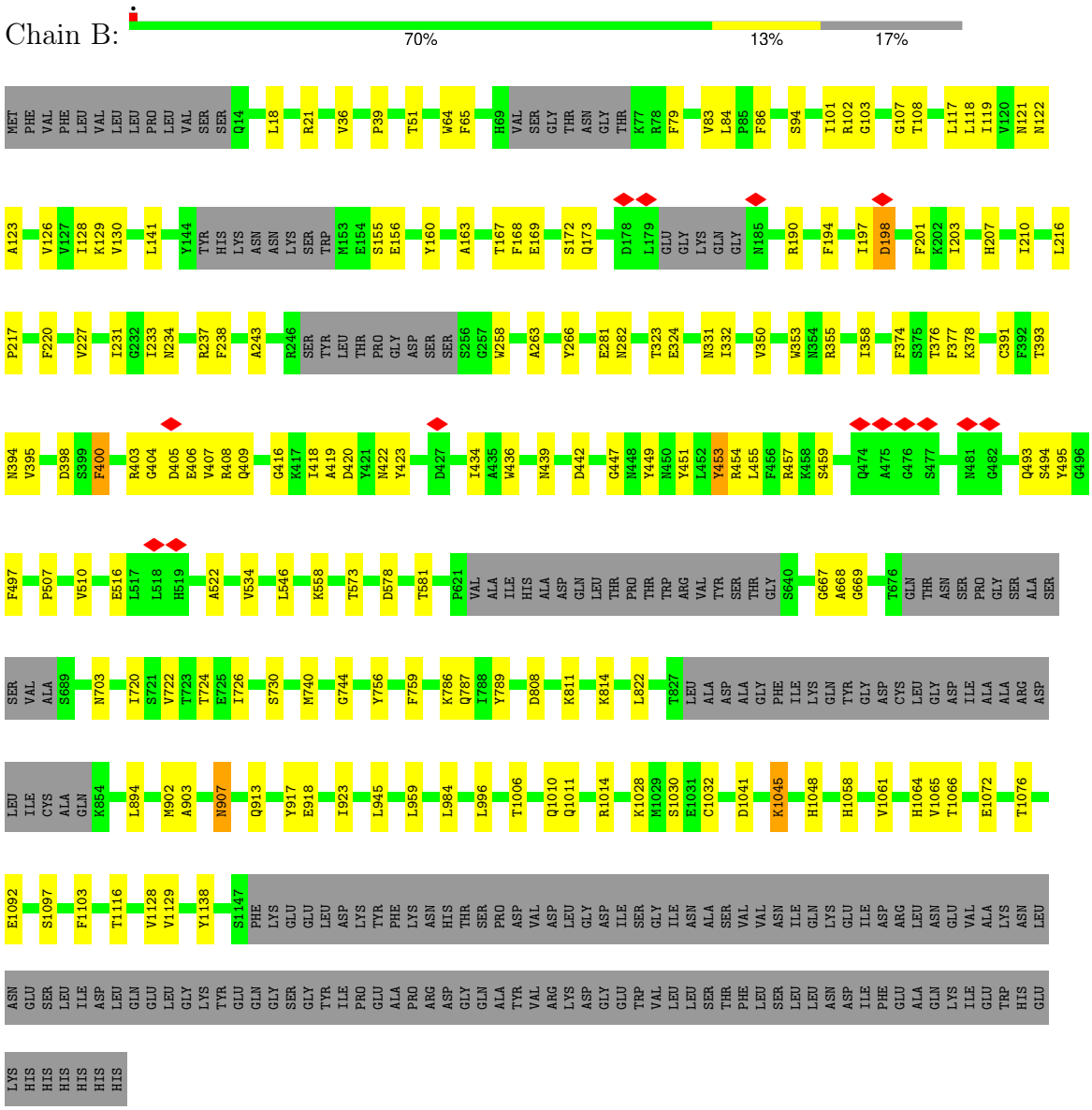
- Molecule 1: Spike glycoprotein

Chain A:



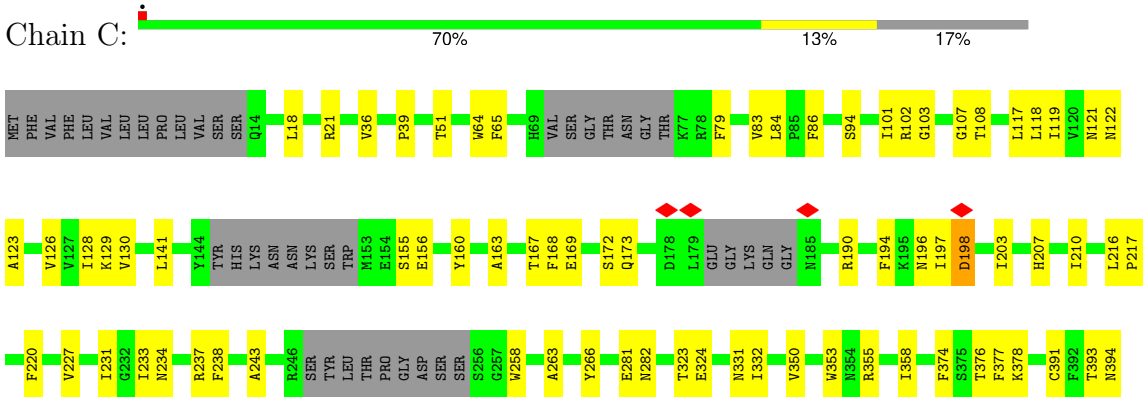
- Molecule 1: Spike glycoprotein

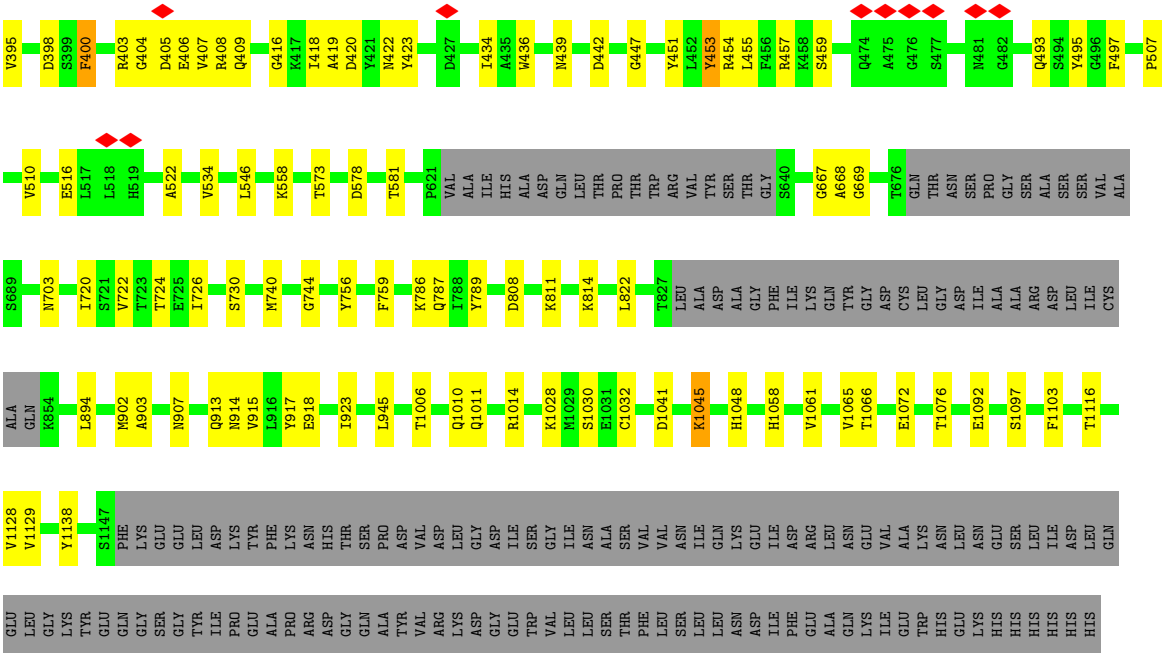
Chain B:



• Molecule 1: Spike glycoprotein

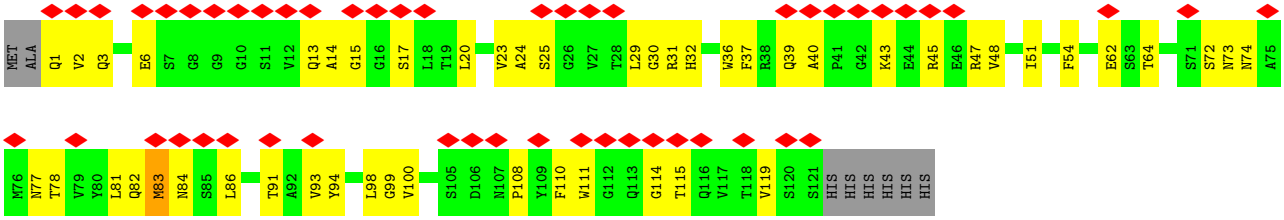
Chain C:





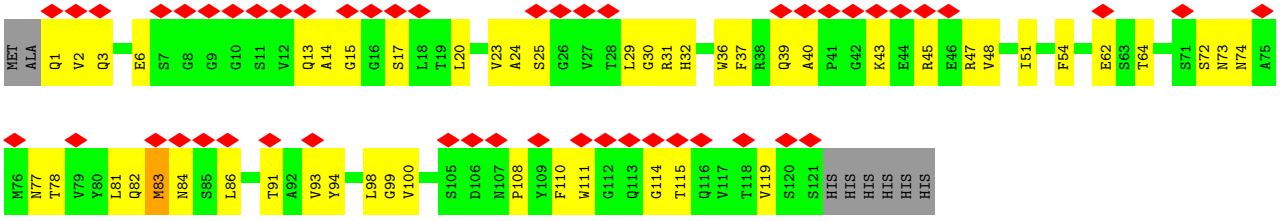
• Molecule 2: immunoglobulin mu heavy chain

Chain F:



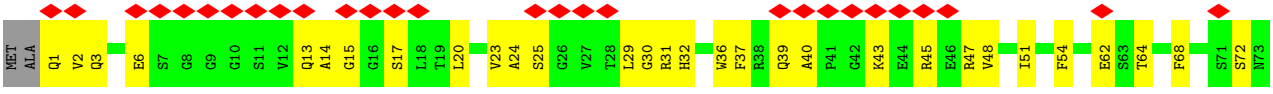
• Molecule 2: immunoglobulin mu heavy chain

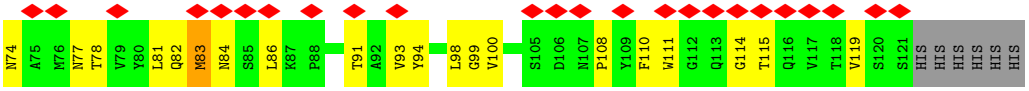
Chain G:



• Molecule 2: immunoglobulin mu heavy chain

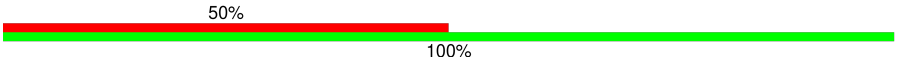
Chain H:





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

Chain D:

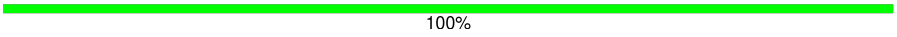


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain I:

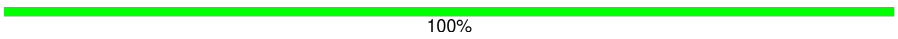


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

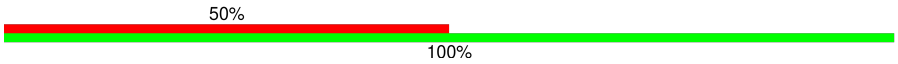
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



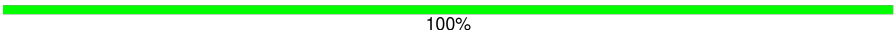
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



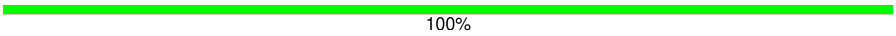
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:

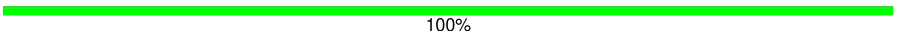


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:

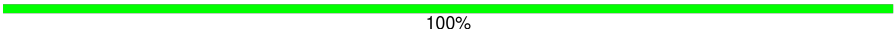


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:



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

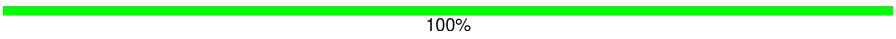
Chain S:

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

Chain T:

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

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	227898	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0099	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.58	0/8379	0.57	0/11401
1	B	0.58	0/8379	0.57	0/11401
1	C	0.58	0/8379	0.57	0/11401
2	F	0.61	0/917	0.63	0/1243
2	G	0.62	0/917	0.63	0/1243
2	H	0.62	0/917	0.63	0/1243
All	All	0.59	0/27888	0.58	0/37932

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	8192	0	7969	121	0
1	B	8192	0	7969	121	0
1	C	8192	0	7969	117	0
2	F	901	0	873	35	0
2	G	901	0	873	36	0
2	H	901	0	873	36	0
3	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
4	A	168	0	156	1	0
4	B	168	0	156	1	0
4	C	168	0	156	1	0
All	All	28203	0	27369	449	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 8.

The worst 5 of 449 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLY:O	1:B:237:ARG:HB3	1.60	1.02
1:A:107:GLY:O	1:A:237:ARG:HB3	1.60	1.02
1:C:107:GLY:O	1:C:237:ARG:HB3	1.60	1.01
2:F:91:THR:HG22	2:F:119:VAL:H	1.42	0.85
2:H:91:THR:HG22	2:H:119:VAL:H	1.42	0.84

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	1033/1260 (82%)	989 (96%)	42 (4%)	2 (0%)	47 82
1	B	1033/1260 (82%)	988 (96%)	43 (4%)	2 (0%)	47 82
1	C	1033/1260 (82%)	989 (96%)	42 (4%)	2 (0%)	47 82
2	F	119/129 (92%)	115 (97%)	4 (3%)	0	100 100
2	G	119/129 (92%)	115 (97%)	4 (3%)	0	100 100
2	H	119/129 (92%)	115 (97%)	4 (3%)	0	100 100
All	All	3456/4167 (83%)	3311 (96%)	139 (4%)	6 (0%)	50 82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	ALA
1	B	668	ALA
1	C	668	ALA
1	A	198	ASP
1	B	198	ASP

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	916/1098 (83%)	905 (99%)	11 (1%)	71 90
1	B	916/1098 (83%)	905 (99%)	11 (1%)	71 90
1	C	916/1098 (83%)	906 (99%)	10 (1%)	73 90
2	F	98/105 (93%)	96 (98%)	2 (2%)	55 83
2	G	98/105 (93%)	96 (98%)	2 (2%)	55 83
2	H	98/105 (93%)	97 (99%)	1 (1%)	76 91
All	All	3042/3609 (84%)	3005 (99%)	37 (1%)	72 90

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	814	LYS
2	G	83	MET
1	C	902	MET
2	F	73	ASN
1	B	323	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	73	ASN
2	F	82	GLN
2	H	82	GLN
2	G	73	ASN
1	B	564	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
3	NAG	D	1	3,1	14,14,15	0.19	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	E	1	3,1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	I	1	3,1	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	J	1	3,1	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	K	1	3,1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	L	1	3,1	14,14,15	0.20	0	17,19,21	0.54	0
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	M	1	3,1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	M	2	3	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	N	1	3,1	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	P	1	3,1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	P	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	Q	1	3,1	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	R	1	3,1	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	R	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	S	1	3,1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	S	2	3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	T	1	3,1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	T	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	U	1	3,1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	U	2	3	14,14,15	0.19	0	17,19,21	0.40	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
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	1	0

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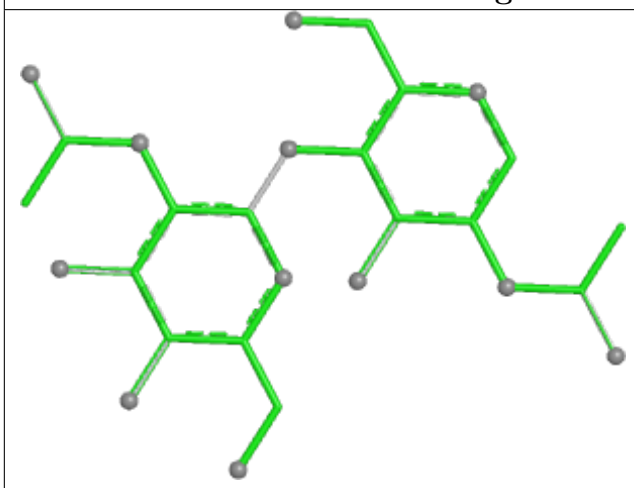
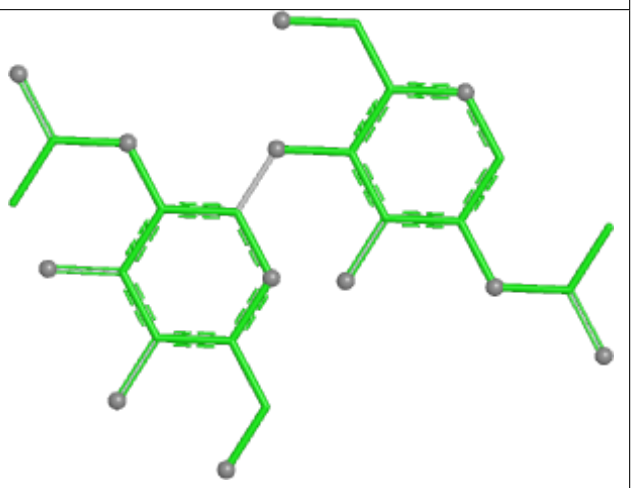
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1	NAG	1	0
3	J	1	NAG	1	0

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

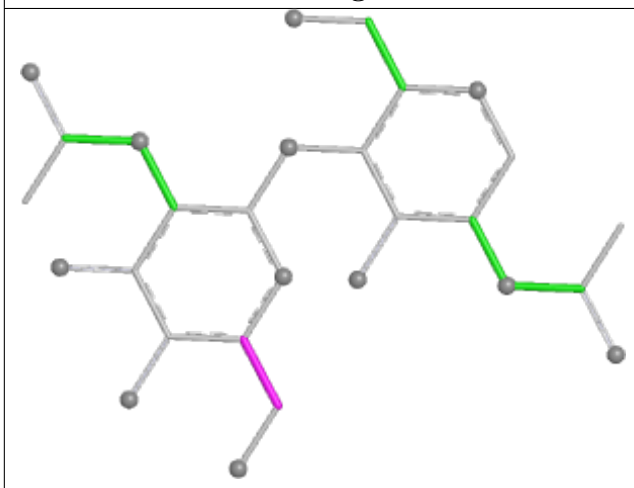
Oligosaccharide Chain D



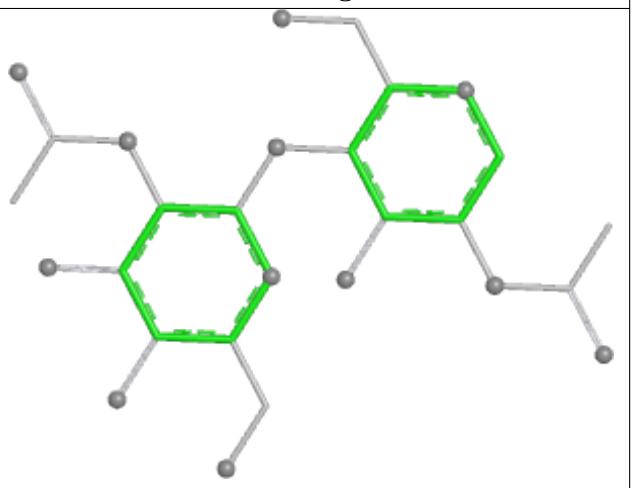
Bond lengths



Bond angles

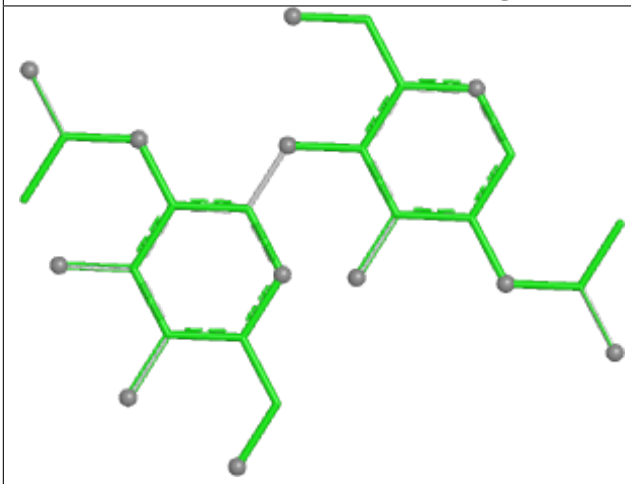


Torsions

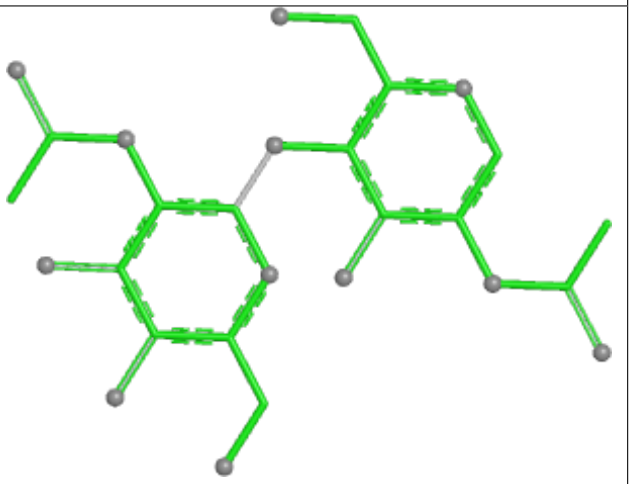


Rings

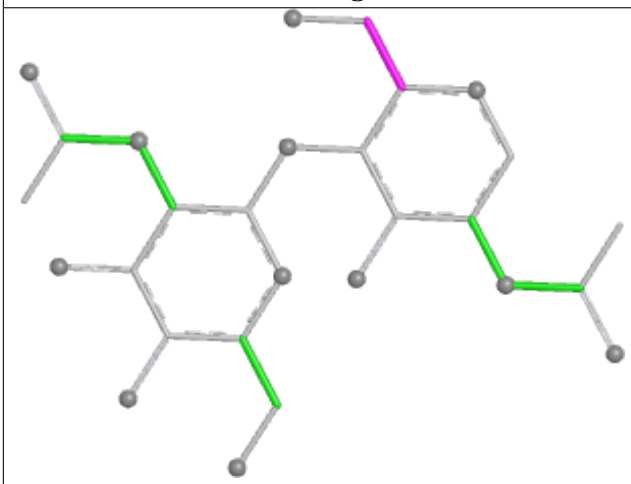
Oligosaccharide Chain E



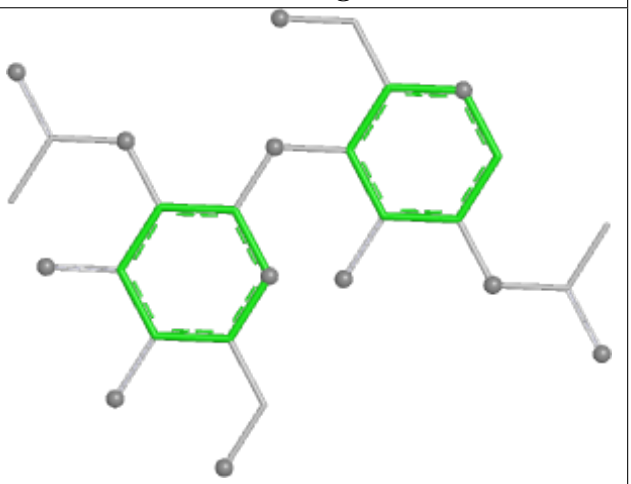
Bond lengths



Bond angles

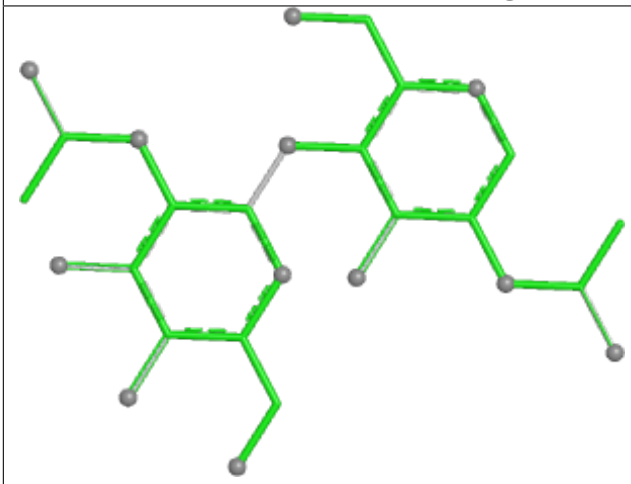


Torsions



Rings

Oligosaccharide Chain I



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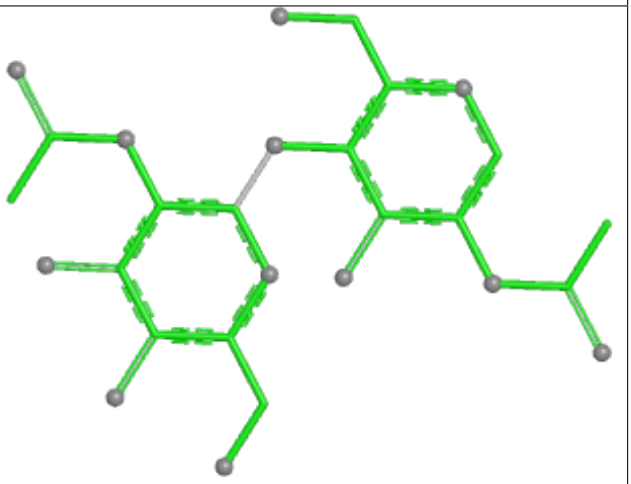
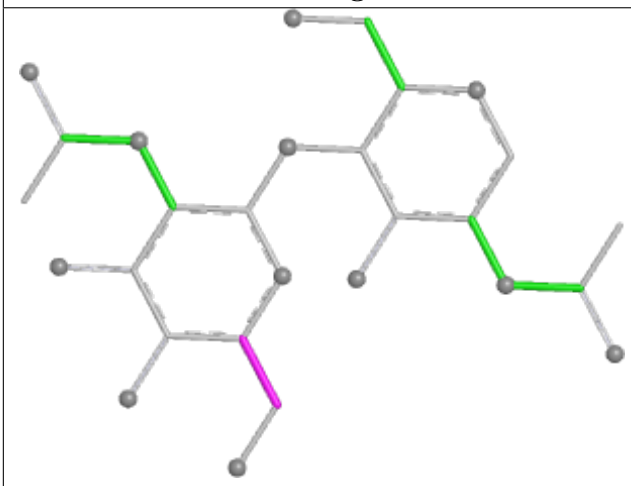


Bond angles



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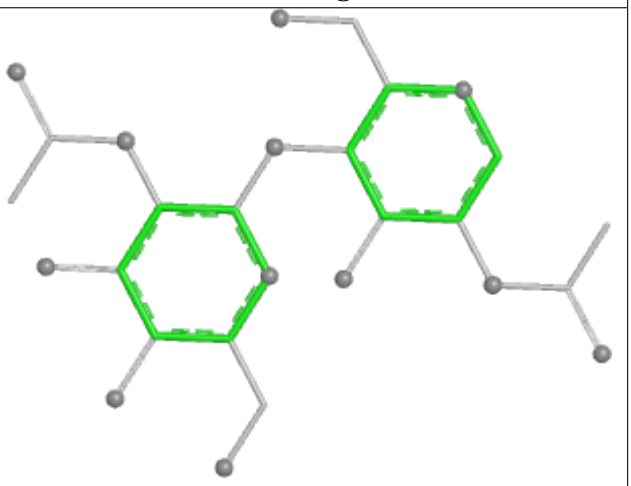
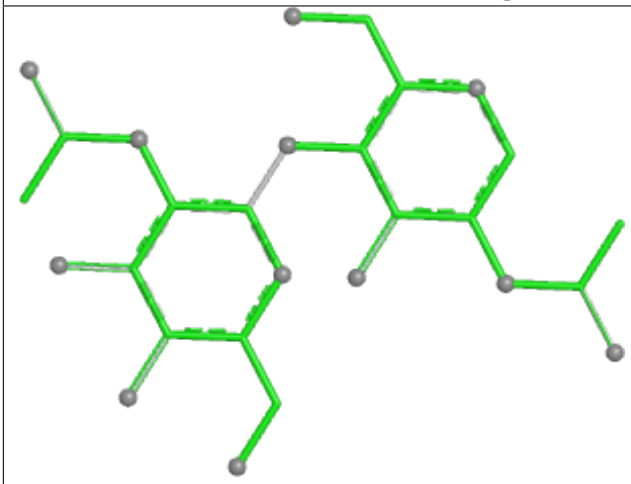


Rings

Oligosaccharide Chain J



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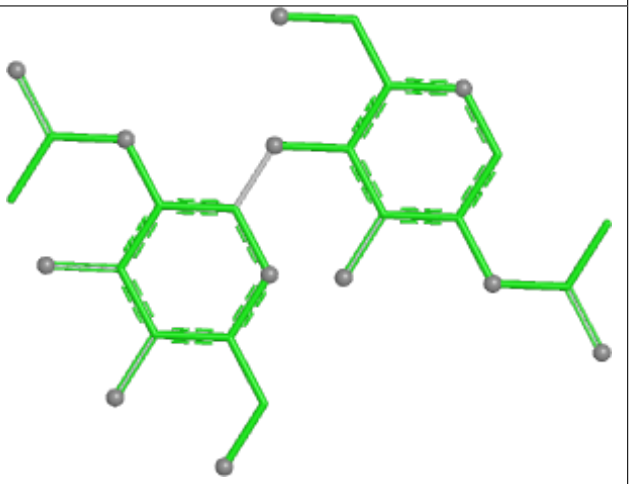

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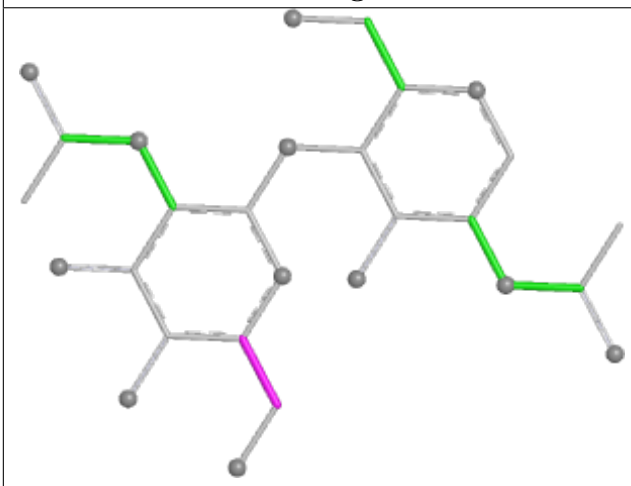

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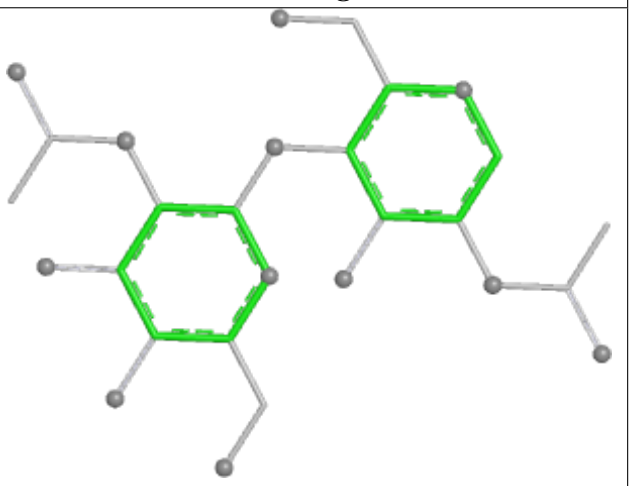
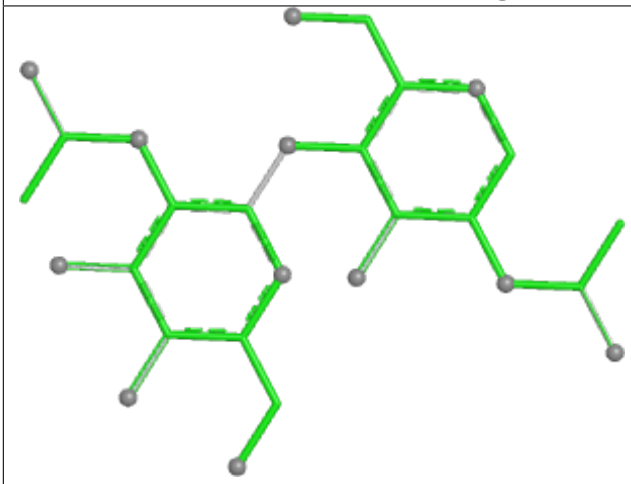


Rings

Oligosaccharide Chain K



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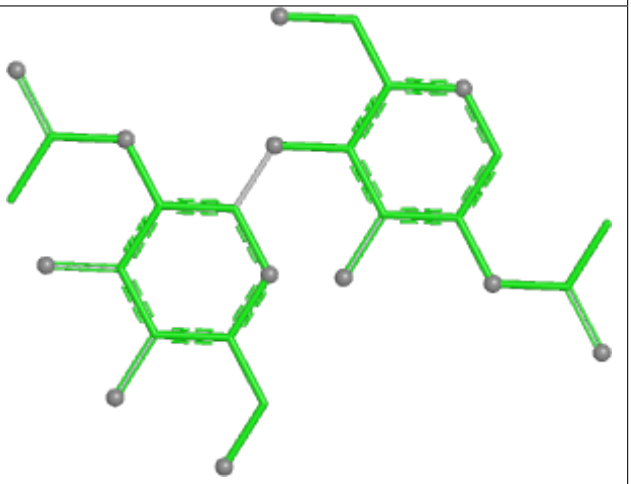
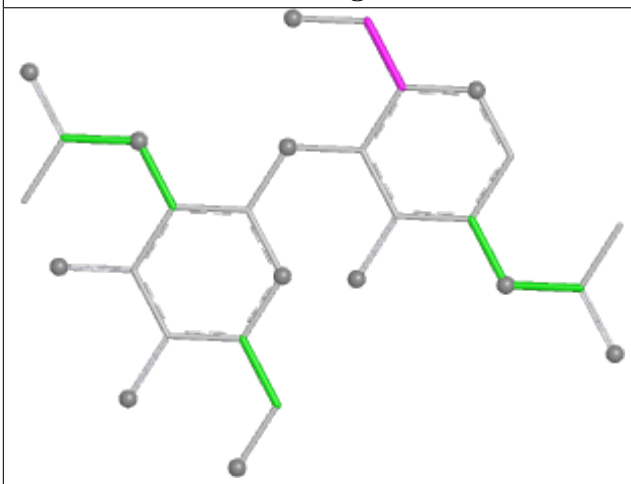


Bond angles



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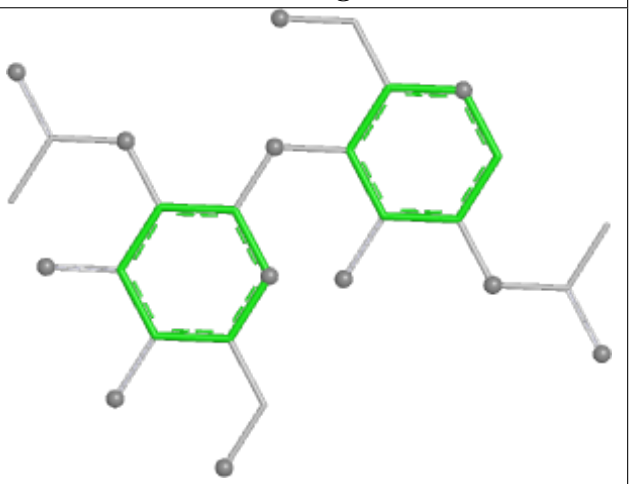
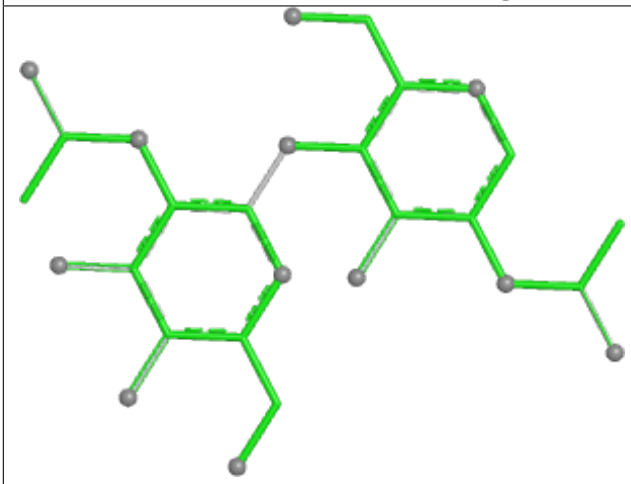
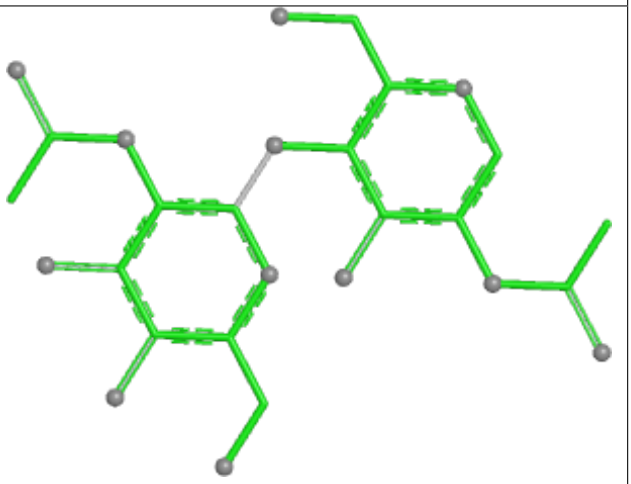


Rings

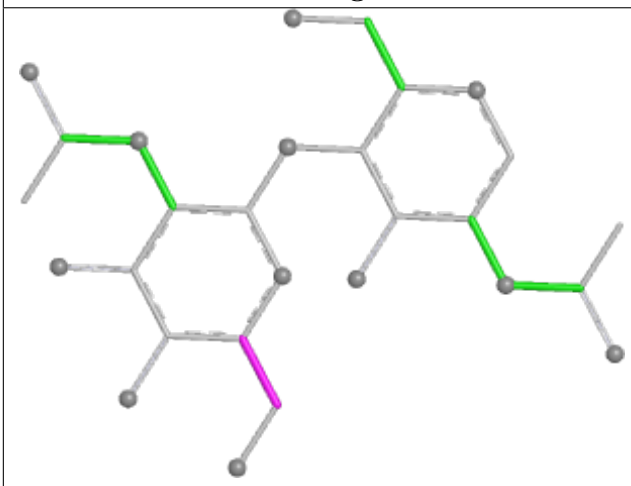
Oligosaccharide Chain L



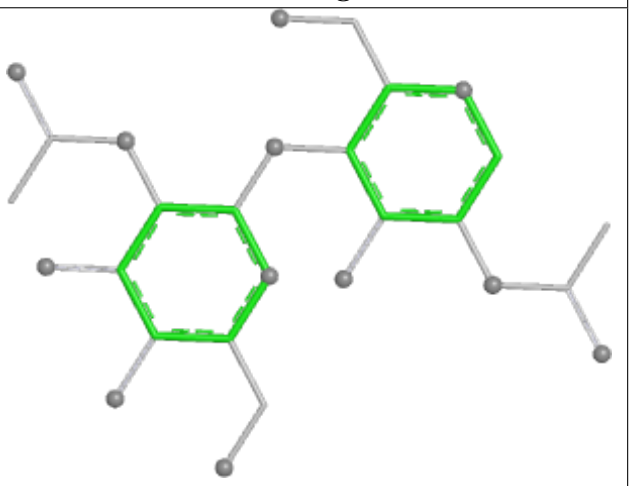
Bond lengths



Bond angles

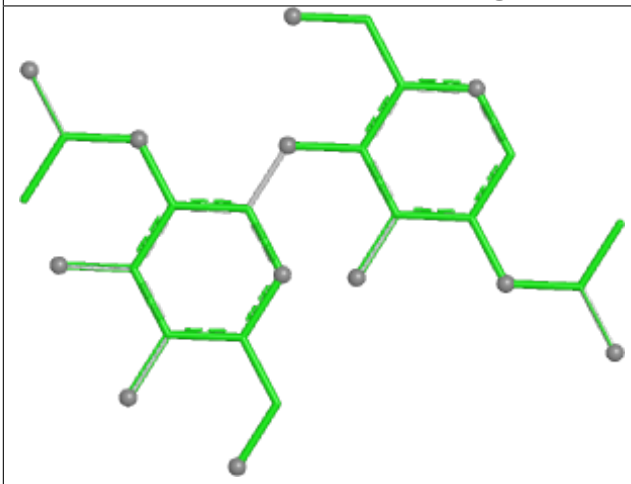


Torsions

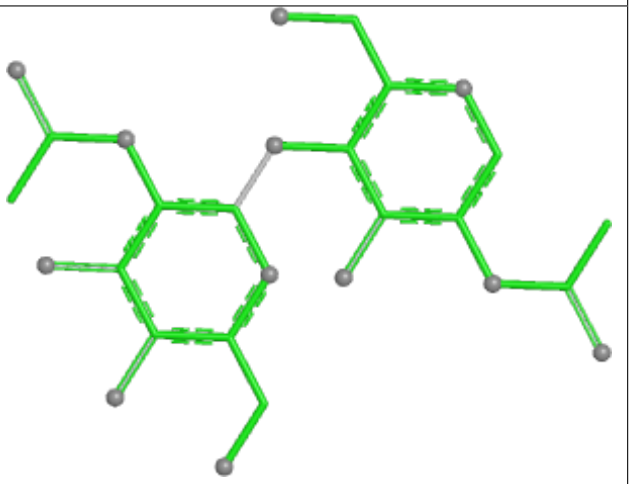


Rings

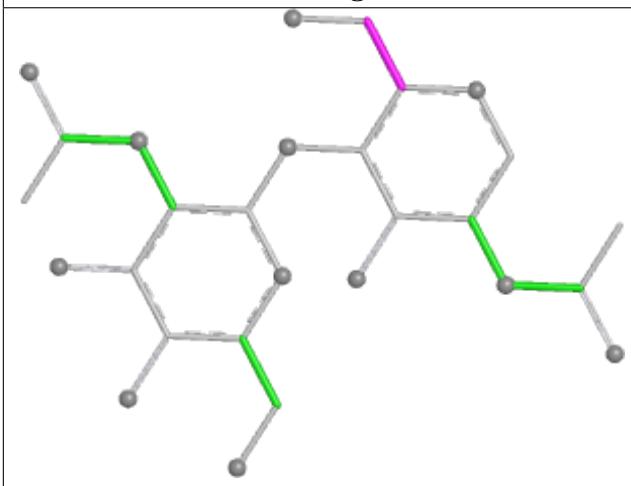
Oligosaccharide Chain M



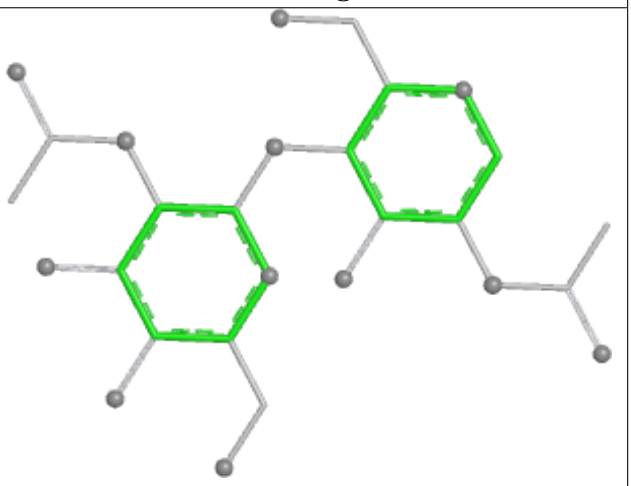
Bond lengths



Bond angles

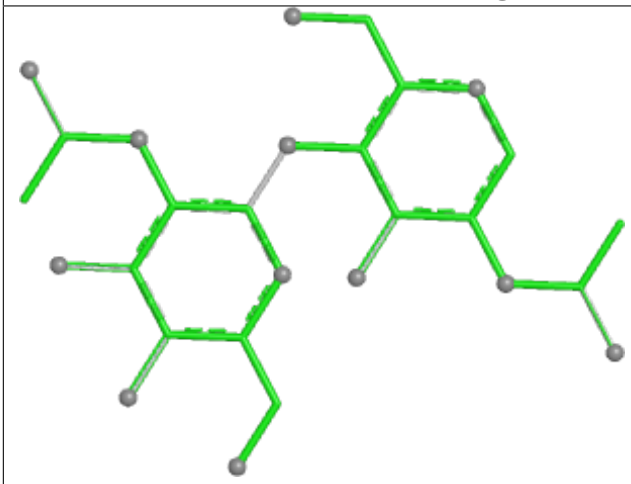


Torsions

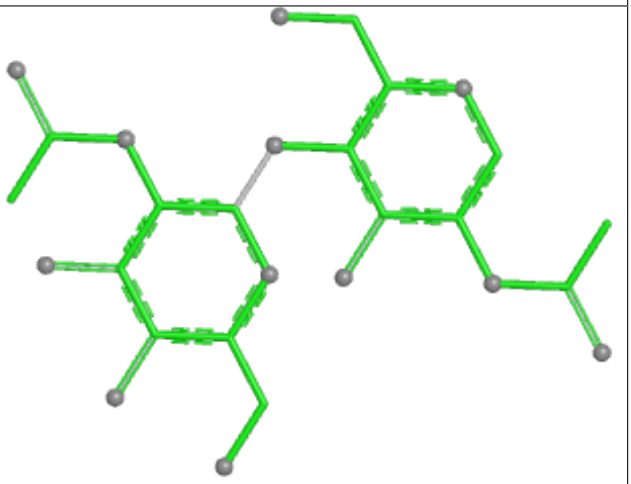


Rings

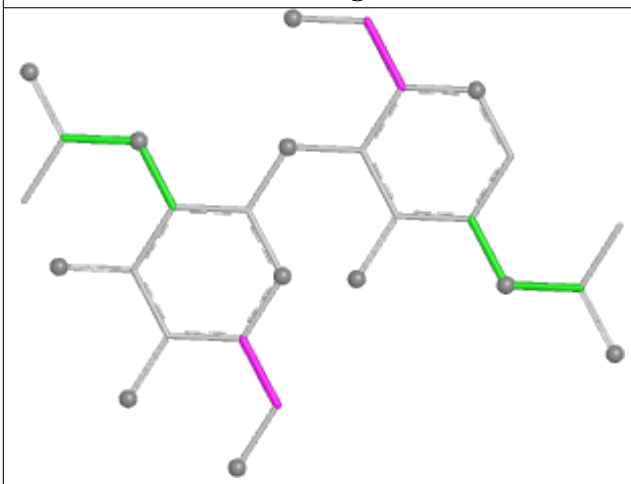
Oligosaccharide Chain N



Bond lengths



Bond angles



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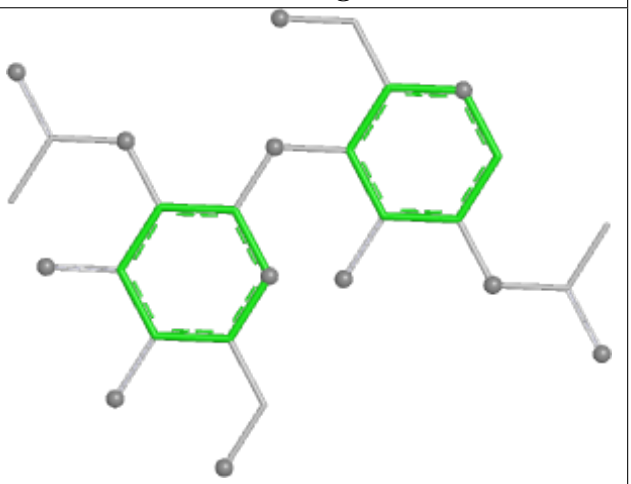
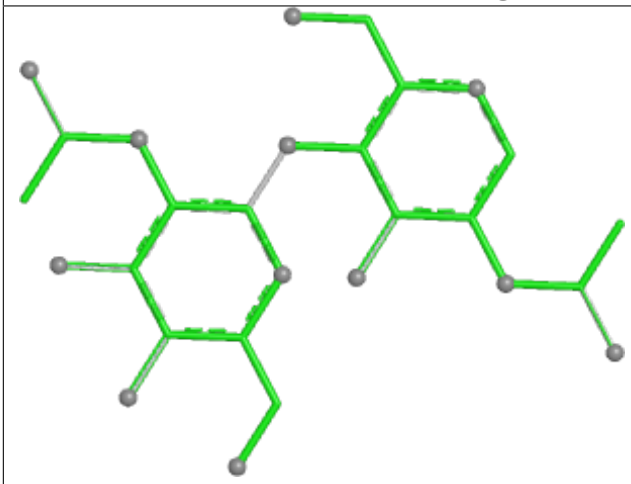
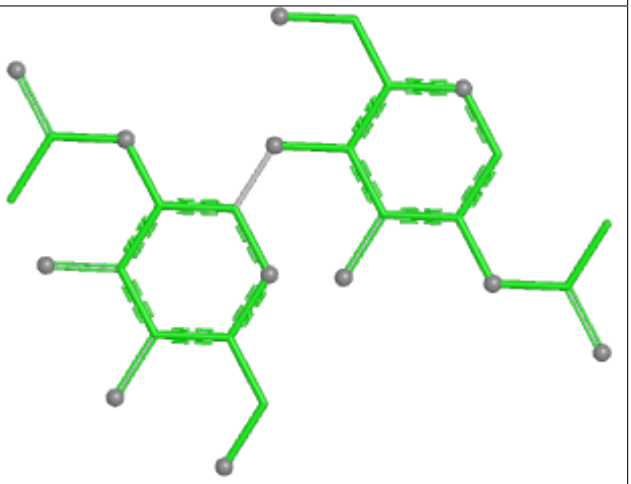


Rings

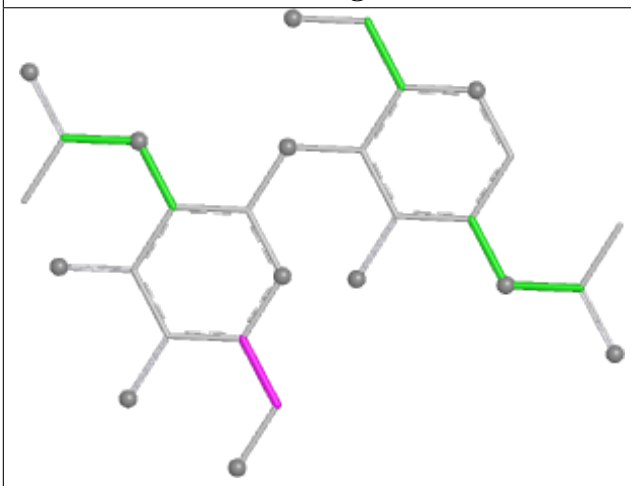
Oligosaccharide Chain O



Bond lengths



Bond angles



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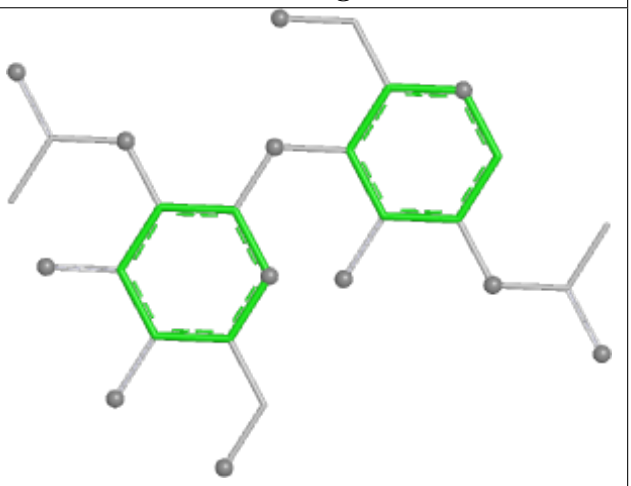
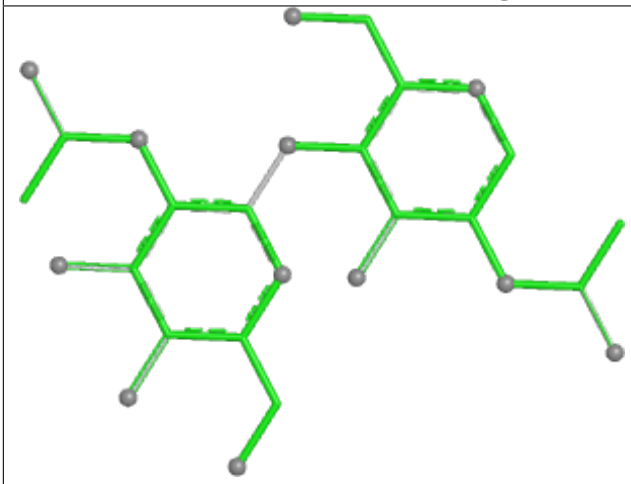
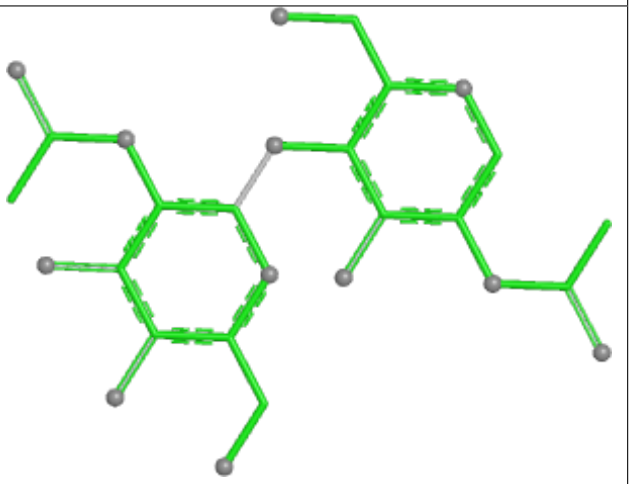


Rings

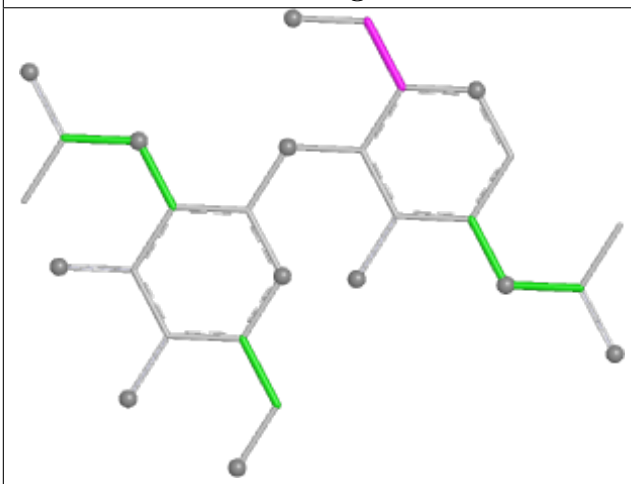
Oligosaccharide Chain P



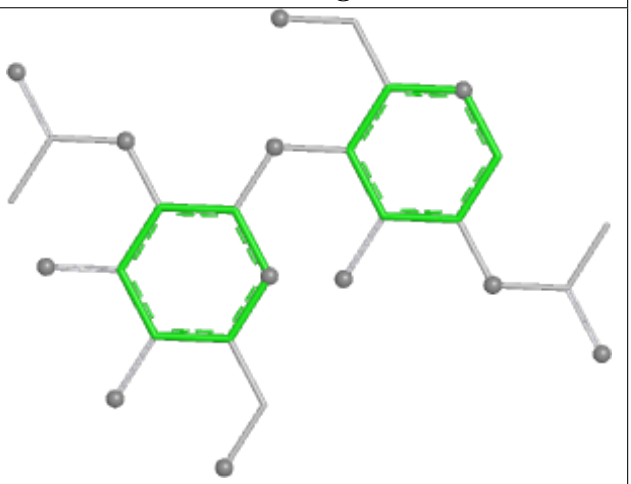
Bond lengths



Bond angles

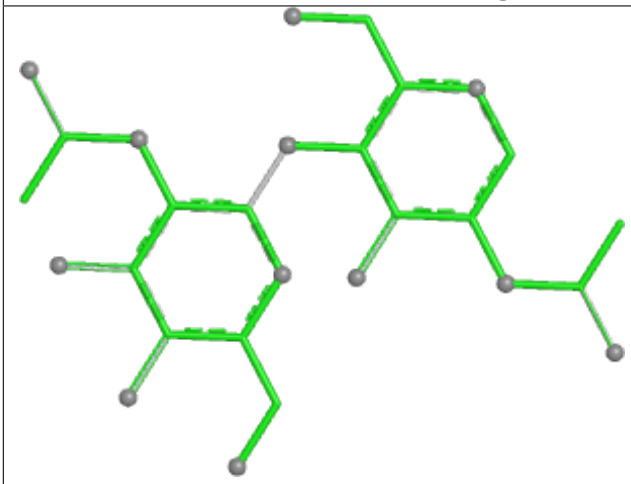


Torsions

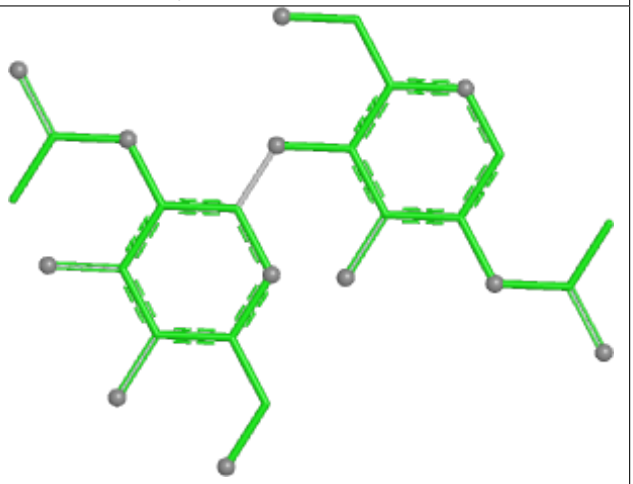


Rings

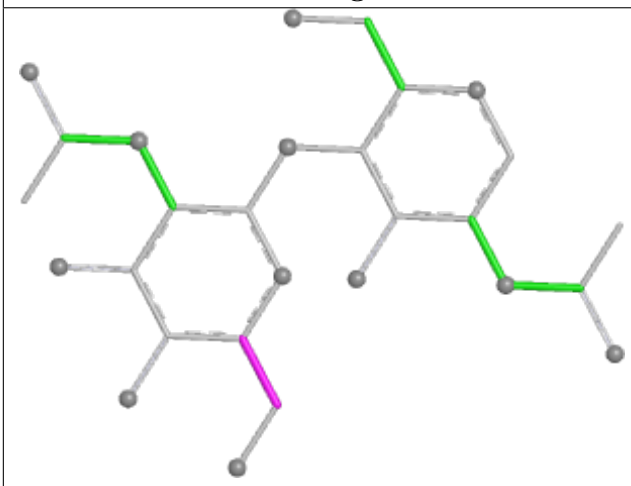
Oligosaccharide Chain Q



Bond lengths



Bond angles



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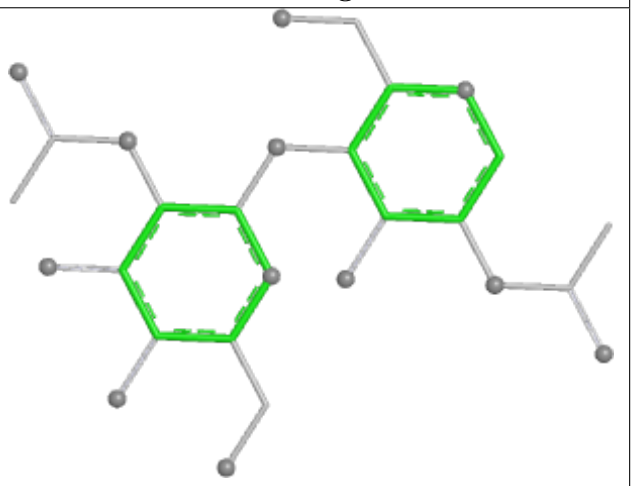
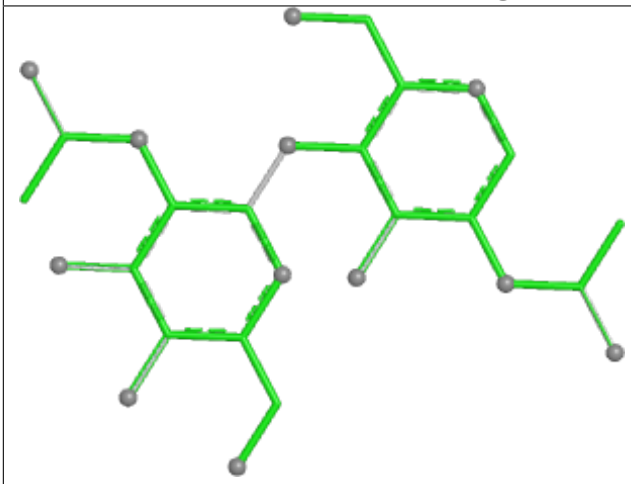
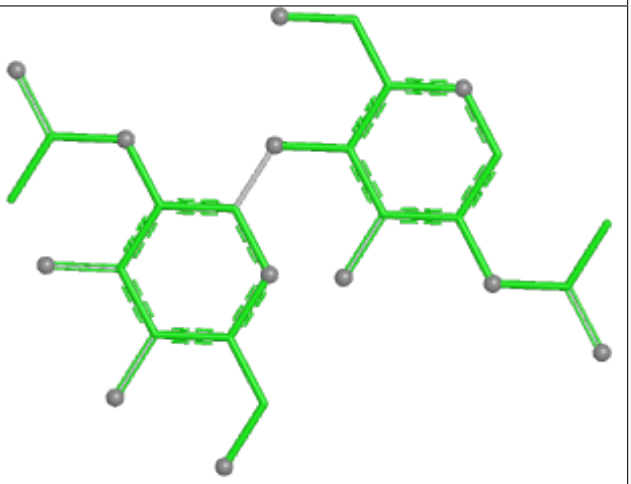


Rings

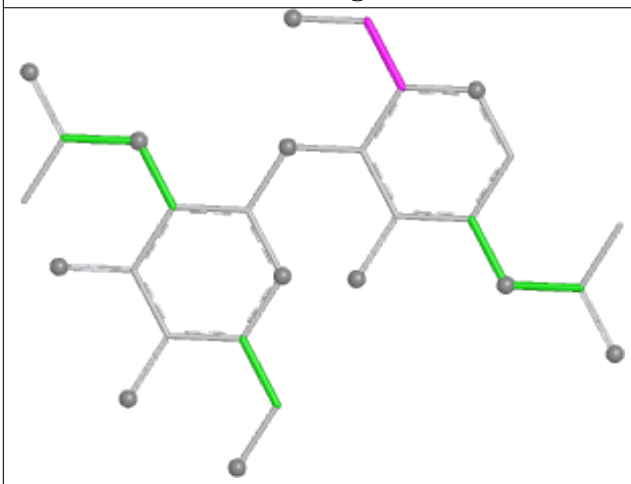
Oligosaccharide Chain R



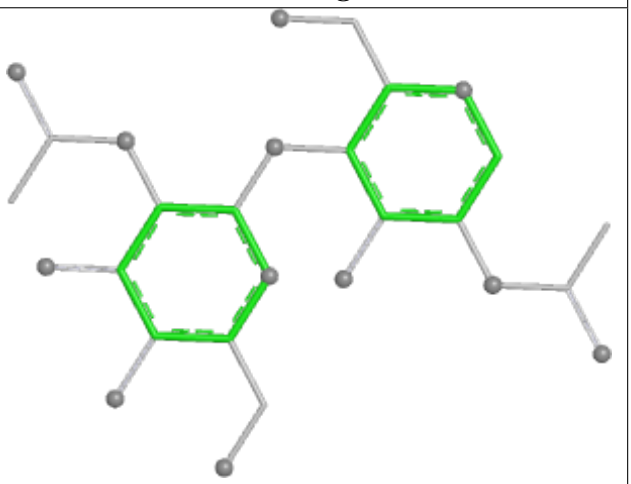
Bond lengths



Bond angles

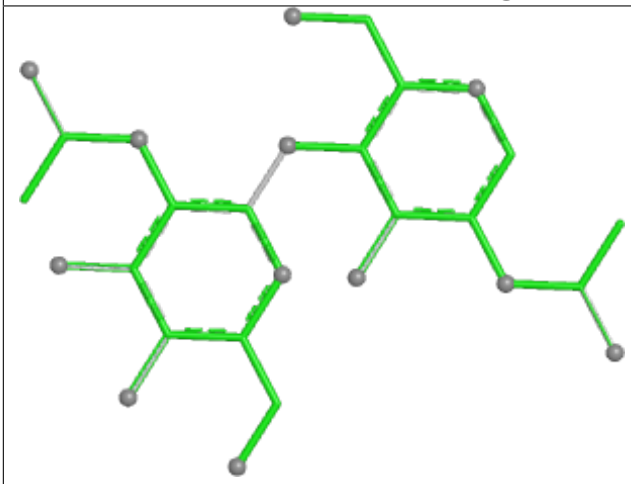


Torsions

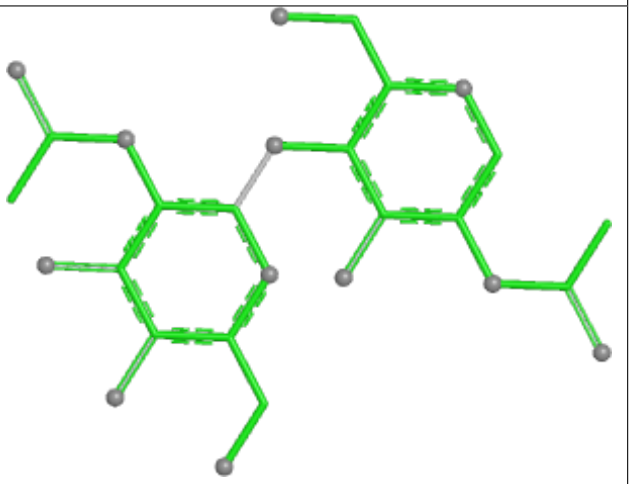


Rings

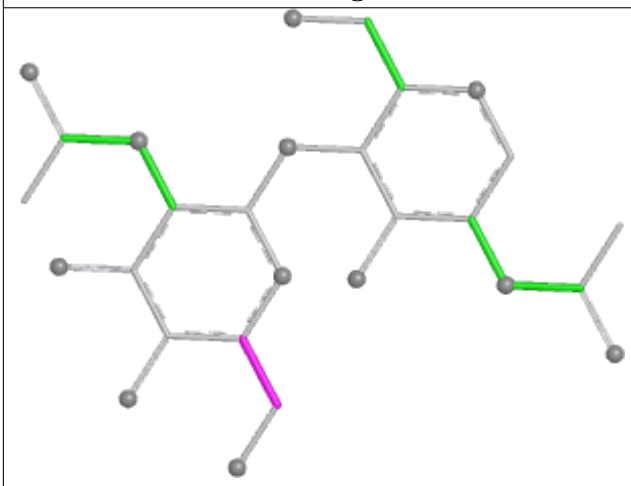
Oligosaccharide Chain S



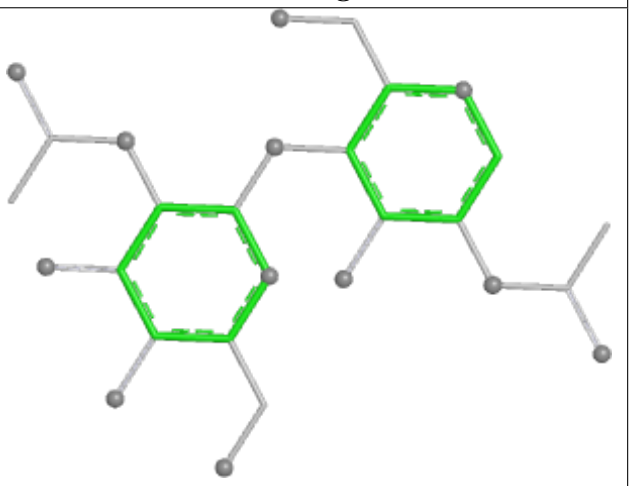
Bond lengths



Bond angles

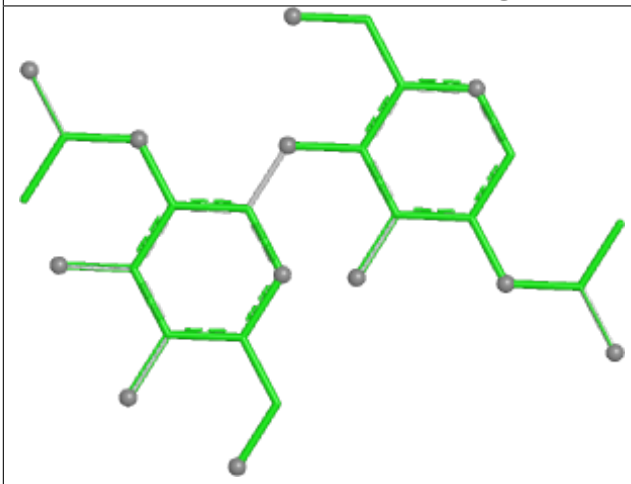


Torsions

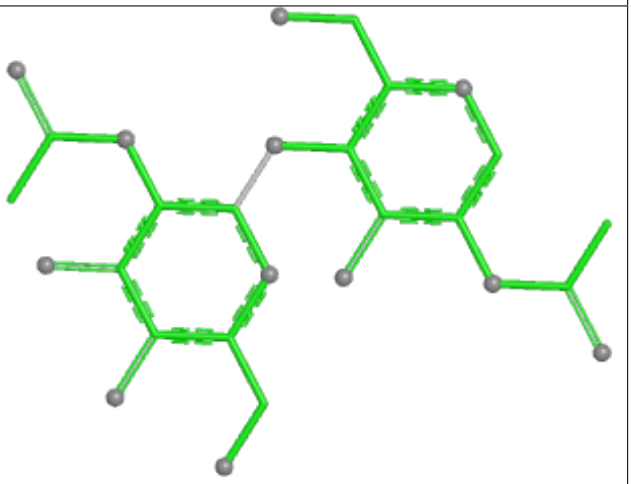


Rings

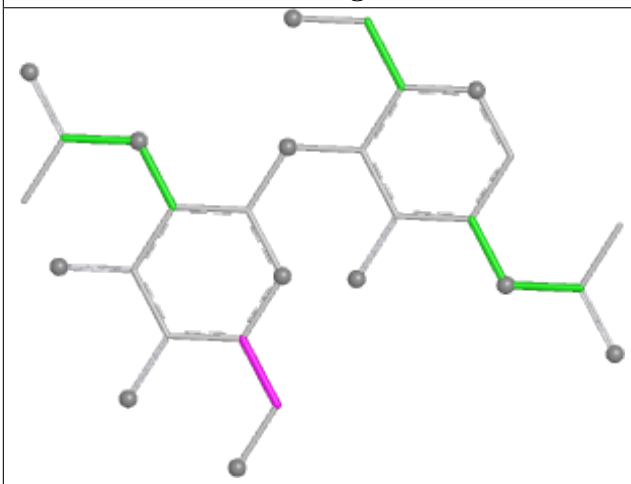
Oligosaccharide Chain T



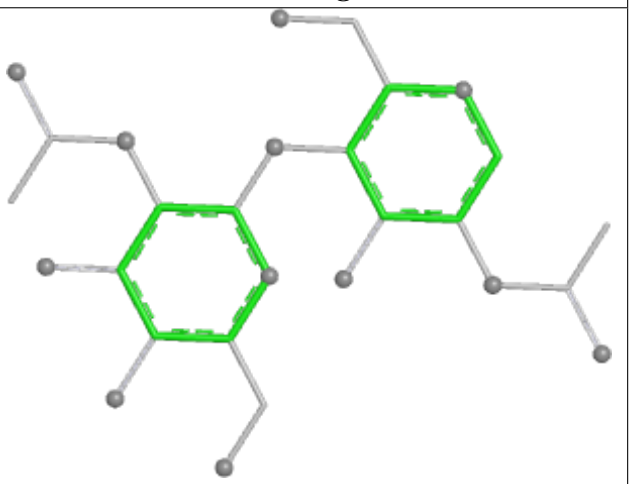
Bond lengths



Bond angles

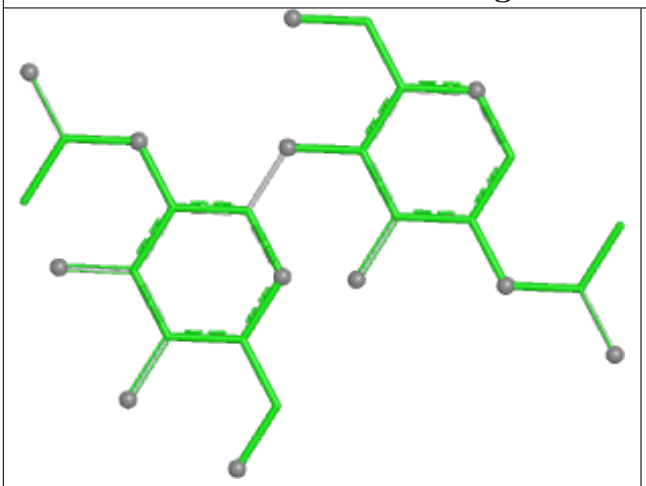


Torsions

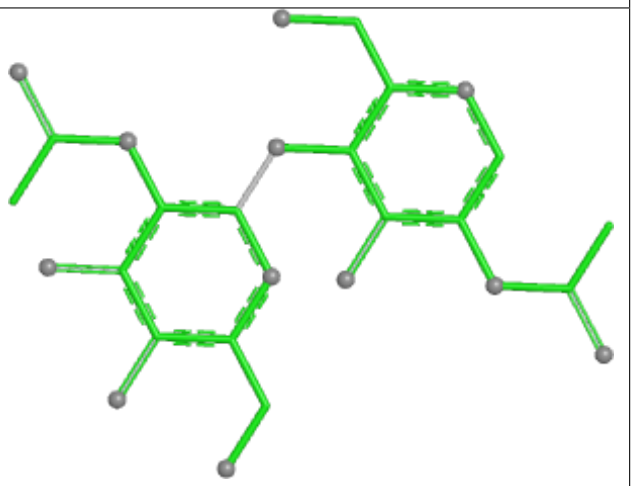


Rings

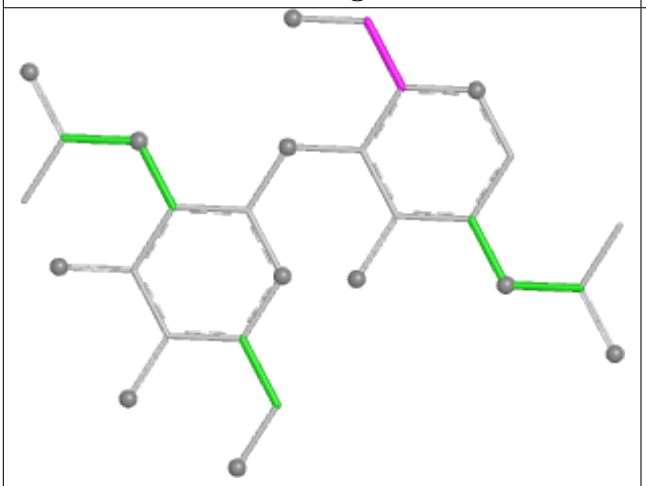
Oligosaccharide Chain U



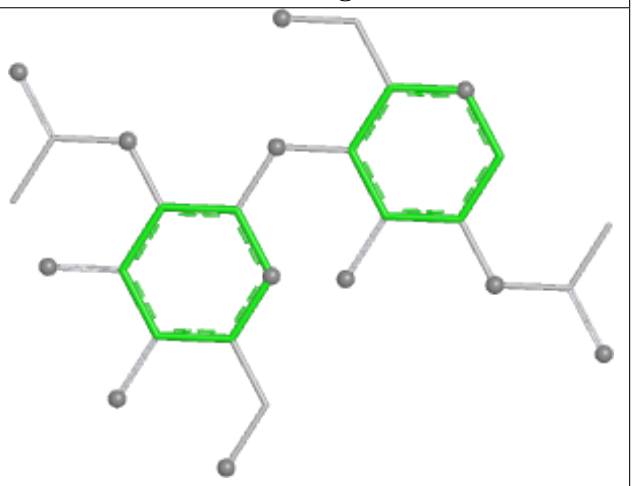
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
4	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.55	0
4	NAG	A	1303	1	14,14,15	0.31	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.31	0
4	NAG	C	1309	1	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	B	1311	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	A	1304	1	14,14,15	0.42	0	17,19,21	0.59	0
4	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	A	1302	1	14,14,15	0.32	0	17,19,21	0.64	0
4	NAG	B	1302	1	14,14,15	0.33	0	17,19,21	0.65	0
4	NAG	C	1303	1	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	B	1301	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	NAG	C	1311	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	B	1309	1	14,14,15	0.17	0	17,19,21	0.46	0
4	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.32	0
4	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.65	0
4	NAG	C	1310	1	14,14,15	0.20	0	17,19,21	0.61	0
4	NAG	B	1303	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	A	1311	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
4	NAG	A	1307	1	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.53	0
4	NAG	B	1304	1	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	C	1312	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.59	0
4	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.32	0
4	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	A	1309	1	14,14,15	0.18	0	17,19,21	0.46	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	A	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1301	NAG	C1-O5-C5	2.78	115.95	112.19
4	B	1301	NAG	C1-O5-C5	2.74	115.91	112.19
4	A	1301	NAG	C1-O5-C5	2.66	115.80	112.19

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1304	NAG	1	0
4	B	1304	NAG	1	0
4	C	1304	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.

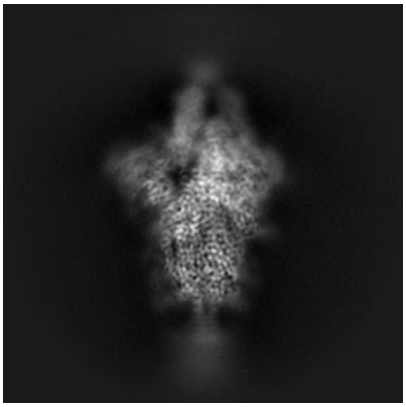
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12777. These allow visual inspection of the internal detail of the map and identification of artifacts.

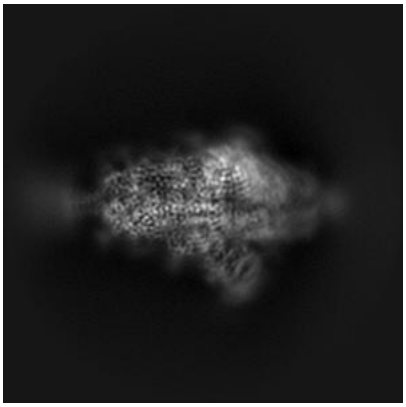
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

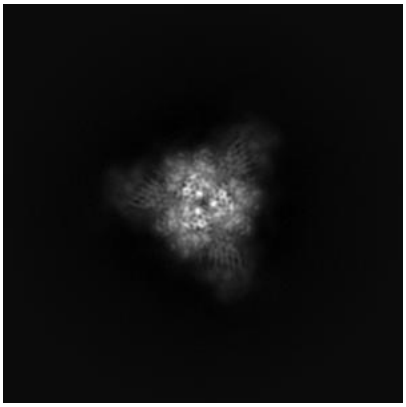
6.1.1 Primary map



X



Y

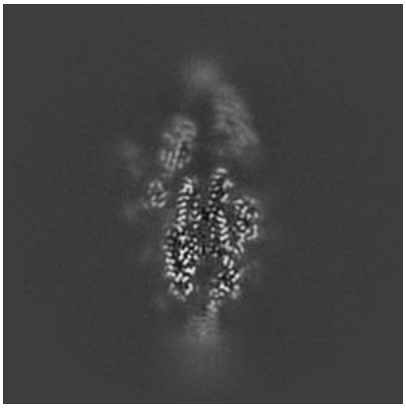


Z

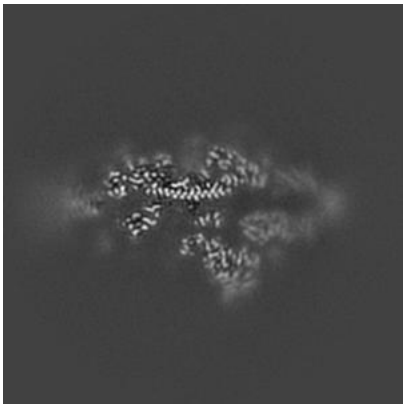
The images above show the map projected in three orthogonal directions.

6.2 Central slices

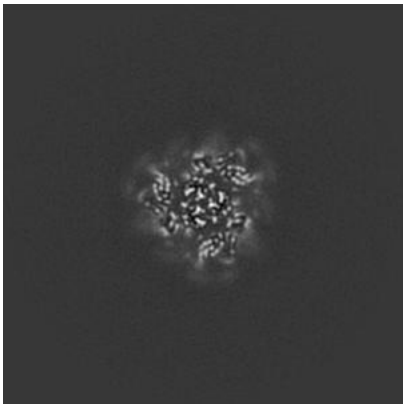
6.2.1 Primary map



X Index: 150



Y Index: 150

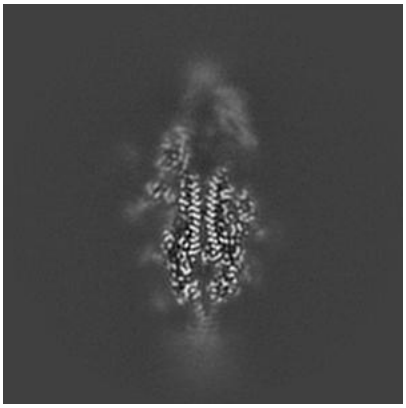


Z Index: 150

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

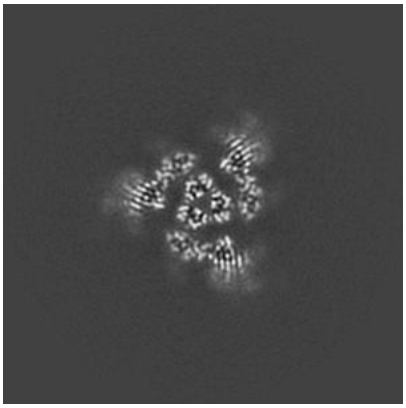
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 146

Y Index: 157

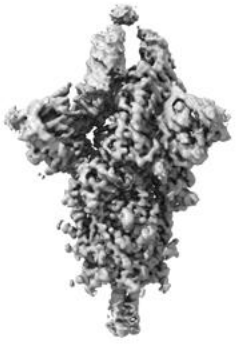


Z Index: 164

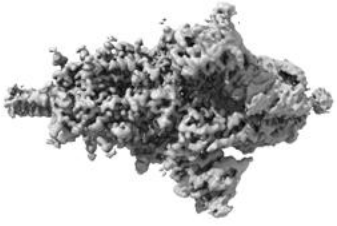
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0099. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

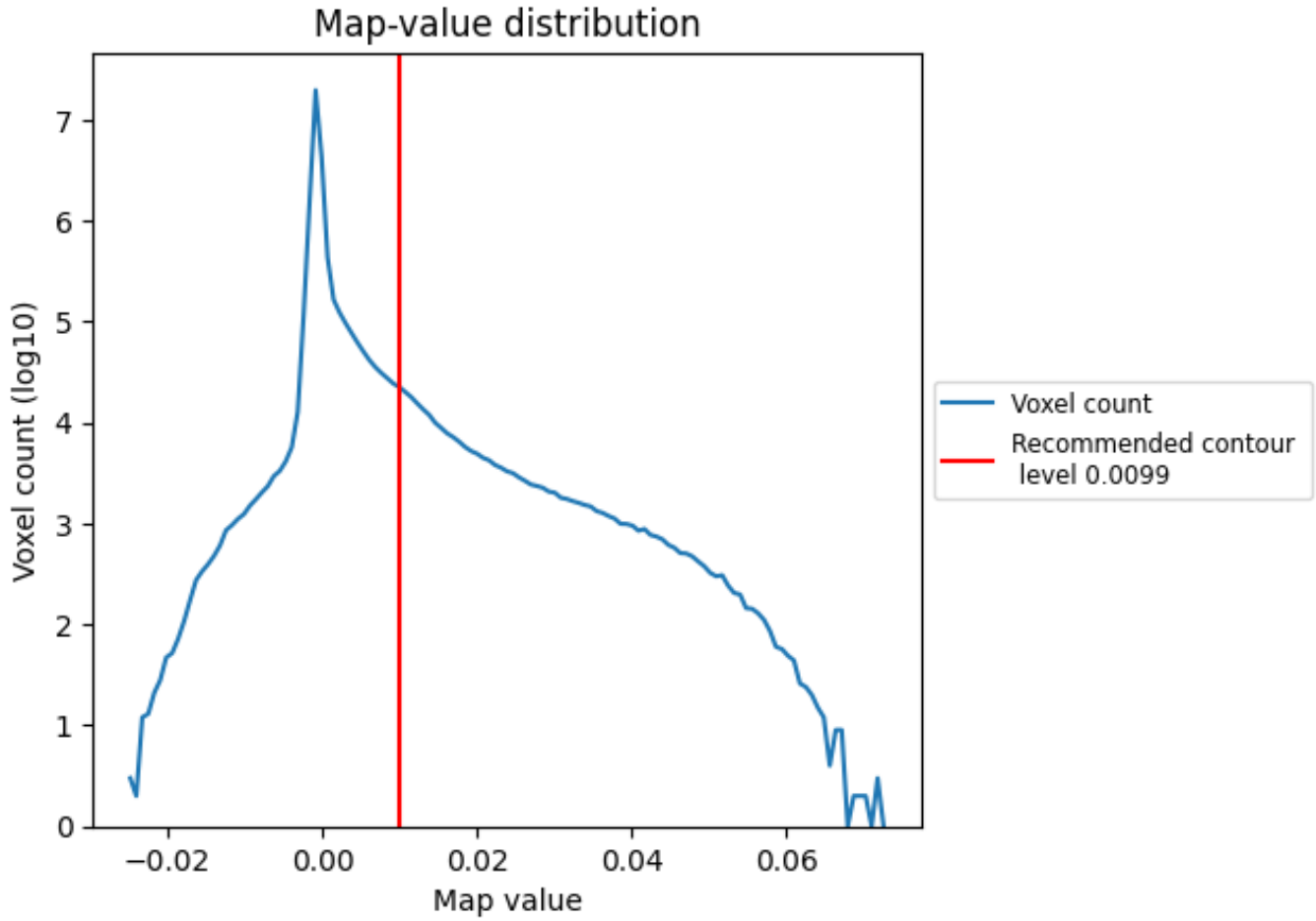
6.5 Mask visualisation (i)

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

7 Map analysis

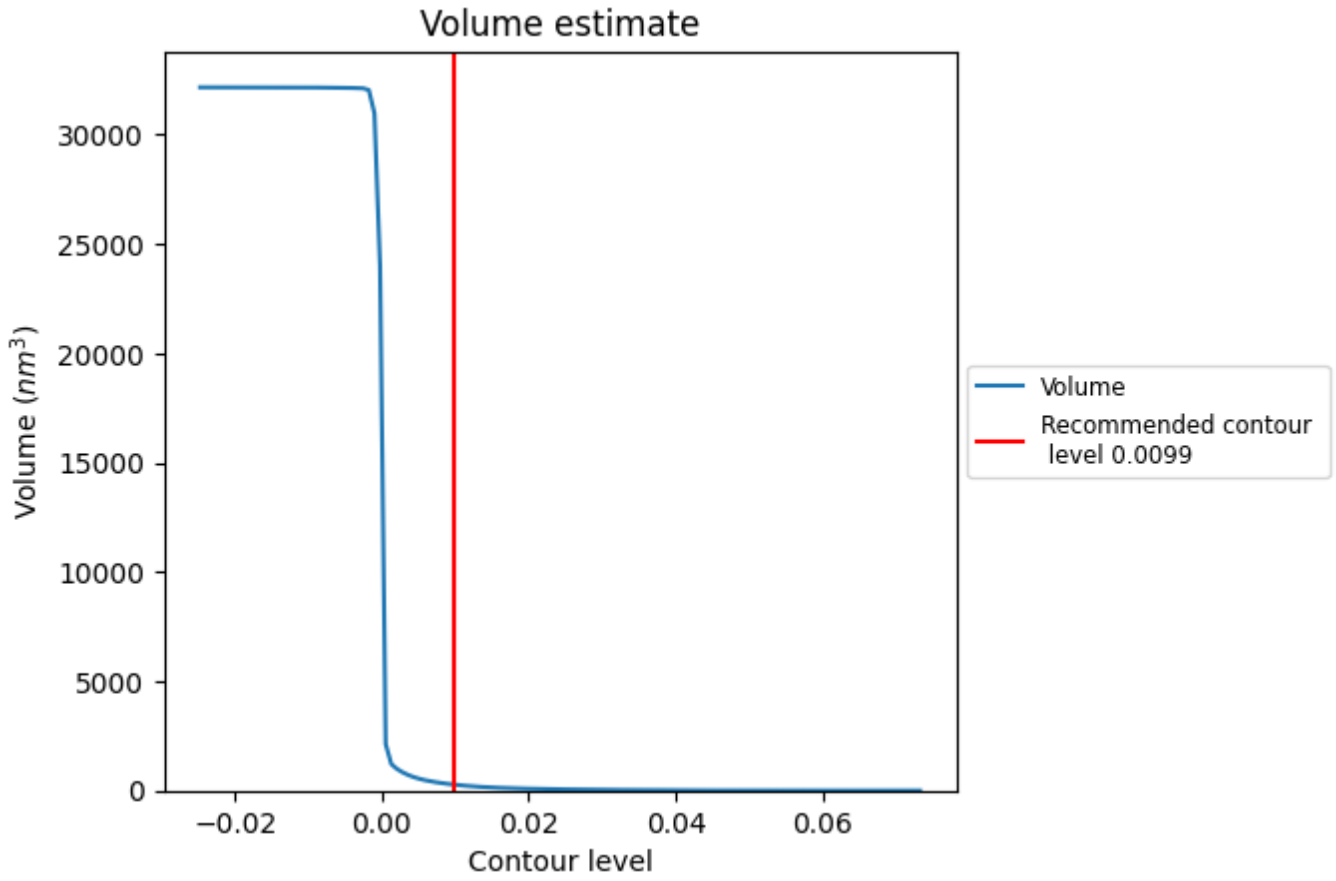
This section contains the results of statistical analysis of the map.

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.

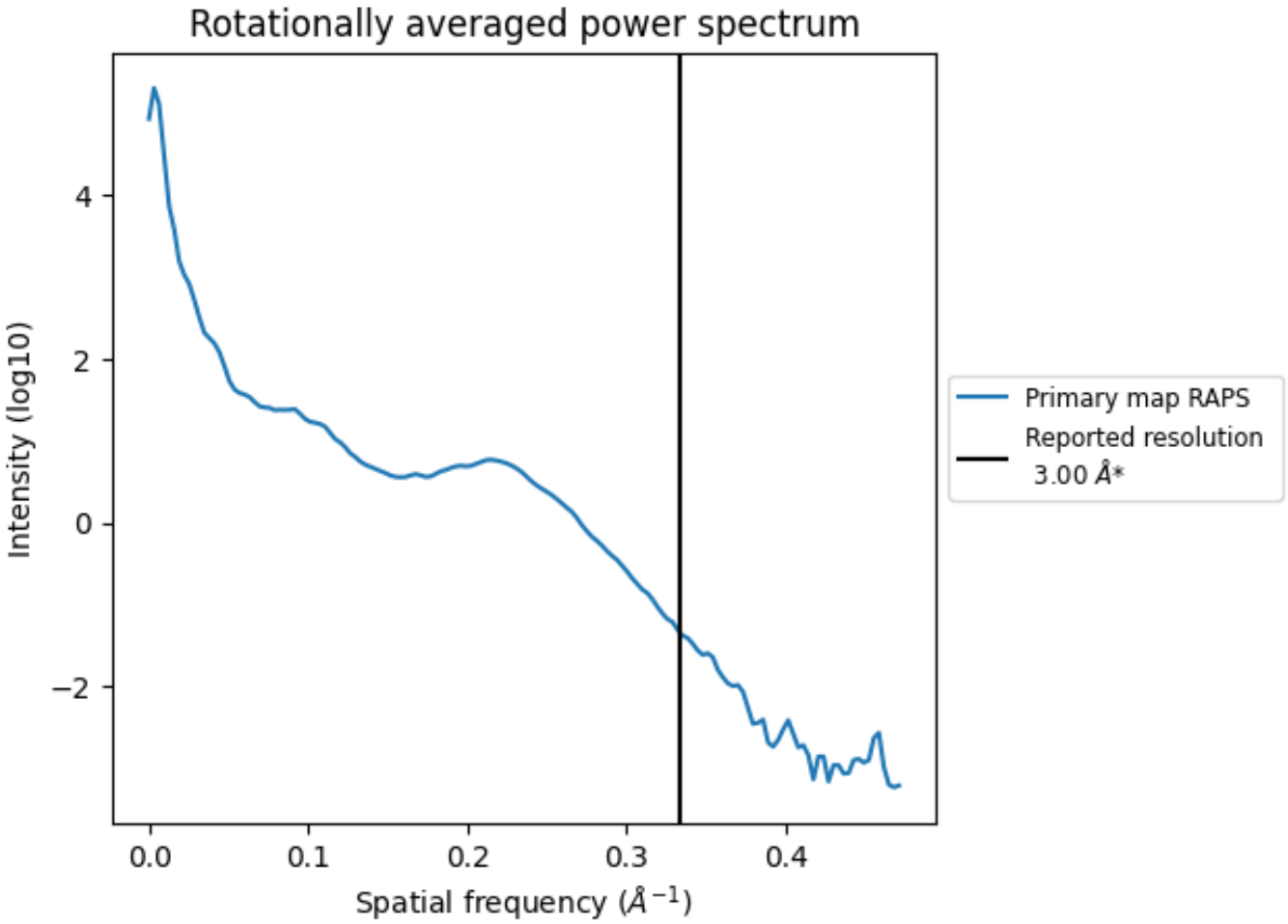
7.2 Volume estimate (i)



The volume at the recommended contour level is 270 nm^3; this corresponds to an approximate mass of 244 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)

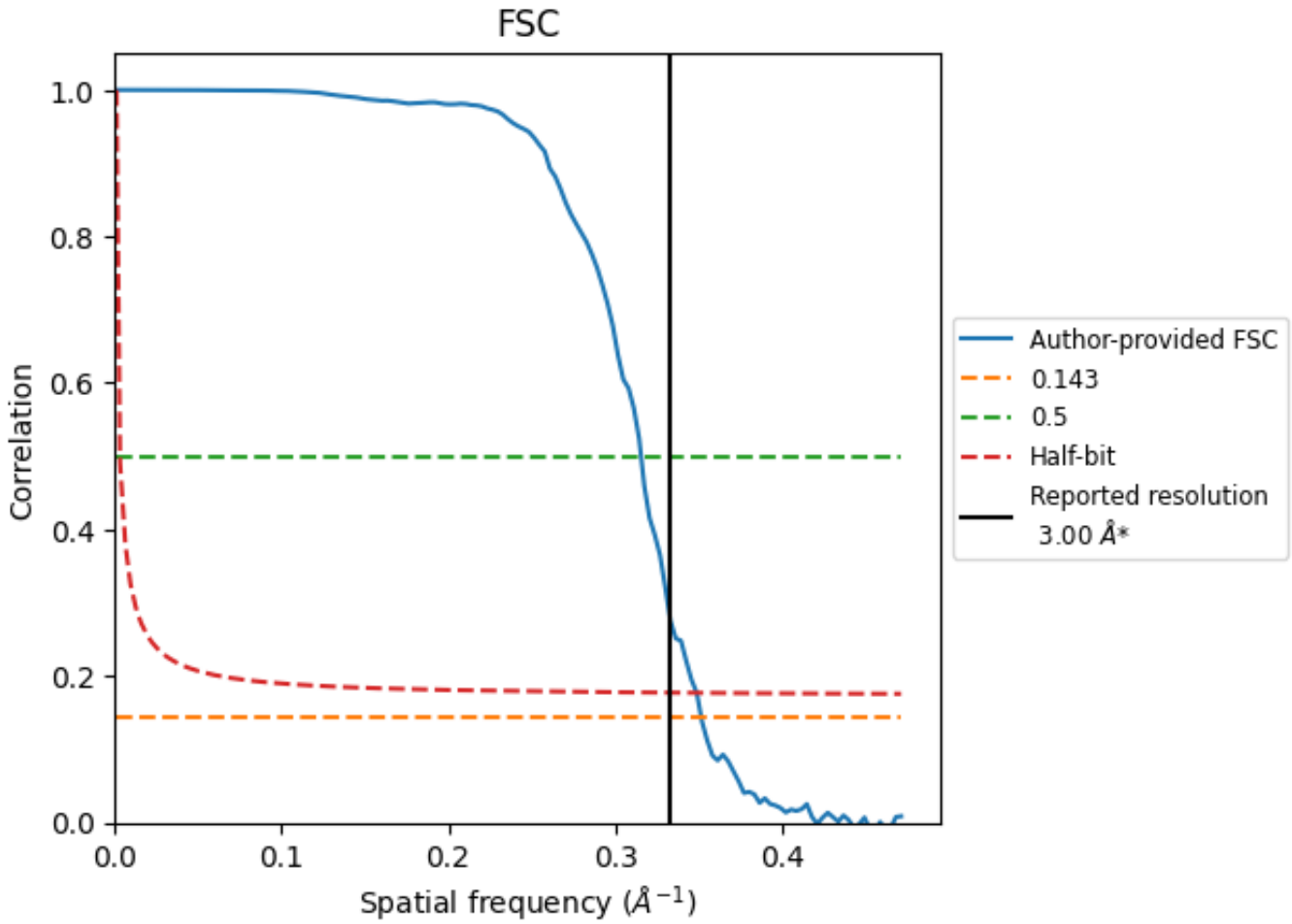


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

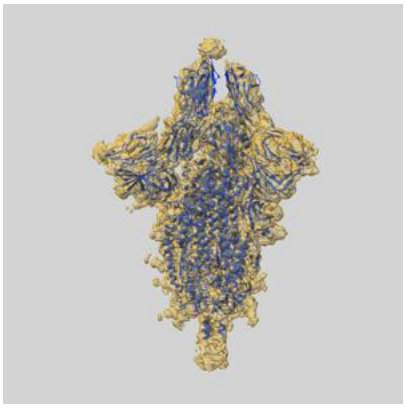
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.84	3.17	2.87
Unmasked-calculated*	-	-	-

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

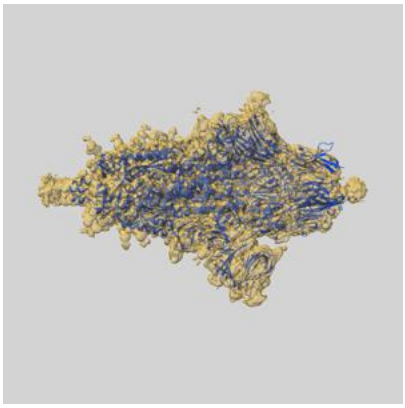
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12777 and PDB model 7OAN. Per-residue inclusion information can be found in section 3 on page 13.

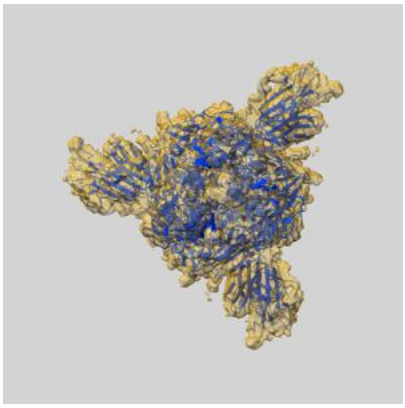
9.1 Map-model overlay



X



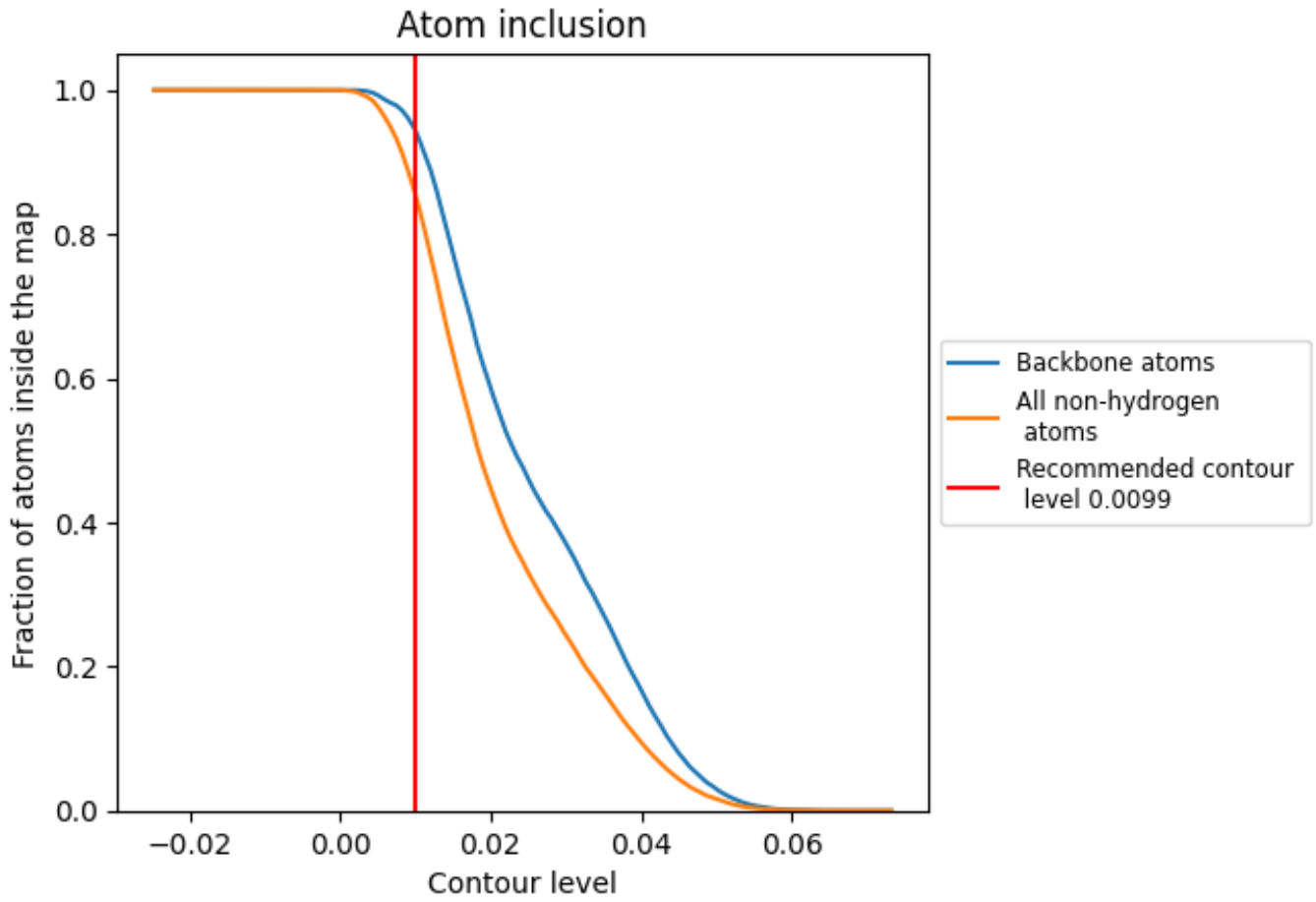
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0099 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.