Full wwPDB EM Validation Report ⓘ

Jan 2, 2024 – 12:24 PM JST

PDB ID	:	8HXJ
EMDB ID	:	EMD-35078
Title	:	BANAL-20-52 Spike trimer
Authors	:	Wang, X.; Xu, G.
Deposited on	:	2023-01-04
Resolution	:	3.50 Å(reported)

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

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

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

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

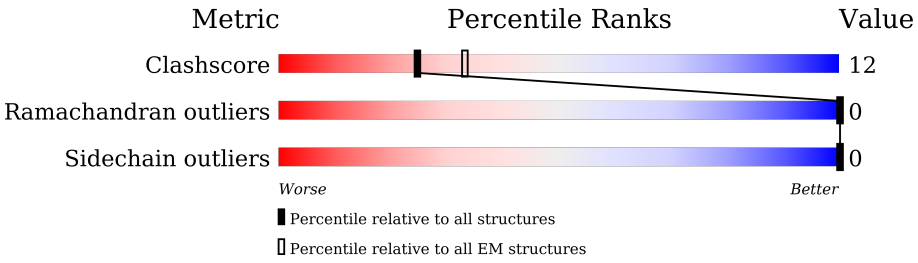
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	1286	66% 22% 12%
1	B	1286	65% 23% 12%
1	C	1286	65% 23% 12%
2	D	2	100%
2	E	2	100% 100%
2	F	2	50% 50%
2	G	2	50% 100%
2	H	2	100%

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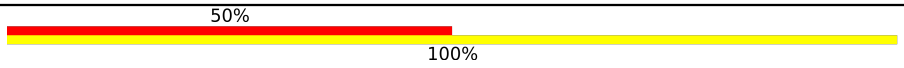
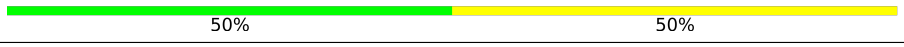
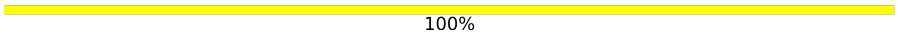
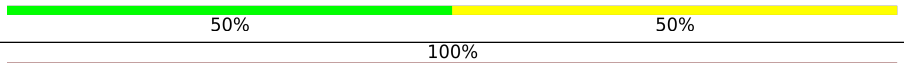
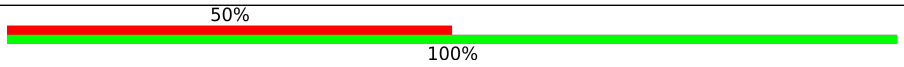
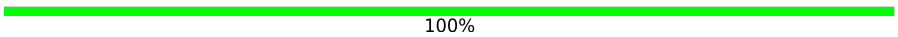
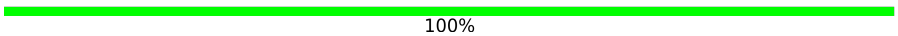
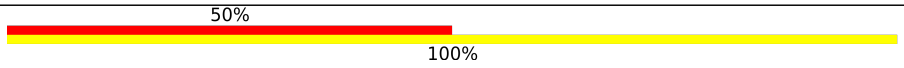
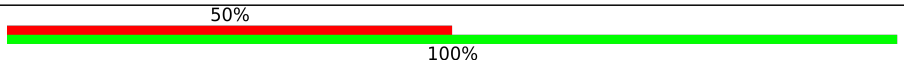
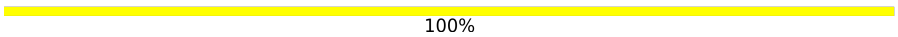
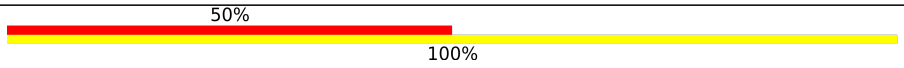
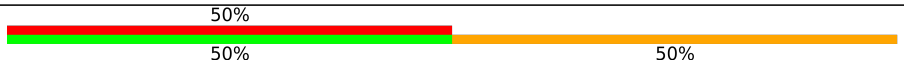
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	
2	a	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27639 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	1133	Total	C	N	O	S	0	0
			8835	5625	1480	1690	40		
1	B	1133	Total	C	N	O	S	0	0
			8835	5625	1480	1690	40		
1	C	1133	Total	C	N	O	S	0	0
			8835	5625	1480	1690	40		

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	PHE	conflict	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	76	ILE	THR	variant	UNP P0DTC2
A	147	ARG	LYS	conflict	UNP P0DTC2
A	218	PRO	GLN	conflict	UNP P0DTC2
A	292	SER	ALA	conflict	UNP P0DTC2
A	346	THR	ARG	conflict	UNP P0DTC2
A	372	THR	ALA	conflict	UNP P0DTC2
A	402	VAL	ILE	conflict	UNP P0DTC2
A	498	HIS	GLN	conflict	UNP P0DTC2
A	519	ASN	HIS	conflict	UNP P0DTC2
A	534	ILE	VAL	conflict	UNP P0DTC2
A	604	ALA	THR	conflict	UNP P0DTC2
A	627	ASN	ASP	conflict	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	789	GLN	PRO	conflict	UNP P0DTC2
A	982	PRO	LYS	conflict	UNP P0DTC2
A	983	PRO	VAL	conflict	UNP P0DTC2
A	1163	SER	GLY	conflict	UNP P0DTC2
A	1205	LEU	-	expression tag	UNP P0DTC2
A	1206	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1207	GLY	-	expression tag	UNP P0DTC2
A	1208	SER	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	TYR	-	expression tag	UNP P0DTC2
A	1211	ILE	-	expression tag	UNP P0DTC2
A	1212	PRO	-	expression tag	UNP P0DTC2
A	1213	GLU	-	expression tag	UNP P0DTC2
A	1214	ALA	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	ASP	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	VAL	-	expression tag	UNP P0DTC2
A	1223	ARG	-	expression tag	UNP P0DTC2
A	1224	LYS	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	TRP	-	expression tag	UNP P0DTC2
A	1229	VAL	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	SER	-	expression tag	UNP P0DTC2
A	1233	THR	-	expression tag	UNP P0DTC2
A	1234	PHE	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	VAL	-	expression tag	UNP P0DTC2
A	1242	LEU	-	expression tag	UNP P0DTC2
A	1243	PHE	-	expression tag	UNP P0DTC2
A	1244	GLN	-	expression tag	UNP P0DTC2
A	1245	GLY	-	expression tag	UNP P0DTC2
A	1246	PRO	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ALA	-	expression tag	UNP P0DTC2
A	1258	TRP	-	expression tag	UNP P0DTC2
A	1259	SER	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	PHE	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	SER	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	SER	-	expression tag	UNP P0DTC2
A	1278	ALA	-	expression tag	UNP P0DTC2
A	1279	TRP	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	PRO	-	expression tag	UNP P0DTC2
A	1283	GLN	-	expression tag	UNP P0DTC2
A	1284	PHE	-	expression tag	UNP P0DTC2
A	1285	GLU	-	expression tag	UNP P0DTC2
A	1286	LYS	-	expression tag	UNP P0DTC2
B	32	SER	PHE	conflict	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	76	ILE	THR	variant	UNP P0DTC2
B	147	ARG	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	218	PRO	GLN	conflict	UNP P0DTC2
B	292	SER	ALA	conflict	UNP P0DTC2
B	346	THR	ARG	conflict	UNP P0DTC2
B	372	THR	ALA	conflict	UNP P0DTC2
B	402	VAL	ILE	conflict	UNP P0DTC2
B	498	HIS	GLN	conflict	UNP P0DTC2
B	519	ASN	HIS	conflict	UNP P0DTC2
B	534	ILE	VAL	conflict	UNP P0DTC2
B	604	ALA	THR	conflict	UNP P0DTC2
B	627	ASN	ASP	conflict	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	789	GLN	PRO	conflict	UNP P0DTC2
B	982	PRO	LYS	conflict	UNP P0DTC2
B	983	PRO	VAL	conflict	UNP P0DTC2
B	1163	SER	GLY	conflict	UNP P0DTC2
B	1205	LEU	-	expression tag	UNP P0DTC2
B	1206	GLU	-	expression tag	UNP P0DTC2
B	1207	GLY	-	expression tag	UNP P0DTC2
B	1208	SER	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	TYR	-	expression tag	UNP P0DTC2
B	1211	ILE	-	expression tag	UNP P0DTC2
B	1212	PRO	-	expression tag	UNP P0DTC2
B	1213	GLU	-	expression tag	UNP P0DTC2
B	1214	ALA	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	ASP	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLN	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	VAL	-	expression tag	UNP P0DTC2
B	1223	ARG	-	expression tag	UNP P0DTC2
B	1224	LYS	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1229	VAL	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	SER	-	expression tag	UNP P0DTC2
B	1233	THR	-	expression tag	UNP P0DTC2
B	1234	PHE	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLU	-	expression tag	UNP P0DTC2
B	1241	VAL	-	expression tag	UNP P0DTC2
B	1242	LEU	-	expression tag	UNP P0DTC2
B	1243	PHE	-	expression tag	UNP P0DTC2
B	1244	GLN	-	expression tag	UNP P0DTC2
B	1245	GLY	-	expression tag	UNP P0DTC2
B	1246	PRO	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ALA	-	expression tag	UNP P0DTC2
B	1258	TRP	-	expression tag	UNP P0DTC2
B	1259	SER	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	PHE	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	SER	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	SER	-	expression tag	UNP P0DTC2
B	1278	ALA	-	expression tag	UNP P0DTC2
B	1279	TRP	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	PRO	-	expression tag	UNP P0DTC2
B	1283	GLN	-	expression tag	UNP P0DTC2
B	1284	PHE	-	expression tag	UNP P0DTC2
B	1285	GLU	-	expression tag	UNP P0DTC2
B	1286	LYS	-	expression tag	UNP P0DTC2
C	32	SER	PHE	conflict	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	76	ILE	THR	variant	UNP P0DTC2
C	147	ARG	LYS	conflict	UNP P0DTC2
C	218	PRO	GLN	conflict	UNP P0DTC2
C	292	SER	ALA	conflict	UNP P0DTC2
C	346	THR	ARG	conflict	UNP P0DTC2
C	372	THR	ALA	conflict	UNP P0DTC2
C	402	VAL	ILE	conflict	UNP P0DTC2
C	498	HIS	GLN	conflict	UNP P0DTC2
C	519	ASN	HIS	conflict	UNP P0DTC2
C	534	ILE	VAL	conflict	UNP P0DTC2
C	604	ALA	THR	conflict	UNP P0DTC2
C	627	ASN	ASP	conflict	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	789	GLN	PRO	conflict	UNP P0DTC2
C	982	PRO	LYS	conflict	UNP P0DTC2
C	983	PRO	VAL	conflict	UNP P0DTC2
C	1163	SER	GLY	conflict	UNP P0DTC2
C	1205	LEU	-	expression tag	UNP P0DTC2
C	1206	GLU	-	expression tag	UNP P0DTC2
C	1207	GLY	-	expression tag	UNP P0DTC2
C	1208	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	TYR	-	expression tag	UNP P0DTC2
C	1211	ILE	-	expression tag	UNP P0DTC2
C	1212	PRO	-	expression tag	UNP P0DTC2
C	1213	GLU	-	expression tag	UNP P0DTC2
C	1214	ALA	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	ASP	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLN	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	VAL	-	expression tag	UNP P0DTC2
C	1223	ARG	-	expression tag	UNP P0DTC2
C	1224	LYS	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	TRP	-	expression tag	UNP P0DTC2
C	1229	VAL	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	THR	-	expression tag	UNP P0DTC2
C	1234	PHE	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	ARG	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	VAL	-	expression tag	UNP P0DTC2
C	1242	LEU	-	expression tag	UNP P0DTC2
C	1243	PHE	-	expression tag	UNP P0DTC2
C	1244	GLN	-	expression tag	UNP P0DTC2
C	1245	GLY	-	expression tag	UNP P0DTC2
C	1246	PRO	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ALA	-	expression tag	UNP P0DTC2
C	1258	TRP	-	expression tag	UNP P0DTC2
C	1259	SER	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	PHE	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	SER	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	SER	-	expression tag	UNP P0DTC2
C	1278	ALA	-	expression tag	UNP P0DTC2
C	1279	TRP	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	PRO	-	expression tag	UNP P0DTC2
C	1283	GLN	-	expression tag	UNP P0DTC2
C	1284	PHE	-	expression tag	UNP P0DTC2
C	1285	GLU	-	expression tag	UNP P0DTC2
C	1286	LYS	-	expression tag	UNP P0DTC2

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

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

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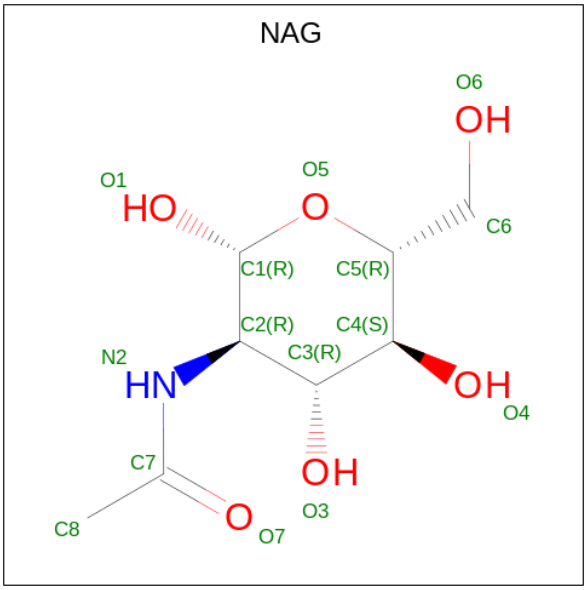
Mol	Chain	Residues	Atoms	AltConf	Trace
2	W	2	Total C N O 28 16 2 10	0	0
2	X	2	Total C N O 28 16 2 10	0	0
2	Y	2	Total C N O 28 16 2 10	0	0
2	Z	2	Total C N O 28 16 2 10	0	0
2	a	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0

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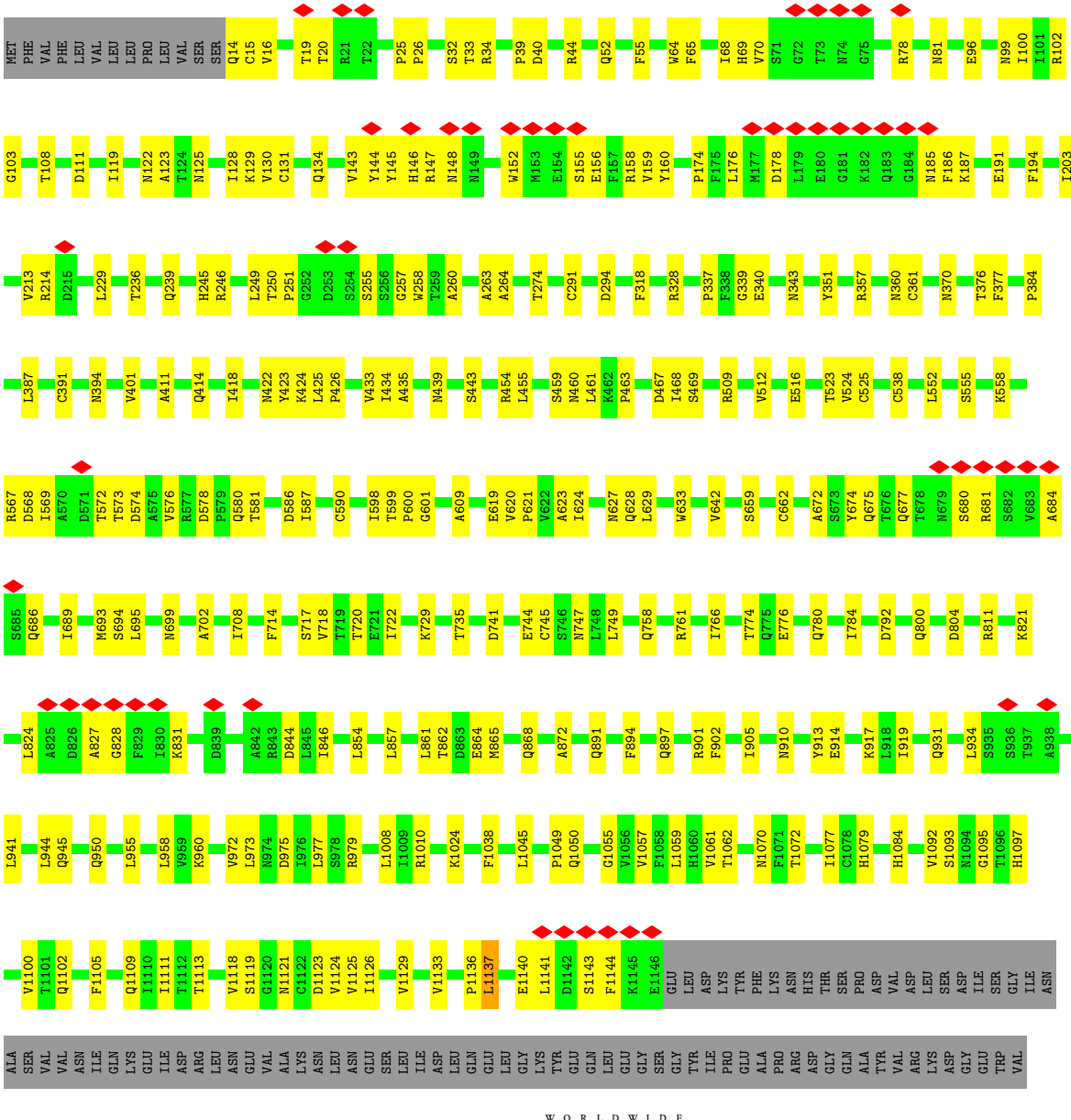
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

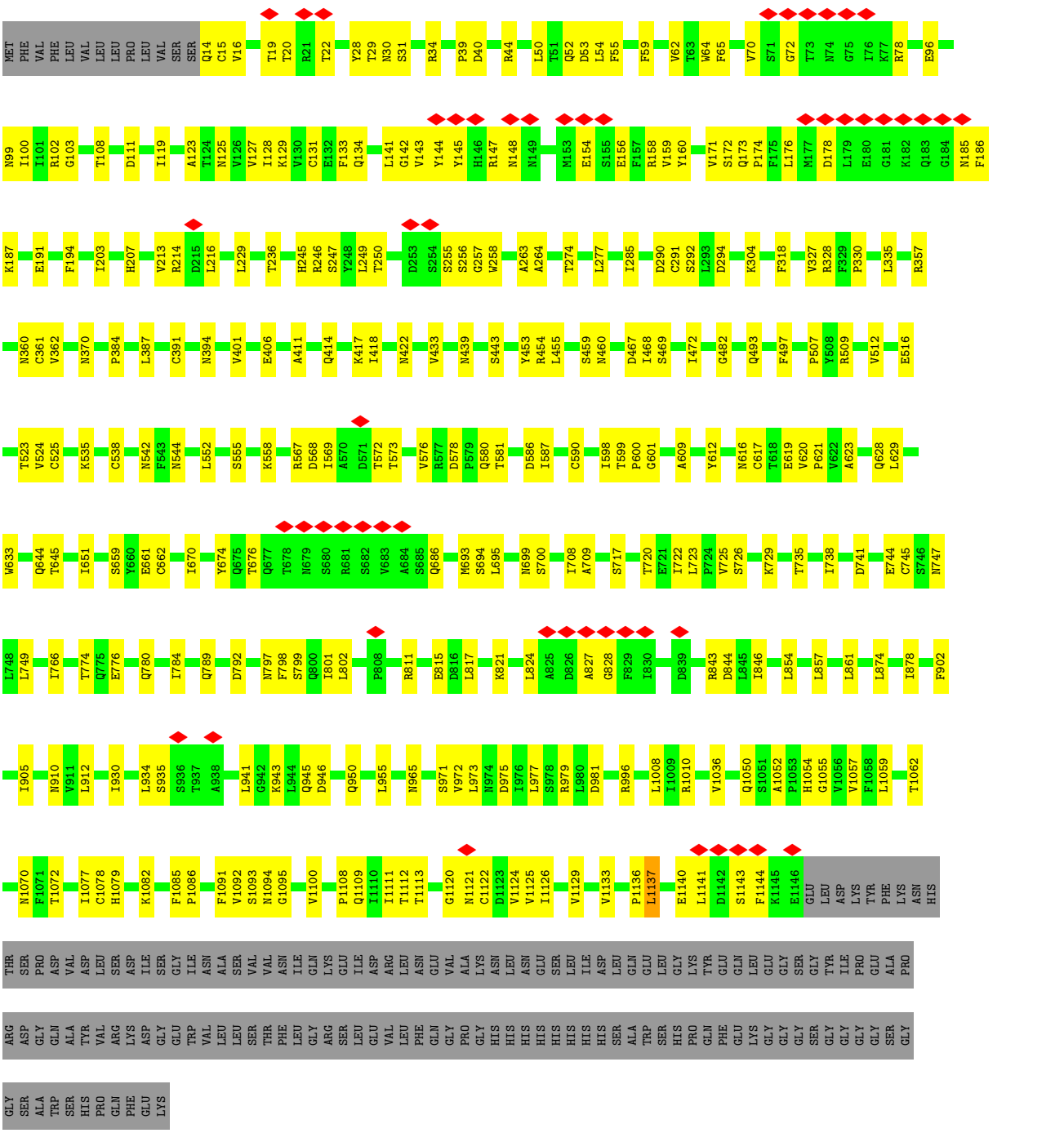
- Molecule 1: Spike glycoprotein

Chain A:



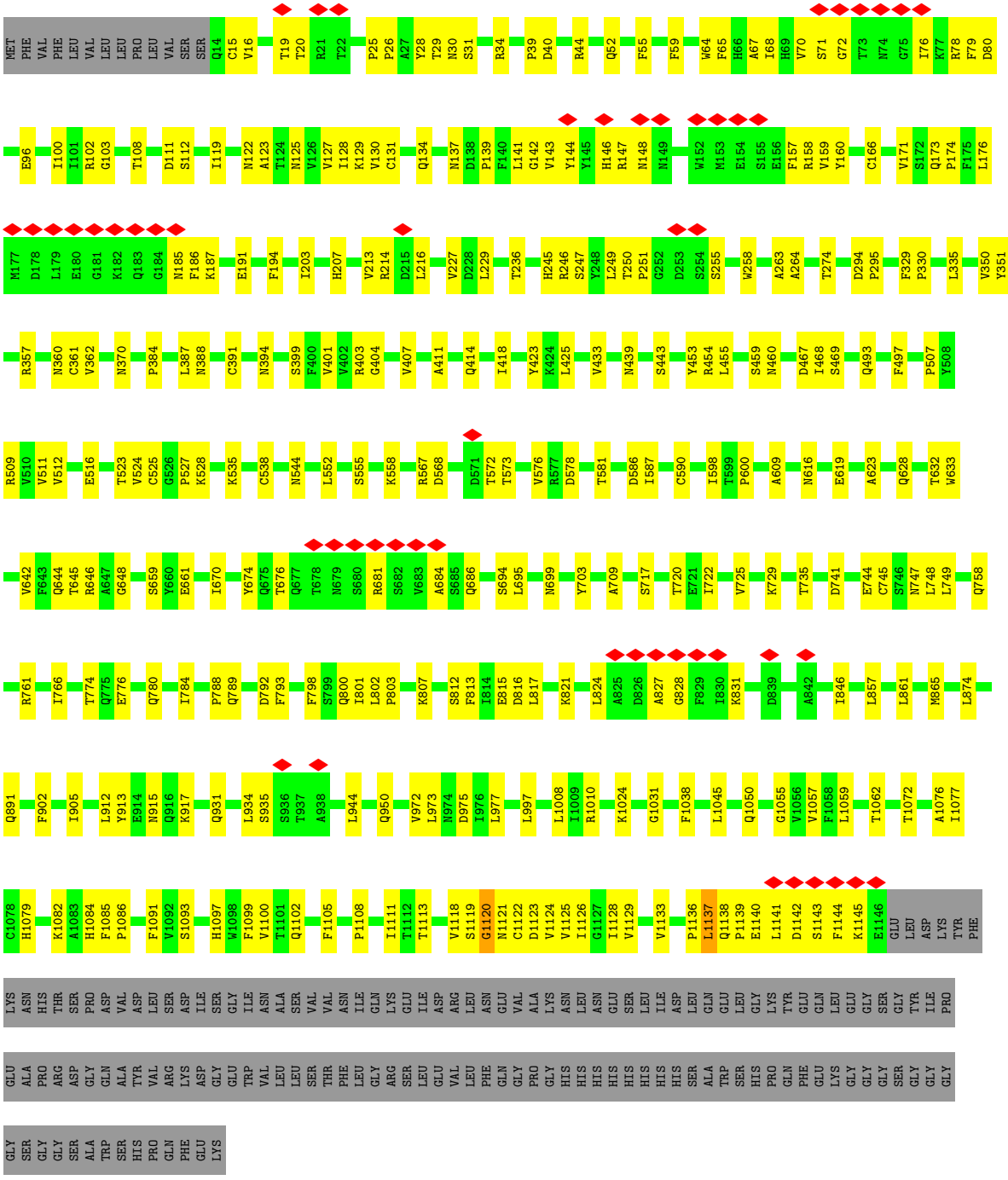
• Molecule 1: Spike glycoprotein

Chain B:



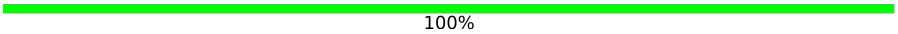
• Molecule 1: Spike glycoprotein

Chain C:



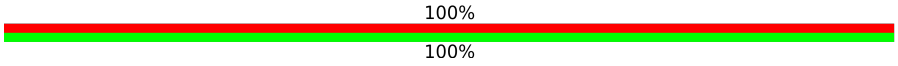
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:

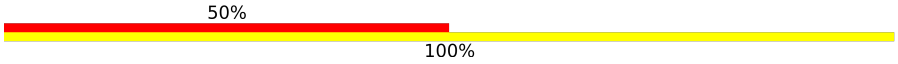


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

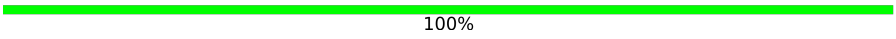
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



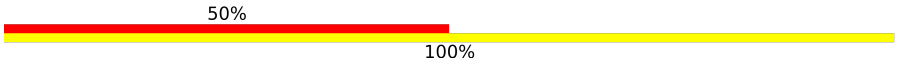
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

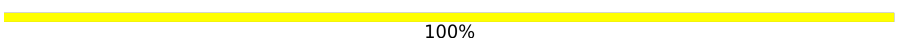


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

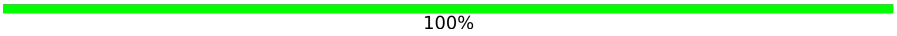
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:



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

Chain M:

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

Chain N:

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

Chain O:

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

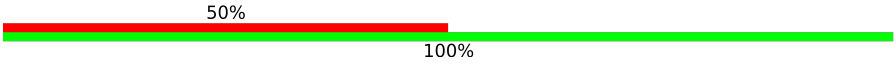
Chain P:

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

Chain Q:

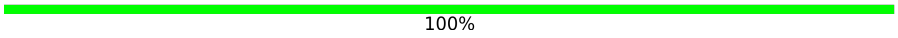
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain S:

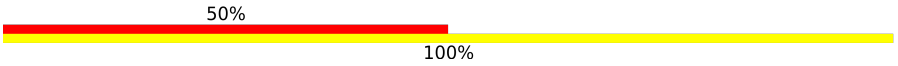


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

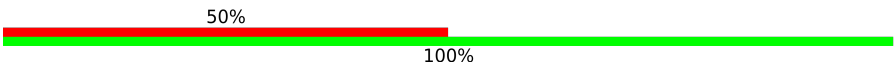
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



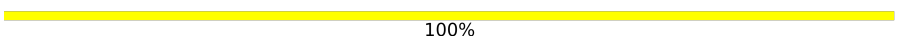
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



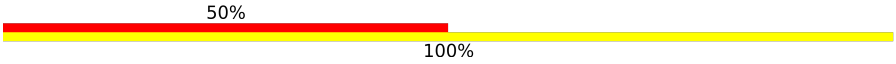
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain X:



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

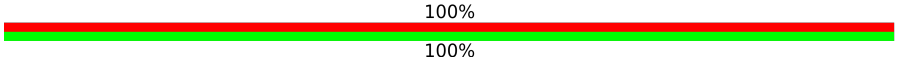
Chain Y:

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

Chain Z:

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

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179587	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	391.03998, 391.03998, 391.03998	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.26	0/9042	0.50	1/12315 (0.0%)
1	B	0.26	0/9042	0.50	1/12315 (0.0%)
1	C	0.26	0/9042	0.50	2/12315 (0.0%)
All	All	0.26	0/27126	0.50	4/36945 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1120	GLY	N-CA-C	6.87	130.26	113.10
1	A	1137	LEU	CA-CB-CG	5.43	127.78	115.30
1	C	1137	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	1137	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8835	0	8596	211	0
1	B	8835	0	8596	225	0
1	C	8835	0	8596	240	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	0	0
2	F	28	0	25	2	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	3	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	1	0
2	V	28	0	25	0	0
2	W	28	0	25	2	0
2	X	28	0	25	1	0
2	Y	28	0	25	0	0
2	Z	28	0	25	3	0
2	a	28	0	25	0	0
3	A	154	0	143	6	0
3	B	154	0	143	6	0
3	C	154	0	143	10	0
All	All	27639	0	26817	635	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 12.

All (635) 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:A:917:LYS:NZ	1:C:1126:ILE:HD11	1.52	1.22
1:B:1126:ILE:HD11	1:C:917:LYS:NZ	1.59	1.14
1:C:1108:PRO:HG2	3:C:1308:NAG:H61	1.18	1.10
1:B:1126:ILE:HD11	1:C:917:LYS:HZ2	1.01	1.10
1:C:1079:HIS:CG	1:C:1133:VAL:HG12	1.88	1.07
1:A:917:LYS:HZ2	1:C:1126:ILE:HD11	0.98	1.05
1:A:1079:HIS:CG	1:A:1133:VAL:HG12	1.95	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:ILE:CD1	1:C:917:LYS:HZ2	1.75	0.99
1:C:1082:LYS:HB3	1:C:1118:VAL:HG11	1.39	0.99
1:A:917:LYS:HZ2	1:C:1126:ILE:CD1	1.76	0.98
1:B:1079:HIS:CG	1:B:1133:VAL:HG12	2.01	0.96
1:C:1082:LYS:HB3	1:C:1118:VAL:CG1	1.95	0.95
1:B:1112:THR:HG23	1:B:1136:PRO:HD3	1.48	0.94
1:C:1079:HIS:CD2	1:C:1133:VAL:CG1	2.52	0.93
1:A:99:ASN:HB3	1:A:102:ARG:HE	1.36	0.89
1:C:1079:HIS:CD2	1:C:1133:VAL:HG12	2.06	0.89
1:A:1079:HIS:CD2	1:A:1133:VAL:HG12	2.08	0.88
1:A:917:LYS:NZ	1:C:1126:ILE:CD1	2.34	0.86
1:A:1079:HIS:CD2	1:A:1133:VAL:CG1	2.58	0.85
1:B:53:ASP:OD1	1:B:54:LEU:N	2.10	0.85
1:B:1094:ASN:OD1	1:B:1095:GLY:N	2.10	0.83
1:B:1108:PRO:HG2	3:B:1307:NAG:H61	1.62	0.82
1:B:1126:ILE:CD1	1:C:917:LYS:NZ	2.39	0.78
1:C:1079:HIS:CG	1:C:1133:VAL:CG1	2.67	0.76
1:B:1112:THR:CG2	1:B:1136:PRO:HD3	2.17	0.75
1:C:1108:PRO:HG2	3:C:1308:NAG:C6	2.08	0.75
1:B:99:ASN:HD21	1:B:178:ASP:HB3	1.50	0.74
1:C:944:LEU:HD21	1:C:1055:GLY:HA3	1.68	0.74
1:A:1072:THR:HG23	1:A:1093:SER:HB3	1.69	0.74
2:U:1:NAG:H62	2:U:2:NAG:HN2	1.49	0.74
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.53	0.74
1:B:1079:HIS:CD2	1:B:1133:VAL:HG12	2.23	0.73
1:B:16:VAL:HG13	1:B:158:ARG:HH22	1.53	0.73
1:A:52:GLN:NE2	1:B:747:ASN:OD1	2.23	0.72
1:C:801:ILE:HG22	1:C:874:LEU:HD21	1.71	0.72
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.55	0.71
1:C:1072:THR:HG23	1:C:1093:SER:HB3	1.72	0.71
1:A:65:PHE:O	1:A:264:ALA:HA	1.91	0.71
1:A:1111:ILE:HG22	1:A:1133:VAL:HG23	1.73	0.71
1:A:1095:GLY:HA3	3:A:1311:NAG:H81	1.72	0.70
1:A:910:ASN:HD22	1:C:1119:SER:CB	2.04	0.70
1:B:1125:VAL:HG22	1:C:913:TYR:HB3	1.73	0.70
1:B:1079:HIS:CD2	1:B:1133:VAL:CG1	2.76	0.69
1:C:1111:ILE:HG22	1:C:1133:VAL:HG23	1.75	0.69
1:B:147:ARG:HE	1:B:148:ASN:H	1.41	0.69
1:A:747:ASN:OD1	1:C:52:GLN:NE2	2.26	0.68
1:C:1084:HIS:CD2	1:C:1118:VAL:HG22	2.28	0.68
1:A:708:ILE:HG21	1:A:1092:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLN:NE2	1:A:931:GLN:OE1	2.27	0.68
1:B:943:LYS:HA	1:B:946:ASP:HB2	1.75	0.68
1:B:250:THR:HA	1:B:257:GLY:HA3	1.76	0.68
1:C:71:SER:HA	1:C:76:ILE:H	1.59	0.67
1:C:1142:ASP:HA	1:C:1145:LYS:HE3	1.77	0.67
1:A:574:ASP:OD2	1:B:843:ARG:NH2	2.28	0.67
1:C:1084:HIS:CD2	1:C:1118:VAL:CG2	2.78	0.66
1:A:20:THR:HG23	1:A:78:ARG:HB3	1.77	0.66
1:A:99:ASN:HD21	1:A:178:ASP:HB3	1.60	0.66
1:B:20:THR:HG23	1:B:78:ARG:HB3	1.78	0.65
1:B:1085:PHE:CZ	1:B:1125:VAL:CG2	2.79	0.65
1:C:147:ARG:HE	1:C:148:ASN:H	1.44	0.65
1:B:96:GLU:HB3	1:B:100:ILE:HD13	1.77	0.65
2:Z:1:NAG:H83	2:Z:1:NAG:H3	1.78	0.65
2:Q:1:NAG:H3	2:Q:1:NAG:H83	1.79	0.65
1:C:246:ARG:HH11	1:C:251:PRO:HG3	1.62	0.65
1:B:1140:GLU:HB3	1:B:1144:PHE:CE2	2.32	0.64
1:B:726:SER:O	1:B:1054:HIS:NE2	2.30	0.64
1:C:798:PHE:HB3	1:C:802:LEU:HD23	1.79	0.64
1:C:803:PRO:HA	1:C:812:SER:HB3	1.78	0.64
1:A:944:LEU:HD21	1:A:1055:GLY:HA3	1.79	0.64
1:B:144:TYR:H	1:B:245:HIS:CE1	2.15	0.64
1:A:1140:GLU:HA	1:A:1143:SER:HB3	1.78	0.64
1:C:1140:GLU:HB3	1:C:1144:PHE:CE2	2.33	0.64
1:A:662:CYS:HB2	1:A:693:MET:HG2	1.80	0.63
1:A:913:TYR:HB3	1:C:1125:VAL:HG22	1.80	0.63
1:C:776:GLU:O	1:C:780:GLN:NE2	2.31	0.63
1:C:1113:THR:HG22	1:C:1136:PRO:HD2	1.81	0.63
1:C:20:THR:HG23	1:C:78:ARG:HB3	1.79	0.63
1:A:144:TYR:H	1:A:245:HIS:CE1	2.16	0.63
1:B:576:VAL:HG22	1:B:587:ILE:HD11	1.81	0.63
1:A:1079:HIS:CG	1:A:1133:VAL:CG1	2.77	0.62
1:C:1097:HIS:CD2	3:C:1308:NAG:C7	2.82	0.62
1:C:137:ASN:H	3:C:1301:NAG:H83	1.64	0.62
1:C:1079:HIS:CD2	1:C:1133:VAL:HG11	2.35	0.62
1:B:824:LEU:HD21	1:B:828:GLY:HA3	1.81	0.62
1:C:1085:PHE:CZ	1:C:1125:VAL:CG2	2.82	0.62
1:A:568:ASP:OD1	1:A:569:ILE:N	2.32	0.61
1:A:776:GLU:O	1:A:780:GLN:NE2	2.33	0.61
1:B:725:VAL:HG22	1:B:1055:GLY:HA2	1.82	0.61
1:C:1140:GLU:HA	1:C:1143:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:824:LEU:HD21	1:C:828:GLY:HA3	1.82	0.61
1:A:576:VAL:HG22	1:A:587:ILE:HD11	1.82	0.61
1:A:1077:ILE:HG22	1:A:1129:VAL:O	2.01	0.61
1:B:717:SER:OG	1:B:1062:THR:OG1	2.18	0.61
1:C:576:VAL:HG22	1:C:587:ILE:HD11	1.81	0.61
1:B:1077:ILE:HG22	1:B:1129:VAL:O	2.00	0.60
1:C:28:TYR:CE2	3:C:1307:NAG:H5	2.36	0.60
1:B:439:ASN:O	1:B:443:SER:OG	2.17	0.60
1:B:776:GLU:O	1:B:780:GLN:NE2	2.33	0.60
1:B:1141:LEU:HA	1:C:1144:PHE:HE1	1.66	0.60
1:A:774:THR:HG22	1:A:861:LEU:HD12	1.83	0.60
1:A:1140:GLU:HB3	1:A:1144:PHE:CE2	2.37	0.60
1:B:255:SER:HG	1:B:258:TRP:HE1	1.49	0.60
1:C:717:SER:OG	1:C:1062:THR:OG1	2.19	0.60
1:B:950:GLN:OE1	1:B:1010:ARG:NH1	2.35	0.60
1:B:1113:THR:HG22	1:B:1136:PRO:HD2	1.82	0.59
1:C:102:ARG:HG3	1:C:141:LEU:HD23	1.83	0.59
1:B:1140:GLU:HA	1:B:1143:SER:HB3	1.83	0.59
1:C:1077:ILE:HA	1:C:1129:VAL:O	2.02	0.59
1:B:1077:ILE:HA	1:B:1129:VAL:O	2.00	0.59
1:A:972:VAL:HG12	1:A:975:ASP:H	1.67	0.59
1:B:708:ILE:HG21	1:B:1092:VAL:HG22	1.84	0.59
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.36	0.59
1:A:717:SER:OG	1:A:1062:THR:OG1	2.20	0.59
1:A:454:ARG:NH2	1:A:467:ASP:O	2.35	0.59
1:A:1144:PHE:CE1	1:C:1141:LEU:HA	2.38	0.59
1:B:1085:PHE:CZ	1:B:1125:VAL:HG21	2.38	0.59
1:A:423:TYR:HE2	1:A:425:LEU:HD13	1.68	0.59
2:M:1:NAG:H5	2:M:2:NAG:H83	1.85	0.59
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.34	0.59
1:A:391:CYS:HA	1:A:525:CYS:HA	1.85	0.59
1:B:1085:PHE:CE1	1:B:1125:VAL:HG21	2.38	0.59
1:C:735:THR:HG22	1:C:749:LEU:HD23	1.85	0.59
1:C:538:CYS:HB3	1:C:628:GLN:HE22	1.69	0.58
1:A:824:LEU:HD21	1:A:828:GLY:HA3	1.84	0.58
1:A:1144:PHE:HE1	1:C:1141:LEU:HA	1.67	0.58
1:C:399:SER:HB3	1:C:511:VAL:HG22	1.84	0.58
1:A:827:ALA:HB2	1:A:846:ILE:HD12	1.83	0.58
1:B:1111:ILE:HG22	1:B:1133:VAL:HG23	1.85	0.58
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.36	0.58
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:HH22	1:B:469:SER:H	1.52	0.58
1:B:1141:LEU:HA	1:C:1144:PHE:CE1	2.38	0.58
1:C:1084:HIS:CG	1:C:1118:VAL:HG22	2.38	0.58
1:C:950:GLN:OE1	1:C:1010:ARG:NH1	2.37	0.57
1:C:1024:LYS:NZ	1:C:1038:PHE:O	2.34	0.57
1:A:735:THR:HG22	1:A:749:LEU:HD23	1.87	0.57
1:A:1113:THR:HG22	1:A:1136:PRO:HD2	1.85	0.57
1:B:972:VAL:HG12	1:B:975:ASP:H	1.68	0.57
1:C:70:VAL:HG12	1:C:72:GLY:H	1.70	0.57
1:C:766:ILE:HD11	1:C:1008:LEU:HD23	1.87	0.57
1:C:827:ALA:HB2	1:C:846:ILE:HD12	1.86	0.57
1:A:568:ASP:HB3	1:A:572:THR:HB	1.87	0.57
1:A:1097:HIS:HD2	3:A:1311:NAG:O7	1.86	0.57
1:B:455:LEU:HD11	1:C:370:ASN:HB2	1.85	0.57
1:C:102:ARG:HH12	1:C:122:ASN:HA	1.69	0.57
1:C:972:VAL:HG12	1:C:975:ASP:H	1.69	0.57
1:C:454:ARG:NH2	1:C:467:ASP:O	2.38	0.57
1:A:158:ARG:HH11	1:A:249:LEU:HD13	1.70	0.57
1:A:1119:SER:CB	1:B:910:ASN:HD22	2.17	0.57
1:C:19:THR:O	1:C:78:ARG:NH1	2.38	0.57
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.36	0.57
1:B:391:CYS:HA	1:B:525:CYS:HA	1.87	0.57
1:C:391:CYS:HA	1:C:525:CYS:HA	1.87	0.57
1:A:766:ILE:HD11	1:A:1008:LEU:HD23	1.87	0.57
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.68	0.56
1:B:774:THR:HG22	1:B:861:LEU:HD12	1.86	0.56
1:B:1079:HIS:CG	1:B:1133:VAL:CG1	2.83	0.56
1:C:1122:CYS:SG	1:C:1123:ASP:N	2.77	0.56
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.87	0.56
1:B:798:PHE:HB3	1:B:802:LEU:HD23	1.86	0.56
1:A:394:ASN:HB3	1:A:516:GLU:HB3	1.86	0.56
1:A:538:CYS:HB3	1:A:628:GLN:HE22	1.70	0.56
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.35	0.56
1:B:616:ASN:HB3	3:B:1302:NAG:HN2	1.70	0.56
1:C:255:SER:HG	1:C:258:TRP:HE1	1.52	0.56
1:B:662:CYS:HB2	1:B:693:MET:HG2	1.88	0.56
1:B:65:PHE:O	1:B:264:ALA:HA	2.04	0.56
1:B:827:ALA:HB2	1:B:846:ILE:HD12	1.87	0.56
1:A:1077:ILE:HA	1:A:1129:VAL:O	2.04	0.56
1:B:246:ARG:HD3	1:B:257:GLY:HA2	1.87	0.56
1:B:797:ASN:OD1	1:B:799:SER:OG	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.37	0.56
1:C:1082:LYS:HB3	1:C:1118:VAL:HG13	1.81	0.56
1:B:411:ALA:HB3	1:B:414:GLN:HB2	1.88	0.56
1:C:127:VAL:HG22	1:C:171:VAL:HG22	1.87	0.56
1:C:1077:ILE:HG22	1:C:1129:VAL:O	2.05	0.56
1:B:123:ALA:HB3	2:Q:1:NAG:O7	2.06	0.56
1:B:538:CYS:HB3	1:B:628:GLN:HE22	1.70	0.56
1:A:854:LEU:HD21	1:A:958:LEU:HB3	1.86	0.55
1:C:439:ASN:O	1:C:443:SER:OG	2.16	0.55
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.89	0.55
1:B:766:ILE:HD11	1:B:1008:LEU:HD23	1.89	0.55
1:B:213:VAL:HG13	1:B:214:ARG:HG2	1.87	0.55
1:B:454:ARG:NH2	1:B:467:ASP:O	2.38	0.55
1:B:1085:PHE:HZ	1:B:1125:VAL:CG2	2.19	0.55
1:B:100:ILE:HD12	1:B:100:ILE:H	1.71	0.55
1:A:620:VAL:HG23	1:A:621:PRO:HD3	1.88	0.55
1:B:52:GLN:NE2	1:C:747:ASN:OD1	2.40	0.55
1:B:277:LEU:HD22	1:B:285:ILE:HD13	1.89	0.55
1:C:29:THR:HG22	1:C:30:ASN:H	1.72	0.55
1:B:357:ARG:NH1	1:B:394:ASN:OD1	2.37	0.54
1:C:1121:ASN:OD1	1:C:1122:CYS:O	2.25	0.54
1:A:147:ARG:HE	1:A:148:ASN:H	1.53	0.54
1:C:1124:VAL:HG13	1:C:1125:VAL:H	1.73	0.54
1:A:411:ALA:HB3	1:A:414:GLN:HB2	1.89	0.54
1:B:651:ILE:H	1:B:651:ILE:HD12	1.72	0.54
1:A:15:CYS:HA	1:A:158:ARG:HH21	1.73	0.54
1:A:722:ILE:HG22	1:A:1057:VAL:HG22	1.89	0.54
1:C:800:GLN:NE2	1:C:931:GLN:OE1	2.35	0.54
1:A:14:GLN:O	1:A:158:ARG:NE	2.41	0.54
1:B:744:GLU:HG2	1:B:977:LEU:HD21	1.90	0.54
1:C:1085:PHE:CE1	1:C:1125:VAL:HG21	2.43	0.54
1:A:384:PRO:HA	1:A:387:LEU:HD12	1.90	0.53
1:A:439:ASN:O	1:A:443:SER:OG	2.18	0.53
1:C:1140:GLU:HB3	1:C:1144:PHE:HE2	1.73	0.53
1:A:1126:ILE:N	1:A:1126:ILE:HD12	2.23	0.53
1:B:15:CYS:HA	1:B:158:ARG:HH21	1.73	0.53
1:B:39:PRO:HG3	1:B:55:PHE:HZ	1.74	0.53
1:B:1108:PRO:HG2	3:B:1307:NAG:C6	2.38	0.53
1:C:676:THR:HA	1:C:686:GLN:HG3	1.91	0.53
1:A:917:LYS:HZ1	1:C:1126:ILE:CG1	2.21	0.53
1:C:411:ALA:HB3	1:C:414:GLN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:1:NAG:H62	2:W:2:NAG:HN2	1.73	0.53
1:A:459:SER:OG	1:A:460:ASN:N	2.42	0.53
1:A:950:GLN:OE1	1:A:1010:ARG:NH1	2.42	0.53
1:A:100:ILE:HG21	1:A:263:ALA:HB2	1.90	0.53
1:A:1141:LEU:HA	1:B:1144:PHE:CE1	2.43	0.53
1:C:813:PHE:O	1:C:815:GLU:N	2.42	0.53
1:A:1095:GLY:O	1:A:1097:HIS:CD2	2.62	0.53
1:C:213:VAL:HG13	1:C:214:ARG:HG2	1.91	0.53
1:A:569:ILE:HG12	1:B:843:ARG:CG	2.38	0.52
1:A:702:ALA:HB2	2:J:2:NAG:H5	1.91	0.52
1:C:96:GLU:HB3	1:C:100:ILE:HD13	1.92	0.52
1:A:454:ARG:HH22	1:A:469:SER:H	1.57	0.52
1:A:862:THR:HG23	1:C:646:ARG:HH22	1.74	0.52
1:B:19:THR:O	1:B:78:ARG:NH1	2.43	0.52
1:C:454:ARG:HH22	1:C:469:SER:H	1.56	0.52
1:A:659:SER:O	1:A:694:SER:HB3	2.10	0.52
1:B:29:THR:HG22	1:B:30:ASN:H	1.75	0.52
1:C:102:ARG:NH2	1:C:144:TYR:HD1	2.08	0.52
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.90	0.52
1:B:616:ASN:HB3	3:B:1302:NAG:N2	2.24	0.52
1:C:28:TYR:HB2	3:C:1307:NAG:H83	1.90	0.52
1:B:102:ARG:HG3	1:B:141:LEU:HD23	1.91	0.52
1:B:418:ILE:HG23	1:B:422:ASN:HB2	1.92	0.52
1:A:39:PRO:HG3	1:A:55:PHE:HZ	1.76	0.51
1:C:1079:HIS:ND1	1:C:1133:VAL:HG12	2.24	0.51
1:C:1085:PHE:CZ	1:C:1125:VAL:HG21	2.44	0.51
1:A:1024:LYS:NZ	1:A:1038:PHE:O	2.43	0.51
1:A:68:ILE:HG22	1:A:70:VAL:H	1.75	0.51
1:C:1085:PHE:HZ	1:C:1125:VAL:CG2	2.24	0.51
1:B:1126:ILE:CG1	1:C:917:LYS:HZ1	2.24	0.51
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.92	0.51
1:A:246:ARG:HD3	1:A:257:GLY:HA2	1.93	0.51
1:A:1095:GLY:CA	3:A:1311:NAG:H81	2.41	0.51
1:A:917:LYS:HZ1	1:C:1126:ILE:HD11	1.67	0.51
1:A:1049:PRO:O	1:A:1050:GLN:NE2	2.41	0.51
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.92	0.51
2:W:1:NAG:C6	2:W:2:NAG:HN2	2.24	0.51
1:A:862:THR:HG22	1:A:864:GLU:H	1.75	0.51
1:B:567:ARG:HA	1:B:573:THR:HA	1.92	0.51
1:A:99:ASN:HB3	1:A:102:ARG:NE	2.16	0.50
1:B:468:ILE:HG13	1:B:468:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.44	0.50
1:C:1121:ASN:O	1:C:1122:CYS:HB3	2.10	0.50
1:B:28:TYR:CE2	3:B:1306:NAG:H5	2.46	0.50
1:B:185:ASN:HB3	1:B:187:LYS:HG3	1.93	0.50
1:B:644:GLN:NE2	1:B:645:THR:O	2.44	0.50
1:B:1078:CYS:SG	1:B:1122:CYS:CB	2.99	0.50
1:C:902:PHE:HA	1:C:905:ILE:HG12	1.93	0.50
1:B:459:SER:OG	1:B:460:ASN:N	2.44	0.50
1:A:52:GLN:HB3	1:A:274:THR:HG23	1.93	0.50
1:B:695:LEU:HD21	1:C:865:MET:SD	2.51	0.50
1:B:975:ASP:OD1	1:B:979:ARG:HD3	2.12	0.50
1:A:681:ARG:HG3	1:A:684:ALA:HB3	1.93	0.50
1:C:459:SER:OG	1:C:460:ASN:N	2.45	0.50
1:B:709:ALA:HB2	1:C:891:GLN:OE1	2.11	0.50
1:C:130:VAL:O	1:C:130:VAL:HG12	2.12	0.50
1:C:1082:LYS:CE	1:C:1118:VAL:HG11	2.42	0.50
1:A:130:VAL:HG12	1:A:130:VAL:O	2.12	0.49
1:A:567:ARG:HA	1:A:573:THR:HA	1.94	0.49
1:B:14:GLN:O	1:B:158:ARG:NE	2.45	0.49
1:A:145:TYR:HA	1:A:152:TRP:HA	1.92	0.49
1:A:213:VAL:HG13	1:A:214:ARG:HG2	1.94	0.49
1:B:40:ASP:OD2	1:B:44:ARG:NH1	2.45	0.49
1:A:1123:ASP:OD1	1:A:1124:VAL:N	2.45	0.49
1:C:578:ASP:OD2	1:C:581:THR:N	2.43	0.49
1:C:774:THR:HG22	1:C:861:LEU:HD12	1.95	0.49
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.95	0.49
1:B:159:VAL:HG13	1:B:160:TYR:CD2	2.46	0.49
1:C:394:ASN:HB3	1:C:516:GLU:HB3	1.94	0.49
1:A:569:ILE:HG12	1:B:843:ARG:HG2	1.95	0.49
1:B:142:GLY:N	1:B:156:GLU:OE2	2.43	0.49
1:A:708:ILE:O	1:A:1070:ASN:HA	2.11	0.49
1:B:811:ARG:O	1:B:815:GLU:HB2	2.13	0.49
1:A:250:THR:HA	1:A:257:GLY:HA3	1.93	0.49
1:B:1077:ILE:HD11	1:B:1111:ILE:HG21	1.93	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.46	0.49
1:B:1082:LYS:C	1:B:1122:CYS:HB3	2.33	0.49
1:C:102:ARG:HH21	1:C:144:TYR:HD1	1.59	0.49
1:C:744:GLU:HG2	1:C:977:LEU:HD21	1.95	0.49
1:C:1099:PHE:HZ	3:C:1308:NAG:H83	1.77	0.49
1:A:185:ASN:HB3	1:A:187:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:HD2	1:B:453:TYR:HE2	1.78	0.48
1:C:567:ARG:HA	1:C:573:THR:HA	1.94	0.48
1:A:255:SER:HG	1:A:258:TRP:HE1	1.60	0.48
1:C:143:VAL:HA	1:C:245:HIS:CD2	2.48	0.48
1:C:807:LYS:NZ	1:C:816:ASP:OD2	2.42	0.48
1:B:125:ASN:OD1	2:Q:1:NAG:H81	2.13	0.48
1:B:659:SER:O	1:B:694:SER:HB3	2.13	0.48
1:C:139:PRO:HB2	1:C:159:VAL:HG23	1.95	0.48
1:C:350:VAL:HG21	1:C:418:ILE:HD12	1.96	0.48
1:A:159:VAL:HG13	1:A:160:TYR:CD2	2.48	0.48
1:A:552:LEU:HD23	1:A:587:ILE:HG13	1.96	0.48
1:A:729:LYS:HG3	1:A:857:LEU:HB2	1.95	0.48
1:B:817:LEU:HD11	1:B:935:SER:HB2	1.96	0.48
1:A:1126:ILE:HD12	1:A:1126:ILE:H	1.79	0.48
1:B:552:LEU:HD23	1:B:587:ILE:HG13	1.96	0.48
1:B:981:ASP:OD1	1:B:981:ASP:N	2.43	0.48
1:C:16:VAL:HG13	1:C:158:ARG:HH22	1.79	0.48
1:A:914:GLU:HA	1:C:1124:VAL:CG2	2.44	0.48
1:C:453:TYR:CE1	1:C:493:GLN:HB3	2.49	0.48
1:C:454:ARG:NH1	1:C:469:SER:OG	2.46	0.48
1:C:817:LEU:HD11	1:C:935:SER:HB2	1.96	0.48
1:A:454:ARG:NH1	1:A:469:SER:OG	2.44	0.48
1:B:143:VAL:HG12	1:B:154:GLU:HB2	1.96	0.48
1:B:433:VAL:HG13	1:B:512:VAL:HG12	1.95	0.48
1:C:15:CYS:HA	1:C:158:ARG:HH21	1.78	0.48
1:B:1072:THR:HG23	1:B:1093:SER:HB3	1.96	0.47
1:C:568:ASP:N	1:C:572:THR:O	2.46	0.47
1:A:155:SER:HB3	2:F:1:NAG:H3	1.96	0.47
1:A:370:ASN:HB2	1:C:455:LEU:HD21	1.95	0.47
1:C:681:ARG:HD3	1:C:684:ALA:HB3	1.95	0.47
1:B:941:LEU:HD12	1:B:945:GLN:HB2	1.96	0.47
1:B:1140:GLU:HB3	1:B:1144:PHE:HE2	1.76	0.47
1:C:102:ARG:NH1	1:C:122:ASN:HA	2.29	0.47
1:C:1102:GLN:NE2	1:C:1105:PHE:HB3	2.28	0.47
2:I:1:NAG:H62	2:I:2:NAG:C7	2.43	0.47
1:B:144:TYR:H	1:B:245:HIS:HE1	1.61	0.47
1:C:143:VAL:HG23	1:C:249:LEU:HG	1.96	0.47
1:C:185:ASN:HB3	1:C:187:LYS:HG3	1.95	0.47
1:A:568:ASP:N	1:A:572:THR:O	2.46	0.47
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.95	0.47
1:B:394:ASN:HB3	1:B:516:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:O	1:A:78:ARG:NH1	2.48	0.47
1:A:568:ASP:CG	1:A:569:ILE:H	2.17	0.47
1:A:744:GLU:HG2	1:A:977:LEU:HD21	1.97	0.47
1:B:52:GLN:HB3	1:B:274:THR:HG23	1.95	0.47
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.80	0.47
1:B:568:ASP:OD1	1:B:569:ILE:N	2.40	0.47
1:B:722:ILE:HG22	1:B:1057:VAL:HG22	1.97	0.47
1:C:616:ASN:HB3	3:C:1309:NAG:O5	2.14	0.47
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.79	0.47
1:B:674:TYR:CZ	1:B:686:GLN:HG2	2.49	0.47
1:A:1079:HIS:CD2	1:A:1133:VAL:HG11	2.46	0.47
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.96	0.47
1:B:568:ASP:N	1:B:572:THR:O	2.47	0.47
1:A:741:ASP:OD2	1:C:590:CYS:HB3	2.14	0.47
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.96	0.47
1:B:290:ASP:OD2	1:B:292:SER:OG	2.27	0.46
1:B:384:PRO:HA	1:B:387:LEU:HD12	1.97	0.46
1:A:975:ASP:OD1	1:A:979:ARG:NH2	2.48	0.46
1:B:568:ASP:HB3	1:B:572:THR:HB	1.97	0.46
1:B:454:ARG:NH1	1:B:469:SER:OG	2.46	0.46
1:B:578:ASP:OD1	1:B:581:THR:N	2.45	0.46
1:C:659:SER:O	1:C:694:SER:HB3	2.15	0.46
1:C:644:GLN:NE2	1:C:645:THR:O	2.47	0.46
1:B:1126:ILE:CG1	1:C:917:LYS:NZ	2.78	0.46
1:C:1124:VAL:HG13	1:C:1125:VAL:N	2.31	0.46
1:A:108:THR:HA	1:A:236:THR:HG22	1.96	0.46
1:A:433:VAL:HG22	1:A:512:VAL:HG12	1.98	0.46
1:A:784:ILE:O	1:C:699:ASN:N	2.48	0.46
1:A:891:GLN:H	1:C:709:ALA:HB3	1.80	0.46
1:B:676:THR:HA	1:B:686:GLN:HG3	1.98	0.46
1:C:361:CYS:HB2	1:C:524:VAL:HG13	1.98	0.46
1:B:108:THR:HA	1:B:236:THR:HG22	1.97	0.46
2:G:1:NAG:H62	2:G:2:NAG:C7	2.46	0.46
1:C:159:VAL:HG13	1:C:160:TYR:CD2	2.51	0.46
1:A:361:CYS:HB2	1:A:524:VAL:HG13	1.98	0.46
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.98	0.46
1:C:433:VAL:HG22	1:C:512:VAL:HG12	1.98	0.46
1:A:246:ARG:HH11	1:A:251:PRO:HG2	1.79	0.45
1:A:960:LYS:HE3	1:A:960:LYS:HB3	1.67	0.45
1:A:1141:LEU:HA	1:B:1144:PHE:HE1	1.81	0.45
1:B:176:LEU:HD13	1:B:207:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1120:GLY:O	1:B:1121:ASN:C	2.54	0.45
1:C:16:VAL:HG21	1:C:250:THR:HG21	1.98	0.45
1:C:661:GLU:OE1	1:C:694:SER:OG	2.33	0.45
1:B:361:CYS:HB2	1:B:524:VAL:HG13	1.98	0.45
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.98	0.45
1:B:472:ILE:HG13	1:B:482:GLY:HA2	1.97	0.45
1:B:558:LYS:HA	1:B:558:LYS:HD3	1.76	0.45
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.98	0.45
1:C:40:ASP:OD2	1:C:44:ARG:NH1	2.48	0.45
1:C:1050:GLN:HB2	1:C:1057:VAL:HB	1.98	0.45
1:B:617:CYS:SG	1:B:651:ILE:HD11	2.56	0.45
1:B:619:GLU:O	1:B:623:ALA:N	2.43	0.45
1:C:108:THR:HA	1:C:236:THR:HG22	1.98	0.45
1:C:1100:VAL:HG23	1:C:1111:ILE:HD13	1.98	0.45
1:A:40:ASP:OD2	1:A:44:ARG:NH1	2.49	0.45
1:B:453:TYR:CE1	1:B:493:GLN:HB3	2.51	0.45
1:B:708:ILE:O	1:B:1070:ASN:HA	2.16	0.45
1:C:360:ASN:H	1:C:523:THR:HG22	1.82	0.45
1:B:245:HIS:CD2	1:B:247:SER:H	2.34	0.45
1:C:905:ILE:HD13	1:C:1045:LEU:HD21	1.99	0.45
1:A:68:ILE:HG13	1:A:260:ALA:HB3	1.98	0.45
1:C:568:ASP:HB3	1:C:572:THR:HB	1.99	0.45
1:C:789:GLN:N	1:C:789:GLN:OE1	2.50	0.45
1:A:125:ASN:HD21	2:F:1:NAG:H62	1.81	0.45
1:A:146:HIS:CE1	1:A:245:HIS:HE2	2.34	0.45
1:A:1097:HIS:CD2	3:A:1311:NAG:O7	2.67	0.45
1:B:629:LEU:HD23	1:B:633:TRP:HB3	1.98	0.45
1:C:146:HIS:HD2	1:C:245:HIS:CE1	2.35	0.45
1:C:157:PHE:CD1	1:C:158:ARG:N	2.84	0.45
1:A:590:CYS:HB3	1:B:741:ASP:OD2	2.17	0.45
1:A:677:GLN:O	1:A:681:ARG:HG2	2.17	0.45
1:A:1102:GLN:NE2	1:A:1105:PHE:HB3	2.32	0.45
1:A:96:GLU:HB3	1:A:100:ILE:HD13	1.99	0.45
1:A:699:ASN:N	1:B:784:ILE:O	2.48	0.45
1:B:255:SER:HG	1:B:256:SER:H	1.63	0.45
1:C:39:PRO:HG3	1:C:55:PHE:HZ	1.81	0.45
1:A:868:GLN:OE1	1:C:695:LEU:HG	2.17	0.44
1:C:142:GLY:HA3	1:C:249:LEU:HD23	1.98	0.44
1:C:423:TYR:HE2	1:C:425:LEU:HD13	1.82	0.44
1:A:424:LYS:HG2	1:A:461:LEU:O	2.17	0.44
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:THR:HB	1:B:670:ILE:HD13	1.98	0.44
1:B:792:ASP:N	1:B:792:ASP:OD1	2.47	0.44
1:B:902:PHE:HA	1:B:905:ILE:HG12	2.00	0.44
1:A:1100:VAL:HG23	1:A:1109:GLN:HB2	1.98	0.44
1:B:745:CYS:HB2	1:B:973:LEU:HD21	1.99	0.44
1:C:404:GLY:O	1:C:407:VAL:HG12	2.18	0.44
1:A:695:LEU:HB3	1:B:784:ILE:HD11	2.00	0.44
1:C:176:LEU:HD13	1:C:207:HIS:HB3	1.99	0.44
1:C:351:TYR:CE2	1:C:468:ILE:HG22	2.53	0.44
1:A:339:GLY:O	1:A:343:ASN:HB3	2.18	0.44
1:A:426:PRO:HB3	1:A:463:PRO:HB3	1.99	0.44
1:A:865:MET:SD	1:C:695:LEU:HD21	2.57	0.44
1:B:720:THR:HG22	1:B:1059:LEU:HD23	2.00	0.44
1:B:789:GLN:N	1:B:789:GLN:OE1	2.50	0.44
1:A:1084:HIS:CE1	1:A:1133:VAL:HG21	2.53	0.44
1:B:612:TYR:HE2	1:B:651:ILE:HD13	1.83	0.44
1:B:902:PHE:CD2	1:B:912:LEU:HB2	2.52	0.44
1:B:1052:ALA:HB2	1:B:1057:VAL:HG23	1.99	0.44
3:C:1308:NAG:C7	3:C:1308:NAG:O3	2.65	0.44
1:A:291:CYS:O	1:A:318:PHE:HB3	2.18	0.44
1:A:1121:ASN:O	1:A:1124:VAL:HG22	2.17	0.44
1:B:661:GLU:OE1	1:B:694:SER:OG	2.35	0.44
1:C:194:PHE:HD1	1:C:203:ILE:HG12	1.81	0.44
1:C:1142:ASP:HA	1:C:1145:LYS:CE	2.46	0.44
1:B:143:VAL:HG23	1:B:249:LEU:HD12	2.00	0.44
1:B:1086:PRO:HB3	1:B:1091:PHE:CE1	2.53	0.44
1:C:619:GLU:O	1:C:623:ALA:N	2.45	0.44
1:C:792:ASP:OD1	1:C:792:ASP:N	2.50	0.44
1:B:70:VAL:HG12	1:B:72:GLY:H	1.83	0.44
1:B:738:ILE:HG22	1:B:996:ARG:HB3	2.00	0.44
1:C:403:ARG:HG2	1:C:404:GLY:N	2.33	0.44
1:C:1084:HIS:CE1	1:C:1133:VAL:HG21	2.52	0.44
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.99	0.43
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.00	0.43
1:C:598:ILE:HB	1:C:609:ALA:HB3	2.00	0.43
1:A:351:TYR:CE2	1:A:468:ILE:HG22	2.53	0.43
1:A:569:ILE:HG12	1:B:843:ARG:HG3	1.99	0.43
1:A:675:GLN:O	1:A:686:GLN:HG3	2.17	0.43
1:B:422:ASN:HD21	1:B:454:ARG:H	1.66	0.43
1:A:821:LYS:HD2	1:A:934:LEU:O	2.19	0.43
1:A:1095:GLY:HA3	3:A:1311:NAG:C8	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PHE:O	1:C:264:ALA:HA	2.17	0.43
1:C:123:ALA:HB3	2:Z:1:NAG:O7	2.18	0.43
1:C:329:PHE:HE2	1:C:528:LYS:HB3	1.83	0.43
1:C:645:THR:HB	1:C:670:ILE:HD13	1.99	0.43
1:C:1137:LEU:HD23	1:C:1137:LEU:O	2.19	0.43
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.01	0.43
1:A:619:GLU:O	1:A:623:ALA:N	2.43	0.43
1:A:674:TYR:CZ	1:A:686:GLN:HG2	2.52	0.43
1:C:68:ILE:HG12	1:C:263:ALA:HB3	2.01	0.43
1:A:804:ASP:N	1:A:811:ARG:O	2.33	0.43
1:B:129:LYS:HD2	1:B:131:CYS:SG	2.58	0.43
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.83	0.43
1:B:406:GLU:HB3	1:B:418:ILE:HD13	1.99	0.43
1:B:590:CYS:HB3	1:C:741:ASP:OD2	2.18	0.43
1:A:629:LEU:HD23	1:A:633:TRP:HB3	1.99	0.43
1:A:902:PHE:HA	1:A:905:ILE:HG12	2.01	0.43
1:B:100:ILE:HG21	1:B:263:ALA:HB2	1.99	0.43
1:B:735:THR:HG22	1:B:749:LEU:HD23	2.00	0.43
1:C:388:ASN:HA	1:C:527:PRO:HD2	2.00	0.43
1:A:599:THR:HG22	1:A:601:GLY:H	1.83	0.43
1:A:1084:HIS:CD2	1:A:1118:VAL:HG12	2.54	0.43
3:A:1306:NAG:H82	1:C:455:LEU:HD23	2.01	0.43
1:B:128:ILE:HD13	1:B:229:LEU:HD11	2.01	0.43
1:C:31:SER:O	1:C:59:PHE:N	2.49	0.43
1:C:335:LEU:HA	1:C:362:VAL:HG22	2.00	0.43
1:C:1086:PRO:HB3	1:C:1091:PHE:CE1	2.53	0.43
1:A:143:VAL:HB	1:A:156:GLU:HG2	2.01	0.43
1:A:69:HIS:CG	1:A:78:ARG:HB2	2.54	0.43
1:C:128:ILE:HD13	1:C:229:LEU:HD11	2.01	0.43
1:C:720:THR:HG22	1:C:1059:LEU:HD23	2.00	0.43
1:C:788:PRO:HG2	1:C:793:PHE:CZ	2.54	0.43
2:X:1:NAG:O6	2:X:2:NAG:H82	2.19	0.43
1:A:1124:VAL:HG23	1:A:1125:VAL:N	2.34	0.43
1:B:1137:LEU:HD23	1:B:1137:LEU:O	2.19	0.43
1:C:52:GLN:HB3	1:C:274:THR:HG23	2.01	0.43
1:C:745:CYS:HB2	1:C:973:LEU:HD21	2.00	0.43
1:A:784:ILE:HG23	1:A:872:ALA:HB2	2.01	0.42
1:B:700:SER:HB2	2:P:2:NAG:H61	2.00	0.42
1:C:173:GLN:HG3	1:C:174:PRO:HD2	2.01	0.42
1:C:295:PRO:HG3	1:C:633:TRP:CH2	2.54	0.42
1:A:662:CYS:HB2	1:A:693:MET:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:CYS:HB2	1:A:973:LEU:HD21	2.00	0.42
1:A:1124:VAL:HG23	1:A:1125:VAL:H	1.84	0.42
1:C:103:GLY:HA3	1:C:119:ILE:O	2.19	0.42
1:C:725:VAL:HG22	1:C:1055:GLY:HA2	2.01	0.42
1:A:16:VAL:HG13	1:A:158:ARG:HH22	1.84	0.42
1:A:128:ILE:HD13	1:A:229:LEU:HD11	2.01	0.42
1:A:897:GLN:HG2	1:A:901:ARG:HE	1.84	0.42
1:B:173:GLN:HG3	1:B:174:PRO:HD2	2.00	0.42
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.55	0.42
1:C:52:GLN:HA	1:C:274:THR:HA	2.01	0.42
1:C:997:LEU:HD12	1:C:997:LEU:HA	1.91	0.42
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.89	0.42
1:A:905:ILE:HD13	1:A:1045:LEU:HD21	2.00	0.42
1:B:699:ASN:N	1:C:784:ILE:O	2.52	0.42
1:C:100:ILE:HG21	1:C:263:ALA:HB2	2.01	0.42
1:C:748:LEU:HD23	1:C:748:LEU:HA	1.86	0.42
1:B:99:ASN:HB3	1:B:102:ARG:HE	1.84	0.42
1:B:291:CYS:O	1:B:318:PHE:HB3	2.19	0.42
1:B:1094:ASN:OD1	3:B:1307:NAG:N2	2.37	0.42
1:C:294:ASP:OD1	1:C:294:ASP:N	2.52	0.42
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.55	0.42
1:C:1082:LYS:HE2	1:C:1118:VAL:HG11	2.01	0.42
1:C:1099:PHE:CE1	3:C:1308:NAG:C1	3.03	0.42
1:A:360:ASN:H	1:A:523:THR:HG22	1.85	0.42
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.85	0.42
1:B:599:THR:HG22	1:B:601:GLY:H	1.84	0.42
1:B:801:ILE:HG23	1:B:1050:GLN:NE2	2.35	0.42
1:C:203:ILE:HB	1:C:227:VAL:HG22	2.02	0.42
1:C:552:LEU:HD23	1:C:587:ILE:HG13	2.01	0.42
1:C:902:PHE:CD2	1:C:912:LEU:HB2	2.55	0.42
1:A:186:PHE:HD2	1:A:213:VAL:O	2.03	0.42
1:A:792:ASP:OD1	1:A:792:ASP:N	2.53	0.42
1:B:216:LEU:HD12	1:B:216:LEU:H	1.85	0.42
1:B:854:LEU:HD23	1:B:955:LEU:HD22	2.01	0.42
1:C:67:ALA:HA	1:C:80:ASP:O	2.20	0.42
1:A:677:GLN:O	1:A:680:SER:N	2.52	0.42
1:A:941:LEU:HD12	1:A:945:GLN:HB2	2.00	0.42
1:B:15:CYS:HA	1:B:158:ARG:NH2	2.33	0.42
1:B:127:VAL:HG22	1:B:171:VAL:HG22	2.02	0.42
1:B:433:VAL:HG22	1:B:512:VAL:HG12	2.01	0.42
1:B:720:THR:HG23	1:B:930:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD12	1:C:216:LEU:H	1.85	0.42
1:C:384:PRO:HA	1:C:387:LEU:HD12	2.02	0.42
1:C:902:PHE:CE2	1:C:912:LEU:HB2	2.55	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.87	0.42
1:A:714:PHE:HE1	1:A:919:ILE:HG12	1.83	0.42
1:A:758:GLN:O	1:A:761:ARG:HB3	2.19	0.42
1:A:1137:LEU:O	1:A:1137:LEU:HD23	2.19	0.42
1:B:29:THR:HG22	1:B:30:ASN:N	2.35	0.42
1:C:758:GLN:O	1:C:761:ARG:HB3	2.19	0.42
1:A:194:PHE:HD1	1:A:203:ILE:HG12	1.84	0.41
1:A:831:LYS:NZ	1:A:844:ASP:OD2	2.53	0.41
1:B:327:VAL:HG22	1:B:542:ASN:HB3	2.01	0.41
1:B:844:ASP:OD1	1:B:844:ASP:N	2.53	0.41
1:C:558:LYS:HD3	1:C:558:LYS:HA	1.80	0.41
1:C:831:LYS:HG3	1:C:846:ILE:HG21	2.02	0.41
1:A:122:ASN:OD1	1:A:123:ALA:N	2.53	0.41
1:A:176:LEU:HD13	1:A:207:HIS:HB3	2.01	0.41
1:A:955:LEU:HD23	1:A:955:LEU:HA	1.90	0.41
1:B:147:ARG:NE	1:B:148:ASN:H	2.13	0.41
1:A:103:GLY:HA3	1:A:119:ILE:O	2.20	0.41
1:A:558:LYS:HD3	1:A:558:LYS:HA	1.76	0.41
1:B:103:GLY:HA3	1:B:119:ILE:O	2.20	0.41
1:B:186:PHE:HD2	1:B:213:VAL:O	2.03	0.41
1:C:144:TYR:HB3	1:C:245:HIS:CE1	2.56	0.41
1:A:81:ASN:O	1:A:239:GLN:NE2	2.52	0.41
1:B:50:LEU:HD13	1:B:304:LYS:HE3	2.01	0.41
1:B:723:LEU:HD23	1:B:723:LEU:HA	1.91	0.41
1:C:294:ASP:HB3	1:C:632:THR:HG21	2.03	0.41
1:B:294:ASP:N	1:B:294:ASP:OD1	2.52	0.41
1:B:729:LYS:HG3	1:B:857:LEU:HB2	2.03	0.41
1:C:112:SER:HB2	1:C:134:GLN:HB2	2.02	0.41
1:A:20:THR:HA	1:A:78:ARG:HD3	2.03	0.41
1:A:578:ASP:OD1	1:A:581:THR:N	2.52	0.41
1:A:917:LYS:HZ1	1:C:1126:ILE:HG12	1.86	0.41
1:A:1140:GLU:HB3	1:A:1144:PHE:HE2	1.82	0.41
1:B:39:PRO:HG3	1:B:55:PHE:CZ	2.53	0.41
1:B:1126:ILE:HG12	1:C:917:LYS:HZ1	1.84	0.41
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.03	0.41
1:C:642:VAL:HG12	1:C:642:VAL:O	2.21	0.41
1:C:729:LYS:HG3	1:C:857:LEU:HB2	2.02	0.41
1:A:894:PHE:N	1:C:703:TYR:OH	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLU:HA	1:C:1124:VAL:HG21	2.03	0.41
1:A:129:LYS:HD2	1:A:131:CYS:SG	2.60	0.41
1:A:337:PRO:HB2	1:A:340:GLU:HB2	2.02	0.41
1:B:454:ARG:NH2	1:B:469:SER:H	2.16	0.41
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.02	0.41
1:B:821:LYS:HD2	1:B:934:LEU:O	2.20	0.41
1:C:146:HIS:CD2	1:C:247:SER:HA	2.55	0.41
1:A:642:VAL:O	1:A:642:VAL:HG12	2.21	0.41
1:A:720:THR:HG22	1:A:1059:LEU:HD23	2.03	0.41
1:B:125:ASN:HB2	1:B:172:SER:O	2.21	0.41
1:B:330:PRO:HD3	1:B:544:ASN:OD1	2.20	0.41
1:B:335:LEU:HA	1:B:362:VAL:HG22	2.03	0.41
1:B:620:VAL:HG23	1:B:621:PRO:HD3	2.02	0.41
1:B:799:SER:HB3	2:N:1:NAG:H61	2.03	0.41
1:B:965:ASN:HA	1:B:971:SER:HB3	2.03	0.41
1:B:1100:VAL:HG23	1:B:1109:GLN:HB2	2.03	0.41
1:C:821:LYS:HD2	1:C:934:LEU:O	2.21	0.41
1:C:1076:ALA:HB3	1:C:1128:ILE:HD13	1.59	0.41
1:C:1138:GLN:N	1:C:1139:PRO:HD2	2.36	0.41
1:A:52:GLN:HA	1:A:274:THR:HA	2.02	0.41
1:A:376:THR:HB	1:A:435:ALA:HB3	2.03	0.41
1:B:31:SER:O	1:B:59:PHE:N	2.52	0.41
1:C:645:THR:OG1	1:C:648:GLY:O	2.34	0.41
1:C:1120:GLY:C	1:C:1122:CYS:H	2.23	0.41
1:B:360:ASN:H	1:B:523:THR:HG22	1.85	0.40
1:B:1121:ASN:O	1:B:1124:VAL:HG22	2.21	0.40
1:B:1124:VAL:HG23	1:B:1125:VAL:N	2.35	0.40
1:C:25:PRO:HA	1:C:26:PRO:HD3	1.90	0.40
1:C:125:ASN:OD1	2:Z:1:NAG:H81	2.21	0.40
1:C:722:ILE:HG22	1:C:1057:VAL:HG22	2.02	0.40
1:A:32:SER:OG	1:A:33:THR:N	2.54	0.40
1:A:455:LEU:HD11	1:B:370:ASN:HB2	2.04	0.40
1:A:620:VAL:O	1:A:624:ILE:HG12	2.22	0.40
1:B:535:LYS:HE3	1:B:535:LYS:HB3	1.97	0.40
1:C:68:ILE:HG22	1:C:79:PHE:CE1	2.56	0.40
1:A:294:ASP:N	1:A:294:ASP:OD1	2.53	0.40
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.57	0.40
1:C:144:TYR:H	1:C:245:HIS:CE1	2.39	0.40
1:C:330:PRO:HD3	1:C:544:ASN:OD1	2.21	0.40
1:A:627:ASN:OD1	1:A:627:ASN:N	2.54	0.40
1:A:672:ALA:HA	1:A:689:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.94	0.40
1:B:22:THR:OG1	1:B:78:ARG:HG3	2.22	0.40
1:B:31:SER:HB3	1:B:62:VAL:HG21	2.04	0.40
1:B:144:TYR:HD1	1:B:145:TYR:HD2	1.68	0.40
1:B:874:LEU:O	1:B:878:ILE:HG12	2.22	0.40
1:B:1036:VAL:HG21	1:C:1031:GLY:HA3	2.02	0.40
1:C:129:LYS:HD2	1:C:131:CYS:SG	2.60	0.40
1:C:131:CYS:HA	1:C:166:CYS:HA	2.03	0.40
1:C:186:PHE:HD2	1:C:213:VAL:O	2.04	0.40
1:C:535:LYS:HE3	1:C:535:LYS:HB3	1.97	0.40
1:A:718:VAL:HG22	1:A:1061:VAL:HG22	2.04	0.40
1:C:454:ARG:NH2	1:C:469:SER:H	2.18	0.40
1:C:915:ASN:OD1	1:C:915:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1131/1286 (88%)	1025 (91%)	106 (9%)	0	100	100
1	B	1131/1286 (88%)	1028 (91%)	103 (9%)	0	100	100
1	C	1131/1286 (88%)	1021 (90%)	110 (10%)	0	100	100
All	All	3393/3858 (88%)	3074 (91%)	319 (9%)	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	986/1115 (88%)	986 (100%)	0	100	100
1	B	986/1115 (88%)	986 (100%)	0	100	100
1	C	986/1115 (88%)	986 (100%)	0	100	100
All	All	2958/3345 (88%)	2958 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	99	ASN
1	A	800	GLN
1	A	931	GLN
1	A	1079	HIS
1	A	1097	HIS
1	B	52	GLN
1	B	99	ASN
1	B	747	ASN
1	B	1079	HIS
1	C	146	HIS
1	C	1079	HIS
1	C	1097	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

48 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	E	1	1,2	14,14,15	0.28	0	17,19,21	0.54	0
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.63	1 (7%)	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	G	1	1,2	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	G	2	2	14,14,15	0.27	0	17,19,21	0.67	0
2	NAG	H	1	1,2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.26	0	17,19,21	0.66	0
2	NAG	I	1	1,2	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	I	2	2	14,14,15	0.27	0	17,19,21	0.66	0
2	NAG	J	1	1,2	14,14,15	0.24	0	17,19,21	0.35	0
2	NAG	J	2	2	14,14,15	0.25	0	17,19,21	0.73	0
2	NAG	K	1	1,2	14,14,15	0.30	0	17,19,21	1.11	1 (5%)
2	NAG	K	2	2	14,14,15	0.30	0	17,19,21	0.81	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	L	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	M	1	1,2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	M	2	2	14,14,15	0.98	2 (14%)	17,19,21	0.51	0
2	NAG	N	1	1,2	14,14,15	0.30	0	17,19,21	0.72	0
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.66	0
2	NAG	O	1	1,2	14,14,15	0.27	0	17,19,21	0.70	0
2	NAG	O	2	2	14,14,15	0.29	0	17,19,21	0.69	0
2	NAG	P	1	1,2	14,14,15	0.25	0	17,19,21	0.89	0
2	NAG	P	2	2	14,14,15	0.27	0	17,19,21	0.68	0
2	NAG	Q	1	1,2	14,14,15	0.45	0	17,19,21	1.16	1 (5%)
2	NAG	Q	2	2	14,14,15	0.30	0	17,19,21	0.40	0
2	NAG	R	1	1,2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	R	2	2	14,14,15	0.27	0	17,19,21	0.72	0
2	NAG	S	1	1,2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	S	2	2	14,14,15	0.25	0	17,19,21	0.67	0
2	NAG	T	1	1,2	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	T	2	2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	U	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	U	2	2	14,14,15	0.26	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	V	1	1,2	14,14,15	0.26	0	17,19,21	0.71	0
2	NAG	V	2	2	14,14,15	0.27	0	17,19,21	0.73	0
2	NAG	W	1	1,2	14,14,15	0.27	0	17,19,21	0.73	0
2	NAG	W	2	2	14,14,15	0.27	0	17,19,21	0.72	0
2	NAG	X	1	1,2	14,14,15	0.32	0	17,19,21	0.55	0
2	NAG	X	2	2	14,14,15	0.28	0	17,19,21	0.65	0
2	NAG	Y	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	Y	2	2	14,14,15	0.47	0	17,19,21	0.45	0
2	NAG	Z	1	1,2	14,14,15	0.41	0	17,19,21	1.25	1 (5%)
2	NAG	Z	2	2	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	a	1	1,2	14,14,15	0.27	0	17,19,21	0.71	0
2	NAG	a	2	2	14,14,15	0.28	0	17,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1	NAG	O5-C1	-4.41	1.36	1.43
2	M	2	NAG	O5-C1	3.01	1.48	1.43
2	F	1	NAG	O5-C1	-2.22	1.40	1.43
2	M	2	NAG	C1-C2	2.02	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	1	NAG	C2-N2-C7	3.97	128.56	122.90
2	Q	1	NAG	C2-N2-C7	3.81	128.33	122.90
2	K	1	NAG	C1-O5-C5	3.12	116.42	112.19
2	Y	1	NAG	C3-C4-C5	2.98	115.55	110.24
2	K	2	NAG	C1-O5-C5	2.16	115.11	112.19
2	Y	1	NAG	O4-C4-C3	-2.09	105.52	110.35

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C3-C2-N2-C7
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	R	2	NAG	C8-C7-N2-C2
2	R	2	NAG	O7-C7-N2-C2
2	U	2	NAG	C3-C2-N2-C7
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	V	1	NAG	C3-C2-N2-C7
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C8-C7-N2-C2
2	V	2	NAG	O7-C7-N2-C2
2	W	1	NAG	C8-C7-N2-C2
2	W	1	NAG	O7-C7-N2-C2
2	W	2	NAG	C3-C2-N2-C7
2	W	2	NAG	C8-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
2	a	2	NAG	C8-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	Z	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C8-C7-N2-C2
2	X	1	NAG	C8-C7-N2-C2
2	X	1	NAG	O7-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C1-C2-N2-C7
2	Z	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
2	W	1	NAG	C1-C2-N2-C7
2	M	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C8-C7-N2-C2
2	R	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	V	2	NAG	C3-C2-N2-C7
2	S	1	NAG	O5-C5-C6-O6
2	X	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Z	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
2	F	2	NAG	O5-C5-C6-O6
2	W	2	NAG	C1-C2-N2-C7

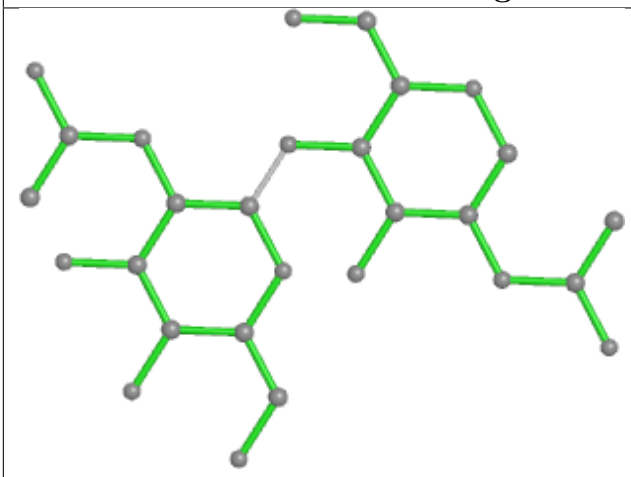
There are no ring outliers.

18 monomers are involved in 18 short contacts:

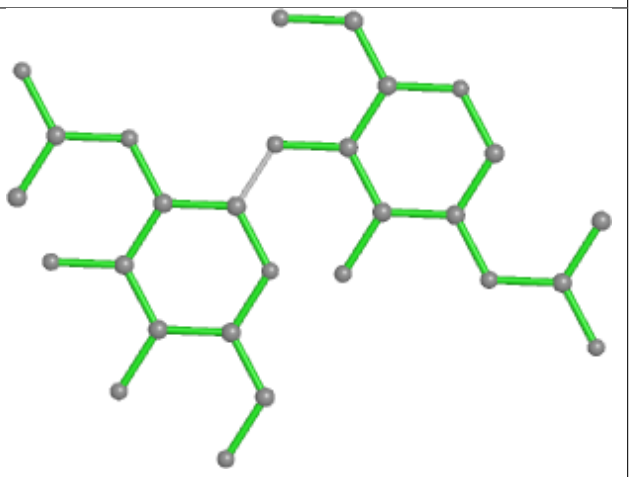
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	3	0
2	W	1	NAG	2	0
2	G	1	NAG	1	0
2	I	1	NAG	1	0
2	U	2	NAG	1	0
2	W	2	NAG	2	0
2	U	1	NAG	1	0
2	I	2	NAG	1	0
2	P	2	NAG	1	0
2	F	1	NAG	2	0
2	G	2	NAG	1	0
2	Z	1	NAG	3	0
2	M	2	NAG	1	0
2	X	2	NAG	1	0
2	J	2	NAG	1	0
2	M	1	NAG	1	0
2	N	1	NAG	1	0
2	X	1	NAG	1	0

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

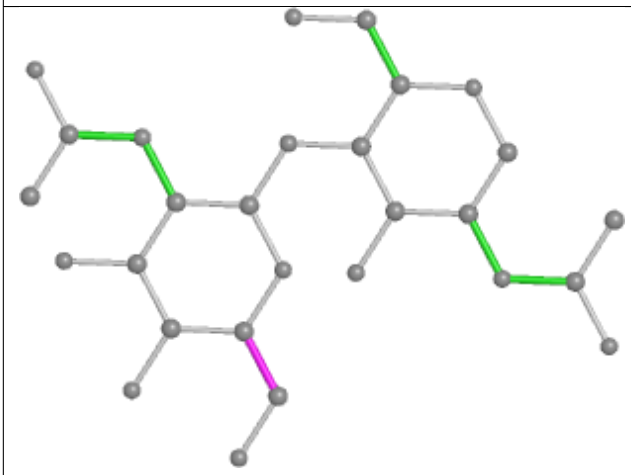
Oligosaccharide Chain D



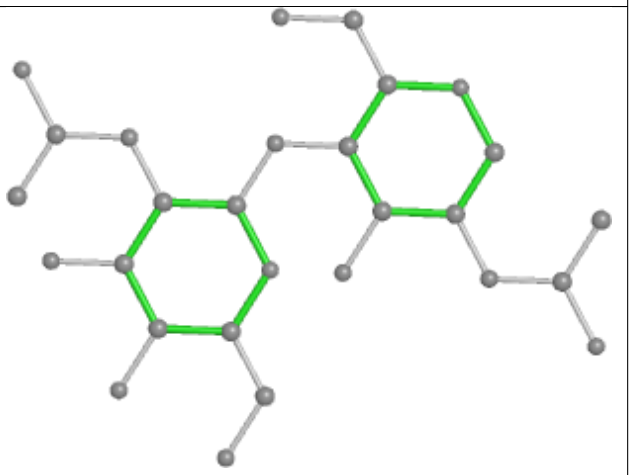
Bond lengths



Bond angles

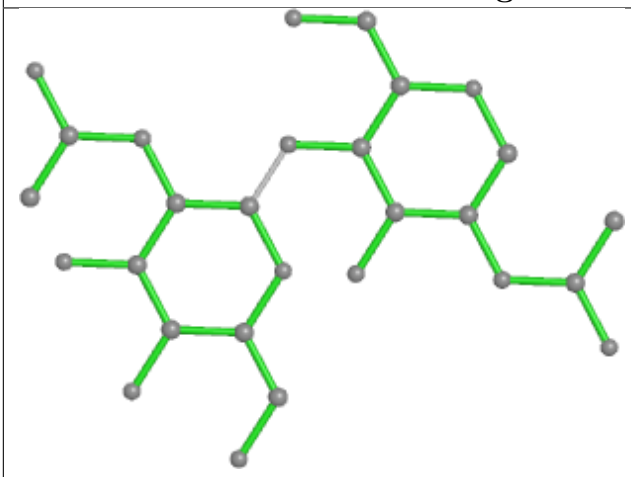


Torsions

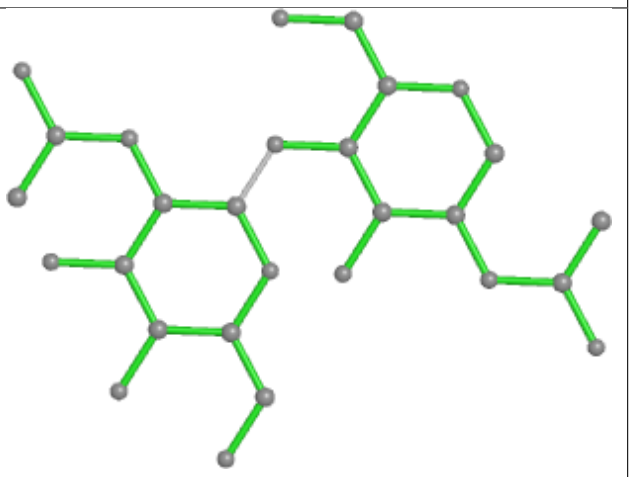


Rings

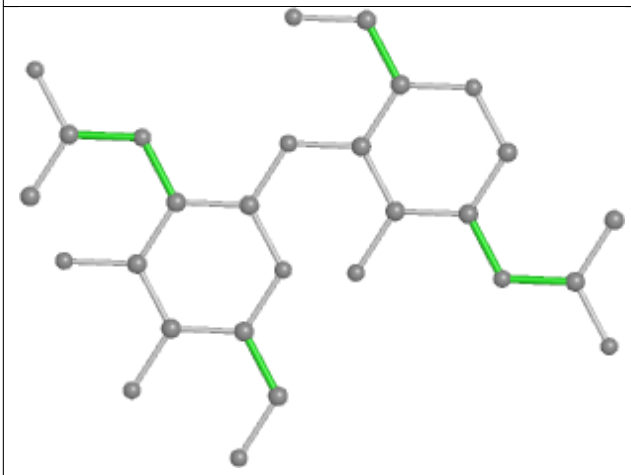
Oligosaccharide Chain E



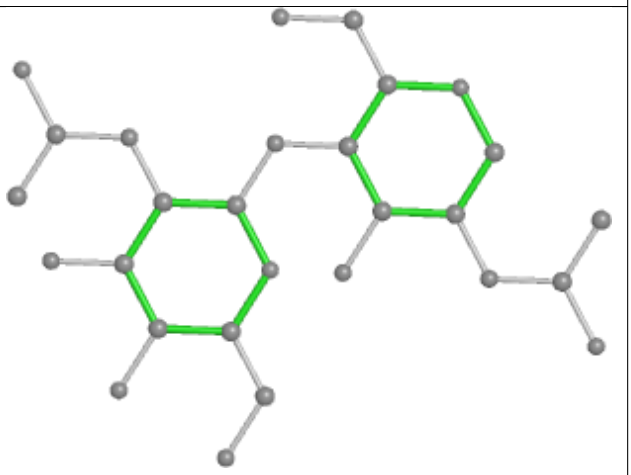
Bond lengths



Bond angles

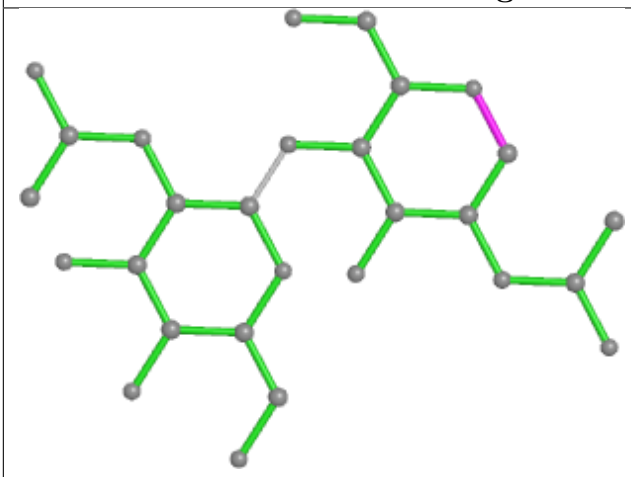


Torsions

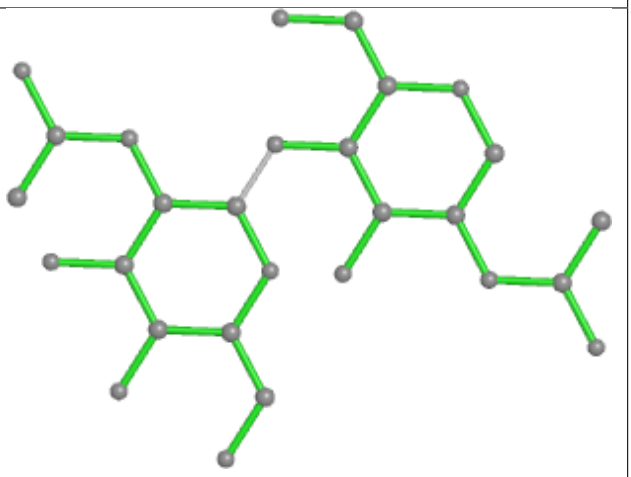


Rings

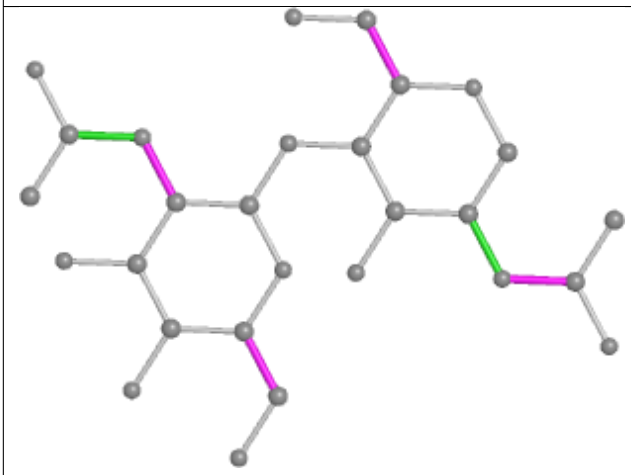
Oligosaccharide Chain F



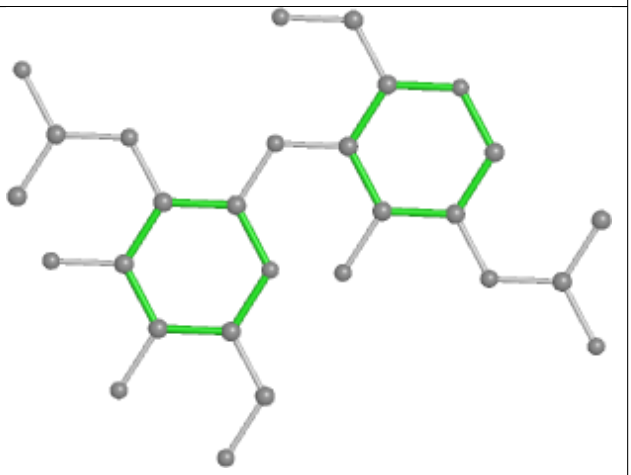
Bond lengths



Bond angles

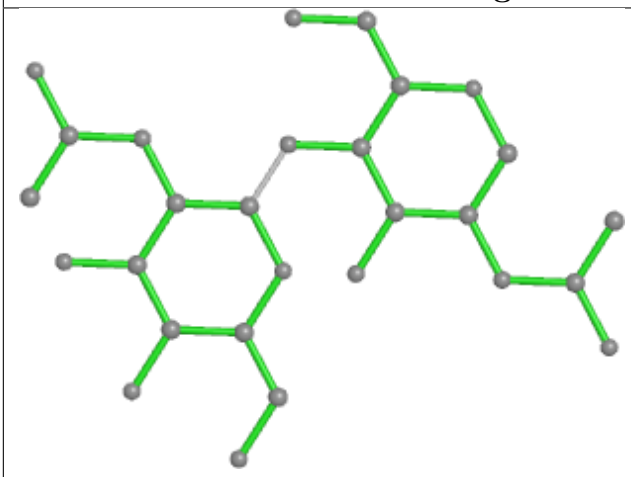


Torsions

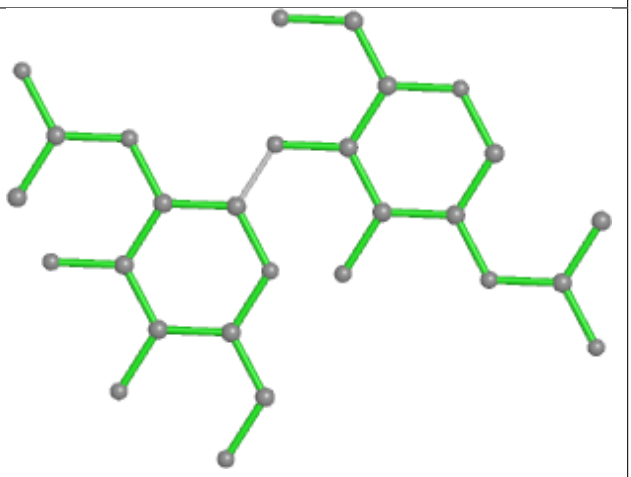


Rings

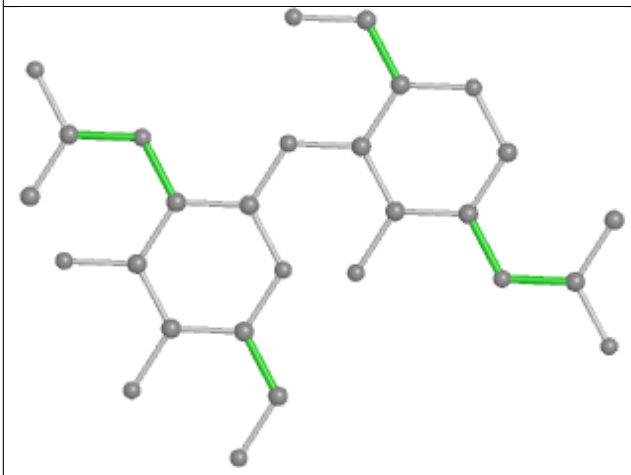
Oligosaccharide Chain G



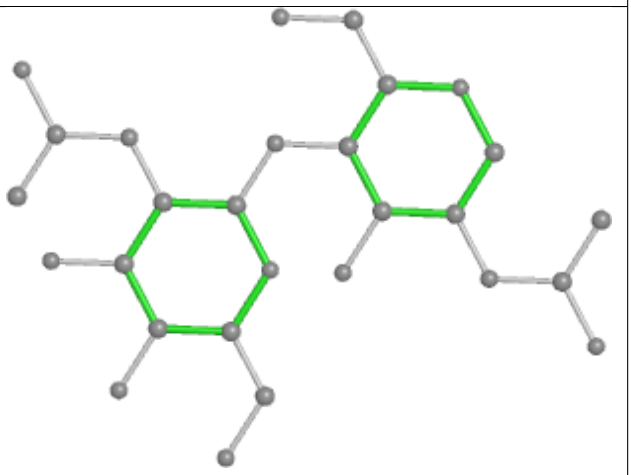
Bond lengths



Bond angles

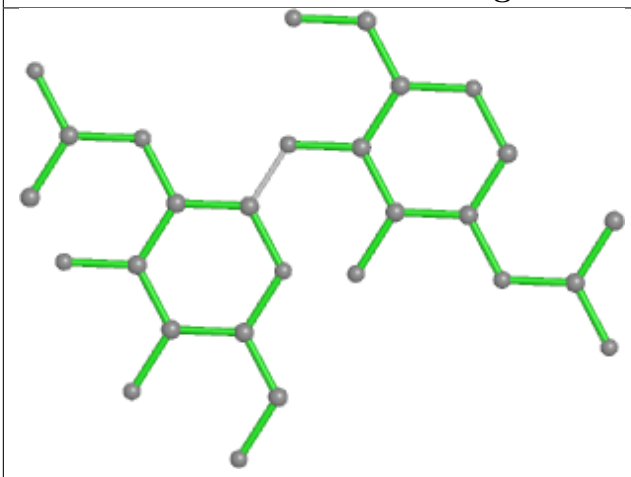


Torsions

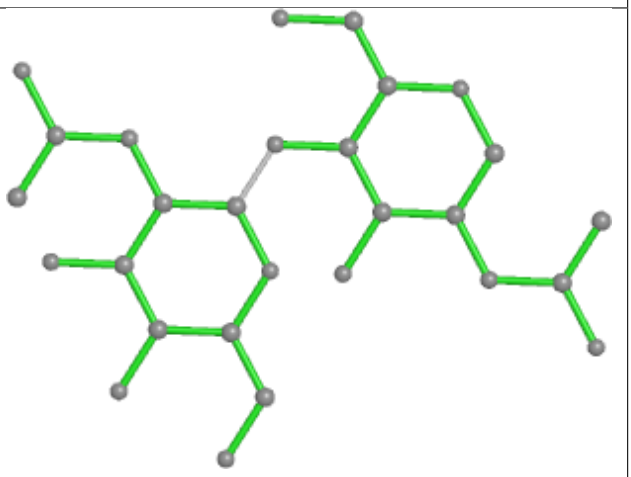


Rings

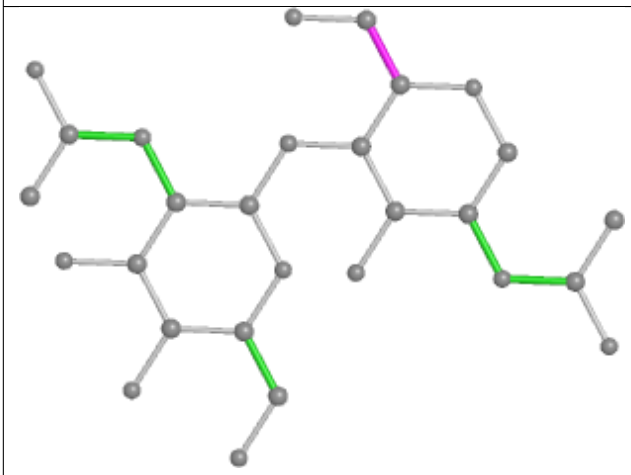
Oligosaccharide Chain H



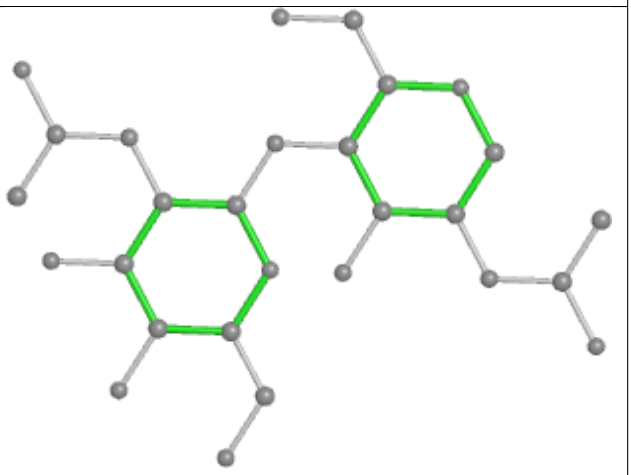
Bond lengths



Bond angles

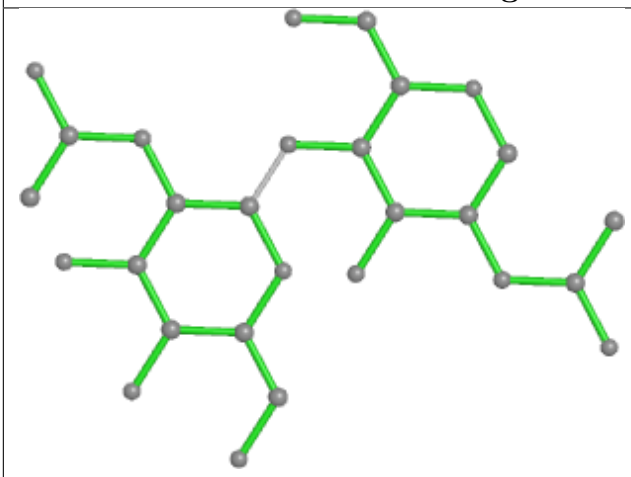


Torsions

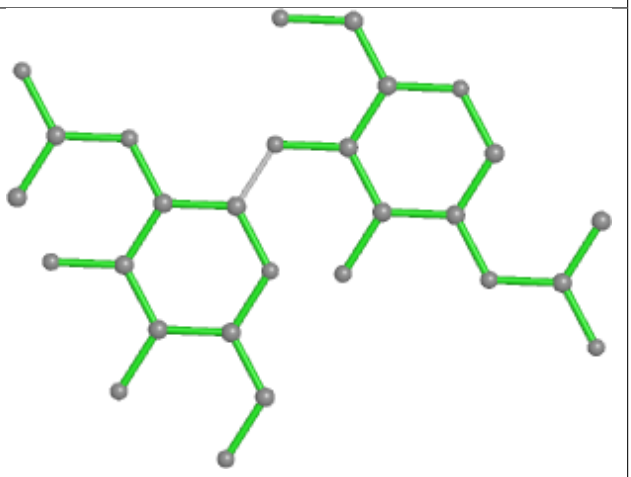


Rings

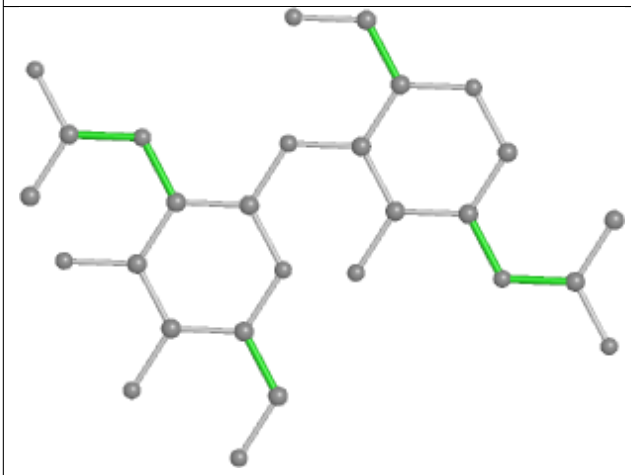
Oligosaccharide Chain I



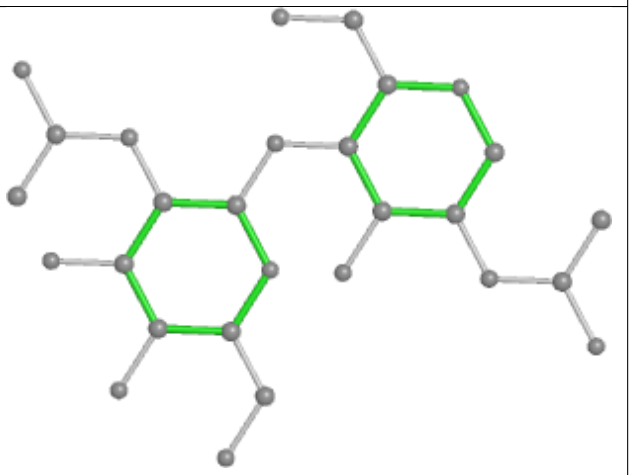
Bond lengths



Bond angles

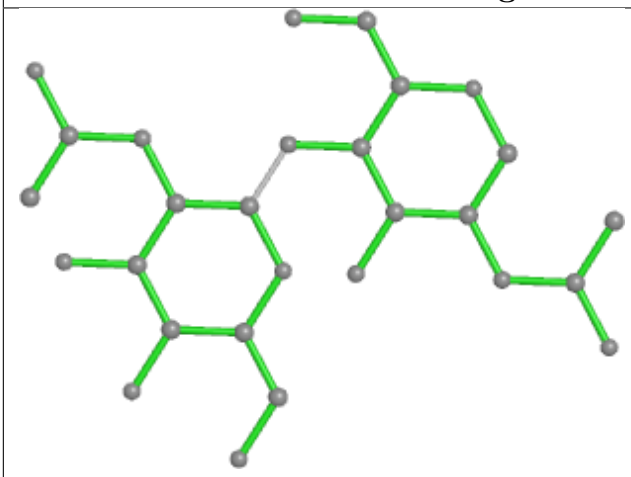


Torsions

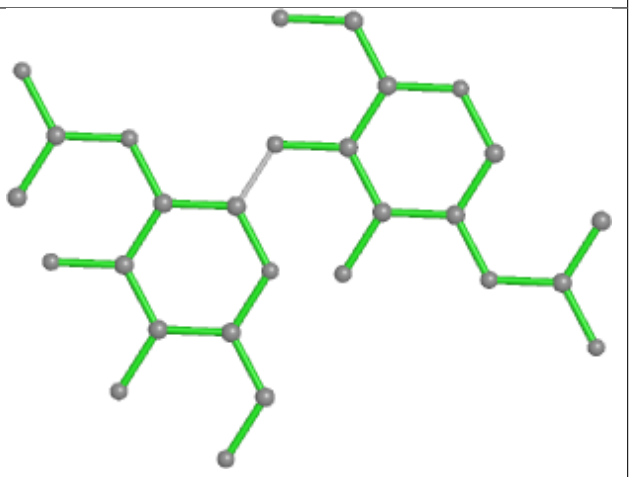


Rings

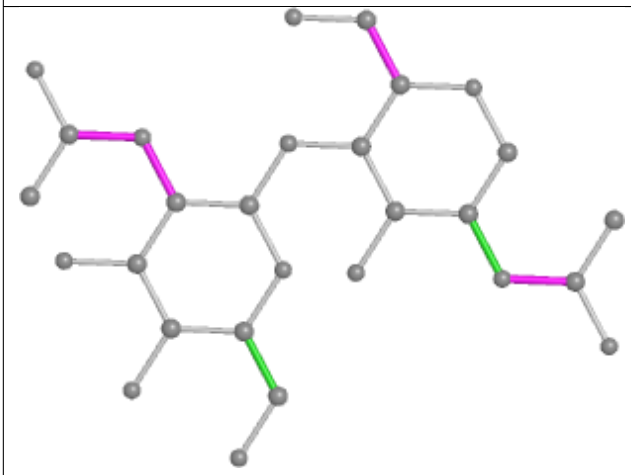
Oligosaccharide Chain J



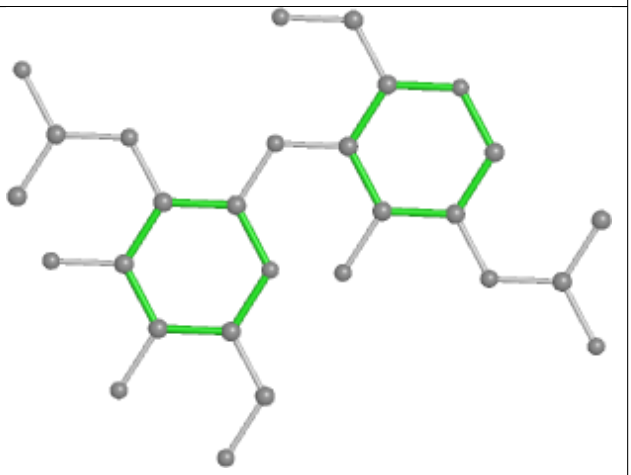
Bond lengths



Bond angles

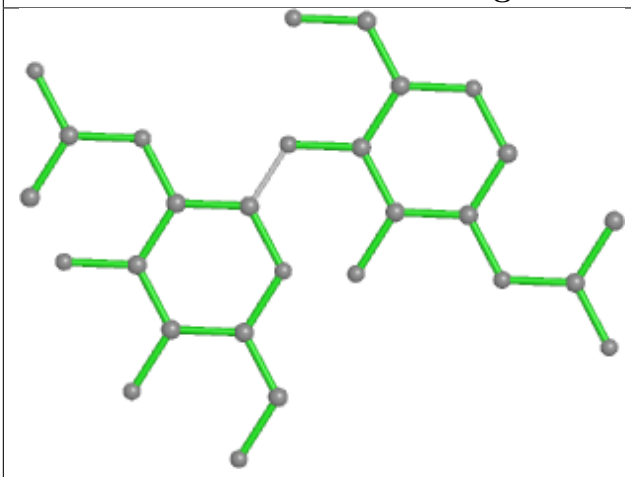


Torsions



Rings

Oligosaccharide Chain K



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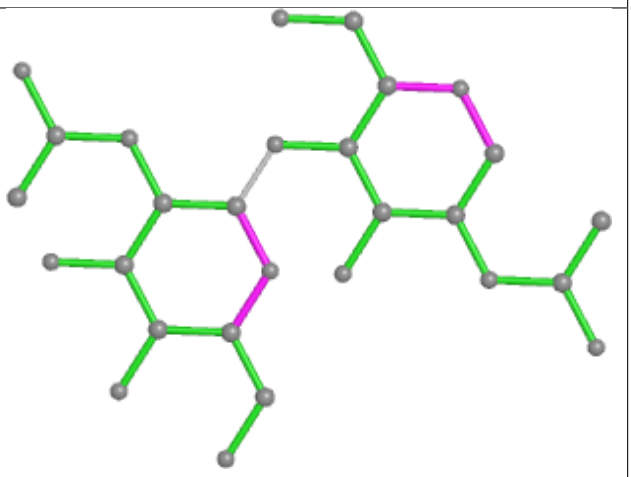

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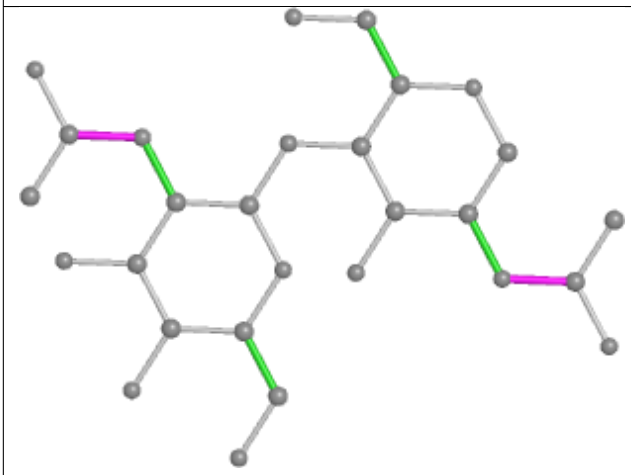

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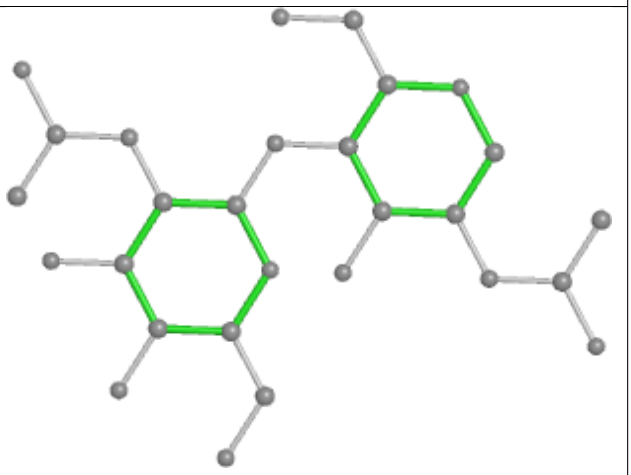
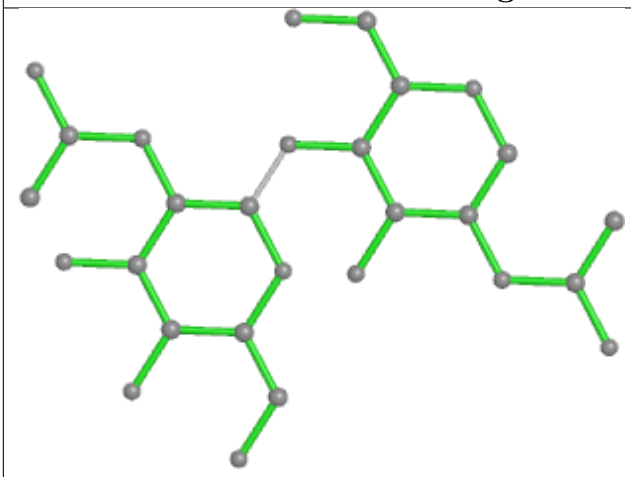


Rings

Oligosaccharide Chain L



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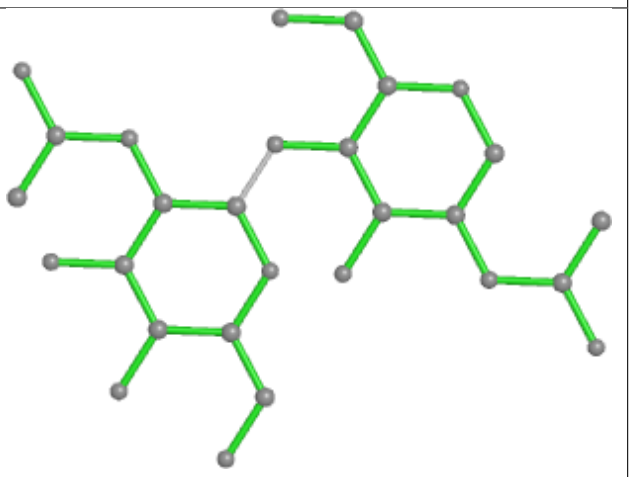
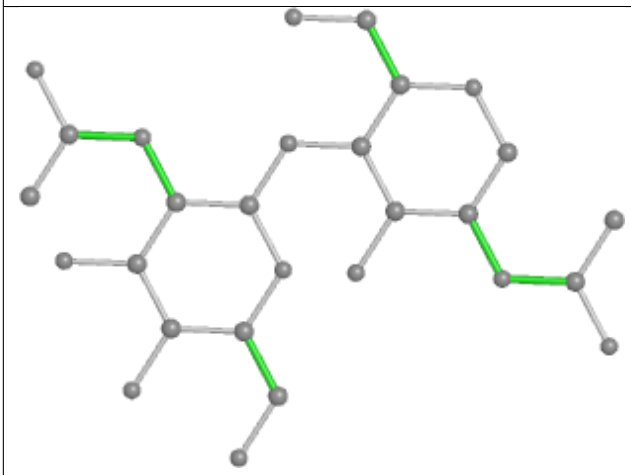


Bond angles



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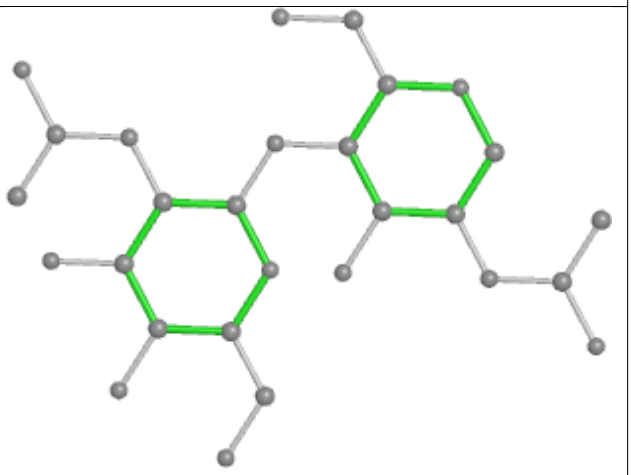
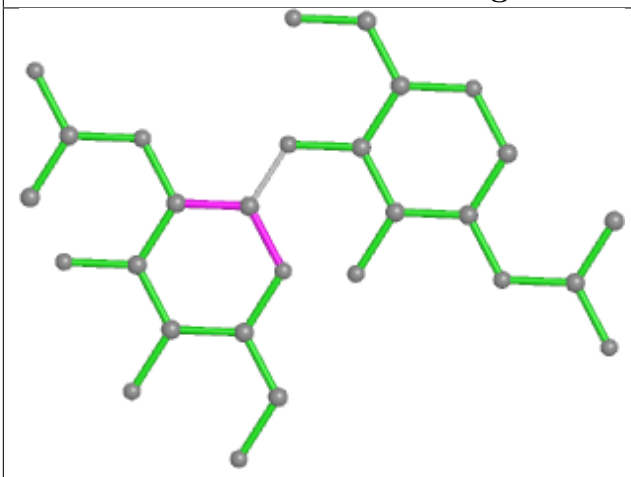
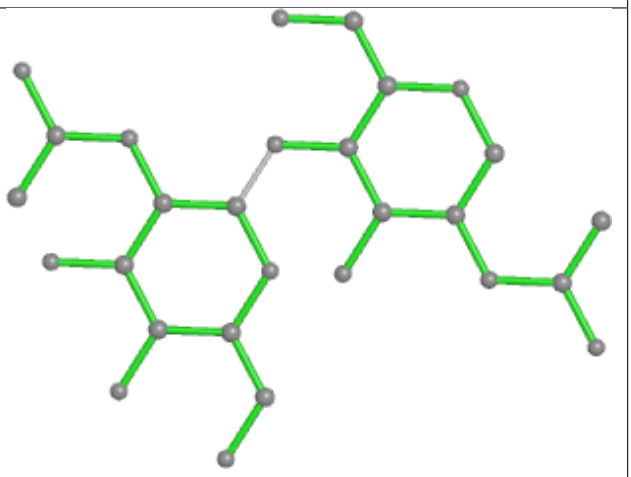
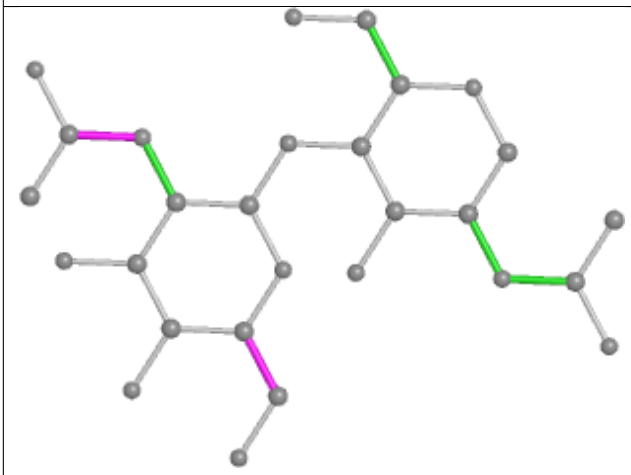
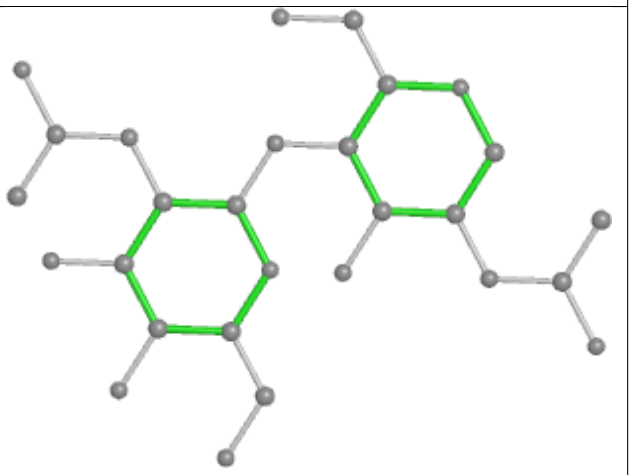
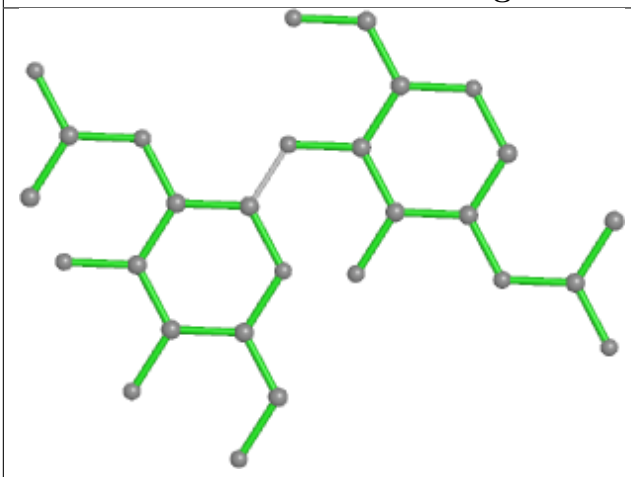


Rings

Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain N



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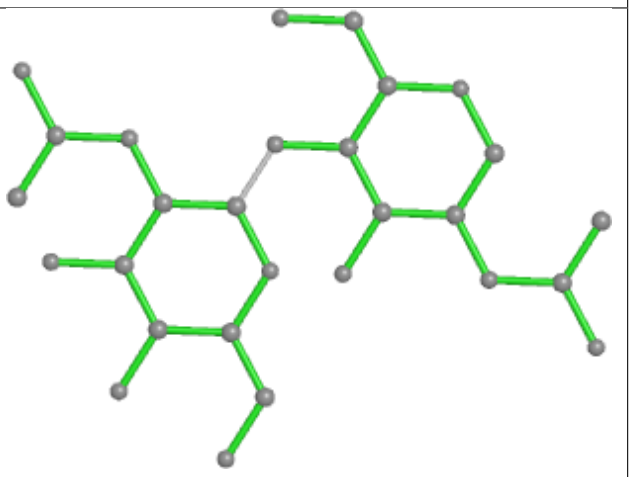

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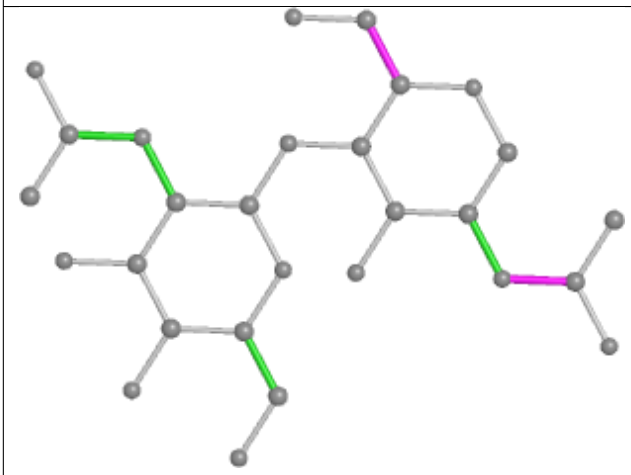

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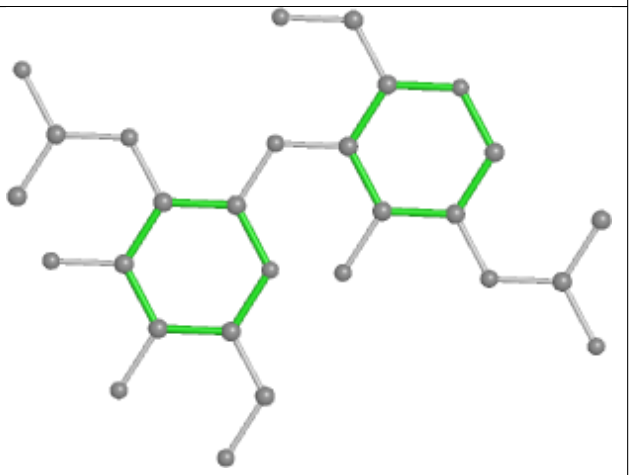
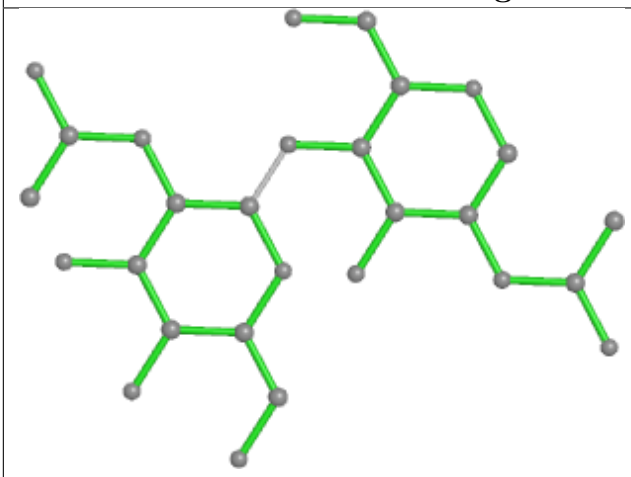


Rings

Oligosaccharide Chain O



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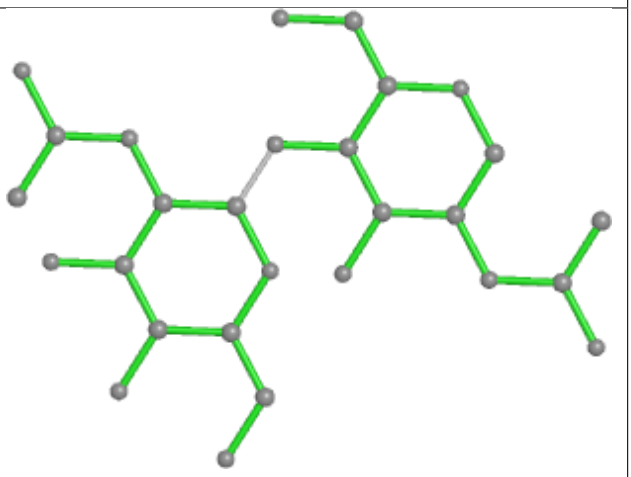

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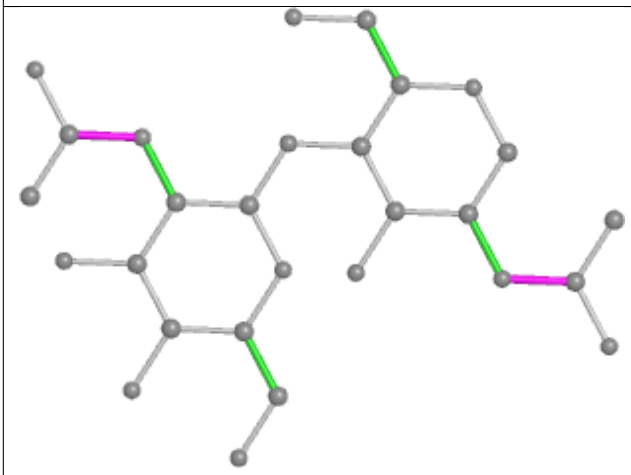

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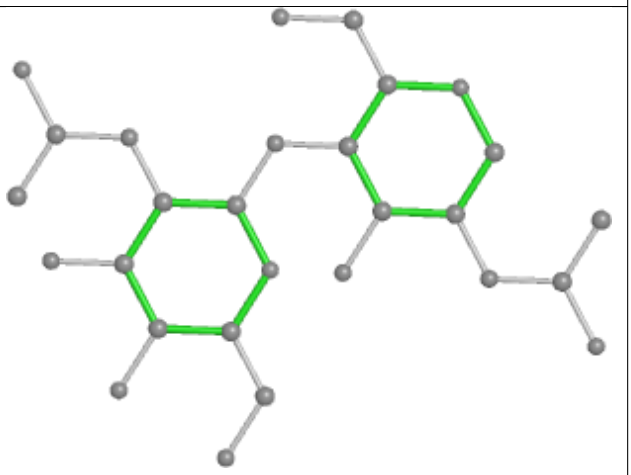
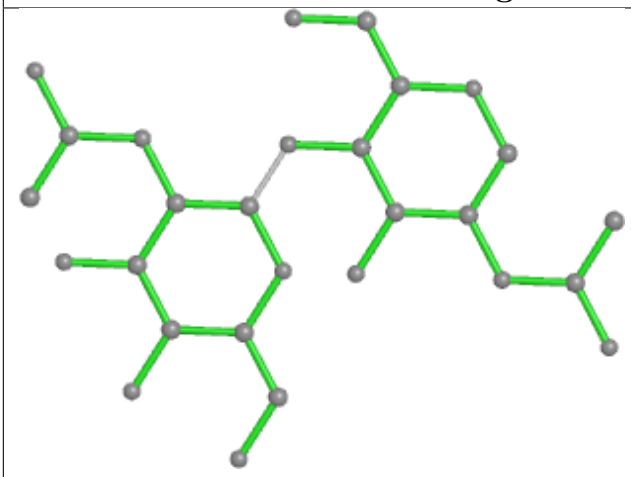


Rings

Oligosaccharide Chain P



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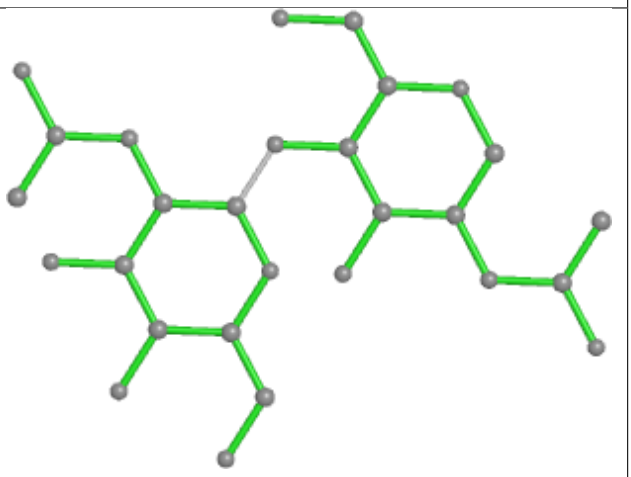
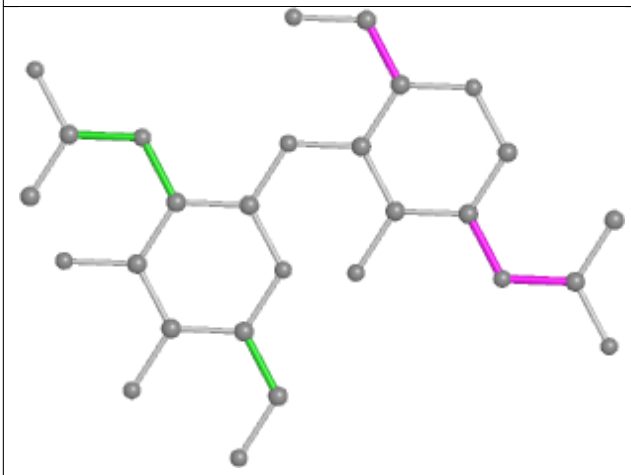


Bond angles



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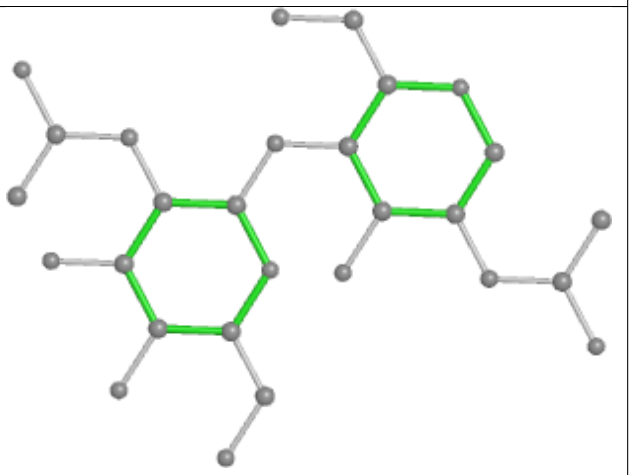
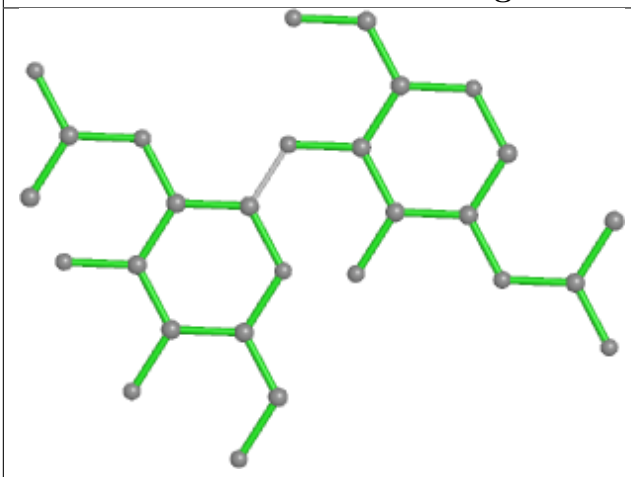


Rings

Oligosaccharide Chain Q



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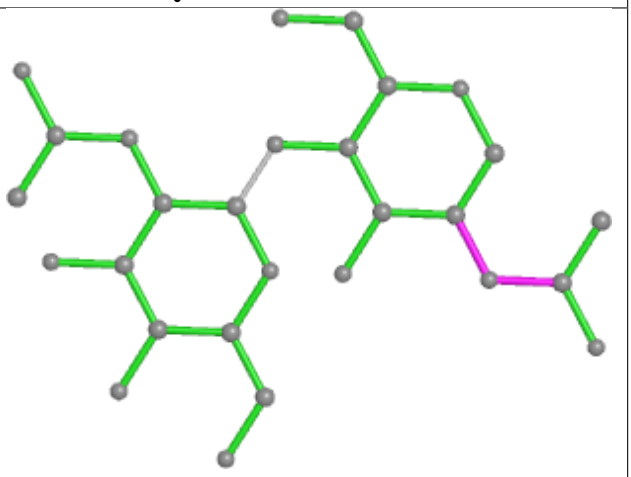
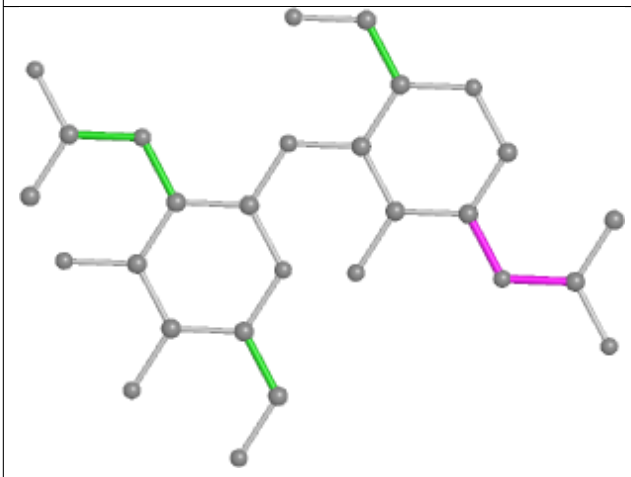


Bond angles



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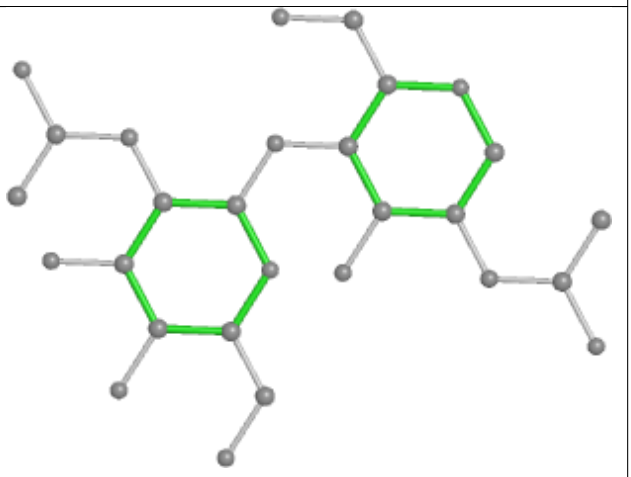
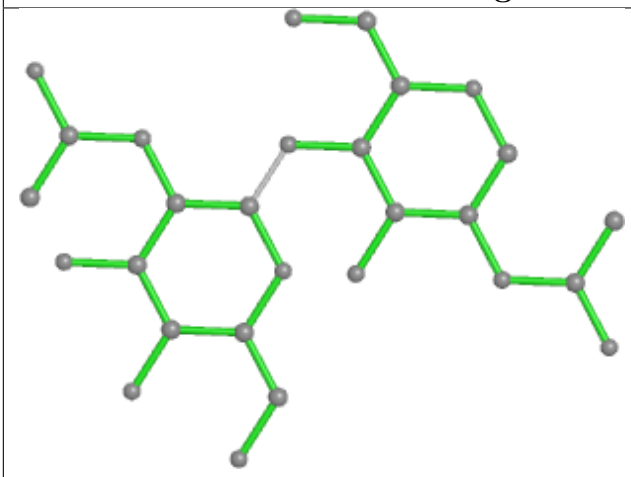


Rings

Oligosaccharide Chain R



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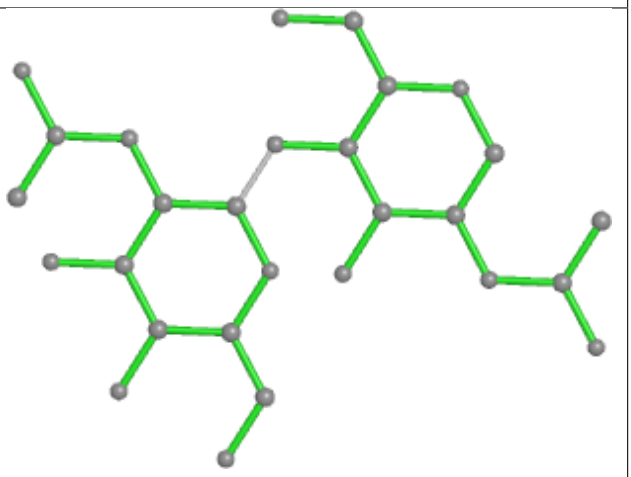
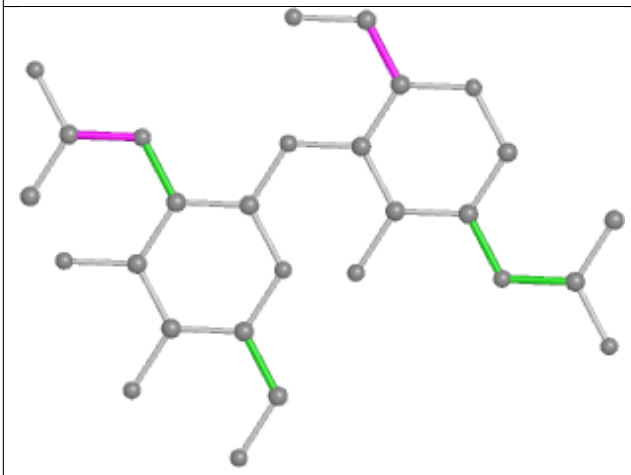


Bond angles



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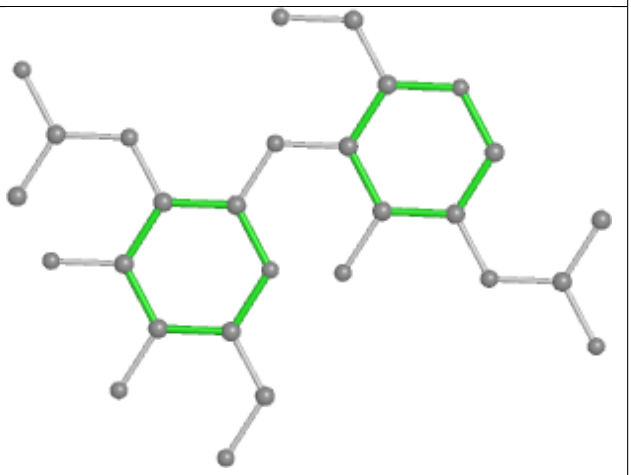
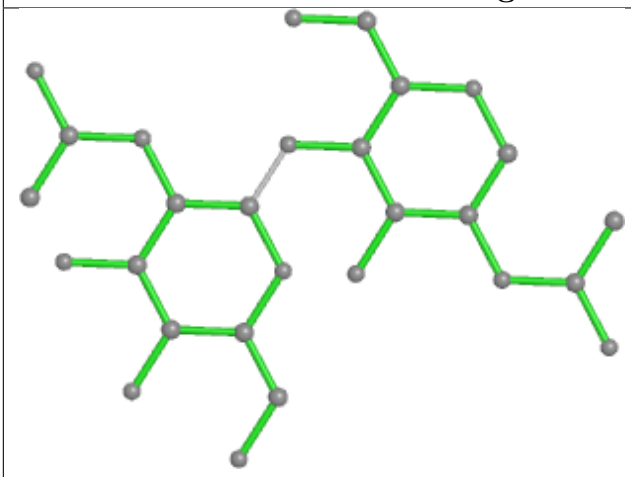


Rings

Oligosaccharide Chain S



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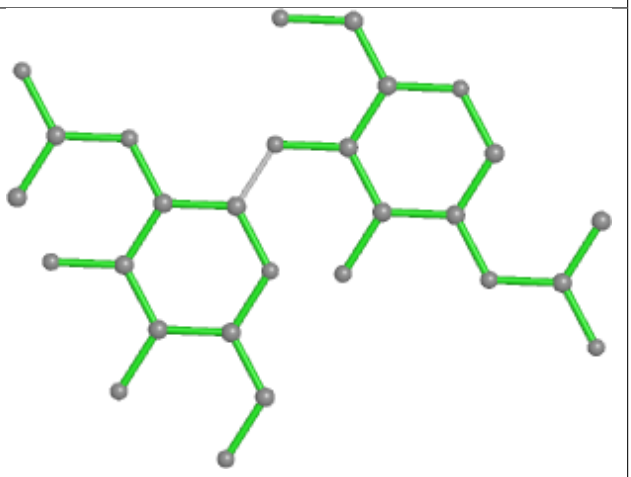

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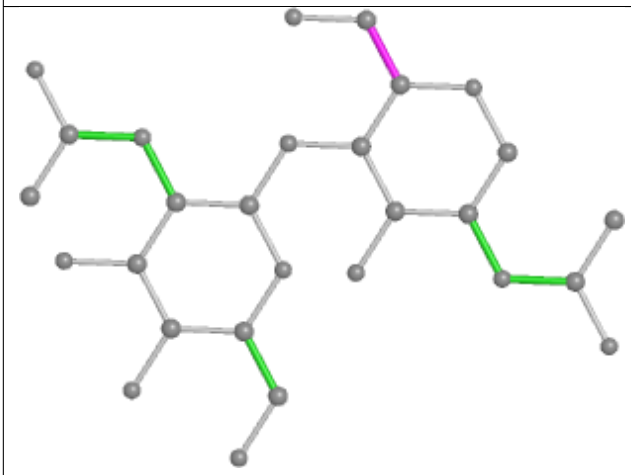

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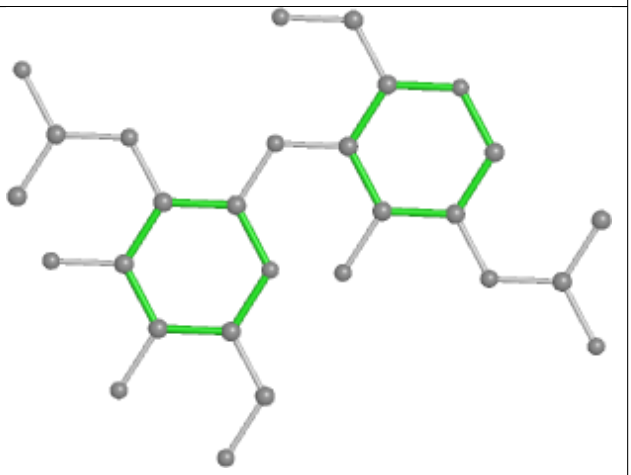
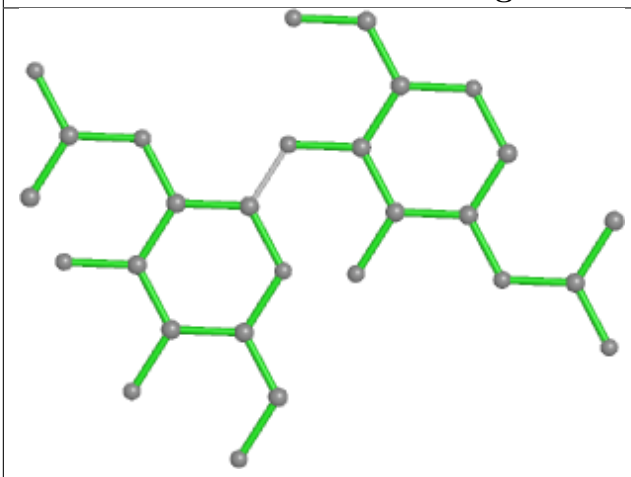


Rings

Oligosaccharide Chain T



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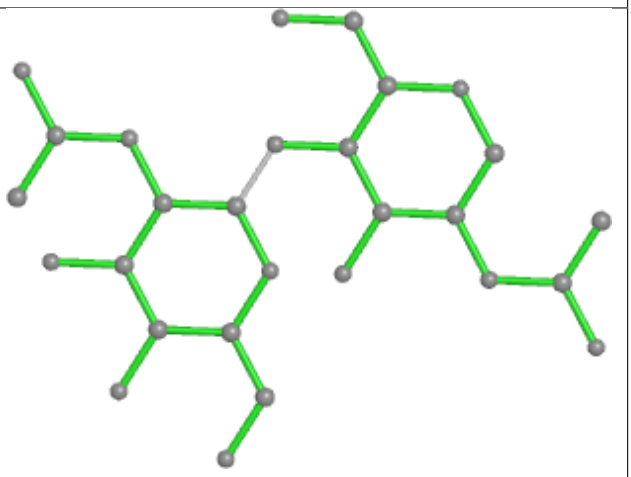
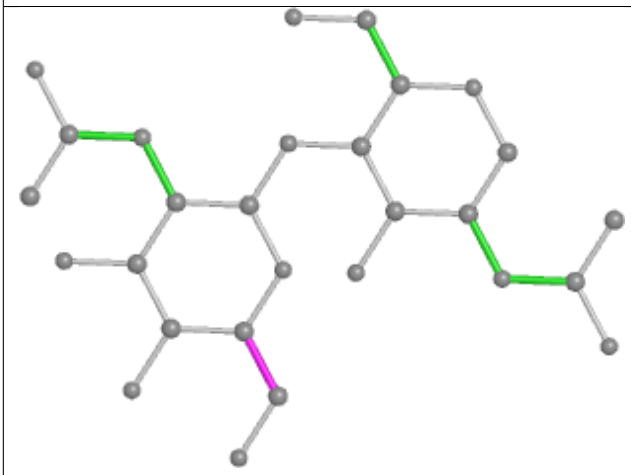


Bond angles



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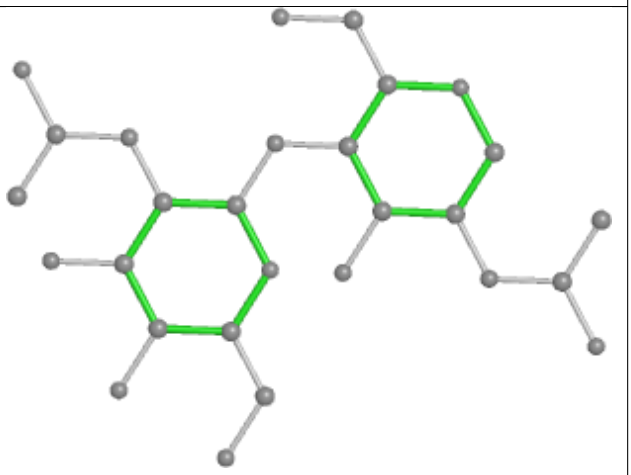
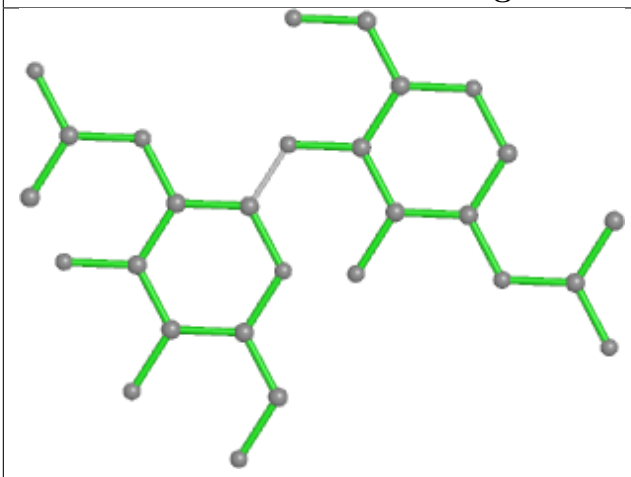


Rings

Oligosaccharide Chain U



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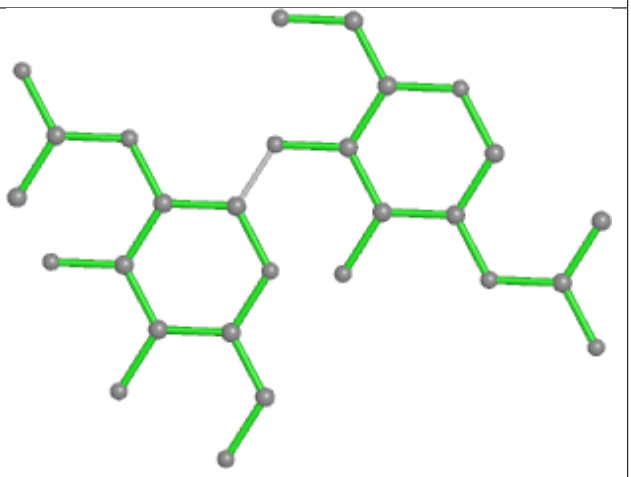

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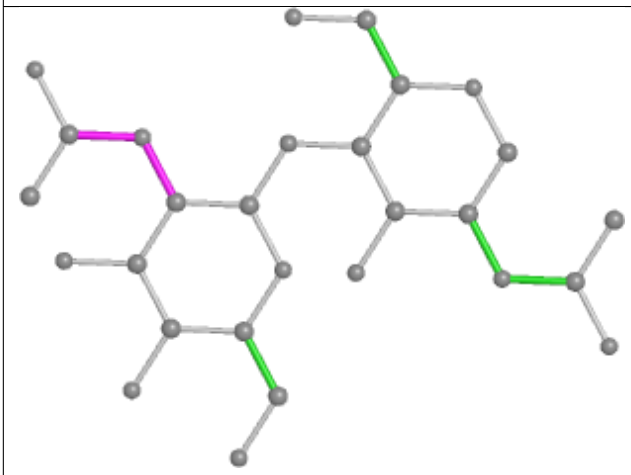

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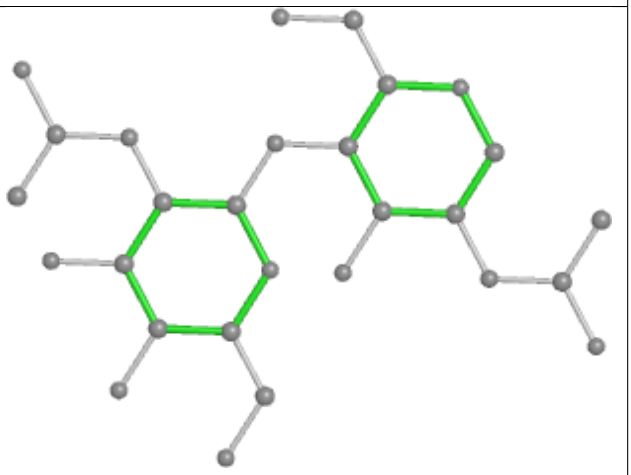
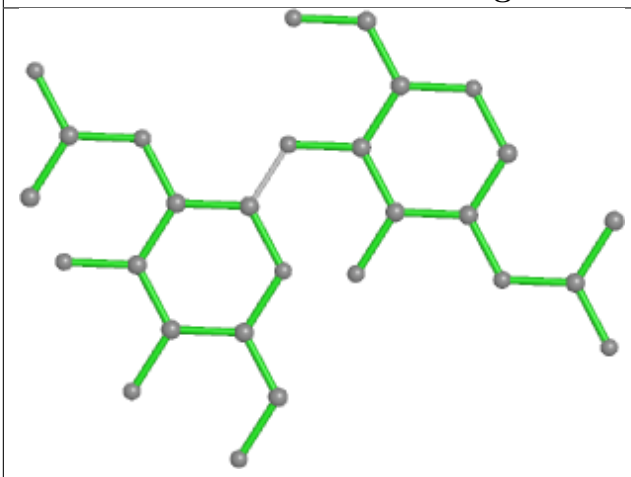


Rings

Oligosaccharide Chain V



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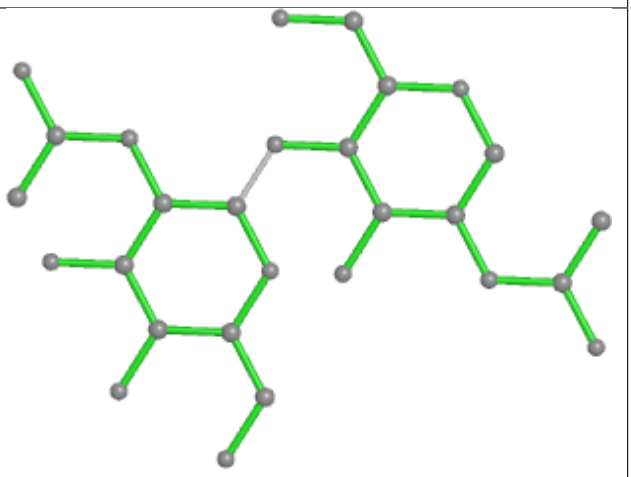
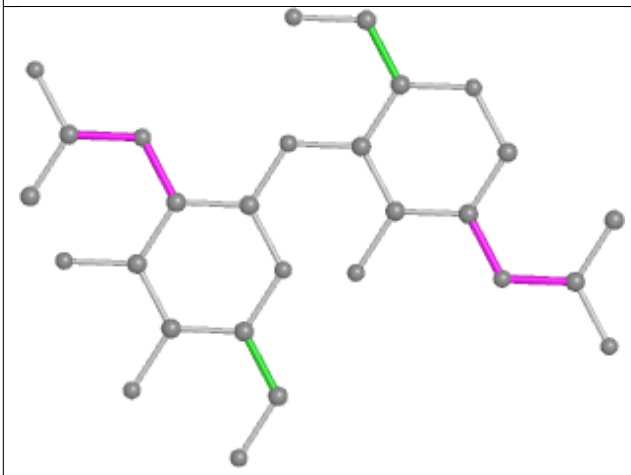


Bond angles



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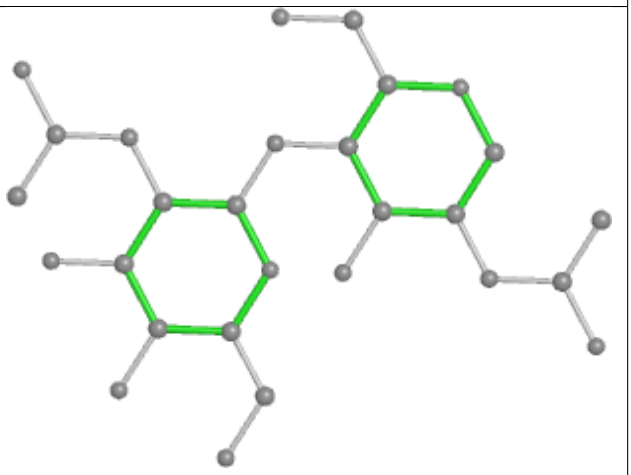
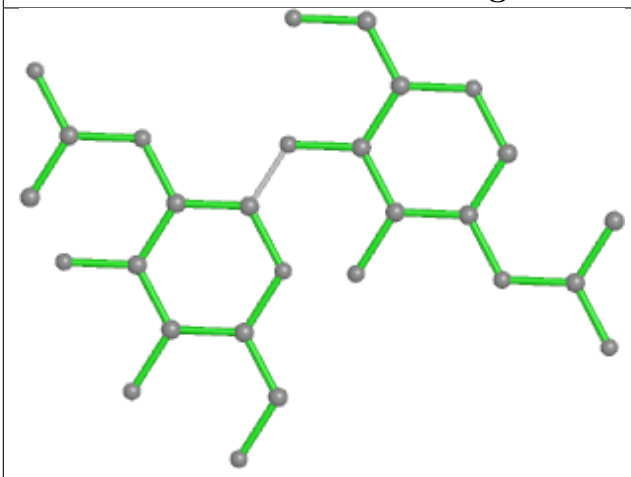


Rings

Oligosaccharide Chain W



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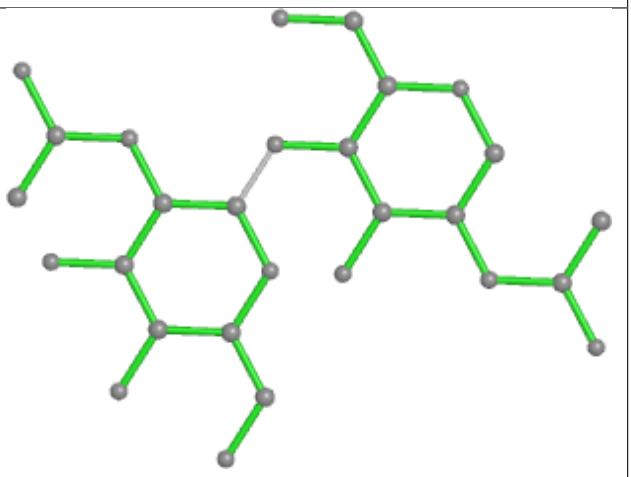
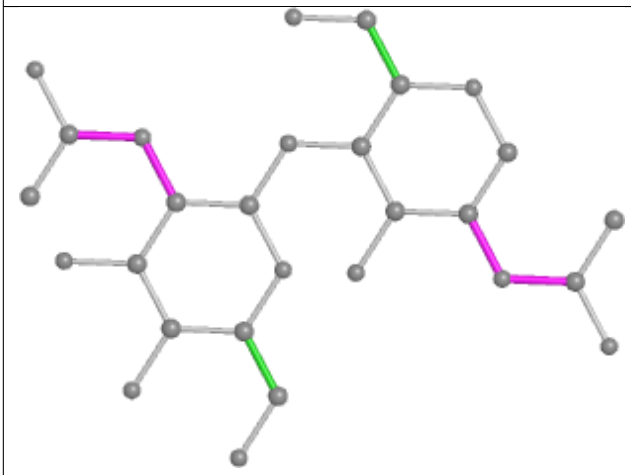


Bond angles



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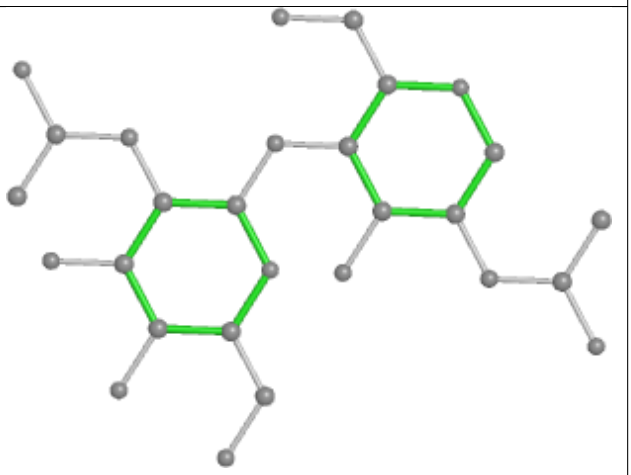
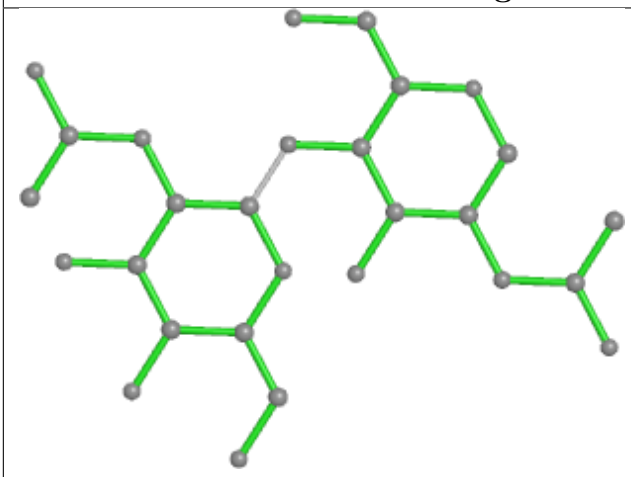
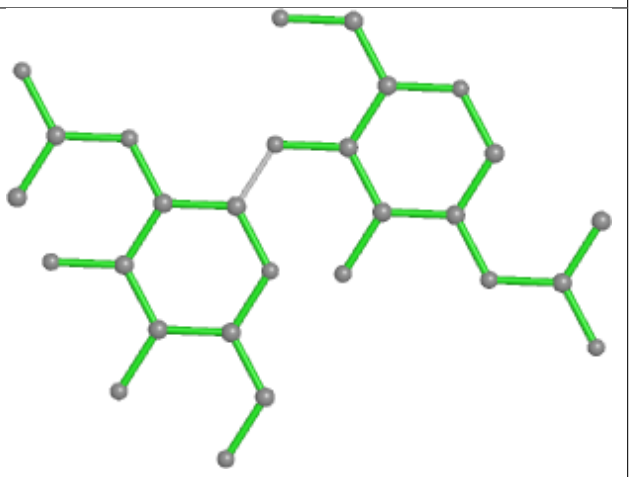


Rings

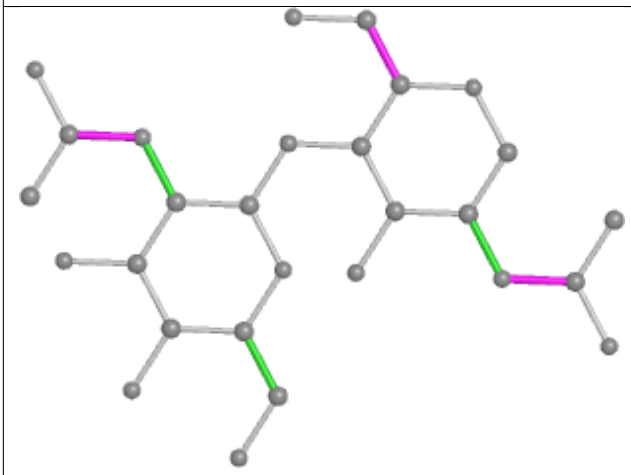
Oligosaccharide Chain X



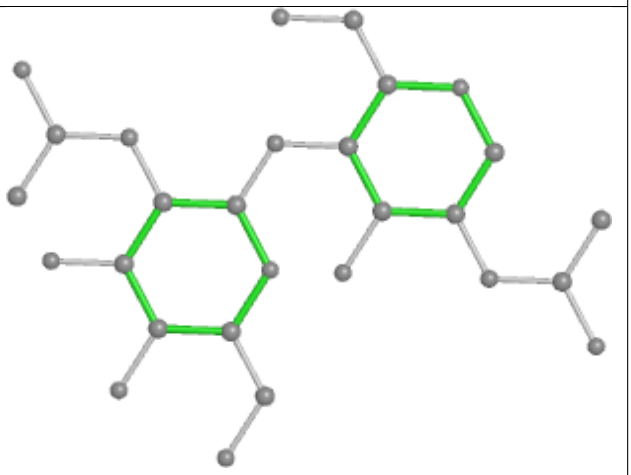
Bond lengths



Bond angles

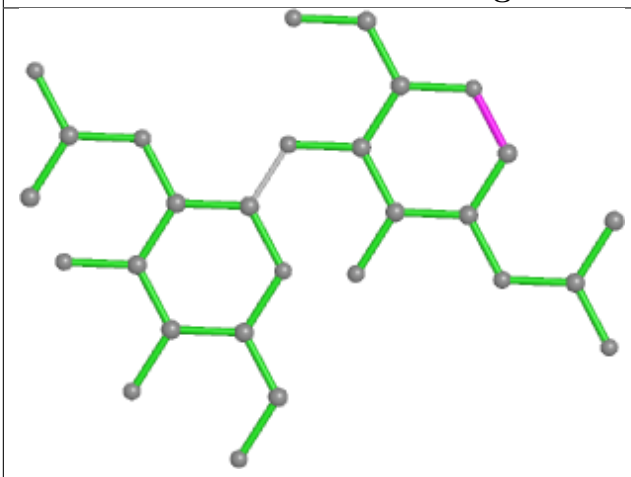


Torsions

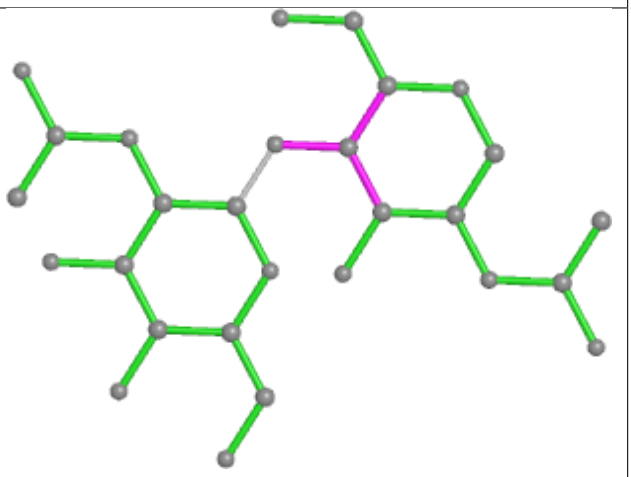


Rings

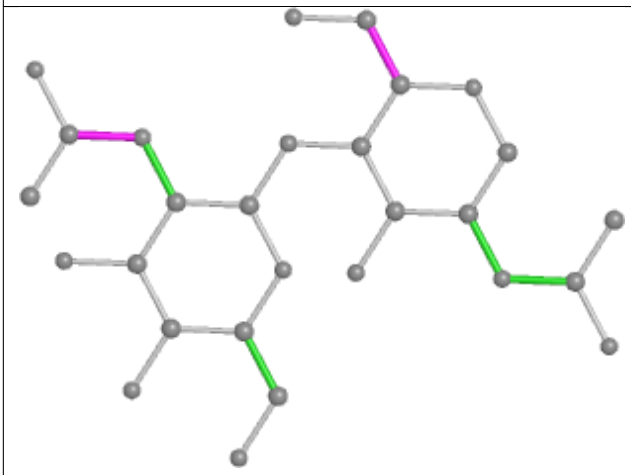
Oligosaccharide Chain Y



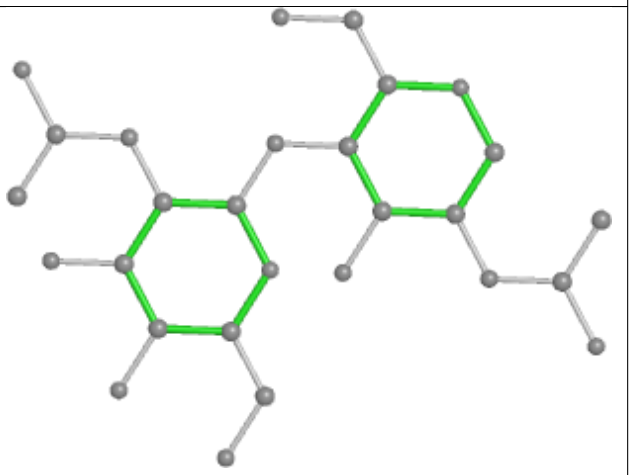
Bond lengths



Bond angles

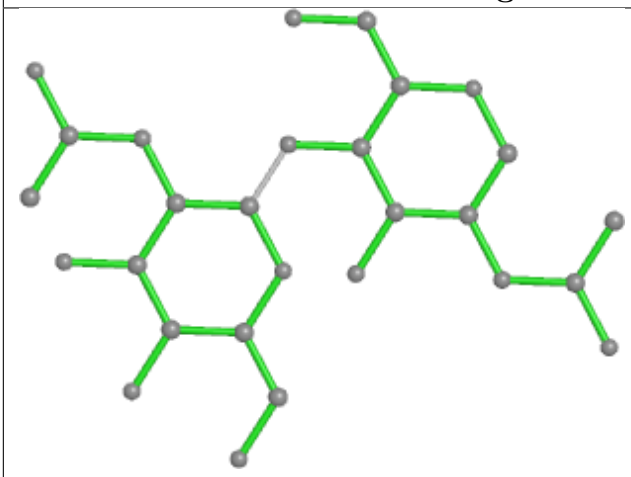


Torsions

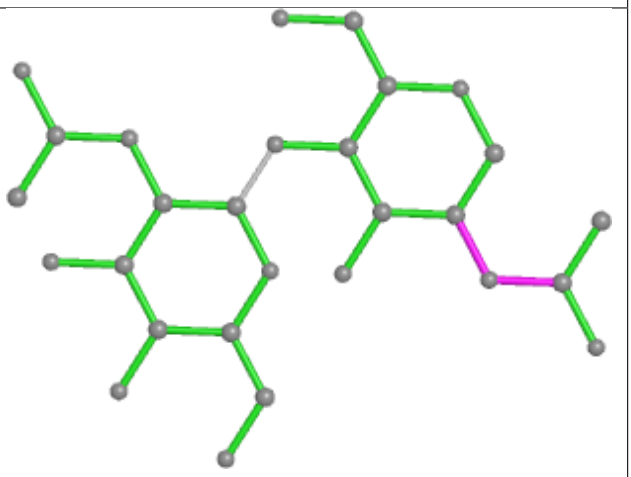


Rings

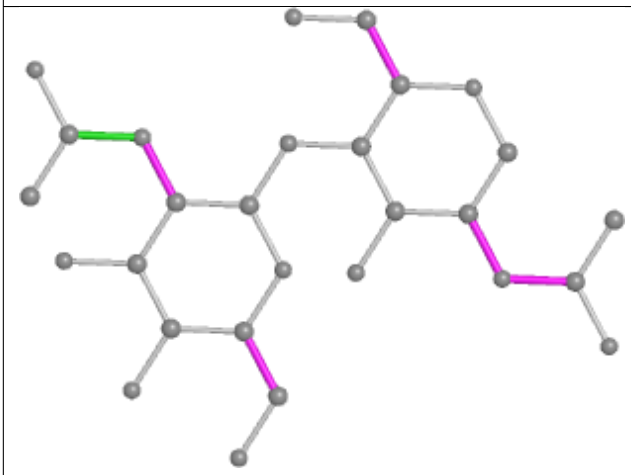
Oligosaccharide Chain Z



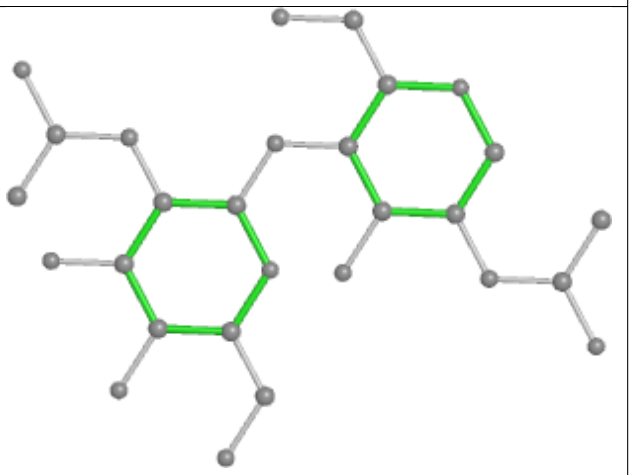
Bond lengths



Bond angles

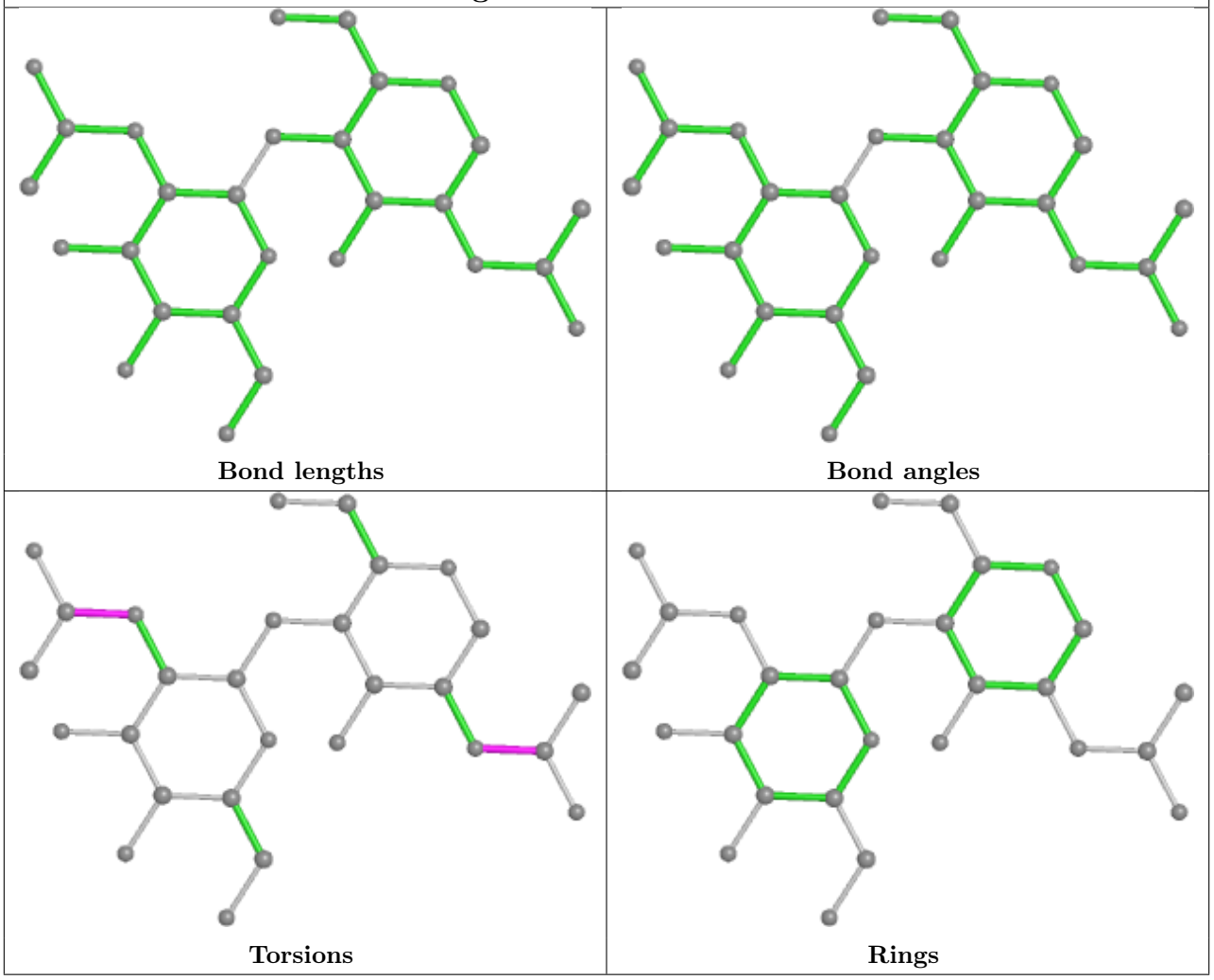


Torsions



Rings

Oligosaccharide Chain a



5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
3	NAG	A	1309	1	14,14,15	0.27	0	17,19,21	0.67	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.66	0
3	NAG	C	1311	1	14,14,15	0.26	0	17,19,21	0.63	0
3	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1309	1	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	A	1310	1	14,14,15	0.27	0	17,19,21	0.70	0
3	NAG	C	1303	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
3	NAG	C	1308	1	14,14,15	0.54	0	17,19,21	1.59	3 (17%)
3	NAG	B	1310	1	14,14,15	0.26	0	17,19,21	0.38	0
3	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.64	0
3	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1309	1	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	B	1311	1	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	A	1302	1	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
3	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1304	1	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.77	0
3	NAG	C	1305	1	14,14,15	0.26	0	17,19,21	0.68	0
3	NAG	A	1311	1	14,14,15	0.29	0	17,19,21	0.69	0
3	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.33	0
3	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.79	0
3	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.75	0
3	NAG	B	1308	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	A	1308	1	14,14,15	0.20	0	17,19,21	0.32	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	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	5/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1308	NAG	C1-O5-C5	4.60	118.42	112.19
3	C	1308	NAG	C6-C5-C4	-2.96	106.07	113.00
3	C	1308	NAG	O5-C1-C2	-2.25	107.73	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1302	NAG	C1-O5-C5	2.21	115.18	112.19
3	B	1307	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1311	NAG	C8-C7-N2-C2
3	A	1311	NAG	O7-C7-N2-C2
3	B	1305	NAG	C3-C2-N2-C7
3	B	1305	NAG	C8-C7-N2-C2
3	B	1305	NAG	O7-C7-N2-C2
3	B	1306	NAG	C8-C7-N2-C2
3	B	1306	NAG	O7-C7-N2-C2
3	B	1307	NAG	C3-C2-N2-C7
3	B	1307	NAG	C8-C7-N2-C2
3	B	1307	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	C	1306	NAG	C3-C2-N2-C7
3	C	1306	NAG	C8-C7-N2-C2
3	C	1306	NAG	O7-C7-N2-C2
3	C	1307	NAG	C3-C2-N2-C7
3	C	1307	NAG	C8-C7-N2-C2
3	C	1307	NAG	O7-C7-N2-C2
3	C	1308	NAG	C3-C2-N2-C7
3	C	1308	NAG	C8-C7-N2-C2
3	C	1308	NAG	O7-C7-N2-C2
3	C	1309	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1309	NAG	C8-C7-N2-C2
3	A	1310	NAG	C8-C7-N2-C2
3	A	1310	NAG	O7-C7-N2-C2
3	B	1304	NAG	C8-C7-N2-C2
3	C	1310	NAG	C8-C7-N2-C2
3	C	1310	NAG	O7-C7-N2-C2
3	C	1311	NAG	C8-C7-N2-C2
3	C	1311	NAG	O7-C7-N2-C2
3	A	1307	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	C4-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	B	1306	NAG	C1-C2-N2-C7
3	C	1304	NAG	C1-C2-N2-C7
3	B	1308	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1303	NAG	C8-C7-N2-C2
3	A	1303	NAG	O7-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	A	1308	NAG	C4-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	C	1305	NAG	C8-C7-N2-C2
3	A	1306	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	B	1303	NAG	C8-C7-N2-C2
3	C	1305	NAG	O7-C7-N2-C2
3	C	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	O7-C7-N2-C2
3	B	1307	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1308	NAG	C1-C2-N2-C7
3	A	1304	NAG	O5-C5-C6-O6
3	C	1306	NAG	C1-C2-N2-C7
3	B	1311	NAG	O5-C5-C6-O6
3	B	1305	NAG	C1-C2-N2-C7
3	B	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1306	NAG	1	0
3	B	1307	NAG	3	0
3	C	1308	NAG	6	0
3	C	1309	NAG	1	0
3	B	1302	NAG	2	0
3	A	1306	NAG	1	0
3	A	1311	NAG	5	0
3	C	1301	NAG	1	0
3	C	1307	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

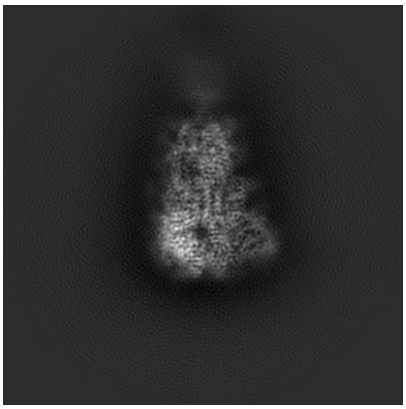
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35078. These allow visual inspection of the internal detail of the map and identification of artifacts.

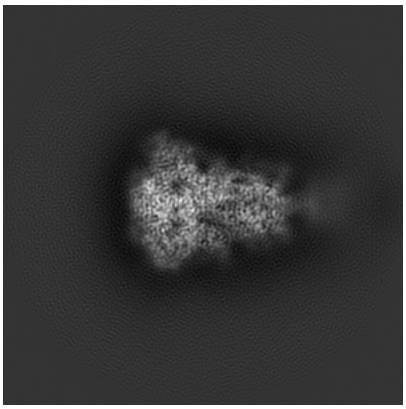
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

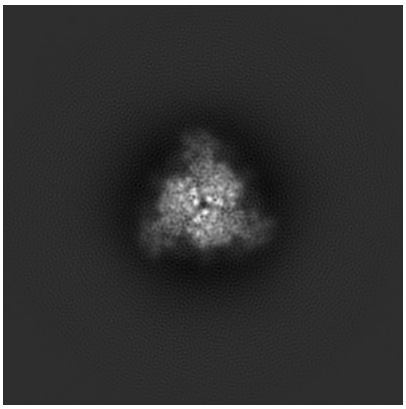
6.1.1 Primary map



X

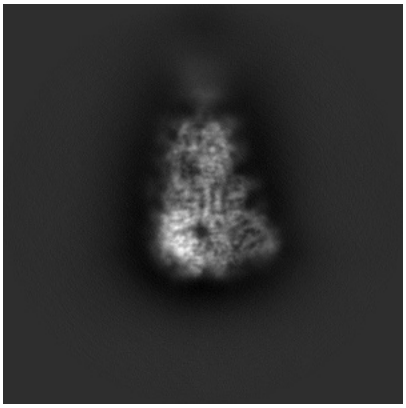


Y

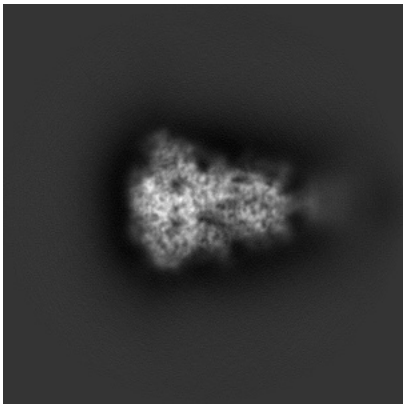


Z

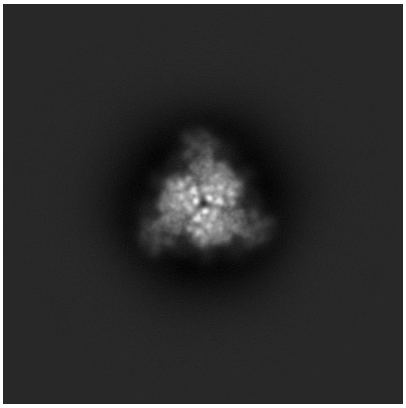
6.1.2 Raw map



X



Y

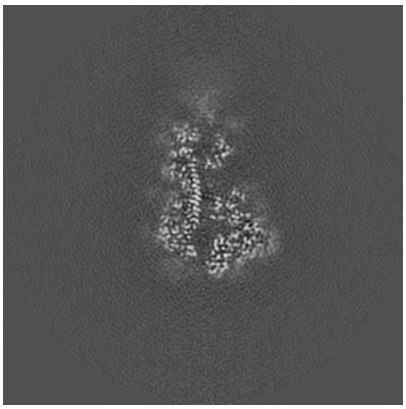


Z

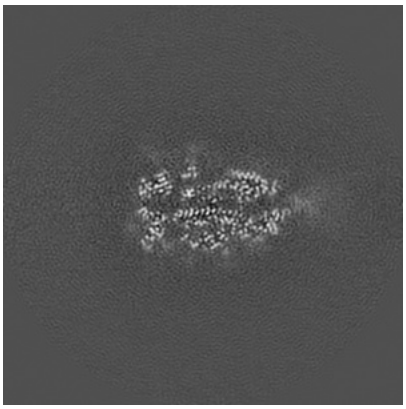
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

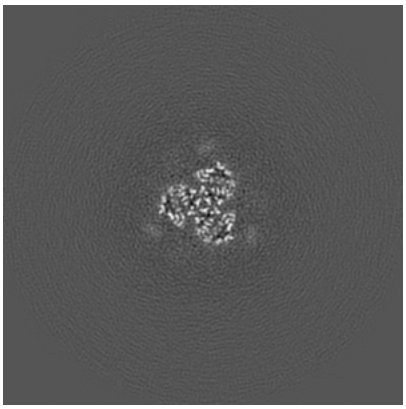
6.2.1 Primary map



X Index: 188

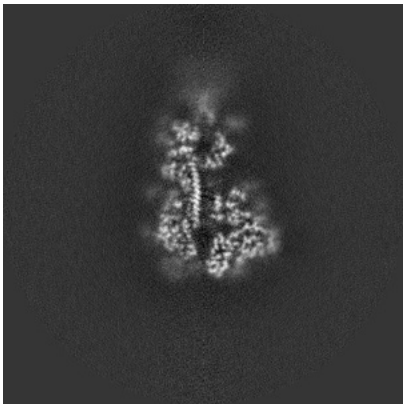


Y Index: 188

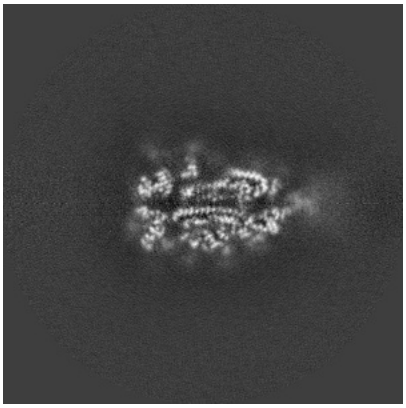


Z Index: 188

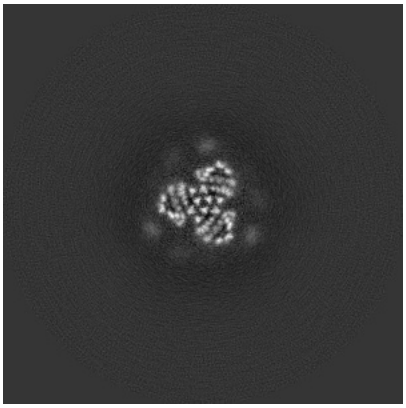
6.2.2 Raw map



X Index: 188



Y Index: 188

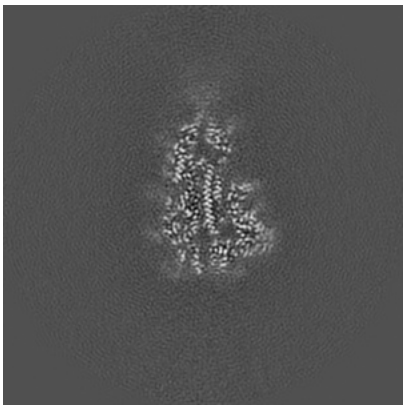


Z Index: 188

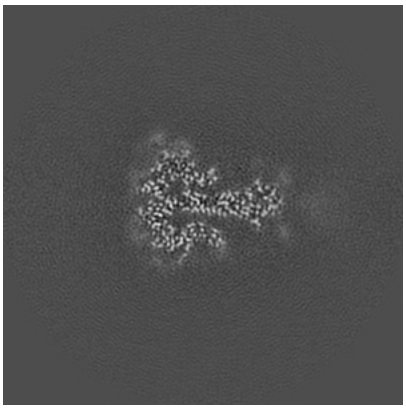
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



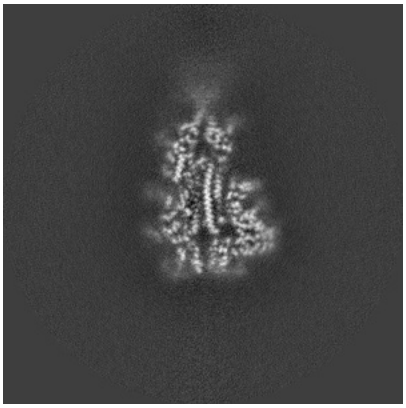
X Index: 193



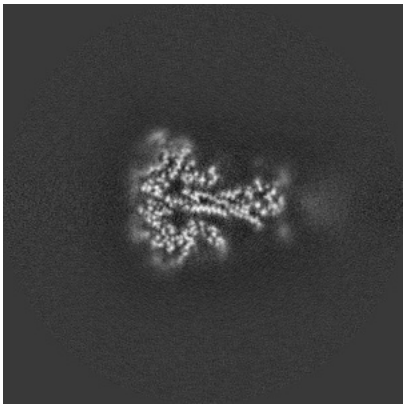
Y Index: 174

Z Index: 150

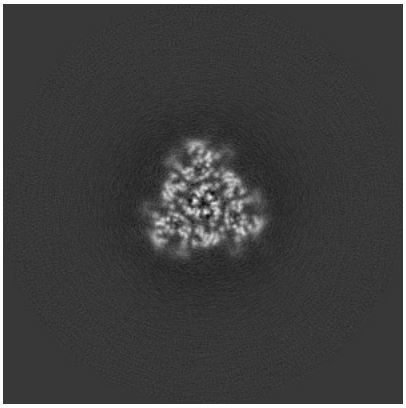
6.3.2 Raw map



X Index: 193



Y Index: 173

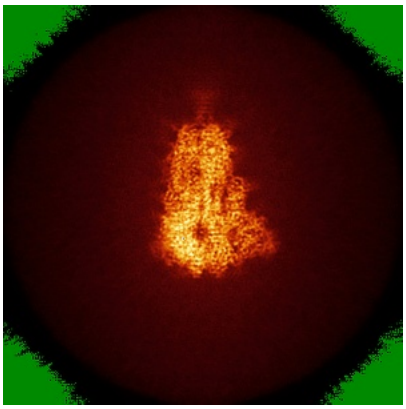


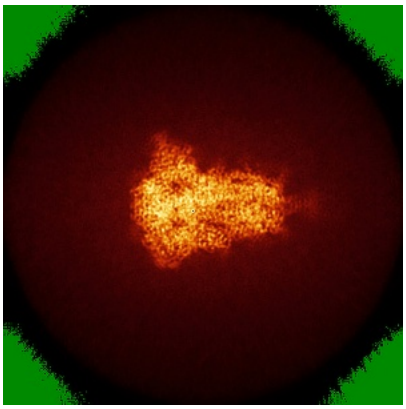
Z Index: 175

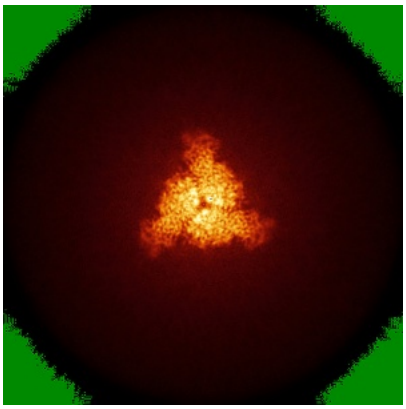
The images above show the largest variance slices of the map in three orthogonal directions.

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

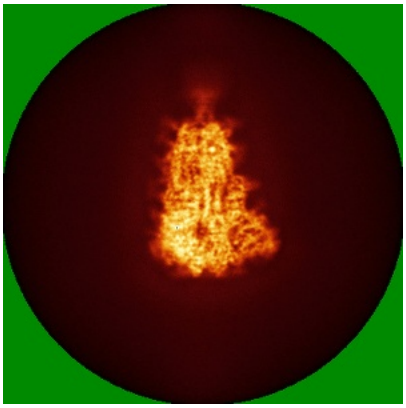
6.4.1 Primary map

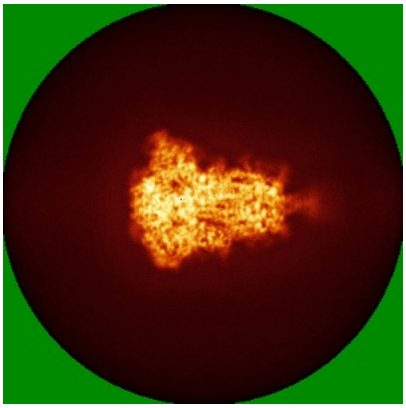

X

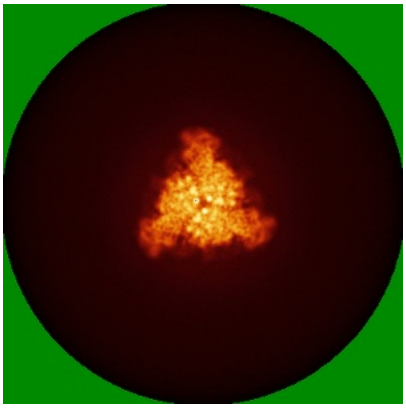

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

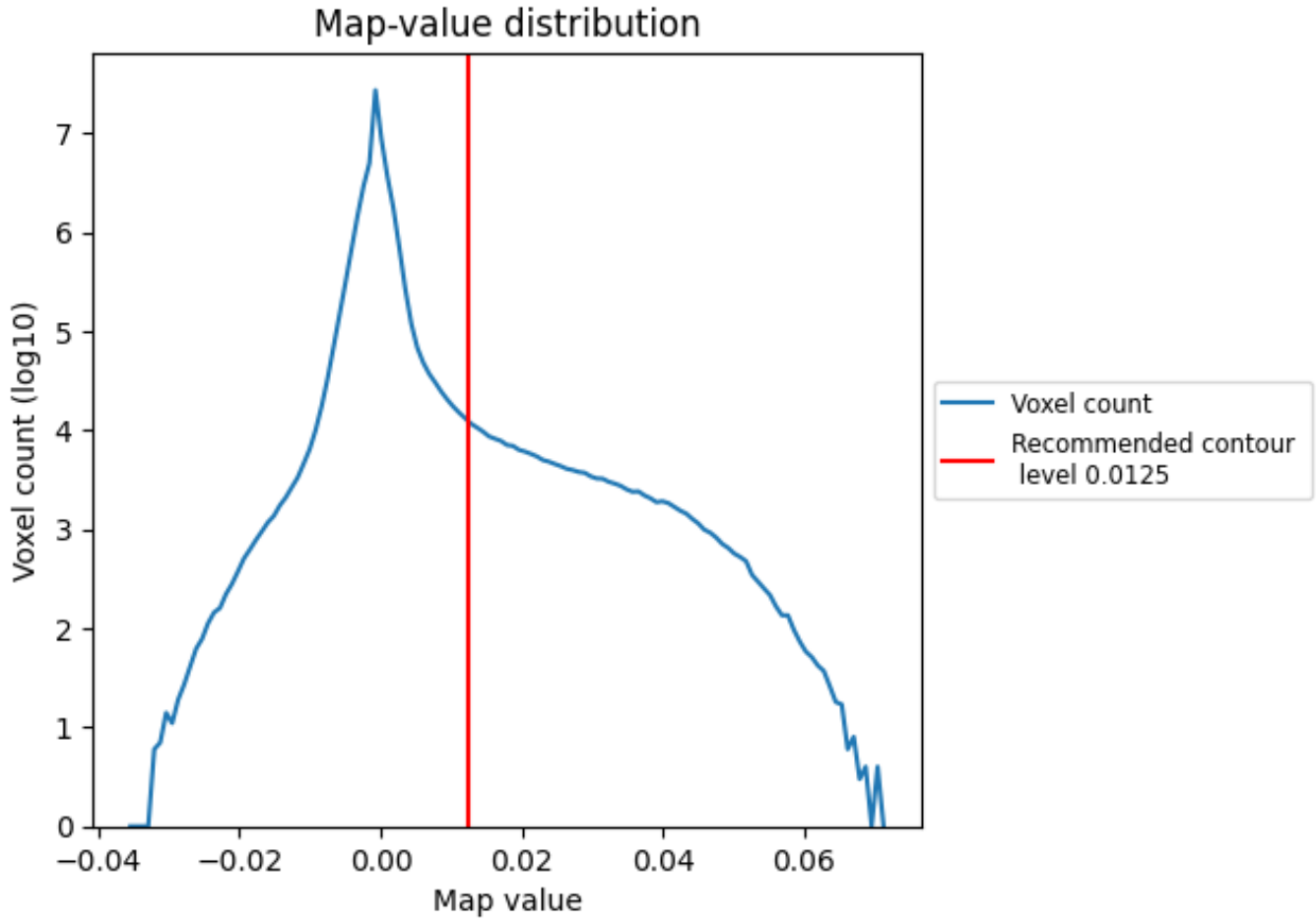
6.6 Mask visualisation (i)

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

7 Map analysis

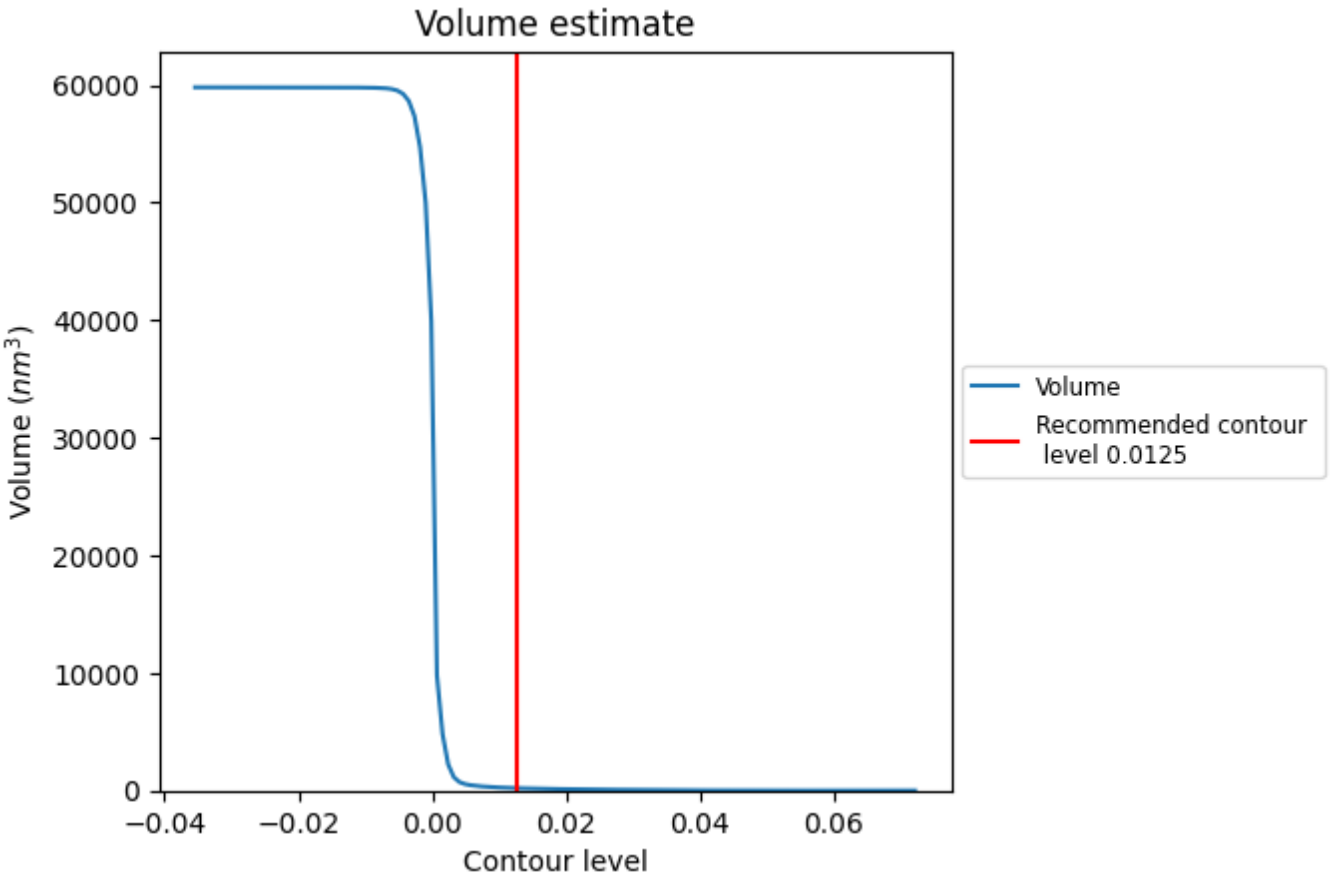
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

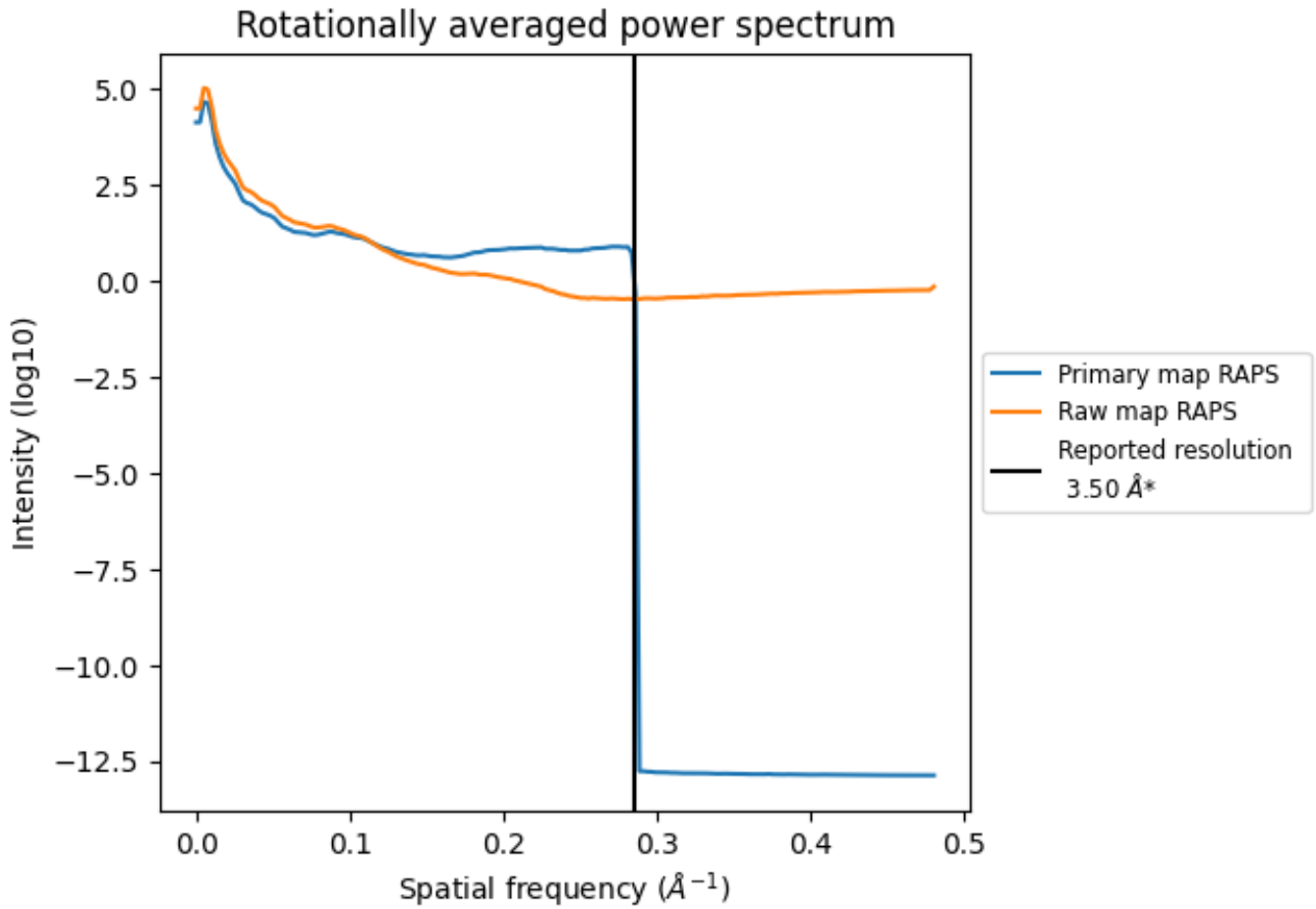
7.2 Volume estimate



The volume at the recommended contour level is 207 nm^3; this corresponds to an approximate mass of 187 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)

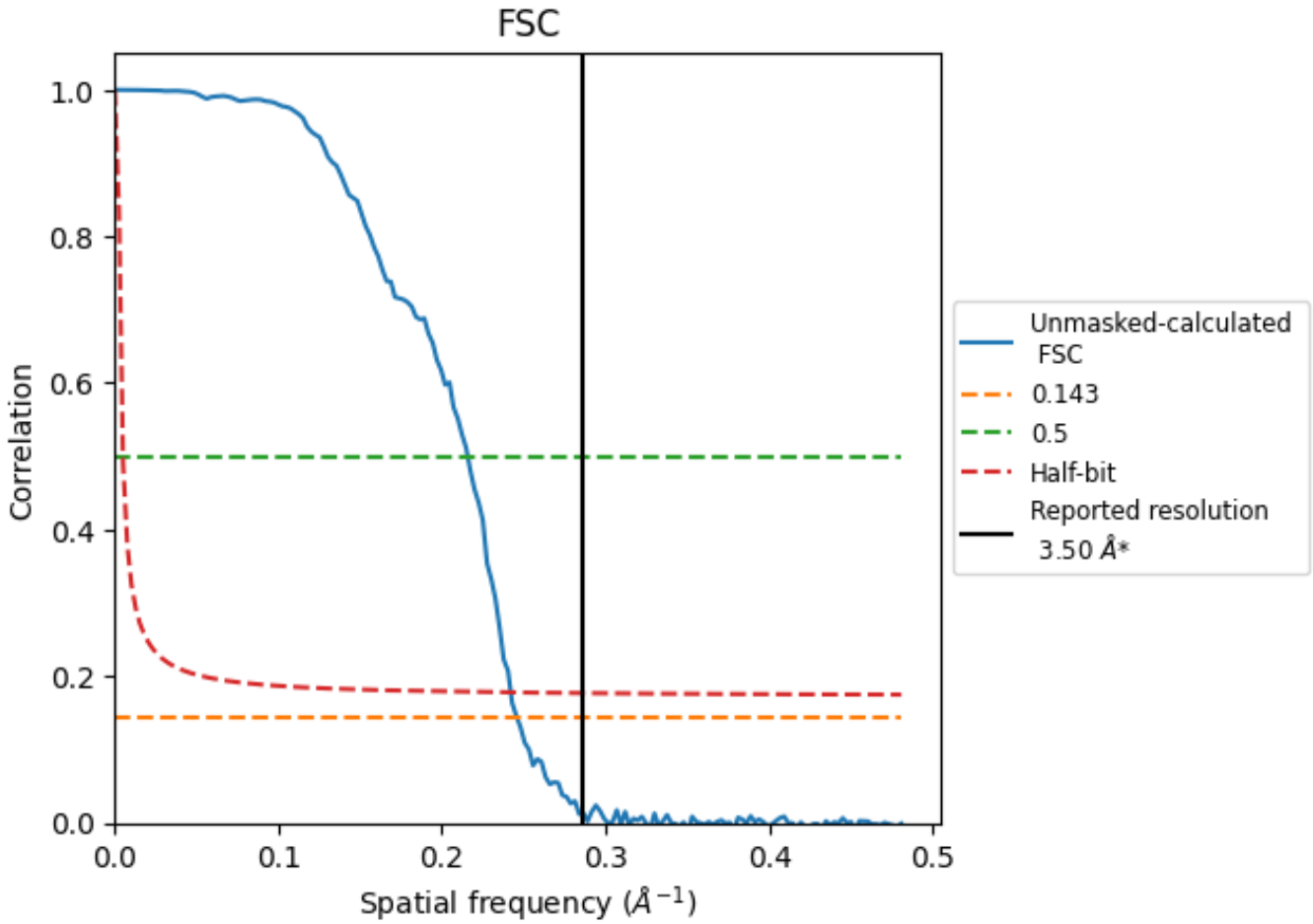


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

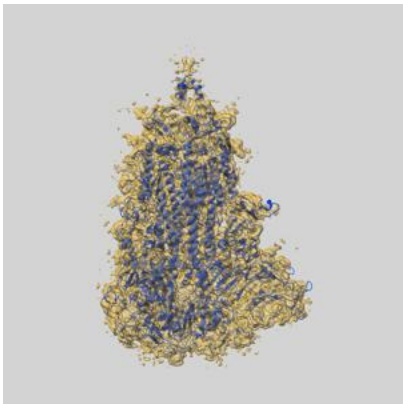
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	4.64	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.5 by more than 10 %

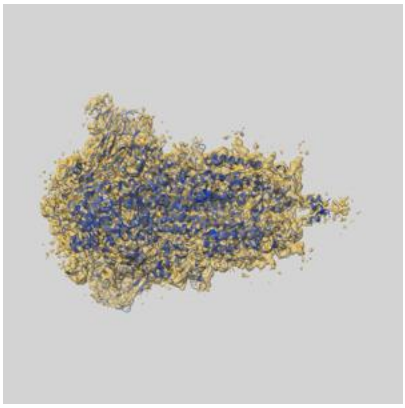
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35078 and PDB model 8HXJ. Per-residue inclusion information can be found in section 3 on page 16.

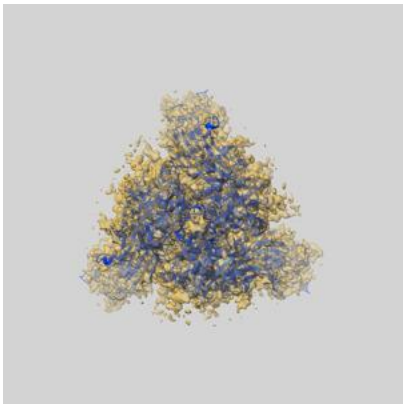
9.1 Map-model overlay



X



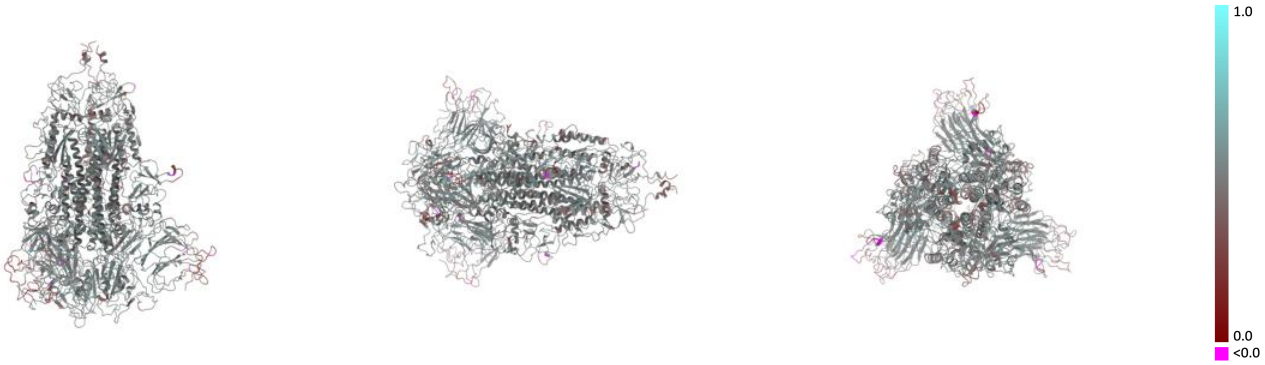
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125 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.

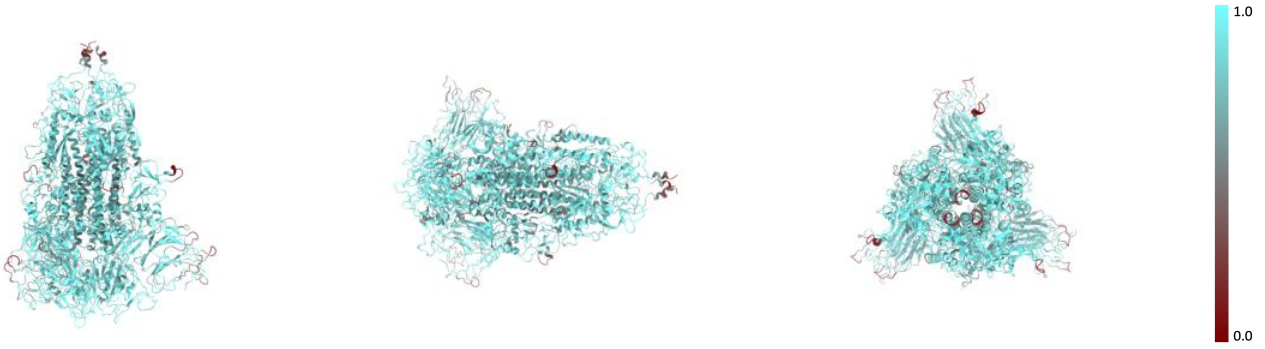
9.2 Q-score mapped to coordinate model (i)



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.

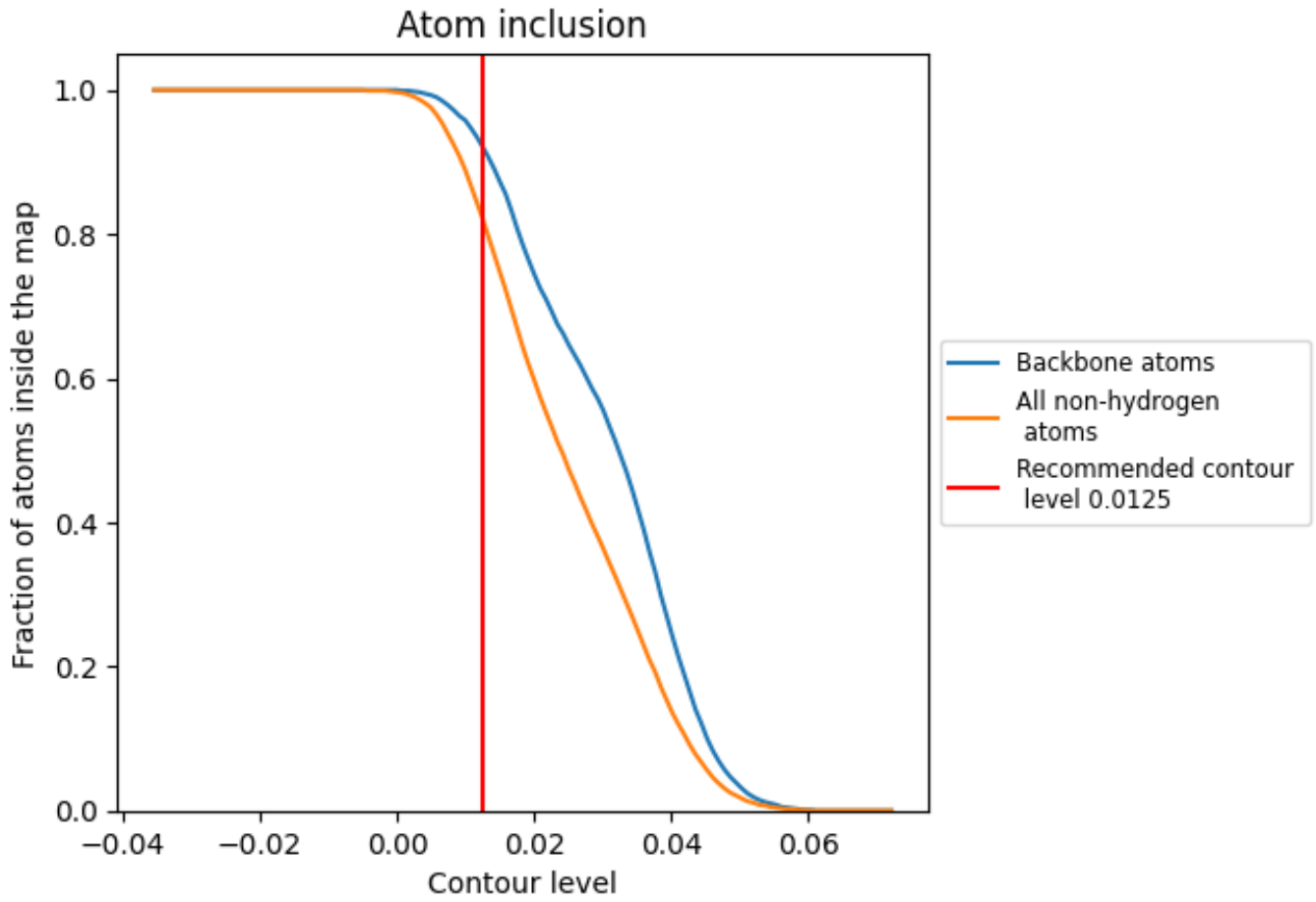
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0125).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.4730
A	0.8260	0.4770
B	0.8290	0.4770
C	0.8280	0.4780
D	0.8210	0.4470
E	0.2860	0.1990
F	0.5710	0.2970
G	0.5360	0.3470
H	0.6430	0.3250
I	0.6430	0.2700
J	0.7140	0.3560
K	0.5710	0.3050
L	0.7860	0.4090
M	0.4640	0.2920
N	0.5000	0.1910
O	0.2860	0.1460
P	0.5710	0.3210
Q	0.5710	0.2970
R	0.6070	0.3580
S	0.6430	0.3220
T	0.7860	0.4700
U	0.5360	0.2500
V	0.5000	0.2670
W	0.5000	0.1970
X	0.5710	0.2420
Y	0.5000	0.3280
Z	0.4290	0.2380
a	0.3210	0.1590