Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 02:52 AM JST

PDB ID	:	7FAE
EMDB ID	:	EMD-31502
Title	:	S protein of SARS-CoV-2 in complex bound with P36-5D2(state2)
Authors	:	Zhang, L.; Wang, X.; Shan, S.; Zhang, S.
Deposited on	:	2021-07-06
Resolution	:	3.65 Å(reported)

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

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

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

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

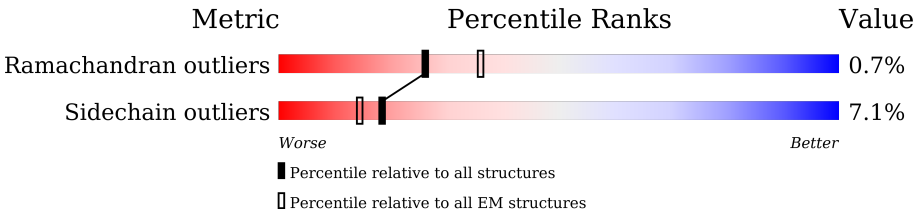
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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.



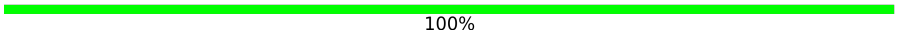
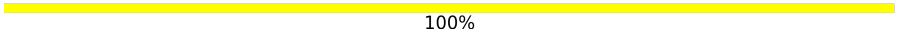
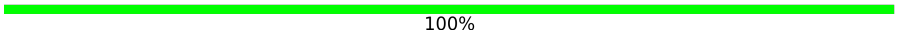
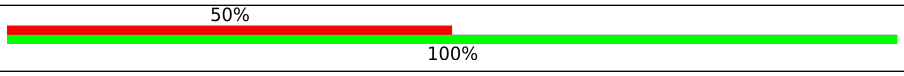
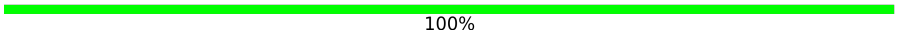
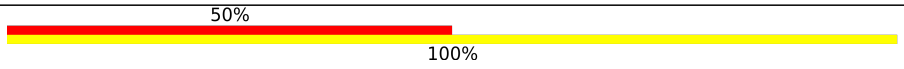
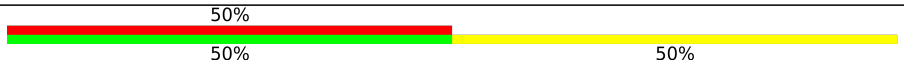
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1298	5% 71% 7% 23%
1	B	1298	8% 70% 7% 22%
1	C	1298	70% 7% 22%
2	H	471	34% 46% 53%
2	e	471	39% 46% 53%
2	h	471	16% 46% 53%
3	L	233	60% 90% 9%
3	d	233	70% 89% 9%
3	g	233	26% 89% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	
4	I	2	
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34352 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	1004	Total	C	N	O	S	0	0
			7853	5014	1307	1496	36		
1	B	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		
1	C	1007	Total	C	N	O	S	0	0
			7866	5020	1309	1501	36		

There are 297 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	SER	-	expression tag	UNP P0DTC2
A	1291	ASP	-	expression tag	UNP P0DTC2
A	1292	TYR	-	expression tag	UNP P0DTC2
A	1293	LYS	-	expression tag	UNP P0DTC2
A	1294	ASP	-	expression tag	UNP P0DTC2
A	1295	ASP	-	expression tag	UNP P0DTC2
A	1296	ASP	-	expression tag	UNP P0DTC2
A	1297	ASP	-	expression tag	UNP P0DTC2
A	1298	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	SER	-	expression tag	UNP P0DTC2
B	1291	ASP	-	expression tag	UNP P0DTC2
B	1292	TYR	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1293	LYS	-	expression tag	UNP P0DTC2
B	1294	ASP	-	expression tag	UNP P0DTC2
B	1295	ASP	-	expression tag	UNP P0DTC2
B	1296	ASP	-	expression tag	UNP P0DTC2
B	1297	ASP	-	expression tag	UNP P0DTC2
B	1298	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
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	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	SER	-	expression tag	UNP P0DTC2
C	1291	ASP	-	expression tag	UNP P0DTC2
C	1292	TYR	-	expression tag	UNP P0DTC2
C	1293	LYS	-	expression tag	UNP P0DTC2
C	1294	ASP	-	expression tag	UNP P0DTC2
C	1295	ASP	-	expression tag	UNP P0DTC2
C	1296	ASP	-	expression tag	UNP P0DTC2
C	1297	ASP	-	expression tag	UNP P0DTC2
C	1298	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called P36-5D2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	222	Total	C	N	O	S	0	0
			1670	1052	285	326	7		
2	e	222	Total	C	N	O	S	0	0
			1666	1048	285	326	7		
2	h	221	Total	C	N	O	S	0	0
			1661	1047	284	323	7		

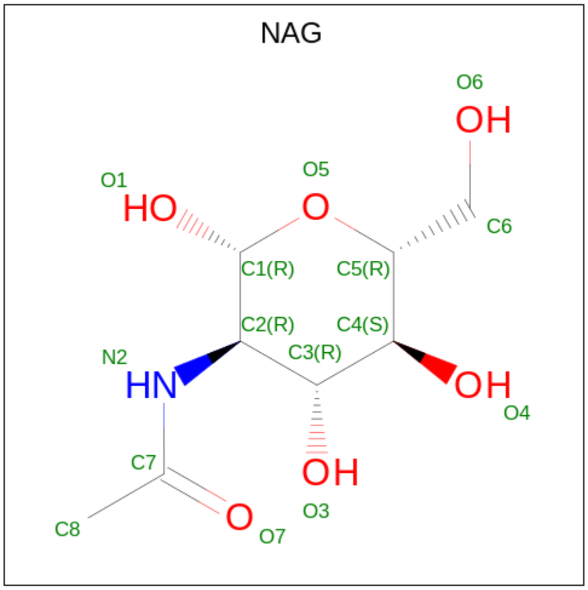
- Molecule 3 is a protein called P36-5D2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		
3	g	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		
3	L	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0

Continued on next page...

Continued from previous page...

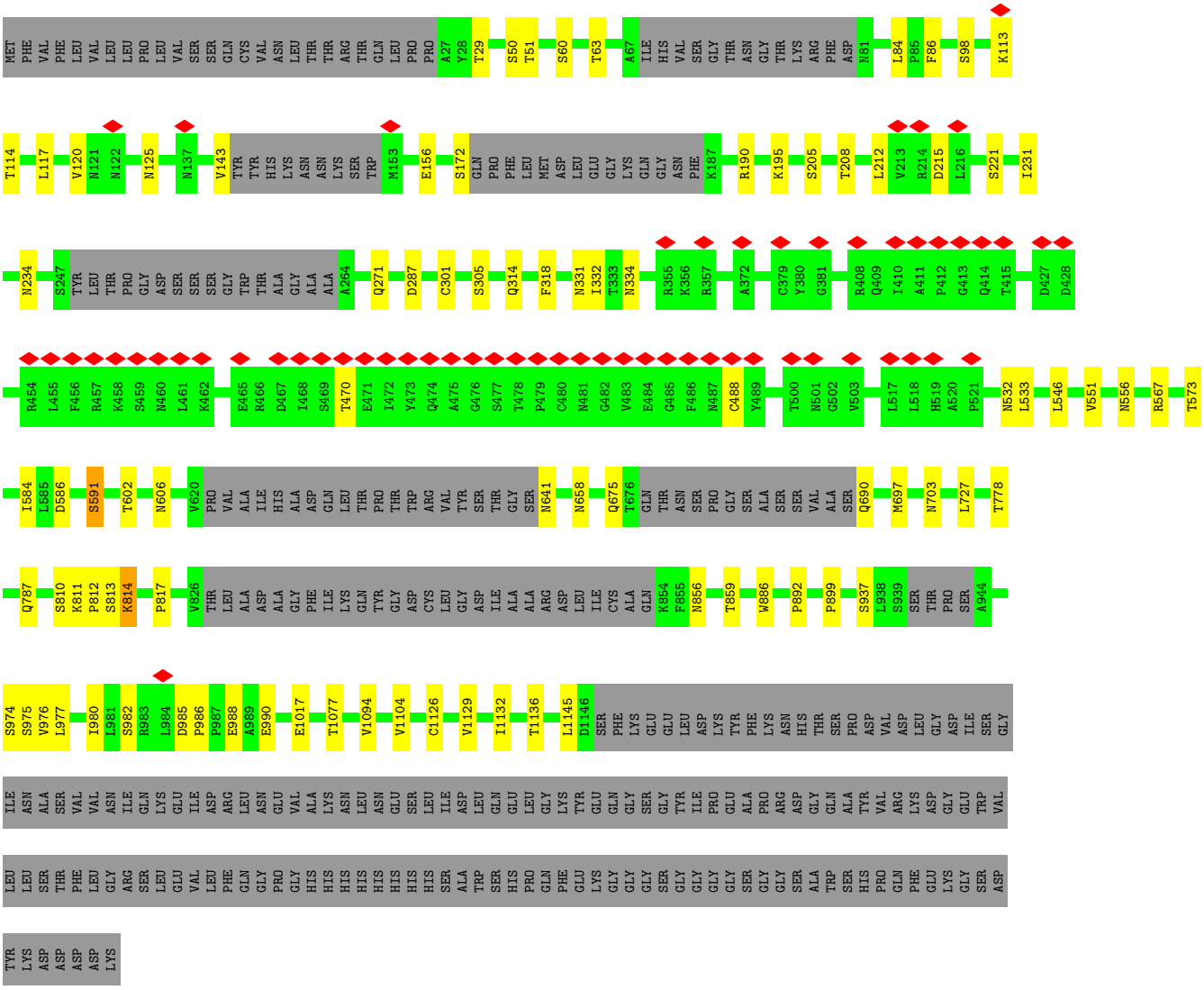
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	B	1	Total C N O 126 72 9 45	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0
5	C	1	Total C N O 154 88 11 55	0

3 Residue-property plots (i)

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

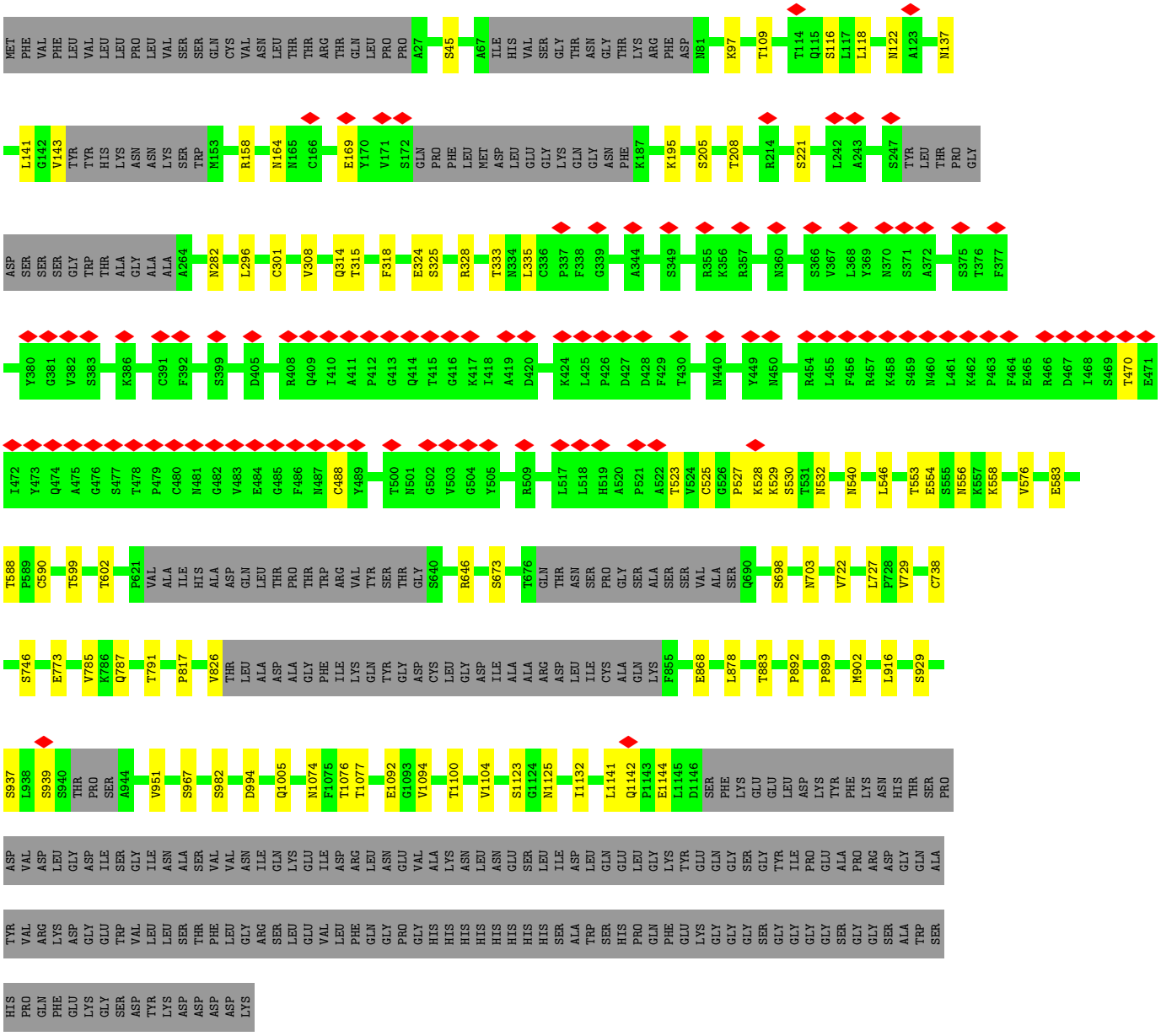
• Molecule 1: Spike glycoprotein

Chain A:



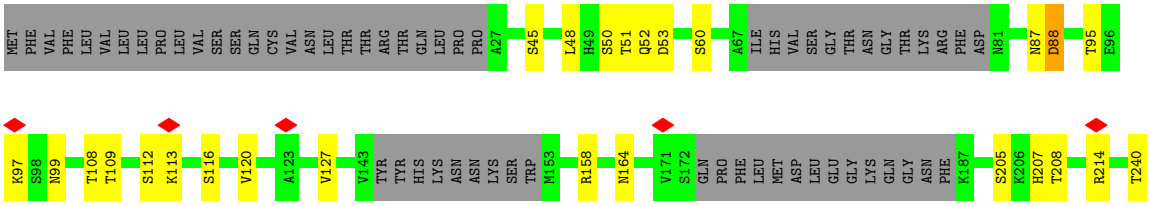
• Molecule 1: Spike glycoprotein

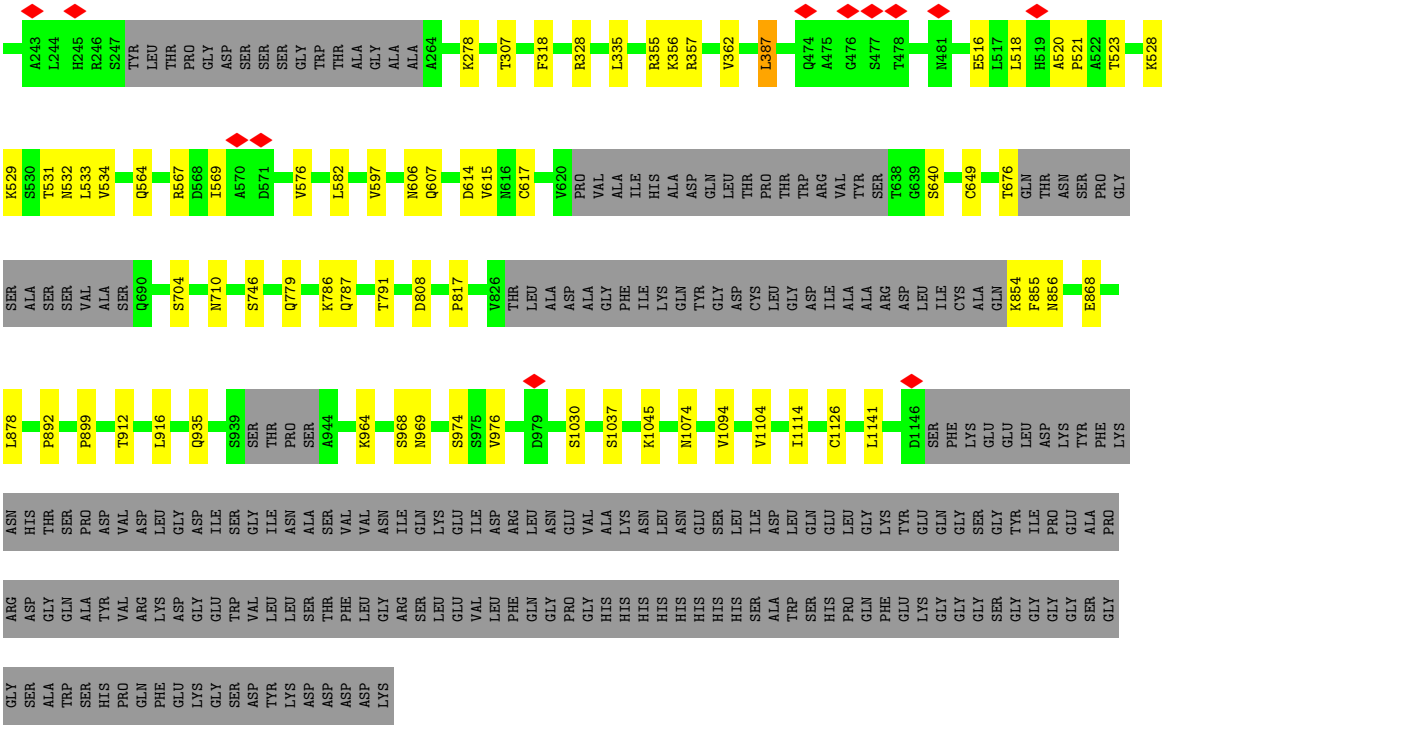
Chain B:



• Molecule 1: Spike glycoprotein

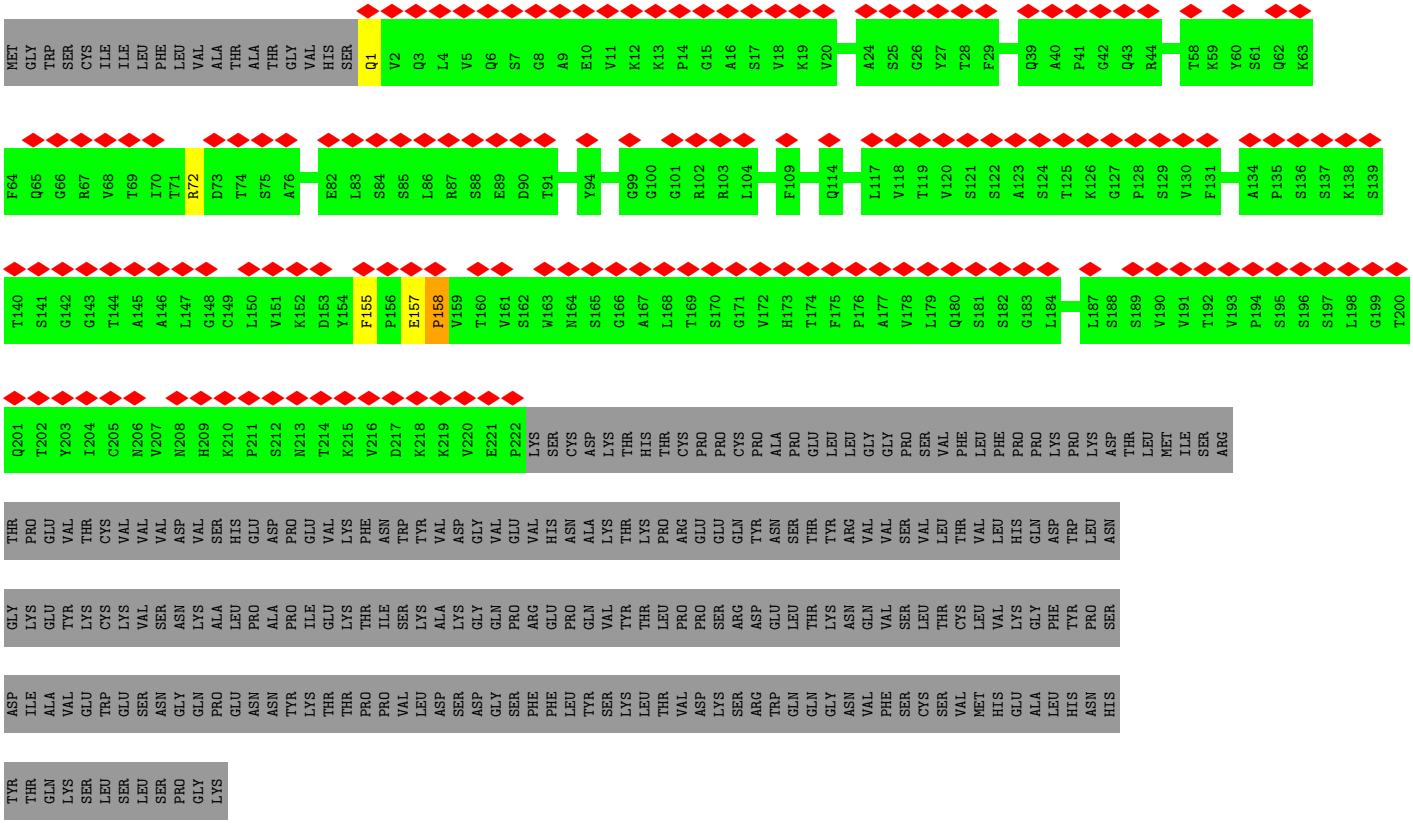
Chain C:





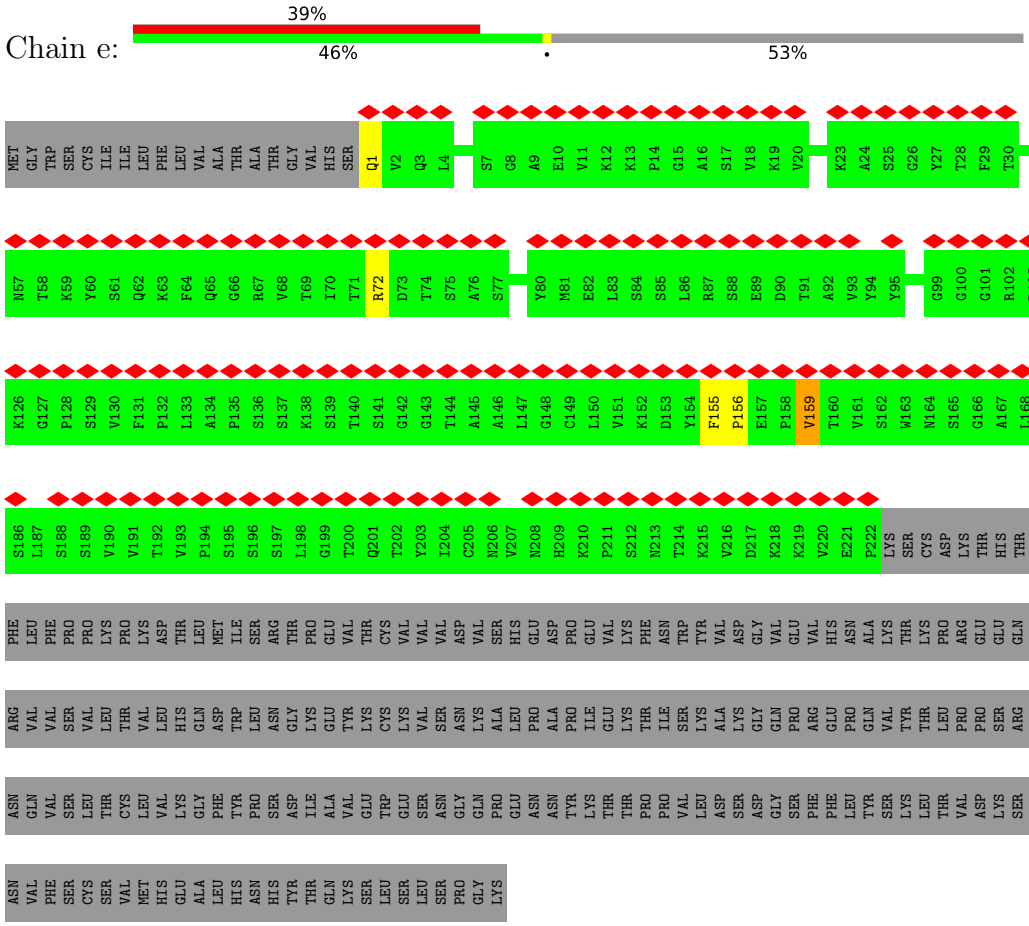
• Molecule 2: P36-5D2 heavy chain

Chain H:



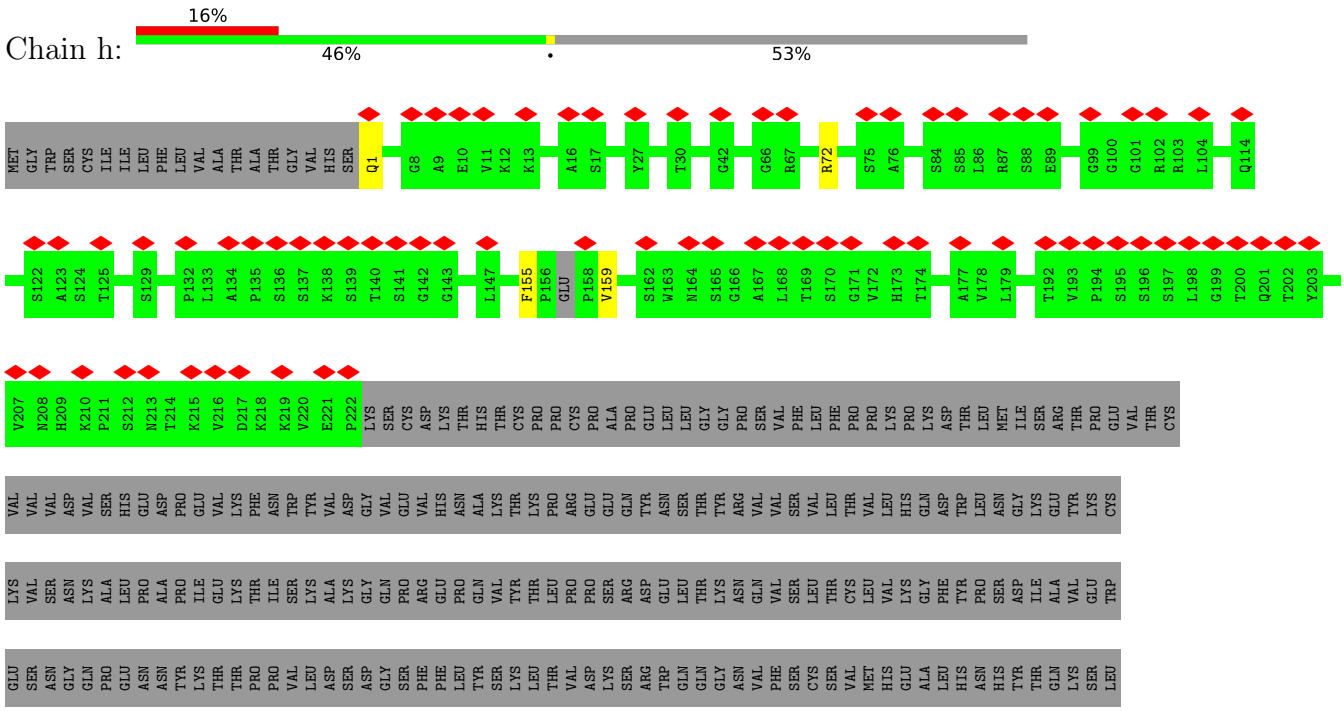
• Molecule 2: P36-5D2 heavy chain

Chain e:



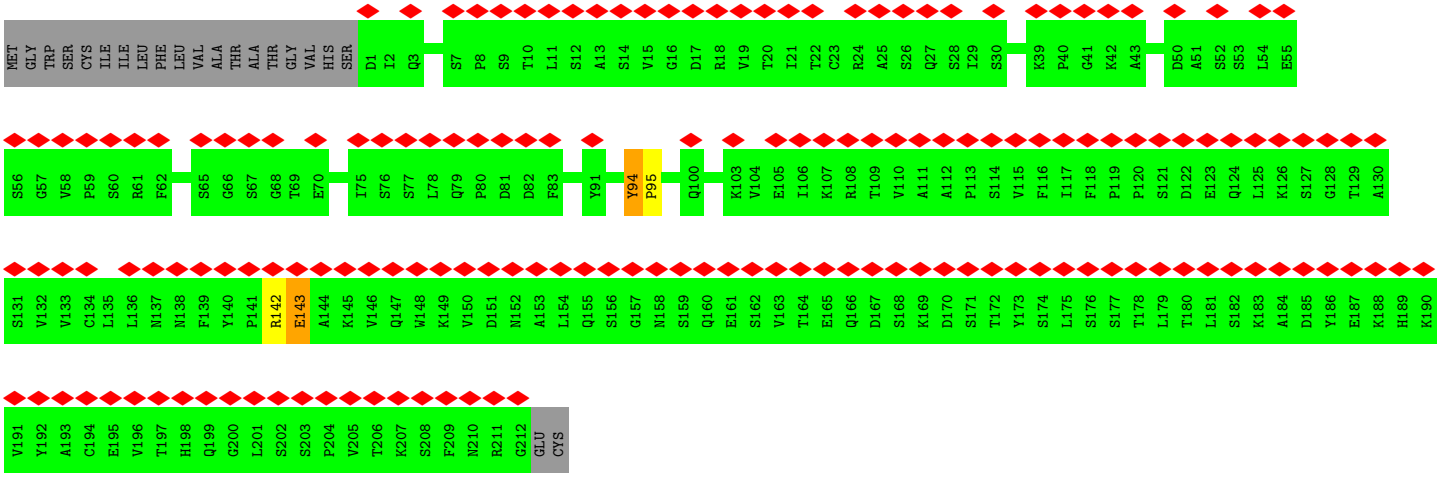
• Molecule 2: P36-5D2 heavy chain

Chain h:



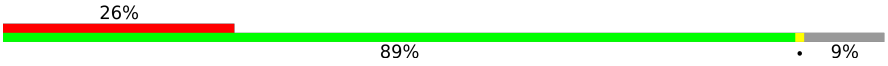
• Molecule 3: P36-5D2 light chain

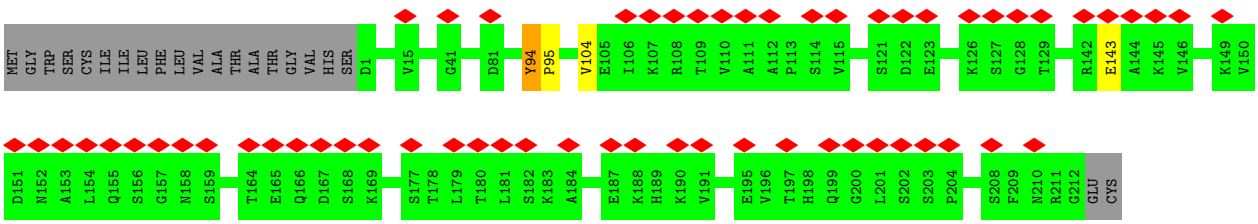
Chain d:



• Molecule 3: P36-5D2 light chain

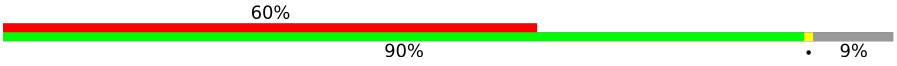
Chain g:

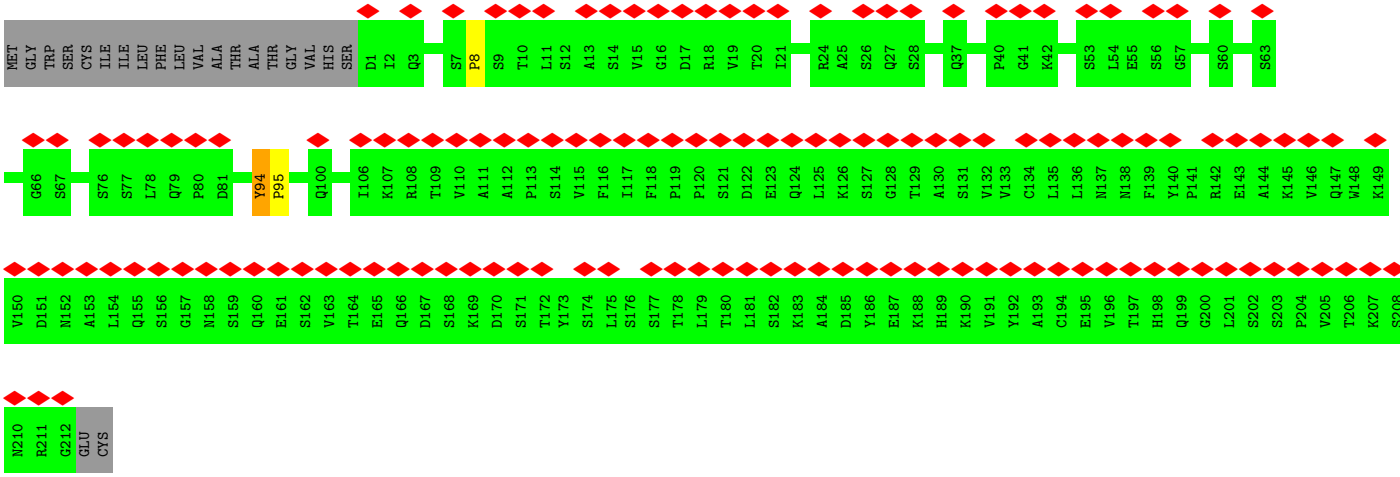




• Molecule 3: P36-5D2 light chain

Chain L:





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

Chain E:

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

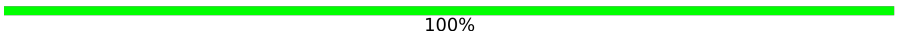
Chain I:

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

Chain J:

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

Chain K:

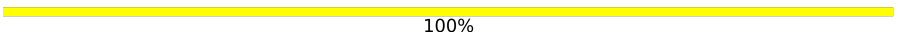


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

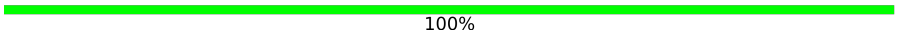
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



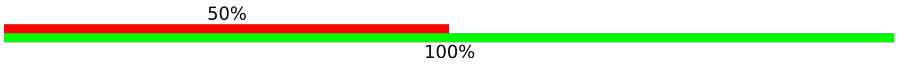
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain Q:



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

Chain R:

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

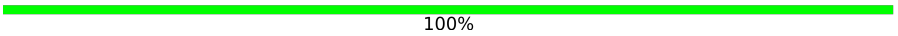
Chain S:

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

Chain T:

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

Chain U:



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

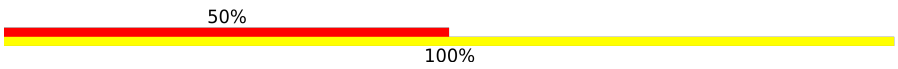
Chain X:

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

Chain Y:

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

Chain Z:



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

Chain a:

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

Chain b:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0077	Depositor
Map size (Å)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9700001, 0.9700001, 0.9700001	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	0.53	0/8030	0.59	3/10925 (0.0%)
1	B	0.53	0/8041	0.58	3/10942 (0.0%)
1	C	0.53	0/8043	0.58	3/10944 (0.0%)
2	H	0.45	0/1711	0.61	1/2328 (0.0%)
2	e	0.45	0/1705	0.58	0/2318
2	h	0.44	0/1701	0.58	0/2312
3	L	0.48	0/1673	0.57	1/2274 (0.0%)
3	d	0.48	0/1673	0.54	0/2274
3	g	0.47	0/1673	0.54	0/2274
All	All	0.51	0/34250	0.58	11/46591 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1
3	d	0	1
3	g	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	8	PRO	CA-N-CD	-9.23	98.58	111.50
1	A	899	PRO	CA-N-CD	-8.73	99.28	111.50
2	H	158	PRO	CA-N-CD	-8.70	99.32	111.50
1	C	899	PRO	CA-N-CD	-8.58	99.49	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	899	PRO	CA-N-CD	-8.56	99.51	111.50
1	C	817	PRO	CA-N-CD	-8.47	99.64	111.50
1	B	817	PRO	CA-N-CD	-8.47	99.64	111.50
1	A	817	PRO	CA-N-CD	-8.43	99.70	111.50
1	B	892	PRO	CA-N-CD	-8.32	99.85	111.50
1	C	892	PRO	CA-N-CD	-8.28	99.91	111.50
1	A	892	PRO	CA-N-CD	-8.27	99.93	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	94	TYR	Peptide
3	d	94	TYR	Peptide
3	g	94	TYR	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	986/1298 (76%)	898 (91%)	81 (8%)	7 (1%)	22	59
1	B	988/1298 (76%)	894 (90%)	91 (9%)	3 (0%)	41	74
1	C	989/1298 (76%)	897 (91%)	87 (9%)	5 (0%)	29	66
2	H	220/471 (47%)	186 (84%)	31 (14%)	3 (1%)	11	45
2	e	220/471 (47%)	186 (84%)	31 (14%)	3 (1%)	11	45
2	h	217/471 (46%)	186 (86%)	30 (14%)	1 (0%)	29	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	210/233 (90%)	195 (93%)	13 (6%)	2 (1%)	15 52
3	d	210/233 (90%)	193 (92%)	13 (6%)	4 (2%)	8 40
3	g	210/233 (90%)	196 (93%)	12 (6%)	2 (1%)	15 52
All	All	4250/6006 (71%)	3831 (90%)	389 (9%)	30 (1%)	26 59

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	814	LYS
1	A	986	PRO
1	C	528	LYS
2	H	155	PHE
2	H	157	GLU
2	H	158	PRO
3	d	142	ARG
3	d	143	GLU
2	e	159	VAL
2	h	155	PHE
1	A	591	SER
1	A	810	SER
1	B	527	PRO
2	e	155	PHE
1	B	324	GLU
1	B	325	SER
1	C	520	ALA
1	C	521	PRO
1	A	813	SER
1	C	387	LEU
1	A	812	PRO
1	C	88	ASP
1	A	811	LYS
3	d	95	PRO
2	e	156	PRO
3	g	95	PRO
3	L	95	PRO
3	g	94	TYR
3	L	94	TYR
3	d	94	TYR

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	881/1125 (78%)	801 (91%)	80 (9%)	9 37
1	B	883/1125 (78%)	797 (90%)	86 (10%)	8 33
1	C	882/1125 (78%)	794 (90%)	88 (10%)	7 32
2	H	184/412 (45%)	182 (99%)	2 (1%)	73 85
2	e	182/412 (44%)	179 (98%)	3 (2%)	62 79
2	h	183/412 (44%)	180 (98%)	3 (2%)	62 79
3	L	186/203 (92%)	186 (100%)	0	100 100
3	d	186/203 (92%)	185 (100%)	1 (0%)	88 94
3	g	186/203 (92%)	184 (99%)	2 (1%)	73 85
All	All	3753/5220 (72%)	3488 (93%)	265 (7%)	18 45

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	50	SER
1	A	51	THR
1	A	60	SER
1	A	63	THR
1	A	84	LEU
1	A	86	PHE
1	A	98	SER
1	A	113	LYS
1	A	114	THR
1	A	117	LEU
1	A	120	VAL
1	A	125	ASN
1	A	143	VAL
1	A	156	GLU
1	A	172	SER
1	A	190	ARG
1	A	195	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	205	SER
1	A	208	THR
1	A	212	LEU
1	A	215	ASP
1	A	221	SER
1	A	231	ILE
1	A	234	ASN
1	A	271	GLN
1	A	287	ASP
1	A	301	CYS
1	A	305	SER
1	A	314	GLN
1	A	318	PHE
1	A	331	ASN
1	A	332	ILE
1	A	334	ASN
1	A	470	THR
1	A	488	CYS
1	A	532	ASN
1	A	533	LEU
1	A	546	LEU
1	A	551	VAL
1	A	556	ASN
1	A	567	ARG
1	A	573	THR
1	A	584	ILE
1	A	586	ASP
1	A	591	SER
1	A	602	THR
1	A	606	ASN
1	A	641	ASN
1	A	658	ASN
1	A	675	GLN
1	A	690	GLN
1	A	697	MET
1	A	703	ASN
1	A	727	LEU
1	A	778	THR
1	A	787	GLN
1	A	814	LYS
1	A	856	ASN
1	A	859	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	886	TRP
1	A	937	SER
1	A	974	SER
1	A	975	SER
1	A	976	VAL
1	A	977	LEU
1	A	980	ILE
1	A	982	SER
1	A	985	ASP
1	A	988	GLU
1	A	990	GLU
1	A	1017	GLU
1	A	1077	THR
1	A	1094	VAL
1	A	1104	VAL
1	A	1126	CYS
1	A	1129	VAL
1	A	1132	ILE
1	A	1136	THR
1	A	1145	LEU
1	B	45	SER
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	314	GLN
1	B	315	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	318	PHE
1	B	328	ARG
1	B	333	THR
1	B	335	LEU
1	B	470	THR
1	B	488	CYS
1	B	523	THR
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	530	SER
1	B	532	ASN
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	576	VAL
1	B	583	GLU
1	B	588	THR
1	B	590	CYS
1	B	599	THR
1	B	602	THR
1	B	646	ARG
1	B	673	SER
1	B	698	SER
1	B	703	ASN
1	B	722	VAL
1	B	727	LEU
1	B	729	VAL
1	B	738	CYS
1	B	746	SER
1	B	773	GLU
1	B	785	VAL
1	B	787	GLN
1	B	791	THR
1	B	826	VAL
1	B	868	GLU
1	B	878	LEU
1	B	883	THR
1	B	902	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	916	LEU
1	B	929	SER
1	B	937	SER
1	B	939	SER
1	B	951	VAL
1	B	967	SER
1	B	982	SER
1	B	994	ASP
1	B	1005	GLN
1	B	1074	ASN
1	B	1076	THR
1	B	1077	THR
1	B	1092	GLU
1	B	1094	VAL
1	B	1100	THR
1	B	1104	VAL
1	B	1123	SER
1	B	1125	ASN
1	B	1132	ILE
1	B	1141	LEU
1	B	1142	GLN
1	B	1144	GLU
1	C	45	SER
1	C	48	LEU
1	C	50	SER
1	C	51	THR
1	C	52	GLN
1	C	53	ASP
1	C	60	SER
1	C	87	ASN
1	C	88	ASP
1	C	95	THR
1	C	97	LYS
1	C	99	ASN
1	C	108	THR
1	C	109	THR
1	C	112	SER
1	C	113	LYS
1	C	116	SER
1	C	120	VAL
1	C	127	VAL
1	C	158	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	164	ASN
1	C	205	SER
1	C	207	HIS
1	C	208	THR
1	C	214	ARG
1	C	240	THR
1	C	278	LYS
1	C	307	THR
1	C	318	PHE
1	C	328	ARG
1	C	335	LEU
1	C	355	ARG
1	C	356	LYS
1	C	357	ARG
1	C	362	VAL
1	C	387	LEU
1	C	516	GLU
1	C	518	LEU
1	C	523	THR
1	C	529	LYS
1	C	531	THR
1	C	532	ASN
1	C	533	LEU
1	C	534	VAL
1	C	564	GLN
1	C	567	ARG
1	C	569	ILE
1	C	576	VAL
1	C	582	LEU
1	C	597	VAL
1	C	606	ASN
1	C	607	GLN
1	C	614	ASP
1	C	615	VAL
1	C	617	CYS
1	C	640	SER
1	C	649	CYS
1	C	676	THR
1	C	704	SER
1	C	710	ASN
1	C	746	SER
1	C	779	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	786	LYS
1	C	787	GLN
1	C	791	THR
1	C	808	ASP
1	C	854	LYS
1	C	855	PHE
1	C	856	ASN
1	C	868	GLU
1	C	878	LEU
1	C	912	THR
1	C	916	LEU
1	C	935	GLN
1	C	964	LYS
1	C	968	SER
1	C	969	ASN
1	C	974	SER
1	C	976	VAL
1	C	1030	SER
1	C	1037	SER
1	C	1045	LYS
1	C	1074	ASN
1	C	1094	VAL
1	C	1104	VAL
1	C	1114	ILE
1	C	1126	CYS
1	C	1141	LEU
2	H	1	GLN
2	H	72	ARG
3	d	143	GLU
2	e	1	GLN
2	e	72	ARG
2	e	159	VAL
3	g	104	VAL
3	g	143	GLU
2	h	1	GLN
2	h	72	ARG
2	h	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	188	ASN
1	A	207	HIS
1	A	271	GLN
1	A	314	GLN
1	A	321	GLN
1	A	331	ASN
1	A	334	ASN
1	A	556	ASN
1	A	606	ASN
1	A	641	ASN
1	A	675	GLN
1	A	690	GLN
1	A	703	ASN
1	A	784	GLN
1	A	804	GLN
1	A	901	GLN
1	A	907	ASN
1	A	914	ASN
1	A	926	GLN
1	A	935	GLN
1	A	992	GLN
1	A	1010	GLN
1	A	1071	GLN
1	A	1101	HIS
1	A	1106	GLN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	540	ASN
1	B	556	ASN
1	B	644	GLN
1	B	690	GLN
1	B	703	ASN
1	B	762	GLN
1	B	787	GLN
1	B	856	ASN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	926	GLN
1	B	955	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	969	ASN
1	B	992	GLN
1	B	1125	ASN
1	B	1142	GLN
1	C	115	GLN
1	C	134	GLN
1	C	164	ASN
1	C	188	ASN
1	C	245	HIS
1	C	532	ASN
1	C	540	ASN
1	C	563	GLN
1	C	606	ASN
1	C	655	HIS
1	C	710	ASN
1	C	804	GLN
1	C	901	GLN
1	C	914	ASN
1	C	919	ASN
1	C	920	GLN
1	C	926	GLN
1	C	992	GLN
1	C	1054	GLN
2	H	1	GLN
2	H	57	ASN
3	d	124	GLN
2	e	1	GLN
2	e	57	ASN
3	g	92	ASN
3	g	124	GLN
2	h	1	GLN
2	h	57	ASN
3	L	92	ASN
3	L	124	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1	4	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	I	1	1,4	14,14,15	0.22	0	17,19,21	1.35	1 (5%)
4	NAG	I	2	4	14,14,15	0.17	0	17,19,21	0.49	0
4	NAG	J	1	1,4	14,14,15	0.51	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	K	1	1,4	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	K	2	4	14,14,15	0.23	0	17,19,21	0.73	0
4	NAG	M	1	1,4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.66	1 (7%)	17,19,21	0.44	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	1.36	2 (11%)
4	NAG	O	1	1,4	14,14,15	0.43	0	17,19,21	0.43	0
4	NAG	O	2	4	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	Q	1	1,4	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	Q	2	4	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	R	1	1,4	14,14,15	0.35	0	17,19,21	1.11	1 (5%)
4	NAG	R	2	4	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	S	1	1,4	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
4	NAG	S	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	T	1	1,4	14,14,15	0.75	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.31	0	17,19,21	0.68	0
4	NAG	U	1	1,4	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	X	1	1,4	14,14,15	0.33	0	17,19,21	0.64	1 (5%)
4	NAG	X	2	4	14,14,15	0.50	0	17,19,21	0.47	0
4	NAG	Y	1	1,4	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	Y	2	4	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.68	1 (7%)	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	Z	2	4	14,14,15	0.40	0	17,19,21	1.39	3 (17%)
4	NAG	a	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	a	2	4	14,14,15	0.32	0	17,19,21	0.64	0
4	NAG	b	1	1,4	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
4	NAG	b	2	4	14,14,15	0.15	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	5/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	3/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	3/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	5/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	3/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-2.70	1.39	1.43
4	a	1	NAG	O5-C1	-2.54	1.39	1.43
4	Z	1	NAG	O5-C1	-2.29	1.40	1.43
4	N	1	NAG	O5-C1	-2.20	1.40	1.43
4	E	1	NAG	O5-C1	-2.07	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	C2-N2-C7	4.66	129.54	122.90
4	N	2	NAG	C2-N2-C7	4.39	129.15	122.90
4	Y	2	NAG	C2-N2-C7	4.34	129.08	122.90
4	M	2	NAG	C2-N2-C7	4.34	129.08	122.90
4	Z	2	NAG	C2-N2-C7	4.32	129.06	122.90
4	R	1	NAG	C1-O5-C5	3.22	116.55	112.19
4	Z	2	NAG	C1-C2-N2	2.41	114.61	110.49
4	T	1	NAG	O4-C4-C3	-2.38	104.84	110.35
4	S	1	NAG	C1-O5-C5	2.29	115.29	112.19
4	J	1	NAG	C1-O5-C5	2.27	115.27	112.19
4	Y	2	NAG	C1-C2-N2	2.26	114.35	110.49
4	N	2	NAG	C1-C2-N2	2.25	114.32	110.49
4	b	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	Z	2	NAG	C1-O5-C5	2.08	115.01	112.19
4	X	1	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	U	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

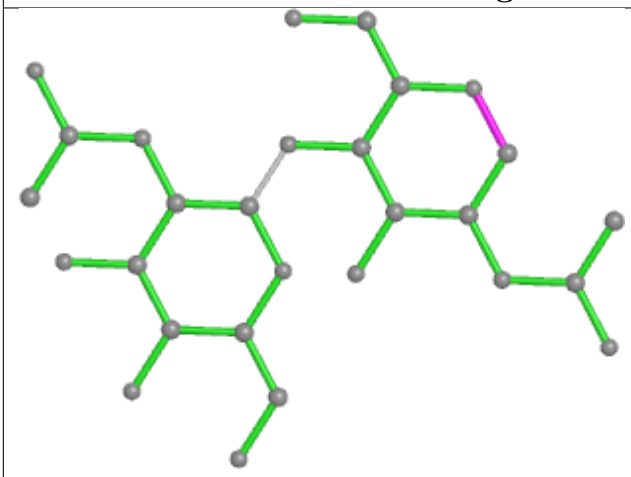
Mol	Chain	Res	Type	Atoms
4	b	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	S	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	Z	2	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7

There are no ring outliers.

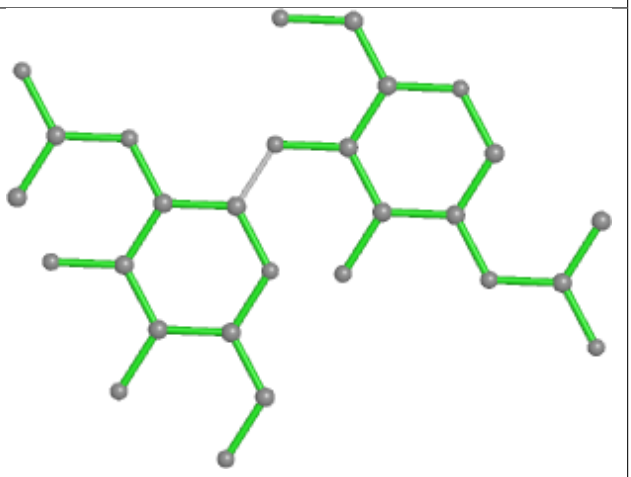
No monomer is involved in short contacts.

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

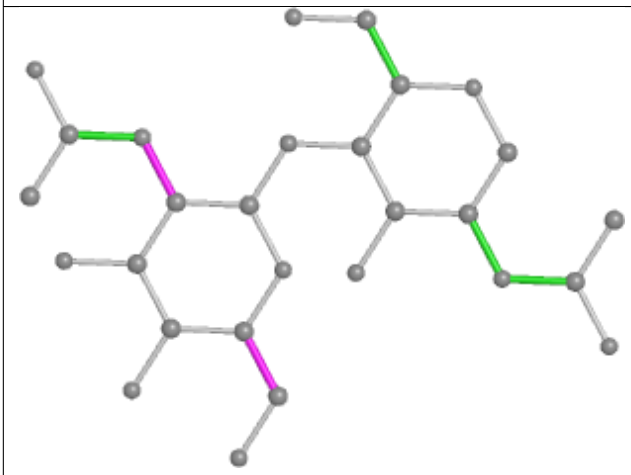
Oligosaccharide Chain E



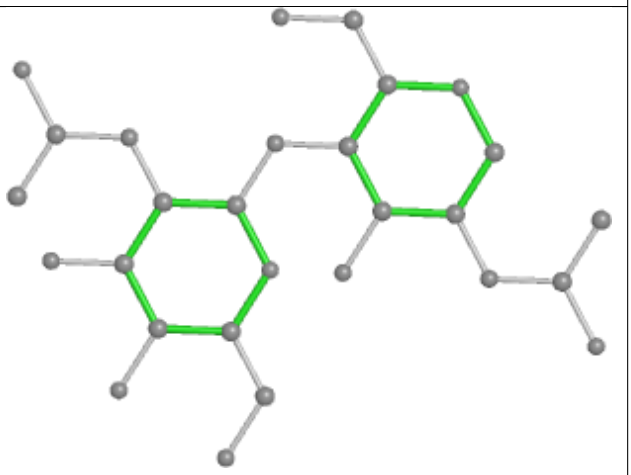
Bond lengths



Bond angles

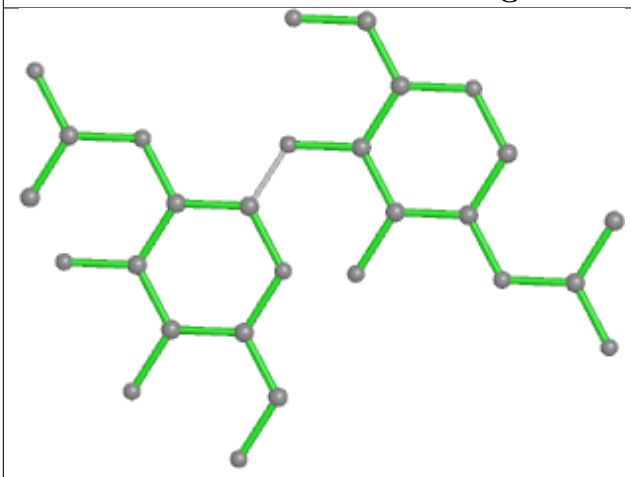


Torsions

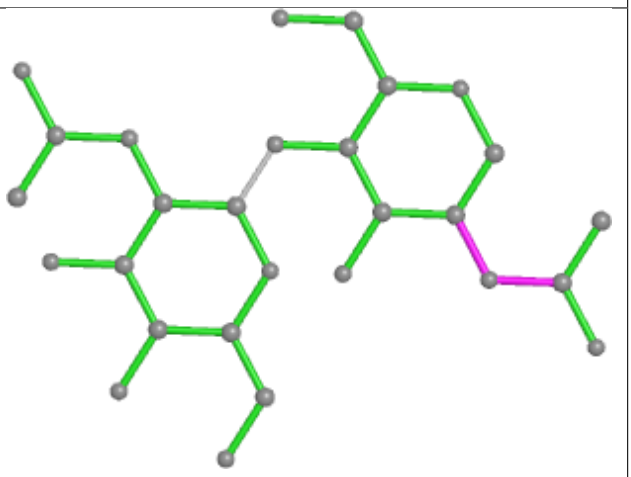


Rings

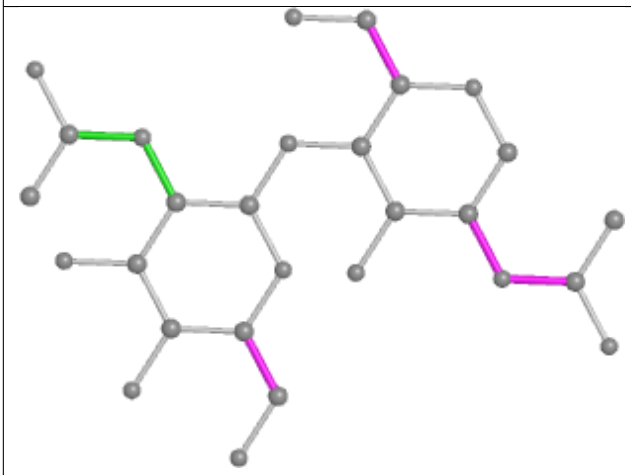
Oligosaccharide Chain I



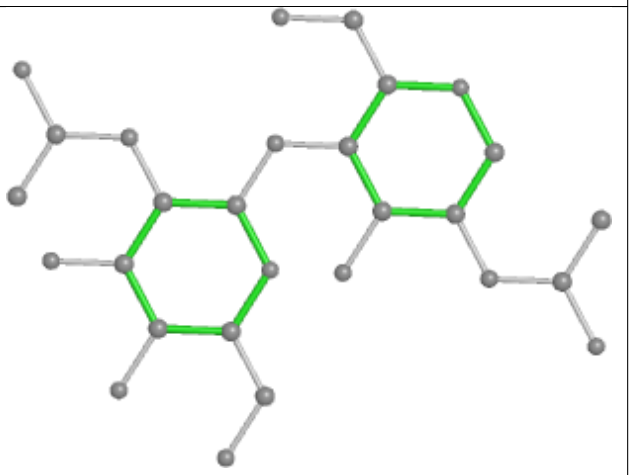
Bond lengths



Bond angles

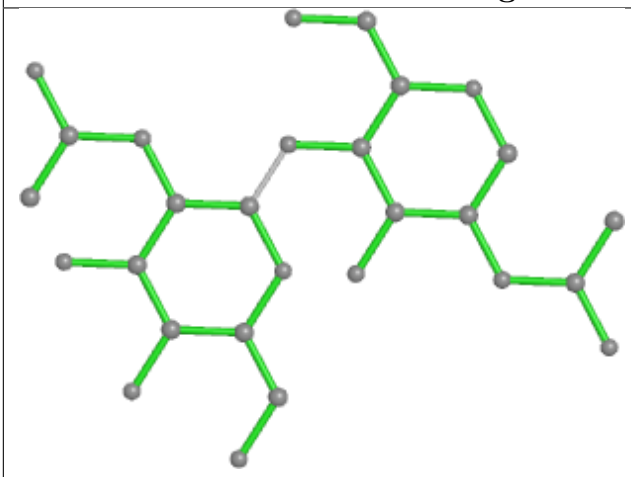


Torsions

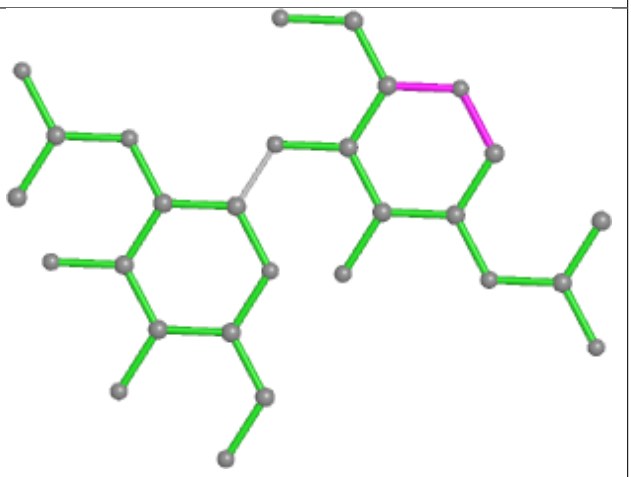


Rings

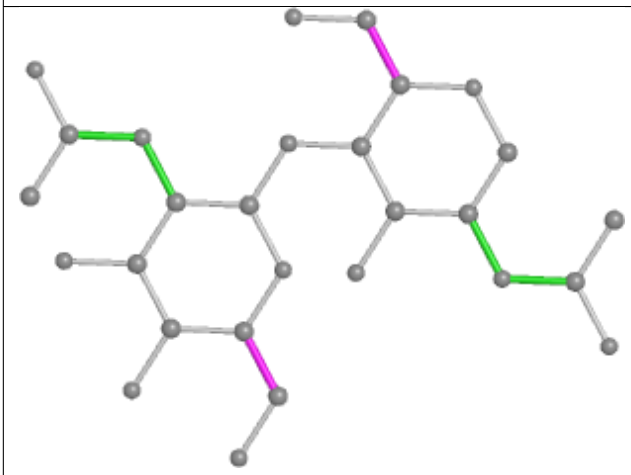
Oligosaccharide Chain J



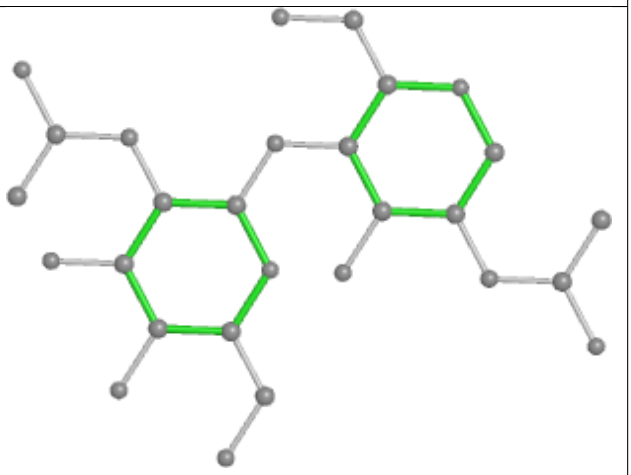
Bond lengths



Bond angles

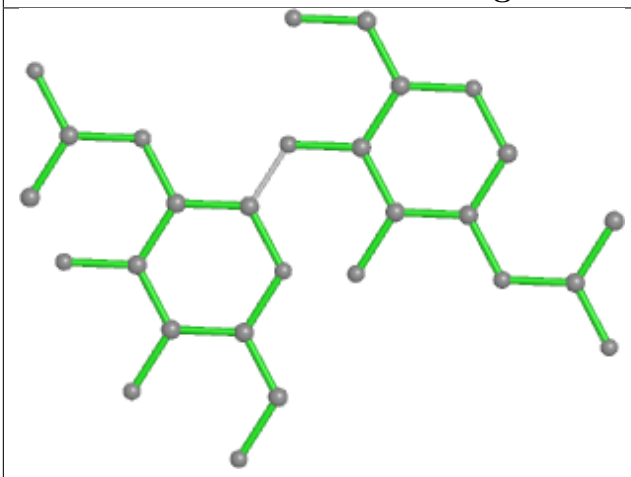


Torsions

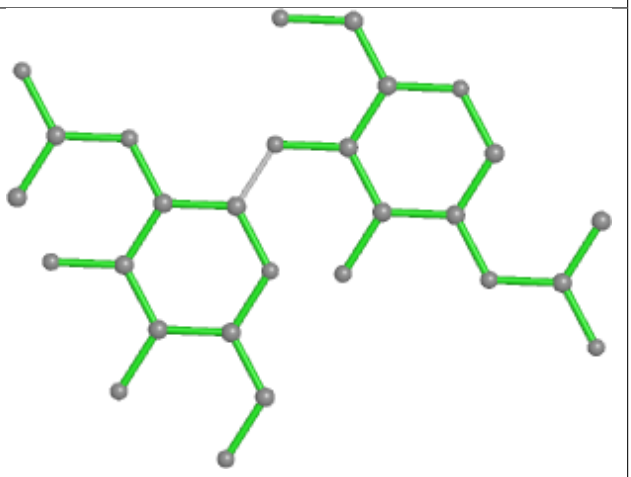


Rings

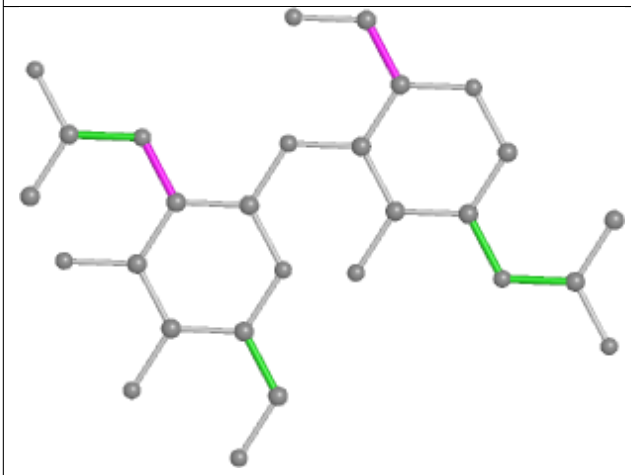
Oligosaccharide Chain K



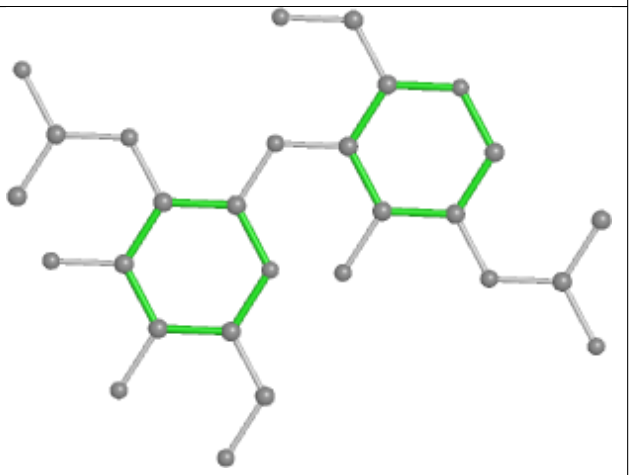
Bond lengths



Bond angles

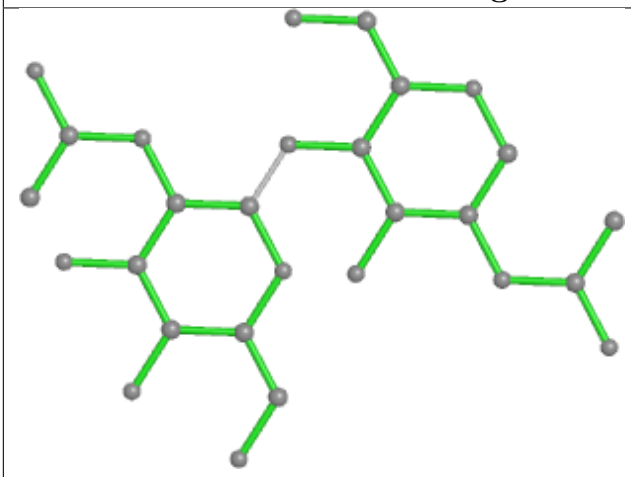


Torsions

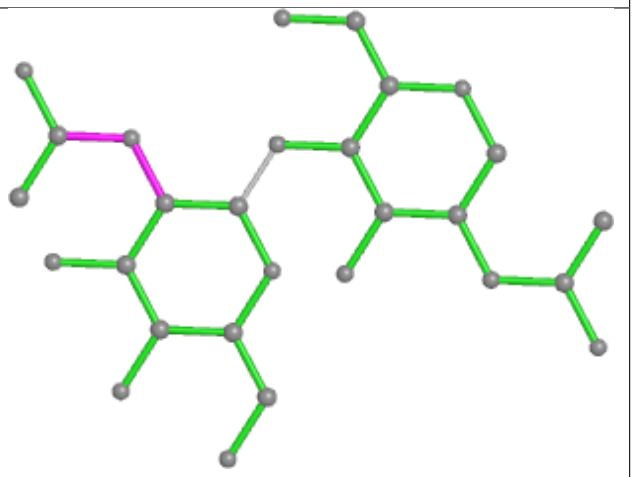


Rings

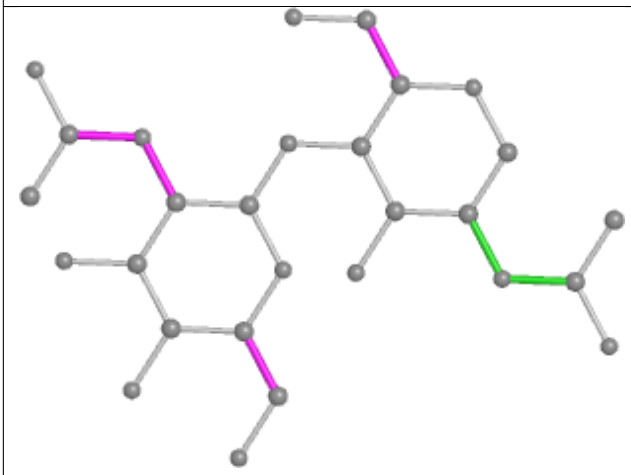
Oligosaccharide Chain M



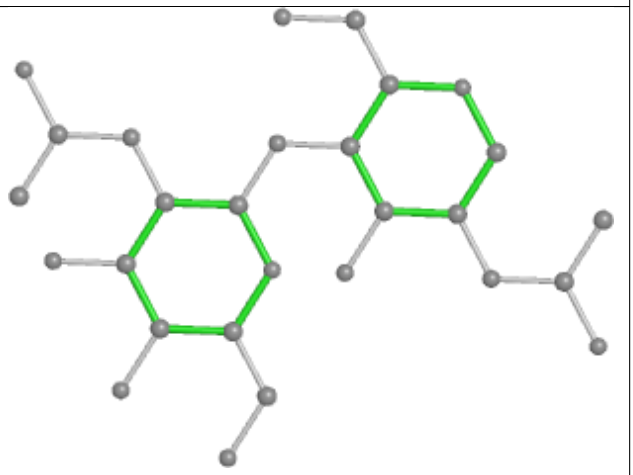
Bond lengths



Bond angles

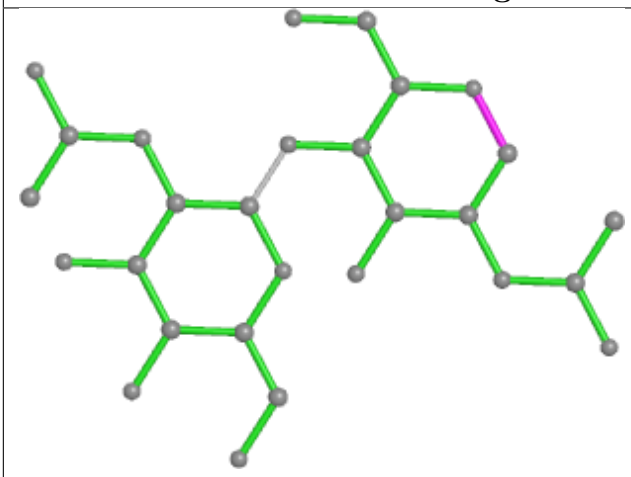


Torsions

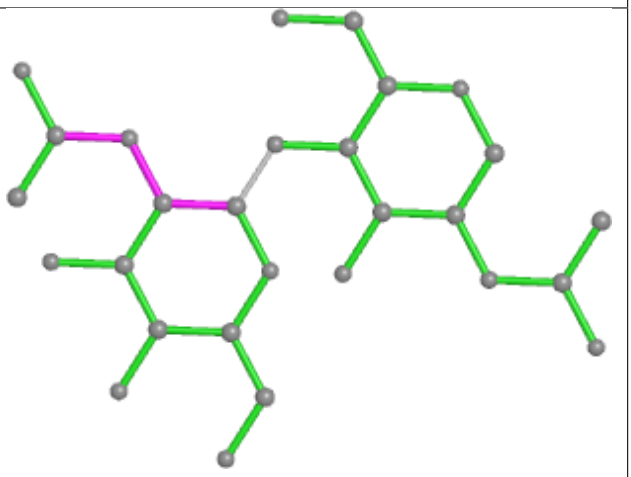


Rings

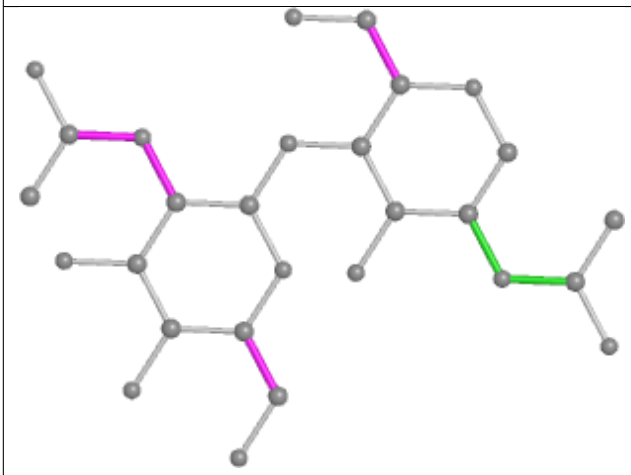
Oligosaccharide Chain N



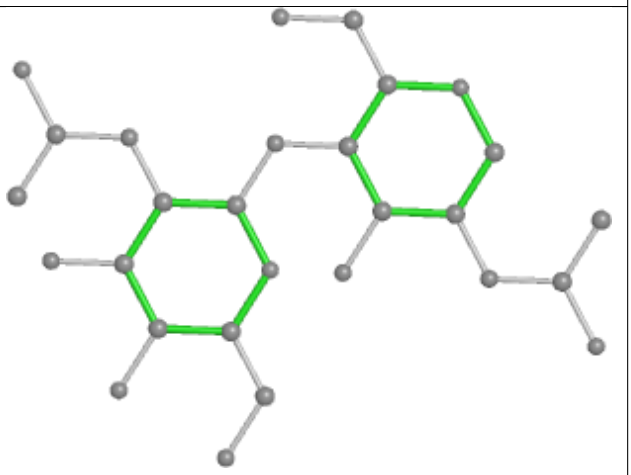
Bond lengths



Bond angles

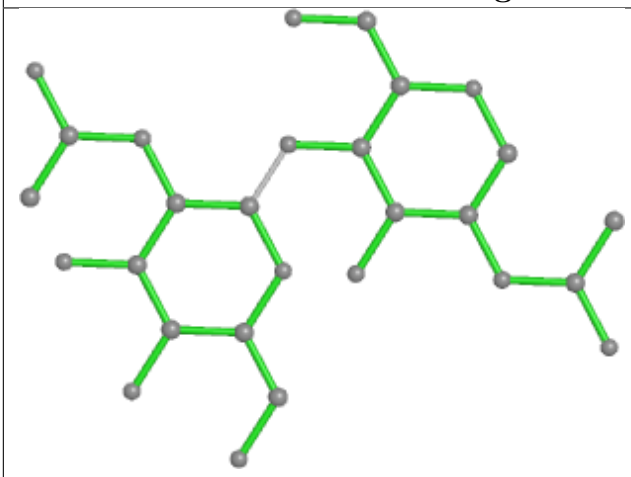


Torsions

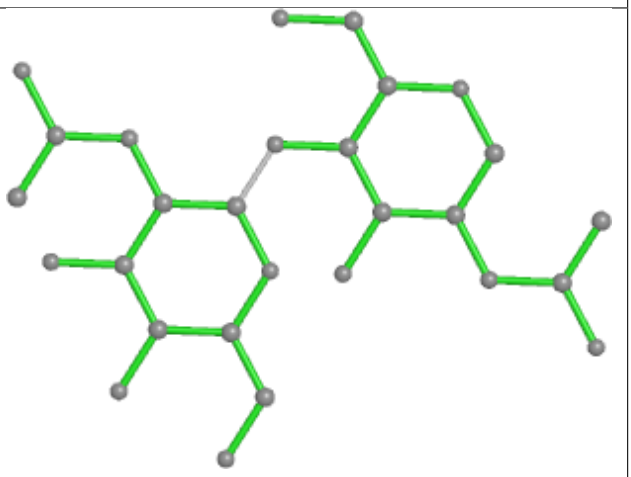


Rings

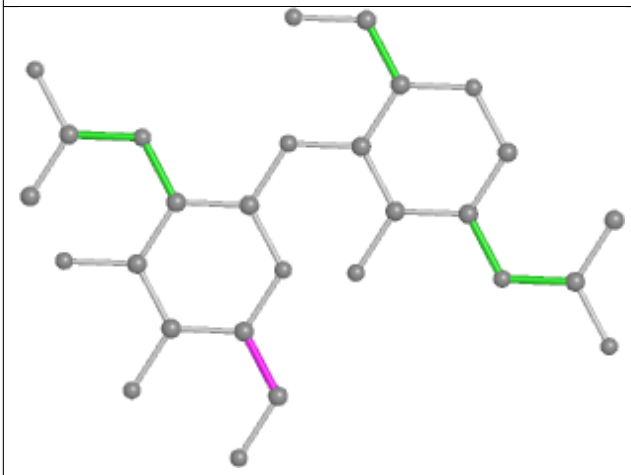
Oligosaccharide Chain O



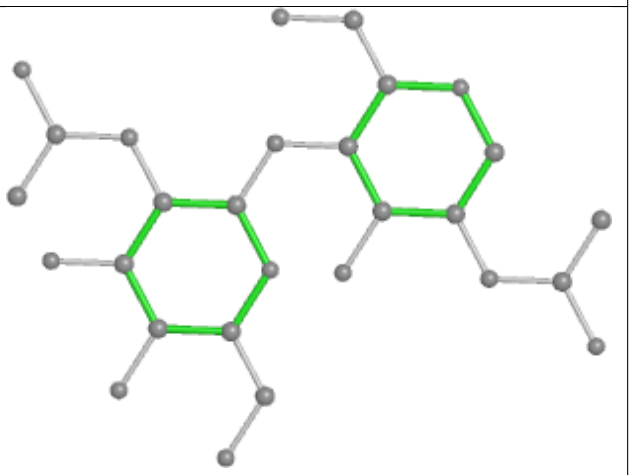
Bond lengths



Bond angles

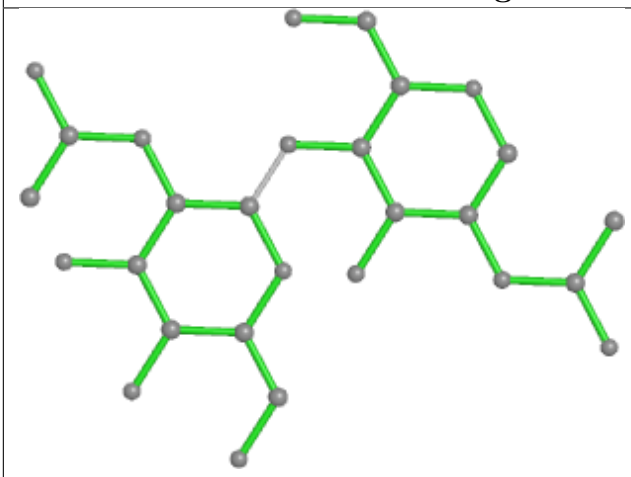


Torsions

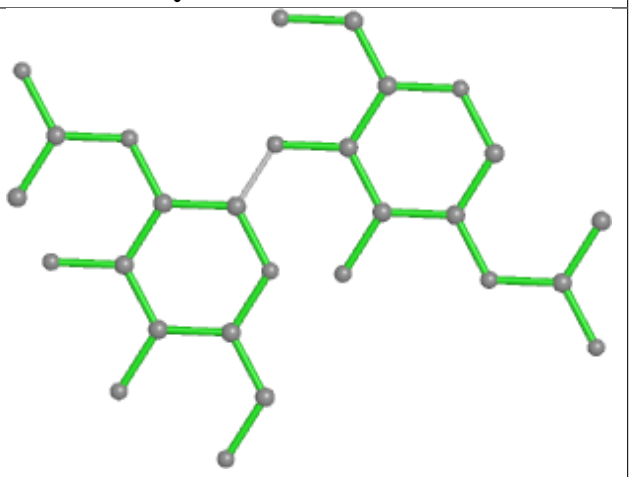


Rings

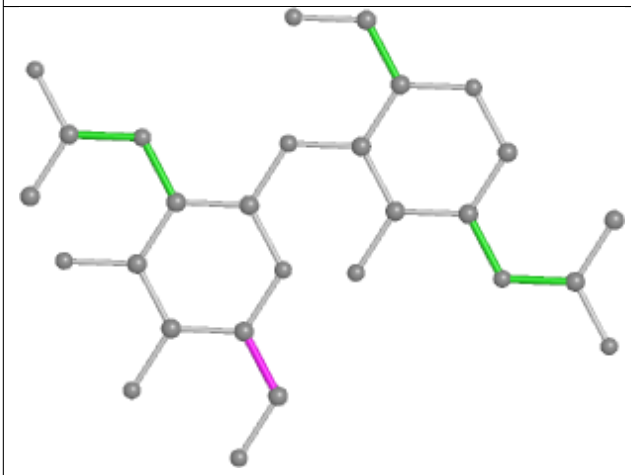
Oligosaccharide Chain Q



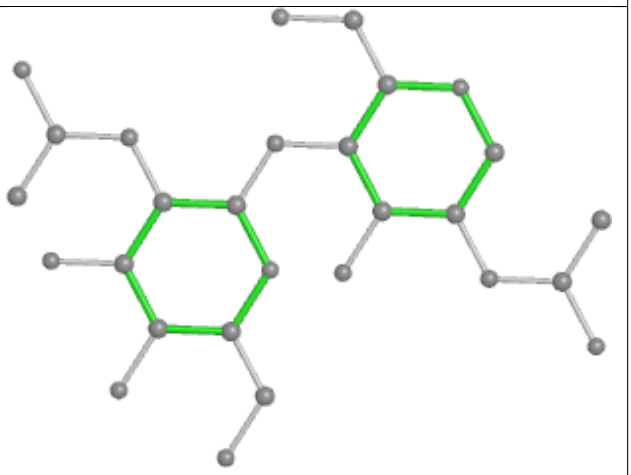
Bond lengths



Bond angles

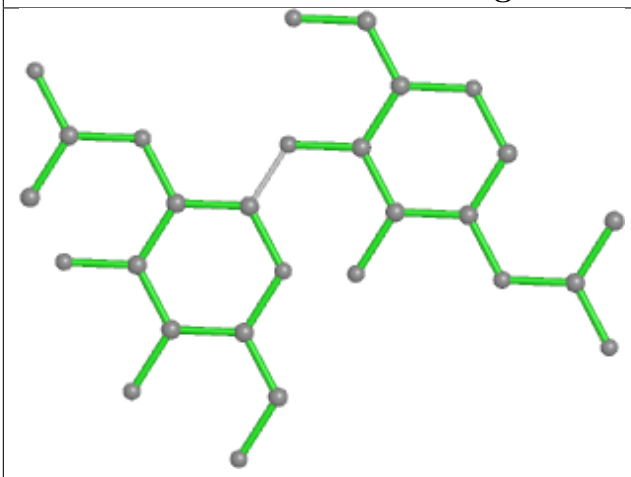


Torsions

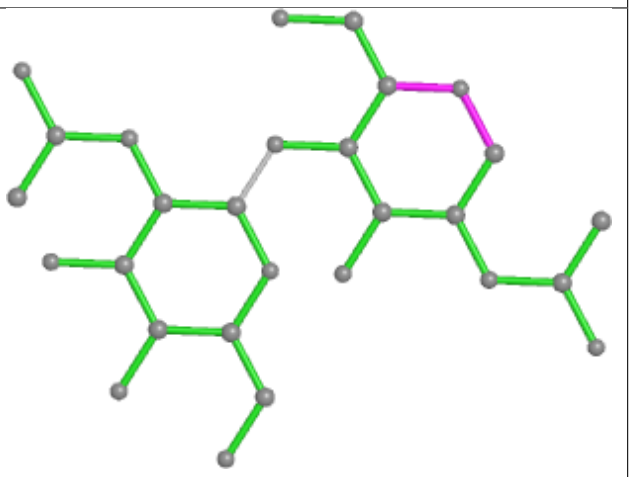


Rings

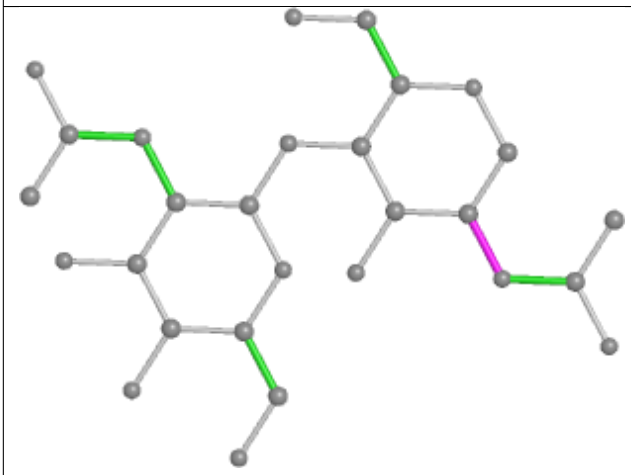
Oligosaccharide Chain R



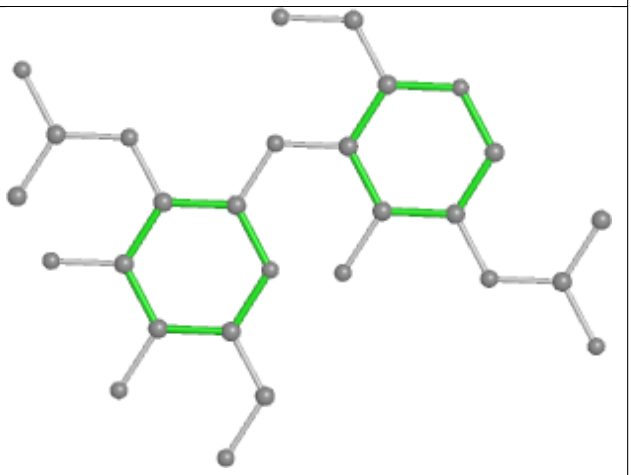
Bond lengths



Bond angles

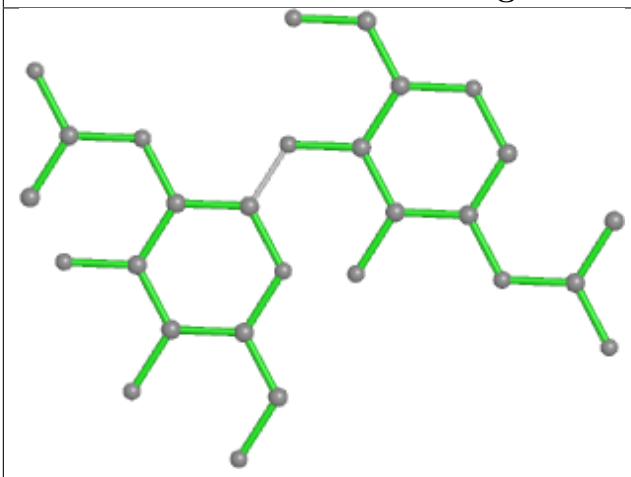


Torsions

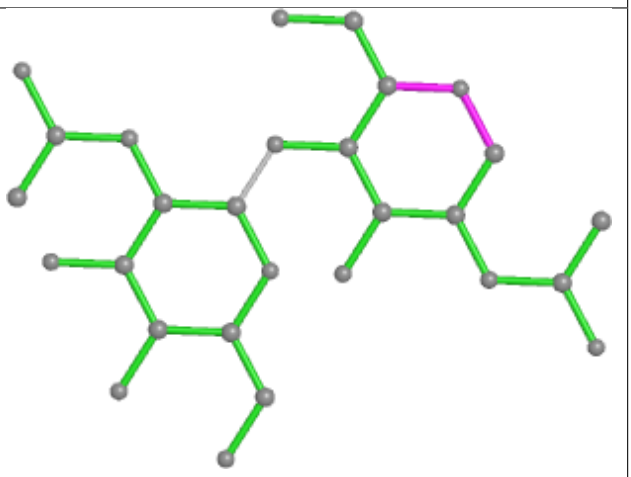


Rings

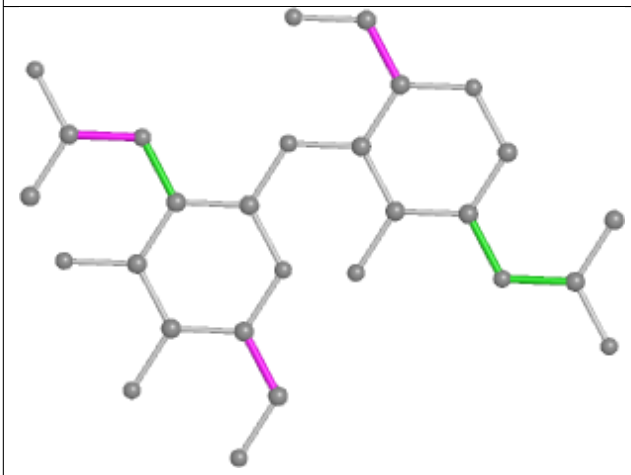
Oligosaccharide Chain S



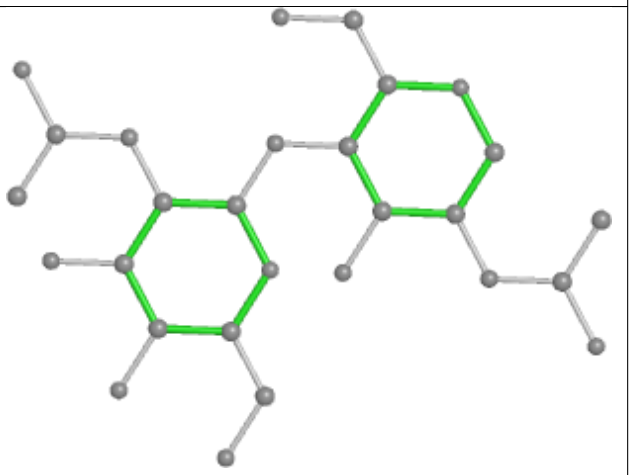
Bond lengths



Bond angles

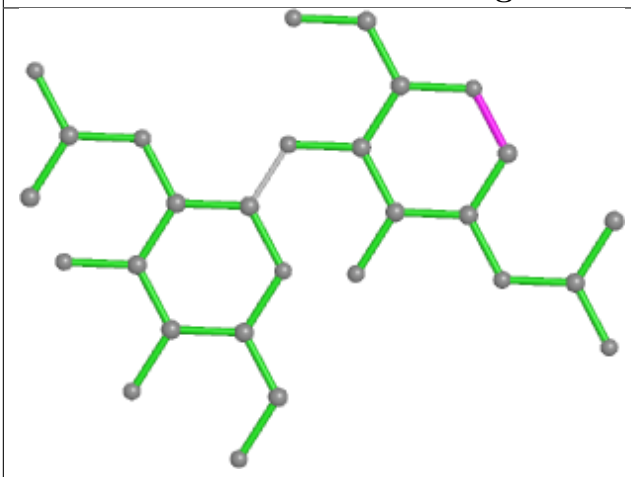


Torsions

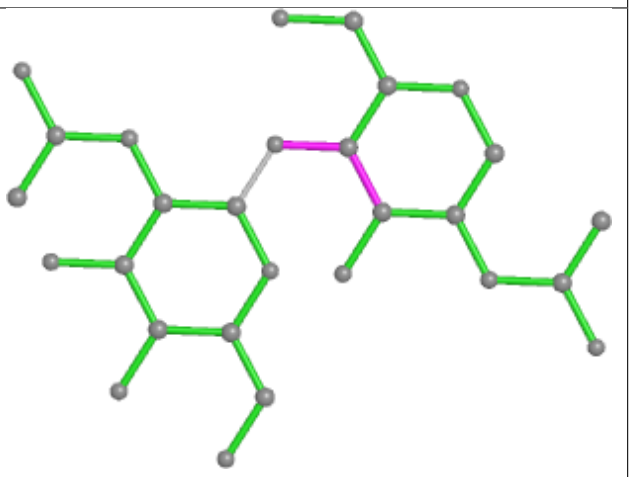


Rings

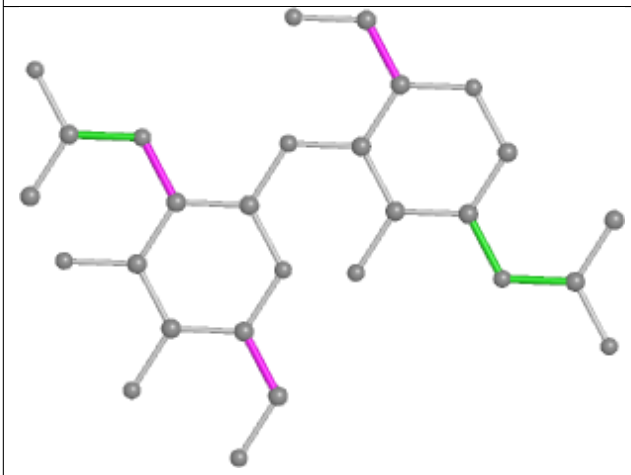
Oligosaccharide Chain T



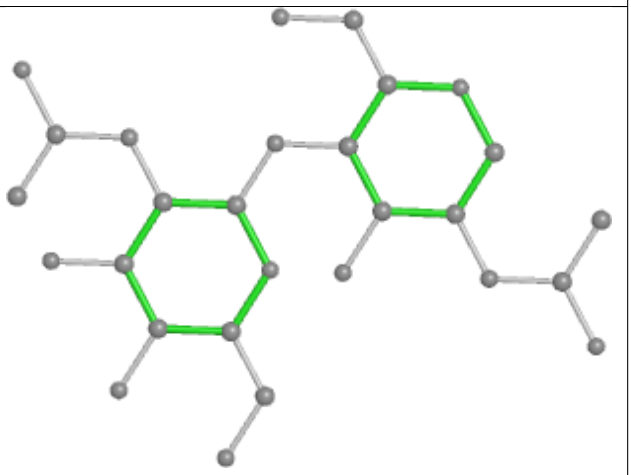
Bond lengths



Bond angles

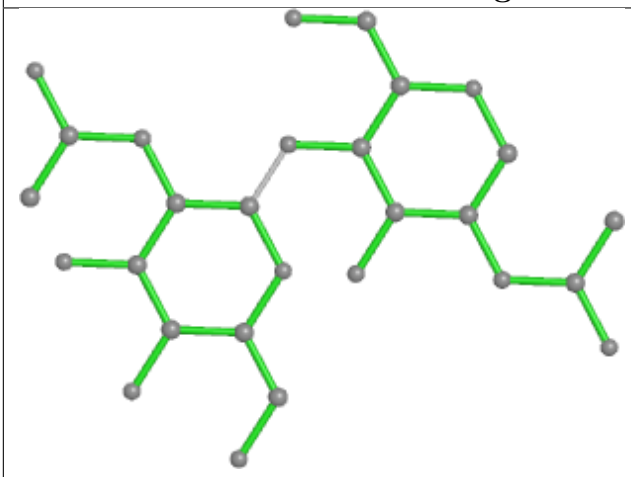


Torsions

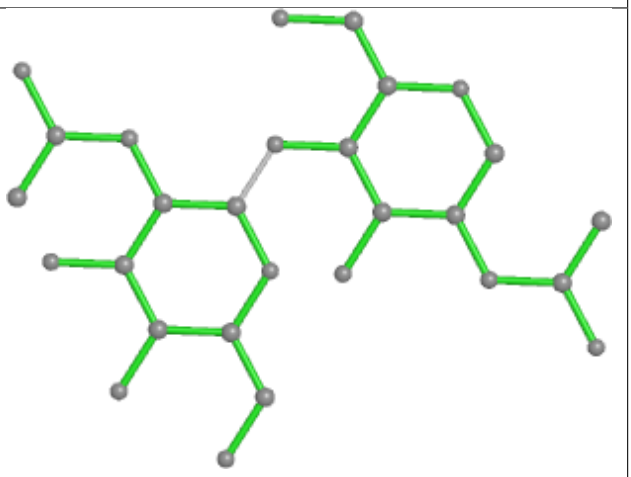


Rings

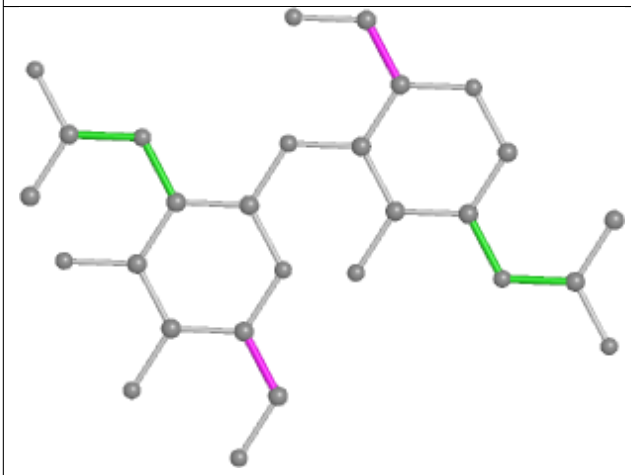
Oligosaccharide Chain U



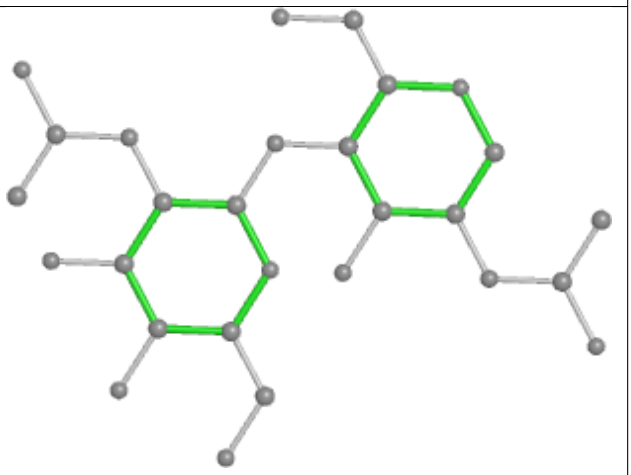
Bond lengths



Bond angles

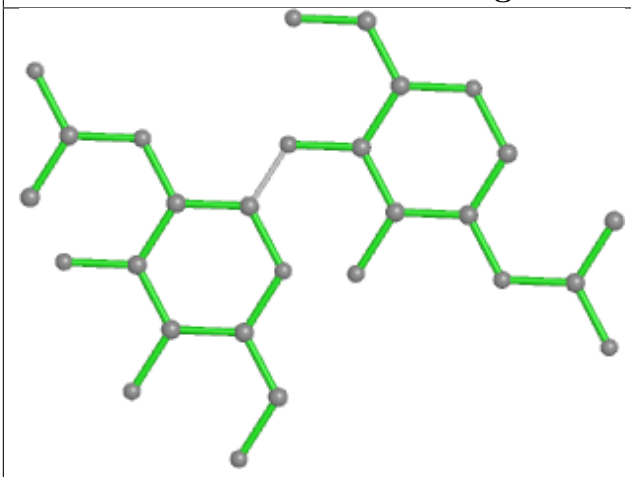


Torsions

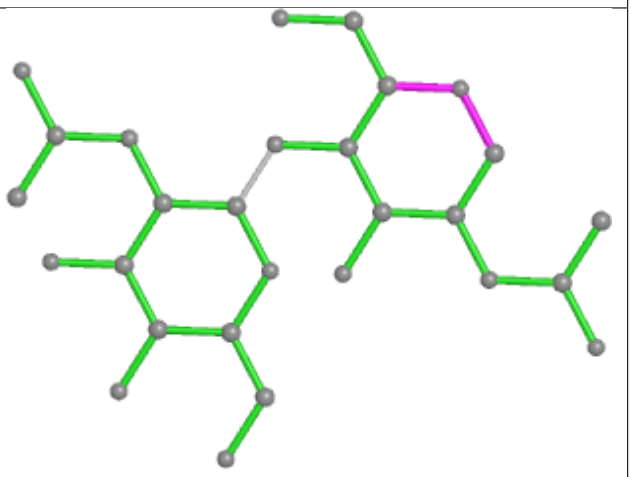


Rings

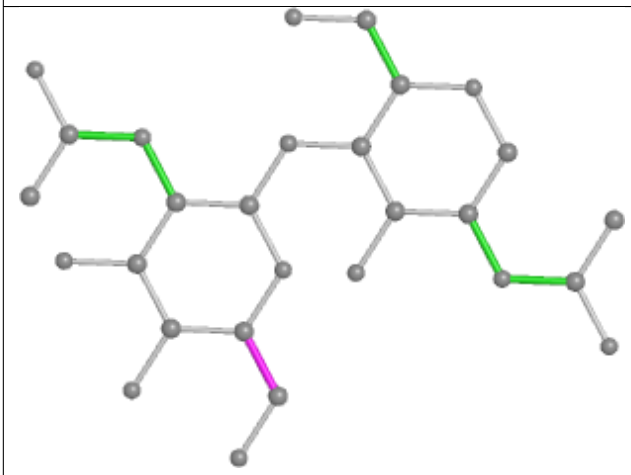
Oligosaccharide Chain X



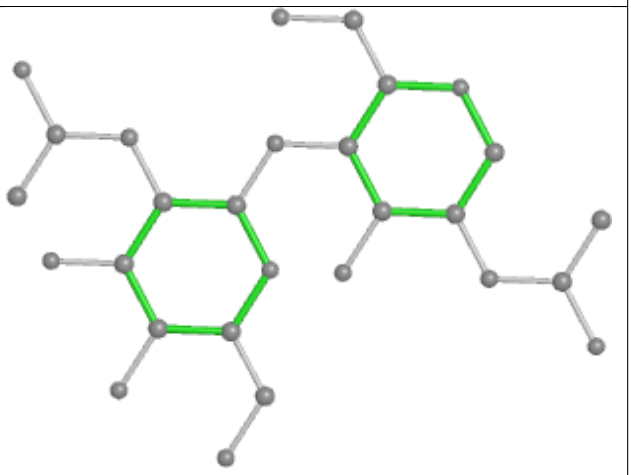
Bond lengths



Bond angles

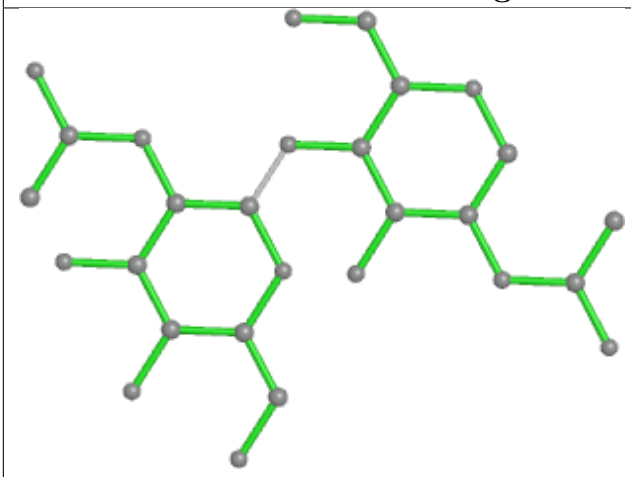


Torsions

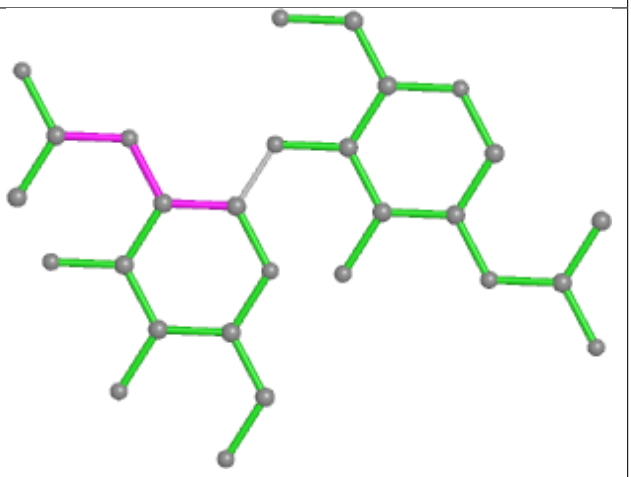


Rings

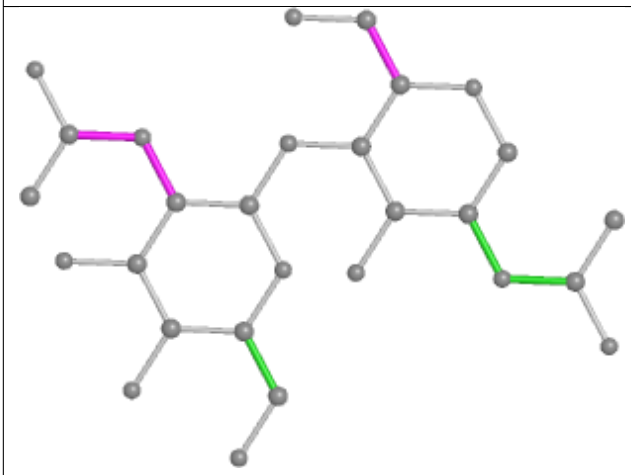
Oligosaccharide Chain Y



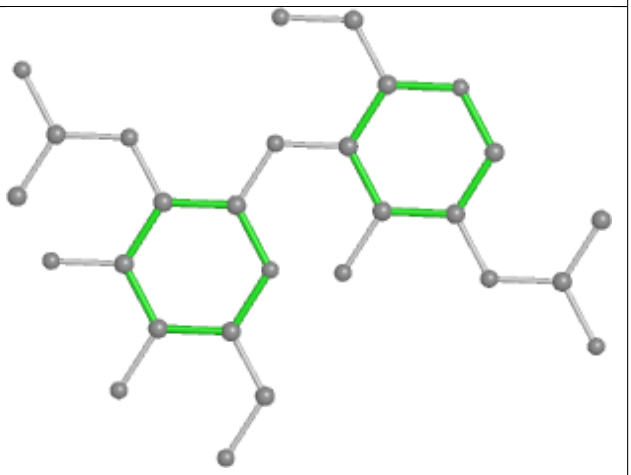
Bond lengths



Bond angles

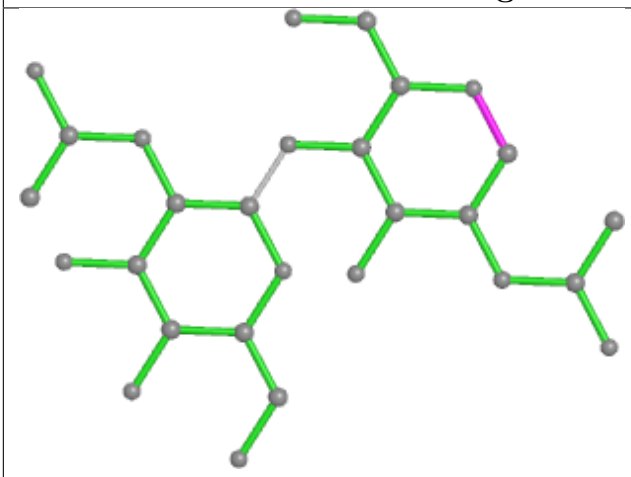


Torsions

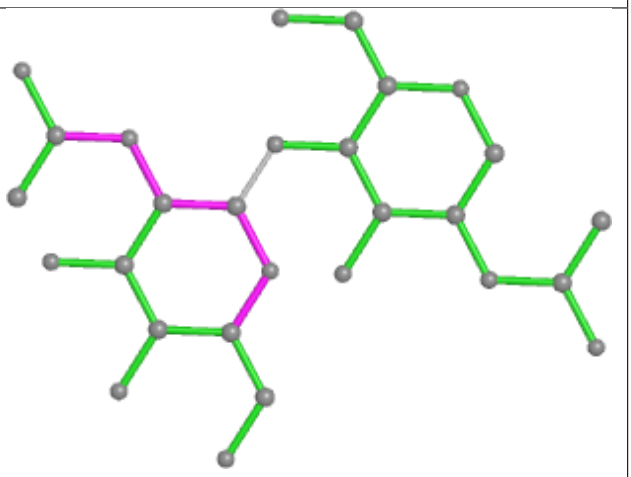


Rings

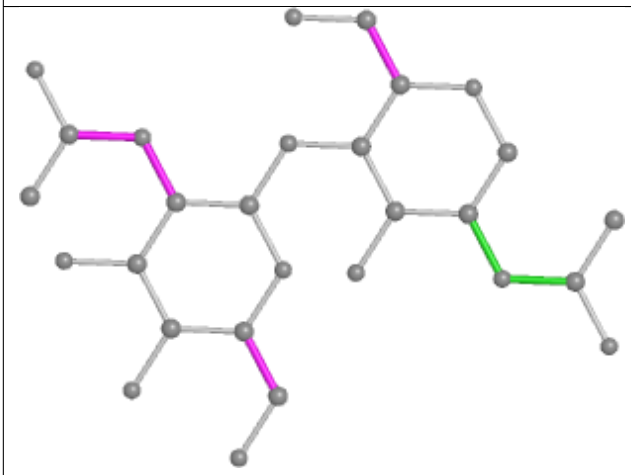
Oligosaccharide Chain Z



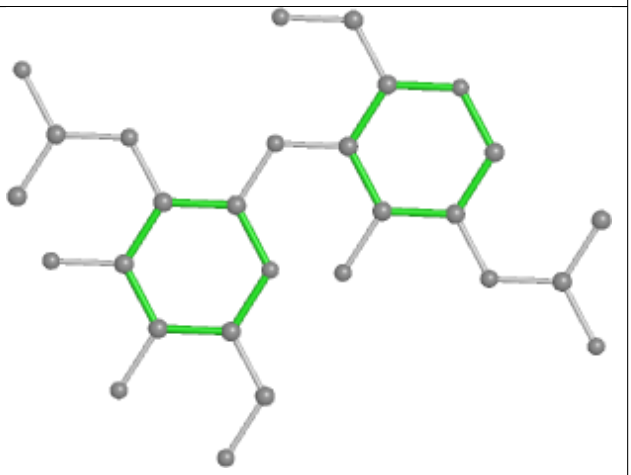
Bond lengths



Bond angles

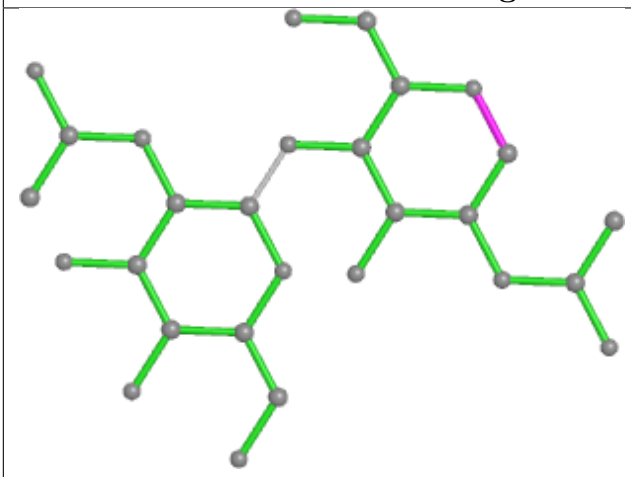


Torsions

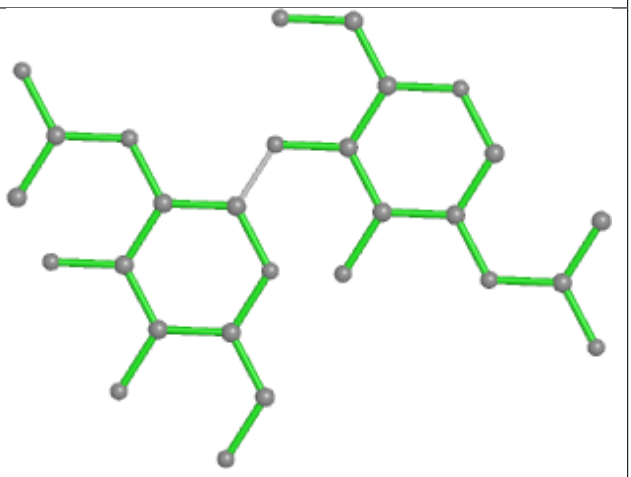


Rings

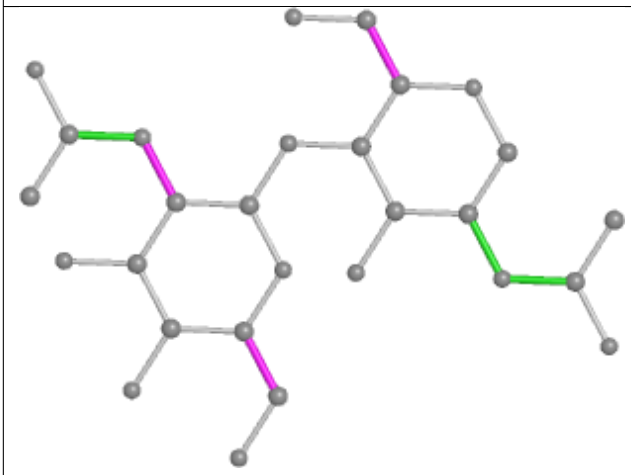
Oligosaccharide Chain a



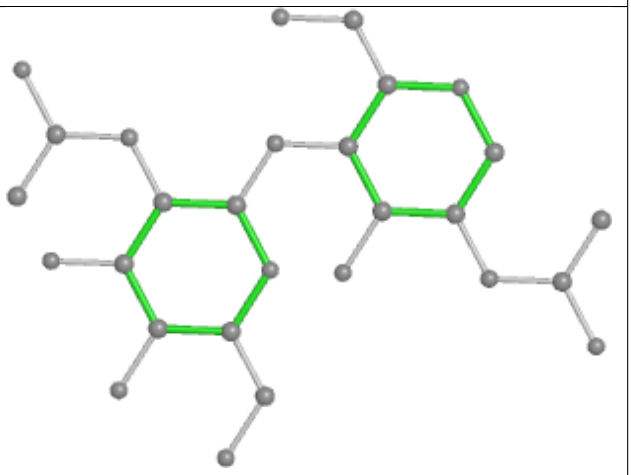
Bond lengths



Bond angles

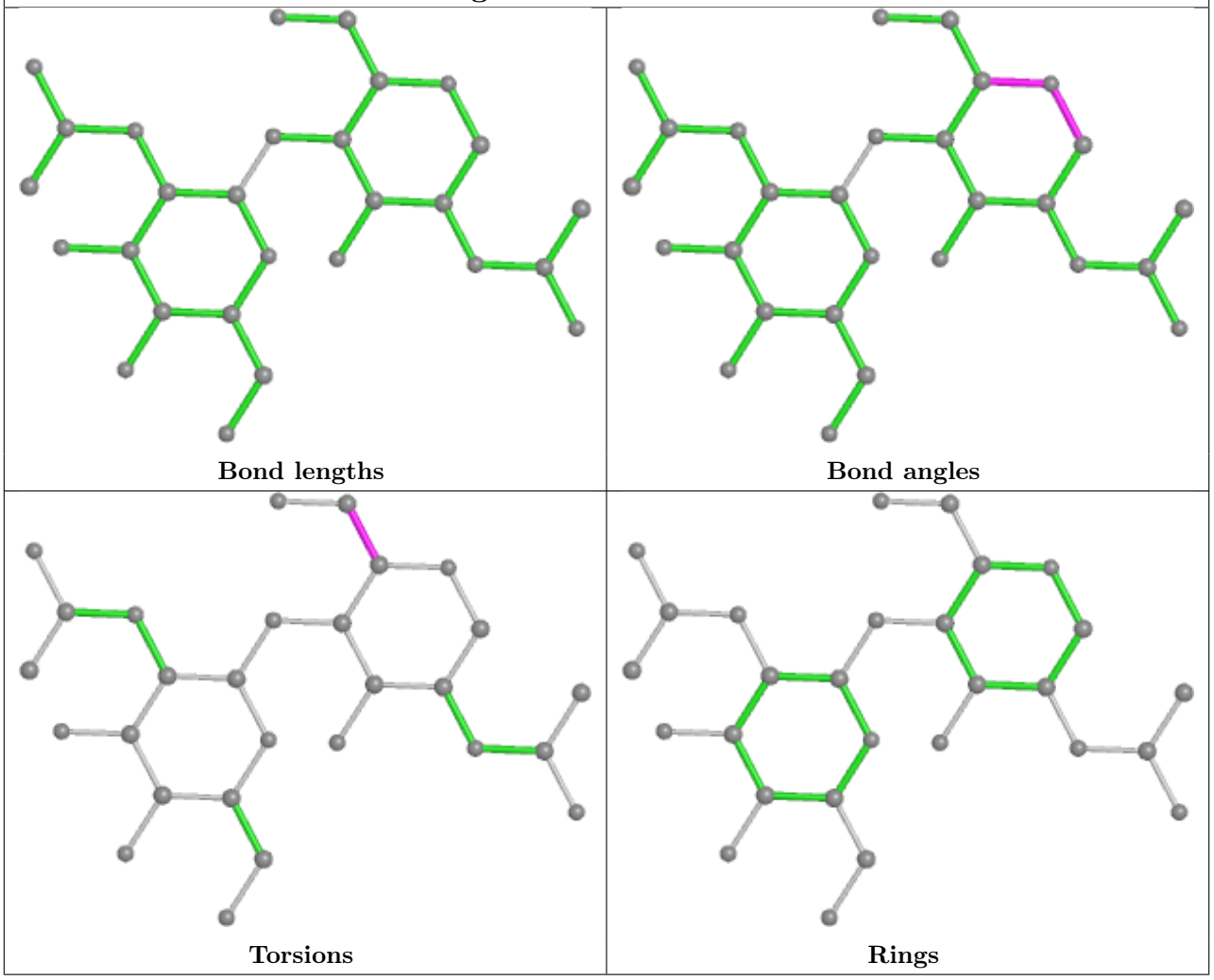


Torsions



Rings

Oligosaccharide Chain b



5.6 Ligand geometry (i)

28 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	$\#\|Z\| > 2$
5	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	B	1409	1	14,14,15	0.50	0	17,19,21	0.35	0
5	NAG	B	1405	1	14,14,15	0.55	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1402	1	14,14,15	0.47	0	17,19,21	0.57	0
5	NAG	A	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	C	1408	1	14,14,15	0.34	0	17,19,21	0.41	0
5	NAG	C	1402	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	A	1404	1	14,14,15	0.31	0	17,19,21	0.37	0
5	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1403	1	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	C	1401	1	14,14,15	0.28	0	17,19,21	0.55	0
5	NAG	A	1406	1	14,14,15	0.20	0	17,19,21	0.37	0
5	NAG	A	1405	1	14,14,15	0.36	0	17,19,21	1.28	2 (11%)
5	NAG	C	1411	-	14,14,15	0.32	0	17,19,21	0.41	0
5	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.64	0
5	NAG	C	1409	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	C	1407	1	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
5	NAG	A	1408	1	14,14,15	0.16	0	17,19,21	0.56	0
5	NAG	B	1401	1	14,14,15	0.28	0	17,19,21	0.34	0
5	NAG	C	1410	1	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
5	NAG	C	1404	1	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
5	NAG	B	1403	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	B	1404	1	14,14,15	0.44	0	17,19,21	0.54	0
5	NAG	B	1408	1	14,14,15	0.32	0	17,19,21	0.38	0
5	NAG	A	1403	1	14,14,15	0.56	0	17,19,21	0.45	0
5	NAG	C	1405	1	14,14,15	0.39	0	17,19,21	1.28	2 (11%)
5	NAG	C	1406	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
5	NAG	A	1407	1	14,14,15	0.36	0	17,19,21	0.63	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
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1405	NAG	C2-N2-C7	4.35	129.09	122.90
5	A	1405	NAG	C2-N2-C7	4.28	129.00	122.90
5	C	1405	NAG	C2-N2-C7	4.14	128.79	122.90
5	A	1401	NAG	C1-O5-C5	2.90	116.12	112.19
5	C	1406	NAG	C1-O5-C5	2.53	115.62	112.19
5	C	1407	NAG	C1-O5-C5	2.36	115.39	112.19
5	C	1410	NAG	C8-C7-N2	2.32	120.02	116.10
5	A	1405	NAG	C1-C2-N2	2.23	114.30	110.49
5	C	1405	NAG	C1-C2-N2	2.08	114.04	110.49
5	C	1410	NAG	C2-N2-C7	-2.06	119.97	122.90
5	C	1404	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1408	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	A	1405	NAG	C8-C7-N2-C2
5	A	1405	NAG	O7-C7-N2-C2
5	A	1406	NAG	C8-C7-N2-C2
5	A	1406	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	B	1409	NAG	O5-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	C	1407	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	C	1409	NAG	C4-C5-C6-O6
5	A	1403	NAG	C1-C2-N2-C7
5	B	1408	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1406	NAG	C4-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	A	1407	NAG	O5-C5-C6-O6
5	C	1409	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	B	1407	NAG	C1-C2-N2-C7
5	A	1407	NAG	C3-C2-N2-C7
5	C	1406	NAG	C3-C2-N2-C7
5	C	1407	NAG	C3-C2-N2-C7
5	A	1403	NAG	C3-C2-N2-C7
5	A	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

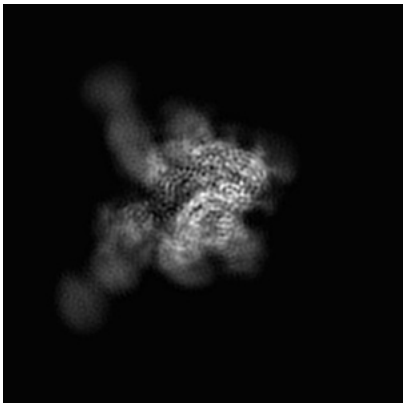
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31502. These allow visual inspection of the internal detail of the map and identification of artifacts.

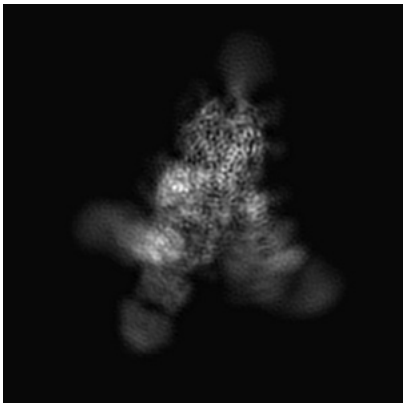
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

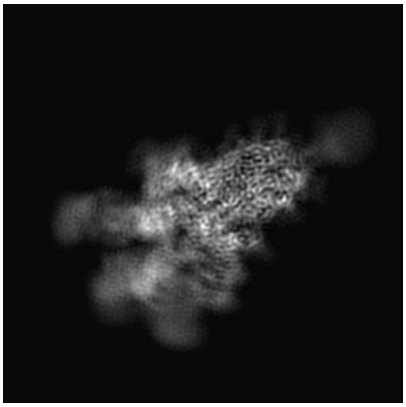
6.1.1 Primary map



X



Y

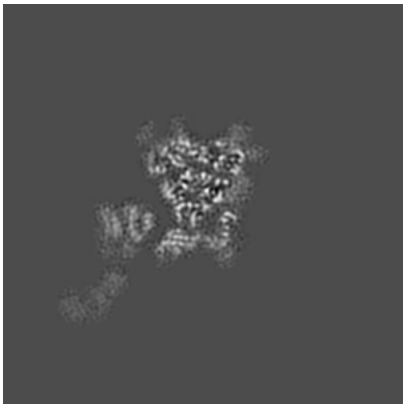


Z

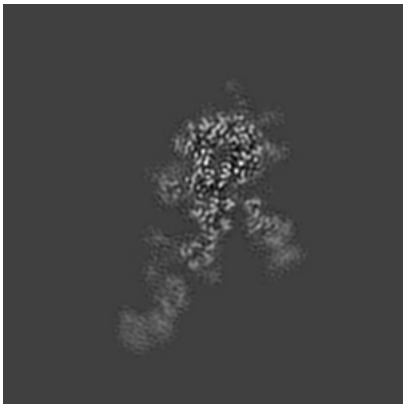
The images above show the map projected in three orthogonal directions.

6.2 Central slices

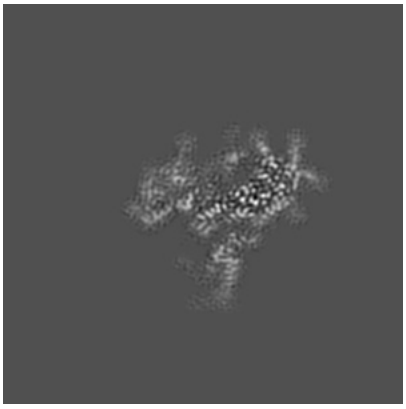
6.2.1 Primary map



X Index: 160



Y Index: 160

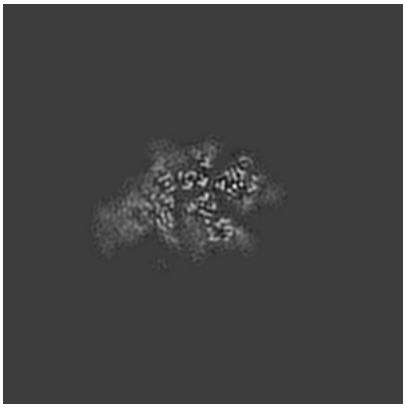


Z Index: 160

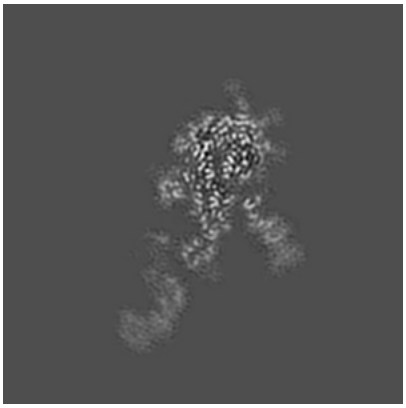
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

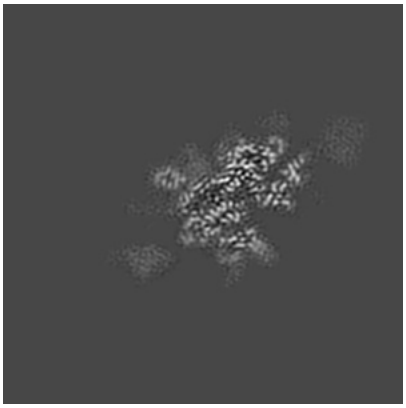
6.3.1 Primary map



X Index: 182



Y Index: 162

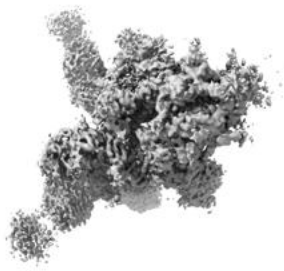


Z Index: 175

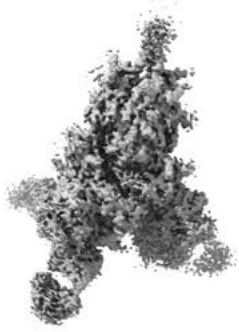
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

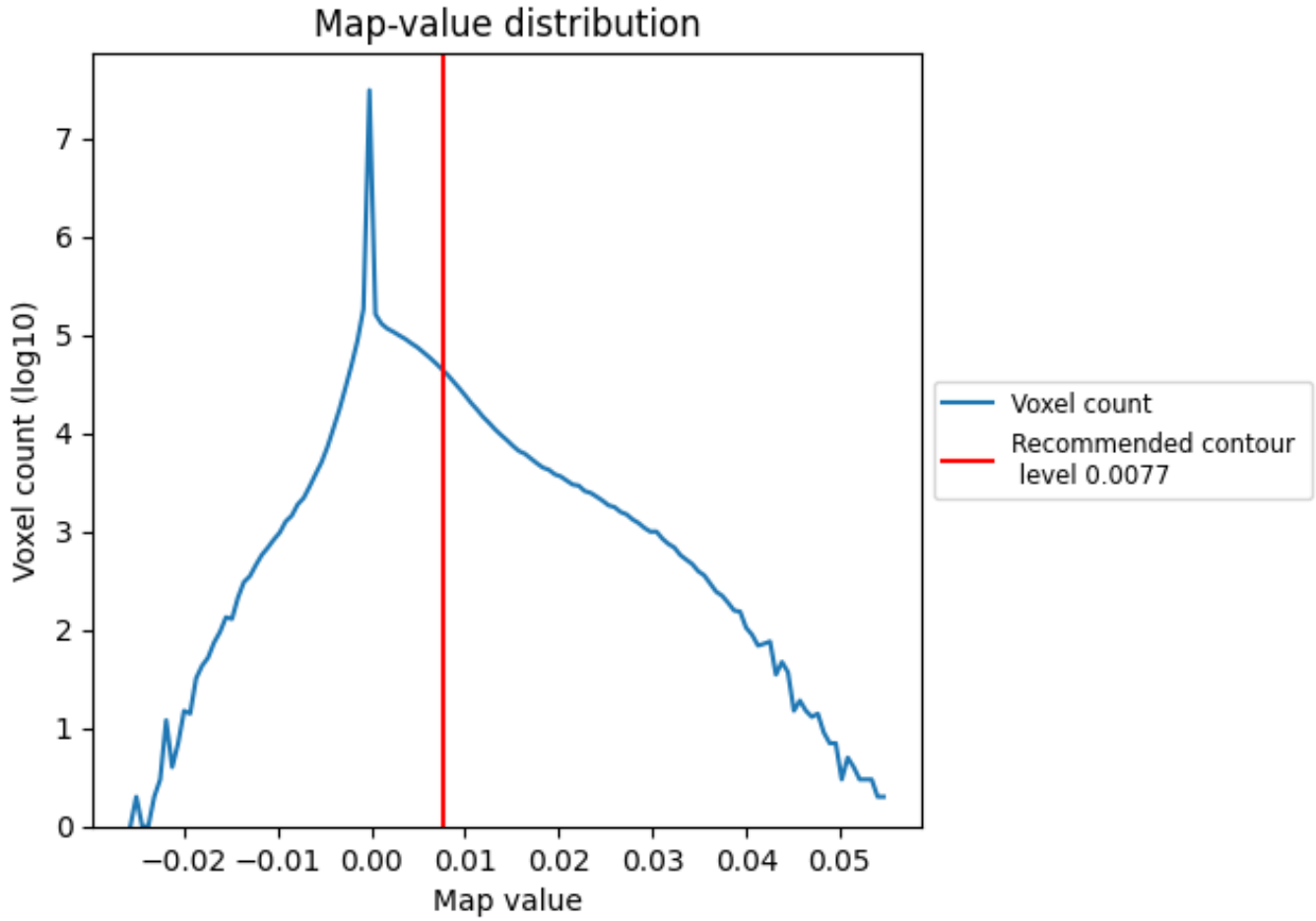
6.5 Mask visualisation (i)

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

7 Map analysis

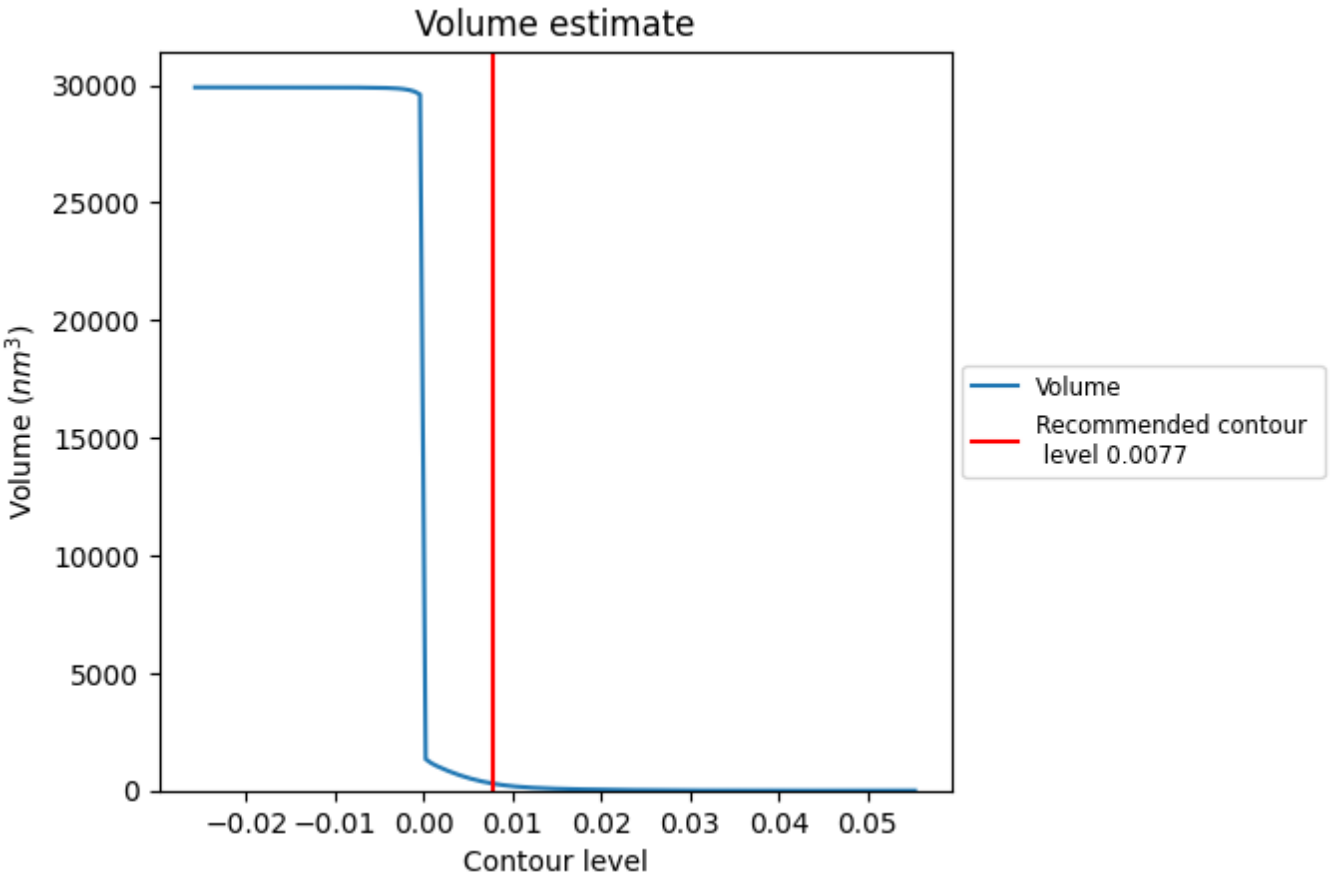
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

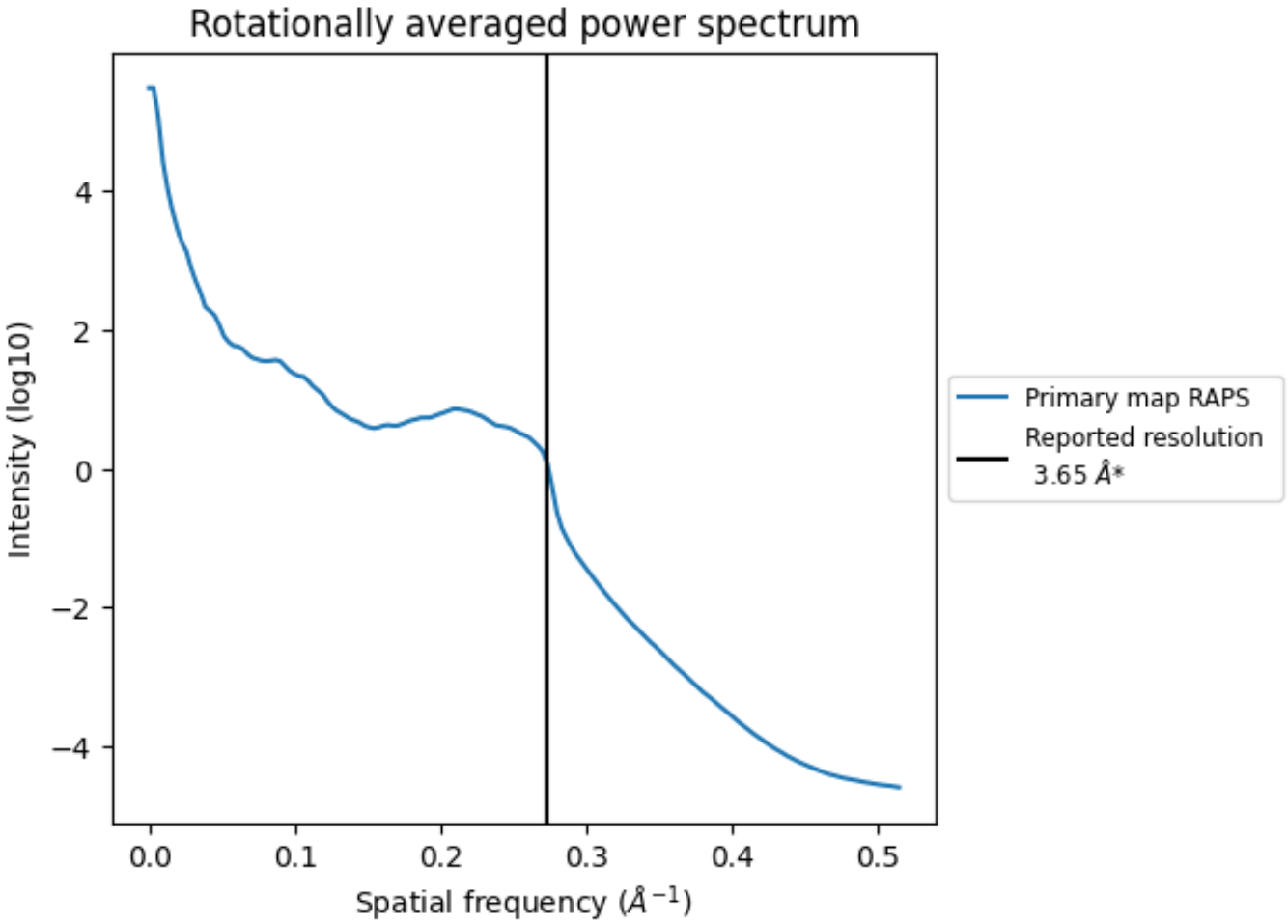
7.2 Volume estimate (i)



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 275 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 0.274 Å^{-1}

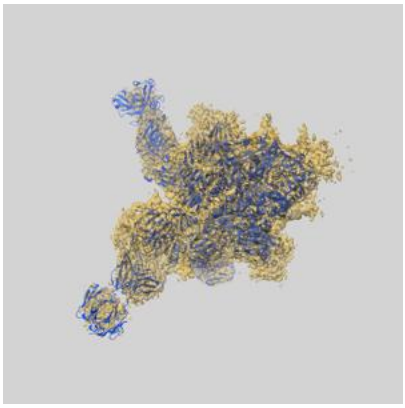
8 Fourier-Shell correlation (i)

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

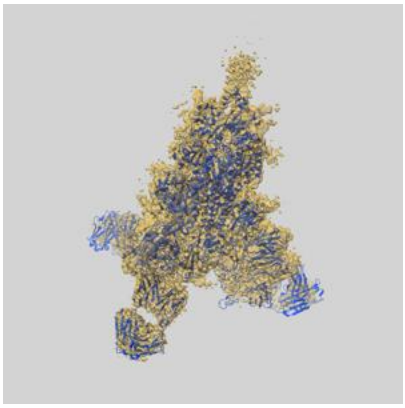
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31502 and PDB model 7FAE. Per-residue inclusion information can be found in section 3 on page 15.

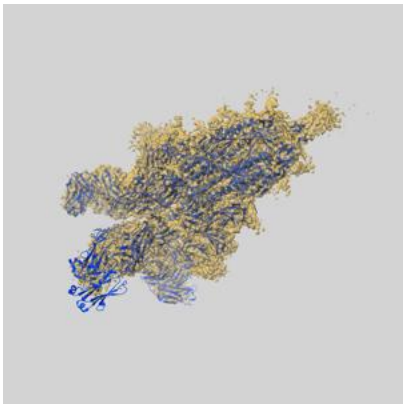
9.1 Map-model overlay



X



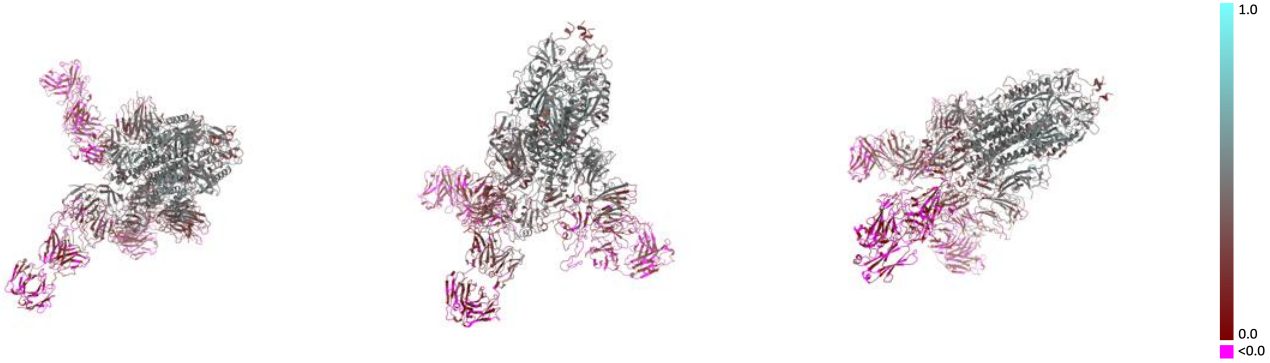
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

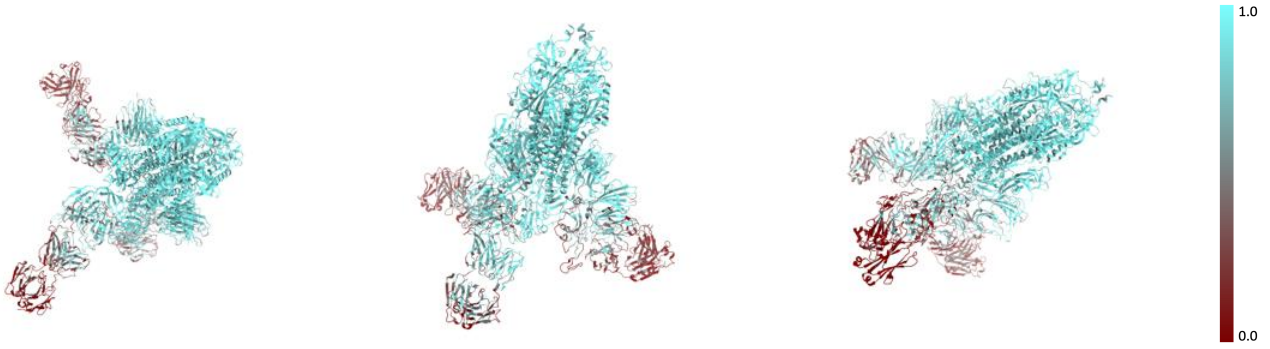
9.2 Q-score mapped to coordinate model



X Y Z

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

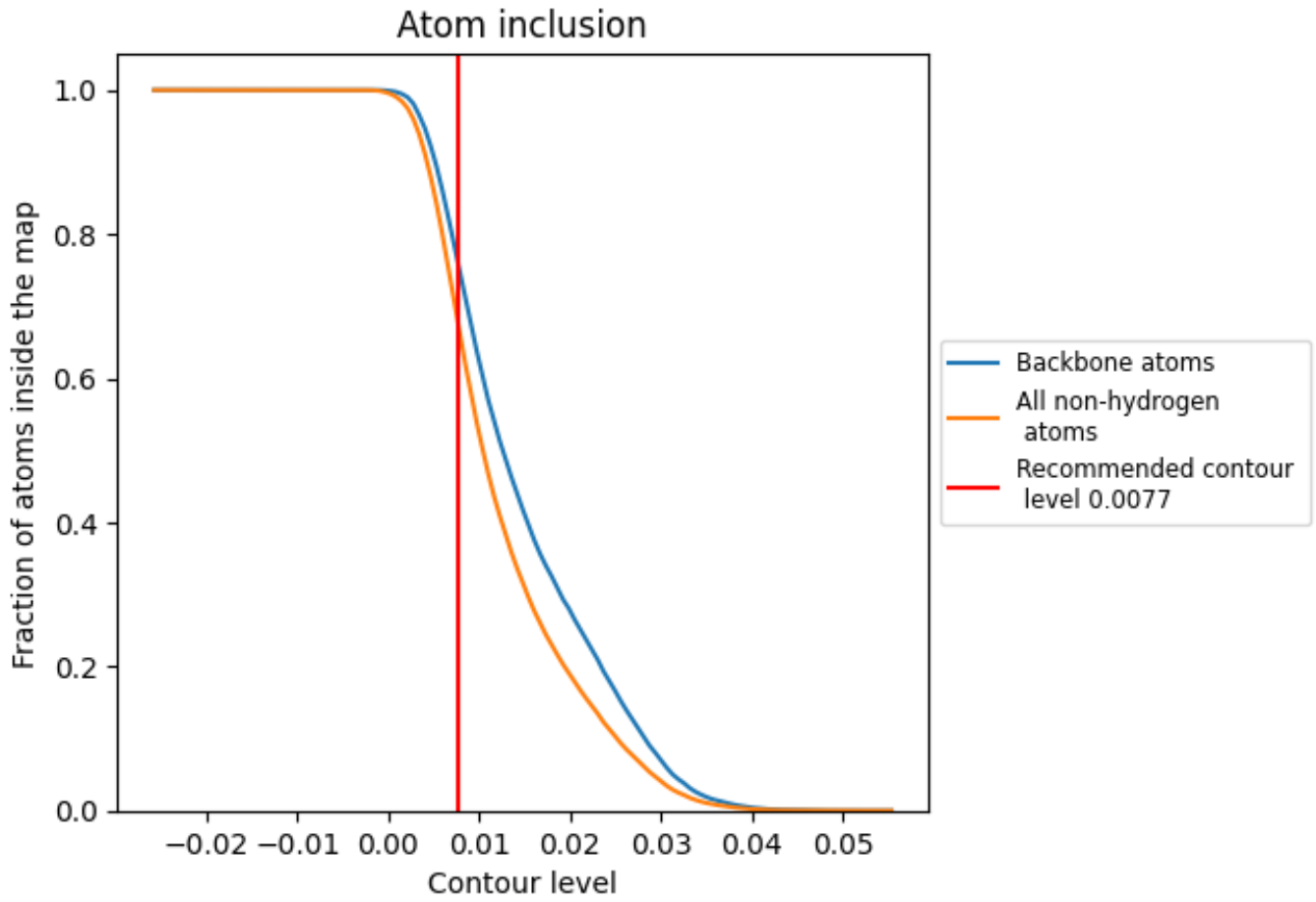
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0077).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.0077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6739	0.2920
A	0.7941	0.3620
B	0.7746	0.3480
C	0.8497	0.4060
E	0.3929	0.0920
H	0.2811	0.0720
I	0.5714	0.3280
J	0.7500	0.3500
K	0.8214	0.3640
L	0.2958	0.0750
M	0.3929	0.2560
N	0.7857	0.2940
O	0.6786	0.2960
Q	0.5357	0.3430
R	0.6429	0.3540
S	0.8214	0.3570
T	0.7857	0.3180
U	0.6786	0.3050
X	0.7500	0.4230
Y	0.7500	0.2560
Z	0.4286	0.3200
a	0.7857	0.3480
b	0.5714	0.2480
d	0.2368	0.0540
e	0.1913	0.0530
g	0.5749	0.1720
h	0.5451	0.1660