Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 08:06 am BST

PDB ID	:	6Z97 / pdb_00006z97
EMDB ID	:	EMD-11119
Title	:	Structure of the prefusion SARS-CoV-2 spike glycoprotein
Authors	:	Duyvesteyn, H.M.E.; Ren, J.; Zhao, Y.; Zhou, D.; Huo, J.; Carrique, L.; Malinauskas, T.; Ruza, R.R.; Shah, P.N.M.; Fry, E.E.; Owens, R.; Stuart, D.I.
Deposited on	:	2020-06-03
Resolution	:	3.40 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:

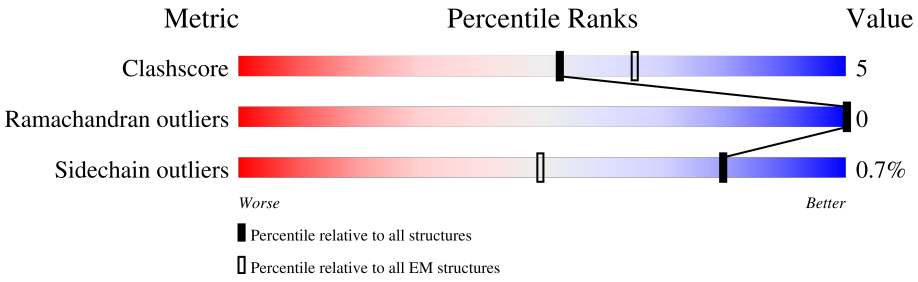
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1288	30% 68% 9% 23%
1	B	1288	34% 67% 9% 23%
1	C	1288	27% 67% 10% 23%
2	D	2	100% 50% 50%
2	E	2	50% 100%
2	F	2	50% 50% 50%
2	G	2	50% 100%
2	H	2	100% 100%

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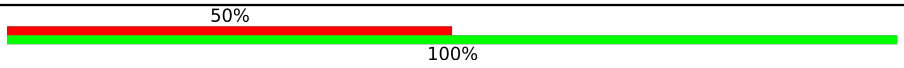
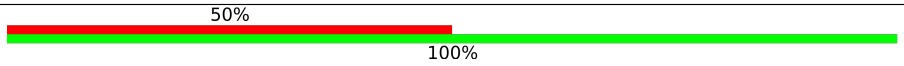
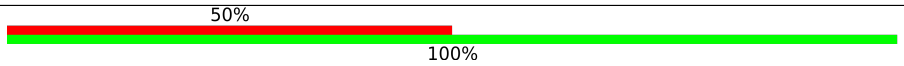
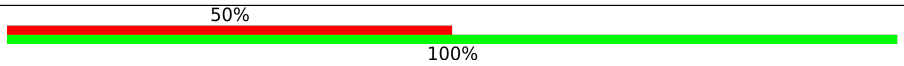
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 45754 atoms, of which 22287 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,Fibritin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	995	Total	C	H	N	O	S	0	0
			14982	4883	7354	1266	1444	35		
1	B	989	Total	C	H	N	O	S	0	0
			14831	4845	7260	1257	1434	35		
1	C	991	Total	C	H	N	O	S	0	0
			14863	4853	7281	1264	1431	34		

There are 177 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	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	conflict	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	GLY	-	expression tag	UNP P10104
A	1259	SER	-	expression tag	UNP P10104
A	1260	ALA	-	expression tag	UNP P10104
A	1261	TRP	-	expression tag	UNP P10104
A	1262	SER	-	expression tag	UNP P10104
A	1263	HIS	-	expression tag	UNP P10104
A	1264	PRO	-	expression tag	UNP P10104
A	1265	GLN	-	expression tag	UNP P10104
A	1266	PHE	-	expression tag	UNP P10104
A	1267	GLU	-	expression tag	UNP P10104
A	1268	LYS	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	GLY	-	expression tag	UNP P10104
A	1272	SER	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104
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	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1232	LEU	PHE	conflict	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	GLY	-	expression tag	UNP P10104
B	1259	SER	-	expression tag	UNP P10104
B	1260	ALA	-	expression tag	UNP P10104
B	1261	TRP	-	expression tag	UNP P10104
B	1262	SER	-	expression tag	UNP P10104
B	1263	HIS	-	expression tag	UNP P10104
B	1264	PRO	-	expression tag	UNP P10104
B	1265	GLN	-	expression tag	UNP P10104
B	1266	PHE	-	expression tag	UNP P10104
B	1267	GLU	-	expression tag	UNP P10104
B	1268	LYS	-	expression tag	UNP P10104
B	1269	GLY	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	GLY	-	expression tag	UNP P10104
B	1272	SER	-	expression tag	UNP P10104
B	1273	GLY	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1279	SER	-	expression tag	UNP P10104
B	1280	ALA	-	expression tag	UNP P10104
B	1281	TRP	-	expression tag	UNP P10104
B	1282	SER	-	expression tag	UNP P10104
B	1283	HIS	-	expression tag	UNP P10104
B	1284	PRO	-	expression tag	UNP P10104
B	1285	GLN	-	expression tag	UNP P10104
B	1286	PHE	-	expression tag	UNP P10104
B	1287	GLU	-	expression tag	UNP P10104
B	1288	LYS	-	expression tag	UNP P10104
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	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	conflict	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104
C	1247	GLY	-	expression tag	UNP P10104
C	1248	PRO	-	expression tag	UNP P10104
C	1249	GLY	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	GLY	-	expression tag	UNP P10104
C	1259	SER	-	expression tag	UNP P10104
C	1260	ALA	-	expression tag	UNP P10104
C	1261	TRP	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1262	SER	-	expression tag	UNP P10104
C	1263	HIS	-	expression tag	UNP P10104
C	1264	PRO	-	expression tag	UNP P10104
C	1265	GLN	-	expression tag	UNP P10104
C	1266	PHE	-	expression tag	UNP P10104
C	1267	GLU	-	expression tag	UNP P10104
C	1268	LYS	-	expression tag	UNP P10104
C	1269	GLY	-	expression tag	UNP P10104
C	1270	GLY	-	expression tag	UNP P10104
C	1271	GLY	-	expression tag	UNP P10104
C	1272	SER	-	expression tag	UNP P10104
C	1273	GLY	-	expression tag	UNP P10104
C	1274	GLY	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	SER	-	expression tag	UNP P10104
C	1277	GLY	-	expression tag	UNP P10104
C	1278	GLY	-	expression tag	UNP P10104
C	1279	SER	-	expression tag	UNP P10104
C	1280	ALA	-	expression tag	UNP P10104
C	1281	TRP	-	expression tag	UNP P10104
C	1282	SER	-	expression tag	UNP P10104
C	1283	HIS	-	expression tag	UNP P10104
C	1284	PRO	-	expression tag	UNP P10104
C	1285	GLN	-	expression tag	UNP P10104
C	1286	PHE	-	expression tag	UNP P10104
C	1287	GLU	-	expression tag	UNP P10104
C	1288	LYS	-	expression tag	UNP P10104

- 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	H	N	O	0	0
			44	16	16	2	10		
2	E	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	F	2	Total	C	H	N	O	0	0
			44	16	16	2	10		

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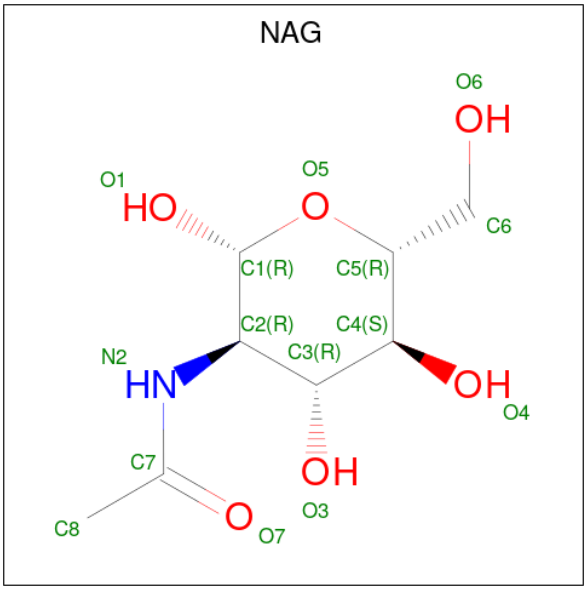
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	H	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	I	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	J	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	K	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	L	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	M	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
2	N	2	Total	C	H	N	O	0	0
			44	16	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			22	8	8	1	5	
3	A	1	Total	C	H	N	O	0
			22	8	8	1	5	
3	A	1	Total	C	H	N	O	0
			22	8	8	1	5	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 22	C 8	H 8	N 1	O 5	0
3	A	1	Total 22	C 8	H 8	N 1	O 5	0
3	A	1	Total 22	C 8	H 8	N 1	O 5	0
3	A	1	Total 22	C 8	H 8	N 1	O 5	0
3	A	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	B	1	Total 22	C 8	H 8	N 1	O 5	0
3	C	1	Total 22	C 8	H 8	N 1	O 5	0
3	C	1	Total 22	C 8	H 8	N 1	O 5	0
3	C	1	Total 22	C 8	H 8	N 1	O 5	0
3	C	1	Total 22	C 8	H 8	N 1	O 5	0
3	C	1	Total 22	C 8	H 8	N 1	O 5	0

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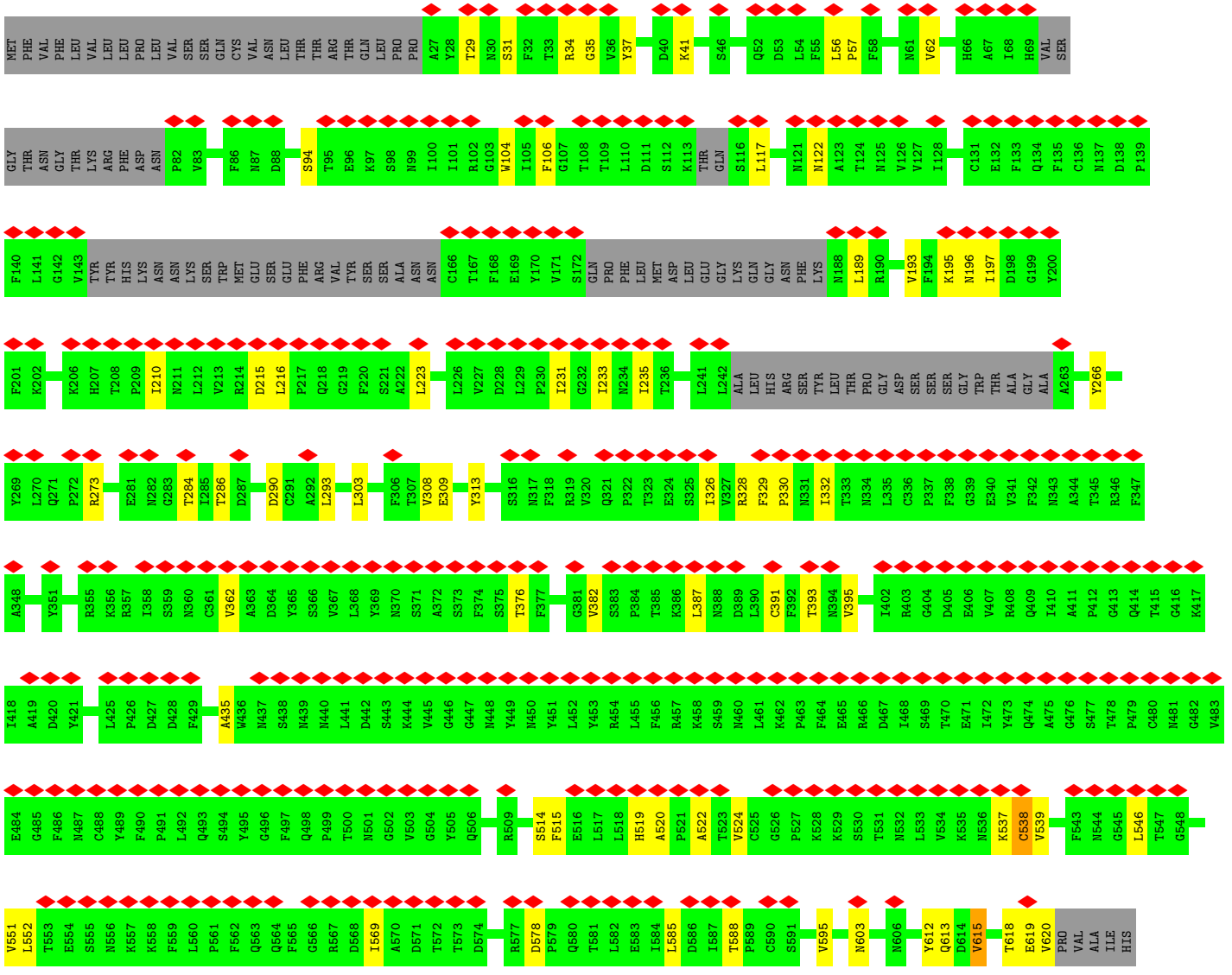
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	N	O	0
			22	8	8	1	5	
3	C	1	Total	C	H	N	O	0
			22	8	8	1	5	
3	C	1	Total	C	H	N	O	0
			22	8	8	1	5	

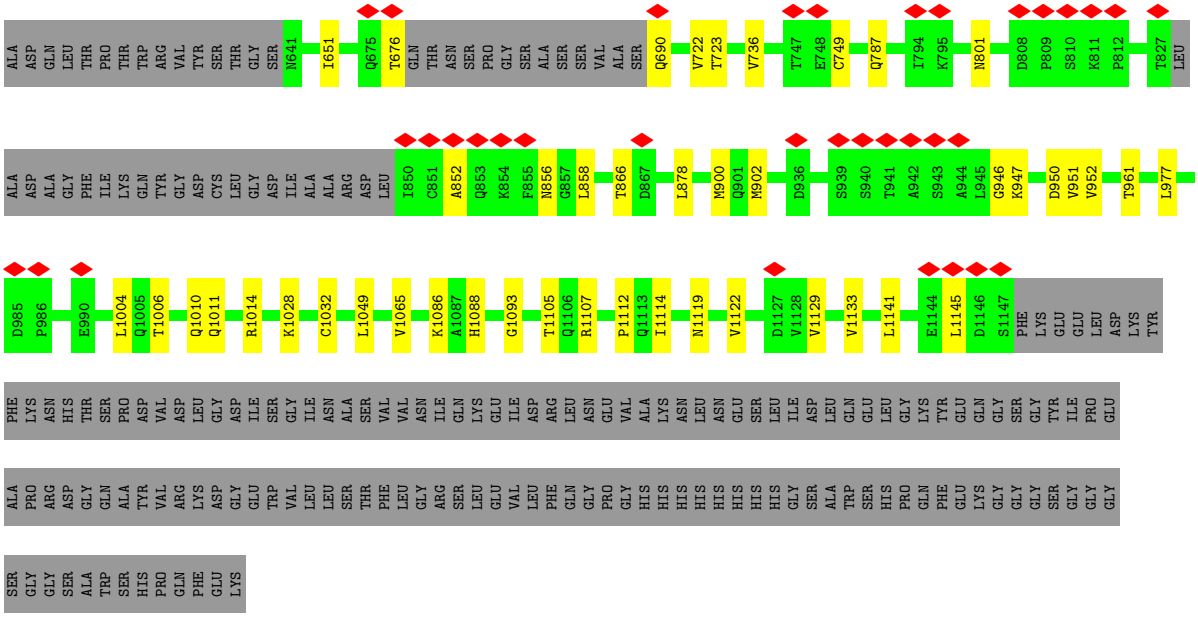
3 Residue-property plots (i)

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,Fibritin

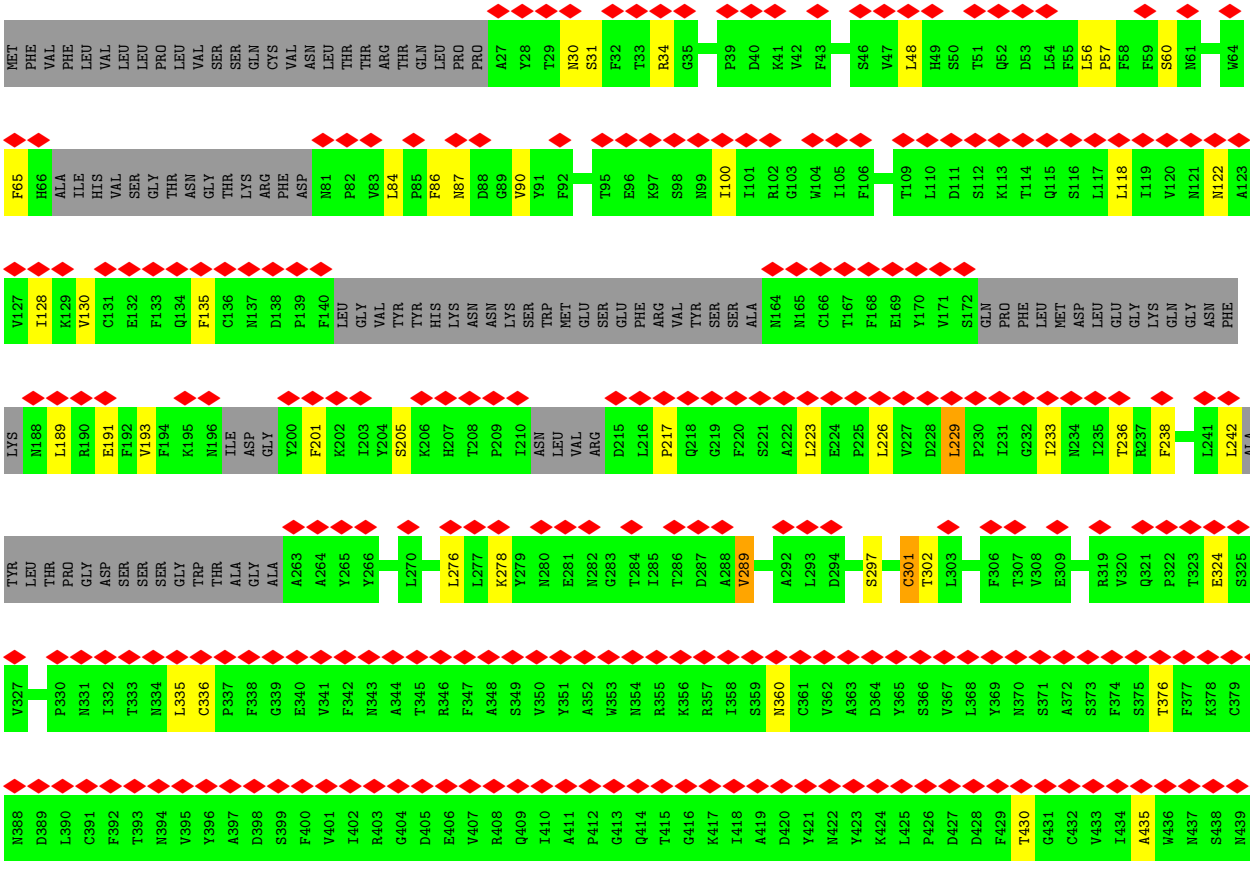
Chain A:

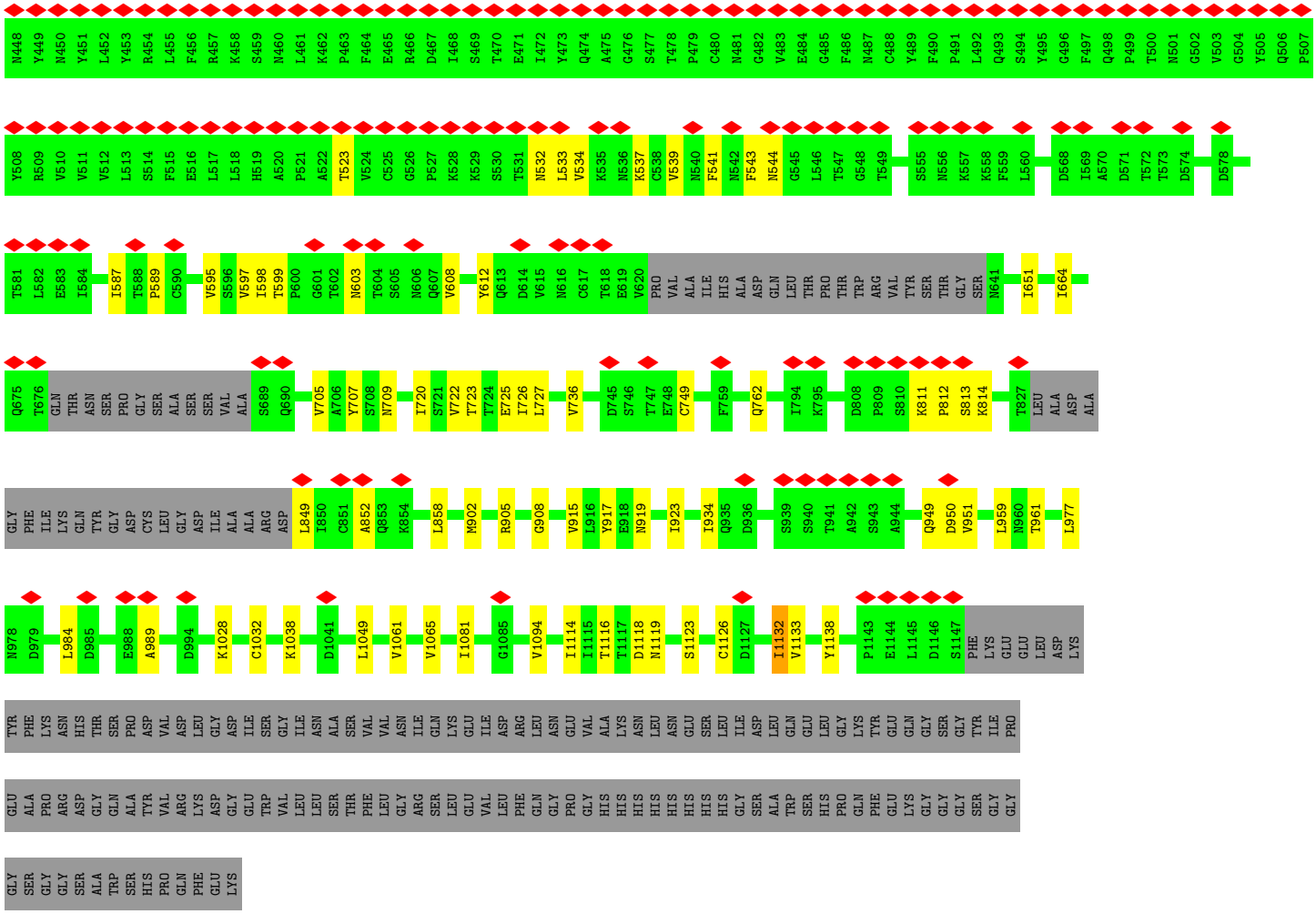




• Molecule 1: Spike glycoprotein,Fibritin

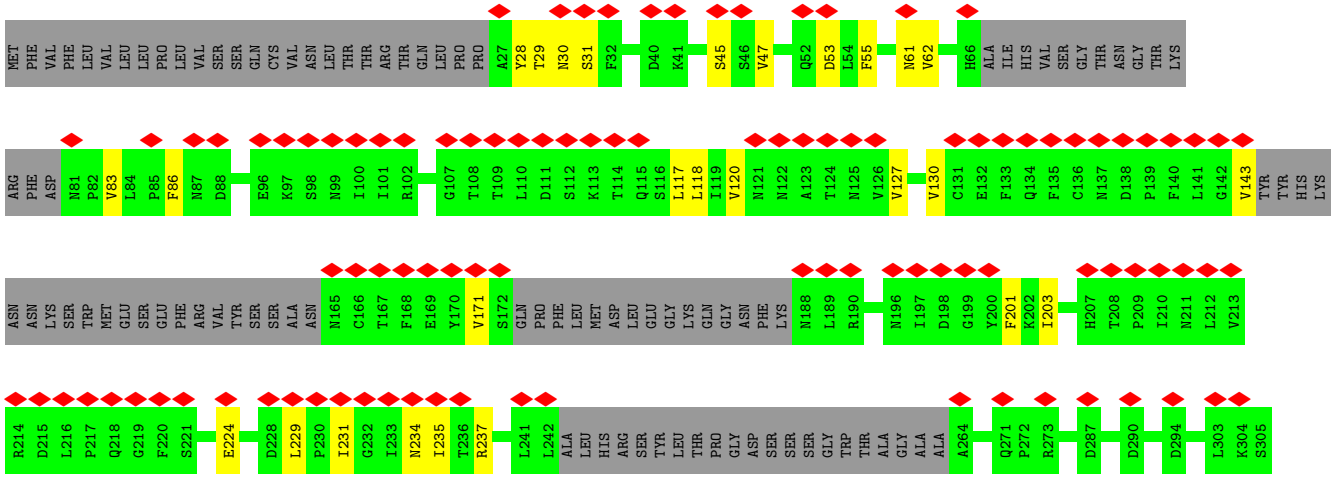
Chain B:

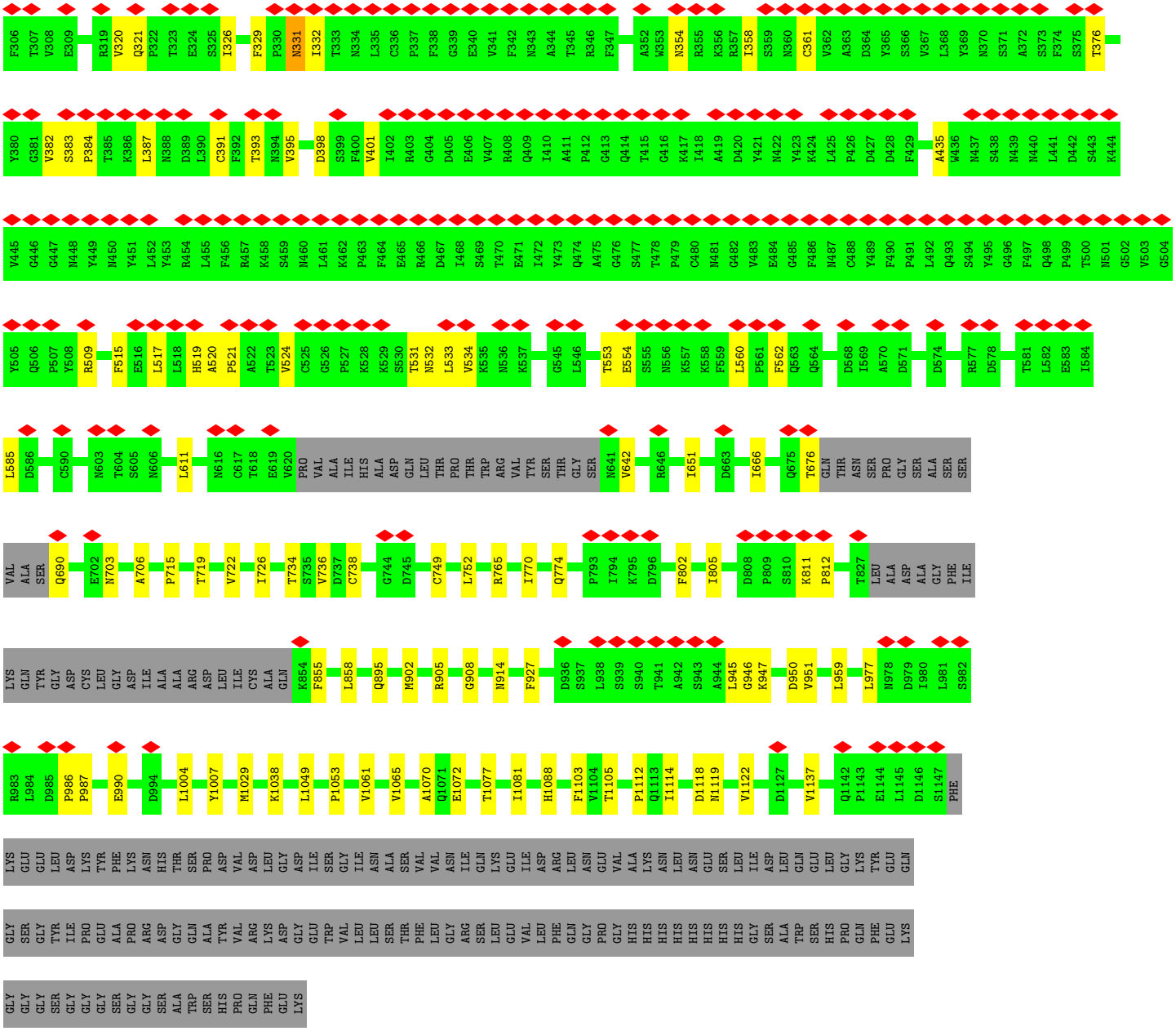




• Molecule 1: Spike glycoprotein,Fibritin

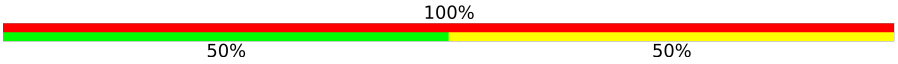
Chain C:





• 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

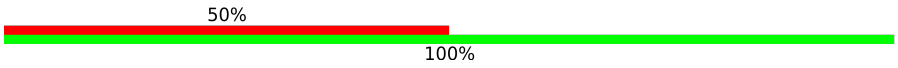
Chain E:

• 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:

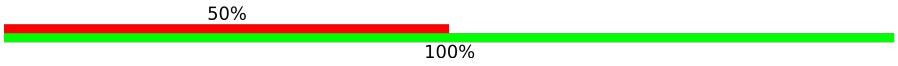


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

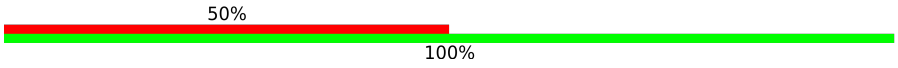
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:

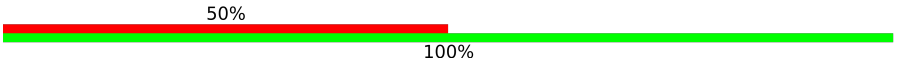


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

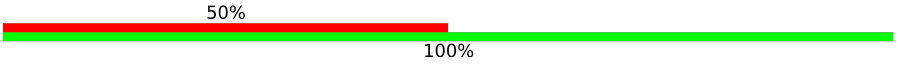
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	328000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	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	4.866	Depositor
Minimum map value	-2.830	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.77	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.18	0/7800	0.34	0/10634
1	B	0.17	0/7742	0.34	0/10557
1	C	0.17	0/7754	0.33	0/10577
All	All	0.17	0/23296	0.34	0/31768

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ASN	Peptide
1	B	814	LYS	Peptide

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	7628	7354	7354	85	0
1	B	7571	7260	7259	79	0
1	C	7582	7281	7280	81	0
2	D	28	16	25	0	0
2	E	28	16	25	0	0
2	F	28	16	25	1	0
2	G	28	16	25	0	0
2	H	28	16	25	0	0
2	I	28	16	25	0	0
2	J	28	16	25	0	0
2	K	28	16	25	0	0
2	L	28	16	25	0	0
2	M	28	16	25	0	0
2	N	28	16	25	1	0
3	A	112	64	104	0	0
3	B	154	88	143	0	0
3	C	112	64	104	1	0
All	All	23467	22287	22519	235	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG11	1:C:387:LEU:HD21	1.42	1.01
1:A:382:VAL:HG11	1:A:387:LEU:HD21	1.56	0.87
1:A:29:THR:HG23	1:A:62:VAL:HG23	1.61	0.82
1:C:117:LEU:HD21	1:C:231:ILE:HD13	1.71	0.73
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.70	0.72
1:B:189:LEU:HD11	1:B:217:PRO:HG2	1.72	0.72
1:B:597:VAL:HG12	1:B:599:THR:HG23	1.73	0.71
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.71	0.70
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.73	0.70
1:A:231:ILE:HD12	1:A:233:ILE:HB	1.79	0.65
1:B:382:VAL:HG11	1:B:387:LEU:HD21	1.77	0.65
1:B:100:ILE:HG22	1:B:242:LEU:HB2	1.77	0.64
1:B:811:LYS:O	1:B:813:SER:N	2.27	0.64
1:B:961:THR:HG21	1:C:765:ARG:HH22	1.62	0.64
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.31	0.63
1:A:195:LYS:HD3	1:A:197:ILE:HD13	1.81	0.63
1:A:326:ILE:HD12	1:A:539:VAL:HG21	1.81	0.62
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.82	0.62
1:A:41:LYS:HD3	1:C:520:ALA:HB2	1.83	0.61
1:B:276:LEU:HB3	1:B:289:VAL:HG23	1.82	0.61
1:B:31:SER:OG	1:B:56:LEU:HD21	1.99	0.61
1:A:961:THR:HG21	1:B:762:GLN:CD	2.26	0.61
1:C:752:LEU:HD21	1:C:990:GLU:HG2	1.82	0.61
1:B:537:LYS:O	1:B:539:VAL:HG23	2.00	0.60
1:A:193:VAL:HG23	1:A:223:LEU:HD23	1.84	0.60
1:C:130:VAL:HG11	1:C:231:ILE:HG22	1.83	0.59
1:C:201:PHE:HB2	1:C:231:ILE:HD11	1.83	0.59
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.36	0.58
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.84	0.58
1:A:736:VAL:HG11	1:A:1004:LEU:HD21	1.86	0.58
1:C:331:ASN:N	1:C:331:ASN:OD1	2.35	0.58
1:A:94:SER:O	1:A:189:LEU:HD12	2.04	0.58
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.86	0.58
1:C:382:VAL:HG11	1:C:387:LEU:CD2	2.27	0.57
1:A:117:LEU:HD21	1:A:231:ILE:HG21	1.87	0.57
1:A:552:LEU:HB3	1:A:585:LEU:HD13	1.86	0.57
1:B:597:VAL:HG12	1:B:599:THR:CG2	2.33	0.57
1:C:332:ILE:HD12	1:C:361:CYS:C	2.30	0.57
1:A:332:ILE:HG22	1:A:362:VAL:HG23	1.85	0.57
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.86	0.56
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.69	0.56
1:B:128:ILE:CG2	1:B:229:LEU:HD21	2.35	0.56
1:C:858:LEU:HD23	1:C:959:LEU:HD22	1.87	0.56
1:B:705:VAL:HG12	1:C:895:GLN:HB3	1.89	0.55
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.88	0.55
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.72	0.55
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.89	0.54
1:B:128:ILE:HG21	1:B:229:LEU:HD21	1.89	0.54
1:B:725:GLU:OE1	1:B:1028:LYS:NZ	2.34	0.54
1:A:382:VAL:HG11	1:A:387:LEU:CD2	2.33	0.53
1:B:599:THR:HG22	1:B:608:VAL:CG1	2.38	0.53
1:B:335:LEU:HD23	1:B:336:CYS:N	2.24	0.53
1:A:196:ASN:C	1:A:197:ILE:HD12	2.34	0.53
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.91	0.53
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:HB2	1:A:332:ILE:HD13	1.91	0.52
1:A:538:CYS:CB	1:A:551:VAL:HG12	2.40	0.52
1:C:229:LEU:HB3	1:C:231:ILE:HG23	1.92	0.52
1:A:1114:ILE:O	1:A:1119:ASN:ND2	2.42	0.52
1:B:1126:CYS:CB	1:B:1132:ILE:HD13	2.39	0.52
1:A:34:ARG:O	1:A:56:LEU:HD23	2.09	0.52
1:B:1123:SER:OG	1:C:914:ASN:ND2	2.43	0.51
1:A:391:CYS:HA	1:A:524:VAL:O	2.11	0.51
1:B:811:LYS:CB	1:B:812:PRO:HD2	2.41	0.50
1:B:1126:CYS:HB2	1:B:1132:ILE:HG21	1.93	0.50
1:A:216:LEU:HD12	1:A:216:LEU:O	2.11	0.50
1:A:329:PHE:HD1	1:A:391:CYS:SG	2.34	0.50
1:A:537:LYS:O	1:A:539:VAL:HG13	2.11	0.50
1:A:309:GLU:O	1:A:313:TYR:OH	2.29	0.49
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.93	0.49
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.95	0.49
1:C:393:THR:HG21	1:C:519:HIS:NE2	2.28	0.49
1:C:127:VAL:HG23	1:C:171:VAL:HG22	1.95	0.49
1:A:749:CYS:HB2	1:A:977:LEU:HD21	1.95	0.48
1:B:236:THR:HG22	1:B:236:THR:O	2.14	0.48
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.95	0.48
1:C:358:ILE:HB	1:C:395:VAL:HB	1.95	0.48
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.94	0.48
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.96	0.48
1:B:30:ASN:OD1	1:B:31:SER:N	2.47	0.48
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.44	0.48
1:C:201:PHE:HE2	1:C:203:ILE:HD11	1.79	0.47
1:B:297:SER:O	1:B:301:CYS:SG	2.72	0.47
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.49	0.47
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.96	0.47
1:A:612:TYR:CE1	1:A:620:VAL:HG21	2.50	0.47
1:A:1093:GLY:O	1:A:1107:ARG:NH2	2.48	0.47
1:B:1114:ILE:O	1:B:1119:ASN:ND2	2.47	0.47
1:C:736:VAL:HG22	1:C:858:LEU:HG	1.96	0.47
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.48	0.47
1:B:324:GLU:OE2	1:B:534:VAL:HG21	2.14	0.47
1:C:28:TYR:HB3	1:C:61:ASN:OD1	2.15	0.47
1:C:29:THR:HG22	1:C:30:ASN:N	2.29	0.47
1:A:37:TYR:HB2	1:A:223:LEU:O	2.15	0.47
1:C:384:PRO:HA	1:C:387:LEU:HG	1.95	0.47
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.97	0.47
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.15	0.47
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.48	0.47
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.97	0.46
1:B:205:SER:HB3	1:B:226:LEU:HD12	1.96	0.46
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.30	0.46
1:C:31:SER:HB3	1:C:62:VAL:HG13	1.96	0.46
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.50	0.46
1:C:560:LEU:HD13	1:C:562:PHE:CE2	2.51	0.46
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.97	0.46
1:A:31:SER:HB2	1:A:56:LEU:HD21	1.98	0.46
1:B:376:THR:HB	1:B:435:ALA:HB3	1.98	0.46
1:B:118:LEU:HD12	1:B:135:PHE:HE2	1.81	0.46
1:A:284:THR:O	1:A:286:THR:HG23	2.16	0.45
1:A:736:VAL:HG13	1:A:858:LEU:HD23	1.97	0.45
1:B:595:VAL:HG22	1:B:612:TYR:CD2	2.50	0.45
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.48	0.45
1:B:90:VAL:HG21	1:B:238:PHE:CE2	2.51	0.45
1:C:83:VAL:HG11	1:C:237:ARG:NH2	2.31	0.45
1:B:589:PRO:HG2	1:C:855:PHE:CB	2.47	0.45
1:B:543:PHE:O	1:B:544:ASN:C	2.60	0.45
1:C:86:PHE:O	1:C:86:PHE:CD2	2.69	0.45
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.99	0.45
1:A:34:ARG:HD2	1:A:216:LEU:HD13	1.99	0.45
1:C:382:VAL:HG12	1:C:383:SER:N	2.31	0.45
1:B:86:PHE:O	1:B:87:ASN:C	2.59	0.45
1:B:722:VAL:O	1:B:934:ILE:HD11	2.17	0.45
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.99	0.45
1:A:595:VAL:HG22	1:A:612:TYR:CD2	2.51	0.45
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.98	0.45
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.98	0.45
1:B:736:VAL:HG13	1:B:858:LEU:HD12	1.98	0.45
1:C:531:THR:HG22	1:C:532:ASN:N	2.32	0.45
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.46	0.44
1:A:391:CYS:CB	1:A:522:ALA:HB1	2.48	0.44
1:A:676:THR:HA	1:A:690:GLN:HA	1.99	0.44
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.16	0.44
1:C:1081:ILE:HD11	1:C:1137:VAL:HG22	1.98	0.44
1:A:603:ASN:C	1:A:603:ASN:OD1	2.61	0.44
1:A:612:TYR:CZ	1:A:620:VAL:HG21	2.52	0.44
1:B:849:LEU:HB2	1:B:852:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ASN:C	1:C:235:ILE:HD12	2.42	0.44
1:A:618:THR:HG23	1:A:619:GLU:N	2.32	0.44
1:C:320:VAL:HG12	1:C:321:GLN:N	2.32	0.44
1:A:395:VAL:HA	1:A:514:SER:O	2.17	0.44
1:A:376:THR:HB	1:A:435:ALA:HB3	1.99	0.44
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.98	0.44
1:B:532:ASN:OD1	1:B:533:LEU:N	2.51	0.44
1:C:143:VAL:HG22	1:C:143:VAL:O	2.17	0.44
1:C:86:PHE:O	1:C:86:PHE:HD2	2.00	0.44
1:C:130:VAL:HG11	1:C:231:ILE:CG2	2.47	0.44
1:C:224:GLU:N	1:C:224:GLU:OE1	2.51	0.44
1:C:719:THR:HG23	1:C:1070:ALA:HB2	2.00	0.44
1:A:749:CYS:CB	1:A:977:LEU:HD21	2.48	0.43
1:B:749:CYS:CB	1:B:977:LEU:HD21	2.48	0.43
1:C:53:ASP:HB2	1:C:55:PHE:CE1	2.53	0.43
1:C:553:THR:HG22	1:C:554:GLU:N	2.33	0.43
1:C:736:VAL:HG11	1:C:1004:LEU:HD21	2.01	0.43
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.83	0.43
1:B:950:ASP:O	1:B:951:VAL:C	2.61	0.43
1:B:122:ASN:O	1:B:124:THR:N	2.39	0.43
1:C:676:THR:HA	1:C:690:GLN:HA	2.00	0.43
1:C:986:PRO:N	1:C:987:PRO:CD	2.82	0.43
1:A:551:VAL:HG22	1:A:588:THR:O	2.18	0.43
1:A:852:ALA:O	1:A:856:ASN:ND2	2.52	0.43
1:B:705:VAL:O	1:B:707:TYR:N	2.48	0.43
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.51	0.43
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.99	0.43
1:B:1081:ILE:HA	1:B:1133:VAL:O	2.19	0.43
1:C:382:VAL:CG1	1:C:387:LEU:HD21	2.30	0.43
1:C:734:THR:HG21	1:C:1007:TYR:OH	2.19	0.43
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.19	0.43
1:A:951:VAL:O	1:A:952:VAL:C	2.62	0.42
1:C:354:ASN:O	1:C:398:ASP:HA	2.19	0.42
1:A:520:ALA:O	1:A:522:ALA:N	2.53	0.42
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.02	0.42
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.51	0.42
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.83	0.42
1:A:946:GLY:O	1:A:947:LYS:C	2.62	0.42
1:B:65:PHE:CE1	1:B:84:LEU:HD11	2.54	0.42
1:C:1029:MET:HE2	1:C:1053:PRO:HB3	2.02	0.42
1:A:551:VAL:HG22	1:A:588:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HD11	1:B:541:PHE:HB3	2.02	0.42
1:C:376:THR:HB	1:C:435:ALA:HB3	2.01	0.42
1:C:533:LEU:HD11	1:C:585:LEU:HD11	2.01	0.42
1:C:927:PHE:HE1	1:C:1065:VAL:HG21	1.85	0.42
1:A:290:ASP:HB3	1:A:293:LEU:HB2	2.01	0.42
1:A:1028:LYS:O	1:A:1032:CYS:CB	2.67	0.42
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.20	0.42
1:B:749:CYS:HB2	1:B:977:LEU:HD21	2.01	0.42
1:C:945:LEU:O	1:C:946:GLY:C	2.63	0.42
1:B:382:VAL:HG23	1:B:430:THR:HG23	2.02	0.42
1:C:329:PHE:CD2	1:C:391:CYS:SG	3.13	0.42
1:C:329:PHE:HD2	1:C:391:CYS:SG	2.42	0.42
1:A:196:ASN:O	1:A:197:ILE:HD12	2.20	0.41
1:A:569:ILE:HD13	1:B:849:LEU:HG	2.02	0.41
1:B:57:PRO:O	1:B:60:SER:OG	2.21	0.41
1:A:900:MET:HE3	1:A:900:MET:HB2	1.91	0.41
1:B:949:GLN:O	1:B:950:ASP:C	2.63	0.41
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.55	0.41
1:B:130:VAL:HB	1:B:233:ILE:HD11	2.01	0.41
1:B:915:VAL:O	1:B:919:ASN:ND2	2.47	0.41
1:B:984:LEU:HB2	1:B:989:ALA:HB2	2.01	0.41
1:B:1116:THR:HG22	1:B:1138:TYR:HD2	1.86	0.41
1:C:946:GLY:O	1:C:947:LYS:C	2.63	0.41
1:A:900:MET:HE1	1:C:1077:THR:HG23	2.03	0.41
1:A:613:GLN:O	1:A:615:VAL:HG13	2.21	0.41
1:A:585:LEU:O	1:A:585:LEU:HD12	2.21	0.41
1:A:801:ASN:ND2	2:F:1:NAG:O7	2.54	0.41
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.69	0.41
1:C:45:SER:O	1:C:47:VAL:HG23	2.21	0.41
1:C:391:CYS:HA	1:C:524:VAL:O	2.21	0.41
1:C:749:CYS:HB2	1:C:977:LEU:HD21	2.02	0.41
1:A:106:PHE:HB3	1:A:235:ILE:CD1	2.51	0.41
1:A:215:ASP:HA	1:A:266:TYR:OH	2.21	0.41
1:B:48:LEU:HD23	1:B:278:LYS:HA	2.02	0.41
1:C:902:MET:HE1	1:C:1049:LEU:HD13	2.03	0.41
1:C:1103:PHE:HZ	2:N:1:NAG:H62	1.85	0.41
1:A:519:HIS:CD2	1:A:546:LEU:HD21	2.56	0.41
1:A:950:ASP:O	1:A:951:VAL:C	2.64	0.41
1:B:86:PHE:O	1:B:86:PHE:CD2	2.75	0.40
1:B:902:MET:HE1	1:B:1049:LEU:HD13	2.03	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:ASP:O	1:C:951:VAL:C	2.64	0.40
1:C:1118:ASP:OD1	1:C:1118:ASP:O	2.39	0.40
1:B:709:ASN:OD1	1:B:709:ASN:N	2.55	0.40
1:C:118:LEU:HG	1:C:120:VAL:HG23	2.02	0.40
1:C:706:ALA:CB	3:C:1311:NAG:H5	2.52	0.40
1:A:538:CYS:HB3	1:A:551:VAL:HG12	2.01	0.40
1:A:1141:LEU:HG	1:A:1145:LEU:HD13	2.02	0.40
1:B:360:ASN:HA	1:B:523:THR:HB	2.01	0.40
1:A:1028:LYS:O	1:A:1032:CYS:HB3	2.22	0.40
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.55	0.40
1:B:335:LEU:HD23	1:B:336:CYS:H	1.86	0.40
1:B:384:PRO:HA	1:B:387:LEU:HD12	2.04	0.40
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.57	0.40
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.86	0.40
1:C:320:VAL:HG12	1:C:321:GLN:H	1.86	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	977/1288 (76%)	932 (95%)	45 (5%)	0	100	100
1	B	969/1288 (75%)	927 (96%)	42 (4%)	0	100	100
1	C	975/1288 (76%)	924 (95%)	51 (5%)	0	100	100
All	All	2921/3864 (76%)	2783 (95%)	138 (5%)	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	834/1113 (75%)	828 (99%)	6 (1%)	81 88
1	B	824/1113 (74%)	816 (99%)	8 (1%)	73 83
1	C	822/1113 (74%)	818 (100%)	4 (0%)	86 91
All	All	2480/3339 (74%)	2462 (99%)	18 (1%)	80 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	CYS
1	A	615	VAL
1	A	723	THR
1	A	866	THR
1	A	878	LEU
1	A	1133	VAL
1	B	229	LEU
1	B	289	VAL
1	B	301	CYS
1	B	302	THR
1	B	603	ASN
1	B	723	THR
1	B	1094	VAL
1	B	1132	ILE
1	C	331	ASN
1	C	515	PHE
1	C	517	LEU
1	C	738	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	544	ASN
1	A	853	GLN

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Mol	Chain	Res	Type
1	A	856	ASN
1	A	1002	GLN
1	B	99	ASN
1	B	321	GLN
1	B	414	GLN
1	B	762	GLN
1	B	1002	GLN
1	B	1101	HIS
1	C	234	ASN
1	C	321	GLN
1	C	414	GLN
1	C	501	ASN
1	C	563	GLN
1	C	703	ASN
1	C	764	ASN
1	C	804	GLN
1	C	856	ASN
1	C	935	GLN
1	C	969	ASN
1	C	1083	HIS
1	C	1108	ASN

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

22 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	0.56	1 (7%)	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	E	1	1,2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	F	1	1,2	14,14,15	0.29	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	G	1	1,2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	G	2	2	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	H	1	1,2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	I	1	1,2	14,14,15	0.31	0	17,19,21	0.42	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	J	1	1,2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	J	2	2	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	K	1	1,2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	L	1	1,2	14,14,15	0.32	0	17,19,21	0.38	0
2	NAG	L	2	2	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	M	1	1,2	14,14,15	0.40	0	17,19,21	0.45	0
2	NAG	M	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	N	1	1,2	14,14,15	0.27	0	17,19,21	0.54	0
2	NAG	N	2	2	14,14,15	0.24	0	17,19,21	0.38	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	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	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	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	-2.04	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

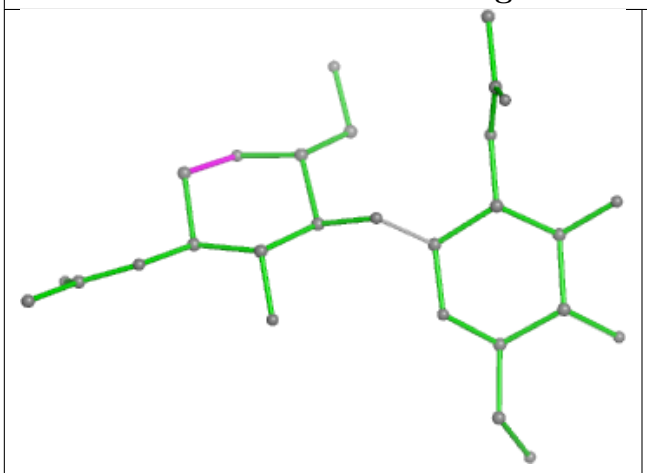
There are no ring outliers.

2 monomers are involved in 2 short contacts:

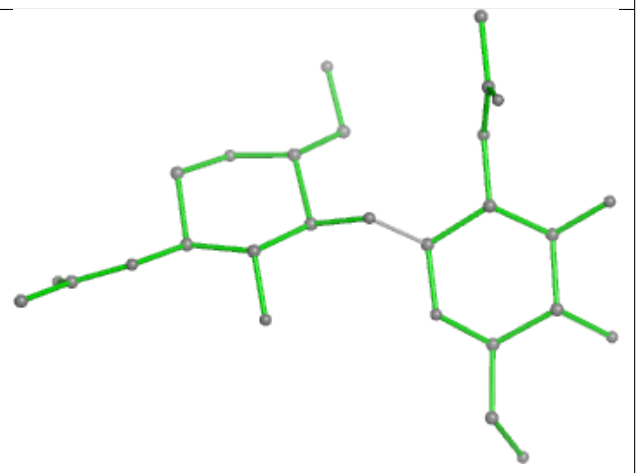
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	NAG	1	0
2	F	1	NAG	1	0

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

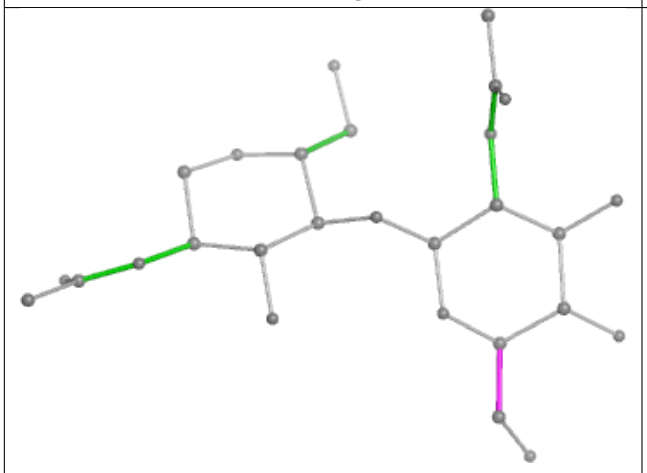
Oligosaccharide Chain D



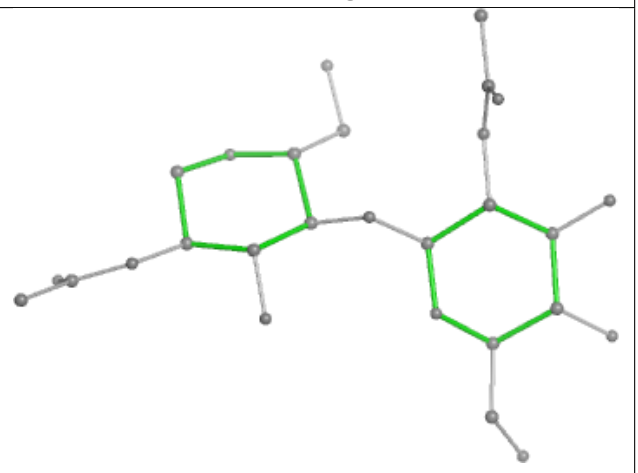
Bond lengths



Bond angles

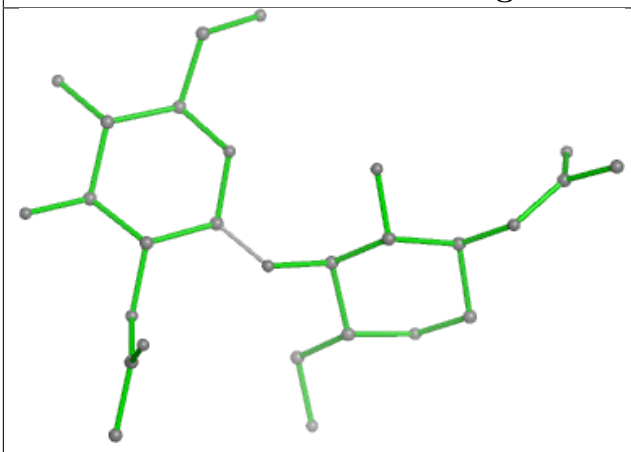


Torsions

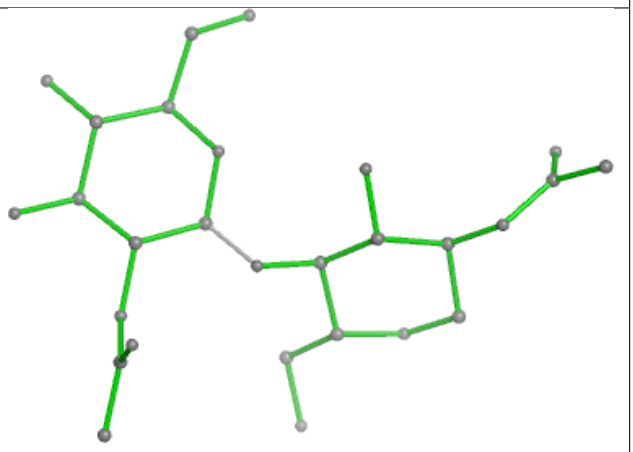


Rings

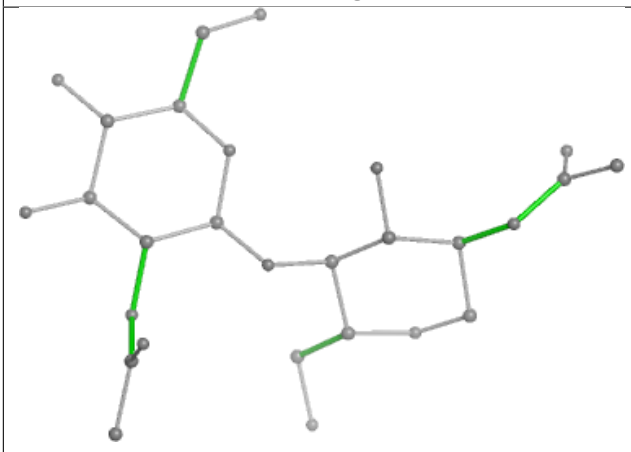
Oligosaccharide Chain E



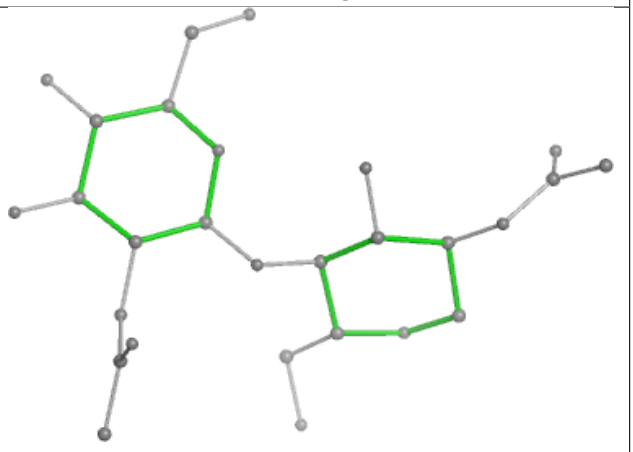
Bond lengths



Bond angles

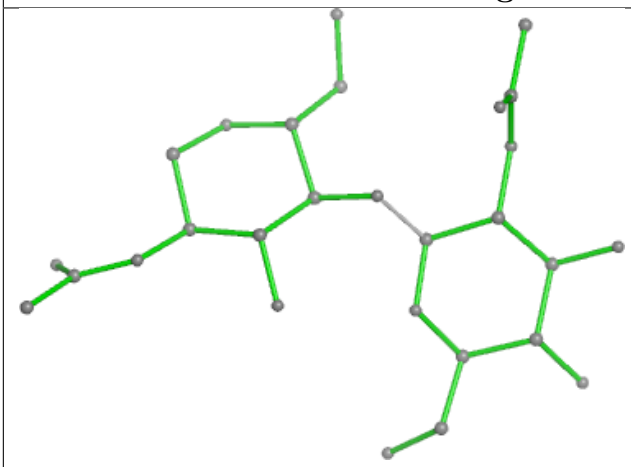


Torsions

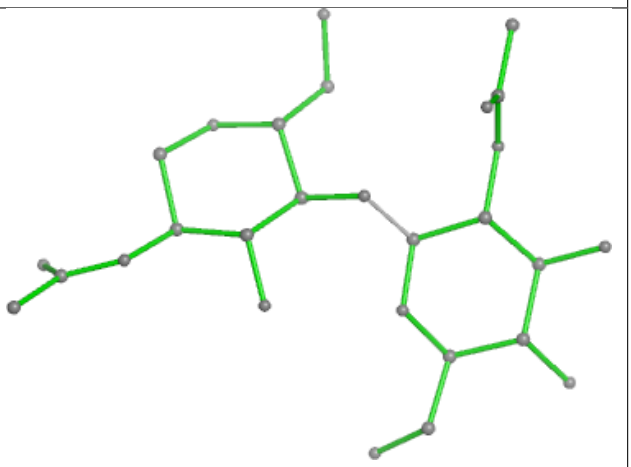


Rings

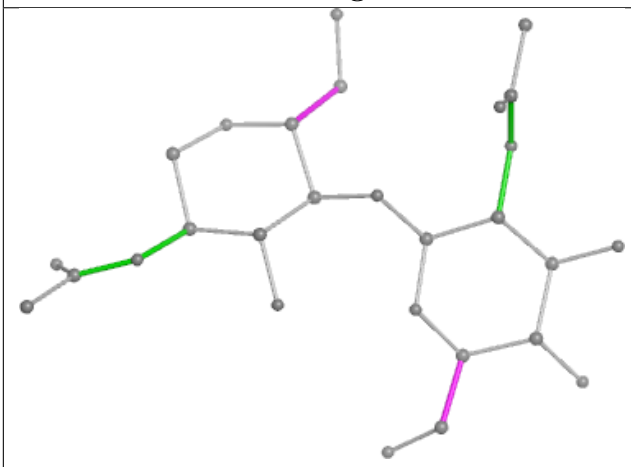
Oligosaccharide Chain F



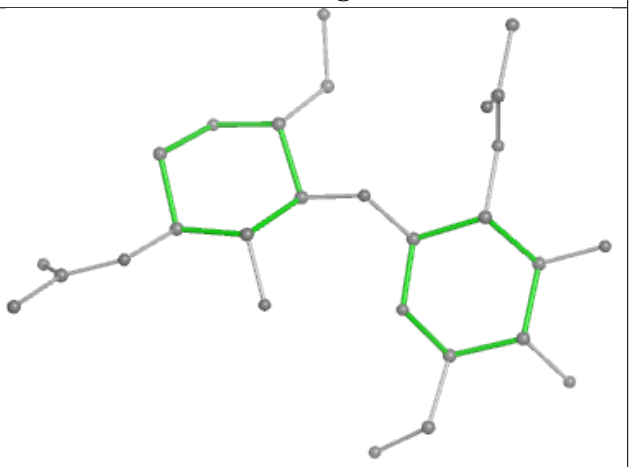
Bond lengths



Bond angles

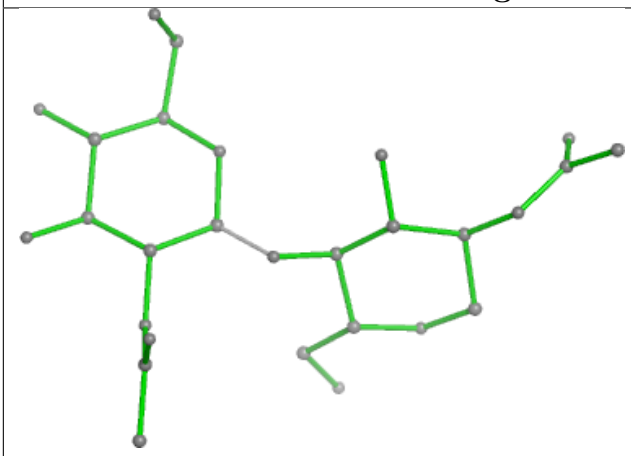


Torsions

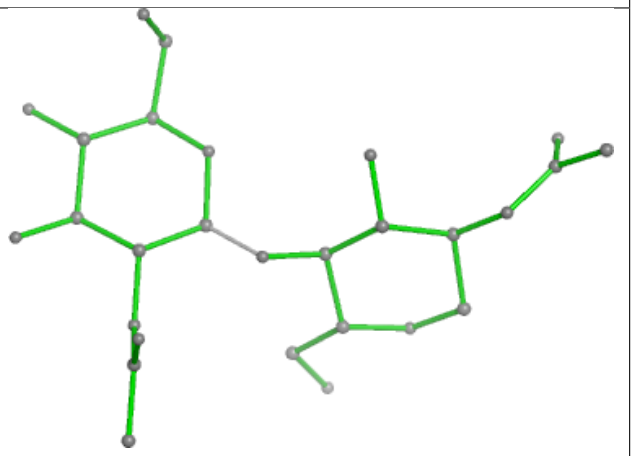


Rings

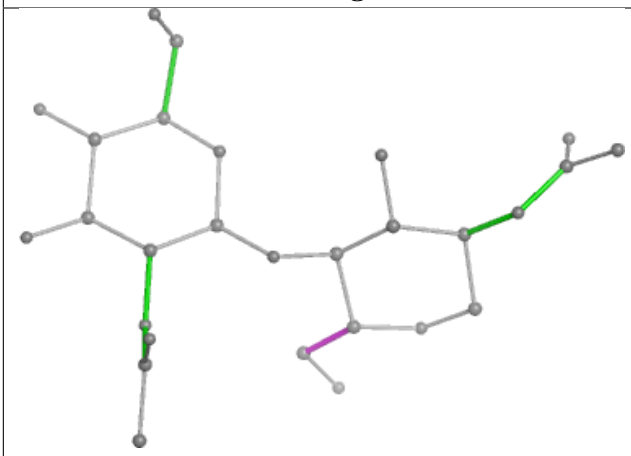
Oligosaccharide Chain G



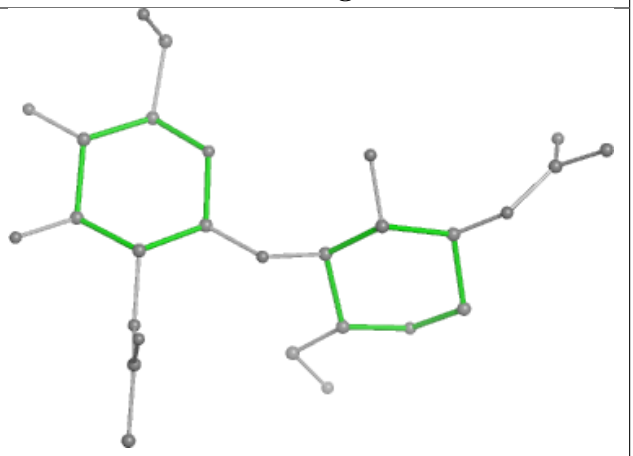
Bond lengths



Bond angles

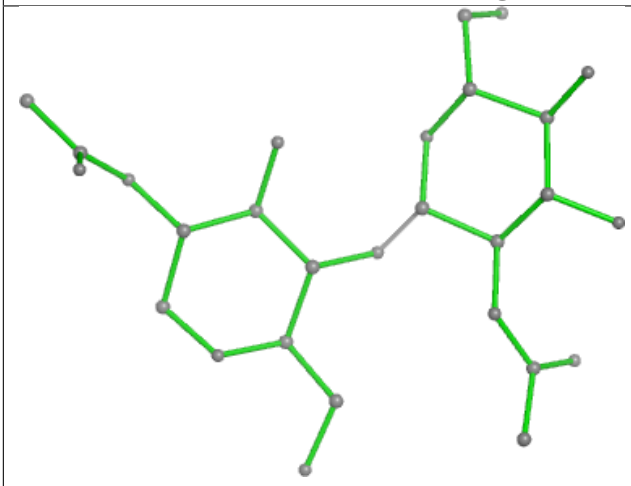


Torsions

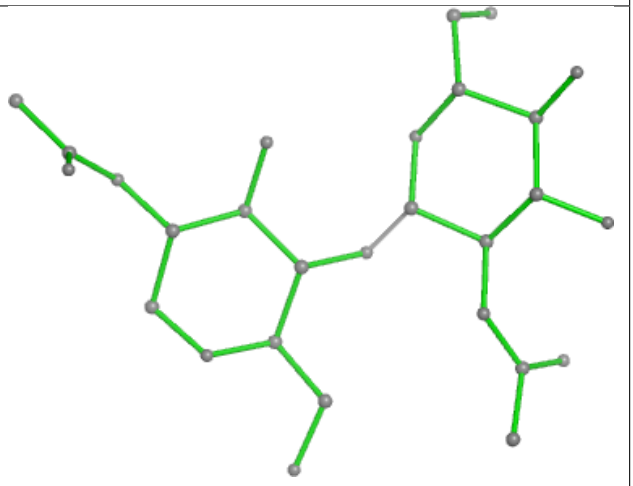


Rings

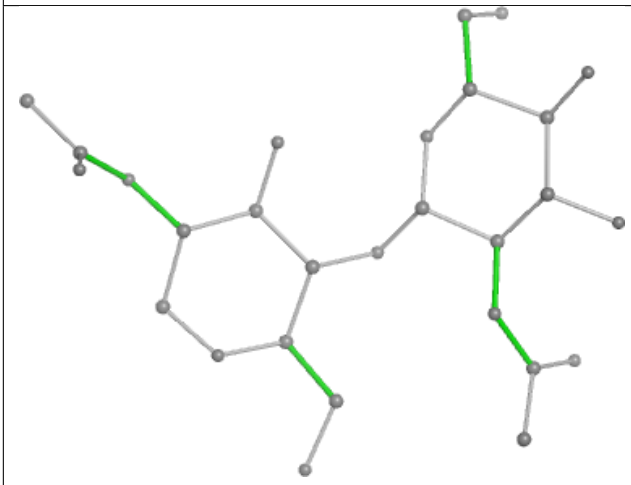
Oligosaccharide Chain H



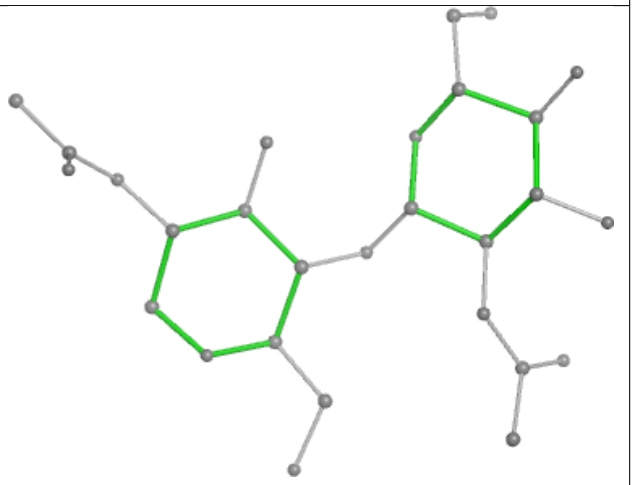
Bond lengths



Bond angles

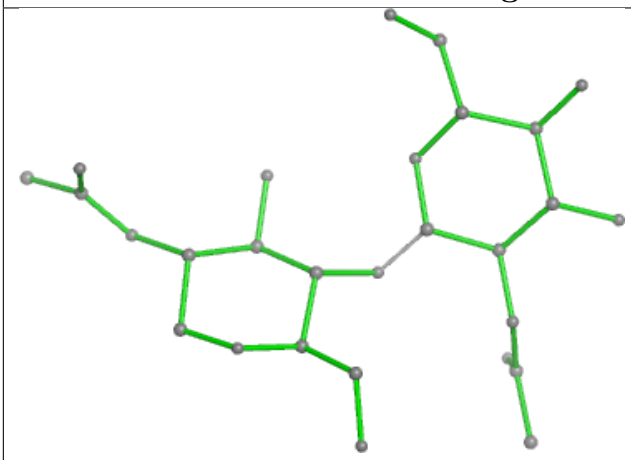


Torsions

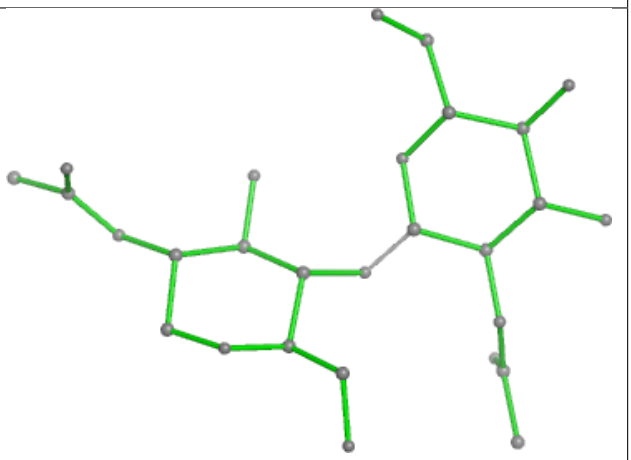


Rings

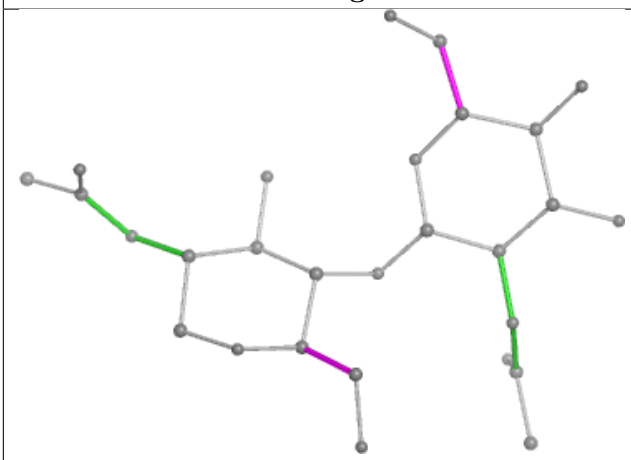
Oligosaccharide Chain I



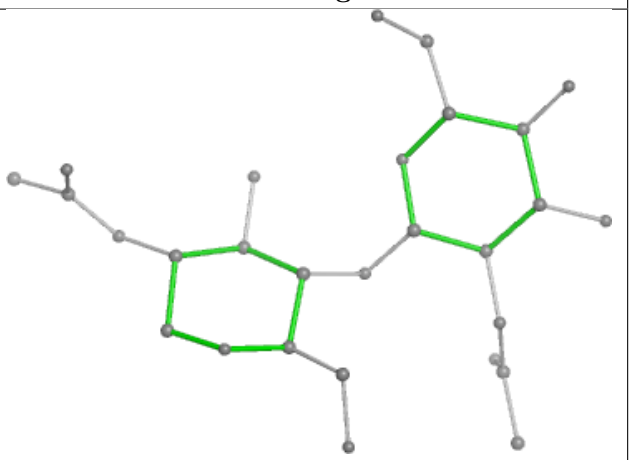
Bond lengths



Bond angles

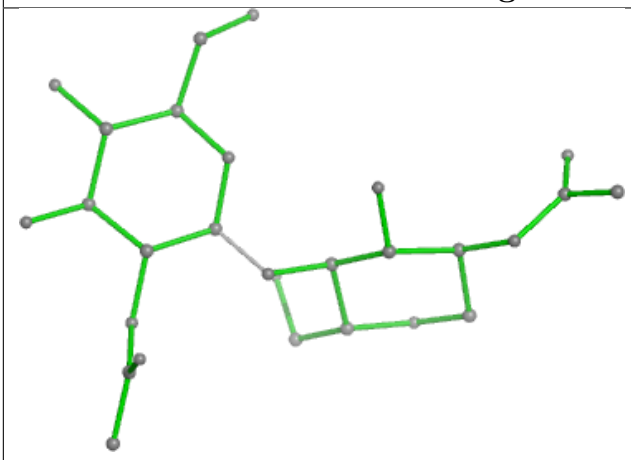


Torsions

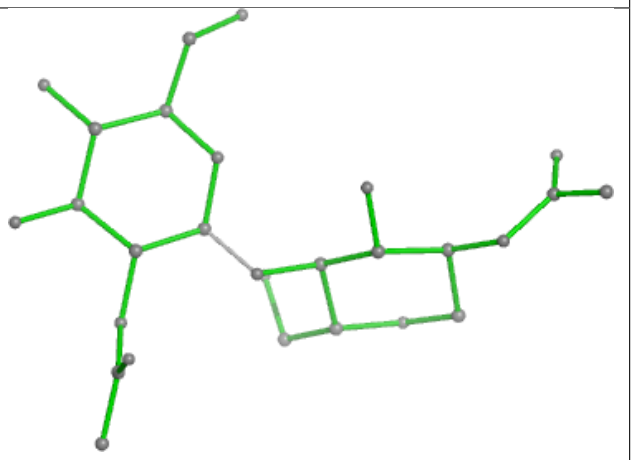


Rings

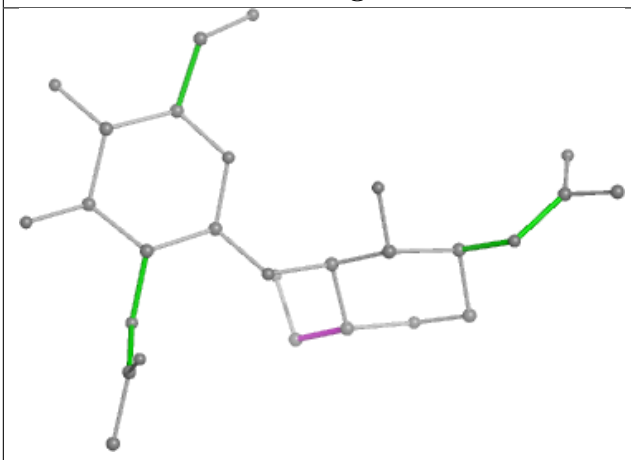
Oligosaccharide Chain J



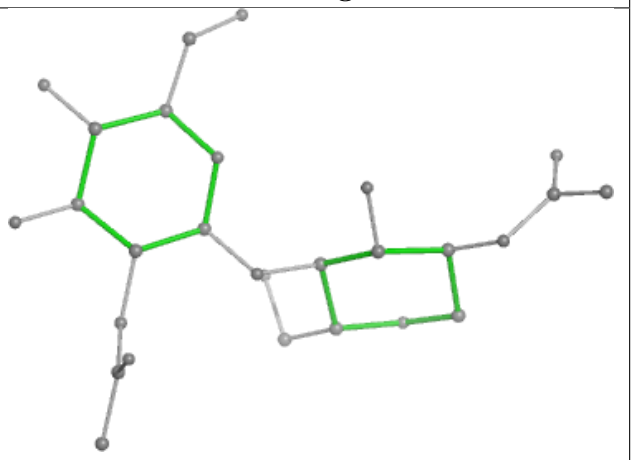
Bond lengths



Bond angles

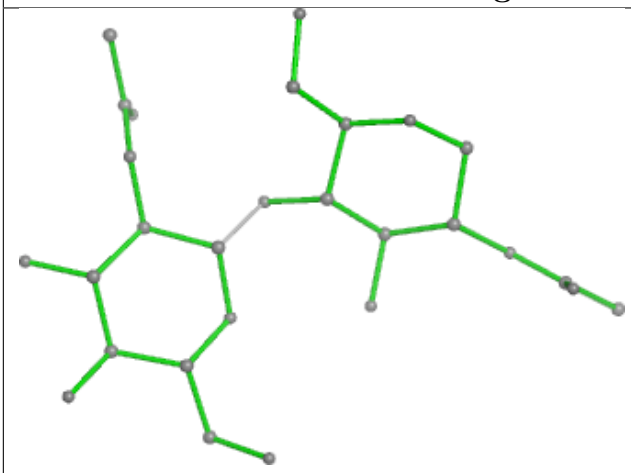


Torsions

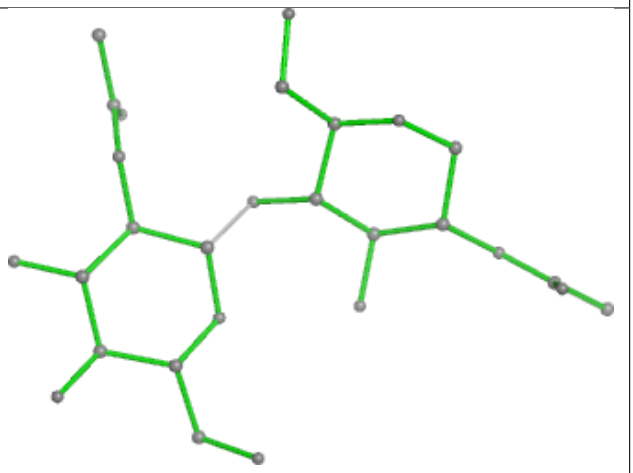


Rings

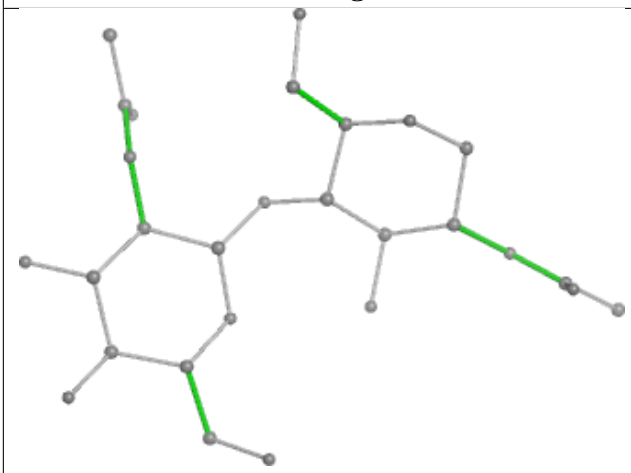
Oligosaccharide Chain K



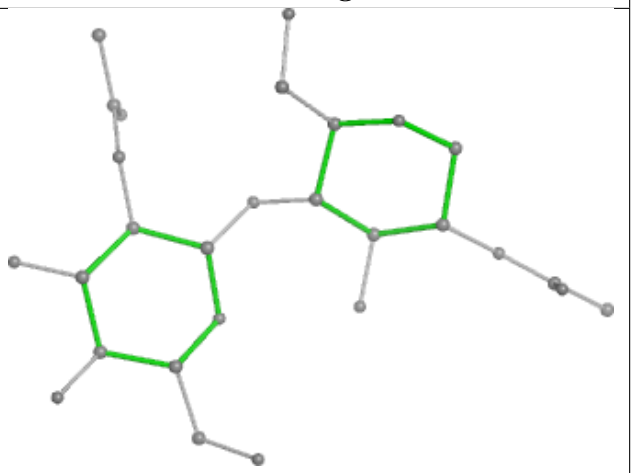
Bond lengths



Bond angles

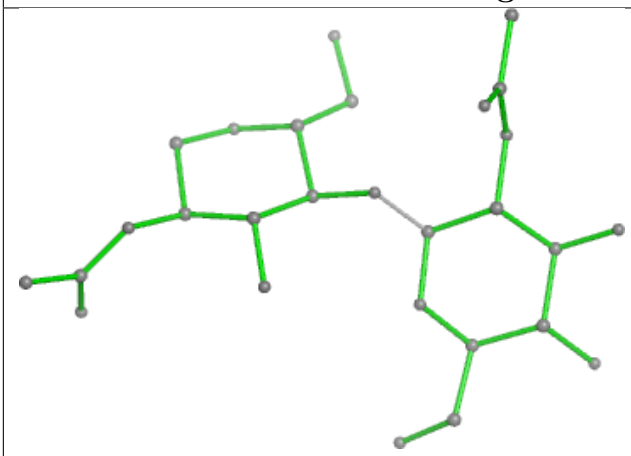


Torsions

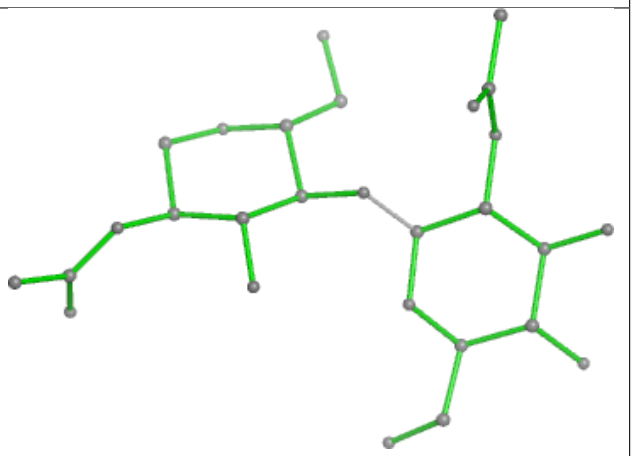


Rings

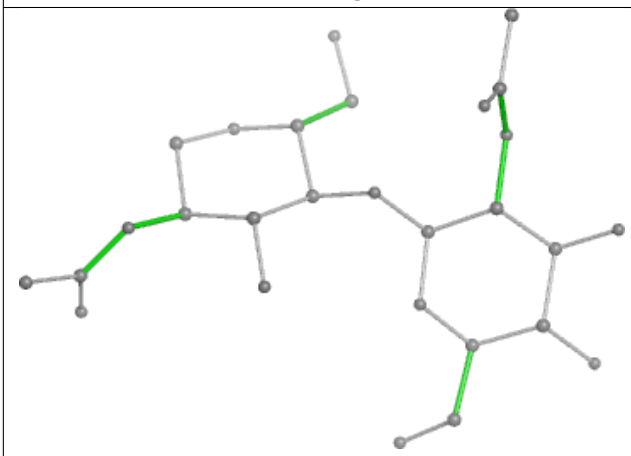
Oligosaccharide Chain L



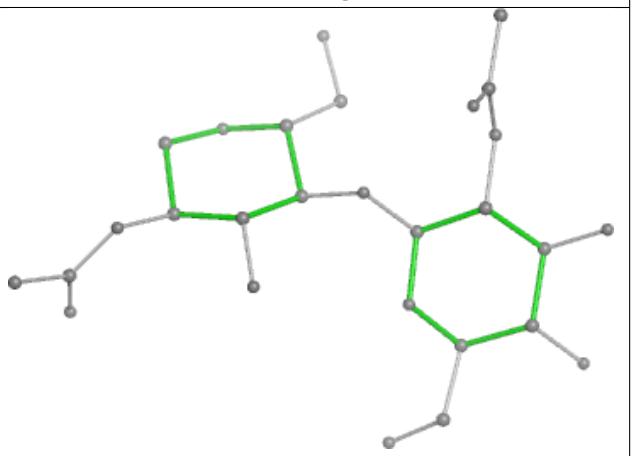
Bond lengths



Bond angles

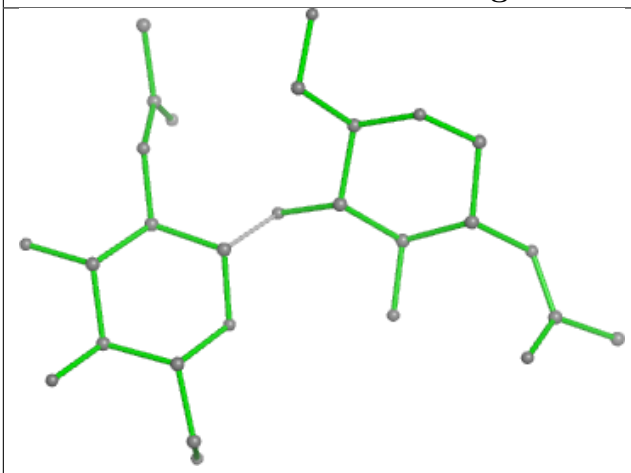


Torsions

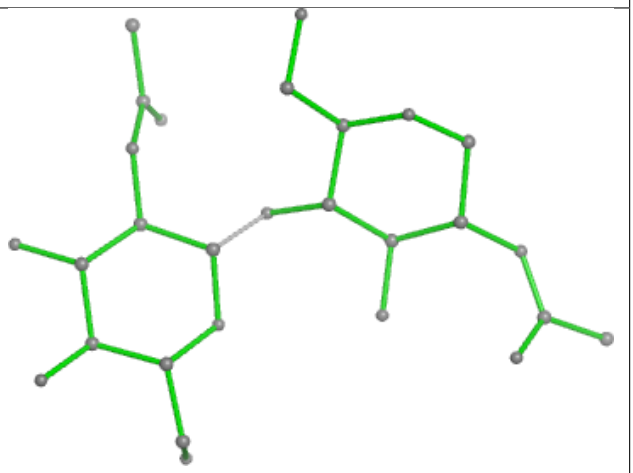


Rings

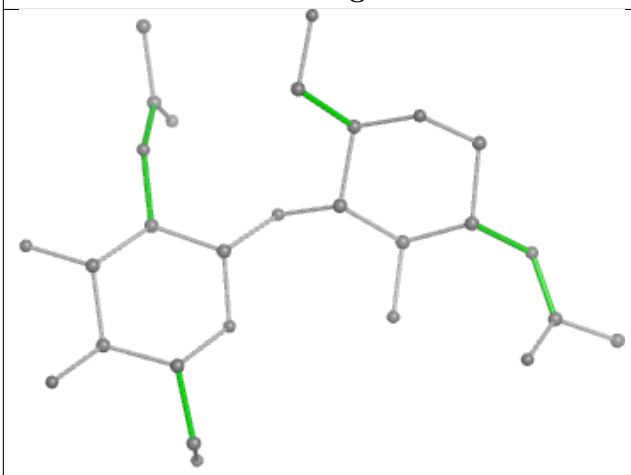
Oligosaccharide Chain M



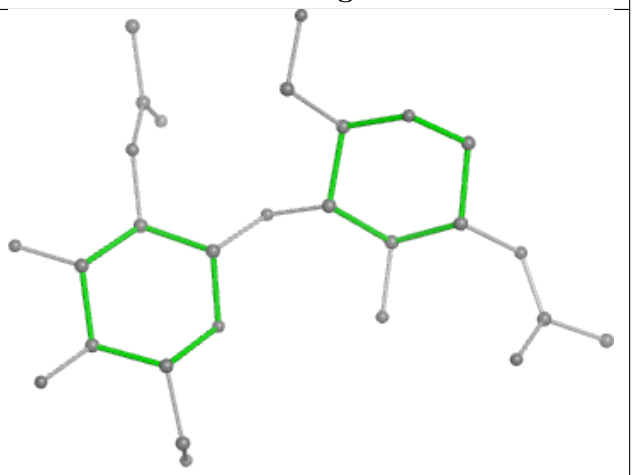
Bond lengths



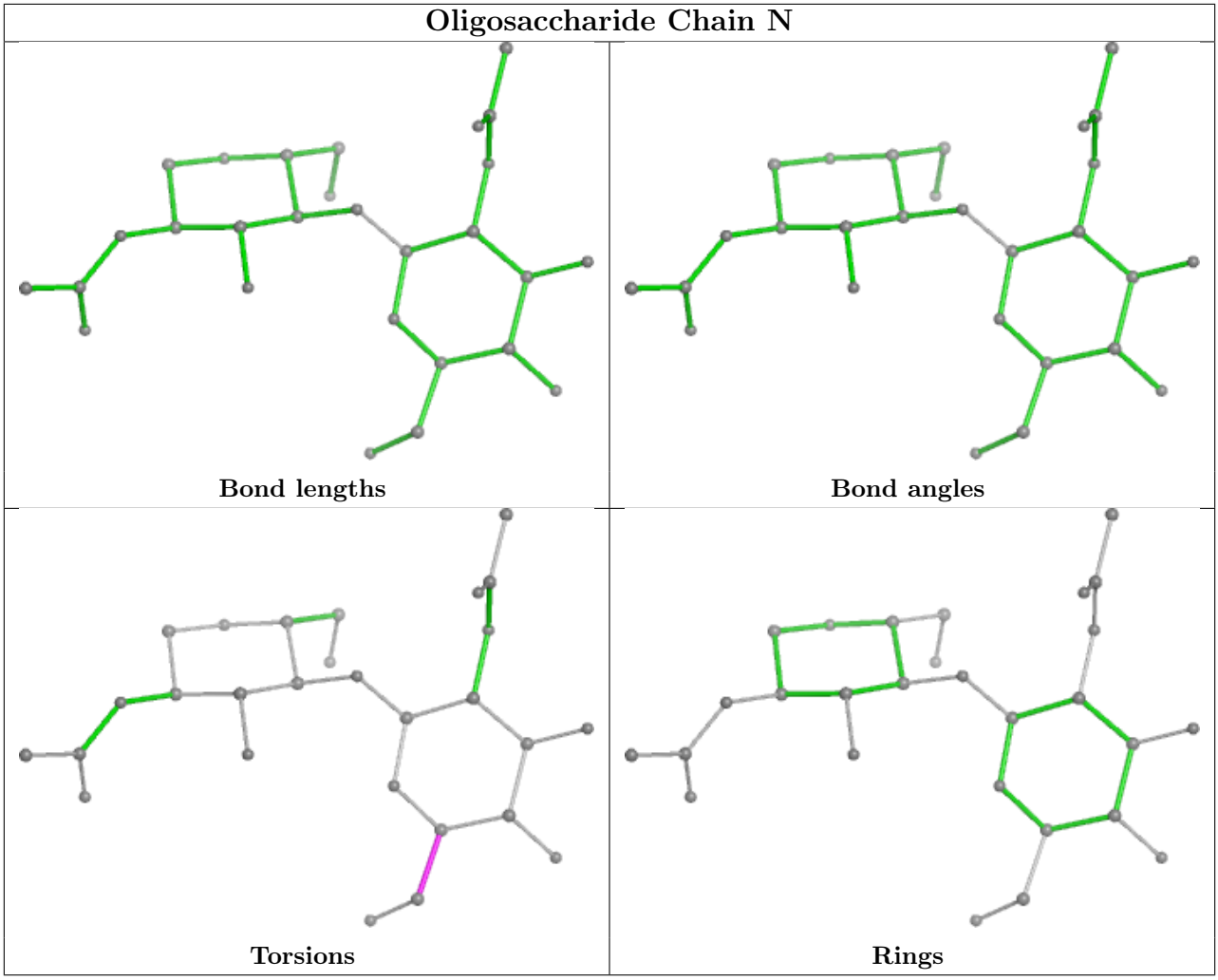
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

27 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	C	1301	1	14,14,15	0.32	0	17,19,21	0.39	0
3	NAG	C	1314	1	14,14,15	0.39	0	17,19,21	0.52	0
3	NAG	B	1301	1	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
3	NAG	B	1304	1	14,14,15	0.31	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1313	1	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.38	0
3	NAG	B	1303	1	14,14,15	0.46	0	17,19,21	0.62	0
3	NAG	B	1309	1	14,14,15	0.17	0	17,19,21	0.40	0
3	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.37	0
3	NAG	A	1305	1	14,14,15	0.79	1 (7%)	17,19,21	0.50	0
3	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.36	0
3	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	A	1308	1	14,14,15	0.40	0	17,19,21	0.33	0
3	NAG	B	1308	1	14,14,15	0.34	0	17,19,21	0.44	0
3	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.34	0
3	NAG	B	1310	1	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.75	1 (5%)
3	NAG	A	1314	1	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	C	1311	1	14,14,15	0.36	0	17,19,21	0.54	0
3	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.58	0
3	NAG	A	1306	1	14,14,15	0.66	1 (7%)	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.18	0	17,19,21	0.40	0
3	NAG	A	1307	1	14,14,15	0.27	0	17,19,21	0.79	1 (5%)
3	NAG	B	1307	1	14,14,15	0.35	0	17,19,21	0.38	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	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	NAG	O5-C1	-2.87	1.39	1.43
3	A	1306	NAG	O5-C1	-2.38	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1301	NAG	C1-O5-C5	3.90	117.48	112.19
3	A	1307	NAG	C1-O5-C5	2.91	116.13	112.19
3	B	1302	NAG	C1-O5-C5	2.70	115.86	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1305	NAG	O5-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	A	1314	NAG	O5-C5-C6-O6
3	B	1313	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1305	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1307	NAG	C1-C2-N2-C7
3	B	1303	NAG	O5-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	A	1314	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6

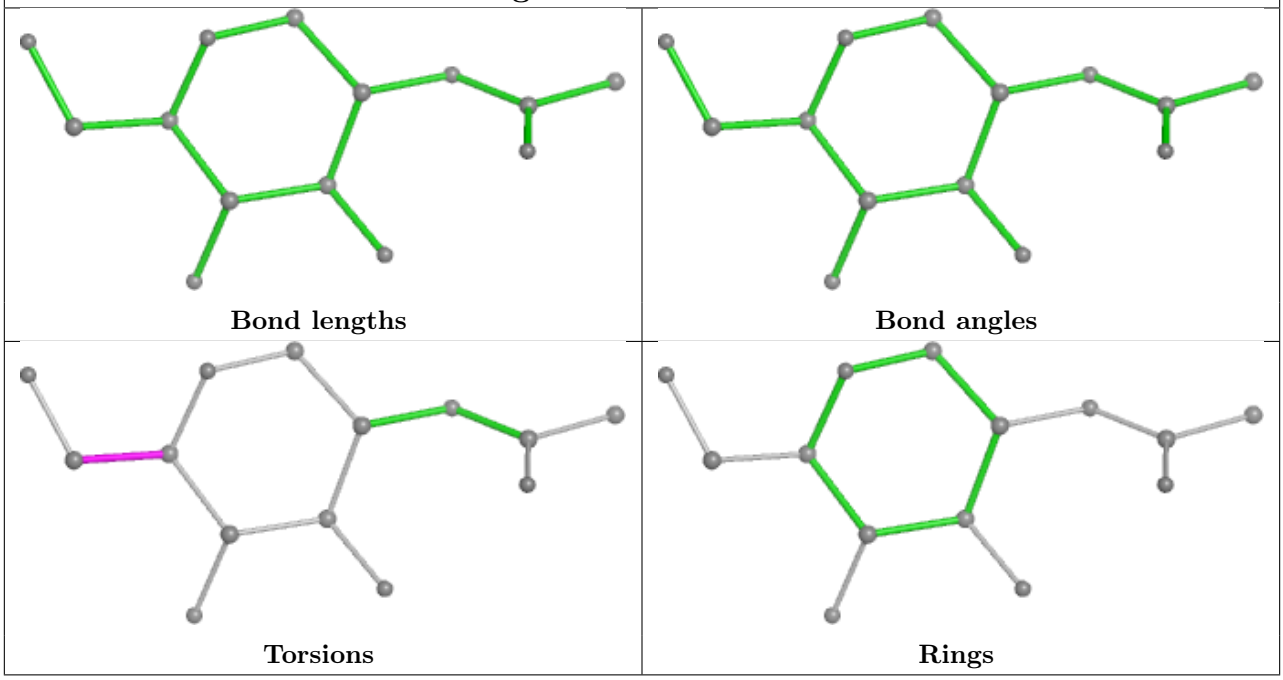
There are no ring outliers.

1 monomer is involved in 1 short contact:

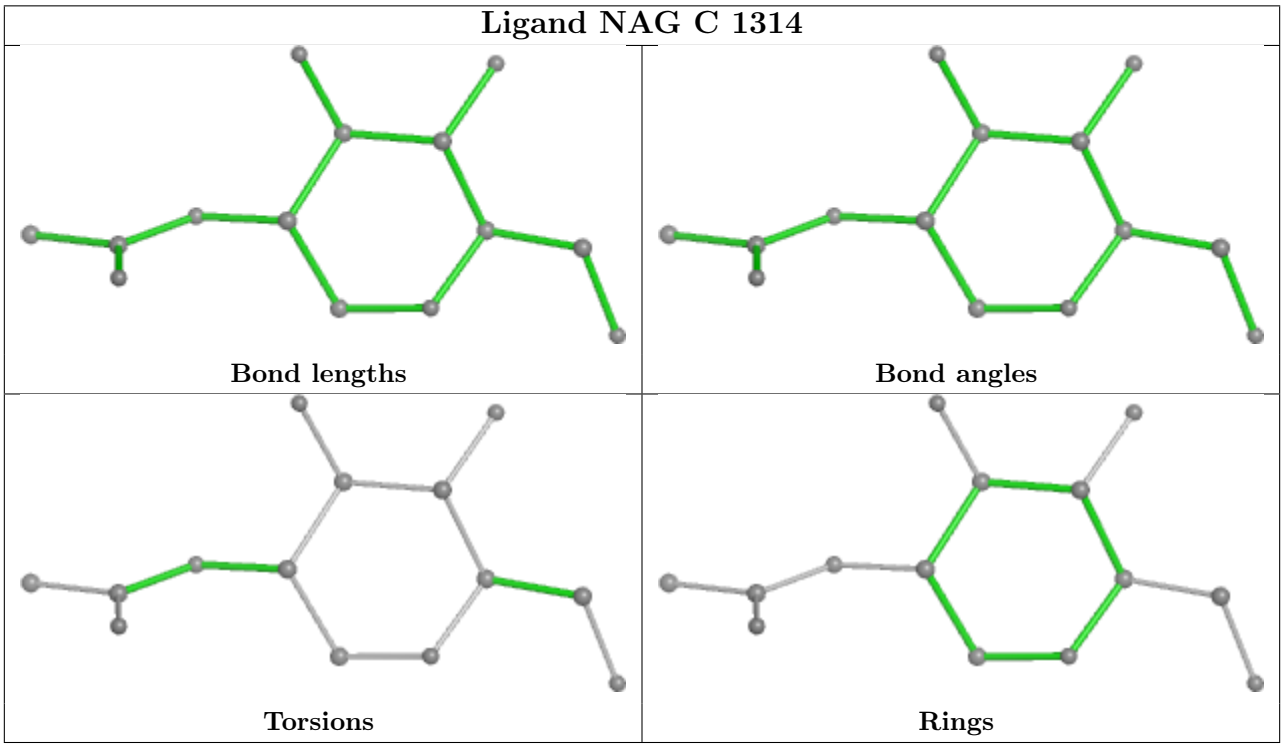
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1311	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

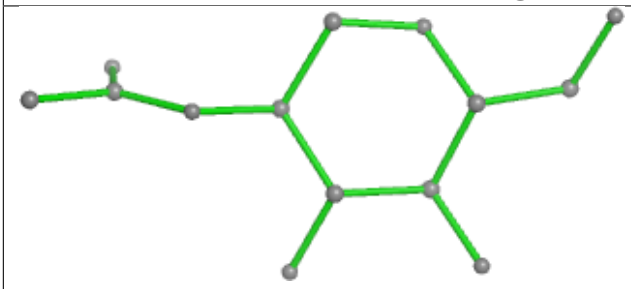
Ligand NAG C 1301



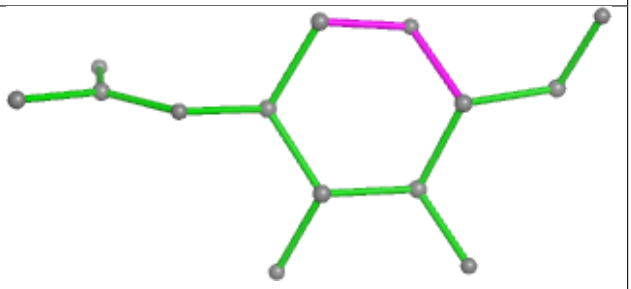
Ligand NAG C 1314



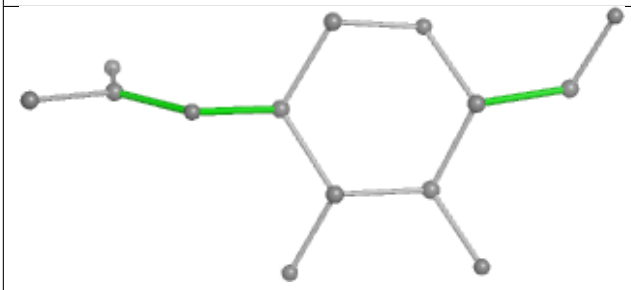
Ligand NAG B 1301



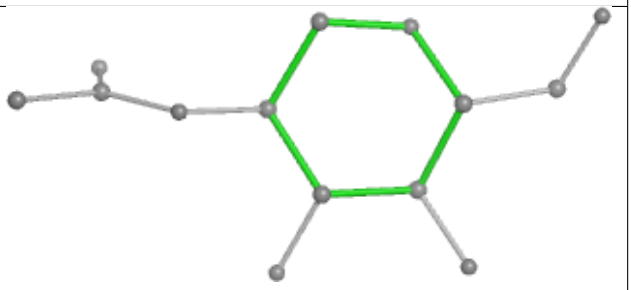
Bond lengths



Bond angles

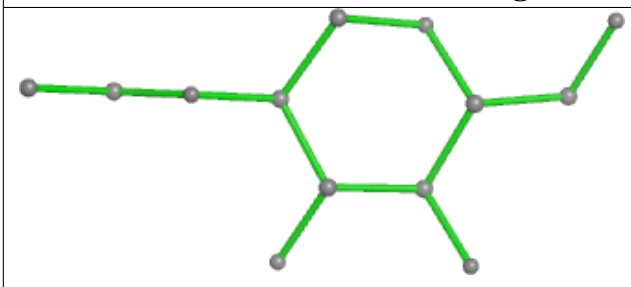


Torsions

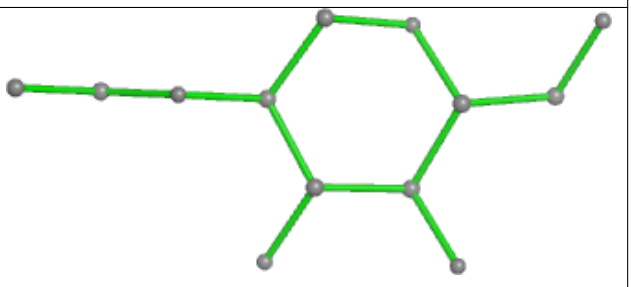


Rings

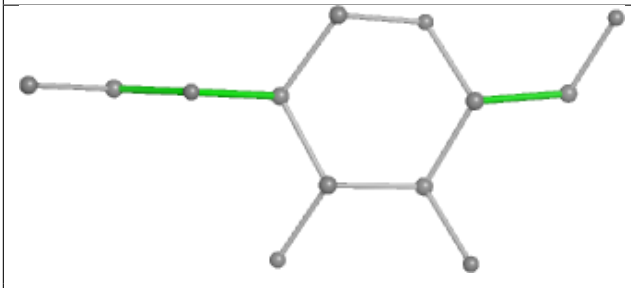
Ligand NAG B 1304



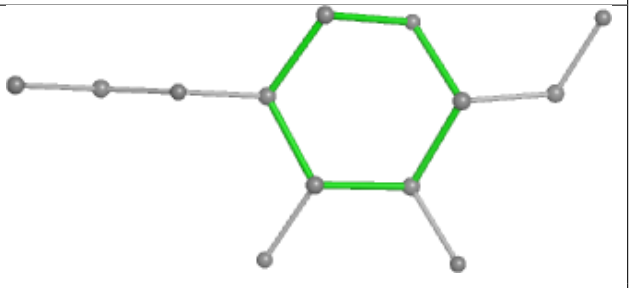
Bond lengths



Bond angles

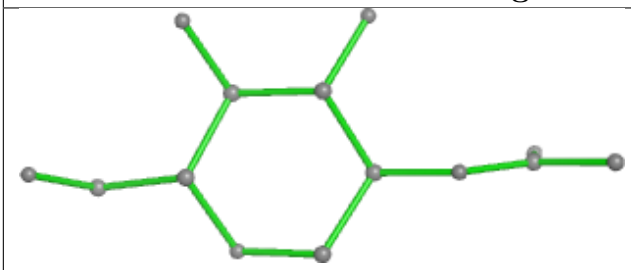


Torsions

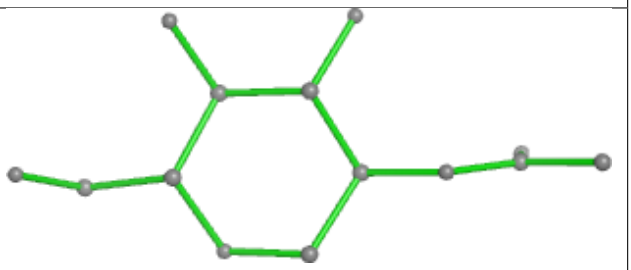


Rings

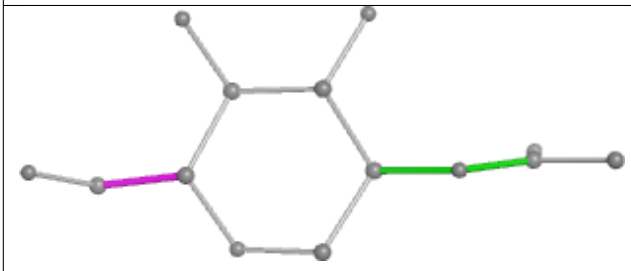
Ligand NAG B 1313



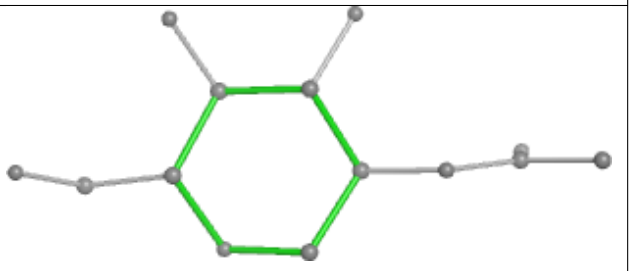
Bond lengths



Bond angles

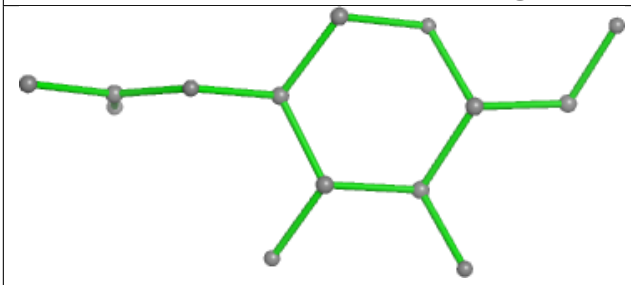


Torsions

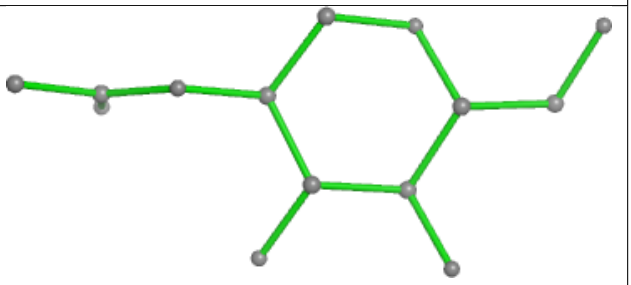


Rings

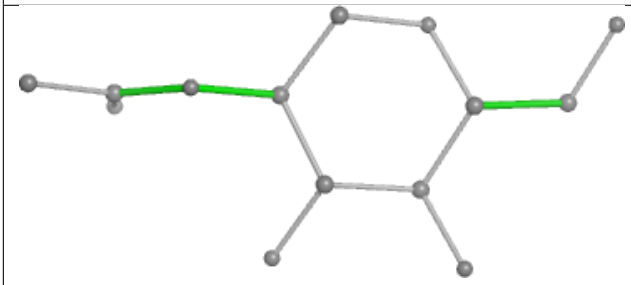
Ligand NAG C 1302



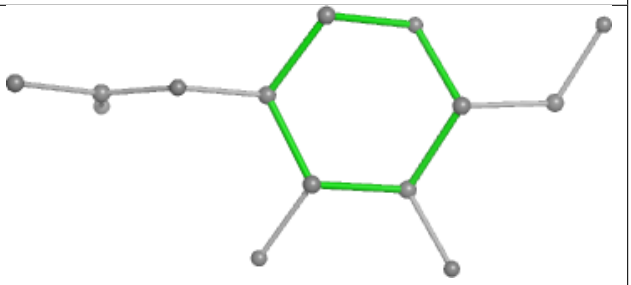
Bond lengths



Bond angles

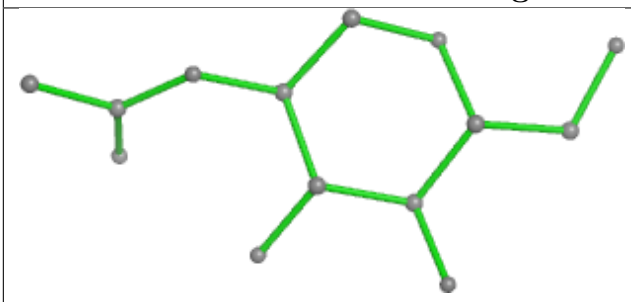


Torsions

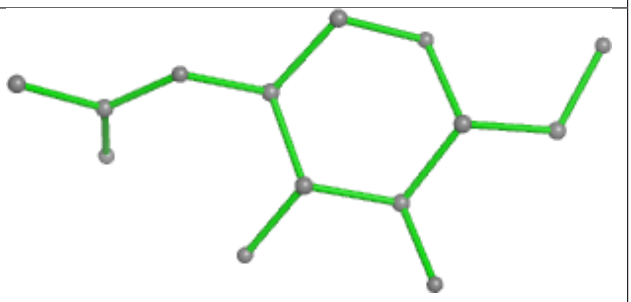


Rings

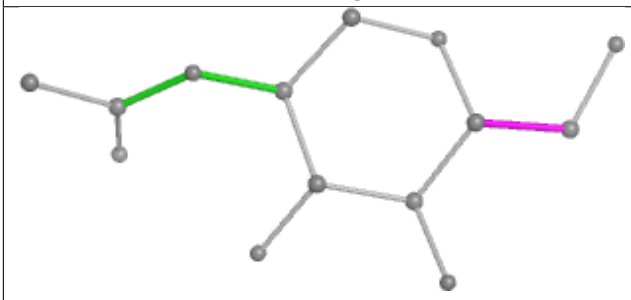
Ligand NAG B 1303



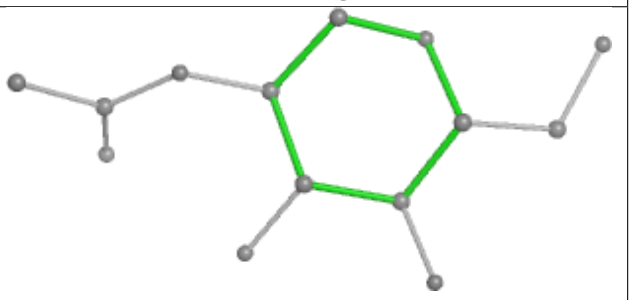
Bond lengths



Bond angles

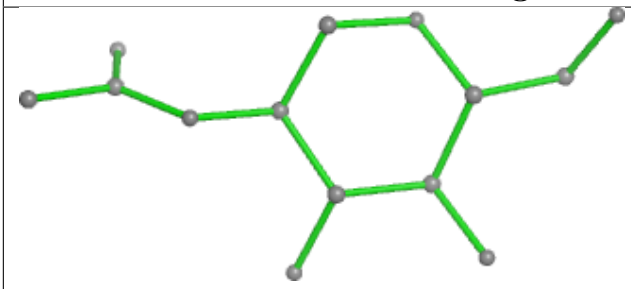


Torsions

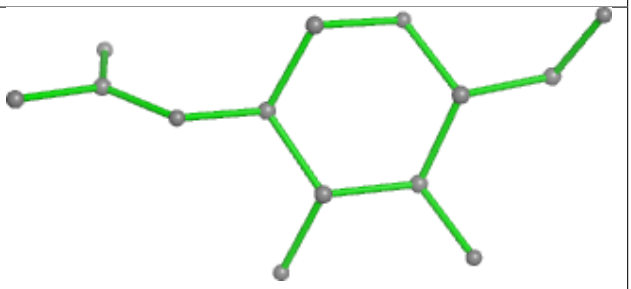


Rings

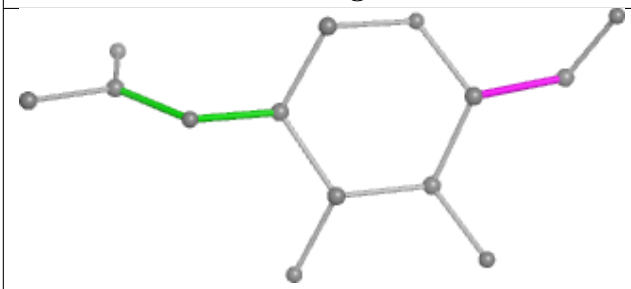
Ligand NAG B 1309



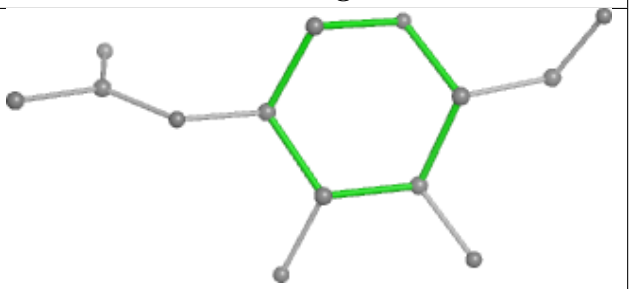
Bond lengths



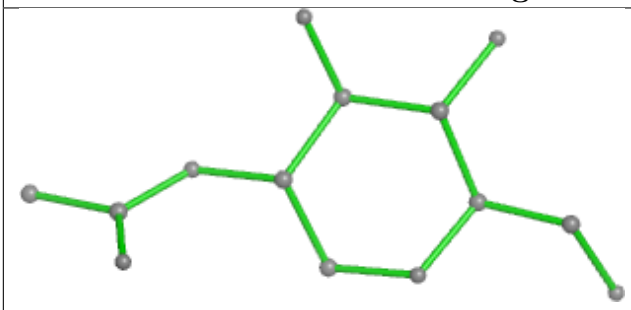
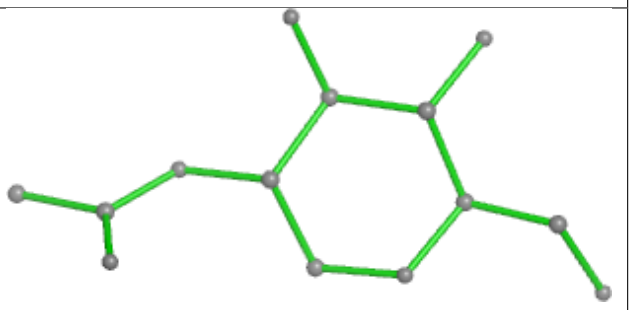
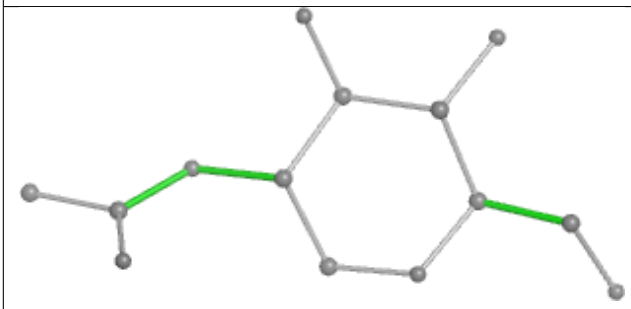
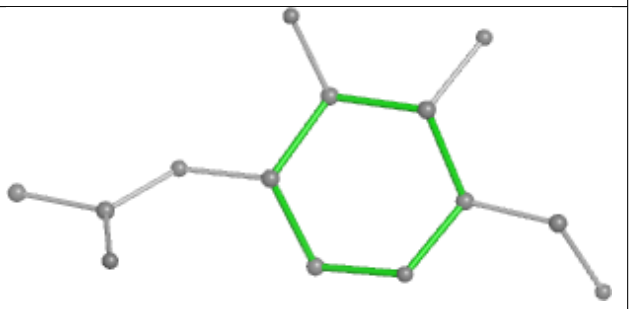
Bond angles

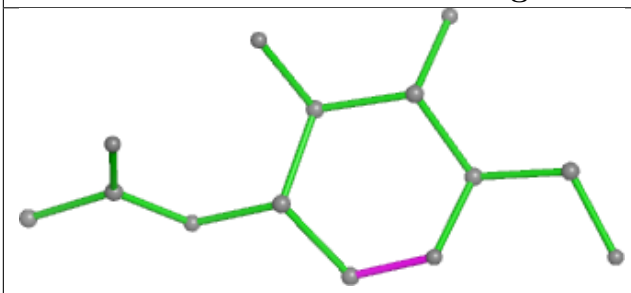
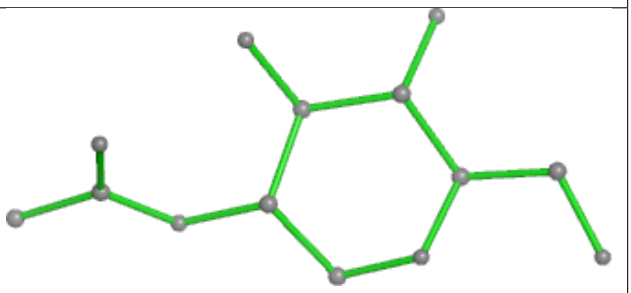
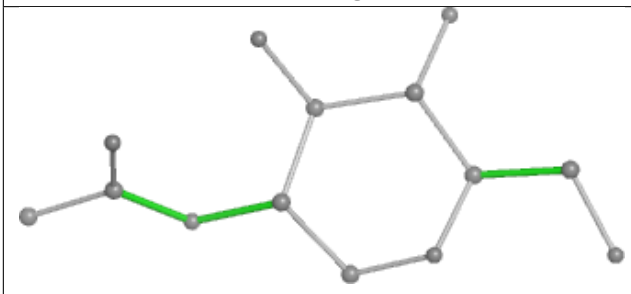
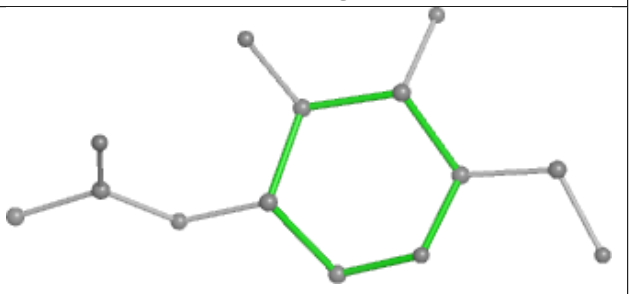


Torsions

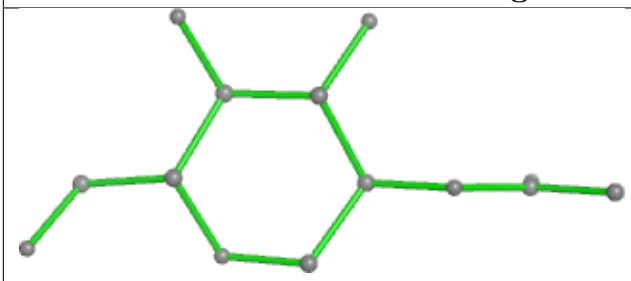


Rings

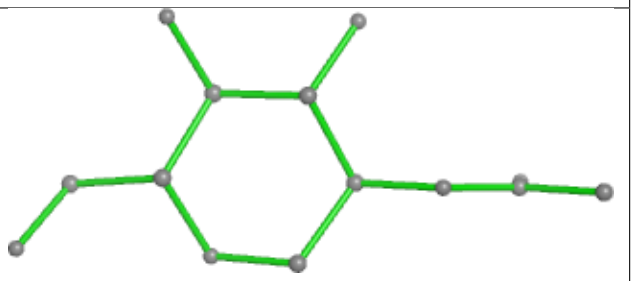
Ligand NAG B 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

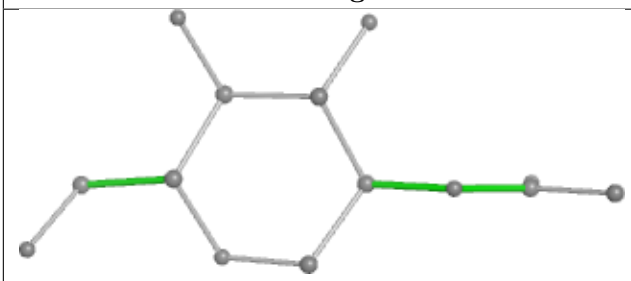
Ligand NAG A 1303



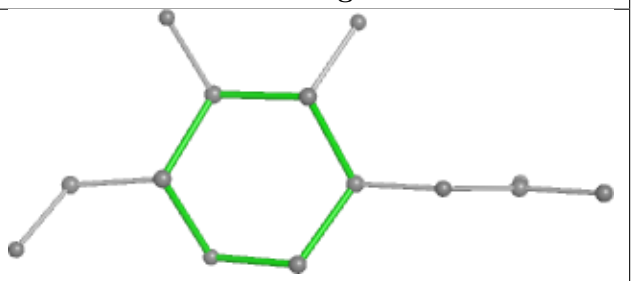
Bond lengths



Bond angles

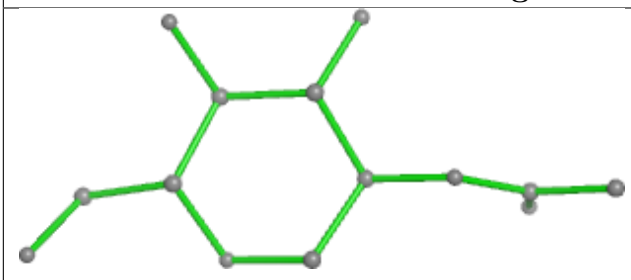


Torsions

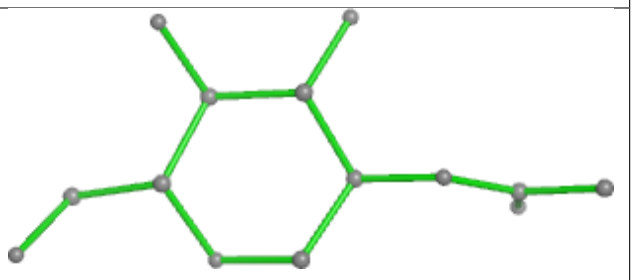


Rings

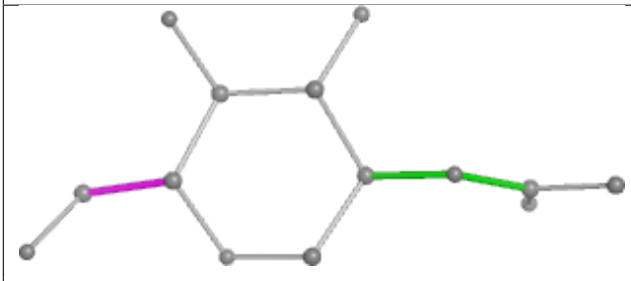
Ligand NAG C 1304



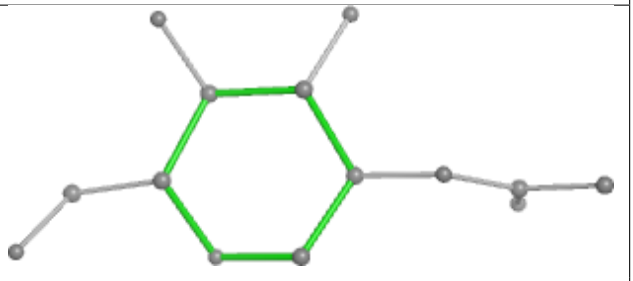
Bond lengths



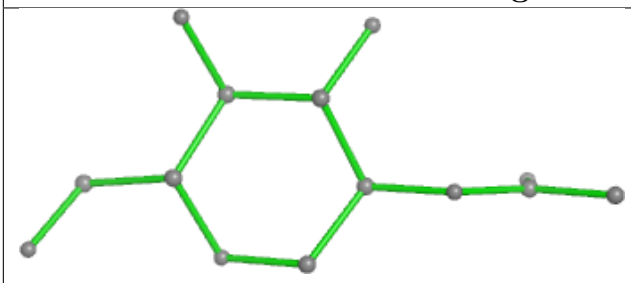
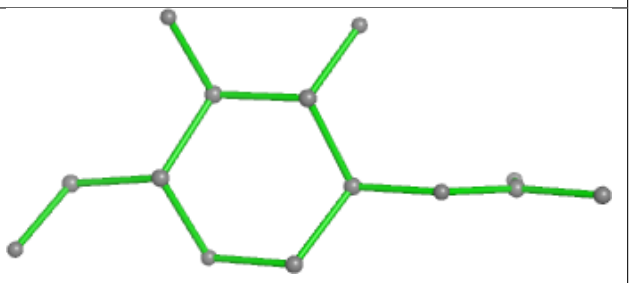
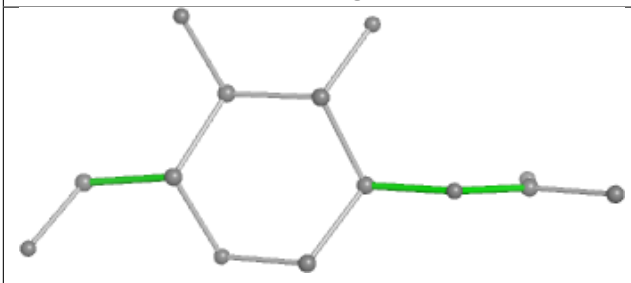
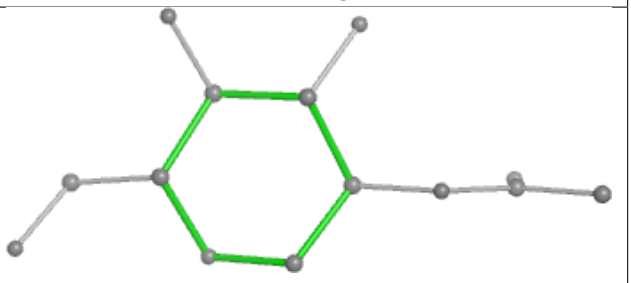
Bond angles

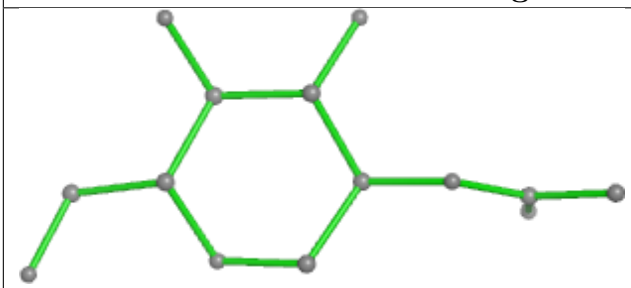
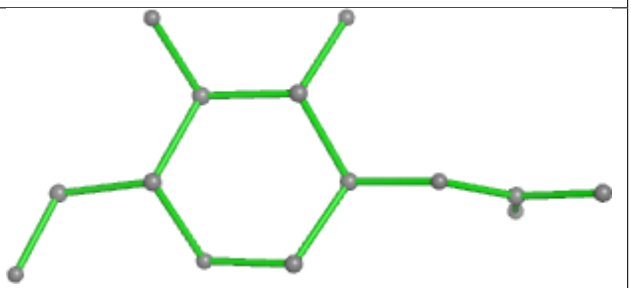
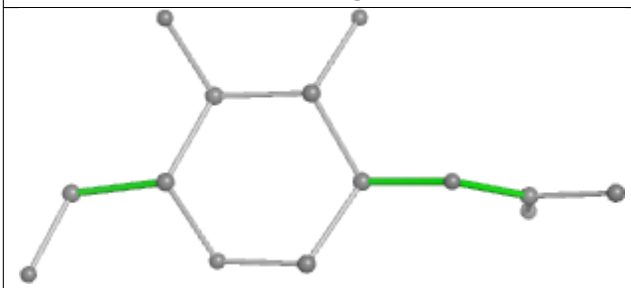
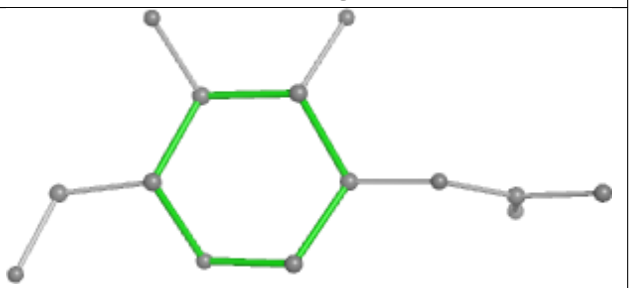


Torsions

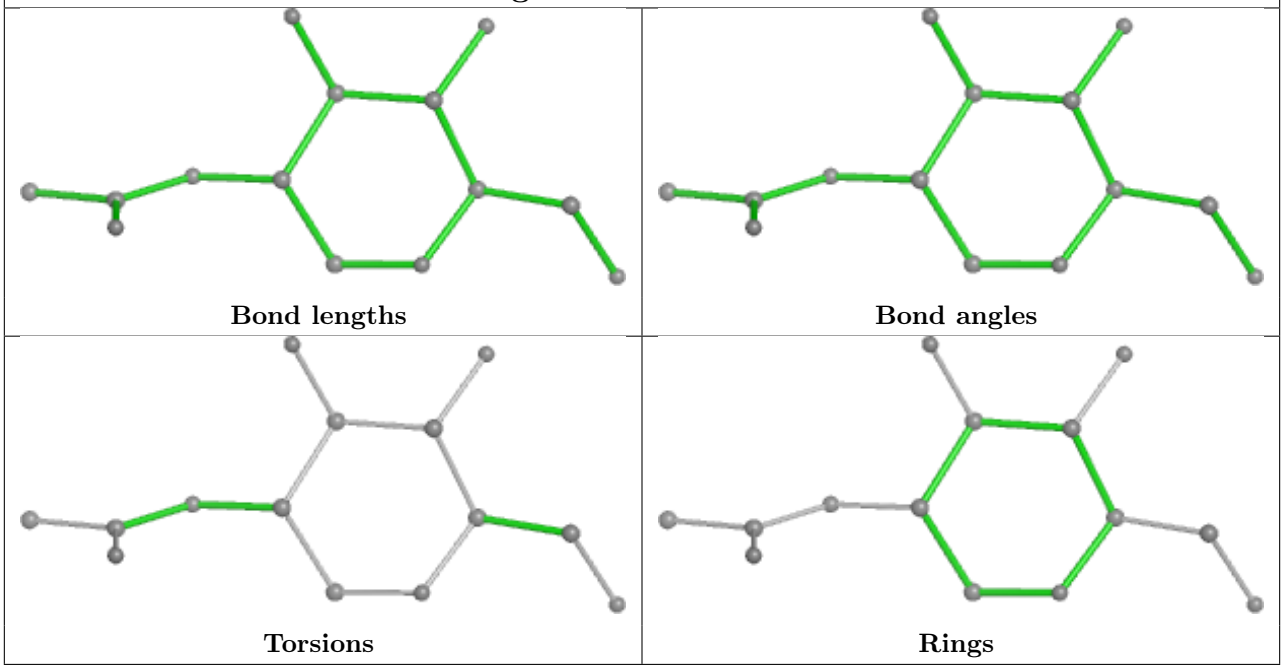


Rings

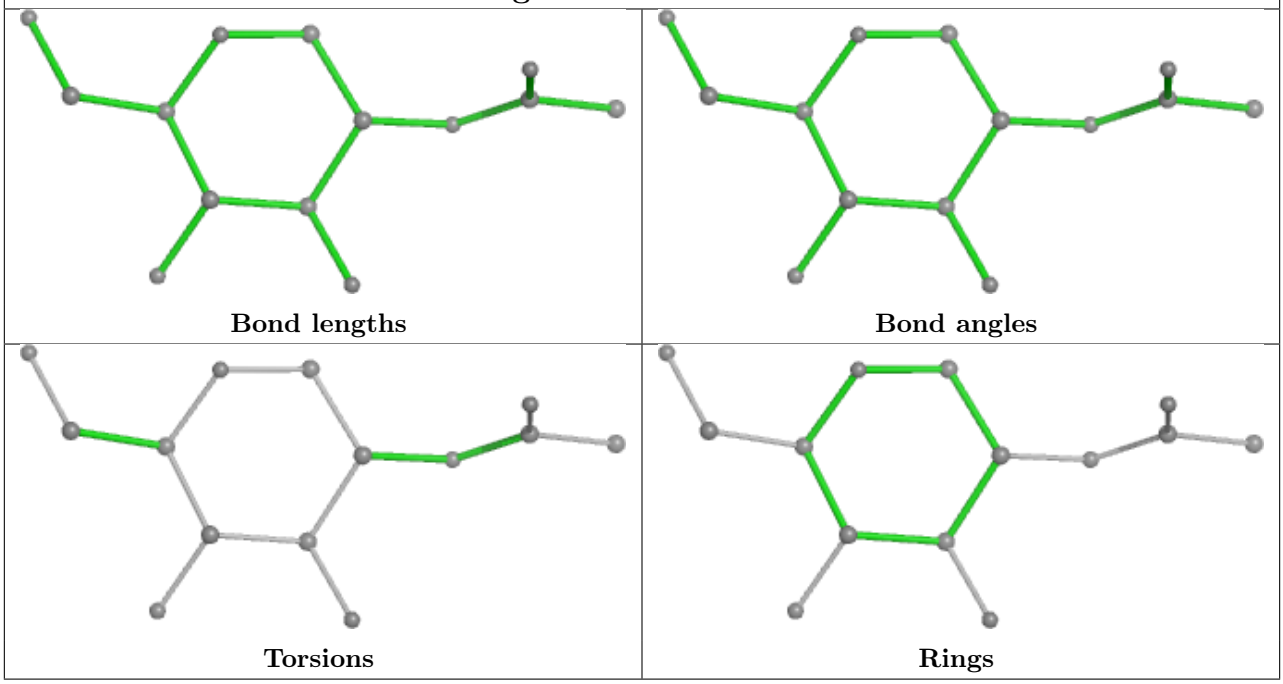
Ligand NAG C 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

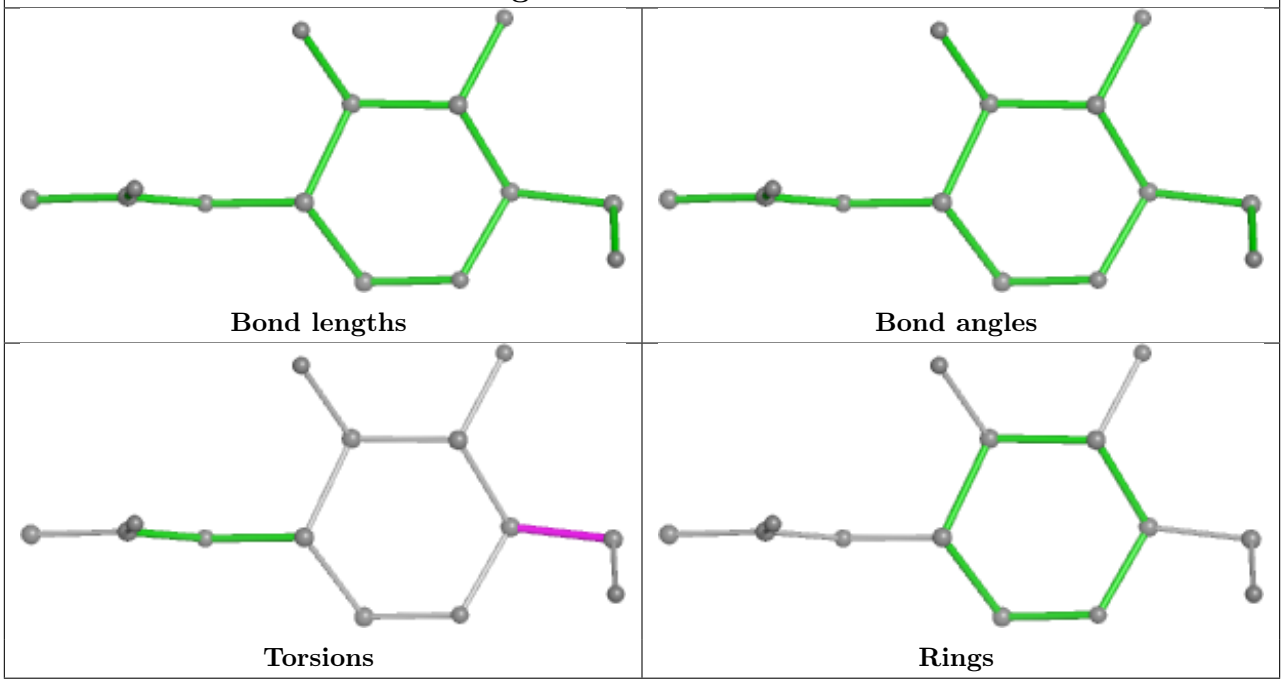
Ligand NAG A 1308



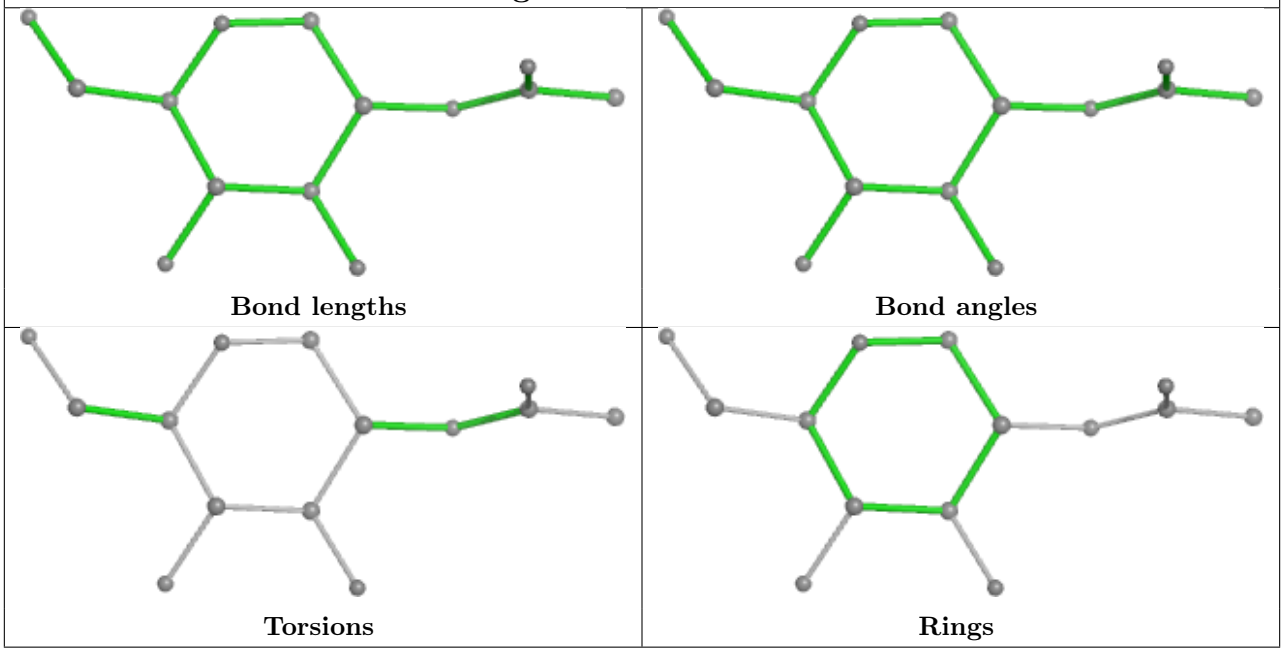
Ligand NAG B 1308



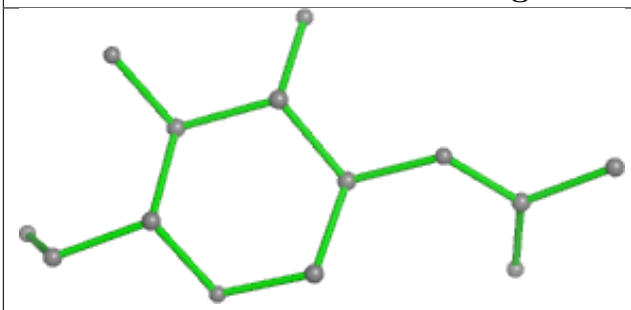
Ligand NAG A 1304



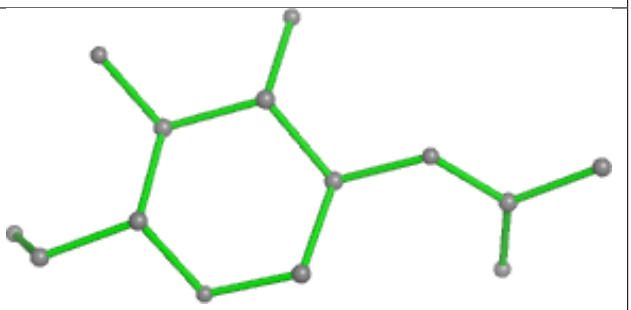
Ligand NAG B 1310



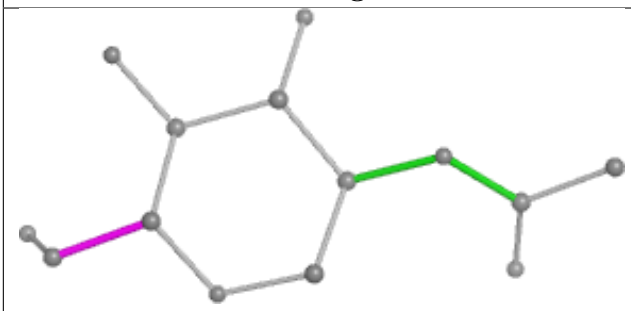
Ligand NAG C 1306



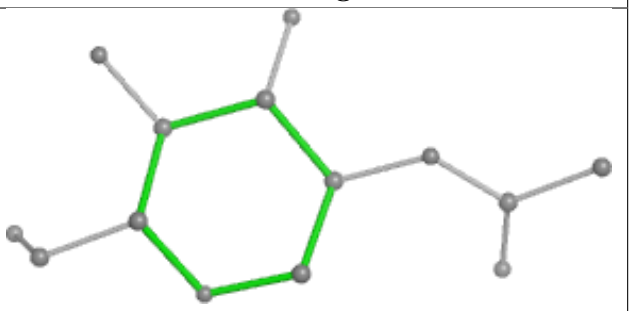
Bond lengths



Bond angles

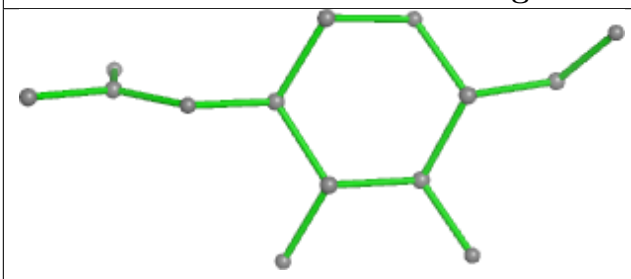


Torsions

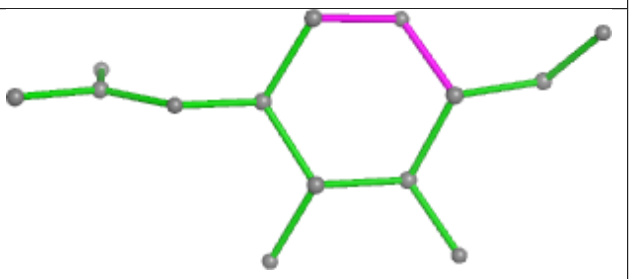


Rings

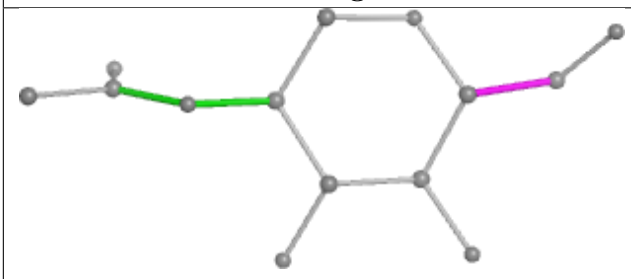
Ligand NAG B 1302



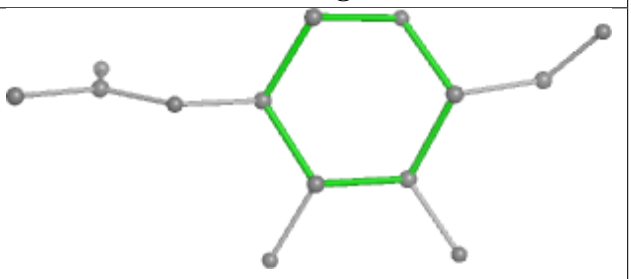
Bond lengths



Bond angles

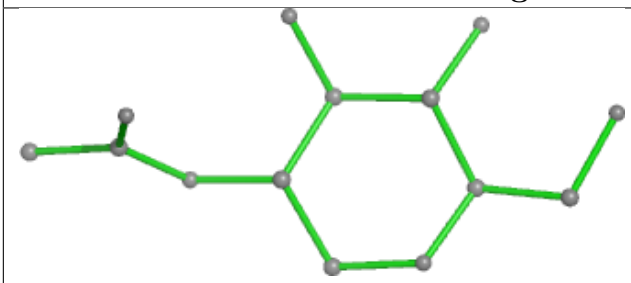


Torsions

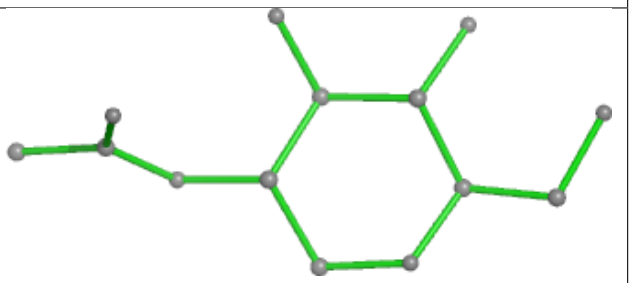


Rings

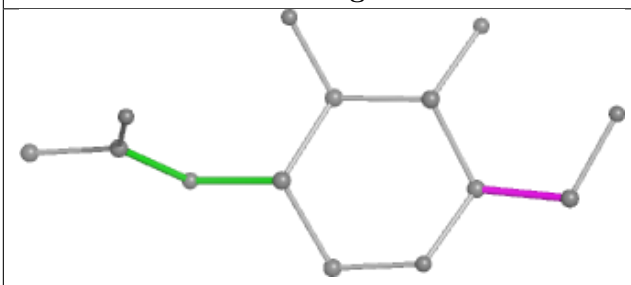
Ligand NAG A 1314



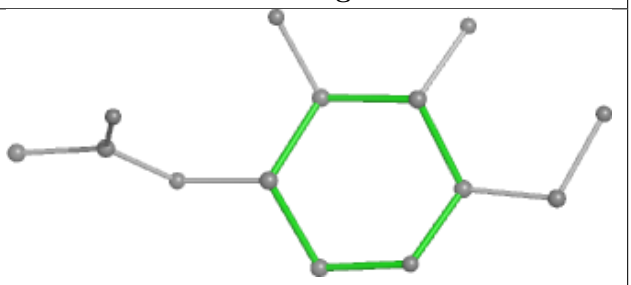
Bond lengths



Bond angles

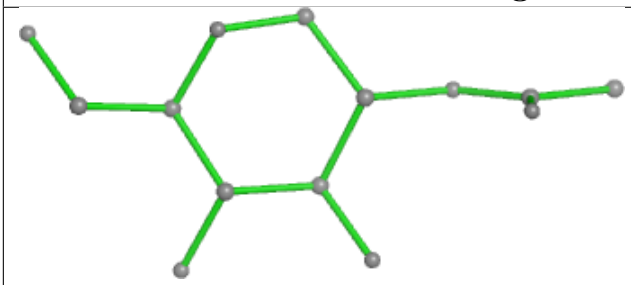


Torsions

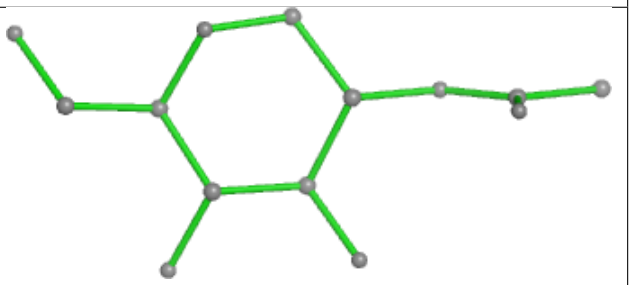


Rings

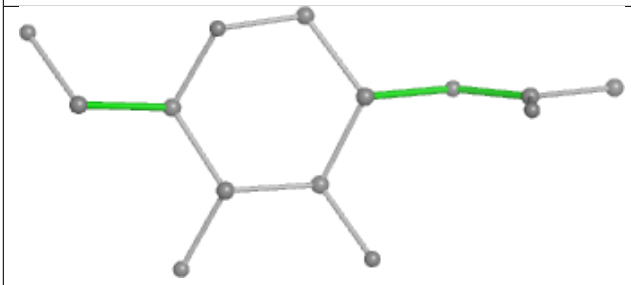
Ligand NAG C 1311



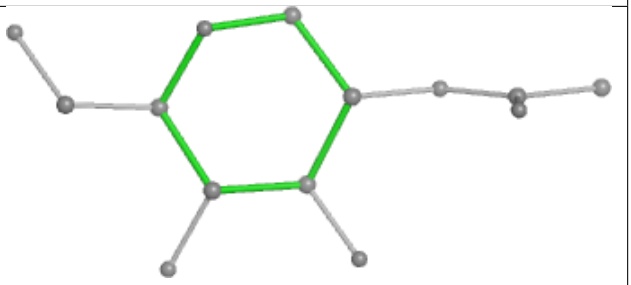
Bond lengths



Bond angles

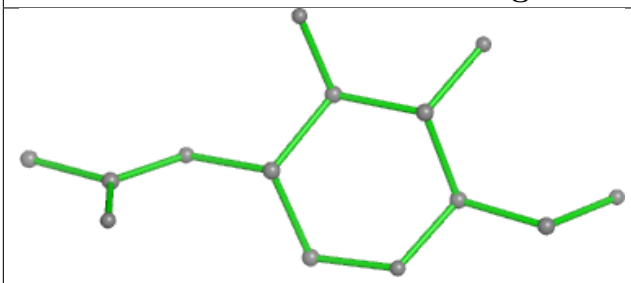


Torsions

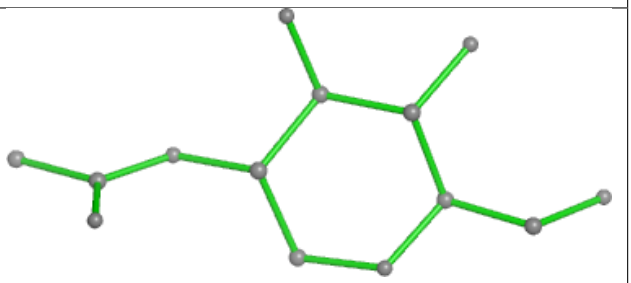


Rings

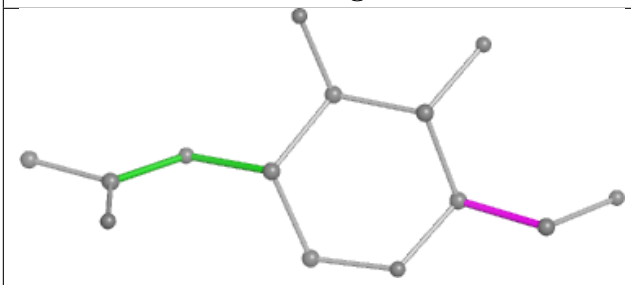
Ligand NAG B 1305



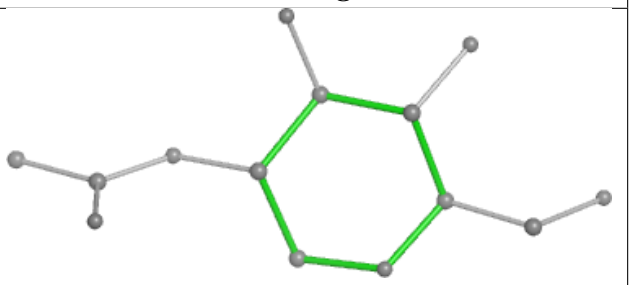
Bond lengths



Bond angles

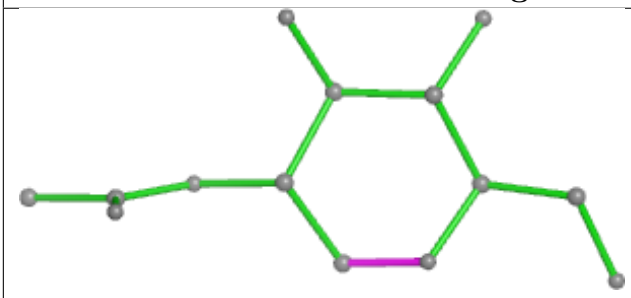


Torsions

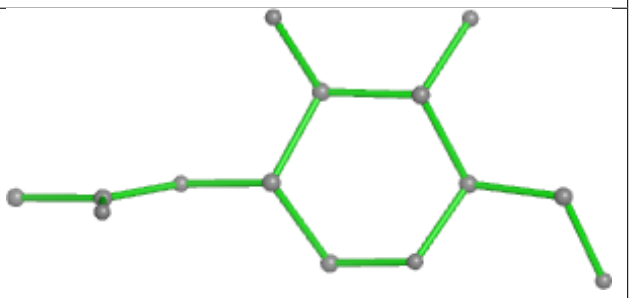


Rings

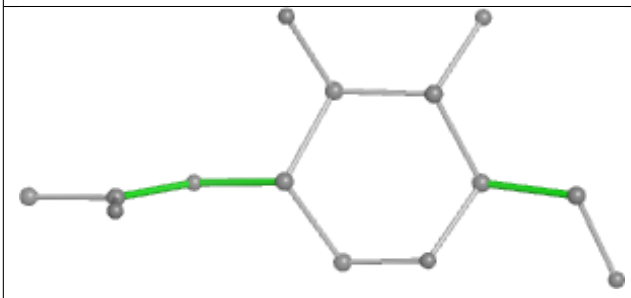
Ligand NAG A 1306



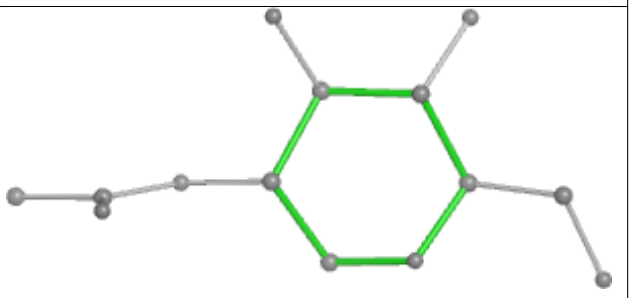
Bond lengths



Bond angles

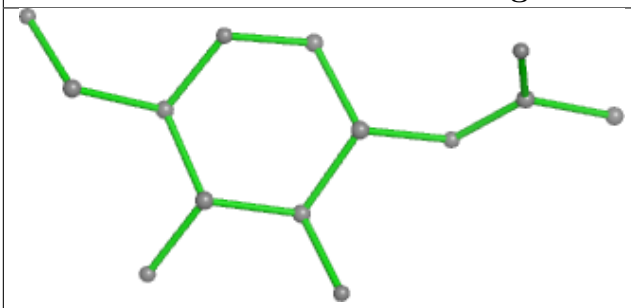


Torsions

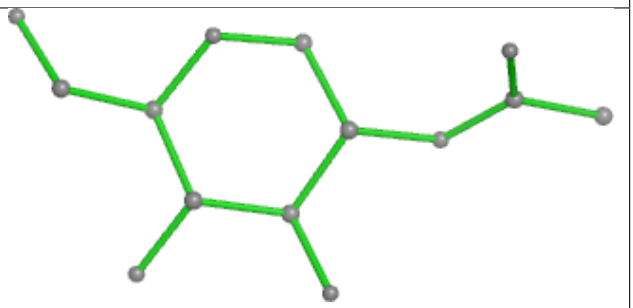


Rings

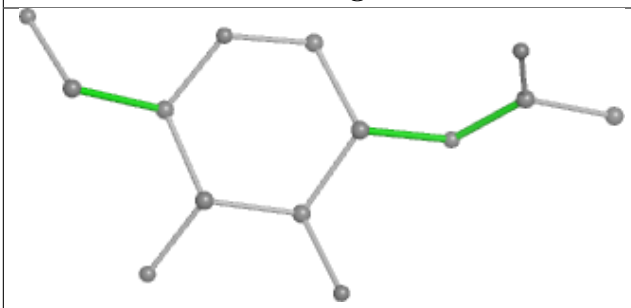
Ligand NAG A 1309



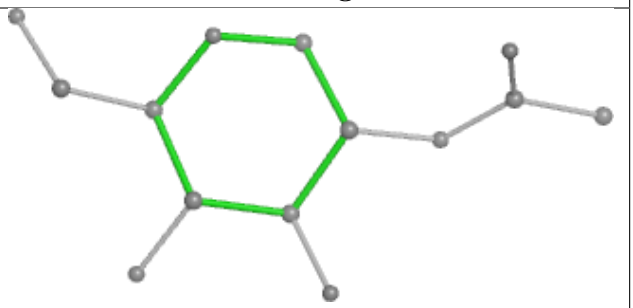
Bond lengths



Bond angles

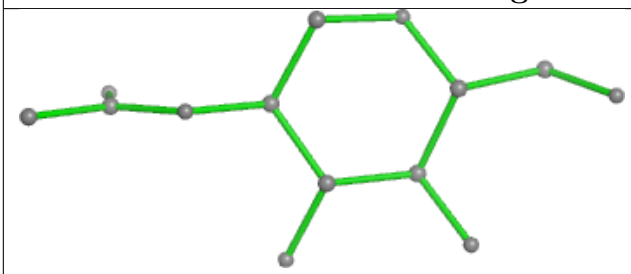


Torsions

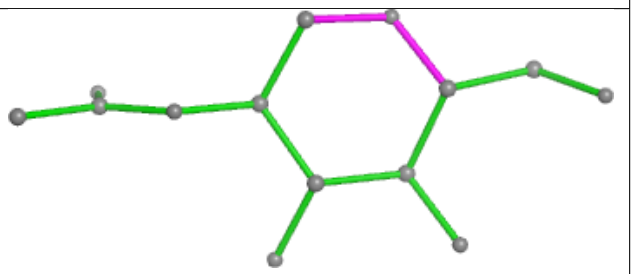


Rings

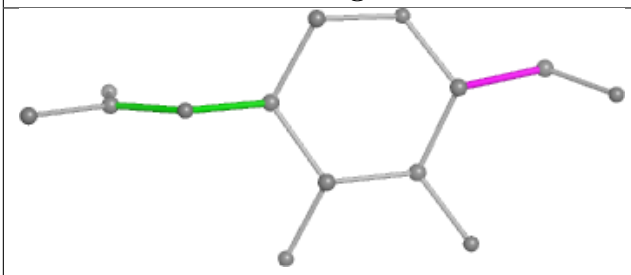
Ligand NAG A 1307



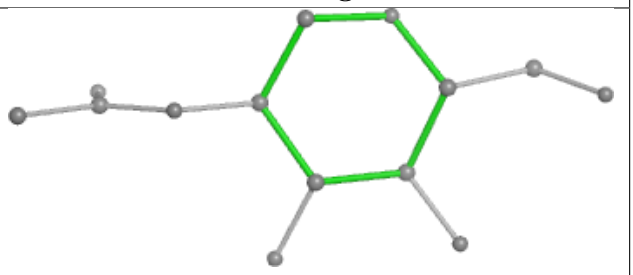
Bond lengths



Bond angles

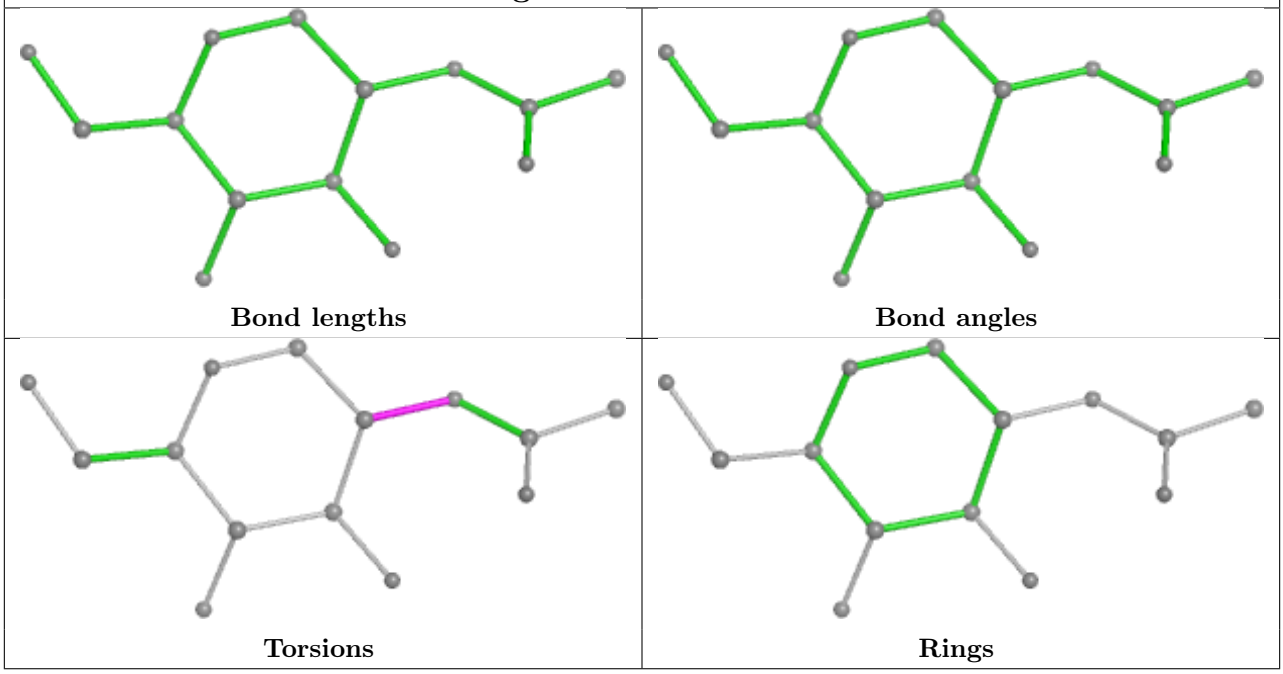


Torsions



Rings

Ligand NAG B 1307



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.

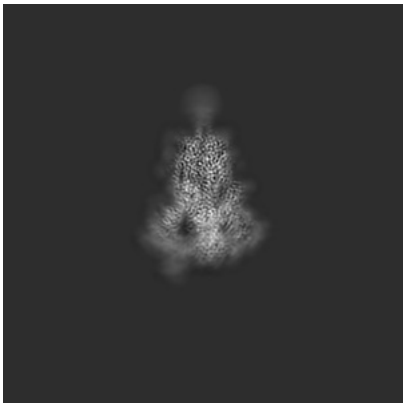
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11119. These allow visual inspection of the internal detail of the map and identification of artifacts.

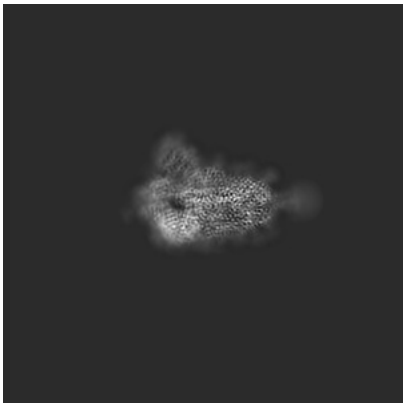
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

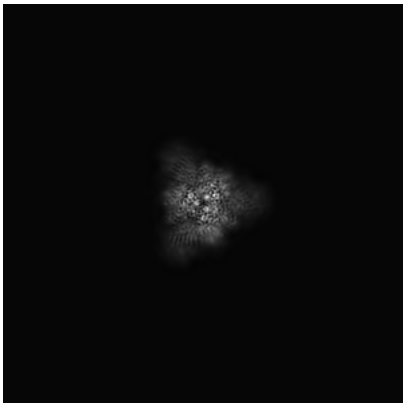
6.1.1 Primary map



X



Y

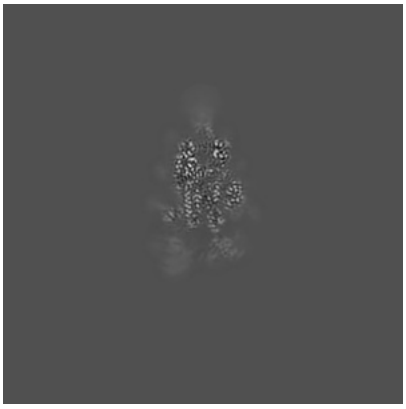


Z

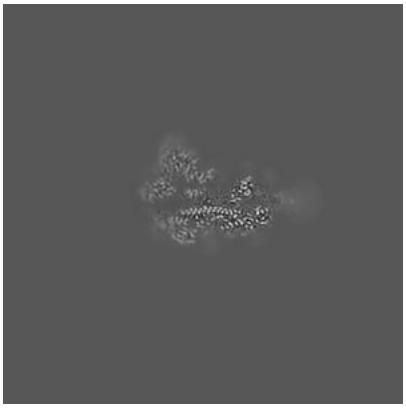
The images above show the map projected in three orthogonal directions.

6.2 Central slices

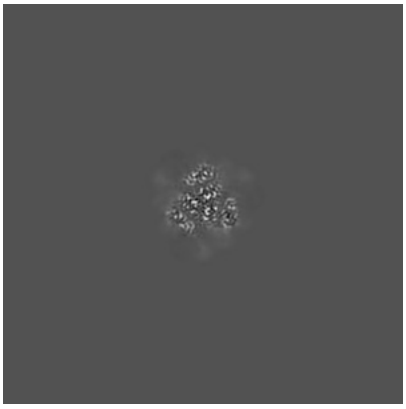
6.2.1 Primary map



X Index: 270



Y Index: 270

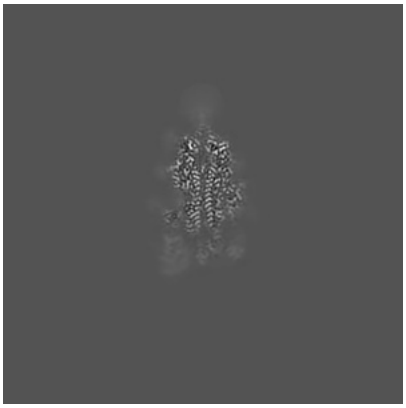


Z Index: 270

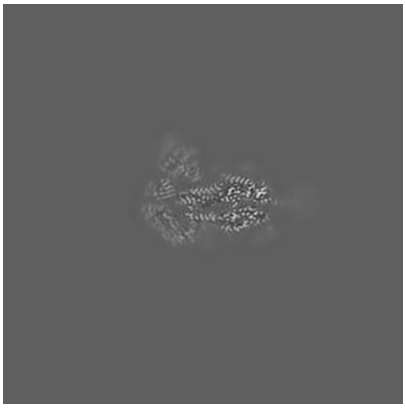
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 276



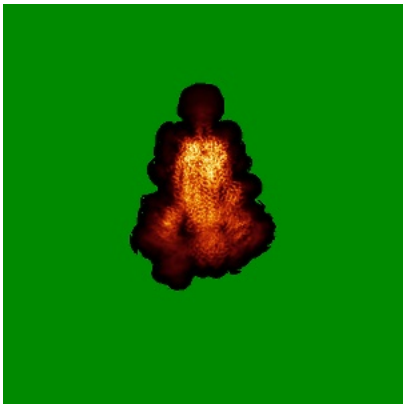
Y Index: 281

Z Index: 332

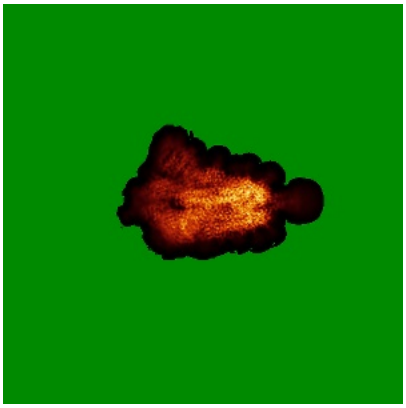
The images above show the largest variance slices of the map in three orthogonal directions.

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

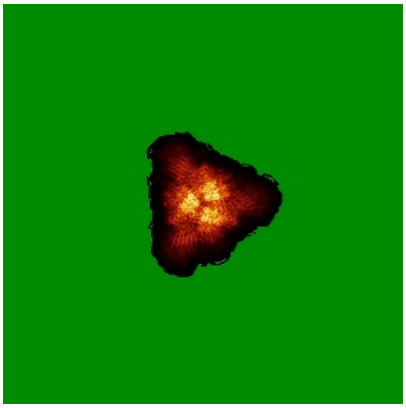
6.4.1 Primary map



X



Y



Z

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

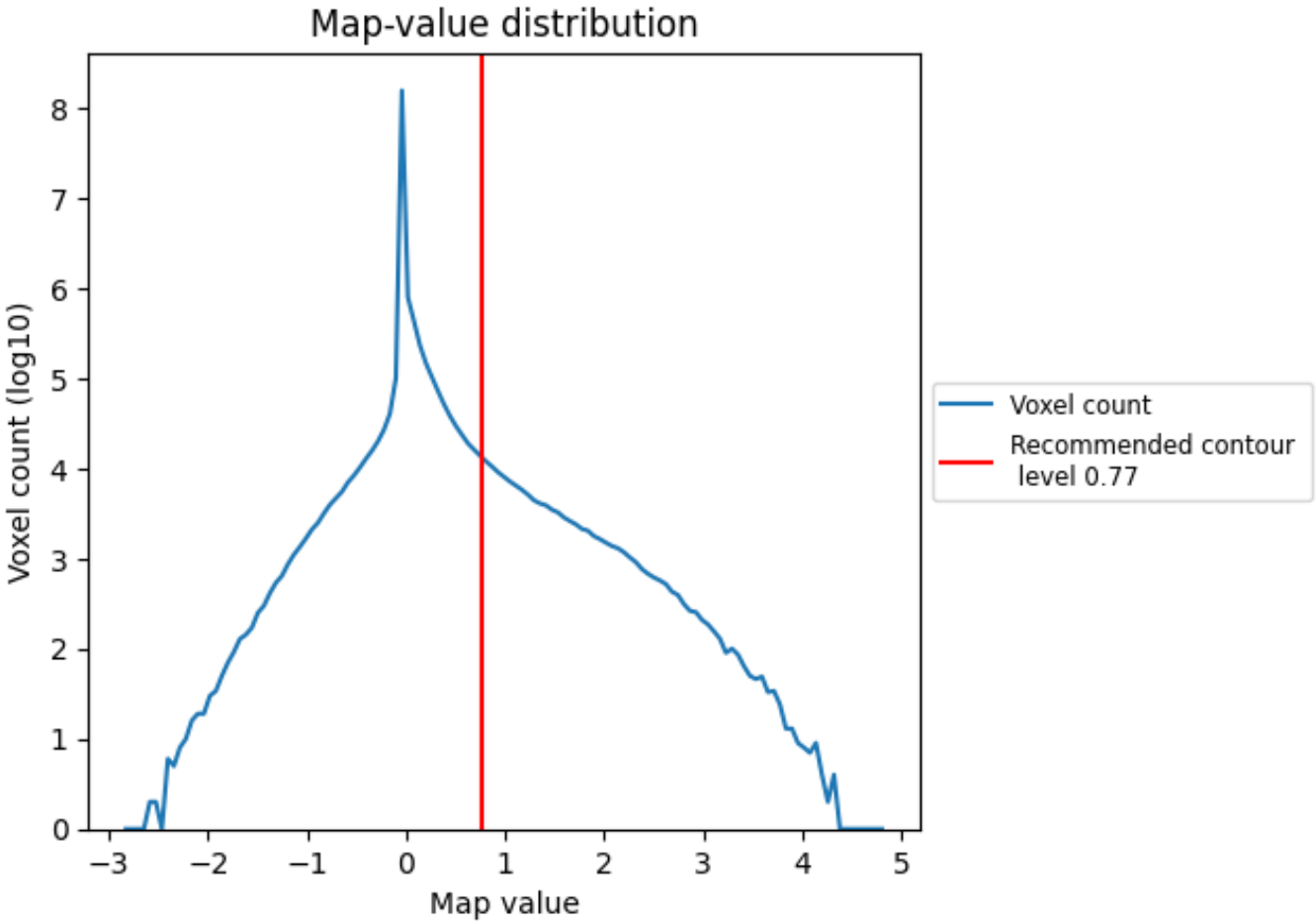
6.6 Mask visualisation (i)

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

7 Map analysis

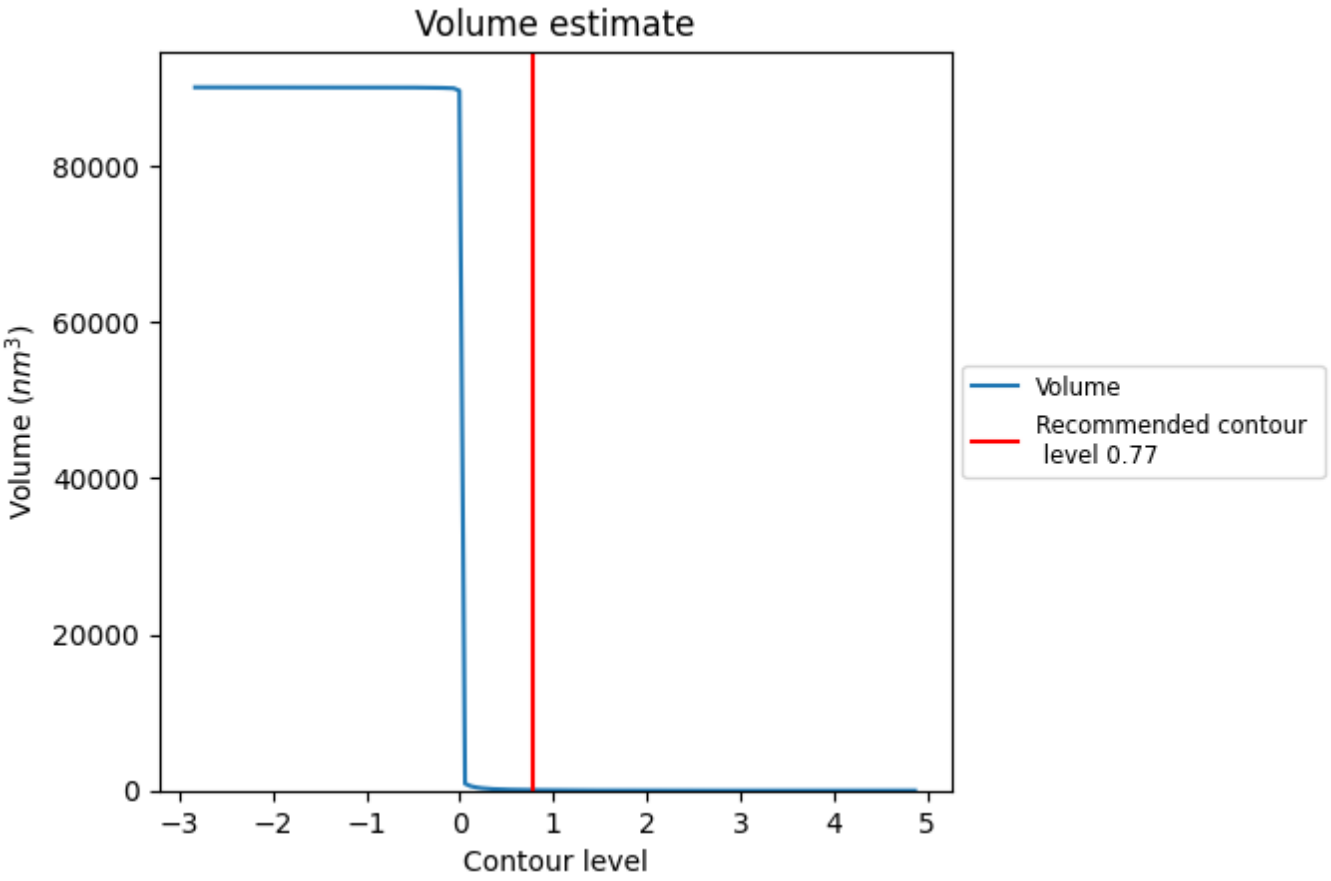
This section contains the results of statistical analysis of the map.

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.

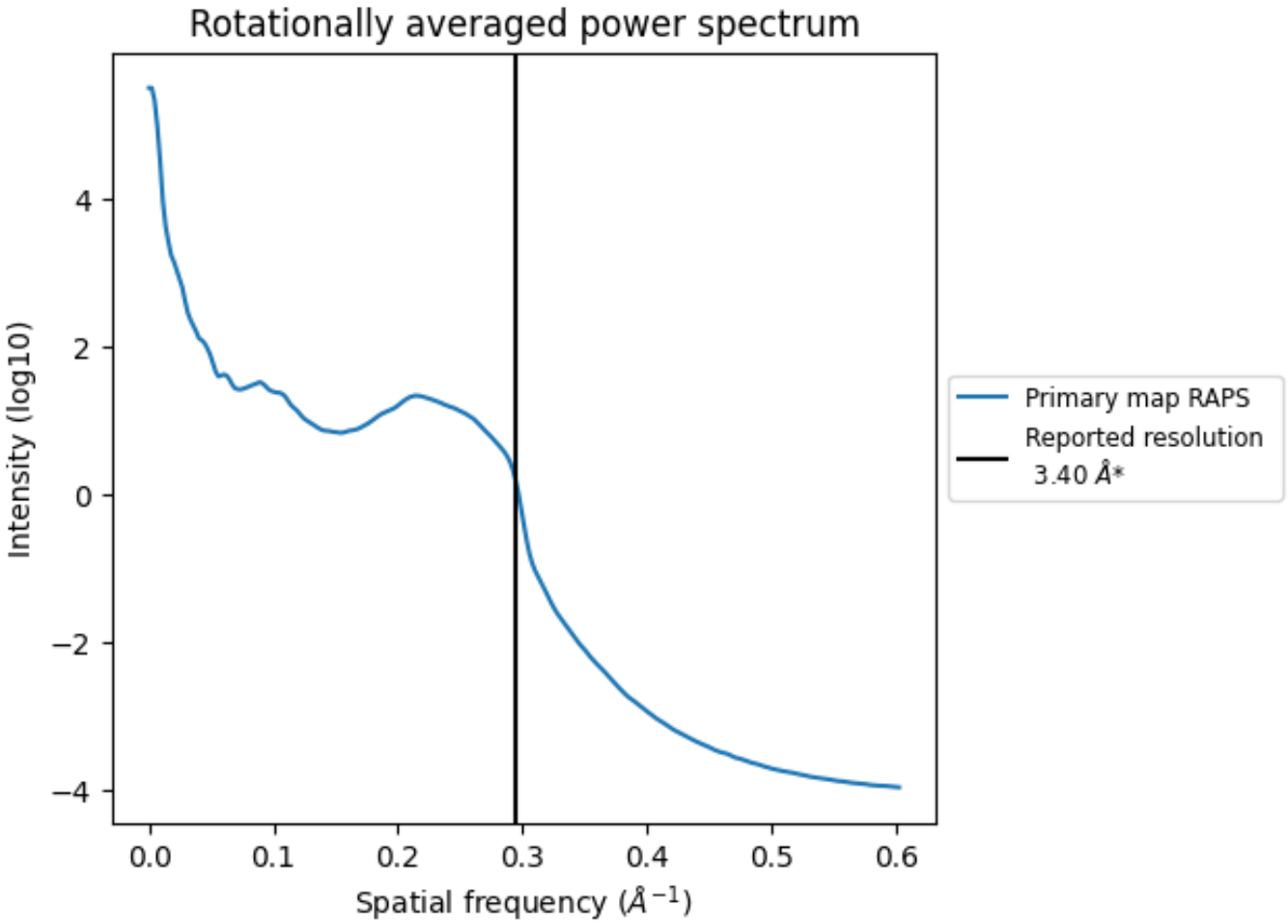
7.2 Volume estimate



The volume at the recommended contour level is 69 nm^3; this corresponds to an approximate mass of 62 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 0.294 Å^{-1}

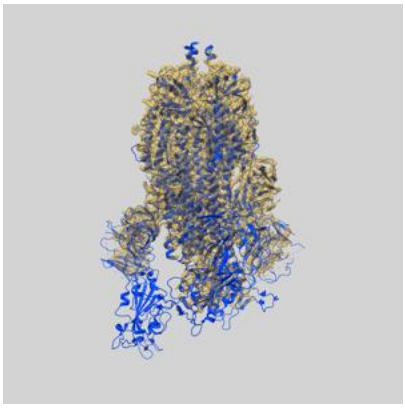
8 Fourier-Shell correlation

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

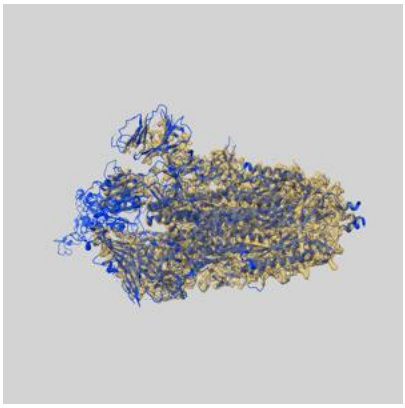
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11119 and PDB model 6Z97. Per-residue inclusion information can be found in section 3 on page 12.

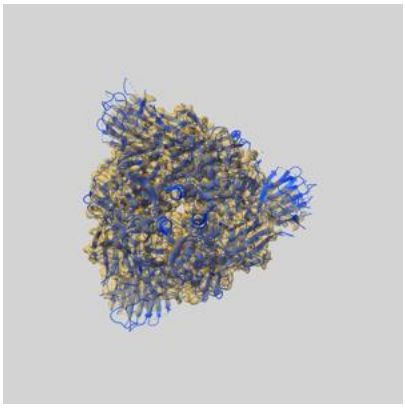
9.1 Map-model overlay



X



Y



Z

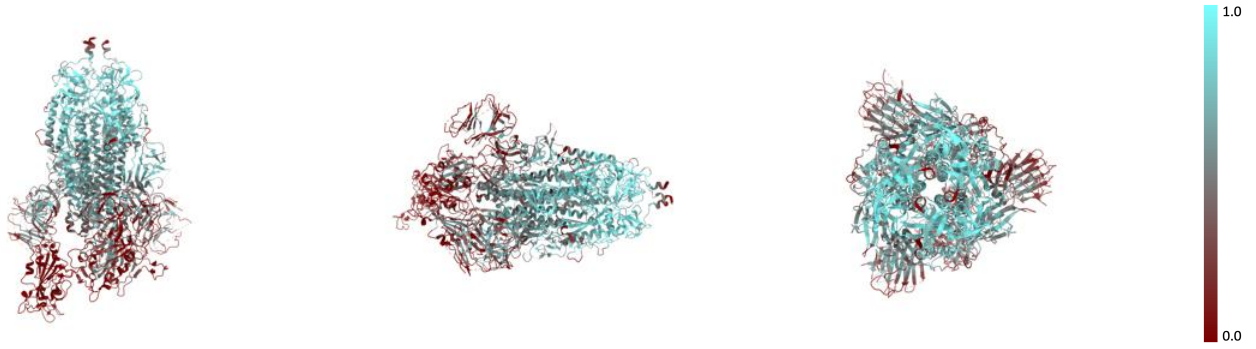
The images above show the 3D surface view of the map at the recommended contour level 0.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

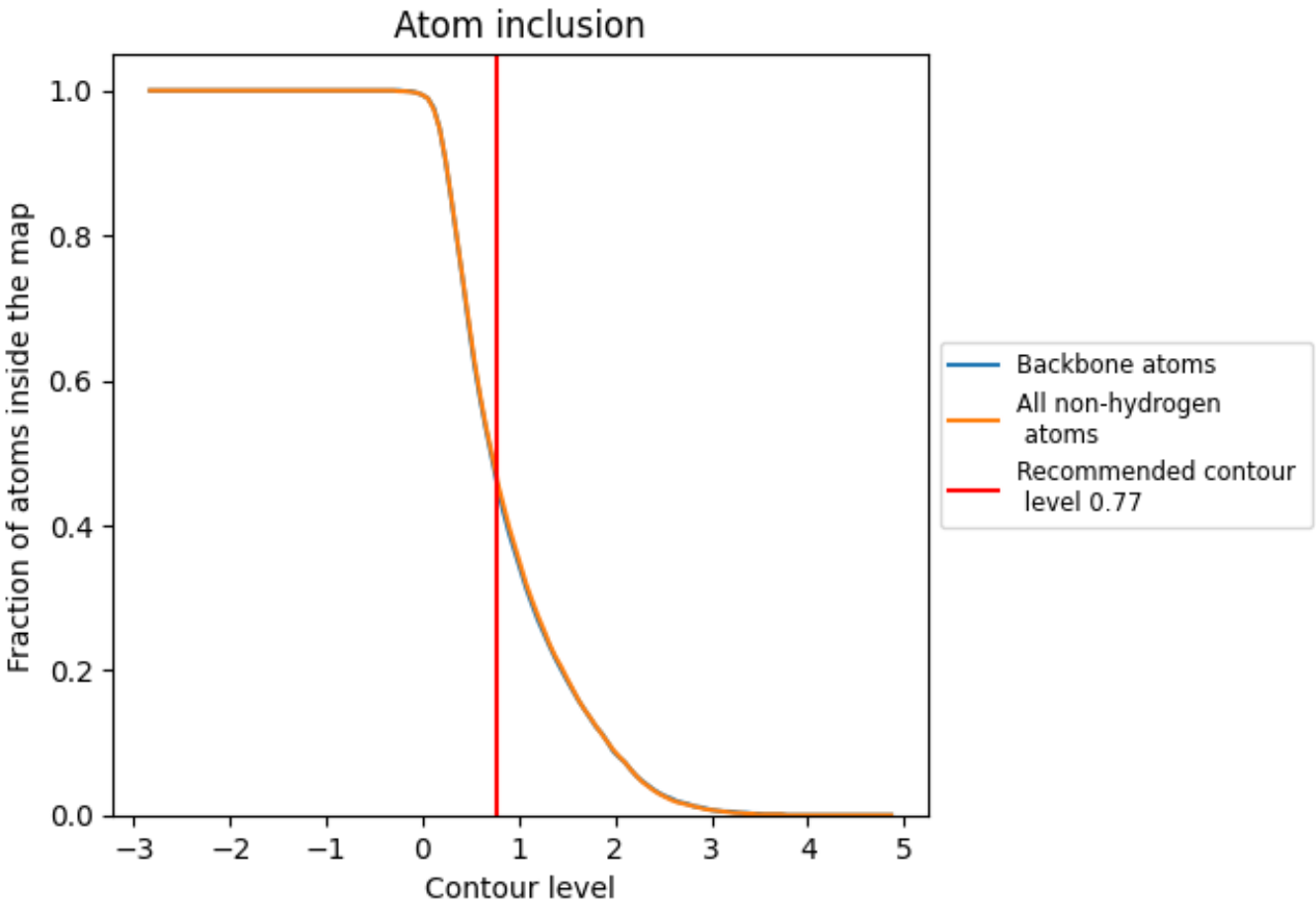
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.77).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 47% 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 (0.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4670	0.4420
A	0.4790	0.4460
B	0.4330	0.4180
C	0.5110	0.4640
D	0.0000	0.2940
E	0.2140	0.5190
F	0.2500	0.3950
G	0.2140	0.3320
H	0.1070	0.4000
I	0.2500	0.4110
J	0.2140	0.4210
K	0.1430	0.3570
L	0.3930	0.4460
M	0.2500	0.3860
N	0.2860	0.4260