wwPDB EM Validation Summary Report

Mar 8, 2026 – 12:43 PM UTC

PDB ID	:	8UUL / pdb_00008uul
EMDB ID	:	EMD-42589
Title	:	Prototypic SARS-CoV-2 spike (containing K417) in the closed conformation
Authors	:	Geng, Q.; Liu, B.; Li, F.
Deposited on	:	2023-11-01
Resolution	:	3.20 Å(reported)
Based on initial model	:	7TGY

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

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

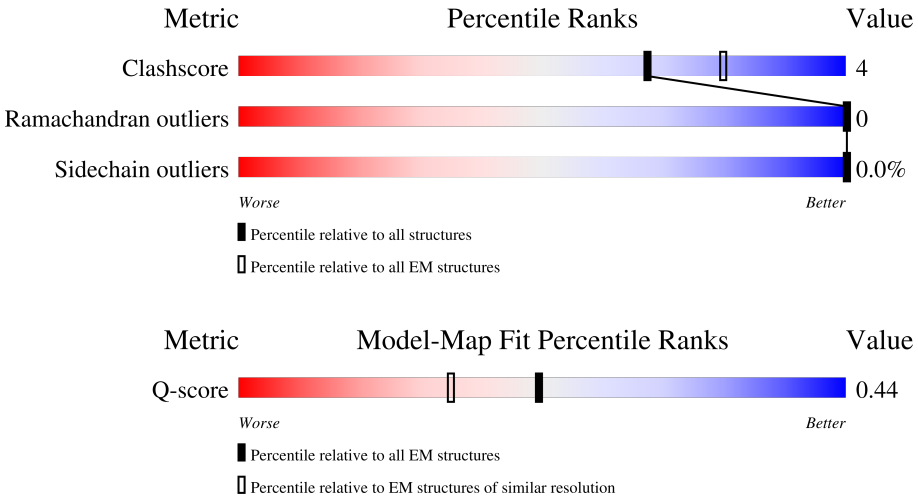
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1211	80% 9% 11%
1	B	1211	79% 10% 10%
1	C	1211	81% 8% 10%
2	D	2	50% 50% 50%

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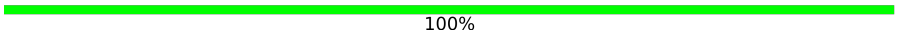
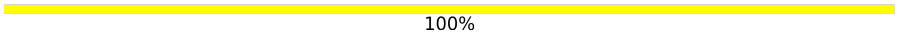
Mol	Chain	Length	Quality of chain
2	E	2	
2	F	2	
2	G	2	
2	H	2	
2	I	2	
2	J	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25891 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	1083	Total	C	N	O	S	0	0
			8460	5399	1410	1612	39		
1	B	1084	Total	C	N	O	S	0	0
			8474	5410	1412	1613	39		
1	C	1087	Total	C	N	O	S	0	0
			8495	5423	1415	1618	39		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	ALA	ARG	conflict	UNP P0DTC2
A	683	GLY	ARG	conflict	UNP P0DTC2
A	685	GLY	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	685	GLY	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	682	ALA	ARG	conflict	UNP P0DTC2
C	683	GLY	ARG	conflict	UNP P0DTC2
C	685	GLY	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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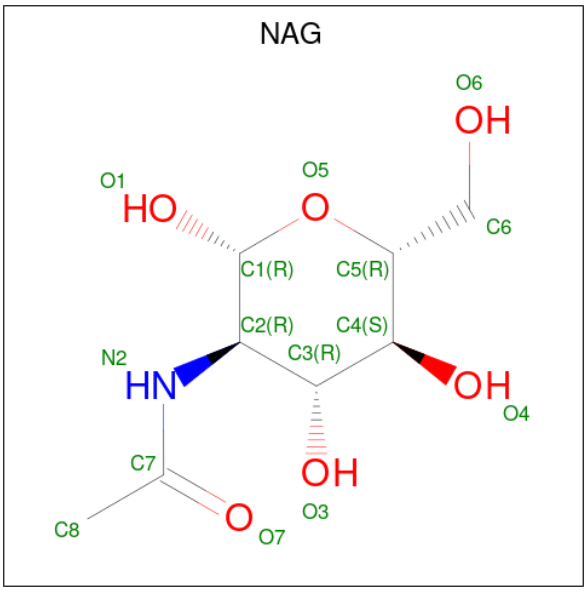
Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

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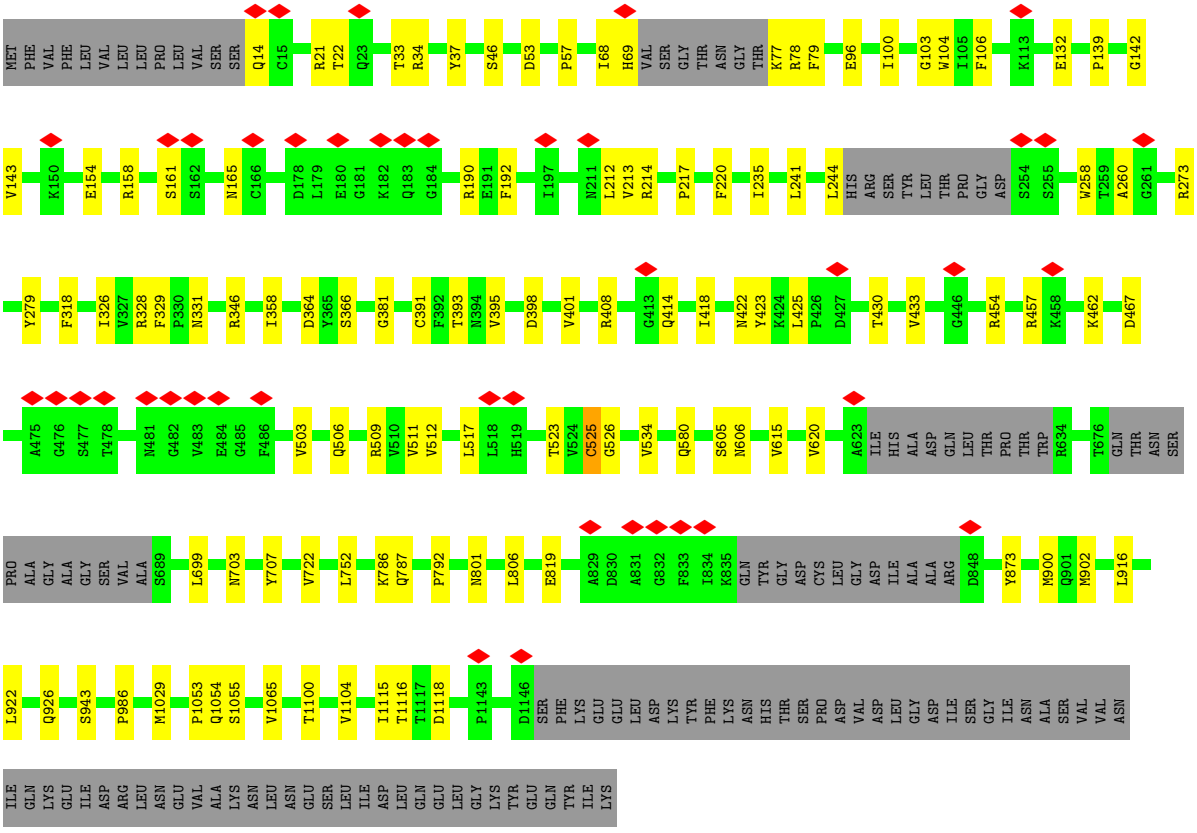
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

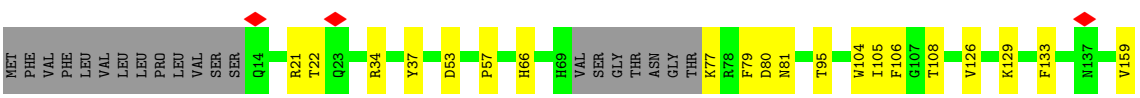
• Molecule 1: Spike glycoprotein

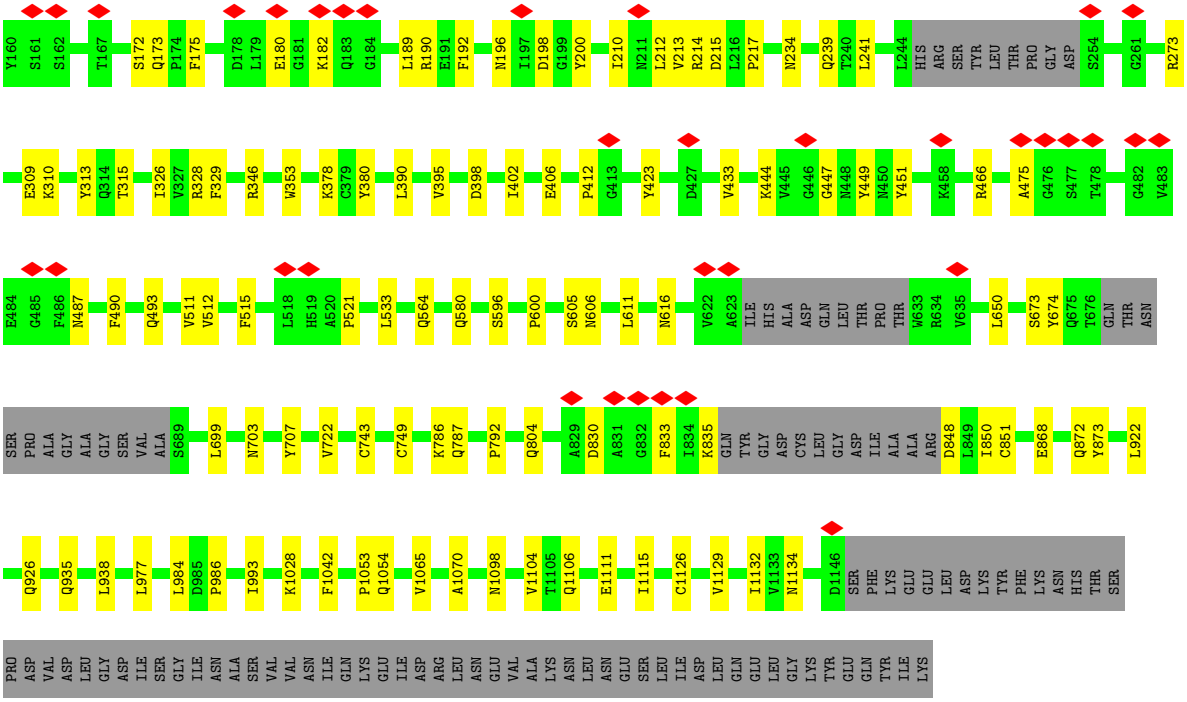
Chain A:



• Molecule 1: Spike glycoprotein

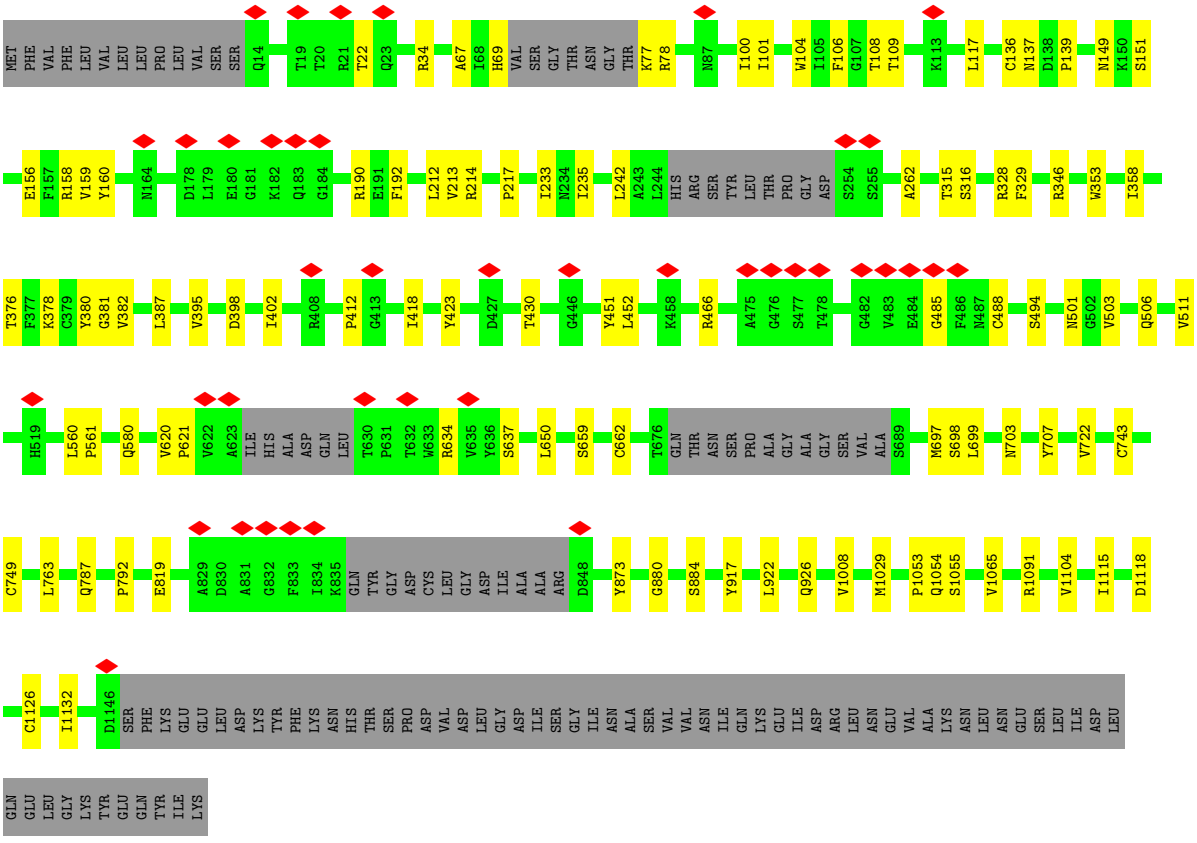
Chain B:





• Molecule 1: Spike glycoprotein

Chain C:



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

Chain D:

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

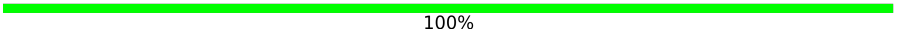
Chain E:

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

Chain F:

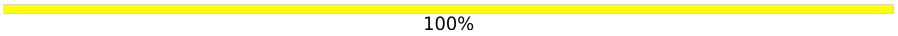
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I:

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	23665	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.559	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	339.96786, 339.96786, 339.96786	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.885333, 0.885333, 0.885333	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	0.40	0/8657	0.64	4/11784 (0.0%)
1	B	0.39	0/8673	0.61	4/11807 (0.0%)
1	C	0.40	0/8695	0.60	0/11839
All	All	0.40	0/26025	0.62	8/35430 (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
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	986	PRO	N-CA-C	5.79	117.76	110.70
1	B	984	LEU	CA-C-N	5.41	128.91	120.68
1	B	984	LEU	C-N-CA	5.41	128.91	120.68
1	B	986	PRO	N-CA-C	5.32	117.19	110.70
1	A	526	GLY	CA-C-N	-5.24	116.36	121.65

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	517	LEU	Peptide
1	A	620	VAL	Peptide
1	B	1070	ALA	Peptide
1	B	315	THR	Peptide

5.2 Too-close contacts (i)

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	8460	0	8261	70	0
1	B	8474	0	8265	72	0
1	C	8495	0	8288	61	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
3	A	84	0	78	1	0
3	B	84	0	78	2	0
3	C	98	0	90	0	0
All	All	25891	0	25235	192	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 4.

The worst 5 of 192 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:67:ALA:O	1:C:262:ALA:HA	1.75	0.86
1:C:213:VAL:HG12	1:C:214:ARG:HG2	1.73	0.69
1:A:213:VAL:HG12	1:A:214:ARG:HG2	1.75	0.68
1:C:101:ILE:HD13	1:C:242:LEU:HB3	1.77	0.66
1:C:100:ILE:HG22	1:C:242:LEU:HB2	1.80	0.64

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	1071/1211 (88%)	1014 (95%)	57 (5%)	0	100	100
1	B	1072/1211 (88%)	1020 (95%)	52 (5%)	0	100	100
1	C	1075/1211 (89%)	1023 (95%)	52 (5%)	0	100	100
All	All	3218/3633 (89%)	3057 (95%)	161 (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	947/1057 (90%)	946 (100%)	1 (0%)	88	91
1	B	948/1057 (90%)	948 (100%)	0	100	100
1	C	951/1057 (90%)	951 (100%)	0	100	100
All	All	2846/3171 (90%)	2845 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	616	ASN
1	C	965	GLN
1	B	935	GLN
1	C	907	ASN
1	B	926	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)

14 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	2	14,14,15	0.80	0	17,19,21	2.30	5 (29%)
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	0.42	0
2	NAG	E	1	1,2	14,14,15	0.71	1 (7%)	17,19,21	1.15	3 (17%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.44	0
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	G	1	1,2	14,14,15	0.43	0	17,19,21	0.64	0
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	0.45	0
2	NAG	H	1	1,2	14,14,15	1.10	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	H	2	2	14,14,15	0.17	0	17,19,21	0.60	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.41	0	17,19,21	0.72	1 (5%)
2	NAG	I	2	2	14,14,15	0.33	0	17,19,21	0.42	0
2	NAG	J	1	1,2	14,14,15	0.53	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	J	2	2	14,14,15	0.44	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
2	NAG	D	1	2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-3.71	1.37	1.43
2	E	1	NAG	C1-C2	2.44	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	6.91	121.44	112.19
2	D	1	NAG	C2-N2-C7	3.50	127.59	122.90
2	D	1	NAG	C3-C4-C5	3.45	116.49	110.23
2	H	1	NAG	C3-C4-C5	2.53	114.83	110.23
2	D	1	NAG	O5-C5-C4	2.51	116.93	110.83

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

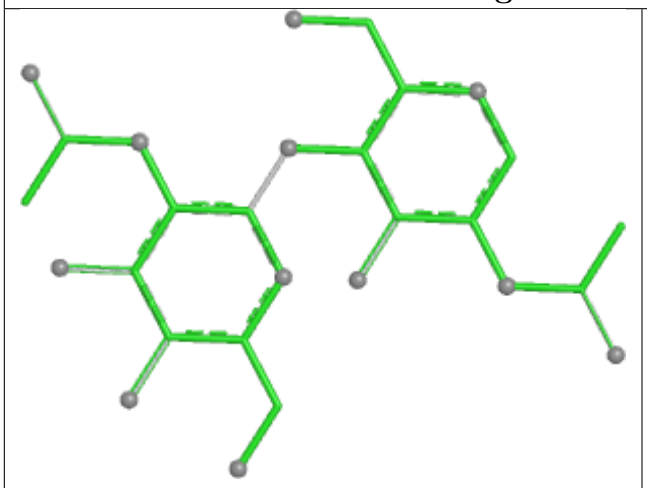
There are no ring outliers.

1 monomer is involved in 1 short contact:

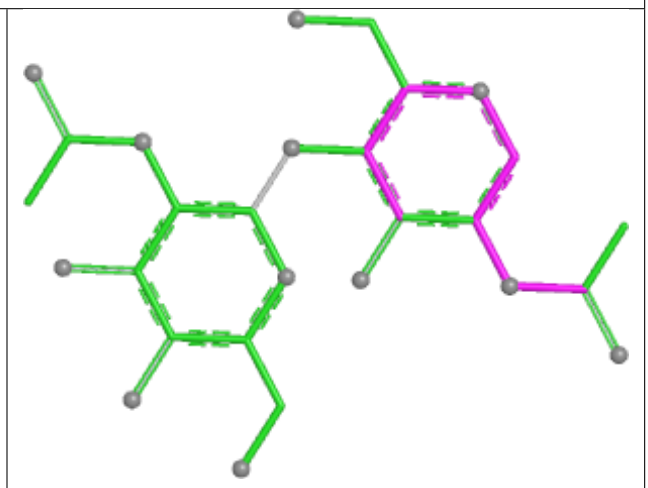
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

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

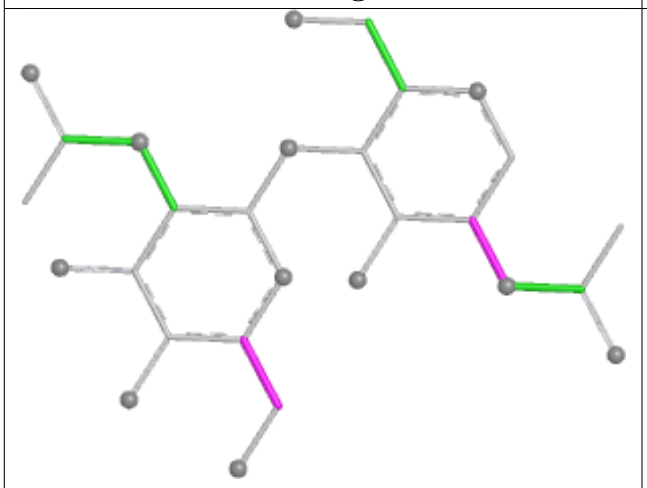
Oligosaccharide Chain D



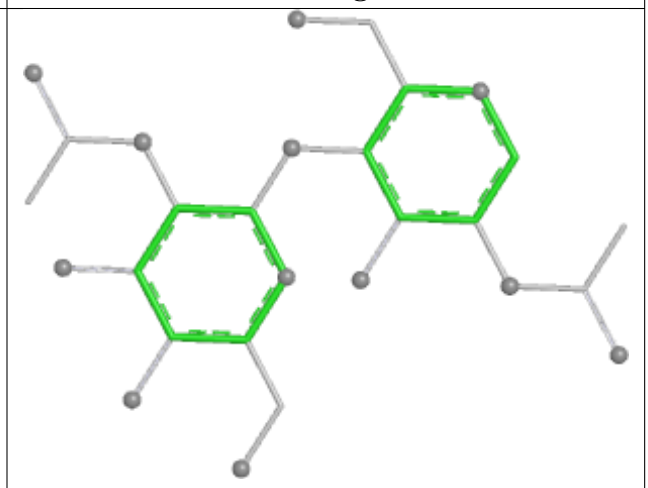
Bond lengths



Bond angles

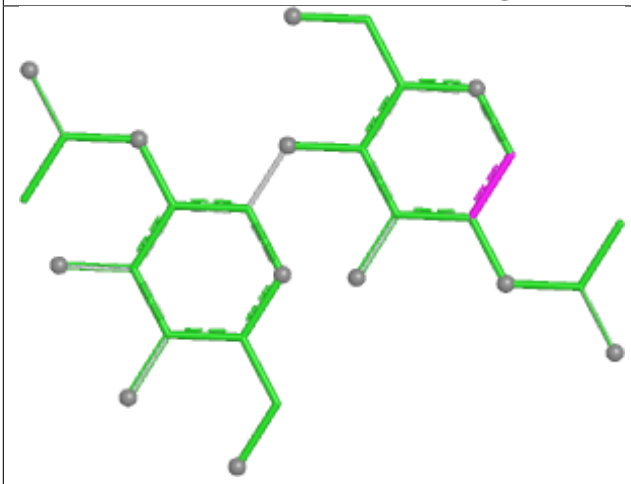


Torsions

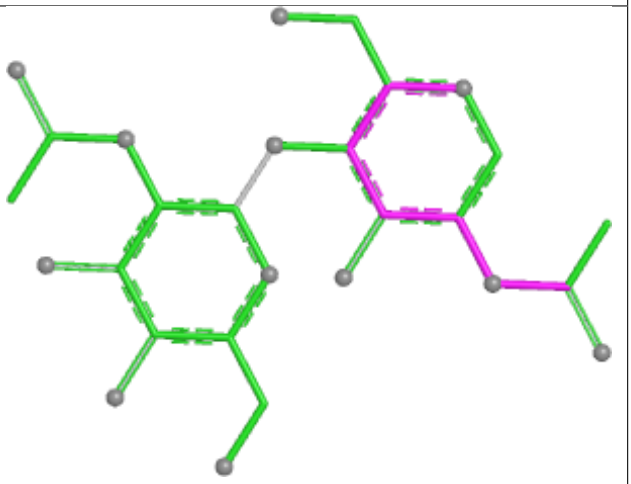


Rings

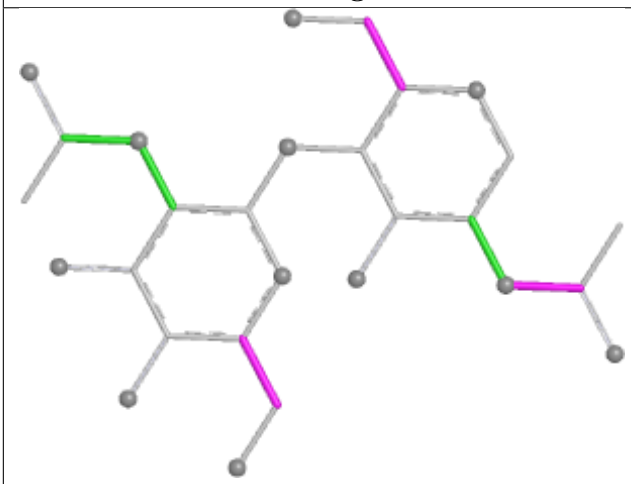
Oligosaccharide Chain E



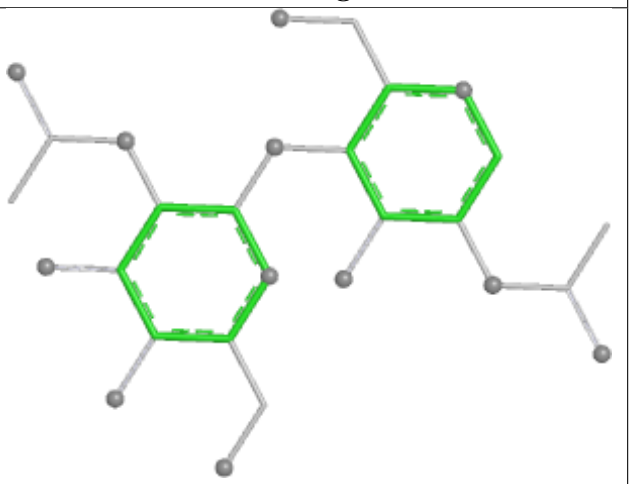
Bond lengths



Bond angles

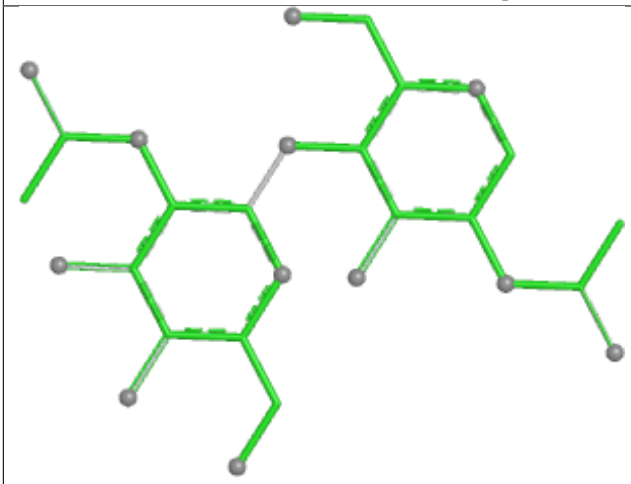


Torsions

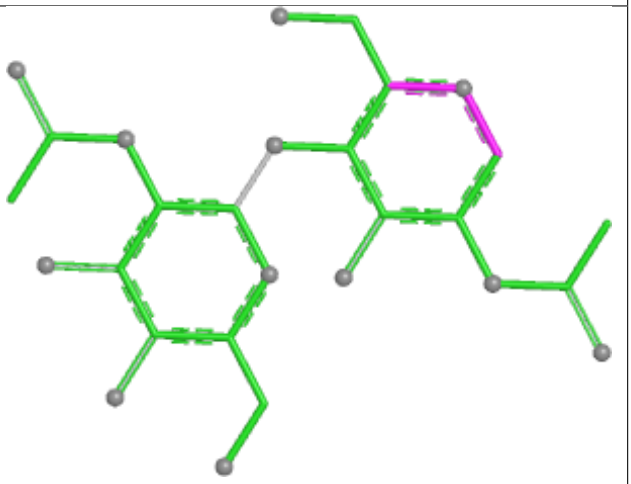


Rings

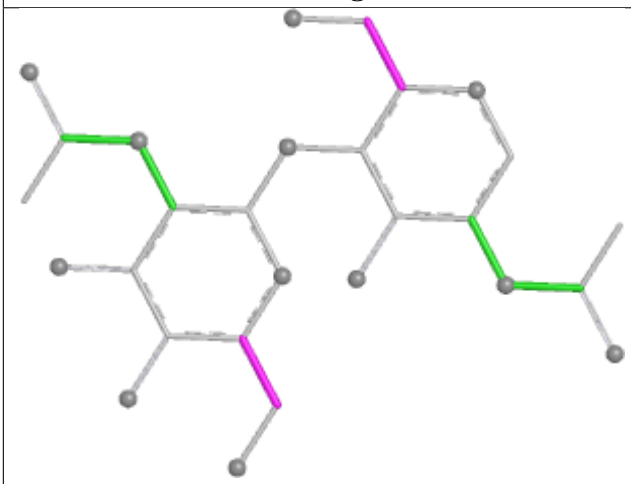
Oligosaccharide Chain F



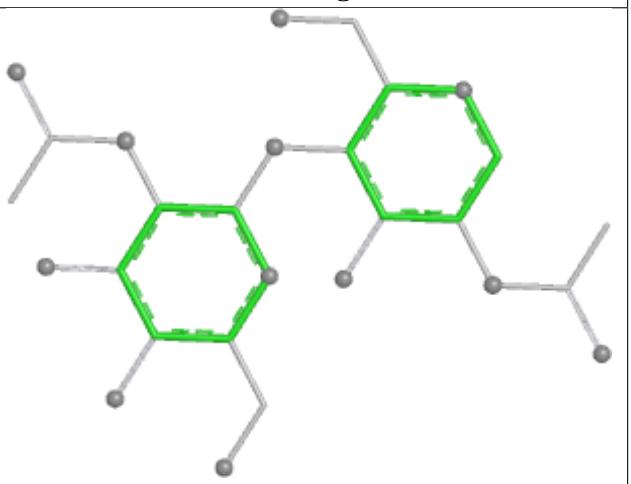
Bond lengths



Bond angles

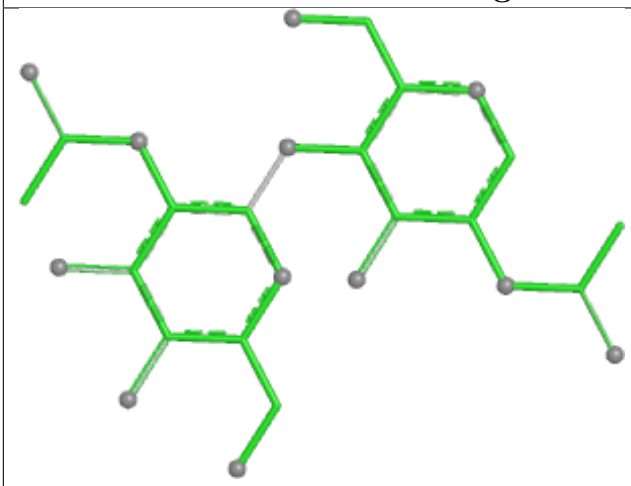


Torsions

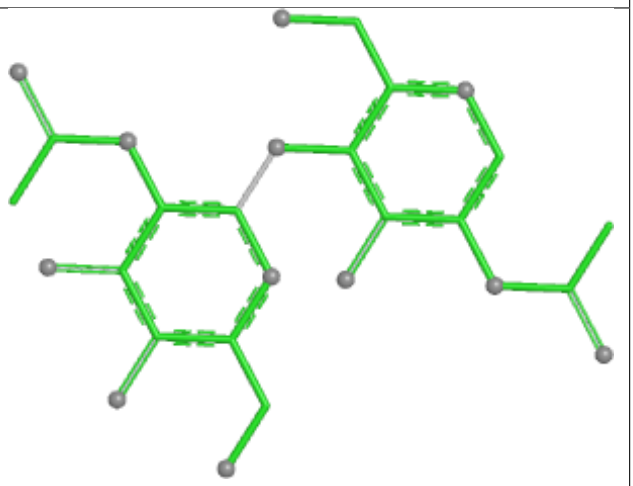


Rings

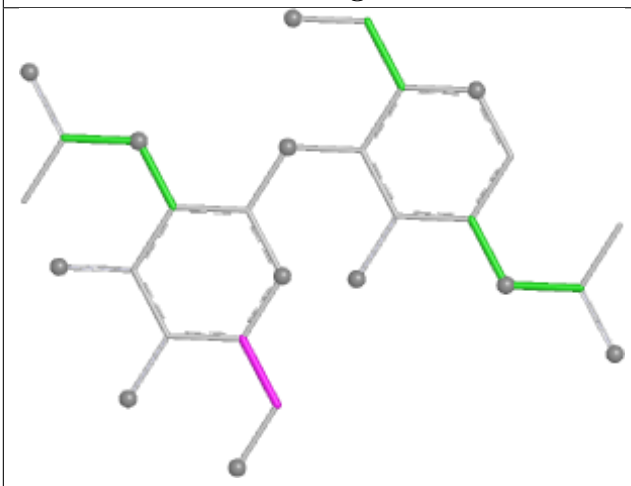
Oligosaccharide Chain G



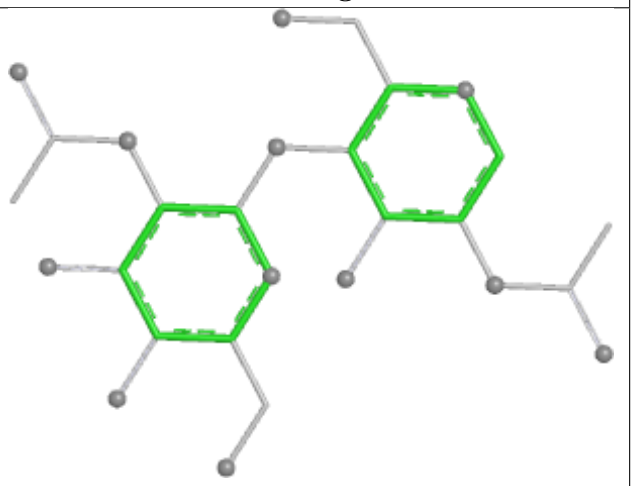
Bond lengths



Bond angles

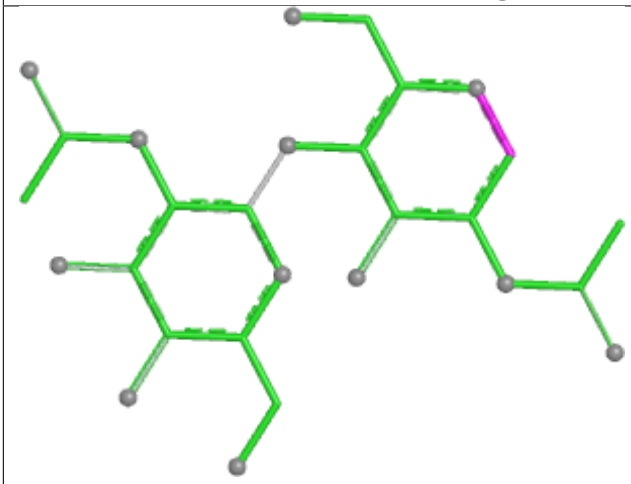


Torsions

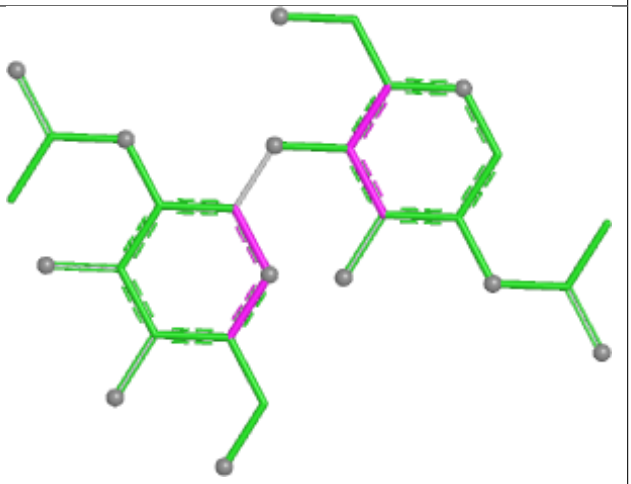


Rings

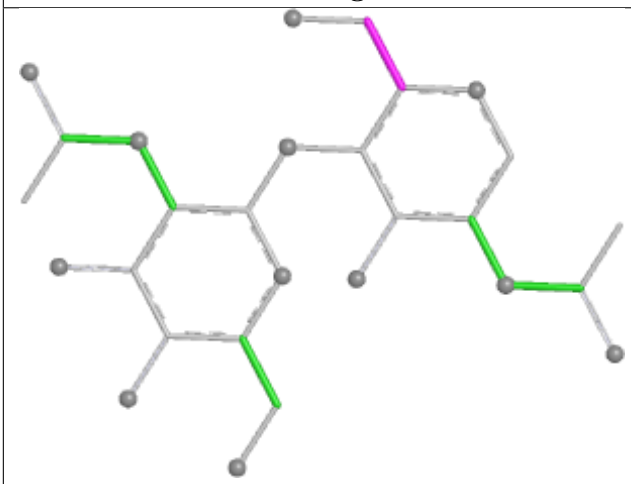
Oligosaccharide Chain H



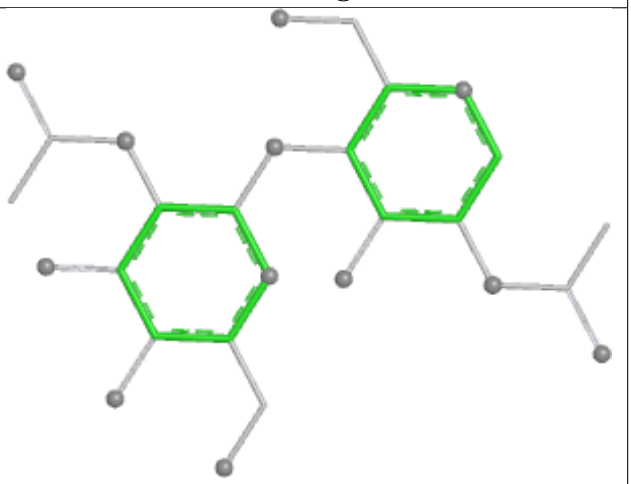
Bond lengths



Bond angles

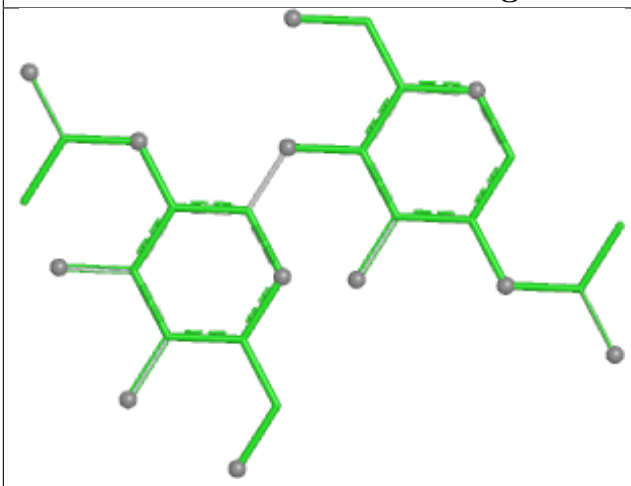


Torsions

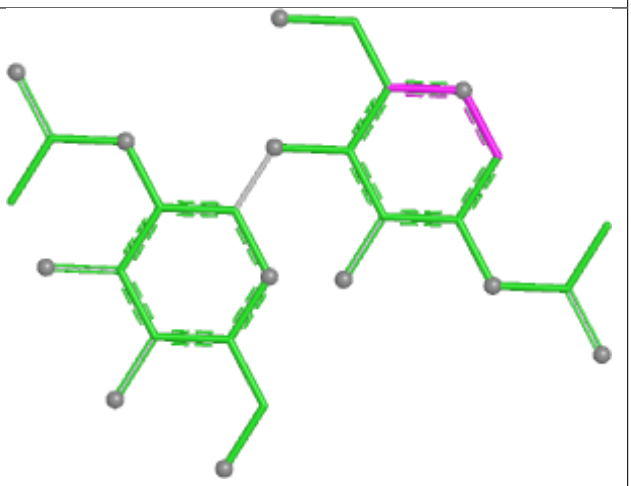


Rings

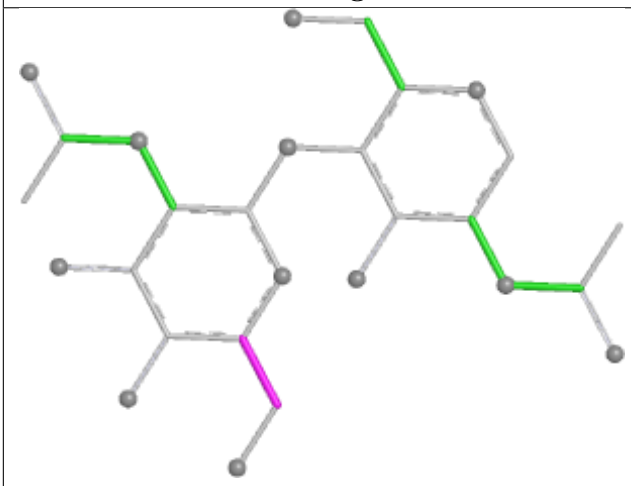
Oligosaccharide Chain I



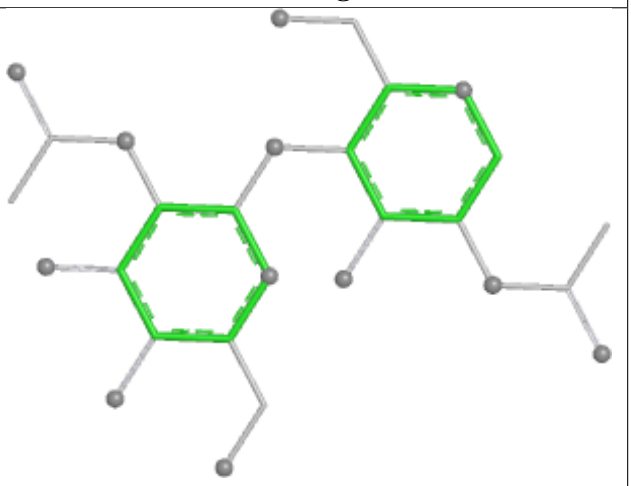
Bond lengths



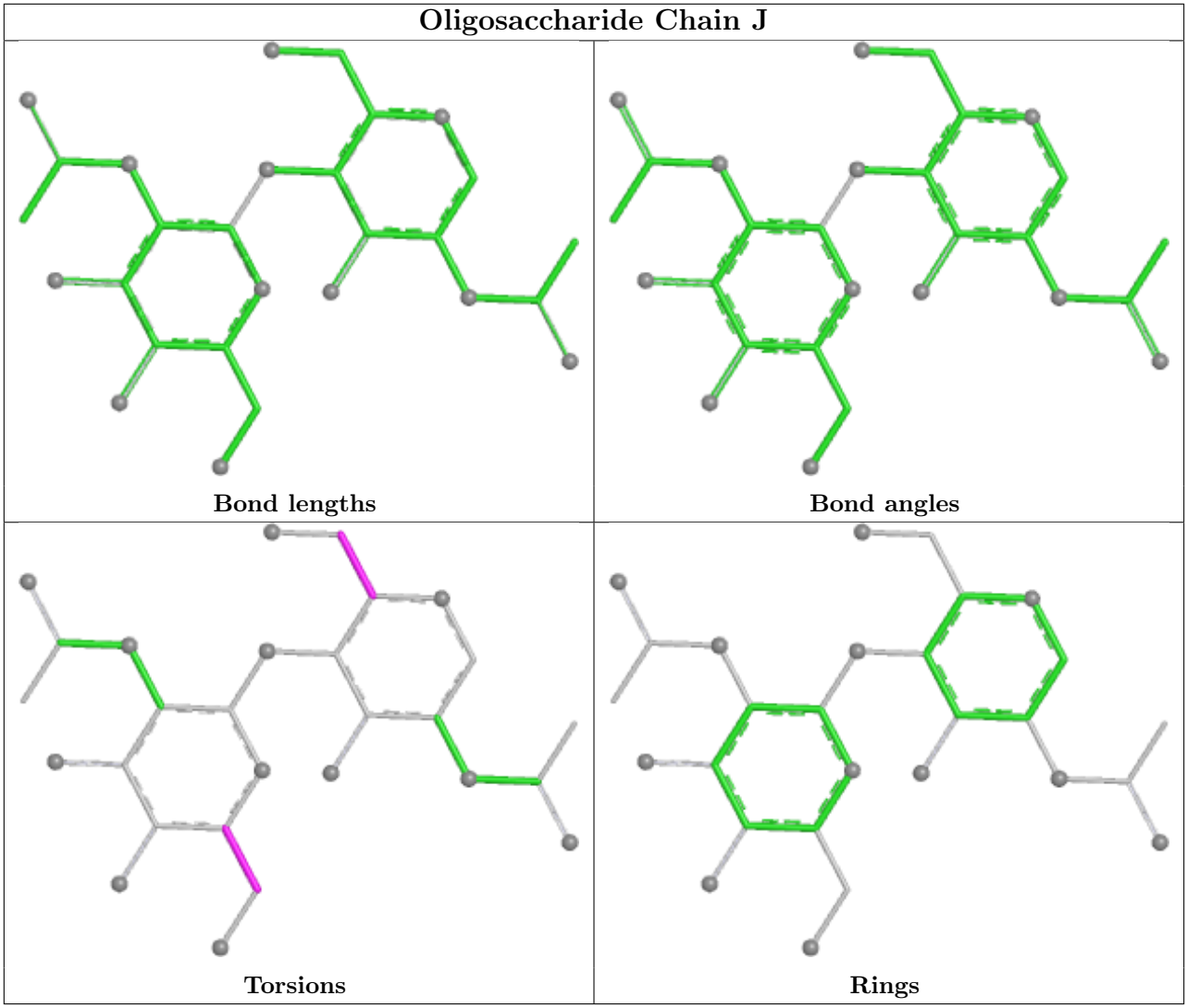
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

19 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	B	1303	1	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	C	1304	-	14,14,15	0.43	0	17,19,21	0.57	0
3	NAG	C	1303	-	14,14,15	2.22	2 (14%)	17,19,21	1.52	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1302	-	14,14,15	0.21	0	17,19,21	0.71	1 (5%)
3	NAG	B	1302	-	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	A	1304	-	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	A	1305	-	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	B	1301	-	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	A	1306	-	14,14,15	0.31	0	17,19,21	0.45	0
3	NAG	C	1301	-	14,14,15	0.53	0	17,19,21	0.87	1 (5%)
3	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	B	1304	-	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
3	NAG	C	1306	-	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	A	1301	-	14,14,15	0.27	0	17,19,21	0.51	0
3	NAG	C	1307	1	14,14,15	0.32	0	17,19,21	0.61	1 (5%)
3	NAG	B	1305	1	14,14,15	0.47	0	17,19,21	0.47	0
3	NAG	C	1302	1	14,14,15	0.69	0	17,19,21	2.37	3 (17%)
3	NAG	C	1305	-	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	B	1306	-	14,14,15	0.27	0	17,19,21	0.46	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	-	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	NAG	O5-C1	6.70	1.54	1.43
3	C	1303	NAG	C1-C2	4.85	1.59	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1302	NAG	C2-N2-C7	8.34	134.08	122.90
3	C	1303	NAG	C1-O5-C5	5.95	120.16	112.19
3	C	1302	NAG	C1-C2-N2	3.91	116.59	110.43
3	C	1301	NAG	C1-O5-C5	3.06	116.29	112.19
3	A	1302	NAG	C1-O5-C5	2.36	115.35	112.19

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

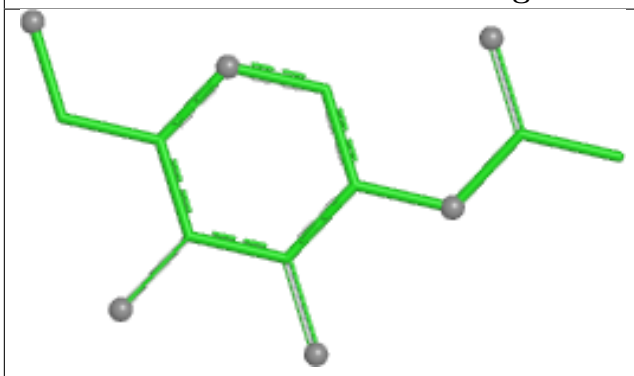
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1304	NAG	1	0
3	A	1301	NAG	1	0
3	B	1306	NAG	1	0

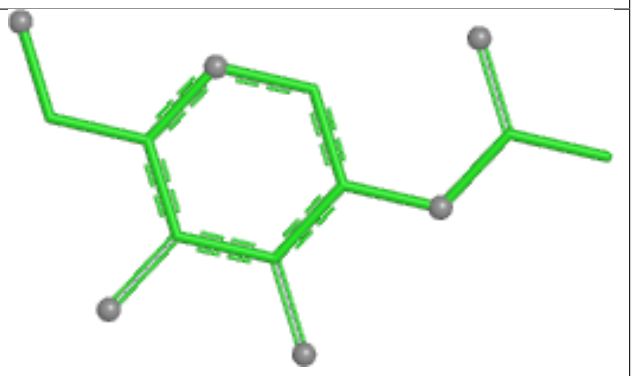
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

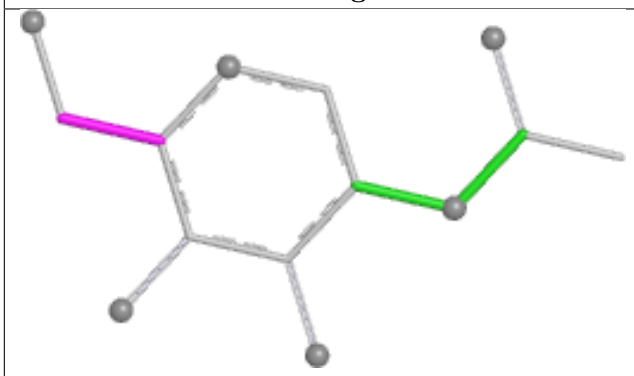
Ligand NAG B 1303



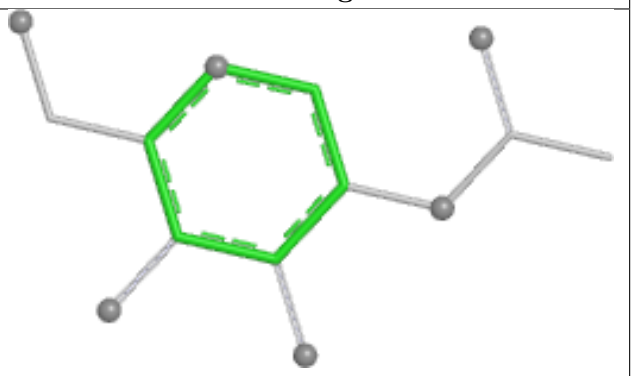
Bond lengths



Bond angles

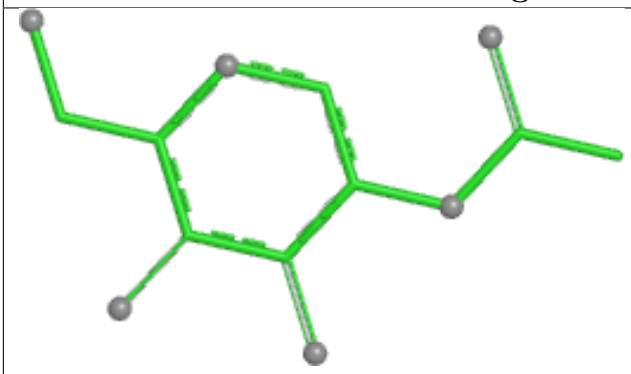


Torsions

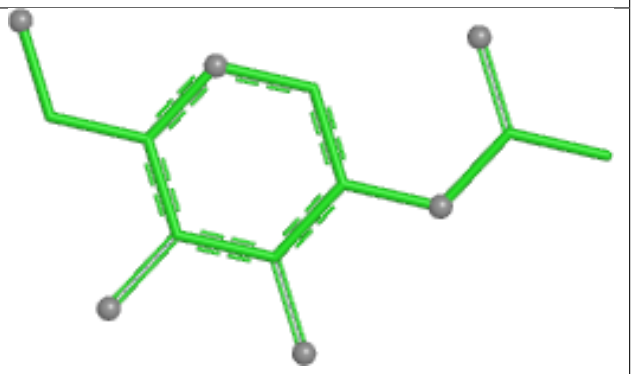


Rings

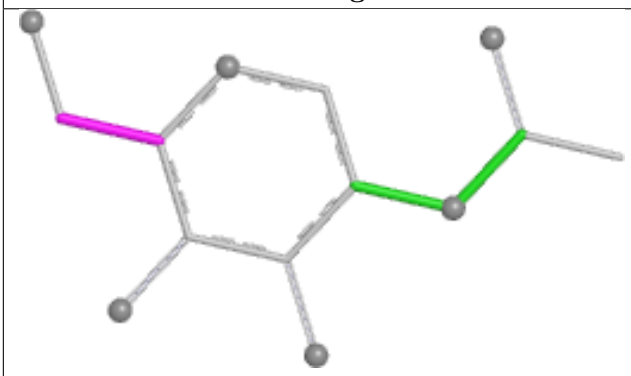
Ligand NAG C 1304



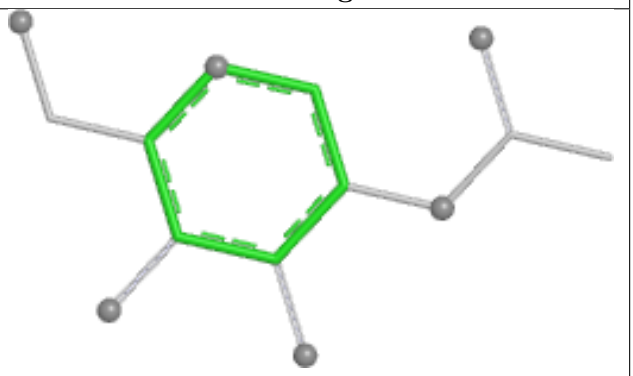
Bond lengths



Bond angles

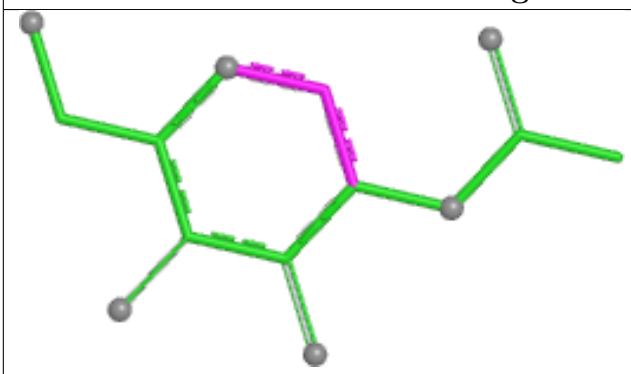


Torsions

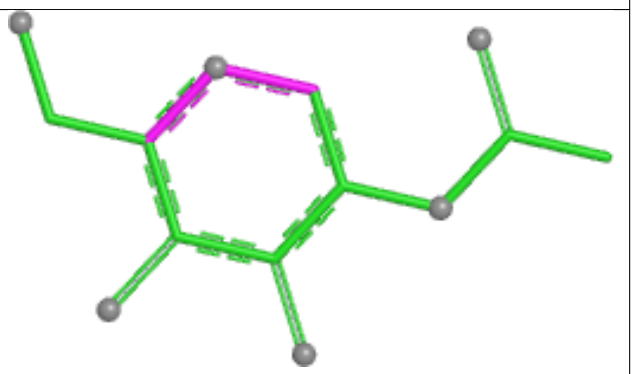


Rings

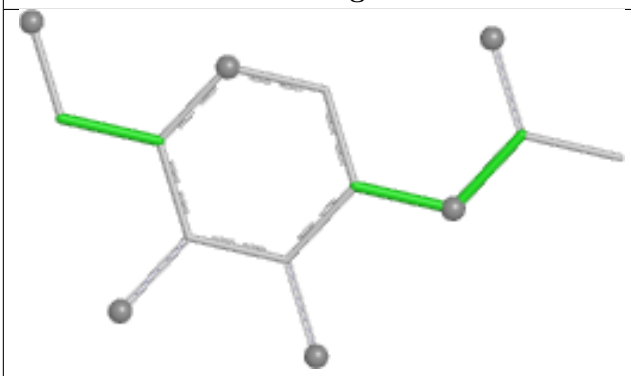
Ligand NAG C 1303



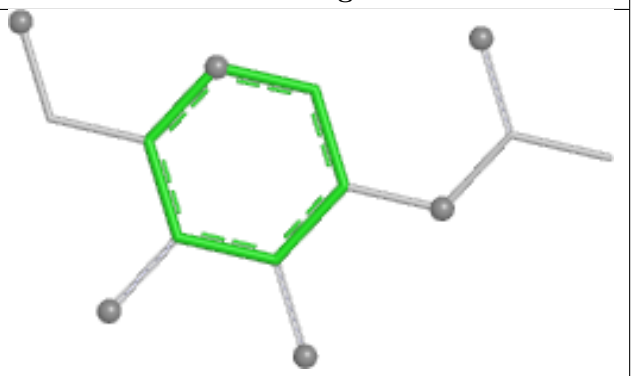
Bond lengths



Bond angles

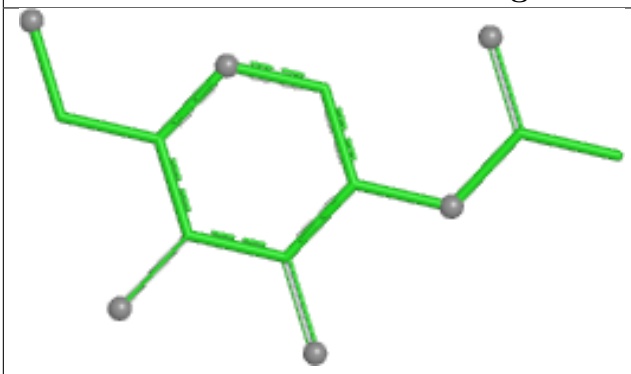


Torsions



Rings

Ligand NAG A 1302



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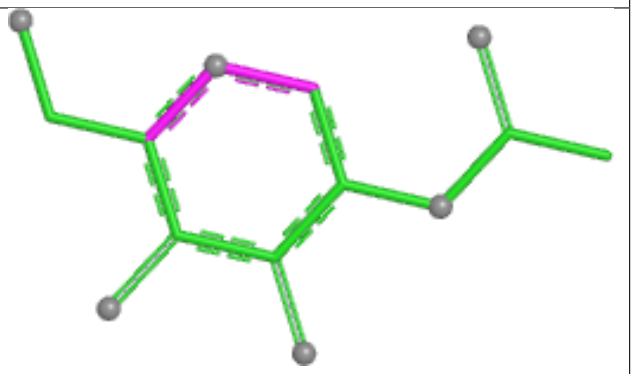
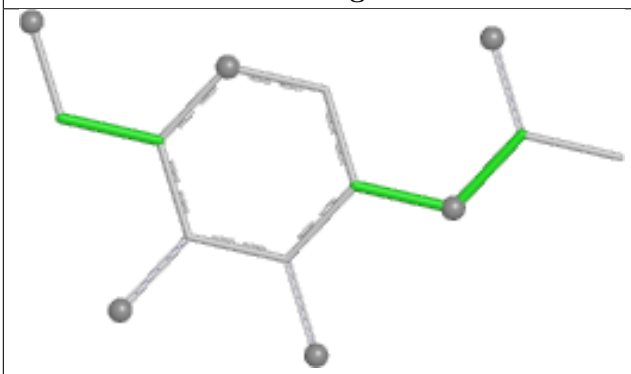
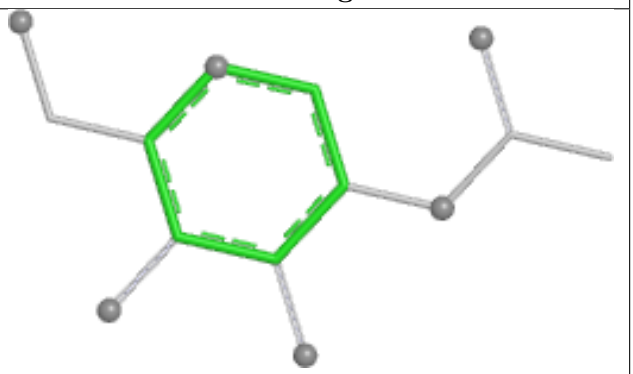


Bond angles

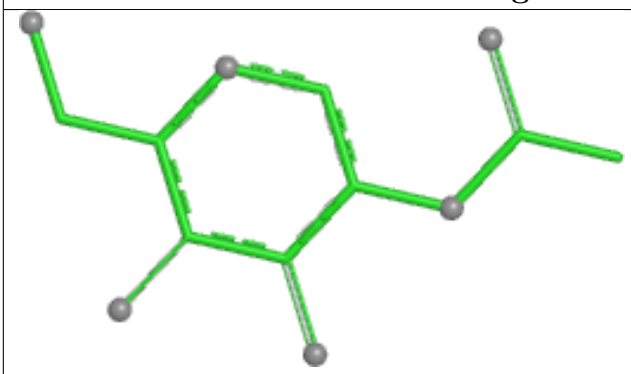


Torsions



Rings

Ligand NAG B 1302



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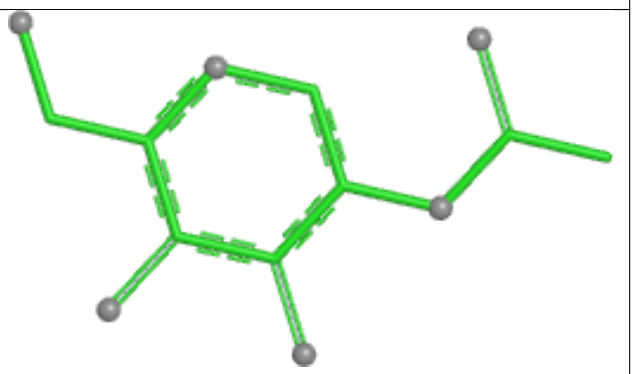
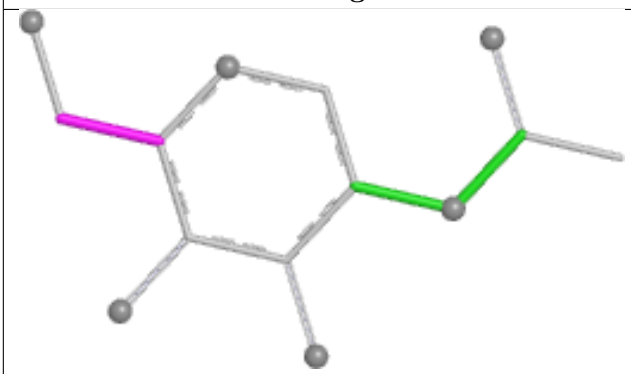


Bond angles



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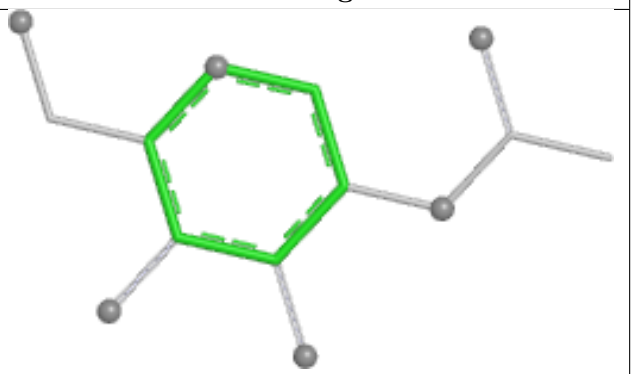
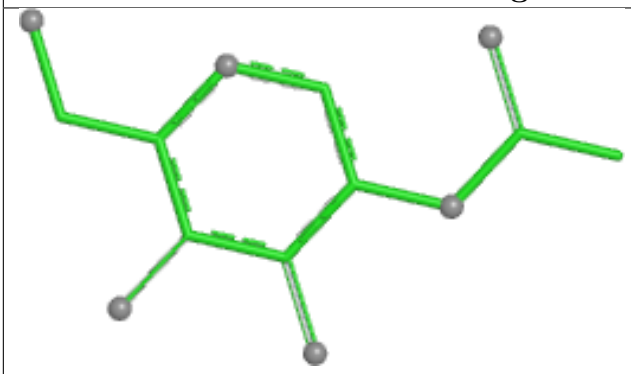


Rings

Ligand NAG A 1304



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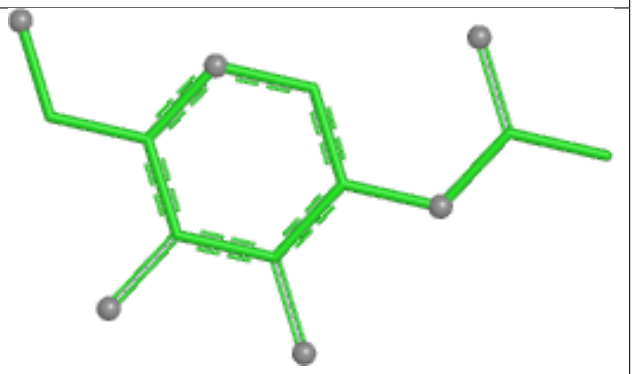
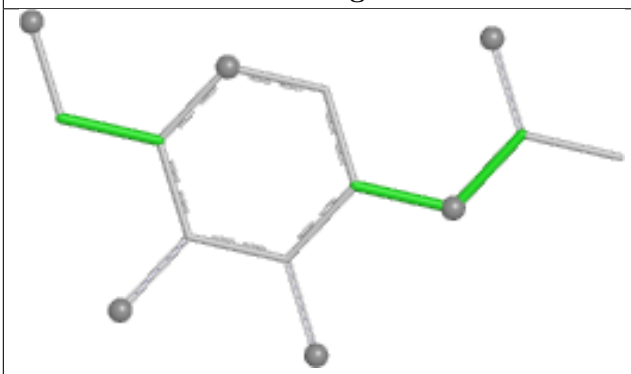


Bond angles



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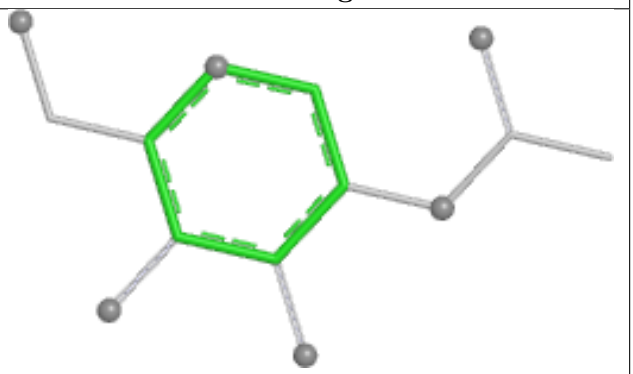
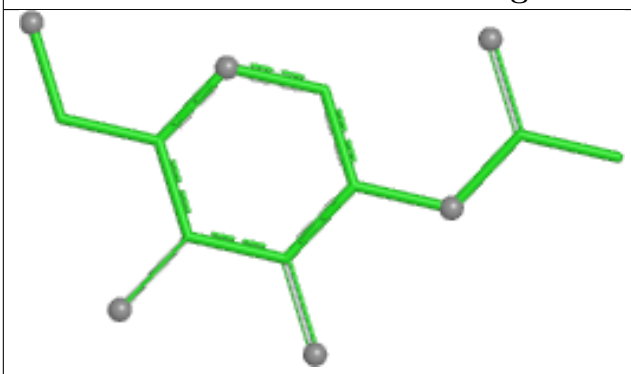


Rings

Ligand NAG A 1305



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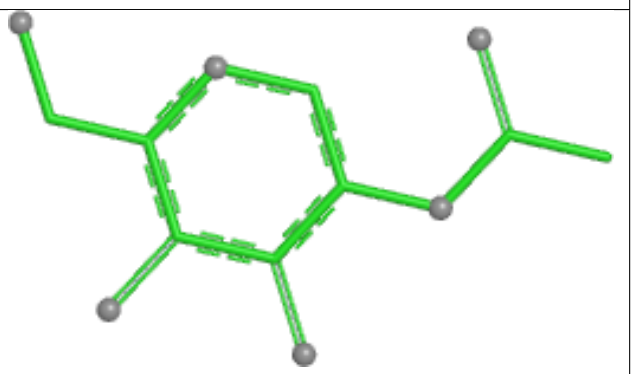
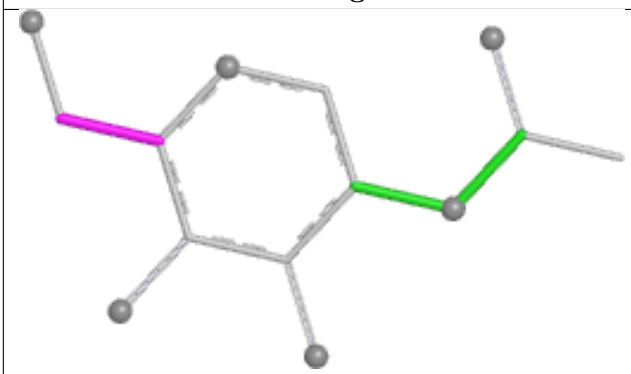


Bond angles



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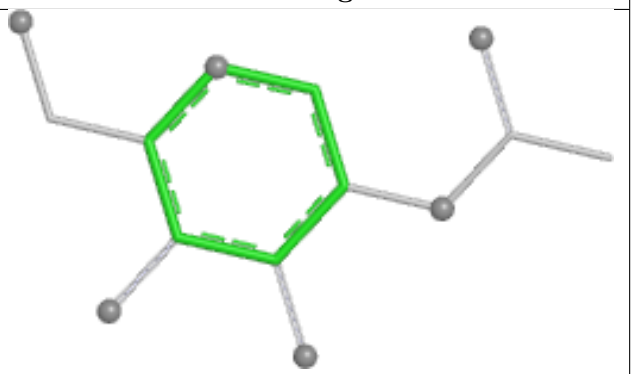
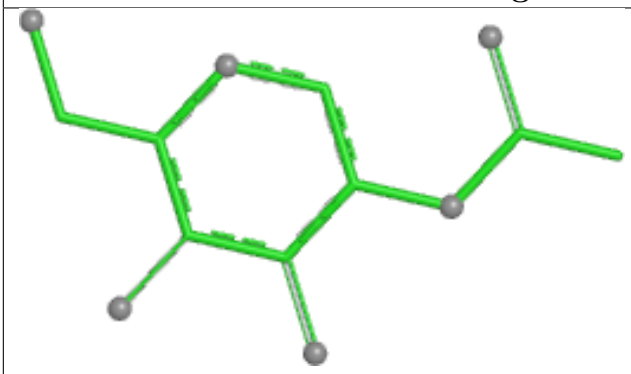


Rings

Ligand NAG B 1301



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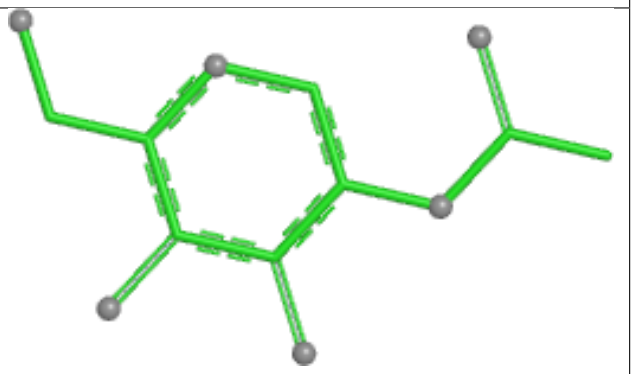
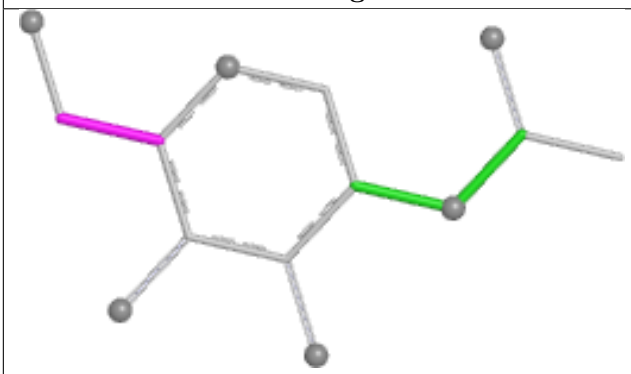


Bond angles



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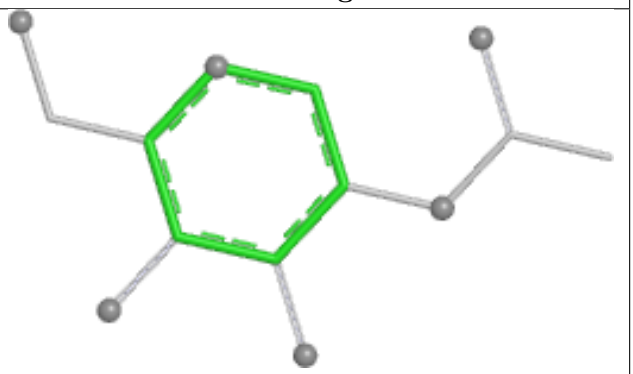
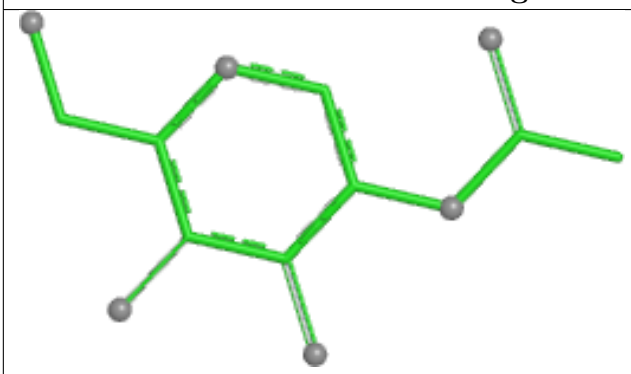


Rings

Ligand NAG A 1306



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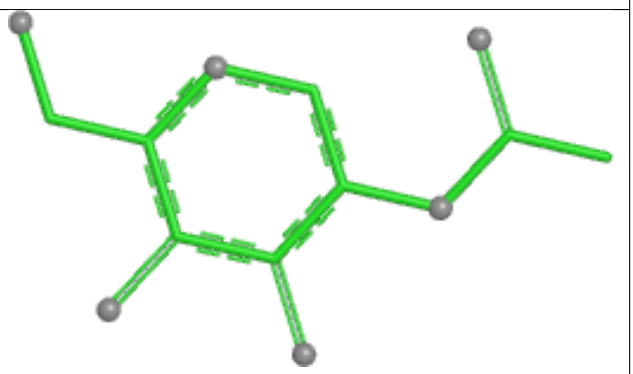
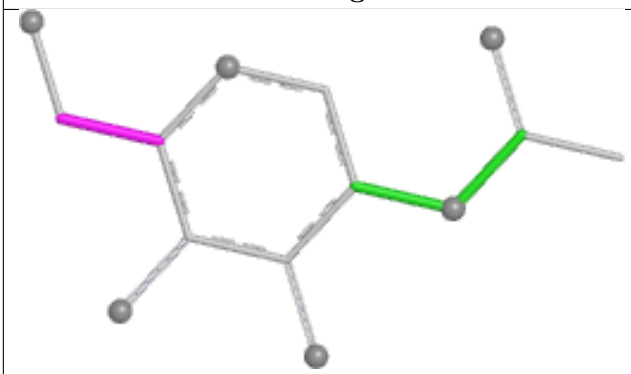


Bond angles



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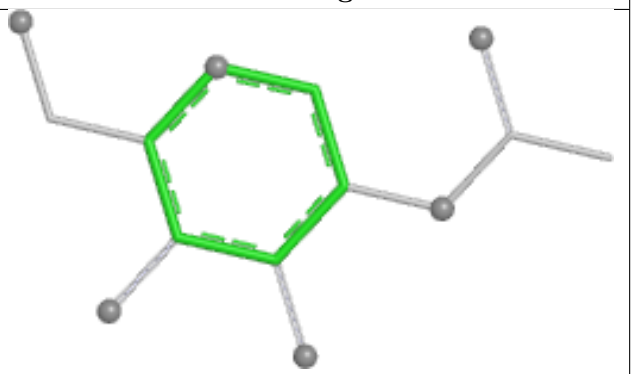
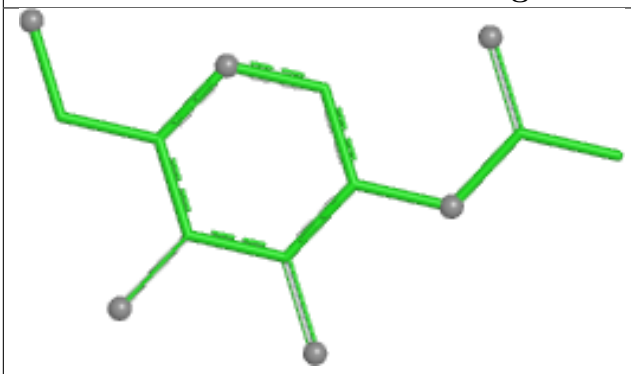


Rings

Ligand NAG C 1301



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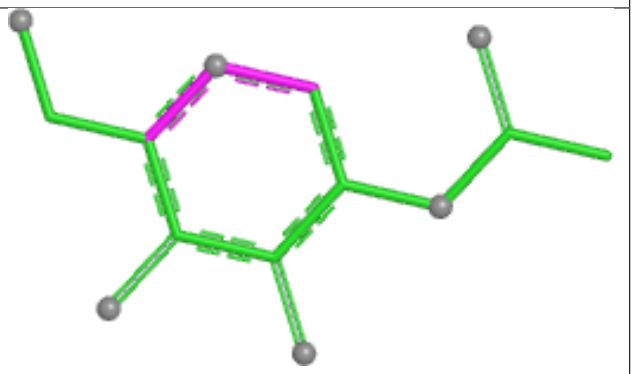
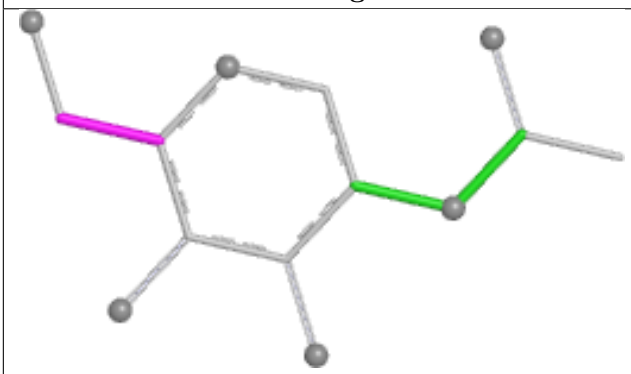


Bond angles



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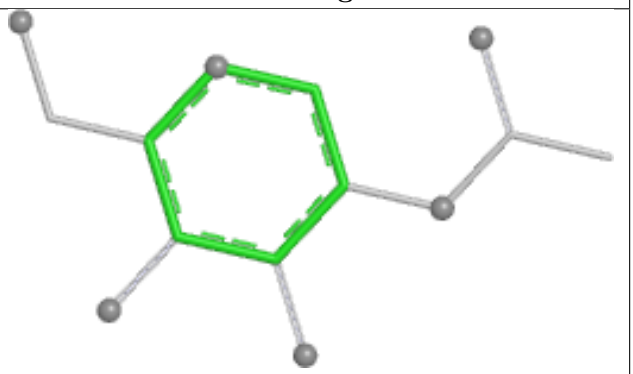
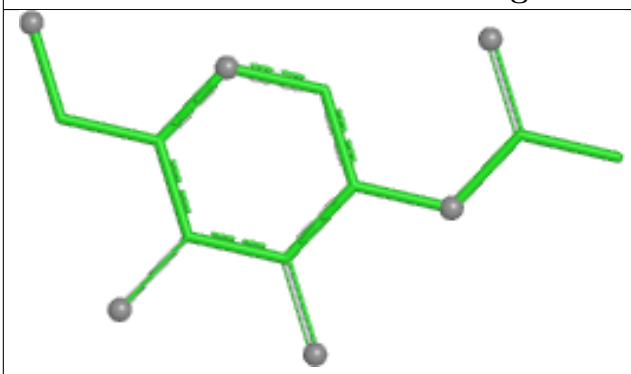


Rings

Ligand NAG A 1303



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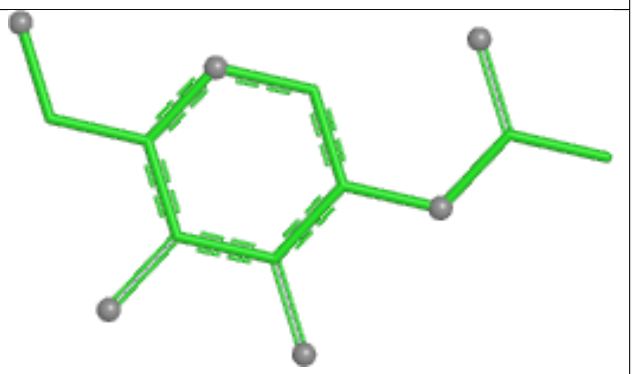
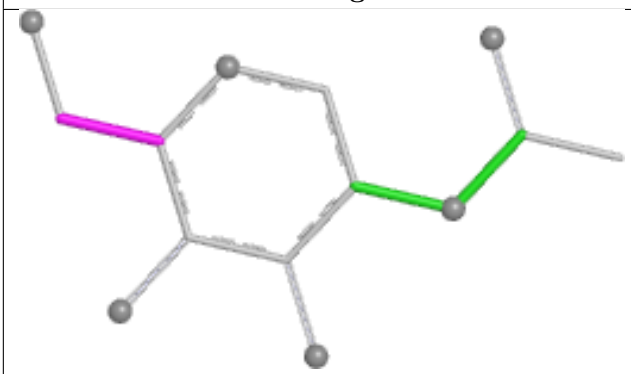


Bond angles



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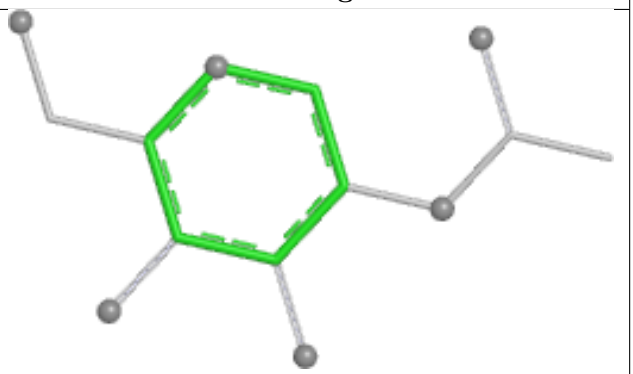
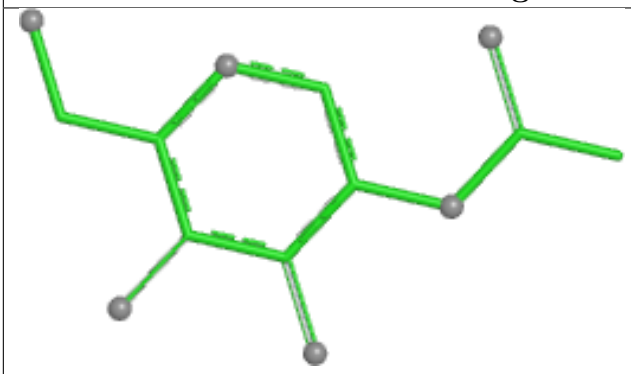


Rings

Ligand NAG B 1304



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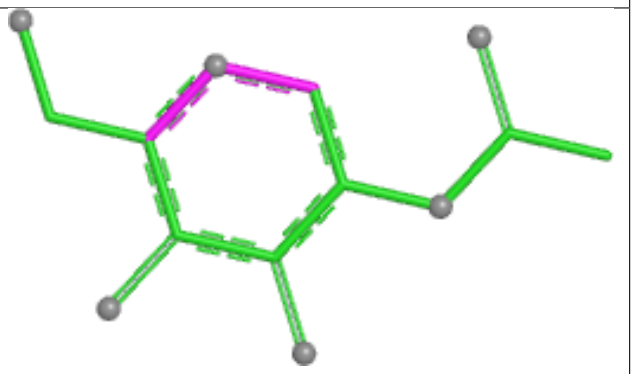

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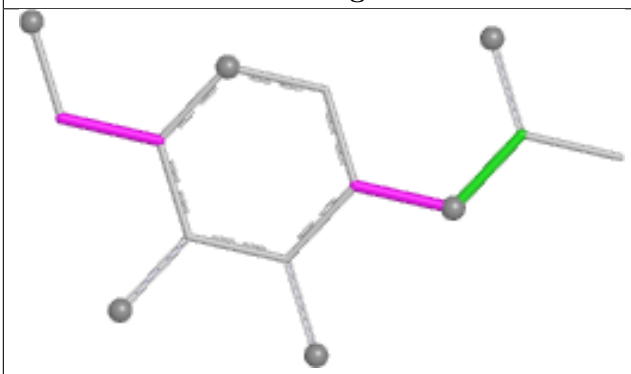

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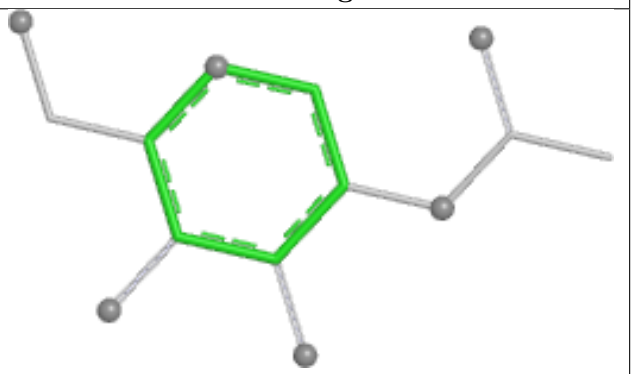
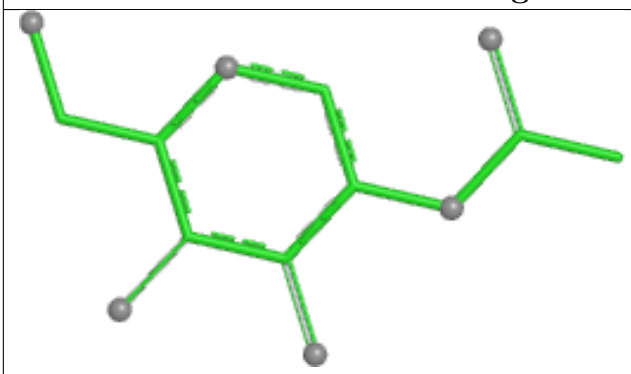


Rings

Ligand NAG C 1306



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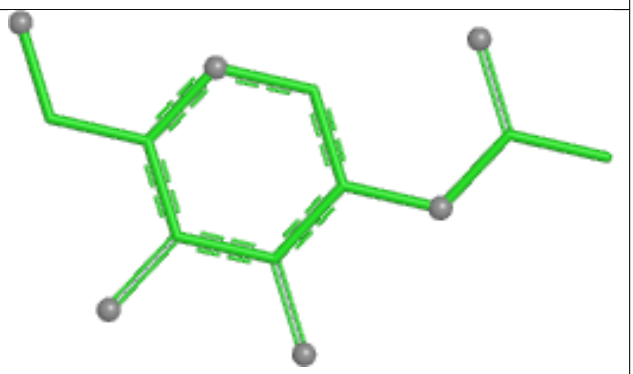
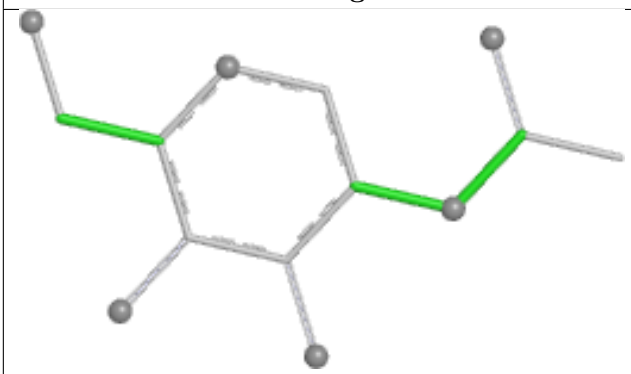


Bond angles



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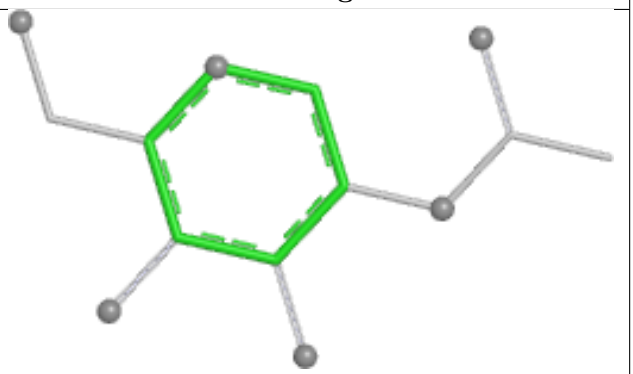
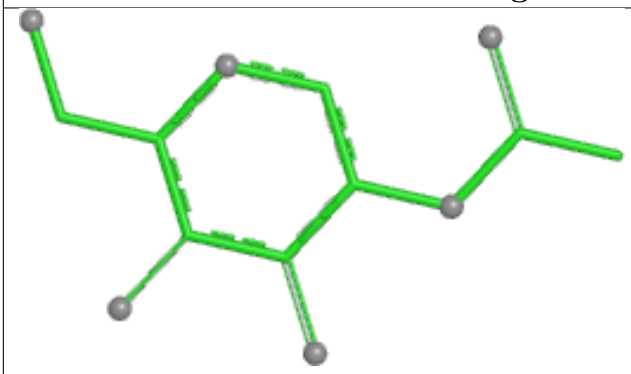
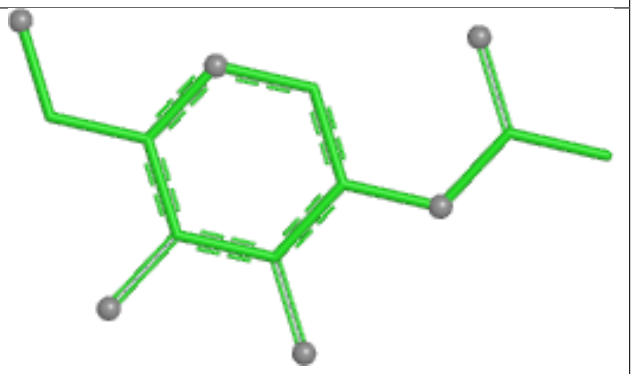


Rings

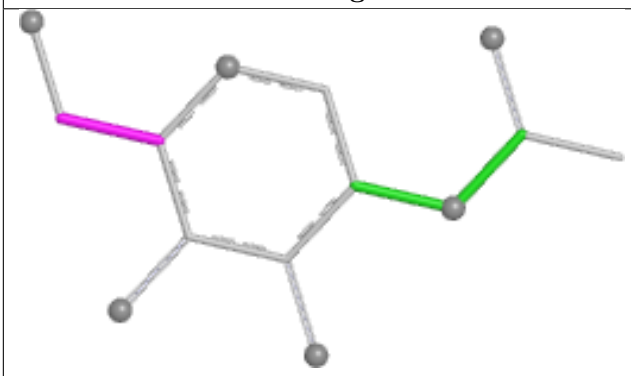
Ligand NAG A 1301



Bond lengths



Bond angles



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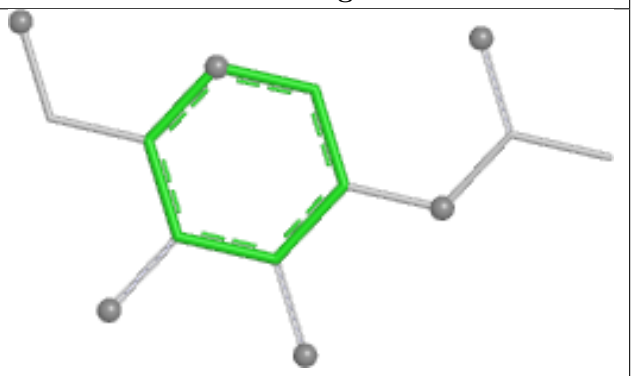
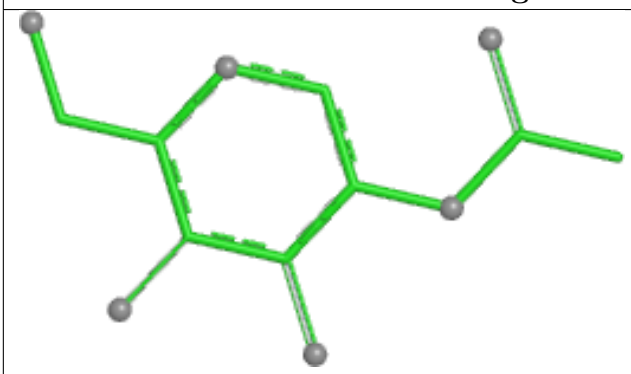


Rings

Ligand NAG C 1307



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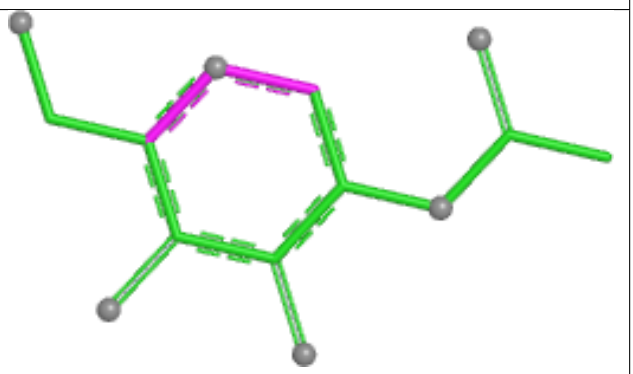
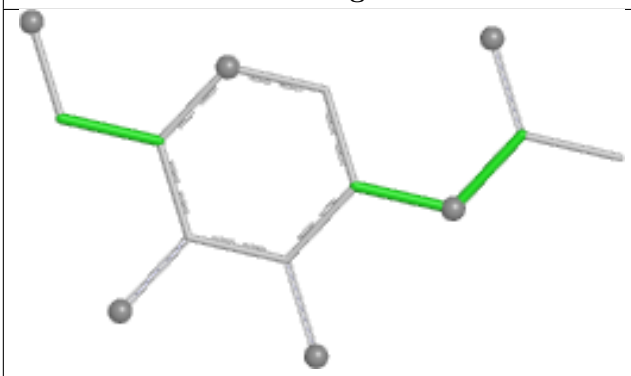


Bond angles



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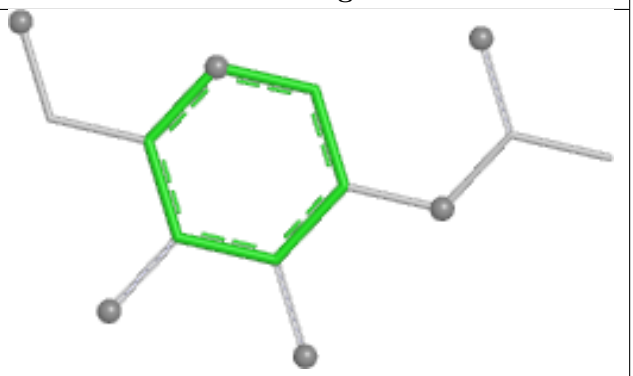
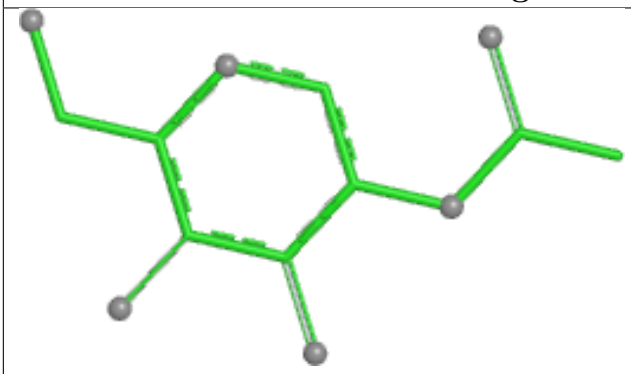
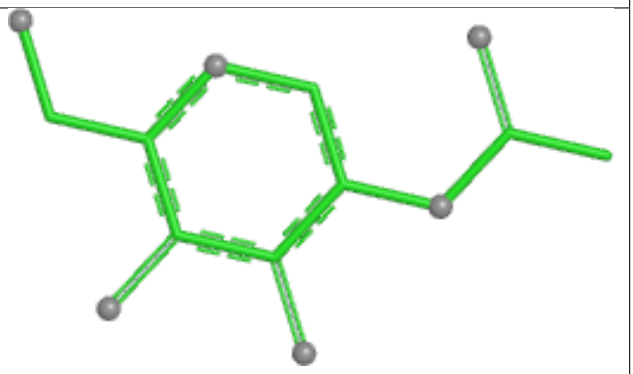


Rings

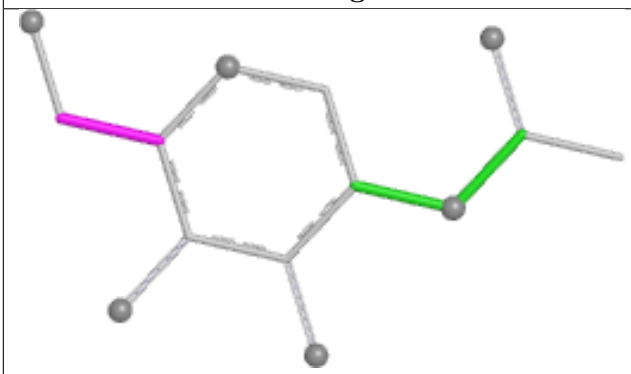
Ligand NAG B 1305



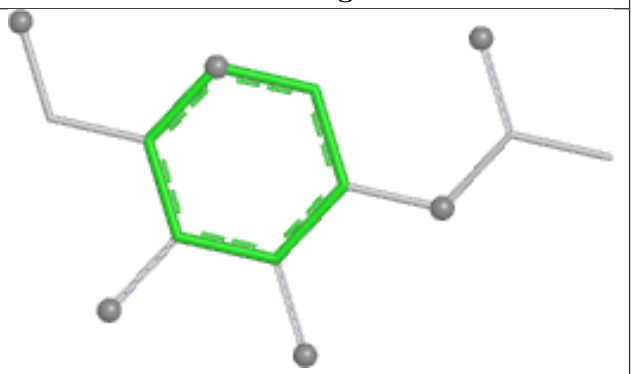
Bond lengths



Bond angles

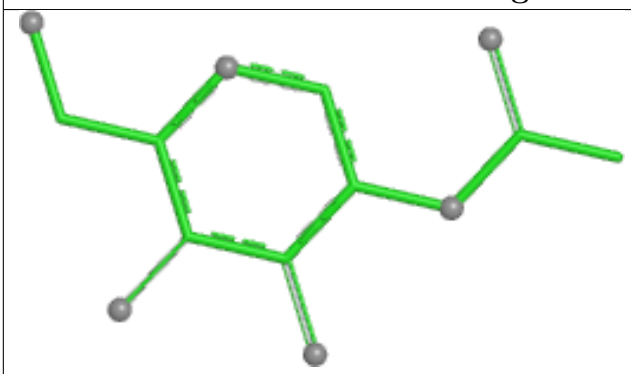


Torsions

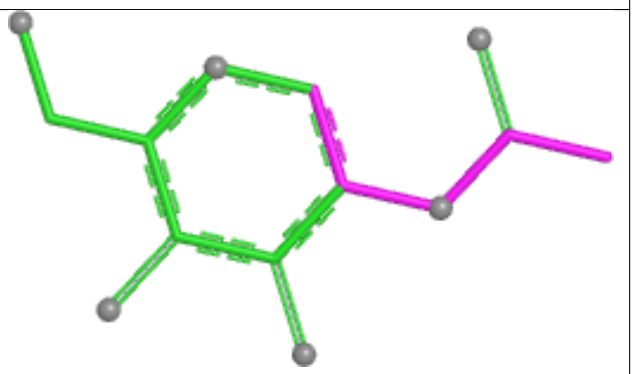


Rings

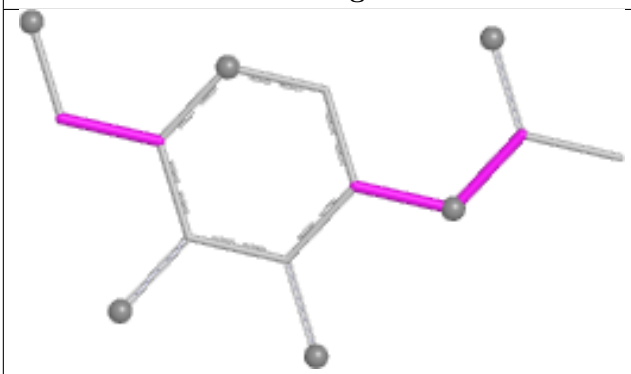
Ligand NAG C 1302



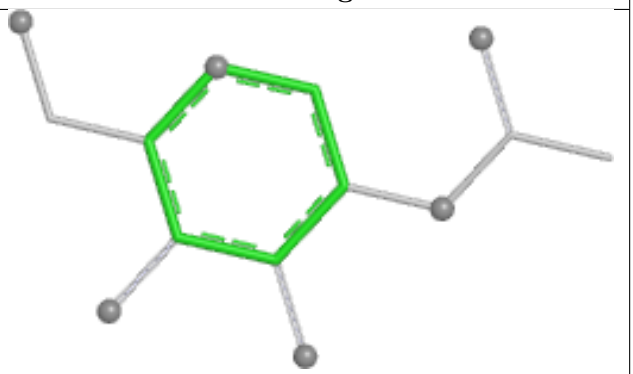
Bond lengths



Bond angles

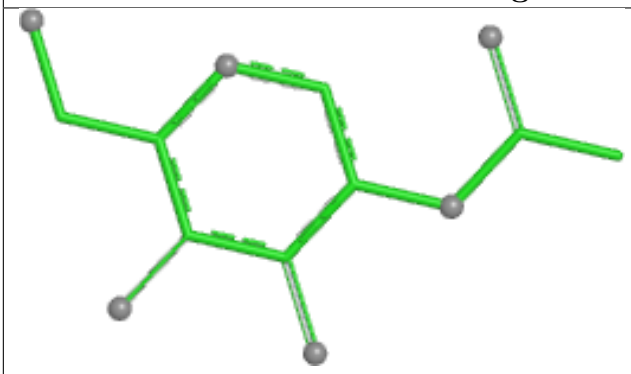


Torsions

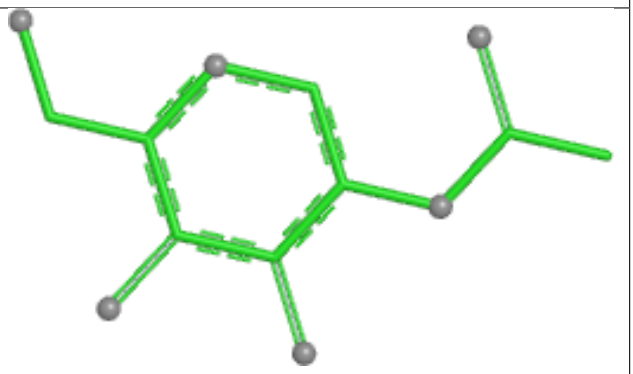


Rings

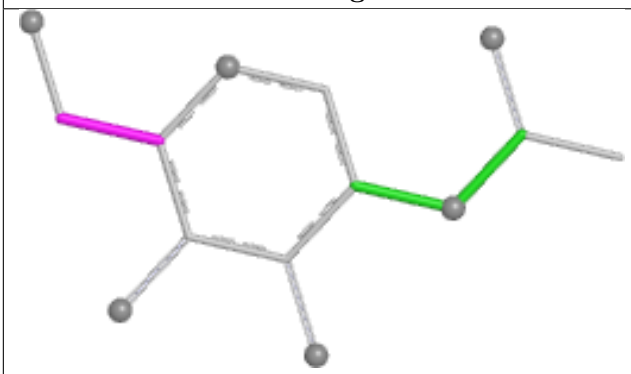
Ligand NAG C 1305



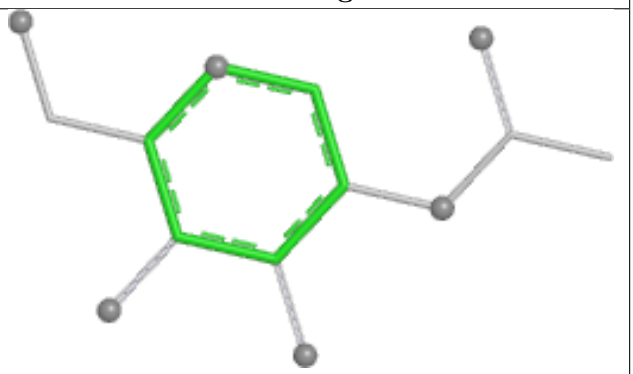
Bond lengths



Bond angles

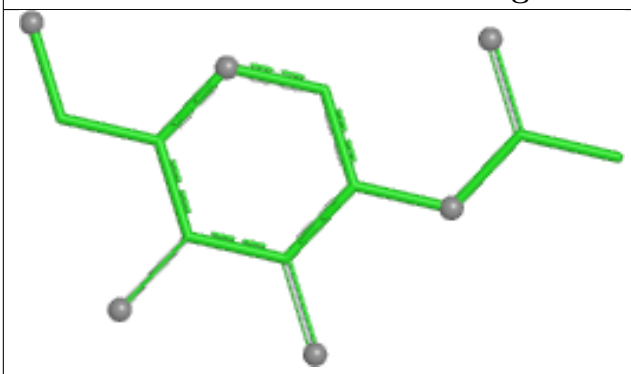


Torsions

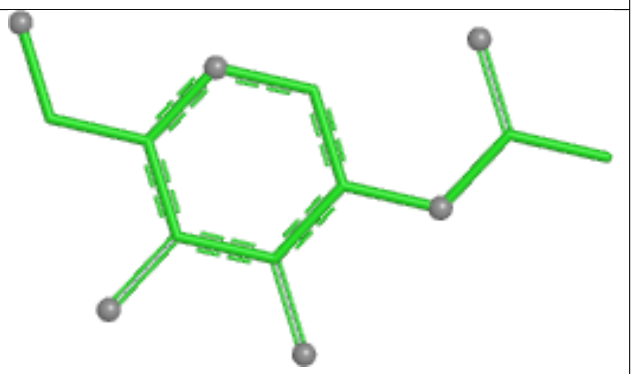


Rings

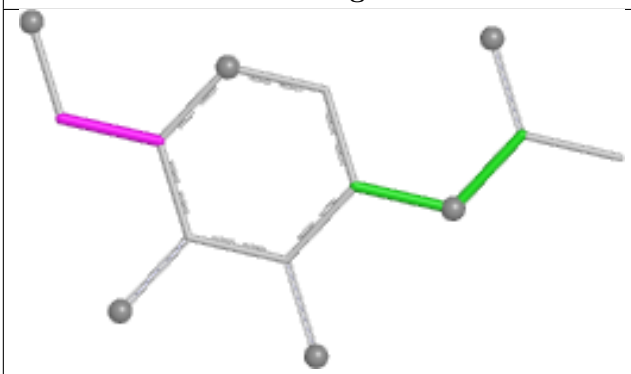
Ligand NAG B 1306



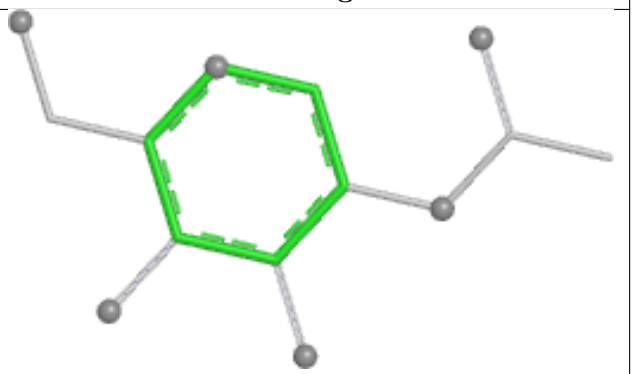
Bond lengths



Bond angles



Torsions



Rings

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.

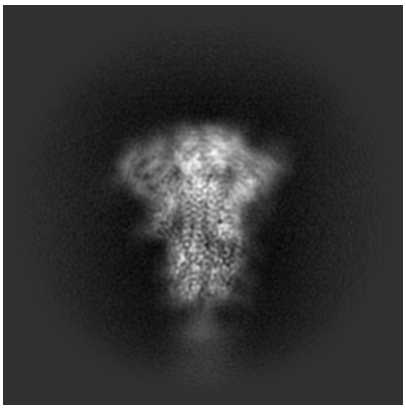
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42589. These allow visual inspection of the internal detail of the map and identification of artifacts.

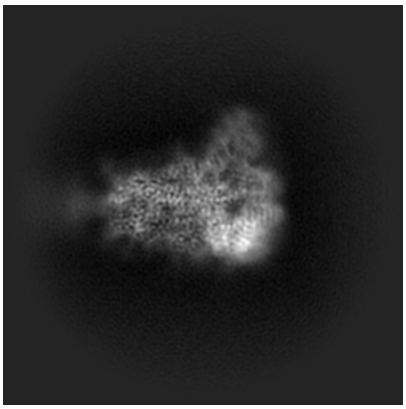
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

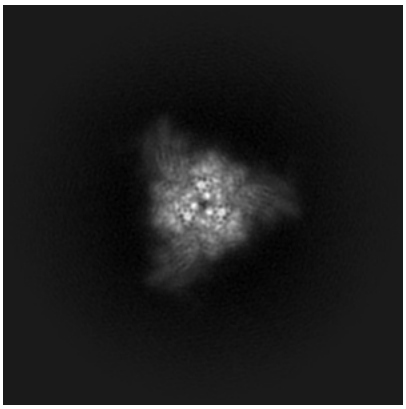
6.1.1 Primary map



X

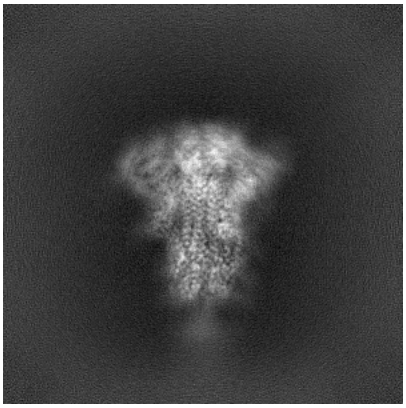


Y

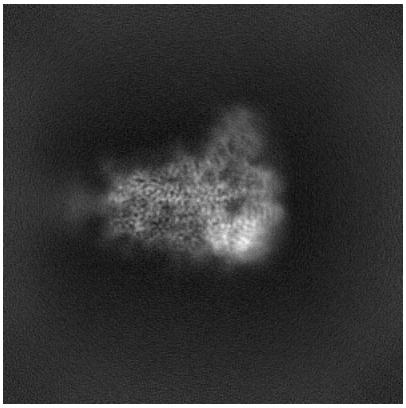


Z

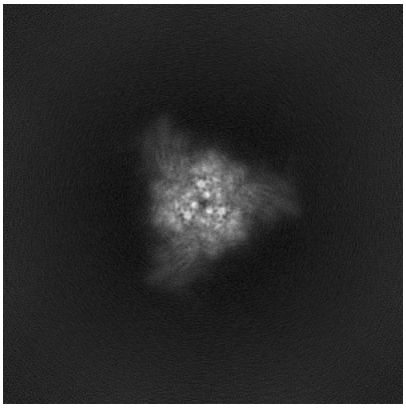
6.1.2 Raw map



X



Y

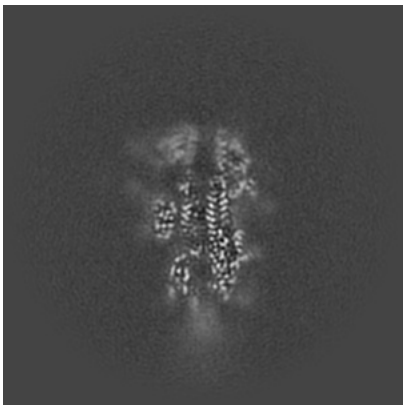


Z

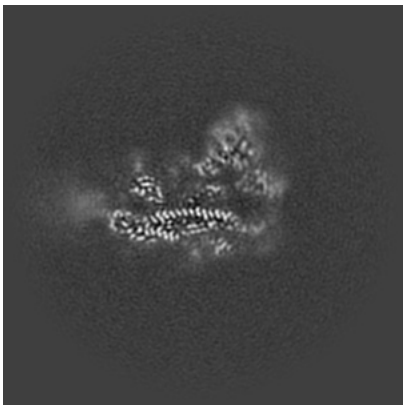
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

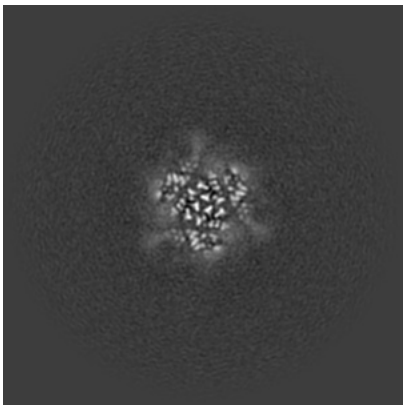
6.2.1 Primary map



X Index: 192

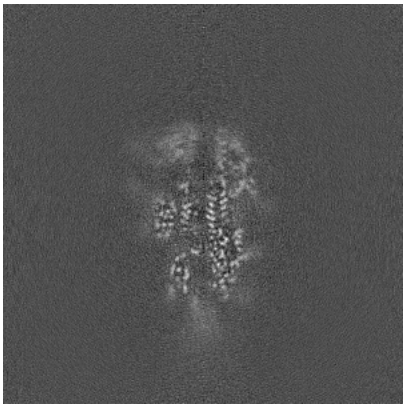


Y Index: 192

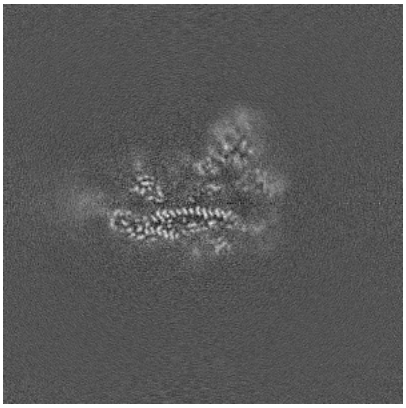


Z Index: 192

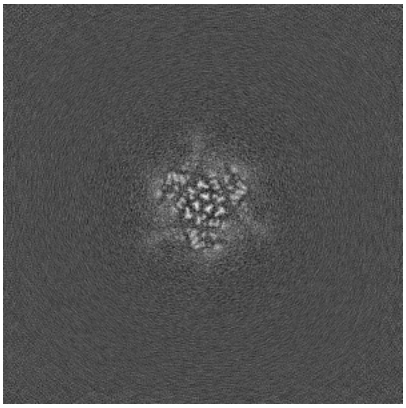
6.2.2 Raw map



X Index: 192



Y Index: 192



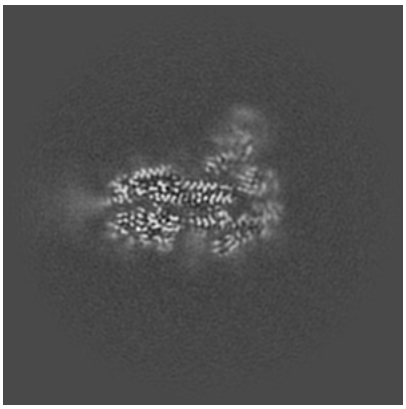
Z Index: 192

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

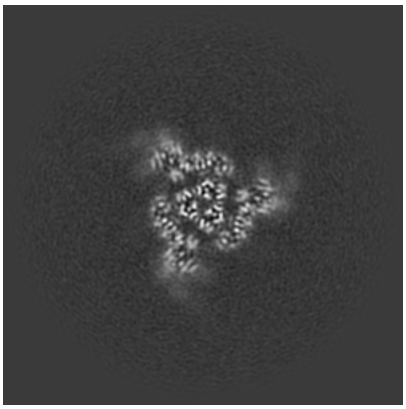
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 197

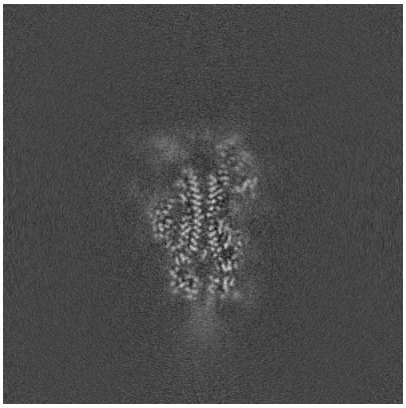


Y Index: 183

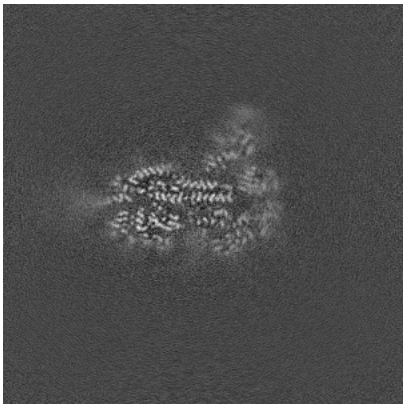


Z Index: 210

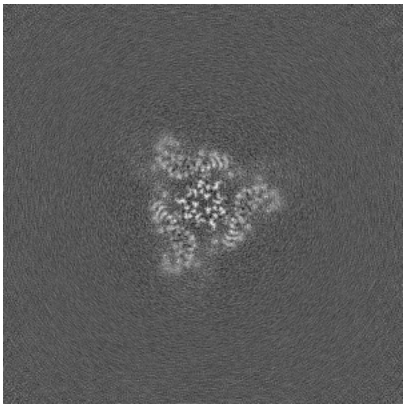
6.3.2 Raw map



X Index: 197



Y Index: 184

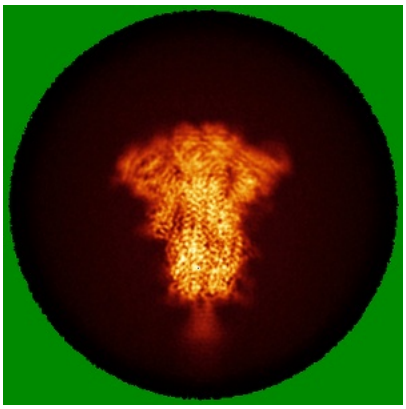


Z Index: 204

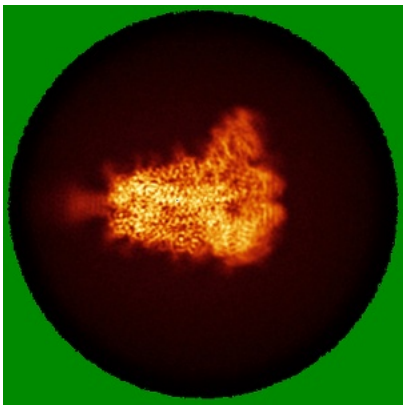
The images above show the largest variance slices of the map in three orthogonal directions.

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

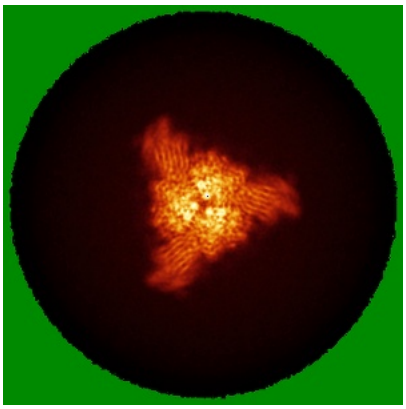
6.4.1 Primary map



X

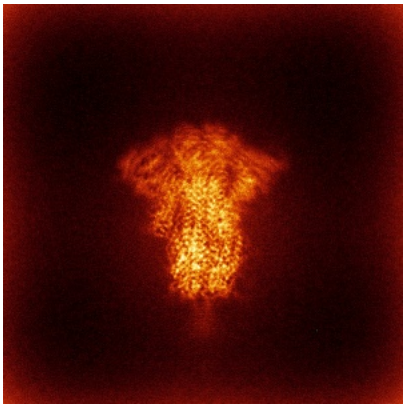


Y

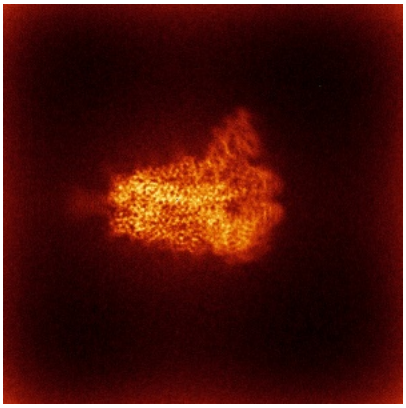


Z

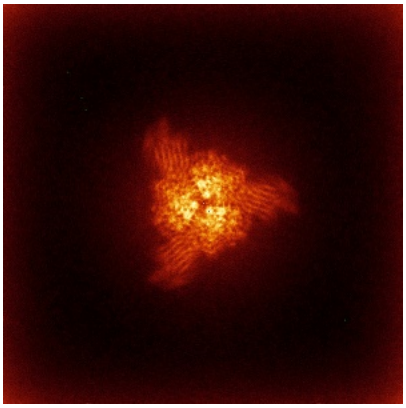
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

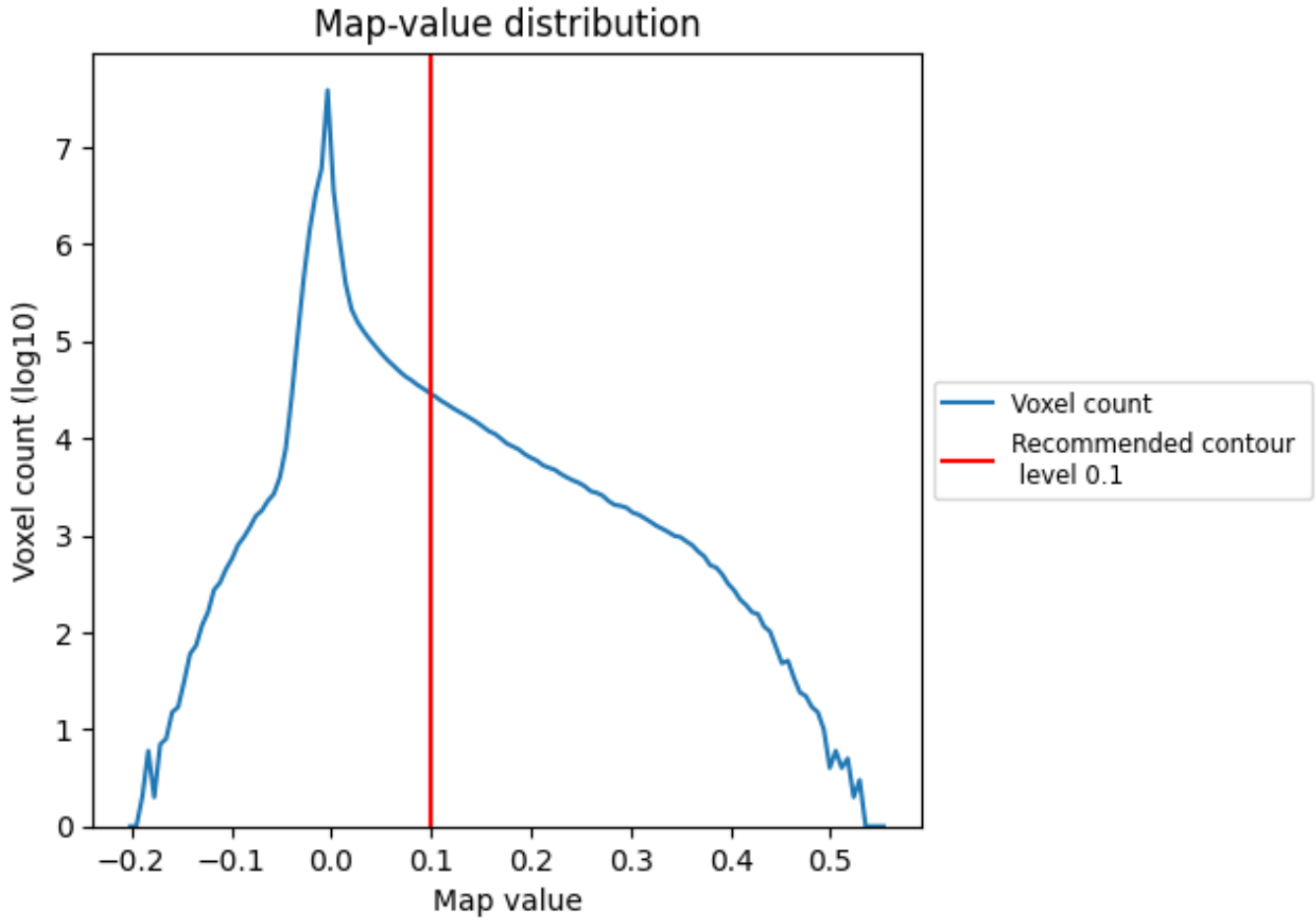
6.6 Mask visualisation (i)

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

7 Map analysis

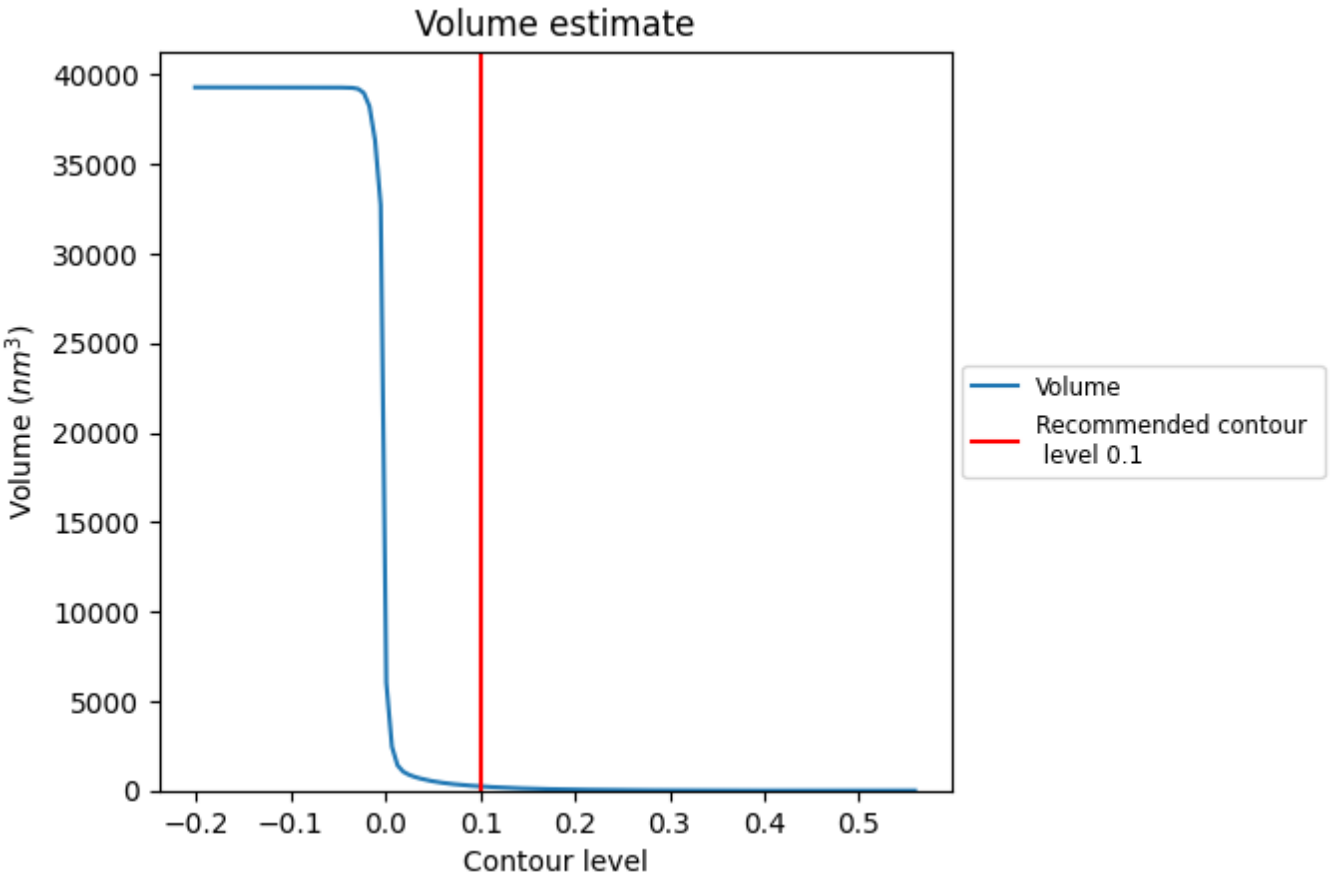
This section contains the results of statistical analysis of the map.

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.

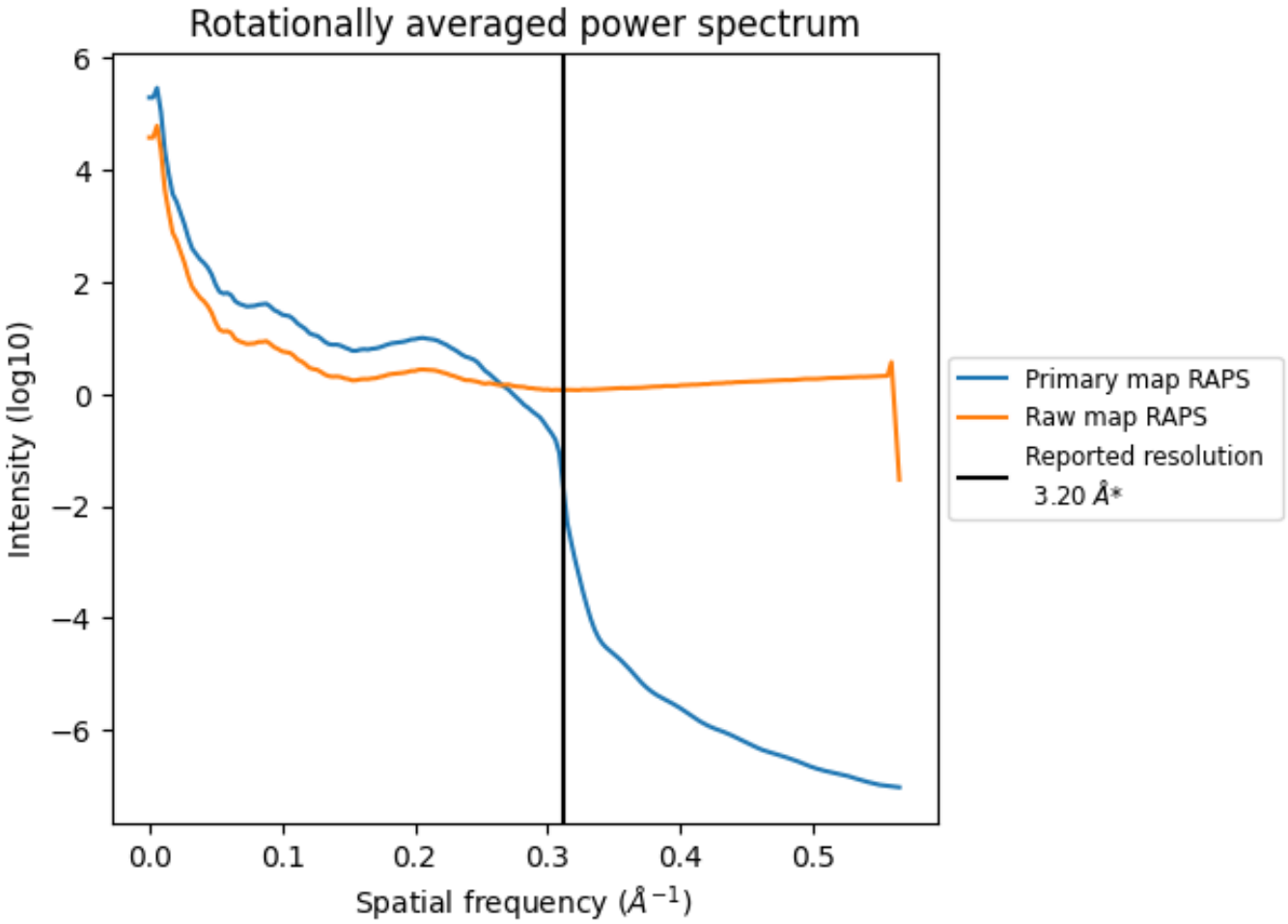
7.2 Volume estimate (i)



The volume at the recommended contour level is 235 nm^3; this corresponds to an approximate mass of 212 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)

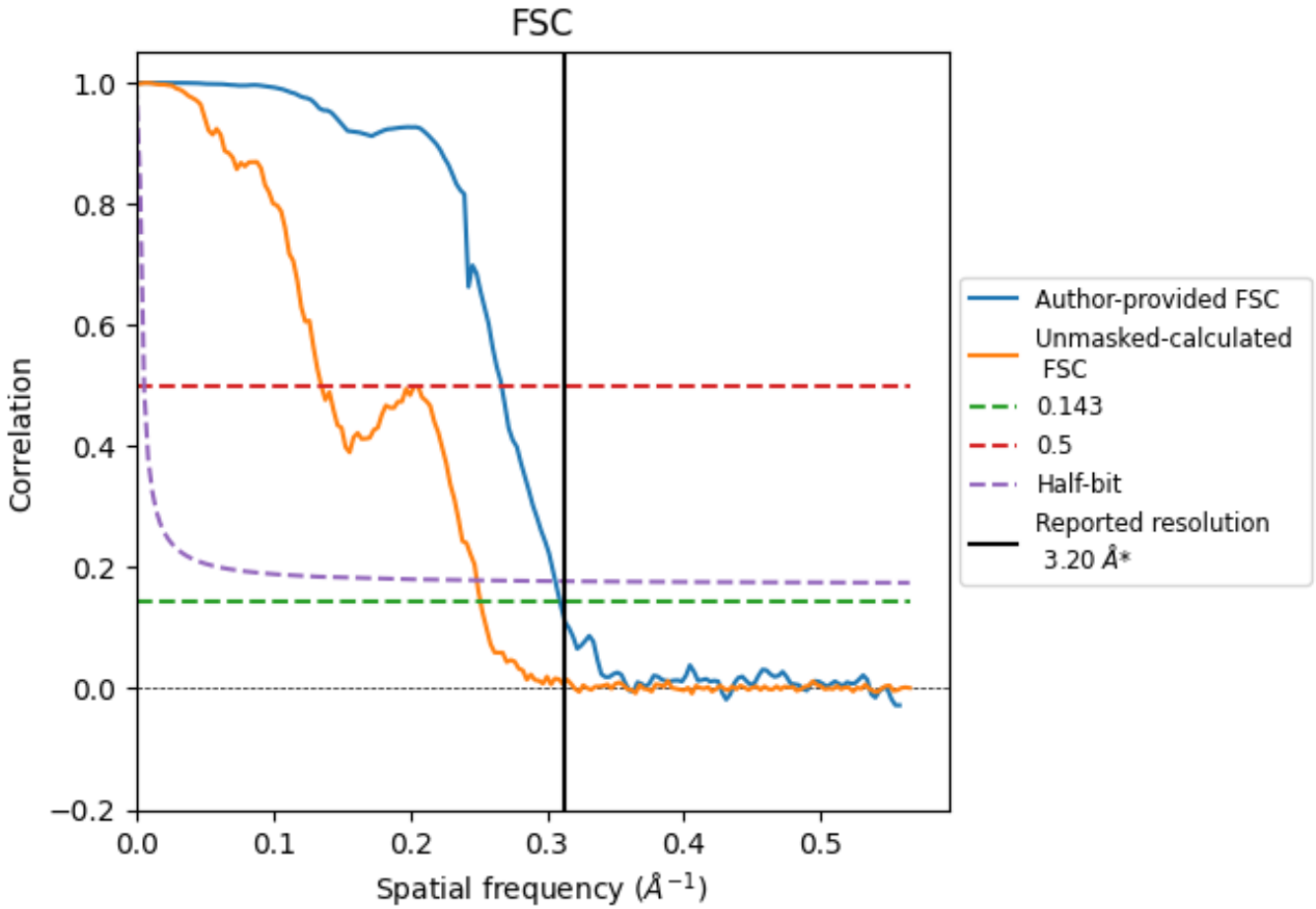


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.75	3.27
Unmasked-calculated*	3.98	7.40	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.2 by more than 10 %

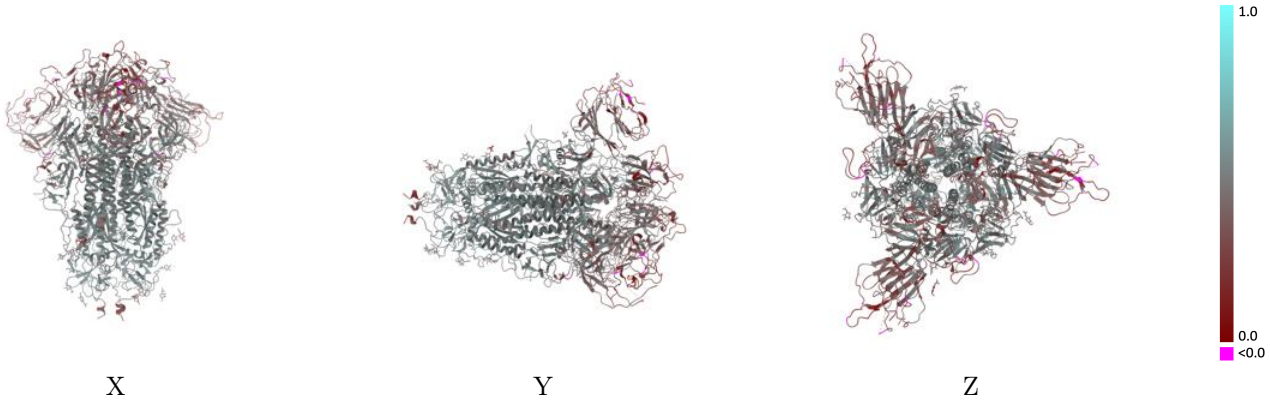
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42589 and PDB model 8UUL. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay

This section was not generated.

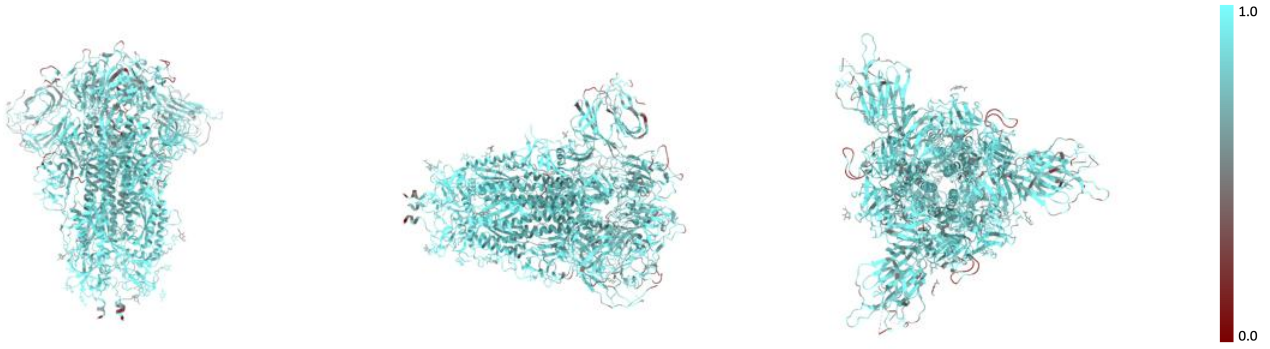
9.2 Q-score mapped to coordinate model



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.

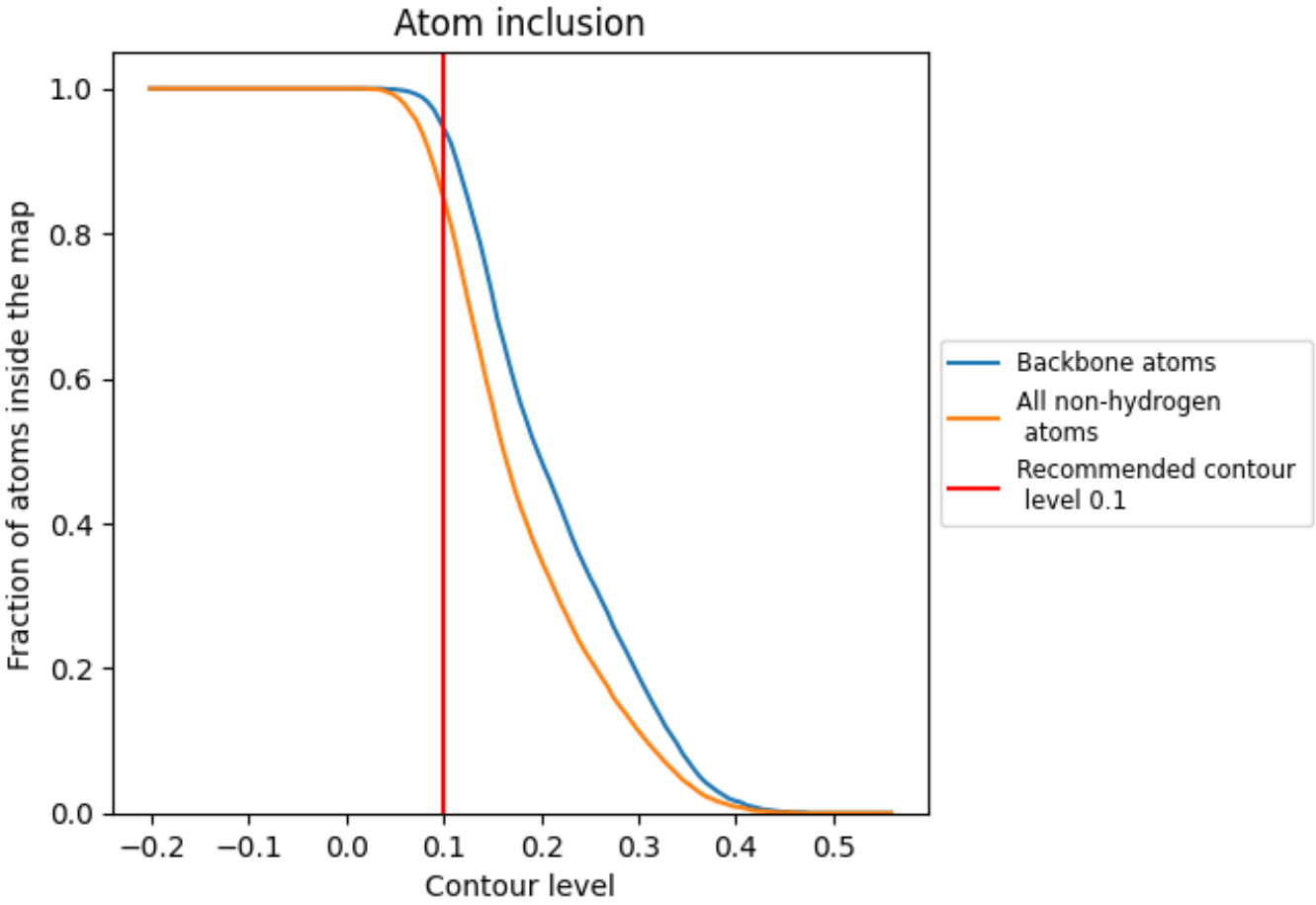
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.4400
A	0.8500	0.4400
B	0.8520	0.4410
C	0.8490	0.4400
D	0.6070	0.2100
E	0.6430	0.3230
F	0.7500	0.4660
G	0.6790	0.3970
H	0.7860	0.4290
I	0.7860	0.4750
J	0.7140	0.3910