Full wwPDB EM Validation Report ⓘ

Jul 4, 2023 – 02:22 PM JST

PDB ID	:	8GTP
EMDB ID	:	EMD-34261
Title	:	cryo-EM structure of Omicron BA.5 S protein in complex with XGv289
Authors	:	Xia, X.Y.; Zhang, Y.Y.; Chi, X.M.; Huang, B.D.; Wu, L.S.; Zhou, Q.
Deposited on	:	2022-09-08
Resolution	:	3.10 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:

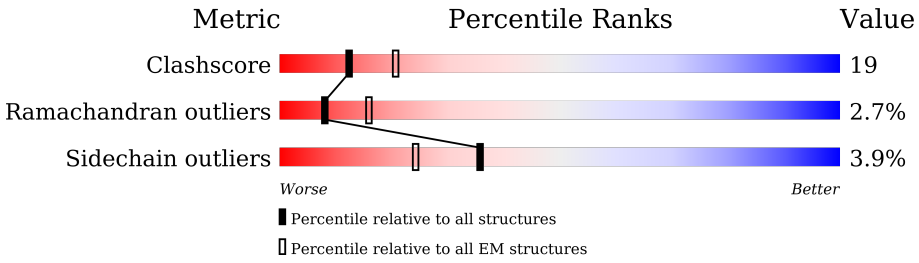
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1271	61% 15% • • 19%
1	B	1271	9% 60% 16% • • 19%
1	C	1271	7% 63% 16% • 19%
2	H	120	21% 76% 24%
2	I	120	99% 77% 23%
2	J	120	88% 77% 23%
3	L	111	34% 69% 25% 5% •
3	M	111	96% 73% 23% • •

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Mol	Chain	Length	Quality of chain
3	N	111	96% 73% 23%
4	D	2	50% 100%
4	E	2	50% 50% 50%
4	F	2	50% 50%
4	G	2	50% 50%
4	K	2	100%
4	O	2	100%
4	P	2	50% 100%
4	Q	2	100% 50% 50%
4	R	2	50% 50%
4	S	2	50% 50%
4	T	2	100%
4	U	2	100%
4	V	2	50% 50%
4	W	2	100% 50% 50%
4	X	2	50% 50%
4	Y	2	50% 50%
4	Z	2	100%
4	a	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	V	1	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30249 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	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		
1	B	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		
1	C	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2

- Molecule 2 is a protein called heavy chain of XGv289.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	120	Total	C	N	O	S	0	0
			902	571	153	173	5		
2	I	120	Total	C	N	O	S	0	0
			902	571	153	173	5		
2	J	120	Total	C	N	O	S	0	0
			902	571	153	173	5		

- Molecule 3 is a protein called light chain of XGv289.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			816	510	139	165	2		
3	M	111	Total	C	N	O	S	0	0
			816	510	139	165	2		
3	N	111	Total	C	N	O	S	0	0
			816	510	139	165	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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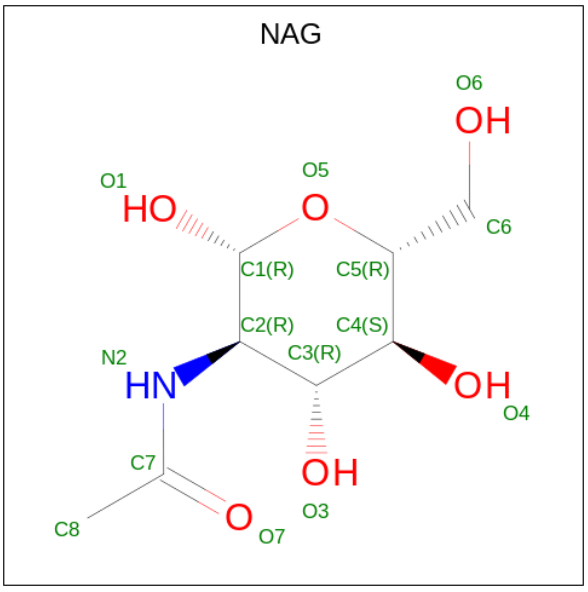
Mol	Chain	Residues	Atoms	AltConf	Trace
4	R	2	Total C N O 28 16 2 10	0	0
4	S	2	Total C N O 28 16 2 10	0	0
4	T	2	Total C N O 28 16 2 10	0	0
4	U	2	Total C N O 28 16 2 10	0	0
4	V	2	Total C N O 28 16 2 10	0	0
4	W	2	Total C N O 28 16 2 10	0	0
4	X	2	Total C N O 28 16 2 10	0	0
4	Y	2	Total C N O 28 16 2 10	0	0
4	Z	2	Total C N O 28 16 2 10	0	0
4	a	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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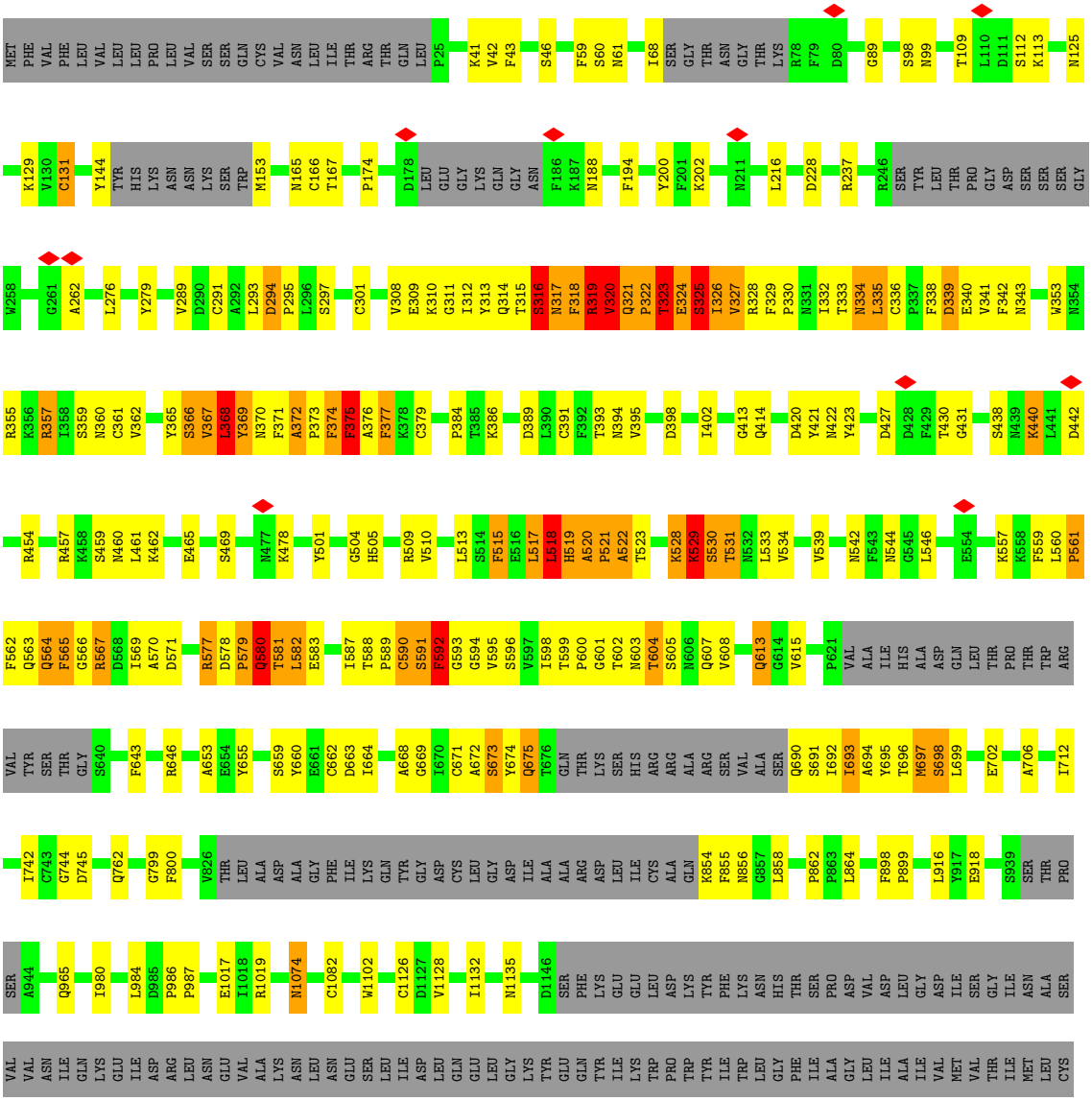
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C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

3 Residue-property plots (i)

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

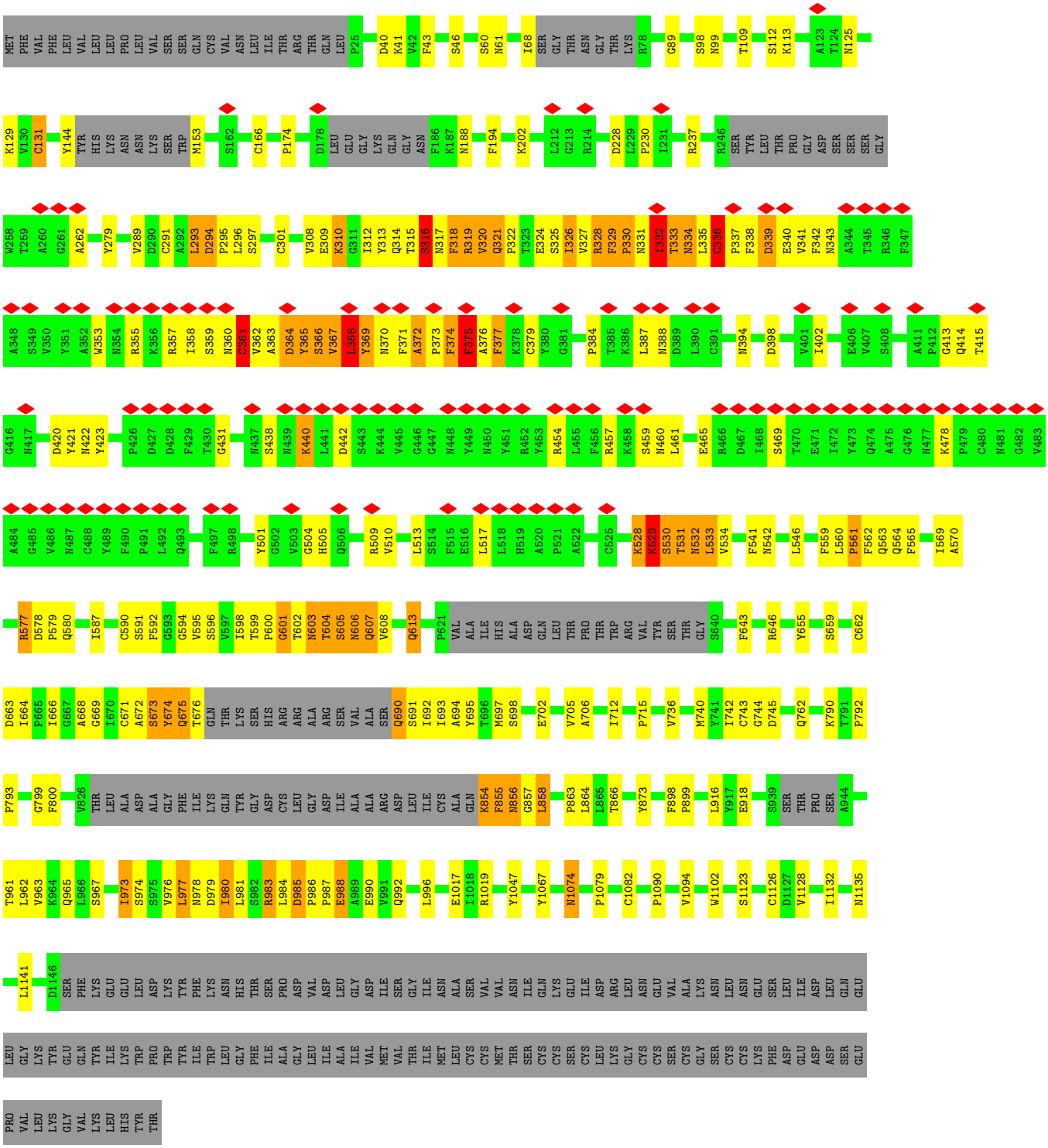
- Molecule 1: Spike glycoprotein

Chain A:



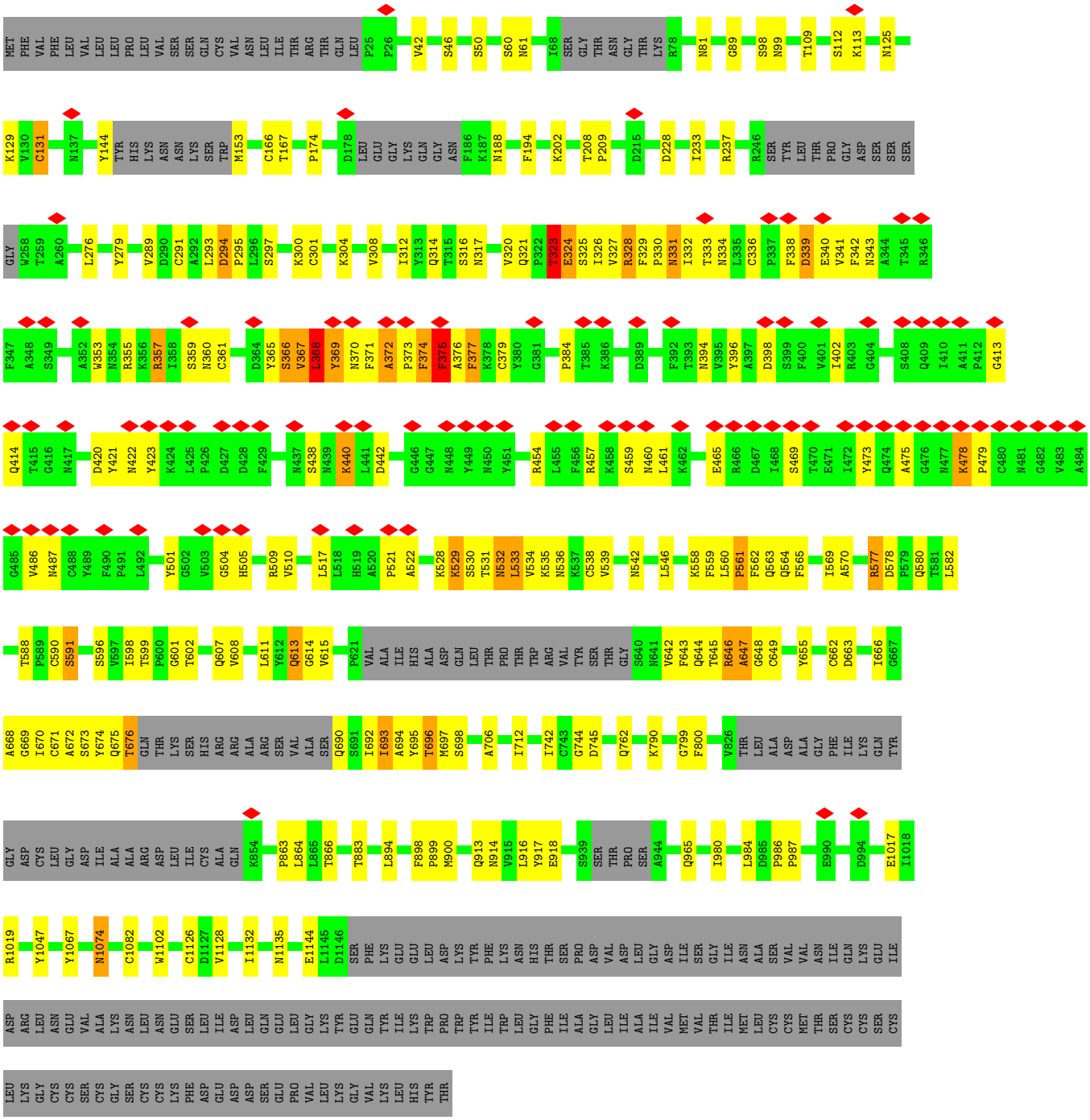
• Molecule 1: Spike glycoprotein

Chain B:



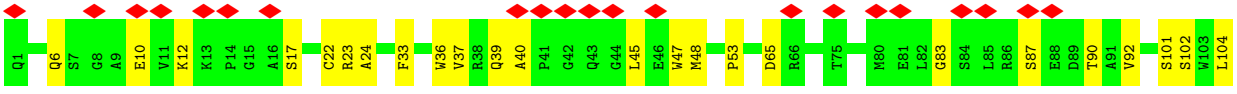
• Molecule 1: Spike glycoprotein

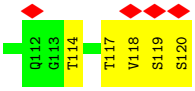
Chain C:



• Molecule 2: heavy chain of XGv289

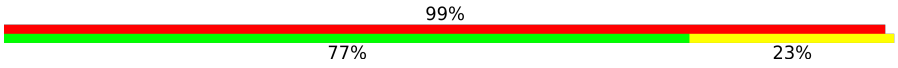
Chain H:

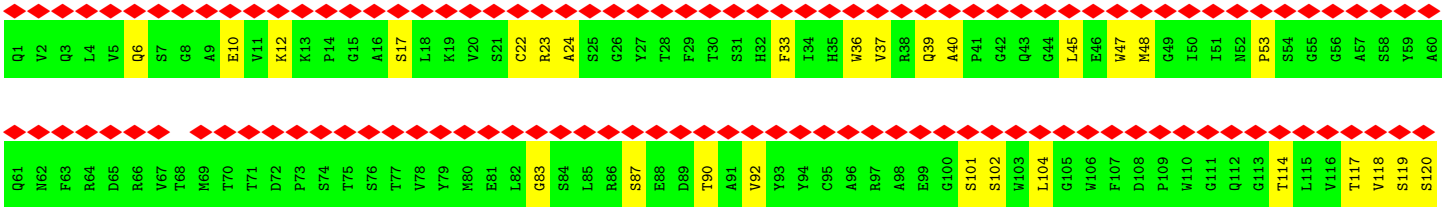




• Molecule 2: heavy chain of XGv289

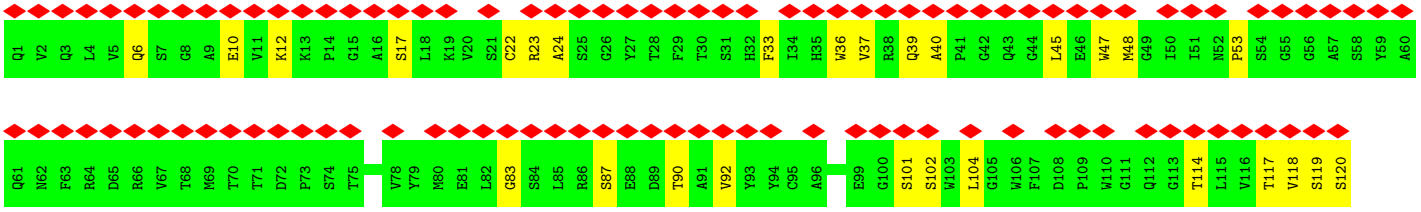
Chain I:





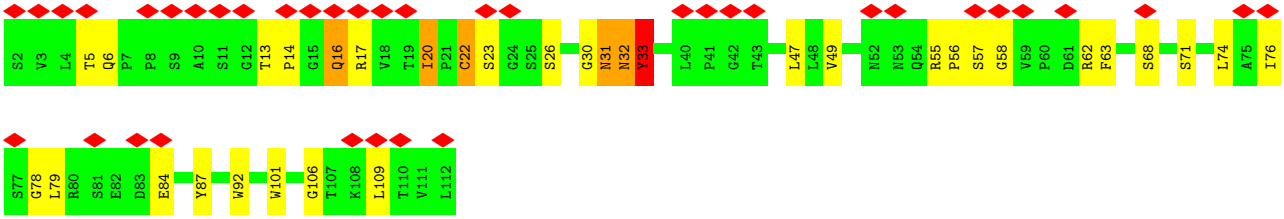
• Molecule 2: heavy chain of XGv289

Chain J:



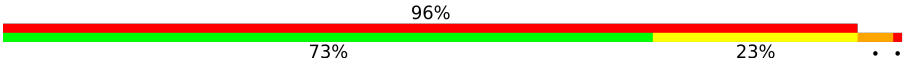
• Molecule 3: light chain of XGv289

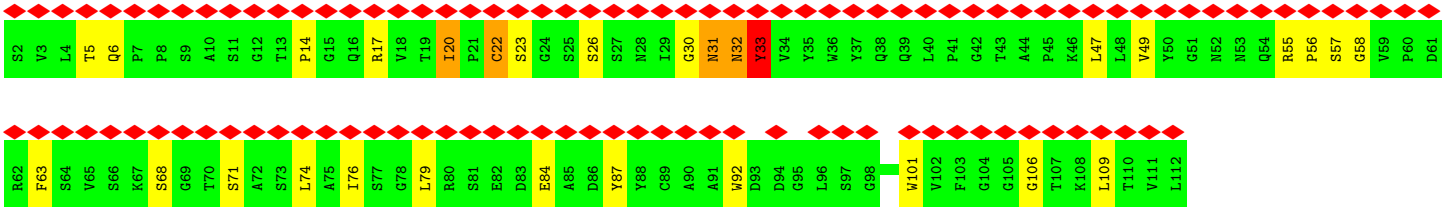
Chain L:



• Molecule 3: light chain of XGv289

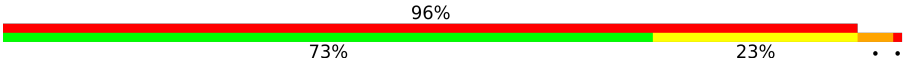
Chain M:

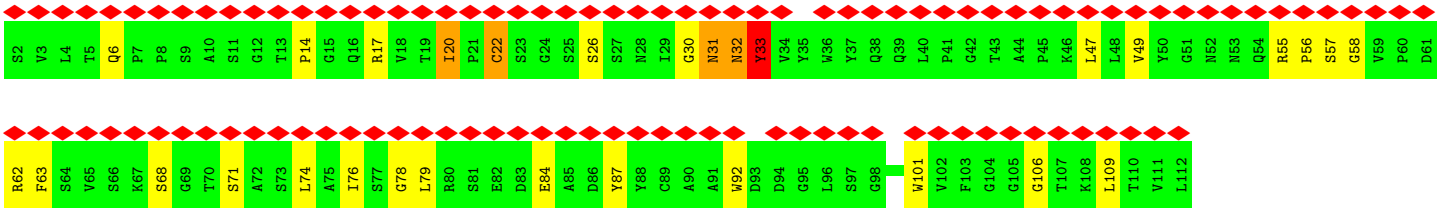




• Molecule 3: light chain of XGv289

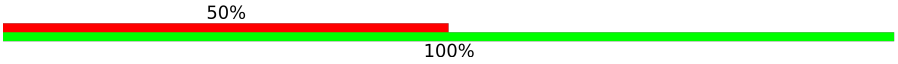
Chain N:





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

Chain D:



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

Chain E:

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

Chain F:

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

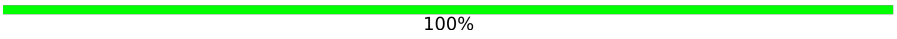
Chain G:

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

Chain K:

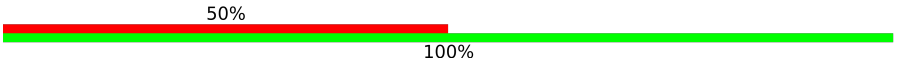
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



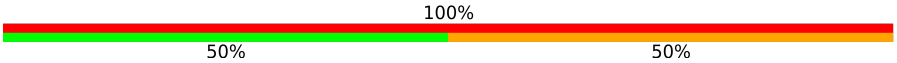
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



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

Chain R:

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

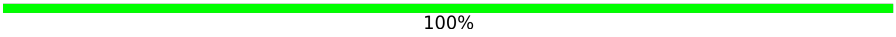
Chain S:

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

Chain T:

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

Chain U:

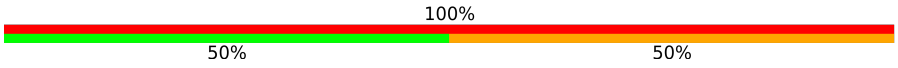


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

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

Chain W:



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

Chain X:

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

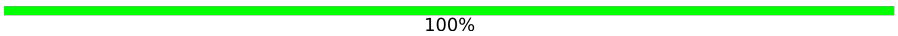
Chain Y:

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

Chain Z:

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

Chain a:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137483	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.136	Depositor
Minimum map value	-2.026	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	310.176, 310.176, 310.176	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	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	0.56	0/8235	0.59	0/11204
1	B	0.55	0/8235	0.59	0/11204
1	C	0.56	0/8235	0.58	0/11204
2	H	0.41	0/927	0.60	0/1264
2	I	0.41	0/927	0.60	0/1264
2	J	0.40	0/927	0.60	0/1264
3	L	0.39	0/837	0.57	0/1143
3	M	0.39	0/837	0.58	0/1143
3	N	0.39	0/837	0.58	0/1143
All	All	0.53	0/29997	0.59	0/40833

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8043	0	7848	384	0
1	B	8043	0	7848	415	0
1	C	8043	0	7846	317	0
2	H	902	0	849	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	902	0	849	16	0
2	J	902	0	849	16	0
3	L	816	0	776	30	0
3	M	816	0	776	23	0
3	N	816	0	776	23	0
4	D	28	0	25	0	0
4	E	28	0	25	2	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	K	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	2	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	7	0
4	W	28	0	25	2	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
5	A	154	0	142	7	0
5	B	154	0	142	9	0
5	C	154	0	142	7	0
All	All	30249	0	29293	1124	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 19.

All (1124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:CD1	1:B:533:LEU:HA	1.30	1.59
1:B:326:ILE:HD11	1:B:533:LEU:CA	1.41	1.50
5:A:1410:NAG:O4	5:A:1411:NAG:C1	1.63	1.45
5:B:1410:NAG:O4	5:B:1411:NAG:C1	1.63	1.44
5:C:1410:NAG:O4	5:C:1411:NAG:C1	1.63	1.44
1:B:365:TYR:CE1	1:B:387:LEU:HD13	1.64	1.31
1:B:332:ILE:O	1:B:333:THR:HG22	1.16	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:HE2	1:A:528:LYS:CG	1.45	1.29
1:B:415:THR:CG2	2:H:65:ASP:HB3	1.61	1.28
1:C:326:ILE:HD11	1:C:539:VAL:CB	1.63	1.25
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.22	1.23
1:A:562:PHE:O	1:B:41:LYS:HB3	1.40	1.21
1:B:334:ASN:ND2	1:B:361:CYS:HA	1.56	1.21
1:A:329:PHE:CD2	1:A:528:LYS:HB2	1.77	1.19
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.25	1.19
1:B:372:ALA:HB1	1:B:373:PRO:HD2	1.21	1.18
1:C:582:LEU:HD11	4:V:1:NAG:C8	1.71	1.18
1:A:372:ALA:HB1	1:A:373:PRO:HD2	1.21	1.18
1:B:365:TYR:HB2	1:B:388:ASN:OD1	1.44	1.17
1:B:367:VAL:HG12	1:B:368:LEU:H	1.08	1.16
1:A:519:HIS:CE1	1:B:40:ASP:HB2	1.79	1.16
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.28	1.16
1:B:336:CYS:SG	1:B:358:ILE:HG23	1.86	1.16
1:C:582:LEU:CD1	4:V:1:NAG:C8	2.22	1.15
1:A:329:PHE:CE2	1:A:528:LYS:HB2	1.80	1.15
1:C:326:ILE:CG2	1:C:533:LEU:HA	1.78	1.14
1:C:372:ALA:HB1	1:C:373:PRO:HD2	1.21	1.14
1:C:357:ARG:HG3	1:C:396:TYR:CE1	1.83	1.13
1:A:329:PHE:CE2	1:A:528:LYS:CG	2.32	1.13
1:A:319:ARG:HH11	1:B:740:MET:HE1	1.12	1.12
1:B:528:LYS:HE2	1:B:528:LYS:HA	1.18	1.12
1:C:329:PHE:O	1:C:580:GLN:HB2	1.47	1.12
1:C:326:ILE:CD1	1:C:539:VAL:HB	1.80	1.11
1:C:326:ILE:HD13	1:C:539:VAL:HG21	1.30	1.11
1:C:308:VAL:O	1:C:601:GLY:HA2	1.51	1.11
1:B:332:ILE:O	1:B:333:THR:CG2	1.98	1.10
1:A:294:ASP:HB2	1:A:295:PRO:HD2	1.23	1.09
1:C:357:ARG:HG3	1:C:396:TYR:HE1	1.10	1.09
1:B:365:TYR:CZ	1:B:387:LEU:HD13	1.86	1.09
1:C:326:ILE:HG21	1:C:533:LEU:HA	1.29	1.08
1:C:582:LEU:CD1	4:V:1:NAG:H83	1.79	1.08
1:C:326:ILE:CD1	1:C:539:VAL:CG2	2.32	1.08
1:B:312:ILE:HG12	1:B:598:ILE:HG12	1.25	1.08
1:B:415:THR:HG21	2:H:65:ASP:O	1.52	1.08
1:C:326:ILE:HD11	1:C:539:VAL:HB	1.14	1.08
1:C:582:LEU:HD12	4:V:1:NAG:H83	1.19	1.07
1:A:360:ASN:HD22	1:A:523:THR:HB	1.20	1.07
1:B:529:LYS:H	1:B:529:LYS:HD3	1.16	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:VAL:HG12	1:C:368:LEU:H	1.08	1.06
1:A:581:THR:HG21	1:A:583:GLU:OE2	1.55	1.06
1:A:367:VAL:HG12	1:A:368:LEU:H	1.08	1.05
1:A:314:GLN:HE22	1:A:594:GLY:HA3	1.23	1.04
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.04
1:A:517:LEU:HD12	1:A:517:LEU:H	1.24	1.03
1:B:308:VAL:O	1:B:601:GLY:HA2	1.58	1.03
1:A:519:HIS:CE1	1:B:41:LYS:H	1.76	1.03
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.37	1.02
1:A:329:PHE:CE2	1:A:528:LYS:HG3	1.92	1.02
1:B:329:PHE:HB3	1:B:330:PRO:CD	1.89	1.01
1:B:334:ASN:O	1:B:362:VAL:HG12	1.61	1.01
1:A:1017:GLU:HG2	1:B:1019:ARG:HH22	1.25	1.01
1:C:326:ILE:CD1	1:C:539:VAL:CB	2.36	1.01
5:A:1410:NAG:C4	5:A:1411:NAG:C1	2.38	1.01
1:C:326:ILE:CD1	1:C:539:VAL:HG21	1.91	1.01
1:A:413:GLY:HA3	1:C:987:PRO:HG2	1.43	1.00
5:B:1410:NAG:C4	5:B:1411:NAG:C1	2.38	1.00
1:C:473:TYR:HE2	3:L:16:GLN:NE2	1.57	1.00
5:C:1410:NAG:C4	5:C:1411:NAG:C1	2.38	1.00
1:A:321:GLN:HA	1:A:321:GLN:HE21	1.26	1.00
1:A:372:ALA:HB1	1:A:373:PRO:CD	1.92	1.00
1:A:329:PHE:CD2	1:A:528:LYS:HB3	1.96	0.99
1:C:357:ARG:CG	1:C:396:TYR:CE1	2.44	0.99
1:A:318:PHE:CZ	1:A:615:VAL:HG21	1.96	0.99
1:A:862:PRO:HG3	1:C:647:ALA:HB1	1.42	0.99
1:B:415:THR:HG22	2:H:65:ASP:HB3	1.40	0.99
1:B:372:ALA:HB1	1:B:373:PRO:CD	1.92	0.99
1:C:372:ALA:HB1	1:C:373:PRO:CD	1.92	0.99
1:A:519:HIS:HE1	1:B:40:ASP:CB	1.75	0.99
1:B:415:THR:HG21	2:H:65:ASP:HB3	1.43	0.99
1:C:534:VAL:CG2	1:C:539:VAL:HG11	1.91	0.99
1:A:167:THR:HG22	1:C:357:ARG:NH1	1.76	0.98
1:A:1017:GLU:HG2	1:B:1019:ARG:NH2	1.79	0.98
1:A:1019:ARG:NH2	1:C:1017:GLU:HG2	1.77	0.97
1:A:312:ILE:HG12	1:A:598:ILE:CG1	1.94	0.97
1:A:360:ASN:ND2	1:A:523:THR:HB	1.80	0.97
1:A:200:TYR:OH	1:C:522:ALA:HB3	1.66	0.96
1:A:329:PHE:HD2	1:A:528:LYS:CB	1.78	0.96
1:A:294:ASP:HB2	1:A:295:PRO:CD	1.93	0.96
1:B:328:ARG:HH22	1:B:580:GLN:HB2	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.48	0.96
1:B:365:TYR:CE1	1:B:387:LEU:CD1	2.49	0.96
1:A:167:THR:HG22	1:C:357:ARG:CZ	1.97	0.95
1:A:312:ILE:HG12	1:A:598:ILE:HG12	1.46	0.95
1:C:320:VAL:HG13	1:C:590:CYS:HB3	1.46	0.95
1:B:856:ASN:O	1:B:856:ASN:ND2	1.99	0.95
1:A:519:HIS:HE1	1:B:40:ASP:HB2	1.19	0.95
1:B:314:GLN:HA	1:B:596:SER:CB	1.96	0.94
1:B:337:PRO:HB2	1:B:339:ASP:OD1	1.68	0.94
1:C:582:LEU:HD11	4:V:1:NAG:H82	1.46	0.94
1:A:289:VAL:HG12	1:A:301:CYS:SG	2.07	0.94
1:B:334:ASN:ND2	1:B:361:CYS:CA	2.29	0.94
1:B:1017:GLU:HG2	1:C:1019:ARG:HH22	1.31	0.93
1:A:1019:ARG:HH22	1:C:1017:GLU:CG	1.82	0.93
1:A:1019:ARG:HH22	1:C:1017:GLU:HG2	1.31	0.92
1:B:674:TYR:CD1	1:B:691:SER:O	2.23	0.92
1:A:314:GLN:HA	1:A:596:SER:HB3	1.49	0.92
1:B:528:LYS:HE2	1:B:528:LYS:CA	1.99	0.92
1:C:326:ILE:HG21	1:C:533:LEU:CA	2.00	0.92
1:C:365:TYR:O	1:C:368:LEU:HD22	1.70	0.92
1:A:329:PHE:HE2	1:A:528:LYS:HG3	1.26	0.92
1:C:326:ILE:HD13	1:C:539:VAL:CG2	1.96	0.91
1:A:365:TYR:O	1:A:368:LEU:HD22	1.70	0.91
1:B:329:PHE:O	1:B:579:PRO:HB2	1.69	0.91
1:C:357:ARG:CG	1:C:396:TYR:HE1	1.80	0.91
1:A:566:GLY:HA3	1:B:43:PHE:HB3	1.53	0.90
1:A:1017:GLU:CG	1:B:1019:ARG:HH22	1.83	0.90
1:A:109:THR:HA	1:A:237:ARG:HH21	1.37	0.89
1:C:308:VAL:HG11	1:C:599:THR:HG21	1.53	0.89
1:A:318:PHE:CE1	1:A:615:VAL:HG21	2.07	0.89
1:A:862:PRO:HG3	1:C:647:ALA:CB	2.03	0.89
1:A:314:GLN:HA	1:A:596:SER:CB	2.02	0.89
1:B:1017:GLU:HG2	1:C:1019:ARG:NH2	1.88	0.89
1:A:389:ASP:OD1	1:A:528:LYS:HE3	1.72	0.88
1:A:762:GLN:HE22	1:C:965:GLN:NE2	1.70	0.88
1:B:530:SER:O	1:B:531:THR:OG1	1.91	0.88
1:C:109:THR:HA	1:C:237:ARG:HH21	1.37	0.88
1:C:367:VAL:HG12	1:C:368:LEU:N	1.88	0.88
1:C:473:TYR:HE2	3:L:16:GLN:HE21	0.94	0.88
1:A:328:ARG:HH21	1:A:328:ARG:HG2	1.39	0.87
1:A:319:ARG:NH1	1:B:740:MET:HE1	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HB2	1:A:562:PHE:CE1	2.10	0.87
1:B:603:ASN:O	1:B:604:THR:OG1	1.92	0.87
1:B:314:GLN:HA	1:B:596:SER:HB3	1.55	0.87
1:A:519:HIS:CD2	1:A:520:ALA:H	1.93	0.86
1:B:109:THR:HA	1:B:237:ARG:HH21	1.37	0.86
1:C:332:ILE:HG22	1:C:333:THR:H	1.40	0.86
1:A:332:ILE:HG23	1:A:362:VAL:HG13	1.55	0.86
1:A:339:ASP:OD1	1:A:340:GLU:N	2.08	0.86
1:B:336:CYS:SG	1:B:358:ILE:CG2	2.62	0.86
1:B:367:VAL:HG12	1:B:368:LEU:N	1.88	0.86
1:A:329:PHE:HE2	1:A:528:LYS:CB	1.72	0.85
1:B:339:ASP:OD1	1:B:340:GLU:N	2.08	0.85
1:C:473:TYR:CE2	3:L:16:GLN:NE2	2.39	0.85
1:B:335:LEU:HD23	1:B:362:VAL:CG1	2.06	0.85
1:C:308:VAL:CG1	1:C:599:THR:HG21	2.06	0.85
1:C:339:ASP:OD1	1:C:340:GLU:N	2.08	0.85
1:C:534:VAL:HG21	1:C:539:VAL:HG11	1.59	0.85
1:C:532:ASN:OD1	1:C:533:LEU:N	2.10	0.85
1:A:312:ILE:CG1	1:A:598:ILE:HG12	2.07	0.84
1:A:367:VAL:HG12	1:A:368:LEU:N	1.88	0.84
1:A:1019:ARG:HH22	1:C:1017:GLU:CD	1.81	0.84
1:A:319:ARG:HH21	1:A:319:ARG:HG3	1.42	0.84
1:C:327:VAL:CG1	1:C:329:PHE:HE1	1.90	0.84
1:C:312:ILE:HG12	1:C:598:ILE:HG12	1.59	0.84
3:N:84:GLU:HA	3:N:109:LEU:O	1.77	0.84
1:B:415:THR:CG2	2:H:65:ASP:CB	2.54	0.84
1:B:646:ARG:NH2	1:C:866:THR:CG2	2.41	0.84
1:A:663:ASP:OD2	1:A:673:SER:HB3	1.76	0.84
3:L:84:GLU:HA	3:L:109:LEU:O	1.77	0.84
1:B:357:ARG:NH2	1:C:167:THR:HG22	1.93	0.83
1:A:318:PHE:CZ	1:A:615:VAL:CG2	2.61	0.83
1:C:529:LYS:N	1:C:529:LYS:HD3	1.91	0.83
1:B:312:ILE:HG12	1:B:598:ILE:CG1	2.08	0.83
1:A:519:HIS:CE1	1:B:41:LYS:N	2.47	0.83
1:B:1017:GLU:CG	1:C:1019:ARG:HH22	1.92	0.83
1:B:668:ALA:H	1:C:864:LEU:HA	1.42	0.83
1:B:357:ARG:HH22	1:C:167:THR:HG22	1.44	0.82
1:A:563:GLN:C	1:A:564:GLN:OE1	2.17	0.82
3:M:84:GLU:HA	3:M:109:LEU:O	1.77	0.82
1:A:308:VAL:O	1:A:601:GLY:HA2	1.79	0.82
1:A:310:LYS:CG	1:A:664:ILE:HD11	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD23	1:B:362:VAL:HG13	1.62	0.82
1:A:646:ARG:NH2	1:B:866:THR:HG22	1.95	0.82
1:B:332:ILE:HD13	1:B:333:THR:H	1.43	0.82
1:A:522:ALA:O	1:A:523:THR:OG1	1.97	0.82
1:A:559:PHE:HE2	1:A:565:PHE:HA	1.43	0.81
1:A:519:HIS:CE1	1:B:40:ASP:CB	2.55	0.81
1:B:326:ILE:HD13	1:B:534:VAL:H	1.45	0.81
1:B:312:ILE:CG1	1:B:598:ILE:HG12	2.09	0.81
1:A:862:PRO:CG	1:C:647:ALA:HB1	2.11	0.80
1:B:365:TYR:CE2	1:B:387:LEU:HB3	2.16	0.80
1:C:326:ILE:HG23	1:C:532:ASN:O	1.81	0.80
1:C:308:VAL:O	1:C:601:GLY:CA	2.30	0.80
1:C:328:ARG:HG2	1:C:578:ASP:OD1	1.82	0.80
3:M:33:TYR:HD1	3:M:33:TYR:H	1.30	0.80
1:B:332:ILE:C	1:B:333:THR:HG22	2.02	0.79
1:C:671:CYS:O	1:C:694:ALA:HA	1.83	0.79
1:A:965:GLN:NE2	1:B:762:GLN:HE22	1.79	0.79
1:B:328:ARG:HG2	1:B:328:ARG:HH21	1.48	0.79
1:B:415:THR:HG21	2:H:65:ASP:CB	2.13	0.79
1:A:646:ARG:NH2	1:B:866:THR:CG2	2.45	0.79
1:B:326:ILE:CD1	1:B:533:LEU:CA	2.24	0.79
1:B:675:GLN:HA	1:B:675:GLN:HE21	1.47	0.79
1:B:334:ASN:HD22	1:B:361:CYS:HB3	1.47	0.79
1:A:342:PHE:HB3	1:A:371:PHE:CE2	2.18	0.79
3:L:33:TYR:HD1	3:L:33:TYR:H	1.30	0.79
1:A:314:GLN:NE2	1:A:594:GLY:HA3	1.99	0.78
1:B:985:ASP:OD1	1:B:988:GLU:HB2	1.82	0.78
1:C:342:PHE:HB3	1:C:371:PHE:CE2	2.18	0.78
3:N:33:TYR:HD1	3:N:33:TYR:H	1.30	0.78
1:A:167:THR:CG2	1:C:357:ARG:NH1	2.46	0.78
1:A:528:LYS:C	1:A:529:LYS:HD2	2.04	0.78
1:A:530:SER:O	1:A:531:THR:OG1	2.00	0.78
1:B:672:ALA:HA	1:B:693:ILE:O	1.84	0.78
1:B:983:ARG:C	1:B:984:LEU:HD12	2.04	0.78
1:B:985:ASP:HB2	1:B:987:PRO:HD2	1.66	0.78
3:L:6:GLN:CG	3:L:22:CYS:SG	2.72	0.78
3:N:6:GLN:CG	3:N:22:CYS:SG	2.72	0.78
1:C:663:ASP:OD2	1:C:673:SER:HB2	1.84	0.78
3:M:6:GLN:CG	3:M:22:CYS:SG	2.72	0.78
1:B:659:SER:CB	1:B:698:SER:HB3	2.14	0.77
1:A:200:TYR:CE2	1:C:521:PRO:HG2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:HE2	1:A:565:PHE:CA	1.96	0.77
1:A:578:ASP:OD1	1:A:579:PRO:HD2	1.85	0.77
1:B:529:LYS:HD3	1:B:529:LYS:N	1.85	0.77
1:A:167:THR:CG2	1:C:357:ARG:CZ	2.62	0.77
1:A:318:PHE:HZ	1:A:615:VAL:CG2	1.96	0.77
1:C:46:SER:HA	1:C:279:TYR:O	1.85	0.77
1:B:342:PHE:HB3	1:B:371:PHE:CE2	2.18	0.77
1:B:372:ALA:CB	1:B:373:PRO:HD2	2.10	0.77
1:A:46:SER:HA	1:A:279:TYR:O	1.85	0.76
1:B:330:PRO:HB2	1:B:332:ILE:HG22	1.65	0.76
1:A:289:VAL:HG13	1:A:297:SER:HB3	1.68	0.76
1:A:372:ALA:CB	1:A:373:PRO:HD2	2.10	0.76
1:B:46:SER:HA	1:B:279:TYR:O	1.85	0.76
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.20	0.76
1:C:329:PHE:O	1:C:580:GLN:CB	2.33	0.76
1:C:693:ILE:HD12	1:C:693:ILE:H	1.50	0.76
1:C:326:ILE:HD11	1:C:539:VAL:CG1	2.16	0.75
1:A:326:ILE:O	1:A:327:VAL:HG23	1.85	0.75
1:C:326:ILE:HD11	1:C:539:VAL:CG2	2.08	0.75
1:A:312:ILE:HG12	1:A:598:ILE:HG13	1.68	0.75
1:A:367:VAL:CG1	1:A:368:LEU:H	1.95	0.75
1:A:603:ASN:O	1:A:604:THR:OG1	2.04	0.75
1:A:289:VAL:CG1	1:A:301:CYS:SG	2.74	0.75
1:C:326:ILE:HG23	1:C:533:LEU:HA	1.65	0.74
1:C:372:ALA:CB	1:C:373:PRO:HD2	2.10	0.74
1:A:592:PHE:CD2	1:B:740:MET:HE2	2.21	0.74
1:B:326:ILE:HD13	1:B:533:LEU:HA	1.59	0.74
1:B:1128:VAL:CG2	1:C:918:GLU:HG2	2.18	0.74
1:A:570:ALA:HB1	1:B:963:VAL:HG12	1.68	0.74
1:B:328:ARG:HG2	1:B:328:ARG:NH2	2.00	0.74
1:B:671:CYS:HB2	1:B:695:TYR:CE1	2.22	0.74
1:A:646:ARG:HH21	1:B:866:THR:HG22	1.52	0.74
1:A:646:ARG:NH2	1:A:668:ALA:O	2.21	0.73
1:B:674:TYR:HD1	1:B:691:SER:O	1.67	0.73
1:A:329:PHE:HD2	1:A:528:LYS:HB3	1.39	0.73
1:A:671:CYS:O	1:A:694:ALA:HA	1.89	0.73
1:B:659:SER:HB3	1:B:698:SER:HB3	1.69	0.73
1:A:324:GLU:HG3	1:A:534:VAL:HG11	1.70	0.72
1:A:581:THR:CG2	1:A:583:GLU:OE2	2.36	0.72
1:A:762:GLN:HE22	1:C:965:GLN:HE21	1.35	0.72
1:B:332:ILE:CD1	1:B:333:THR:H	2.00	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ARG:NH2	1:B:668:ALA:O	2.21	0.72
1:C:332:ILE:HG22	1:C:333:THR:N	2.03	0.72
1:A:319:ARG:HH11	1:B:740:MET:CE	1.96	0.72
1:B:646:ARG:NH2	1:C:866:THR:HG22	2.04	0.72
1:C:326:ILE:CG2	1:C:533:LEU:CA	2.61	0.72
1:A:295:PRO:HG2	1:A:608:VAL:HG21	1.71	0.72
1:A:357:ARG:NH1	1:B:230:PRO:HG3	2.03	0.72
1:C:475:ALA:HB3	1:C:487:ASN:O	1.89	0.72
1:A:315:THR:N	1:A:595:VAL:O	2.22	0.72
1:B:985:ASP:CG	1:B:988:GLU:HB2	2.10	0.72
1:A:328:ARG:HG2	1:A:328:ARG:NH2	1.97	0.71
1:B:332:ILE:HD13	1:B:333:THR:N	2.04	0.71
1:B:669:GLY:N	1:C:864:LEU:O	2.23	0.71
5:A:1410:NAG:H4	5:A:1411:NAG:C1	2.21	0.71
3:L:6:GLN:HG3	3:L:22:CYS:SG	2.31	0.71
1:A:321:GLN:HA	1:A:321:GLN:NE2	2.02	0.71
1:A:1017:GLU:CD	1:B:1019:ARG:HH22	1.93	0.71
1:A:393:THR:HG22	1:A:522:ALA:HA	1.74	0.70
1:A:562:PHE:O	1:B:41:LYS:CB	2.33	0.70
1:B:327:VAL:O	1:B:328:ARG:HG3	1.91	0.70
3:N:6:GLN:HG3	3:N:22:CYS:SG	2.31	0.70
1:A:366:SER:O	1:A:369:TYR:HB2	1.91	0.70
1:A:580:GLN:O	1:A:581:THR:OG1	2.09	0.70
1:B:606:ASN:N	1:B:606:ASN:HD22	1.90	0.70
1:C:534:VAL:HG23	1:C:539:VAL:HG11	1.73	0.70
1:C:366:SER:O	1:C:369:TYR:HB2	1.91	0.70
3:M:6:GLN:HG3	3:M:22:CYS:SG	2.31	0.70
1:A:310:LYS:CD	1:A:664:ILE:HD11	2.22	0.70
1:A:564:GLN:OE1	1:A:564:GLN:N	2.23	0.70
1:B:367:VAL:CG1	1:B:368:LEU:H	1.95	0.70
1:A:317:ASN:HA	1:A:595:VAL:HG23	1.72	0.70
1:B:334:ASN:HD21	1:B:361:CYS:HA	1.53	0.70
1:A:291:CYS:HG	1:A:301:CYS:CB	2.04	0.70
1:B:668:ALA:HA	1:C:863:PRO:O	1.91	0.69
1:C:326:ILE:HG21	1:C:533:LEU:CB	2.22	0.69
3:L:87:TYR:O	3:L:106:GLY:HA2	1.93	0.69
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.23	0.69
1:A:690:GLN:OE1	1:A:690:GLN:N	2.25	0.69
5:C:1410:NAG:H4	5:C:1411:NAG:C1	2.21	0.69
1:B:965:GLN:NE2	1:C:762:GLN:HE22	1.90	0.69
5:B:1410:NAG:H4	5:B:1411:NAG:C1	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:VAL:O	1:C:369:TYR:N	2.26	0.69
1:B:319:ARG:HB2	1:B:319:ARG:NH2	2.08	0.69
1:A:167:THR:HG21	1:C:357:ARG:NH2	2.08	0.69
1:B:326:ILE:HD11	1:B:532:ASN:O	1.93	0.69
1:A:367:VAL:O	1:A:369:TYR:N	2.25	0.69
1:B:326:ILE:HD11	1:B:533:LEU:N	2.07	0.68
1:B:560:LEU:O	1:B:562:PHE:N	2.27	0.68
1:C:320:VAL:CG1	1:C:590:CYS:HB3	2.22	0.68
3:M:87:TYR:O	3:M:106:GLY:HA2	1.93	0.68
1:C:646:ARG:NH1	1:C:646:ARG:HG2	2.07	0.68
1:A:519:HIS:HE1	1:B:40:ASP:CA	2.06	0.68
1:B:359:SER:O	1:B:361:CYS:SG	2.51	0.68
1:B:367:VAL:O	1:B:369:TYR:N	2.26	0.68
3:N:87:TYR:O	3:N:106:GLY:HA2	1.93	0.68
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.17	0.68
1:B:332:ILE:CG1	1:B:333:THR:H	2.07	0.68
1:B:743:CYS:HA	1:B:977:LEU:CD2	2.24	0.68
1:C:560:LEU:O	1:C:562:PHE:N	2.27	0.68
1:A:368:LEU:C	1:A:368:LEU:HD23	2.14	0.68
1:B:321:GLN:CD	1:B:321:GLN:H	1.96	0.68
1:B:368:LEU:HD23	1:B:368:LEU:C	2.14	0.68
1:A:357:ARG:HH11	1:B:230:PRO:HG3	1.58	0.68
1:B:371:PHE:CE1	4:Q:1:NAG:H82	2.29	0.68
1:C:371:PHE:CE1	4:W:1:NAG:H82	2.29	0.68
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.76	0.67
1:C:533:LEU:HD13	1:C:533:LEU:O	1.93	0.67
3:L:13:THR:HG22	3:L:16:GLN:OE1	1.94	0.67
1:A:320:VAL:HG13	1:A:590:CYS:HB3	1.76	0.67
1:B:328:ARG:HD3	1:B:578:ASP:OD1	1.94	0.67
1:C:368:LEU:C	1:C:368:LEU:HD23	2.14	0.67
1:A:371:PHE:CE1	4:E:1:NAG:H82	2.29	0.67
1:B:326:ILE:CD1	1:B:532:ASN:O	2.42	0.67
1:C:611:LEU:HD12	1:C:649:CYS:H	1.57	0.67
1:C:308:VAL:CG1	1:C:599:THR:CG2	2.72	0.67
1:B:314:GLN:HA	1:B:596:SER:CA	2.23	0.67
1:C:328:ARG:HG3	1:C:329:PHE:N	2.10	0.67
1:B:371:PHE:HE1	4:Q:1:NAG:H82	1.60	0.67
1:B:605:SER:OG	1:B:607:GLN:HG3	1.95	0.66
1:C:533:LEU:CD1	1:C:533:LEU:H	2.09	0.66
3:L:32:ASN:O	3:L:33:TYR:O	2.13	0.66
1:A:310:LYS:HG2	1:A:664:ILE:CD1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ASN:C	1:C:332:ILE:HG12	2.15	0.66
1:B:326:ILE:CD1	1:B:534:VAL:H	2.09	0.66
1:A:519:HIS:HD2	1:A:520:ALA:H	1.39	0.66
1:B:315:THR:N	1:B:595:VAL:O	2.29	0.66
1:A:519:HIS:NE2	1:B:41:LYS:N	2.42	0.66
1:B:329:PHE:CB	1:B:330:PRO:HD2	2.18	0.66
1:B:607:GLN:O	1:B:608:VAL:HG13	1.96	0.66
1:B:1128:VAL:HG23	1:C:918:GLU:HG2	1.77	0.66
1:C:367:VAL:C	1:C:369:TYR:H	1.99	0.66
1:A:560:LEU:O	1:A:562:PHE:N	2.28	0.66
1:A:391:CYS:SG	1:A:544:ASN:OD1	2.54	0.66
1:B:973:ILE:HG22	1:B:992:GLN:OE1	1.96	0.66
3:M:32:ASN:O	3:M:33:TYR:O	2.13	0.66
1:A:291:CYS:HG	1:A:301:CYS:HG	1.16	0.65
1:B:308:VAL:CG1	1:B:313:TYR:CE2	2.79	0.65
1:C:367:VAL:CG1	1:C:368:LEU:H	1.95	0.65
3:N:31:ASN:O	3:N:32:ASN:ND2	2.30	0.65
1:B:333:THR:OG1	1:B:362:VAL:HG11	1.96	0.65
3:L:31:ASN:O	3:L:32:ASN:ND2	2.30	0.65
1:B:668:ALA:N	1:C:864:LEU:HA	2.11	0.65
3:M:31:ASN:O	3:M:32:ASN:ND2	2.30	0.65
1:A:440:LYS:NZ	2:H:104:LEU:HD11	2.12	0.65
1:C:327:VAL:CG1	1:C:329:PHE:CE1	2.77	0.65
1:B:440:LYS:NZ	2:I:104:LEU:HD11	2.12	0.65
1:C:371:PHE:HE1	4:W:1:NAG:H82	1.60	0.65
3:N:32:ASN:O	3:N:33:TYR:O	2.13	0.65
1:A:144:TYR:HB3	1:A:153:MET:HB3	1.79	0.65
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.29	0.65
1:B:986:PRO:O	1:B:990:GLU:HG3	1.96	0.65
1:C:440:LYS:NZ	2:J:104:LEU:HD11	2.12	0.64
1:A:560:LEU:HD12	1:A:562:PHE:CZ	2.31	0.64
3:M:30:GLY:O	3:M:31:ASN:HB3	1.98	0.64
1:A:522:ALA:C	1:A:523:THR:HG1	1.99	0.64
1:A:567:ARG:HD3	1:A:571:ASP:OD1	1.96	0.64
1:C:644:GLN:HG3	1:C:644:GLN:O	1.96	0.64
1:A:328:ARG:O	1:A:579:PRO:HG3	1.96	0.64
1:A:367:VAL:C	1:A:369:TYR:H	1.99	0.64
1:A:371:PHE:HE1	4:E:1:NAG:H82	1.60	0.64
1:C:144:TYR:HB3	1:C:153:MET:HB3	1.79	0.64
3:L:6:GLN:HG2	3:L:22:CYS:SG	2.37	0.64
1:A:371:PHE:O	1:A:372:ALA:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:30:GLY:O	3:N:31:ASN:HB3	1.98	0.64
1:B:144:TYR:HB3	1:B:153:MET:HB3	1.79	0.64
3:M:6:GLN:HG2	3:M:22:CYS:SG	2.37	0.64
3:L:30:GLY:O	3:L:31:ASN:HB3	1.98	0.64
1:A:200:TYR:HE2	1:C:521:PRO:HG2	1.62	0.63
1:A:319:ARG:NH1	1:B:740:MET:CE	2.58	0.63
3:N:6:GLN:HG2	3:N:22:CYS:SG	2.37	0.63
1:A:577:ARG:O	1:A:577:ARG:HG3	1.98	0.63
1:B:332:ILE:O	1:B:333:THR:CB	2.46	0.63
1:B:367:VAL:C	1:B:369:TYR:H	1.99	0.63
1:C:611:LEU:HD11	1:C:648:GLY:HA3	1.78	0.63
1:A:566:GLY:CA	1:B:43:PHE:HB3	2.27	0.63
1:A:799:GLY:O	1:A:800:PHE:C	2.37	0.63
1:B:334:ASN:HD22	1:B:361:CYS:CB	2.11	0.63
1:C:582:LEU:CD1	4:V:1:NAG:H82	2.11	0.63
1:B:371:PHE:O	1:B:372:ALA:HB2	1.98	0.63
1:C:646:ARG:HG2	1:C:646:ARG:HH11	1.62	0.63
1:B:415:THR:CB	2:H:65:ASP:HB3	2.27	0.63
1:B:799:GLY:O	1:B:800:PHE:C	2.37	0.63
1:A:310:LYS:HG3	1:A:600:PRO:CA	2.21	0.63
1:A:517:LEU:HD12	1:A:517:LEU:N	2.04	0.63
1:A:559:PHE:CE2	1:A:566:GLY:N	2.67	0.63
1:B:646:ARG:HH21	1:C:866:THR:HG22	1.62	0.63
1:C:328:ARG:O	1:C:329:PHE:CD1	2.51	0.63
1:A:334:ASN:O	1:A:335:LEU:HG	1.99	0.62
1:B:314:GLN:HA	1:B:596:SER:HA	1.81	0.62
1:C:357:ARG:HG2	1:C:396:TYR:CE1	2.32	0.62
1:C:643:PHE:CZ	1:C:655:TYR:CD1	2.88	0.62
1:A:579:PRO:O	1:A:580:GLN:HG2	1.98	0.62
1:B:974:SER:O	1:B:980:ILE:HD11	1.99	0.62
1:C:367:VAL:C	1:C:369:TYR:N	2.52	0.62
1:C:799:GLY:O	1:C:800:PHE:C	2.37	0.62
1:A:646:ARG:HH22	1:B:866:THR:CG2	2.12	0.62
1:B:858:LEU:CD2	1:B:962:LEU:HD23	2.29	0.62
1:B:1017:GLU:CD	1:C:1019:ARG:HH22	2.03	0.62
1:C:300:LYS:HE2	1:C:602:THR:HG21	1.82	0.62
1:C:371:PHE:O	1:C:372:ALA:HB2	1.98	0.62
3:M:17:ARG:HA	3:M:76:ILE:O	2.00	0.62
1:B:367:VAL:C	1:B:369:TYR:N	2.53	0.62
3:L:17:ARG:HA	3:L:76:ILE:O	2.00	0.62
1:C:366:SER:C	1:C:367:VAL:O	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CB	1:B:330:PRO:CD	2.65	0.61
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.33	0.61
1:A:559:PHE:CE2	1:A:565:PHE:HA	2.31	0.61
2:I:101:SER:OG	2:I:102:SER:N	2.33	0.61
2:J:101:SER:OG	2:J:102:SER:N	2.33	0.61
1:A:672:ALA:HA	1:A:693:ILE:O	2.01	0.61
1:C:643:PHE:CZ	1:C:655:TYR:CG	2.89	0.61
1:A:310:LYS:HD2	1:A:664:ILE:HD11	1.82	0.61
3:N:17:ARG:HA	3:N:76:ILE:O	2.00	0.61
1:A:322:PRO:O	1:A:323:THR:HG23	1.99	0.61
1:A:690:GLN:HG2	1:A:690:GLN:O	2.00	0.61
1:A:328:ARG:HH21	1:A:328:ARG:CG	2.13	0.61
1:A:389:ASP:CG	1:A:528:LYS:HE3	2.21	0.61
1:A:333:THR:HG22	1:A:333:THR:O	2.01	0.60
1:A:335:LEU:O	1:A:336:CYS:SG	2.59	0.60
1:B:659:SER:HB2	1:B:698:SER:HB3	1.82	0.60
1:B:671:CYS:O	1:B:694:ALA:HA	2.00	0.60
1:B:328:ARG:HH21	1:B:328:ARG:CG	2.14	0.60
1:A:308:VAL:CG1	1:A:313:TYR:CE2	2.84	0.60
1:A:366:SER:C	1:A:367:VAL:O	2.35	0.60
1:B:607:GLN:O	1:B:608:VAL:CG1	2.49	0.60
1:A:367:VAL:C	1:A:369:TYR:N	2.52	0.60
1:B:109:THR:HA	1:B:237:ARG:NH2	2.15	0.60
1:A:43:PHE:CE1	1:C:558:LYS:O	2.54	0.60
1:B:675:GLN:HG3	1:B:676:THR:N	2.17	0.60
1:B:706:ALA:CB	5:B:1410:NAG:H5	2.32	0.60
1:A:515:PHE:HD2	1:A:515:PHE:O	1.85	0.60
1:A:557:LYS:HD3	1:B:43:PHE:CE2	2.36	0.60
1:B:319:ARG:HH21	1:B:319:ARG:CG	2.14	0.60
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.32	0.60
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.84	0.60
1:A:706:ALA:CB	5:A:1410:NAG:H5	2.32	0.60
1:B:319:ARG:HH21	1:B:319:ARG:HG3	1.67	0.60
1:C:312:ILE:HG12	1:C:598:ILE:CG1	2.29	0.60
1:B:326:ILE:HD13	1:B:534:VAL:N	2.17	0.59
1:B:565:PHE:O	1:C:42:VAL:HA	2.02	0.59
1:B:858:LEU:HD22	1:B:962:LEU:HD23	1.83	0.59
1:A:1128:VAL:CG2	1:B:918:GLU:HG2	2.32	0.59
1:A:592:PHE:HD1	1:A:592:PHE:N	2.00	0.59
2:H:87:SER:HA	2:H:118:VAL:HG11	1.84	0.59
2:J:37:VAL:HA	2:J:47:TRP:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:THR:O	1:A:604:THR:N	2.33	0.59
1:C:440:LYS:HZ2	2:J:104:LEU:HD11	1.68	0.59
1:C:643:PHE:CE1	1:C:655:TYR:CG	2.91	0.59
1:C:706:ALA:CB	5:C:1410:NAG:H5	2.32	0.59
1:C:289:VAL:HG12	1:C:301:CYS:SG	2.42	0.59
2:J:87:SER:HA	2:J:118:VAL:HG11	1.84	0.59
1:A:376:ALA:O	1:A:377:PHE:HB2	2.02	0.59
1:A:560:LEU:CB	1:A:562:PHE:CE1	2.85	0.59
1:B:1128:VAL:HG21	1:C:918:GLU:HG2	1.83	0.58
1:A:318:PHE:HZ	1:A:615:VAL:HG22	1.65	0.58
1:A:560:LEU:N	1:A:563:GLN:OE1	2.31	0.58
1:C:353:TRP:HZ3	1:C:355:ARG:HD2	1.69	0.58
1:C:376:ALA:O	1:C:377:PHE:HB2	2.02	0.58
2:I:87:SER:HA	2:I:118:VAL:HG11	1.84	0.58
1:A:353:TRP:HZ3	1:A:355:ARG:HD2	1.69	0.58
1:B:318:PHE:O	1:B:592:PHE:HA	2.03	0.58
1:C:109:THR:HA	1:C:237:ARG:NH2	2.15	0.58
1:B:327:VAL:HG12	1:B:328:ARG:N	2.18	0.58
1:B:973:ILE:CG2	1:B:992:GLN:OE1	2.51	0.58
1:A:109:THR:HA	1:A:237:ARG:NH2	2.15	0.58
1:B:376:ALA:O	1:B:377:PHE:HB2	2.02	0.58
1:C:300:LYS:CE	1:C:602:THR:HG21	2.34	0.58
1:B:337:PRO:O	1:B:338:PHE:C	2.41	0.58
1:C:533:LEU:H	1:C:533:LEU:HD12	1.68	0.58
1:B:359:SER:OG	1:B:360:ASN:N	2.37	0.58
1:C:323:THR:OG1	1:C:538:CYS:O	2.20	0.58
1:A:965:GLN:HE21	1:B:762:GLN:HE22	1.52	0.58
1:C:646:ARG:HH11	1:C:646:ARG:CG	2.16	0.58
1:A:309:GLU:HG2	1:A:313:TYR:OH	2.04	0.58
2:H:37:VAL:HA	2:H:47:TRP:HA	1.85	0.58
1:A:295:PRO:CG	1:A:608:VAL:HG21	2.33	0.57
1:A:310:LYS:CG	1:A:600:PRO:HA	2.25	0.57
1:A:324:GLU:HB2	1:A:539:VAL:HG12	1.86	0.57
1:A:359:SER:OG	1:A:360:ASN:N	2.37	0.57
1:A:592:PHE:N	1:A:592:PHE:CD1	2.72	0.57
1:B:702:GLU:OE2	1:C:790:LYS:CE	2.51	0.57
1:C:325:SER:C	1:C:326:ILE:HG13	2.24	0.57
2:I:37:VAL:HA	2:I:47:TRP:HA	1.85	0.57
1:B:663:ASP:OD2	1:B:673:SER:HB2	2.05	0.57
1:C:326:ILE:HD12	1:C:539:VAL:HB	1.83	0.57
1:C:359:SER:OG	1:C:360:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HD11	1:B:532:ASN:C	2.24	0.57
1:B:353:TRP:HZ3	1:B:355:ARG:HD2	1.69	0.57
2:H:101:SER:OG	2:H:102:SER:N	2.33	0.57
1:A:395:VAL:HA	1:A:515:PHE:HB3	1.86	0.57
1:B:326:ILE:HG13	1:B:532:ASN:O	2.04	0.57
1:A:374:PHE:HB3	1:A:376:ALA:O	2.05	0.57
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.86	0.57
1:B:374:PHE:HB3	1:B:376:ALA:O	2.05	0.57
1:B:980:ILE:CD1	1:B:996:LEU:HD11	2.34	0.57
1:A:864:LEU:HA	1:C:668:ALA:H	1.68	0.57
1:C:374:PHE:HB3	1:C:376:ALA:O	2.05	0.57
1:B:308:VAL:O	1:B:601:GLY:CA	2.45	0.57
1:B:334:ASN:HD22	1:B:361:CYS:CA	2.15	0.57
1:C:308:VAL:HG11	1:C:599:THR:CG2	2.31	0.57
1:C:582:LEU:HD11	4:V:1:NAG:H81	1.79	0.57
3:N:49:VAL:HG23	3:N:55:ARG:HG3	1.87	0.57
1:B:599:THR:C	1:B:601:GLY:H	2.08	0.56
3:M:49:VAL:HG23	3:M:55:ARG:HG3	1.87	0.56
1:B:308:VAL:HG12	1:B:313:TYR:CE2	2.41	0.56
1:B:531:THR:HG22	1:B:532:ASN:N	2.21	0.56
1:B:976:VAL:O	1:B:978:ASN:N	2.38	0.56
1:B:314:GLN:CA	1:B:596:SER:CB	2.79	0.56
1:B:980:ILE:HD11	1:B:996:LEU:HD11	1.86	0.56
1:B:313:TYR:O	1:B:315:THR:HG23	2.04	0.56
3:L:33:TYR:HD1	3:L:33:TYR:N	2.01	0.56
1:A:675:GLN:OE1	1:A:693:ILE:HD11	2.06	0.56
1:B:321:GLN:HB3	1:B:322:PRO:HD2	1.88	0.56
1:C:332:ILE:CG2	1:C:333:THR:H	2.15	0.56
1:C:308:VAL:HG12	1:C:599:THR:CG2	2.36	0.56
2:H:36:TRP:O	2:H:48:MET:N	2.38	0.56
1:B:672:ALA:O	1:B:673:SER:HB3	2.05	0.56
1:B:983:ARG:HB3	1:B:984:LEU:HD12	1.88	0.56
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.88	0.56
3:M:63:PHE:HB3	3:M:74:LEU:HD11	1.88	0.56
1:B:981:LEU:O	1:B:983:ARG:N	2.36	0.56
1:B:326:ILE:CD1	1:B:534:VAL:N	2.69	0.55
1:C:672:ALA:HA	1:C:693:ILE:O	2.06	0.55
3:L:63:PHE:HB3	3:L:74:LEU:HD11	1.88	0.55
1:A:42:VAL:HA	1:C:565:PHE:O	2.06	0.55
1:A:564:GLN:C	1:A:565:PHE:HD1	2.09	0.55
1:C:478:LYS:HD2	1:C:478:LYS:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:VAL:HG23	3:L:55:ARG:HG3	1.87	0.55
1:A:591:SER:O	1:A:592:PHE:HB3	2.07	0.55
1:B:979:ASP:O	1:B:981:LEU:N	2.39	0.55
2:I:17:SER:HA	2:I:83:GLY:HA2	1.89	0.55
1:B:314:GLN:CA	1:B:596:SER:HB3	2.32	0.55
1:A:864:LEU:O	1:C:669:GLY:N	2.40	0.55
2:I:36:TRP:O	2:I:48:MET:N	2.38	0.55
3:L:13:THR:CG2	3:L:16:GLN:OE1	2.55	0.55
2:J:17:SER:HA	2:J:83:GLY:HA2	1.89	0.55
1:A:440:LYS:HZ2	2:H:104:LEU:HD11	1.72	0.54
1:A:659:SER:HA	1:A:696:THR:O	2.07	0.54
1:B:319:ARG:CB	1:B:319:ARG:CZ	2.85	0.54
1:B:854:LYS:C	1:B:856:ASN:H	2.10	0.54
1:C:328:ARG:HG3	1:C:329:PHE:H	1.72	0.54
2:J:10:GLU:OE1	2:J:12:LYS:NZ	2.40	0.54
1:A:328:ARG:HD2	1:A:533:LEU:HD13	1.89	0.54
1:A:592:PHE:CD2	1:B:740:MET:CE	2.90	0.54
1:B:334:ASN:ND2	1:B:360:ASN:O	2.41	0.54
2:H:10:GLU:OE1	2:H:12:LYS:NZ	2.40	0.54
2:I:23:ARG:NH1	2:I:24:ALA:O	2.39	0.54
3:N:63:PHE:HB3	3:N:74:LEU:HD11	1.88	0.54
1:B:321:GLN:OE1	1:B:321:GLN:N	2.40	0.54
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.89	0.54
1:A:529:LYS:O	1:A:530:SER:O	2.25	0.54
1:B:289:VAL:HG13	1:B:297:SER:HB3	1.90	0.54
1:B:440:LYS:HZ2	2:I:104:LEU:HD11	1.70	0.54
1:B:973:ILE:CG2	1:B:992:GLN:HG3	2.37	0.54
1:C:357:ARG:NE	1:C:396:TYR:OH	2.40	0.54
1:C:646:ARG:HG3	1:C:646:ARG:O	2.07	0.54
3:M:33:TYR:HD1	3:M:33:TYR:N	2.01	0.54
1:A:167:THR:CG2	1:C:357:ARG:NH2	2.70	0.54
1:C:312:ILE:CG1	1:C:598:ILE:HG12	2.36	0.54
1:C:534:VAL:HG21	1:C:539:VAL:CG1	2.33	0.54
1:B:702:GLU:OE2	1:C:790:LYS:HE3	2.07	0.54
1:C:366:SER:O	1:C:367:VAL:O	2.26	0.54
2:I:10:GLU:OE1	2:I:12:LYS:NZ	2.40	0.54
1:B:854:LYS:HB2	1:B:858:LEU:O	2.08	0.54
2:H:17:SER:HA	2:H:83:GLY:HA2	1.89	0.54
1:A:855:PHE:HB2	1:A:858:LEU:HB2	1.89	0.53
1:A:366:SER:O	1:A:367:VAL:O	2.26	0.53
1:C:532:ASN:OD1	1:C:533:LEU:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:OD2	1:A:509:ARG:NE	2.41	0.53
1:A:1019:ARG:NH2	1:C:1017:GLU:CG	2.52	0.53
1:C:327:VAL:HG12	1:C:329:PHE:CE1	2.43	0.53
1:A:319:ARG:HG3	1:A:319:ARG:NH2	2.17	0.53
1:B:605:SER:HG	1:B:607:GLN:HG3	1.71	0.53
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.41	0.53
1:A:517:LEU:O	1:A:518:LEU:HD12	2.09	0.53
2:H:23:ARG:NH1	2:H:24:ALA:O	2.39	0.53
1:A:276:LEU:HD22	1:A:301:CYS:HA	1.90	0.53
3:N:33:TYR:HD1	3:N:33:TYR:N	2.01	0.53
1:C:316:SER:OG	1:C:317:ASN:N	2.42	0.53
1:A:308:VAL:HG12	1:A:313:TYR:CE2	2.44	0.53
1:A:339:ASP:O	1:A:343:ASN:HB2	2.09	0.53
1:A:762:GLN:NE2	1:C:965:GLN:HE21	2.05	0.53
1:B:980:ILE:O	1:B:980:ILE:HG22	2.08	0.53
1:B:980:ILE:CD1	1:B:996:LEU:CD1	2.87	0.52
1:B:663:ASP:HB3	1:B:673:SER:HB3	1.91	0.52
2:J:36:TRP:O	2:J:48:MET:N	2.38	0.52
3:N:20:ILE:HG23	3:N:74:LEU:HB3	1.91	0.52
1:A:564:GLN:O	1:A:565:PHE:HB3	2.09	0.52
1:A:599:THR:HG23	1:A:599:THR:O	2.08	0.52
1:A:918:GLU:HG2	1:C:1128:VAL:CG2	2.39	0.52
1:B:339:ASP:O	1:B:343:ASN:HB2	2.10	0.52
1:B:531:THR:HG22	1:B:532:ASN:O	2.09	0.52
1:C:611:LEU:HD12	1:C:649:CYS:N	2.25	0.52
1:B:316:SER:OG	1:B:317:ASN:N	2.43	0.52
1:C:328:ARG:HG2	1:C:578:ASP:CG	2.29	0.52
1:C:339:ASP:O	1:C:343:ASN:HB2	2.10	0.52
1:C:643:PHE:CG	1:C:655:TYR:HB2	2.44	0.52
1:B:415:THR:CG2	2:H:65:ASP:O	2.42	0.52
1:A:319:ARG:HH21	1:A:319:ARG:CG	2.14	0.52
1:B:326:ILE:CG1	1:B:532:ASN:O	2.58	0.52
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.45	0.52
1:A:308:VAL:HG12	1:A:313:TYR:HE2	1.75	0.52
1:A:372:ALA:CB	1:A:373:PRO:CD	2.66	0.52
1:A:521:PRO:O	1:A:522:ALA:HB2	2.09	0.52
1:B:309:GLU:HG2	1:B:313:TYR:OH	2.10	0.52
1:B:858:LEU:HD21	1:B:962:LEU:CD2	2.39	0.52
3:M:33:TYR:N	3:M:33:TYR:CD1	2.72	0.52
1:B:319:ARG:NH2	1:B:319:ARG:CB	2.73	0.52
1:C:314:GLN:HA	1:C:596:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:PRO:O	1:C:331:ASN:O	2.28	0.52
1:A:855:PHE:N	1:A:855:PHE:CD1	2.77	0.52
1:A:898:PHE:N	1:A:899:PRO:CD	2.73	0.52
1:C:332:ILE:CG2	1:C:333:THR:N	2.73	0.52
1:B:898:PHE:N	1:B:899:PRO:CD	2.73	0.51
1:B:442:ASP:OD2	1:B:509:ARG:NE	2.41	0.51
1:A:200:TYR:OH	1:C:522:ALA:CB	2.51	0.51
1:B:736:VAL:HA	1:B:857:GLY:O	2.10	0.51
1:A:560:LEU:HD12	1:A:562:PHE:CE1	2.46	0.51
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.46	0.51
1:C:672:ALA:O	1:C:673:SER:HB3	2.10	0.51
1:C:898:PHE:N	1:C:899:PRO:CD	2.73	0.51
3:M:20:ILE:HG23	3:M:74:LEU:HB3	1.91	0.51
1:A:589:PRO:HG2	1:B:855:PHE:HB3	1.92	0.51
3:L:20:ILE:HG23	3:L:74:LEU:HB3	1.91	0.51
1:B:690:GLN:O	1:B:690:GLN:HG2	2.10	0.51
1:A:318:PHE:O	1:A:319:ARG:HB3	2.11	0.51
1:B:333:THR:OG1	1:B:362:VAL:CG1	2.59	0.51
1:C:454:ARG:NH2	1:C:469:SER:O	2.43	0.51
1:A:313:TYR:O	1:A:315:THR:HG23	2.10	0.51
1:B:308:VAL:HG12	1:B:313:TYR:HE2	1.74	0.51
1:B:415:THR:HG21	2:H:65:ASP:C	2.28	0.51
1:C:372:ALA:CB	1:C:373:PRO:CD	2.66	0.51
2:H:90:THR:HG23	2:H:117:THR:HA	1.93	0.51
2:J:90:THR:HG23	2:J:117:THR:HA	1.93	0.51
1:A:1128:VAL:HG23	1:B:918:GLU:HG2	1.93	0.50
1:C:294:ASP:OD1	1:C:294:ASP:N	2.43	0.50
1:A:367:VAL:CG1	1:A:368:LEU:N	2.61	0.50
2:I:90:THR:HG23	2:I:117:THR:HA	1.93	0.50
1:B:375:PHE:CD1	1:B:375:PHE:C	2.85	0.50
1:A:98:SER:OG	1:A:99:ASN:N	2.45	0.50
1:A:319:ARG:NH2	1:A:319:ARG:CG	2.73	0.50
1:A:375:PHE:CD1	1:A:375:PHE:C	2.85	0.50
1:A:461:LEU:HB3	1:A:465:GLU:HB3	1.94	0.50
1:A:579:PRO:C	1:A:580:GLN:CG	2.78	0.50
1:B:325:SER:O	1:B:327:VAL:HG23	2.12	0.50
1:C:294:ASP:HB2	1:C:295:PRO:CD	2.40	0.50
1:A:321:GLN:HE21	1:A:322:PRO:HD2	1.77	0.50
1:C:327:VAL:O	1:C:531:THR:N	2.41	0.50
1:A:579:PRO:O	1:A:580:GLN:CB	2.59	0.50
1:B:98:SER:OG	1:B:99:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:SER:OG	1:B:692:ILE:N	2.44	0.50
1:C:338:PHE:O	1:C:341:VAL:N	2.45	0.50
1:A:317:ASN:N	1:A:317:ASN:ND2	2.60	0.50
1:A:454:ARG:NH2	1:A:469:SER:O	2.43	0.50
1:A:520:ALA:CB	1:A:521:PRO:HD2	2.22	0.50
1:A:570:ALA:CB	1:B:963:VAL:CG1	2.90	0.50
1:B:325:SER:O	1:B:325:SER:OG	2.28	0.50
1:C:375:PHE:CD1	1:C:375:PHE:C	2.85	0.50
1:A:565:PHE:CD1	1:A:565:PHE:N	2.79	0.50
1:B:461:LEU:HB3	1:B:465:GLU:HB3	1.94	0.50
1:B:663:ASP:OD2	1:B:673:SER:CB	2.60	0.50
1:A:528:LYS:O	1:A:529:LYS:HD2	2.11	0.49
1:C:314:GLN:HA	1:C:596:SER:CB	2.42	0.49
1:A:112:SER:OG	1:A:113:LYS:N	2.45	0.49
1:A:338:PHE:O	1:A:341:VAL:N	2.45	0.49
1:A:534:VAL:HG21	1:A:539:VAL:HG11	1.94	0.49
1:A:560:LEU:HD12	1:A:562:PHE:HZ	1.77	0.49
1:A:646:ARG:NH2	1:B:866:THR:HG21	2.26	0.49
1:B:112:SER:OG	1:B:113:LYS:N	2.45	0.49
1:B:328:ARG:C	1:B:329:PHE:CD1	2.86	0.49
1:B:858:LEU:CD2	1:B:962:LEU:CD2	2.89	0.49
1:C:98:SER:OG	1:C:99:ASN:N	2.45	0.49
1:A:515:PHE:CD2	1:A:515:PHE:N	2.78	0.49
1:A:519:HIS:CD2	1:A:520:ALA:N	2.73	0.49
1:B:338:PHE:O	1:B:341:VAL:N	2.45	0.49
1:B:854:LYS:O	1:B:856:ASN:N	2.45	0.49
2:H:39:GLN:HB2	2:H:45:LEU:HG	1.94	0.49
2:J:23:ARG:NH1	2:J:24:ALA:O	2.39	0.49
1:A:294:ASP:CB	1:A:295:PRO:CD	2.71	0.49
1:A:332:ILE:O	1:A:333:THR:OG1	2.26	0.49
1:C:614:GLY:H	1:C:648:GLY:HA2	1.77	0.49
1:C:695:TYR:CD1	1:C:695:TYR:C	2.85	0.49
1:A:579:PRO:O	1:A:580:GLN:CG	2.59	0.49
1:A:643:PHE:CE1	1:A:655:TYR:CD2	3.01	0.49
1:A:695:TYR:C	1:A:695:TYR:CD2	2.85	0.49
1:B:705:VAL:HG11	1:C:883:THR:OG1	2.13	0.49
1:C:744:GLY:O	1:C:745:ASP:HB2	2.13	0.49
2:J:39:GLN:HB2	2:J:45:LEU:HG	1.94	0.49
1:A:314:GLN:HG3	1:A:315:THR:N	2.27	0.49
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.94	0.49
2:I:39:GLN:HB2	2:I:45:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:HG22	1:B:341:VAL:O	2.12	0.49
1:B:643:PHE:CE1	1:B:655:TYR:CD2	3.01	0.49
1:C:329:PHE:CZ	1:C:528:LYS:HG2	2.47	0.49
1:C:475:ALA:HB2	3:L:16:GLN:NE2	2.27	0.49
1:C:112:SER:OG	1:C:113:LYS:N	2.45	0.49
1:B:607:GLN:C	1:B:608:VAL:HG13	2.33	0.49
1:B:986:PRO:N	1:B:987:PRO:CD	2.76	0.49
1:C:329:PHE:HB2	1:C:530:SER:OG	2.12	0.49
1:C:615:VAL:O	1:C:649:CYS:HB2	2.13	0.49
1:A:587:ILE:O	1:A:588:THR:HG22	2.13	0.49
1:B:420:ASP:OD1	1:B:421:TYR:N	2.42	0.49
1:A:592:PHE:CE2	1:B:740:MET:HE2	2.47	0.48
1:A:646:ARG:HH22	1:B:866:THR:HG21	1.76	0.48
1:A:1128:VAL:HG21	1:B:918:GLU:HG2	1.93	0.48
1:B:334:ASN:HD21	1:B:361:CYS:CA	2.13	0.48
1:B:744:GLY:O	1:B:745:ASP:HB2	2.13	0.48
1:B:663:ASP:CB	1:B:673:SER:HB3	2.43	0.48
1:C:341:VAL:HG22	1:C:341:VAL:O	2.12	0.48
1:A:564:GLN:C	1:A:565:PHE:CD1	2.86	0.48
1:B:333:THR:O	1:B:333:THR:HG23	2.12	0.48
1:B:454:ARG:NH2	1:B:469:SER:O	2.43	0.48
1:C:461:LEU:HB3	1:C:465:GLU:HB3	1.94	0.48
1:A:341:VAL:HG22	1:A:341:VAL:O	2.12	0.48
1:B:326:ILE:HG23	1:B:326:ILE:O	2.13	0.48
1:A:321:GLN:HE21	1:A:322:PRO:CD	2.25	0.48
1:A:327:VAL:O	1:A:327:VAL:HG12	2.12	0.48
1:B:529:LYS:H	1:B:529:LYS:CD	2.05	0.48
1:A:41:LYS:HB3	1:C:562:PHE:O	2.13	0.48
1:A:393:THR:HA	1:A:522:ALA:O	2.12	0.48
1:B:315:THR:OG1	1:B:316:SER:N	2.42	0.48
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.13	0.48
1:B:332:ILE:CG1	1:B:333:THR:N	2.75	0.48
1:C:326:ILE:HG12	1:C:534:VAL:HG22	1.94	0.48
1:B:327:VAL:CG1	1:B:328:ARG:N	2.77	0.48
1:B:438:SER:O	1:B:438:SER:OG	2.31	0.48
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.71	0.48
3:N:14:PRO:HA	3:N:79:LEU:HB2	1.96	0.48
1:A:744:GLY:O	1:A:745:ASP:HB2	2.12	0.48
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.54	0.48
1:C:357:ARG:HG3	1:C:396:TYR:CD1	2.45	0.48
1:B:336:CYS:HB2	1:B:361:CYS:HB2	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HD11	1:C:539:VAL:HG11	1.94	0.48
1:B:372:ALA:CB	1:B:373:PRO:CD	2.66	0.47
1:B:564:GLN:O	1:B:577:ARG:HB3	2.14	0.47
1:C:325:SER:O	1:C:326:ILE:HG13	2.13	0.47
1:C:342:PHE:HB3	1:C:371:PHE:HE2	1.78	0.47
2:H:6:GLN:NE2	2:H:22:CYS:SG	2.87	0.47
2:I:119:SER:OG	2:I:120:SER:N	2.47	0.47
1:B:592:PHE:CD1	1:B:592:PHE:C	2.87	0.47
1:C:294:ASP:HB2	1:C:295:PRO:HD2	1.96	0.47
1:C:670:ILE:HG22	1:C:671:CYS:N	2.27	0.47
1:A:314:GLN:CA	1:A:596:SER:CB	2.86	0.47
1:A:427:ASP:CG	1:C:987:PRO:HG3	2.35	0.47
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.47	0.47
1:C:202:LYS:NZ	1:C:228:ASP:OD2	2.47	0.47
1:C:333:THR:OG1	1:C:334:ASN:OD1	2.29	0.47
1:C:564:GLN:O	1:C:577:ARG:HB3	2.14	0.47
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.54	0.47
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.96	0.47
2:H:119:SER:OG	2:H:120:SER:N	2.47	0.47
2:I:6:GLN:NE2	2:I:22:CYS:SG	2.87	0.47
2:J:119:SER:OG	2:J:120:SER:N	2.47	0.47
1:B:986:PRO:N	1:B:987:PRO:HD2	2.29	0.47
1:B:1123:SER:OG	1:C:914:ASN:ND2	2.47	0.47
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.96	0.47
1:B:308:VAL:H	1:B:602:THR:HG23	1.79	0.47
1:B:320:VAL:HG22	1:B:320:VAL:O	2.14	0.47
1:B:715:PRO:HD3	1:C:894:LEU:CD1	2.44	0.47
2:H:92:VAL:HA	2:H:114:THR:O	2.15	0.47
1:A:314:GLN:HA	1:A:596:SER:CA	2.44	0.47
1:B:338:PHE:O	1:B:341:VAL:HG12	2.15	0.47
1:C:331:ASN:O	1:C:332:ILE:HG12	2.14	0.47
1:C:338:PHE:O	1:C:341:VAL:HG12	2.15	0.47
1:C:535:LYS:O	1:C:536:ASN:HB2	2.15	0.47
1:C:1082:CYS:SG	1:C:1132:ILE:HD13	2.54	0.47
2:H:33:PHE:HA	2:H:53:PRO:HD3	1.97	0.47
2:H:39:GLN:NE2	2:H:40:ALA:O	2.48	0.47
2:I:33:PHE:HA	2:I:53:PRO:HD3	1.97	0.47
1:A:291:CYS:HG	1:A:301:CYS:HB3	1.79	0.47
2:J:33:PHE:HA	2:J:53:PRO:HD3	1.97	0.47
1:A:706:ALA:HB1	5:A:1410:NAG:H5	1.97	0.47
1:C:332:ILE:O	1:C:333:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:92:VAL:HA	2:I:114:THR:O	2.14	0.47
2:J:6:GLN:NE2	2:J:22:CYS:SG	2.87	0.47
1:A:338:PHE:O	1:A:341:VAL:HG12	2.15	0.47
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.32	0.47
1:B:983:ARG:O	1:B:984:LEU:HG	2.14	0.47
1:C:420:ASP:OD1	1:C:421:TYR:N	2.42	0.47
3:L:14:PRO:HA	3:L:79:LEU:HB2	1.96	0.47
2:J:39:GLN:NE2	2:J:40:ALA:O	2.48	0.47
2:J:92:VAL:HA	2:J:114:THR:O	2.15	0.47
1:A:329:PHE:HE2	1:A:528:LYS:HG2	1.60	0.46
1:B:327:VAL:CG1	1:B:329:PHE:HE1	2.27	0.46
1:B:331:ASN:O	1:B:332:ILE:O	2.33	0.46
1:B:531:THR:CG2	1:B:532:ASN:N	2.78	0.46
1:B:706:ALA:HB1	5:B:1410:NAG:H5	1.97	0.46
3:M:14:PRO:HA	3:M:79:LEU:HB2	1.96	0.46
1:A:430:THR:O	1:A:430:THR:OG1	2.31	0.46
1:B:977:LEU:HD12	1:B:977:LEU:HA	1.77	0.46
1:C:611:LEU:CD1	1:C:649:CYS:H	2.25	0.46
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.47	0.46
1:C:368:LEU:HD23	1:C:368:LEU:O	2.15	0.46
1:C:642:VAL:HG12	1:C:642:VAL:O	2.15	0.46
2:I:39:GLN:NE2	2:I:40:ALA:O	2.48	0.46
1:B:674:TYR:HA	1:B:691:SER:O	2.16	0.46
1:B:973:ILE:HG22	1:B:992:GLN:CD	2.35	0.46
1:A:462:LYS:NZ	5:B:1404:NAG:H62	2.31	0.46
1:B:602:THR:O	1:B:604:THR:N	2.46	0.46
1:C:643:PHE:CD1	1:C:655:TYR:CB	2.99	0.46
1:A:321:GLN:NE2	1:A:322:PRO:HD2	2.30	0.46
1:A:368:LEU:HD23	1:A:368:LEU:O	2.15	0.46
1:C:289:VAL:HG13	1:C:297:SER:HB3	1.96	0.46
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.96	0.46
1:A:321:GLN:NE2	1:A:321:GLN:CA	2.72	0.46
1:A:653:ALA:HA	1:A:692:ILE:O	2.16	0.46
1:B:328:ARG:CD	1:B:578:ASP:OD1	2.62	0.46
1:C:607:GLN:O	1:C:608:VAL:HG13	2.15	0.46
1:A:519:HIS:HE1	1:B:41:LYS:N	2.07	0.46
1:B:291:CYS:HG	1:B:301:CYS:CB	2.24	0.46
1:B:371:PHE:O	1:B:372:ALA:CB	2.64	0.46
1:A:334:ASN:O	1:A:335:LEU:CB	2.62	0.46
1:A:607:GLN:O	1:A:608:VAL:HG13	2.15	0.46
1:B:328:ARG:HE	1:B:533:LEU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:HD23	1:B:368:LEU:O	2.15	0.46
1:B:604:THR:O	1:B:605:SER:HB2	2.16	0.46
1:A:165:ASN:OD1	1:C:357:ARG:NH1	2.49	0.46
1:B:89:GLY:HA2	1:B:194:PHE:O	2.16	0.46
1:B:363:ALA:O	1:B:365:TYR:N	2.48	0.46
1:B:675:GLN:HA	1:B:675:GLN:NE2	2.24	0.46
1:B:983:ARG:O	1:B:984:LEU:HD12	2.14	0.46
1:A:394:ASN:O	1:A:515:PHE:HA	2.15	0.45
1:B:319:ARG:HB2	1:B:319:ARG:CZ	2.45	0.45
3:L:32:ASN:O	3:L:33:TYR:C	2.55	0.45
1:B:310:LYS:HA	1:B:599:THR:O	2.16	0.45
1:B:613:GLN:H	1:B:613:GLN:HG2	1.48	0.45
1:B:672:ALA:O	1:B:673:SER:CB	2.64	0.45
3:M:68:SER:O	3:M:71:SER:OG	2.34	0.45
3:N:32:ASN:O	3:N:33:TYR:C	2.55	0.45
1:A:321:GLN:HE21	1:A:321:GLN:CA	2.02	0.45
1:A:374:PHE:N	1:A:374:PHE:CD1	2.85	0.45
1:A:660:TYR:O	1:A:697:MET:HA	2.17	0.45
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.45
1:C:374:PHE:N	1:C:374:PHE:CD1	2.85	0.45
3:L:33:TYR:N	3:L:33:TYR:CD1	2.72	0.45
1:A:167:THR:HG21	1:C:357:ARG:HH22	1.80	0.45
1:A:542:ASN:HA	1:A:546:LEU:O	2.17	0.45
1:A:668:ALA:HA	1:B:863:PRO:O	2.16	0.45
1:A:669:GLY:N	1:B:864:LEU:O	2.49	0.45
1:C:542:ASN:HA	1:C:546:LEU:O	2.17	0.45
1:B:973:ILE:CG2	1:B:992:GLN:CD	2.85	0.45
1:C:89:GLY:HA2	1:C:194:PHE:O	2.17	0.45
1:C:413:GLY:O	1:C:414:GLN:NE2	2.50	0.45
1:C:706:ALA:HB1	5:C:1410:NAG:H5	1.97	0.45
1:A:587:ILE:C	1:A:588:THR:CG2	2.85	0.45
1:A:918:GLU:HG2	1:C:1128:VAL:HG23	1.99	0.45
1:B:978:ASN:O	1:B:979:ASP:C	2.54	0.45
1:C:60:SER:OG	1:C:61:ASN:N	2.50	0.45
1:C:370:ASN:O	1:C:371:PHE:CD1	2.70	0.45
1:C:669:GLY:O	1:C:696:THR:HG22	2.16	0.45
1:A:592:PHE:HD2	1:B:740:MET:HE2	1.76	0.45
1:B:328:ARG:O	1:B:329:PHE:CD1	2.70	0.45
1:C:324:GLU:HB2	1:C:325:SER:H	1.58	0.45
1:C:332:ILE:C	1:C:333:THR:CG2	2.86	0.45
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:VAL:O	1:C:487:ASN:HB2	2.17	0.45
1:C:613:GLN:H	1:C:613:GLN:HG2	1.48	0.45
1:C:643:PHE:CE2	1:C:655:TYR:CD1	3.05	0.45
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.99	0.45
1:A:332:ILE:CG2	1:A:362:VAL:HG13	2.38	0.45
1:A:559:PHE:HB3	1:A:563:GLN:CB	2.47	0.45
1:A:565:PHE:O	1:A:565:PHE:CD2	2.70	0.45
1:A:570:ALA:CB	1:B:963:VAL:HG12	2.44	0.45
1:A:693:ILE:H	1:A:693:ILE:HG12	1.68	0.45
1:B:334:ASN:HD21	1:B:360:ASN:C	2.20	0.45
1:A:342:PHE:CB	1:A:371:PHE:CE2	2.97	0.44
1:A:375:PHE:CD1	1:A:375:PHE:O	2.70	0.44
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.99	0.44
1:C:569:ILE:O	1:C:570:ALA:HB3	2.16	0.44
1:C:331:ASN:O	1:C:332:ILE:HD13	2.17	0.44
3:N:68:SER:O	3:N:71:SER:OG	2.34	0.44
1:A:89:GLY:HA2	1:A:194:PHE:O	2.16	0.44
1:A:564:GLN:CB	1:A:565:PHE:HD1	2.31	0.44
1:A:571:ASP:HB3	1:B:967:SER:OG	2.17	0.44
1:B:375:PHE:CD1	1:B:375:PHE:O	2.70	0.44
1:B:569:ILE:O	1:B:570:ALA:HB3	2.16	0.44
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.83	0.44
1:C:375:PHE:CD1	1:C:375:PHE:O	2.70	0.44
1:A:60:SER:OG	1:A:61:ASN:N	2.50	0.44
1:A:530:SER:OG	1:A:531:THR:N	2.50	0.44
1:A:675:GLN:HB2	1:A:693:ILE:HD11	2.00	0.44
1:B:318:PHE:O	1:B:318:PHE:CD2	2.70	0.44
1:B:318:PHE:O	1:B:318:PHE:CG	2.70	0.44
1:B:413:GLY:O	1:B:414:GLN:NE2	2.50	0.44
1:B:705:VAL:HG11	1:C:883:THR:CB	2.48	0.44
1:A:413:GLY:O	1:A:414:GLN:NE2	2.50	0.44
1:A:569:ILE:O	1:A:570:ALA:HB3	2.16	0.44
1:B:370:ASN:O	1:B:371:PHE:CD1	2.70	0.44
3:L:26:SER:O	3:L:31:ASN:CG	2.56	0.44
1:A:357:ARG:HH11	1:B:230:PRO:CG	2.27	0.44
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.00	0.44
1:B:973:ILE:HG21	1:B:992:GLN:HG3	2.00	0.44
1:C:371:PHE:O	1:C:372:ALA:CB	2.64	0.44
1:C:712:ILE:O	1:C:1074:ASN:HA	2.18	0.44
5:C:1410:NAG:O4	5:C:1411:NAG:O5	2.28	0.44
1:A:420:ASP:OD1	1:A:421:TYR:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:HD21	1:A:454:ARG:H	1.66	0.44
1:A:560:LEU:C	1:A:562:PHE:H	2.20	0.44
1:B:542:ASN:HA	1:B:546:LEU:O	2.17	0.44
1:B:976:VAL:C	1:B:978:ASN:H	2.21	0.44
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.58	0.44
1:A:311:GLY:HA2	1:A:664:ILE:HG23	2.00	0.44
1:A:370:ASN:O	1:A:371:PHE:CD1	2.70	0.44
1:A:564:GLN:HB3	1:A:565:PHE:HD1	1.82	0.44
1:B:364:ASP:O	1:B:366:SER:N	2.49	0.44
1:B:402:ILE:HD11	1:B:510:VAL:HG21	2.00	0.44
1:B:559:PHE:HE2	1:B:565:PHE:HA	1.82	0.44
1:C:81:ASN:OD1	1:C:81:ASN:N	2.51	0.44
3:M:26:SER:O	3:M:31:ASN:CG	2.56	0.44
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.45	0.44
1:B:394:ASN:OD1	1:B:394:ASN:N	2.49	0.44
1:A:699:LEU:HD22	1:B:873:TYR:OH	2.17	0.43
1:B:675:GLN:CG	1:B:676:THR:N	2.81	0.43
1:C:233:ILE:HD13	1:C:233:ILE:HA	1.87	0.43
1:C:394:ASN:OD1	1:C:394:ASN:N	2.49	0.43
1:C:422:ASN:HD21	1:C:454:ARG:H	1.66	0.43
1:C:559:PHE:HE2	1:C:565:PHE:HA	1.82	0.43
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.51	0.43
1:A:371:PHE:O	1:A:372:ALA:CB	2.64	0.43
1:A:593:GLY:O	1:A:594:GLY:C	2.53	0.43
1:A:862:PRO:CG	1:C:647:ALA:CB	2.83	0.43
1:B:60:SER:OG	1:B:61:ASN:N	2.50	0.43
1:B:294:ASP:HB2	1:B:295:PRO:CD	2.48	0.43
1:B:342:PHE:HB3	1:B:371:PHE:HE2	1.78	0.43
1:B:606:ASN:N	1:B:606:ASN:ND2	2.60	0.43
1:B:973:ILE:CG2	1:B:992:GLN:CG	2.96	0.43
1:C:533:LEU:N	1:C:533:LEU:CD1	2.73	0.43
1:C:670:ILE:CG2	1:C:671:CYS:N	2.80	0.43
1:C:675:GLN:HG3	1:C:676:THR:H	1.83	0.43
3:N:33:TYR:N	3:N:33:TYR:CD1	2.72	0.43
1:A:334:ASN:HB2	1:A:361:CYS:HA	2.00	0.43
1:A:1126:CYS:SG	1:A:1132:ILE:HD13	2.58	0.43
1:B:916:LEU:C	1:B:916:LEU:HD23	2.39	0.43
3:N:26:SER:O	3:N:31:ASN:CG	2.56	0.43
1:A:702:GLU:OE2	1:B:790:LYS:CE	2.66	0.43
1:A:712:ILE:O	1:A:1074:ASN:HA	2.18	0.43
1:B:320:VAL:O	1:B:321:GLN:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ILE:O	1:B:1074:ASN:HA	2.18	0.43
1:B:979:ASP:C	1:B:981:LEU:N	2.72	0.43
1:C:980:ILE:O	1:C:984:LEU:HB3	2.18	0.43
3:M:32:ASN:O	3:M:33:TYR:C	2.55	0.43
1:A:316:SER:HB2	1:A:317:ASN:H	1.64	0.43
1:A:613:GLN:H	1:A:613:GLN:HG2	1.48	0.43
1:B:315:THR:H	1:B:596:SER:HA	1.83	0.43
1:B:367:VAL:O	1:B:368:LEU:C	2.57	0.43
1:A:368:LEU:C	1:A:368:LEU:CD2	2.85	0.43
1:A:438:SER:O	1:A:438:SER:OG	2.31	0.43
1:B:319:ARG:NH2	1:B:319:ARG:CG	2.73	0.43
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.32	0.43
1:B:422:ASN:HD21	1:B:454:ARG:H	1.66	0.43
1:C:374:PHE:C	1:C:376:ALA:N	2.72	0.43
3:M:5:THR:OG1	3:M:23:SER:O	2.33	0.43
1:A:188:ASN:OD1	1:A:188:ASN:N	2.52	0.43
1:A:528:LYS:O	1:A:529:LYS:HB2	2.18	0.43
1:B:961:THR:HG21	1:C:762:GLN:NE2	2.33	0.43
1:C:402:ILE:HD11	1:C:510:VAL:HG21	2.00	0.43
1:C:1126:CYS:SG	1:C:1132:ILE:HD13	2.58	0.43
1:A:379:CYS:HB2	1:A:384:PRO:HG3	2.01	0.43
1:A:659:SER:HB3	1:A:696:THR:O	2.19	0.43
1:B:374:PHE:N	1:B:374:PHE:CD1	2.85	0.43
1:C:916:LEU:C	1:C:916:LEU:HD23	2.39	0.43
4:K:1:NAG:H4	4:K:2:NAG:C7	2.49	0.43
1:B:296:LEU:HD13	1:B:608:VAL:HG11	2.01	0.43
1:B:334:ASN:HD21	1:B:361:CYS:N	2.17	0.43
1:B:599:THR:C	1:B:601:GLY:N	2.72	0.43
1:B:690:GLN:O	1:B:691:SER:HB2	2.19	0.43
1:B:985:ASP:C	1:B:987:PRO:HD2	2.39	0.43
1:C:611:LEU:CD1	1:C:649:CYS:N	2.80	0.43
1:A:374:PHE:C	1:A:376:ALA:N	2.72	0.43
1:C:379:CYS:HB2	1:C:384:PRO:HG3	2.01	0.43
3:N:47:LEU:HB3	3:N:56:PRO:HG3	2.01	0.43
3:N:92:TRP:HE3	3:N:101:TRP:HE3	1.66	0.43
4:T:1:NAG:H4	4:T:2:NAG:C7	2.49	0.43
1:A:522:ALA:HB3	1:A:544:ASN:HD21	1.84	0.42
1:B:599:THR:O	1:B:601:GLY:N	2.51	0.42
1:C:188:ASN:OD1	1:C:188:ASN:N	2.52	0.42
1:C:374:PHE:O	1:C:376:ALA:N	2.52	0.42
4:Z:1:NAG:H4	4:Z:2:NAG:C7	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:HB3	1:A:563:GLN:HB2	2.01	0.42
1:A:980:ILE:O	1:A:984:LEU:HB3	2.19	0.42
1:C:342:PHE:CB	1:C:371:PHE:CE2	2.97	0.42
1:C:367:VAL:O	1:C:368:LEU:C	2.57	0.42
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.87	0.42
1:A:374:PHE:O	1:A:376:ALA:N	2.52	0.42
1:A:560:LEU:C	1:A:562:PHE:N	2.73	0.42
1:A:581:THR:C	1:A:582:LEU:HG	2.39	0.42
1:A:602:THR:C	1:A:604:THR:N	2.72	0.42
1:B:129:LYS:HG2	1:B:131:CYS:SG	2.60	0.42
1:B:330:PRO:CB	1:B:332:ILE:HG22	2.42	0.42
1:B:364:ASP:HB3	1:B:367:VAL:HG23	2.01	0.42
1:B:379:CYS:HB2	1:B:384:PRO:HG3	2.01	0.42
3:L:92:TRP:HE3	3:L:101:TRP:HE3	1.66	0.42
1:A:916:LEU:C	1:A:916:LEU:HD23	2.39	0.42
1:C:109:THR:CA	1:C:237:ARG:HH21	2.21	0.42
1:C:129:LYS:HG2	1:C:131:CYS:SG	2.60	0.42
1:C:560:LEU:HB2	1:C:563:GLN:OE1	2.20	0.42
1:C:693:ILE:HD12	1:C:693:ILE:N	2.17	0.42
3:L:57:SER:OG	3:L:58:GLY:N	2.52	0.42
3:N:62:ARG:NH2	3:N:78:GLY:O	2.47	0.42
1:A:316:SER:C	1:A:317:ASN:ND2	2.72	0.42
1:A:565:PHE:O	1:A:565:PHE:CG	2.72	0.42
1:A:602:THR:C	1:A:604:THR:H	2.20	0.42
1:B:374:PHE:C	1:B:376:ALA:N	2.72	0.42
1:A:394:ASN:OD1	1:A:394:ASN:N	2.49	0.42
1:A:660:TYR:O	1:A:698:SER:N	2.50	0.42
1:B:328:ARG:CZ	1:B:578:ASP:OD2	2.67	0.42
1:B:976:VAL:C	1:B:978:ASN:N	2.72	0.42
1:B:986:PRO:O	1:B:990:GLU:CG	2.66	0.42
3:N:57:SER:OG	3:N:58:GLY:N	2.52	0.42
1:A:336:CYS:HB3	1:A:361:CYS:HB3	1.83	0.42
1:A:918:GLU:HG2	1:C:1128:VAL:HG21	2.01	0.42
1:B:374:PHE:O	1:B:376:ALA:N	2.52	0.42
1:C:457:ARG:NH1	1:C:460:ASN:O	2.52	0.42
1:C:898:PHE:HB3	1:C:899:PRO:HD3	2.01	0.42
1:B:308:VAL:CG1	1:B:599:THR:HG21	2.49	0.42
1:C:643:PHE:CD1	1:C:655:TYR:HB2	2.55	0.42
3:L:68:SER:O	3:L:71:SER:OG	2.34	0.42
1:A:459:SER:OG	1:A:460:ASN:N	2.53	0.42
1:A:534:VAL:CG2	1:A:539:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASN:N	1:B:188:ASN:OD1	2.52	0.42
1:B:457:ARG:NH1	1:B:460:ASN:O	2.52	0.42
1:B:743:CYS:O	1:B:977:LEU:HD22	2.20	0.42
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.91	0.42
1:C:374:PHE:N	1:C:374:PHE:HD1	2.18	0.42
3:L:62:ARG:NH2	3:L:78:GLY:O	2.47	0.42
3:M:47:LEU:HB3	3:M:56:PRO:HG3	2.01	0.42
3:M:57:SER:OG	3:M:58:GLY:N	2.52	0.42
1:A:457:ARG:NH1	1:A:460:ASN:O	2.52	0.42
1:B:1141:LEU:CD2	1:C:1144:GLU:OE1	2.68	0.42
1:A:129:LYS:HG2	1:A:131:CYS:SG	2.60	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.92	0.41
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.85	0.41
1:B:364:ASP:C	1:B:366:SER:N	2.73	0.41
1:C:276:LEU:HD22	1:C:301:CYS:HA	2.02	0.41
1:C:649:CYS:O	1:C:649:CYS:SG	2.78	0.41
3:L:47:LEU:HB3	3:L:56:PRO:HG3	2.01	0.41
1:A:43:PHE:CD1	1:C:559:PHE:HA	2.55	0.41
1:A:324:GLU:O	1:A:325:SER:CB	2.67	0.41
1:A:369:TYR:HD1	1:A:369:TYR:HA	1.70	0.41
1:B:342:PHE:CB	1:B:371:PHE:HE2	2.33	0.41
1:B:854:LYS:C	1:B:856:ASN:N	2.73	0.41
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.35	0.41
3:M:92:TRP:HE3	3:M:101:TRP:HE3	1.66	0.41
1:B:125:ASN:HD21	5:B:1402:NAG:H5	1.86	0.41
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.01	0.41
5:B:1410:NAG:O4	5:B:1411:NAG:O5	2.28	0.41
1:C:50:SER:HB2	1:C:304:LYS:HE3	2.03	0.41
1:C:607:GLN:HE21	1:C:607:GLN:HB3	1.68	0.41
1:C:670:ILE:O	1:C:671:CYS:SG	2.78	0.41
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.36	0.41
3:L:5:THR:OG1	3:L:23:SER:O	2.33	0.41
1:A:579:PRO:C	1:A:580:GLN:HG2	2.41	0.41
1:A:582:LEU:HD23	1:A:582:LEU:N	2.36	0.41
1:A:898:PHE:HB3	1:A:899:PRO:HD3	2.01	0.41
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.36	0.41
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.20	0.41
1:B:668:ALA:CA	1:C:863:PRO:O	2.65	0.41
1:A:515:PHE:O	1:A:515:PHE:CD2	2.70	0.41
1:B:459:SER:OG	1:B:460:ASN:N	2.52	0.41
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:LYS:C	1:C:529:LYS:HD3	2.41	0.41
1:C:986:PRO:N	1:C:987:PRO:CD	2.83	0.41
1:A:986:PRO:N	1:A:987:PRO:CD	2.83	0.41
1:C:504:GLY:O	1:C:505:HIS:ND1	2.54	0.41
1:A:59:PHE:CD2	1:A:293:LEU:HD21	2.56	0.41
1:A:342:PHE:CB	1:A:371:PHE:HE2	2.33	0.41
1:B:504:GLY:O	1:B:505:HIS:ND1	2.54	0.41
1:B:979:ASP:C	1:B:981:LEU:H	2.24	0.41
1:B:980:ILE:HD12	1:B:996:LEU:CD1	2.51	0.41
1:C:50:SER:CB	1:C:304:LYS:HE3	2.51	0.41
1:C:459:SER:OG	1:C:460:ASN:N	2.52	0.41
1:C:643:PHE:CE1	1:C:655:TYR:CD2	3.09	0.41
1:B:68:ILE:HG21	1:B:262:ALA:HA	2.03	0.41
1:B:294:ASP:N	1:B:294:ASP:OD1	2.52	0.41
1:B:374:PHE:N	1:B:374:PHE:HD1	2.18	0.41
1:A:68:ILE:HG21	1:A:262:ALA:HA	2.03	0.41
1:A:374:PHE:N	1:A:374:PHE:HD1	2.18	0.41
1:A:462:LYS:HZ2	5:B:1404:NAG:H62	1.85	0.41
1:A:504:GLY:O	1:A:505:HIS:ND1	2.54	0.41
1:A:559:PHE:HE2	1:A:565:PHE:N	2.19	0.41
1:A:566:GLY:HA2	1:B:43:PHE:O	2.21	0.41
1:B:362:VAL:HG13	1:B:362:VAL:O	2.19	0.41
1:B:431:GLY:HA3	1:B:513:LEU:O	2.21	0.41
1:B:675:GLN:HE21	1:B:675:GLN:CA	2.17	0.41
1:B:858:LEU:HD21	1:B:962:LEU:HD21	2.02	0.41
1:C:208:THR:HA	1:C:209:PRO:HD3	1.96	0.41
1:C:327:VAL:HG13	1:C:329:PHE:HE1	1.78	0.41
1:C:438:SER:O	1:C:438:SER:OG	2.31	0.41
1:A:320:VAL:CG2	1:A:321:GLN:N	2.84	0.41
1:A:431:GLY:HA3	1:A:513:LEU:O	2.20	0.41
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.86	0.41
1:A:125:ASN:HD21	5:A:1402:NAG:H5	1.86	0.40
1:A:602:THR:HA	1:A:605:SER:O	2.21	0.40
1:A:603:ASN:OD1	5:A:1406:NAG:C7	2.69	0.40
1:B:326:ILE:HD11	1:B:533:LEU:HA	0.54	0.40
1:C:334:ASN:OD1	1:C:334:ASN:N	2.54	0.40
1:C:342:PHE:CB	1:C:371:PHE:HE2	2.33	0.40
1:B:743:CYS:O	1:B:977:LEU:CD2	2.69	0.40
1:C:478:LYS:HA	1:C:479:PRO:HD3	1.92	0.40
1:B:294:ASP:HB2	1:B:295:PRO:HD2	2.04	0.40
1:B:669:GLY:O	1:B:697:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.04	0.40
1:B:983:ARG:O	1:B:984:LEU:CD1	2.70	0.40
1:C:125:ASN:HD21	5:C:1402:NAG:H5	1.86	0.40
1:C:293:LEU:HD12	1:C:293:LEU:HA	1.80	0.40
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.04	0.40
1:A:200:TYR:HH	1:C:522:ALA:HB3	1.79	0.40
1:B:326:ILE:O	1:B:326:ILE:CG2	2.70	0.40
1:B:1094:VAL:HG23	1:C:900:MET:CE	2.51	0.40
1:C:334:ASN:CG	1:C:361:CYS:HA	2.42	0.40
1:C:646:ARG:CG	1:C:646:ARG:O	2.69	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	1007/1271 (79%)	893 (89%)	75 (7%)	39 (4%)	3 18
1	B	1007/1271 (79%)	892 (89%)	79 (8%)	36 (4%)	3 20
1	C	1007/1271 (79%)	912 (91%)	78 (8%)	17 (2%)	9 36
2	H	118/120 (98%)	107 (91%)	11 (9%)	0	100 100
2	I	118/120 (98%)	107 (91%)	11 (9%)	0	100 100
2	J	118/120 (98%)	107 (91%)	11 (9%)	0	100 100
3	L	109/111 (98%)	98 (90%)	8 (7%)	3 (3%)	5 25
3	M	109/111 (98%)	98 (90%)	8 (7%)	3 (3%)	5 25
3	N	109/111 (98%)	98 (90%)	8 (7%)	3 (3%)	5 25
All	All	3702/4506 (82%)	3312 (90%)	289 (8%)	101 (3%)	8 25

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	A	323	THR
1	A	327	VAL
1	A	335	LEU
1	A	367	VAL
1	A	372	ALA
1	A	377	PHE
1	A	518	LEU
1	A	521	PRO
1	A	522	ALA
1	A	530	SER
1	A	580	GLN
1	B	316	SER
1	B	329	PHE
1	B	332	ILE
1	B	333	THR
1	B	372	ALA
1	B	377	PHE
1	B	529	LYS
1	B	561	PRO
1	B	591	SER
1	B	604	THR
1	C	331	ASN
1	C	367	VAL
1	C	372	ALA
1	C	377	PHE
1	C	561	PRO
3	L	31	ASN
3	L	33	TYR
3	M	31	ASN
3	M	33	TYR
3	N	31	ASN
3	N	33	TYR
1	A	174	PRO
1	A	316	SER
1	A	322	PRO
1	A	325	SER
1	A	334	ASN
1	A	368	LEU
1	A	519	HIS
1	A	561	PRO
1	A	565	PHE
1	A	581	THR

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Mol	Chain	Res	Type
1	A	590	CYS
1	A	604	THR
1	B	174	PRO
1	B	293	LEU
1	B	368	LEU
1	B	594	GLY
1	B	855	PHE
1	B	977	LEU
1	B	980	ILE
1	B	983	ARG
1	C	174	PRO
1	C	368	LEU
1	C	647	ALA
3	L	32	ASN
3	M	32	ASN
3	N	32	ASN
1	A	324	GLU
1	A	374	PHE
1	B	361	CYS
1	B	365	TYR
1	B	374	PHE
1	B	531	THR
1	B	673	SER
1	C	291	CYS
1	C	323	THR
1	C	374	PHE
1	C	532	ASN
1	A	294	ASP
1	A	318	PHE
1	A	326	ILE
1	A	339	ASP
1	A	375	PHE
1	A	529	LYS
1	B	336	CYS
1	B	339	ASP
1	B	375	PHE
1	B	603	ASN
1	B	605	SER
1	C	294	ASP
1	C	339	ASP
1	C	375	PHE
1	C	591	SER

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Mol	Chain	Res	Type
1	A	330	PRO
1	A	520	ALA
1	A	592	PHE
1	B	321	GLN
1	B	367	VAL
1	B	530	SER
1	B	601	GLY
1	A	531	THR
1	B	294	ASP
1	A	320	VAL
1	B	330	PRO
1	B	326	ILE
1	A	579	PRO
1	A	742	ILE
1	B	742	ILE
1	C	742	ILE

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	896/1111 (81%)	854 (95%)	42 (5%)	26	59
1	B	896/1111 (81%)	854 (95%)	42 (5%)	26	59
1	C	896/1111 (81%)	863 (96%)	33 (4%)	34	66
2	H	94/98 (96%)	94 (100%)	0	100	100
2	I	94/98 (96%)	94 (100%)	0	100	100
2	J	94/98 (96%)	94 (100%)	0	100	100
3	L	89/89 (100%)	85 (96%)	4 (4%)	27	60
3	M	89/89 (100%)	86 (97%)	3 (3%)	37	69
3	N	89/89 (100%)	86 (97%)	3 (3%)	37	69
All	All	3237/3894 (83%)	3110 (96%)	127 (4%)	36	65

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	CYS
1	A	166	CYS
1	A	316	SER
1	A	317	ASN
1	A	319	ARG
1	A	320	VAL
1	A	321	GLN
1	A	323	THR
1	A	325	SER
1	A	357	ARG
1	A	366	SER
1	A	368	LEU
1	A	369	TYR
1	A	375	PHE
1	A	386	LYS
1	A	440	LYS
1	A	478	LYS
1	A	515	PHE
1	A	517	LEU
1	A	518	LEU
1	A	528	LYS
1	A	529	LYS
1	A	561	PRO
1	A	564	GLN
1	A	567	ARG
1	A	577	ARG
1	A	580	GLN
1	A	582	LEU
1	A	591	SER
1	A	592	PHE
1	A	613	GLN
1	A	662	CYS
1	A	673	SER
1	A	674	TYR
1	A	675	GLN
1	A	691	SER
1	A	693	ILE
1	A	697	MET
1	A	698	SER
1	A	854	LYS
1	A	856	ASN
1	A	1074	ASN
1	B	131	CYS

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Mol	Chain	Res	Type
1	B	166	CYS
1	B	310	LYS
1	B	316	SER
1	B	318	PHE
1	B	319	ARG
1	B	320	VAL
1	B	324	GLU
1	B	328	ARG
1	B	332	ILE
1	B	334	ASN
1	B	336	CYS
1	B	361	CYS
1	B	364	ASP
1	B	366	SER
1	B	368	LEU
1	B	369	TYR
1	B	375	PHE
1	B	440	LYS
1	B	478	LYS
1	B	517	LEU
1	B	528	LYS
1	B	529	LYS
1	B	532	ASN
1	B	533	LEU
1	B	561	PRO
1	B	577	ARG
1	B	590	CYS
1	B	606	ASN
1	B	607	GLN
1	B	613	GLN
1	B	662	CYS
1	B	674	TYR
1	B	675	GLN
1	B	690	GLN
1	B	854	LYS
1	B	856	ASN
1	B	858	LEU
1	B	973	ILE
1	B	985	ASP
1	B	988	GLU
1	B	1074	ASN
1	C	131	CYS

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Mol	Chain	Res	Type
1	C	166	CYS
1	C	321	GLN
1	C	323	THR
1	C	324	GLU
1	C	328	ARG
1	C	357	ARG
1	C	366	SER
1	C	368	LEU
1	C	369	TYR
1	C	375	PHE
1	C	440	LYS
1	C	478	LYS
1	C	517	LEU
1	C	529	LYS
1	C	533	LEU
1	C	561	PRO
1	C	577	ARG
1	C	588	THR
1	C	591	SER
1	C	613	GLN
1	C	645	THR
1	C	646	ARG
1	C	662	CYS
1	C	674	TYR
1	C	676	THR
1	C	690	GLN
1	C	692	ILE
1	C	693	ILE
1	C	696	THR
1	C	697	MET
1	C	698	SER
1	C	1074	ASN
3	L	16	GLN
3	L	20	ILE
3	L	22	CYS
3	L	33	TYR
3	M	20	ILE
3	M	22	CYS
3	M	33	TYR
3	N	20	ILE
3	N	22	CYS
3	N	33	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	173	GLN
1	A	314	GLN
1	A	317	ASN
1	A	321	GLN
1	A	360	ASN
1	A	414	GLN
1	A	422	ASN
1	A	450	ASN
1	A	519	HIS
1	A	607	GLN
1	A	690	GLN
1	A	965	GLN
1	B	164	ASN
1	B	173	GLN
1	B	334	ASN
1	B	414	GLN
1	B	422	ASN
1	B	450	ASN
1	B	606	ASN
1	B	607	GLN
1	B	675	GLN
1	B	690	GLN
1	B	913	GLN
1	B	965	GLN
1	C	164	ASN
1	C	173	GLN
1	C	414	GLN
1	C	422	ASN
1	C	450	ASN
1	C	607	GLN
1	C	913	GLN
1	C	914	ASN
1	C	965	GLN

5.3.3 RNA

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)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	1	4,1	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	E	1	4,1	14,14,15	0.18	0	17,19,21	0.81	1 (5%)
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	F	1	4,1	14,14,15	0.34	0	17,19,21	1.14	1 (5%)
4	NAG	F	2	4	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	G	1	4,1	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	K	1	4,1	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	K	2	4	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	O	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	P	1	4,1	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	P	2	4	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	Q	1	4,1	14,14,15	0.17	0	17,19,21	0.81	1 (5%)
4	NAG	Q	2	4	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	R	1	4,1	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
4	NAG	R	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	S	1	4,1	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
4	NAG	S	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	T	1	4,1	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.33	0	17,19,21	0.71	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	V	1	4,1	14,14,15	0.33	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	V	2	4	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	W	1	4,1	14,14,15	0.16	0	17,19,21	0.82	1 (5%)
4	NAG	W	2	4	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	X	1	4,1	14,14,15	0.35	0	17,19,21	1.14	1 (5%)
4	NAG	X	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	Y	1	4,1	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
4	NAG	Y	2	4	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	Z	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	Z	2	4	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	a	2	4	14,14,15	0.29	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	1	NAG	O5-C1	-2.77	1.39	1.43
4	T	1	NAG	O5-C1	-2.72	1.39	1.43
4	K	1	NAG	O5-C1	-2.67	1.39	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	1	NAG	C1-O5-C5	3.34	116.72	112.19
4	X	1	NAG	C1-O5-C5	3.33	116.71	112.19
4	F	1	NAG	C1-O5-C5	3.32	116.69	112.19
4	W	1	NAG	C1-O5-C5	2.77	115.95	112.19
4	Q	1	NAG	C1-O5-C5	2.76	115.93	112.19
4	E	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	K	1	NAG	O4-C4-C3	-2.38	104.84	110.35
4	Z	1	NAG	O4-C4-C3	-2.37	104.86	110.35
4	T	1	NAG	O4-C4-C3	-2.37	104.87	110.35
4	S	1	NAG	C1-O5-C5	2.26	115.26	112.19
4	G	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	Y	1	NAG	C1-O5-C5	2.20	115.17	112.19
4	K	2	NAG	C1-O5-C5	2.13	115.07	112.19
4	T	2	NAG	C1-O5-C5	2.11	115.05	112.19
4	Z	2	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6

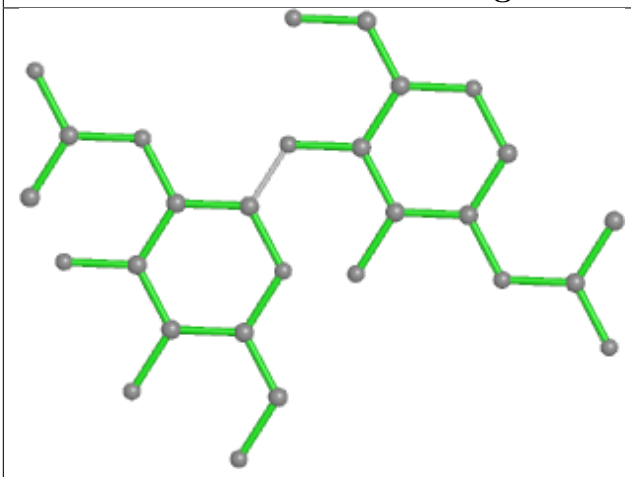
There are no ring outliers.

10 monomers are involved in 16 short contacts:

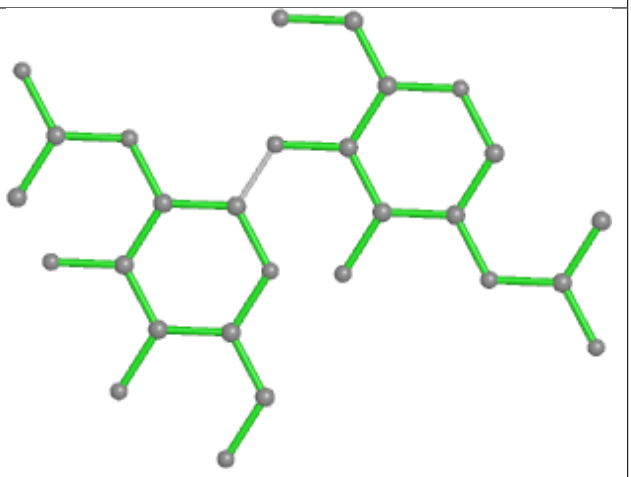
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0
4	K	2	NAG	1	0
4	K	1	NAG	1	0
4	Z	1	NAG	1	0
4	Z	2	NAG	1	0
4	Q	1	NAG	2	0
4	W	1	NAG	2	0
4	T	1	NAG	1	0
4	T	2	NAG	1	0
4	V	1	NAG	7	0

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

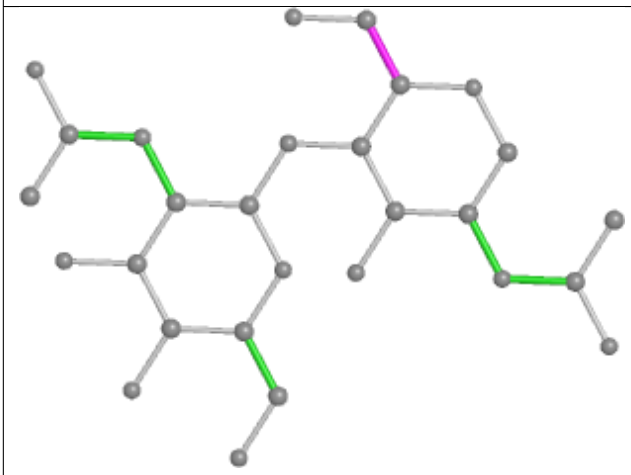
Oligosaccharide Chain D



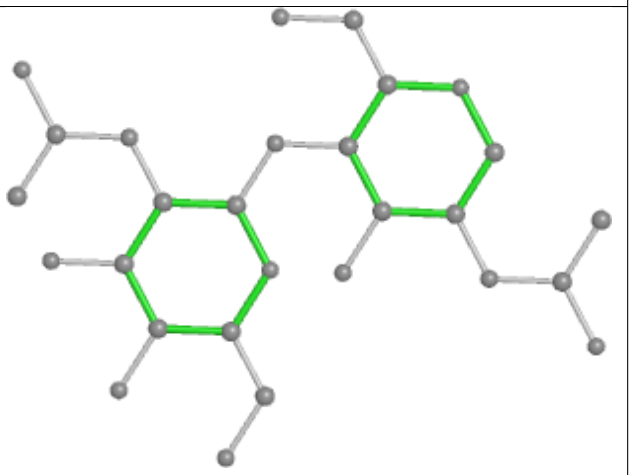
Bond lengths



Bond angles

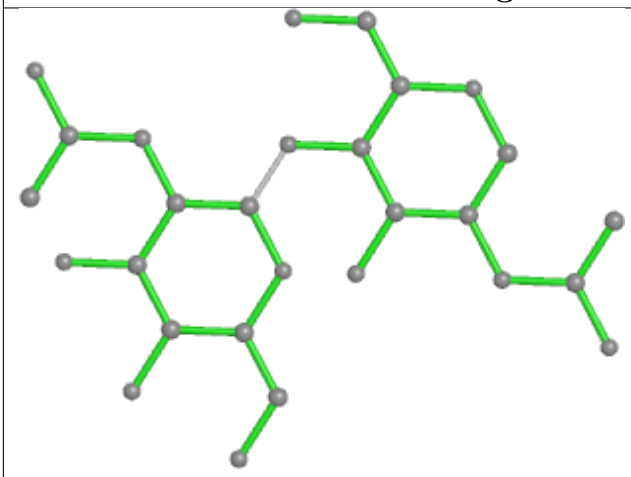


Torsions

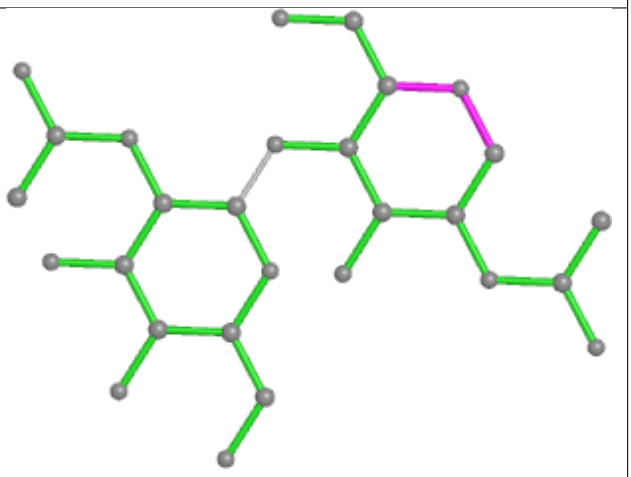


Rings

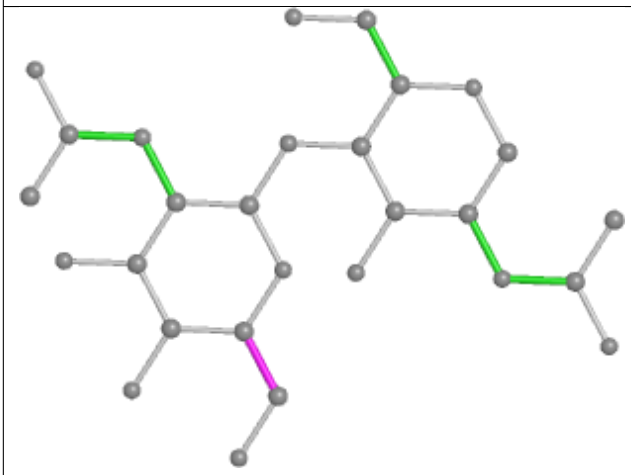
Oligosaccharide Chain E



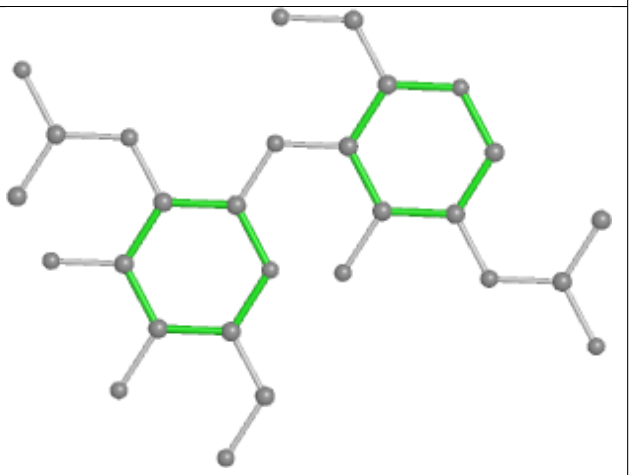
Bond lengths



Bond angles

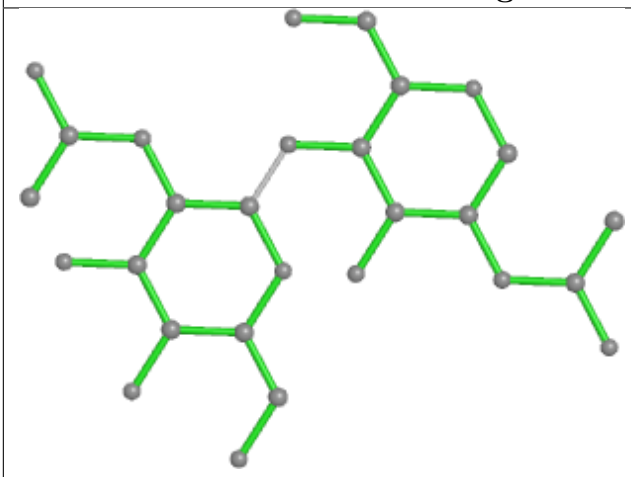


Torsions

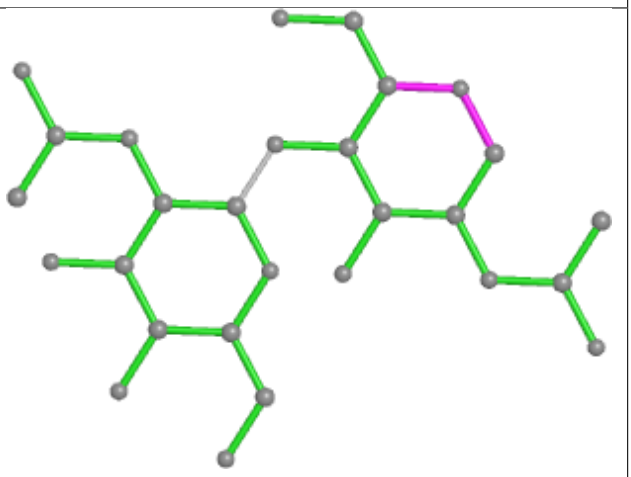


Rings

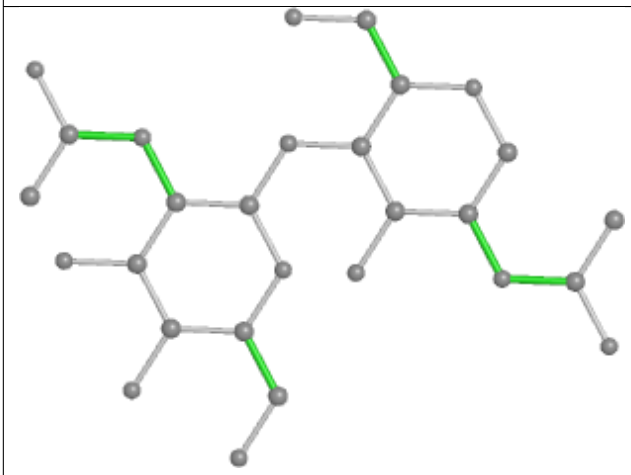
Oligosaccharide Chain F



Bond lengths



Bond angles



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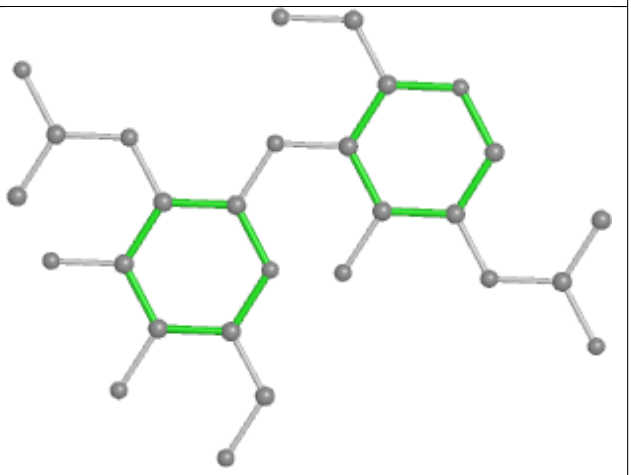
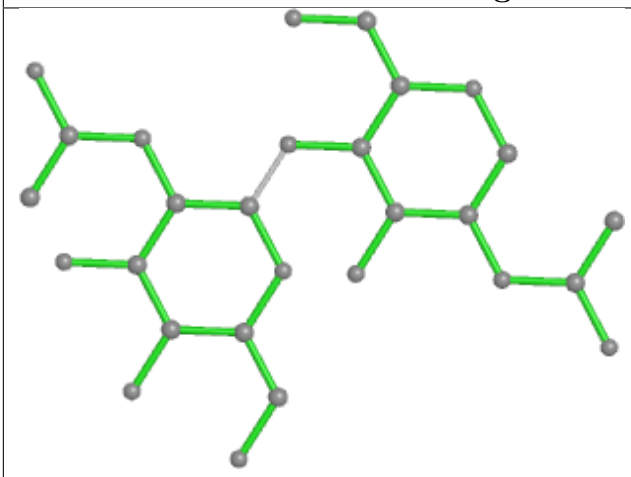


Rings

Oligosaccharide Chain G



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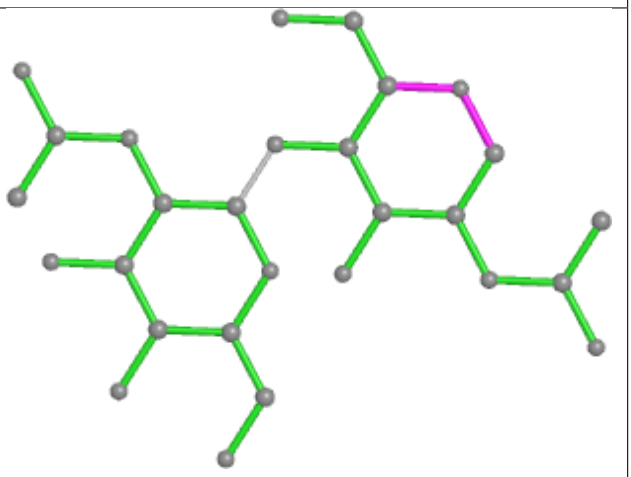
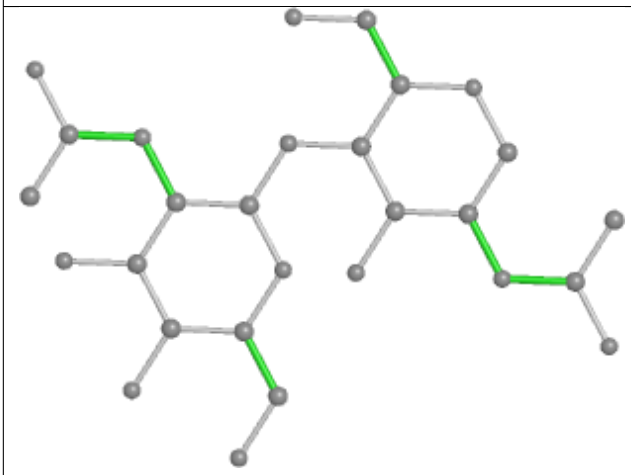


Bond angles



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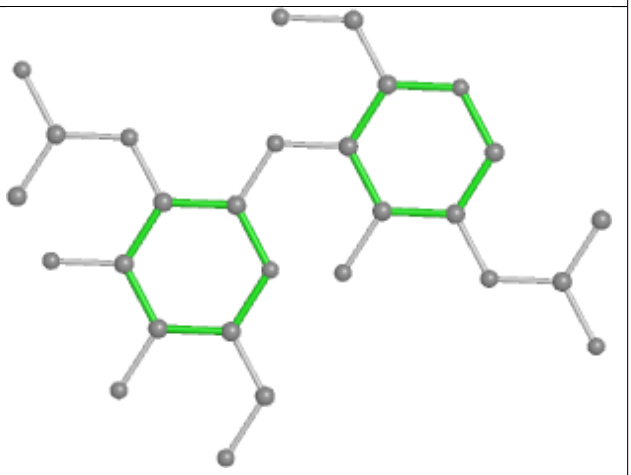
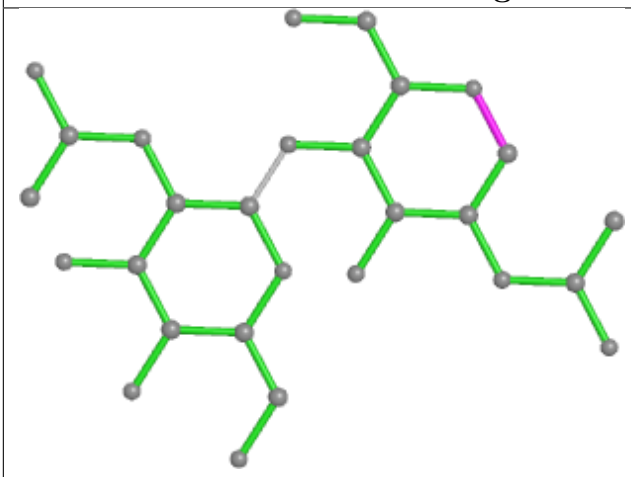


Rings

Oligosaccharide Chain K



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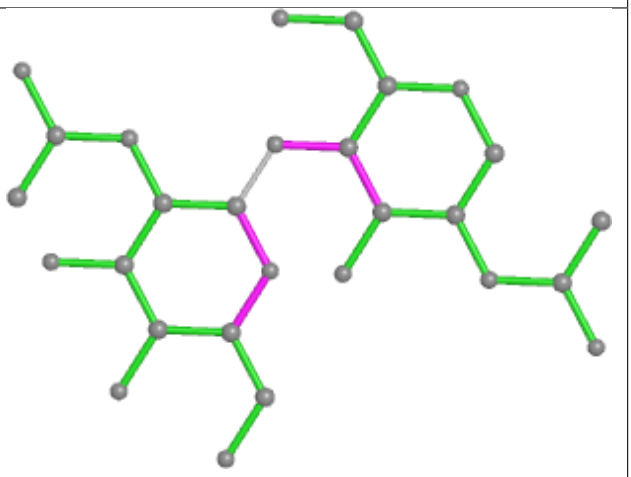
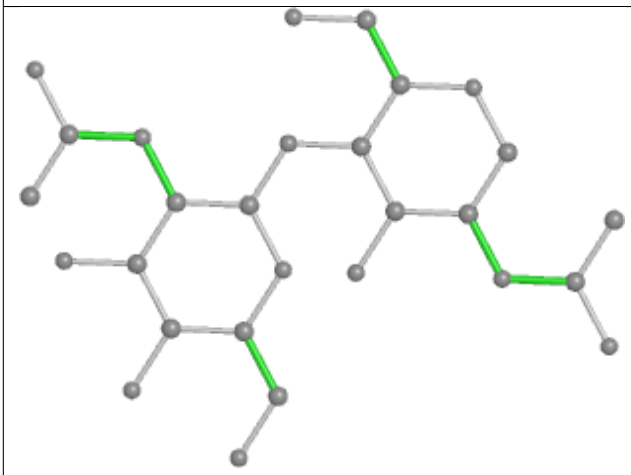


Bond angles



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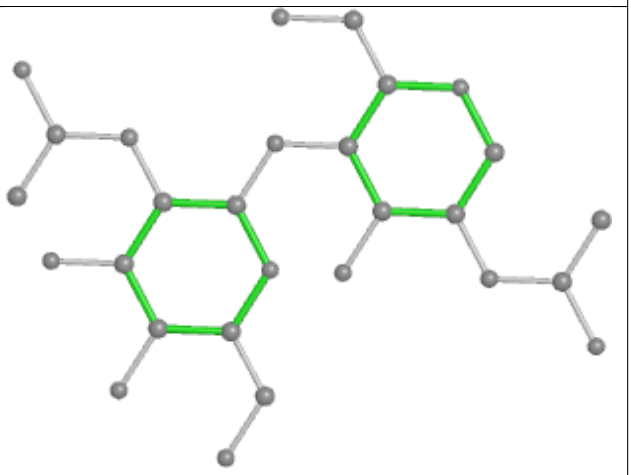
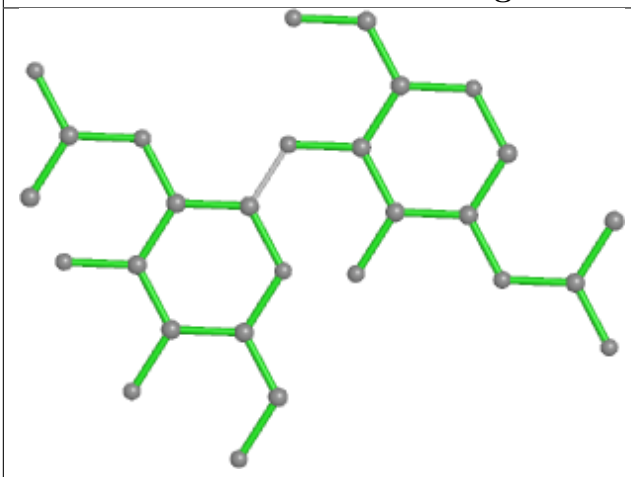


Rings

Oligosaccharide Chain O



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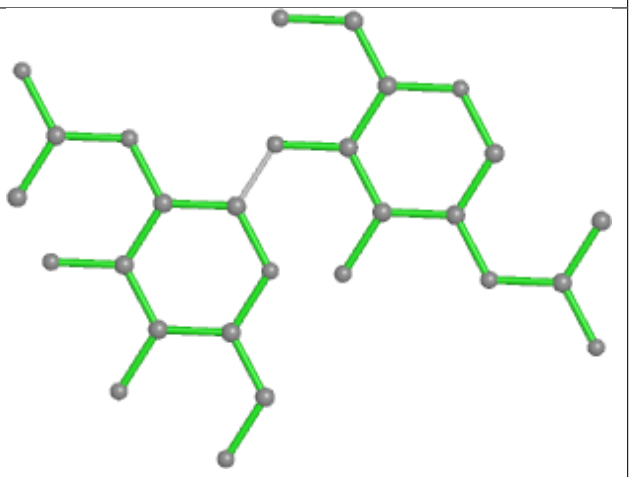
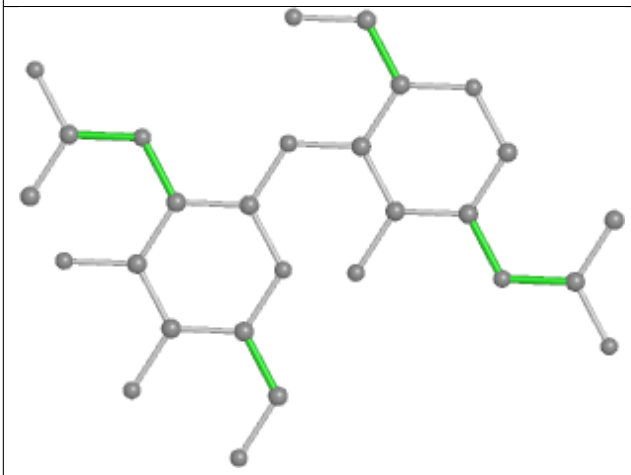


Bond angles



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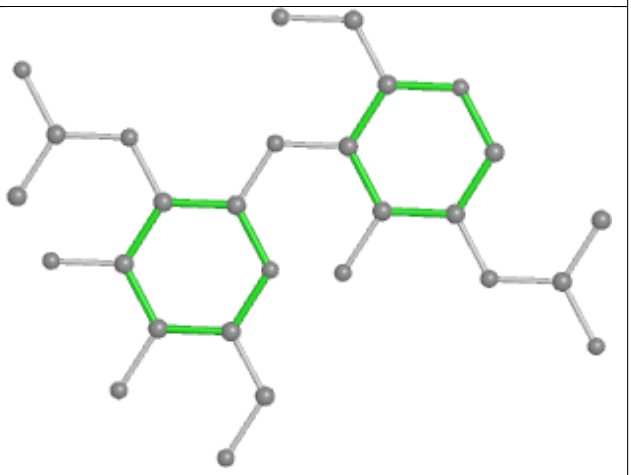
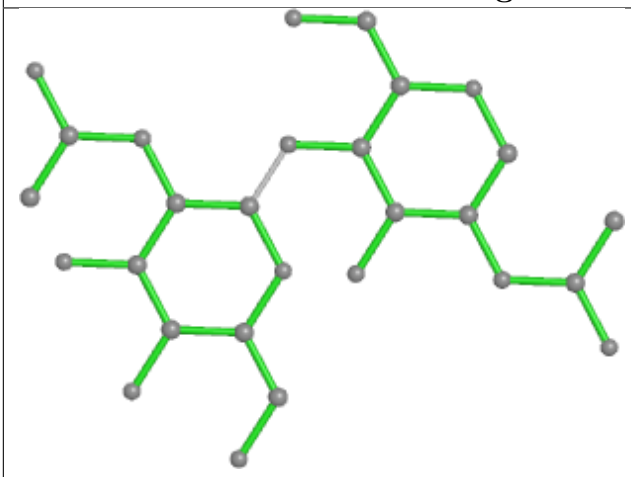


Rings

Oligosaccharide Chain P



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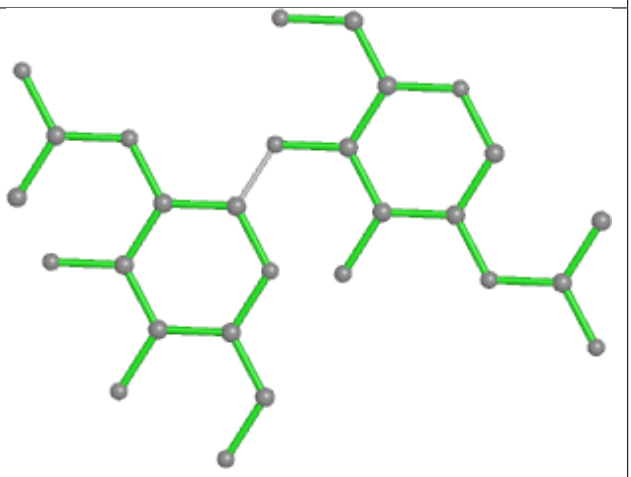

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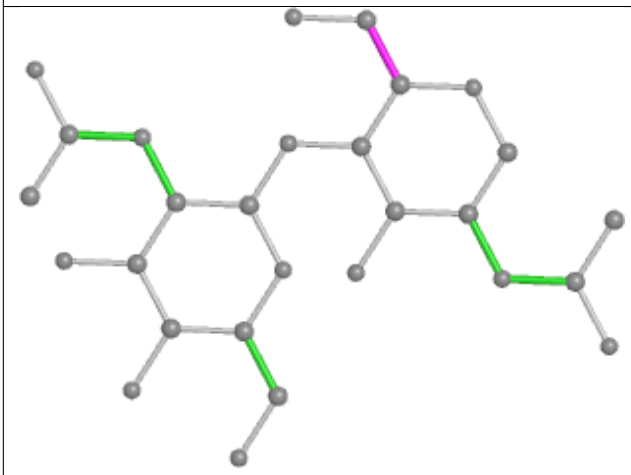

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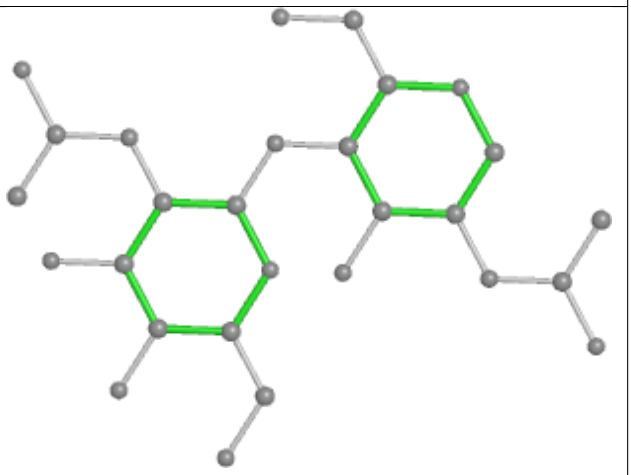
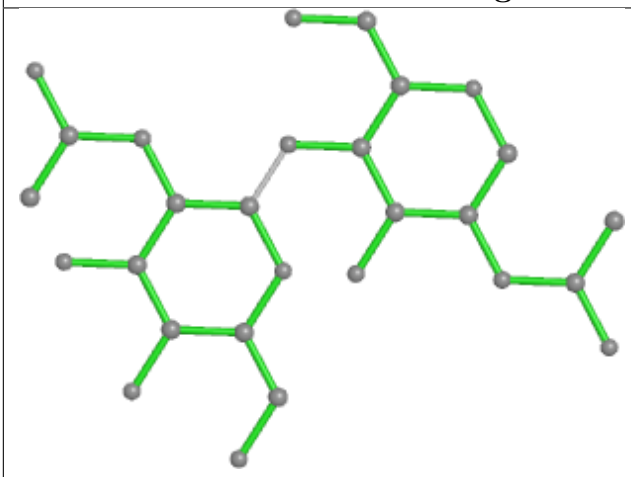


Rings

Oligosaccharide Chain Q



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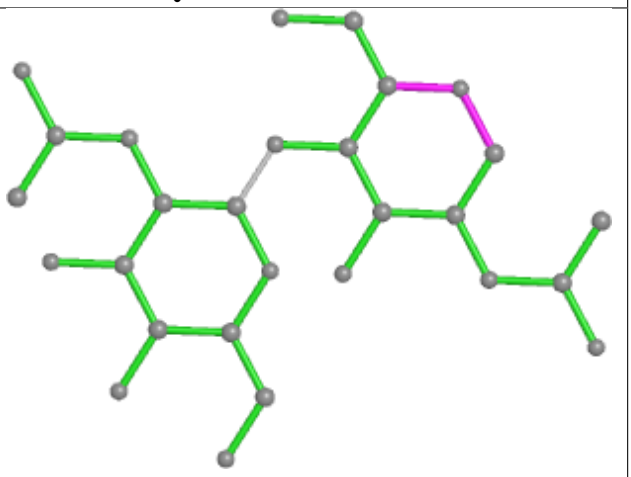
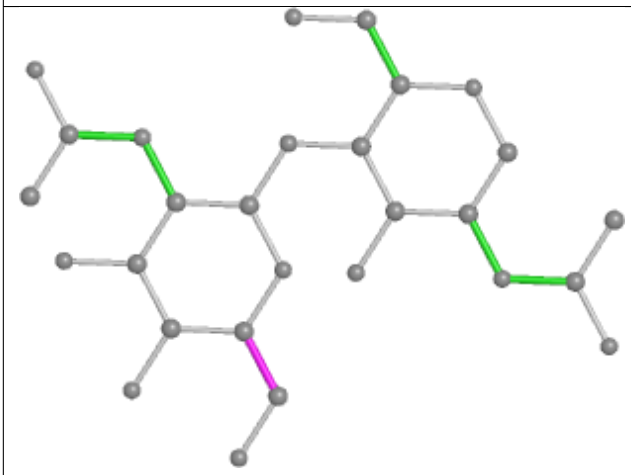


Bond angles



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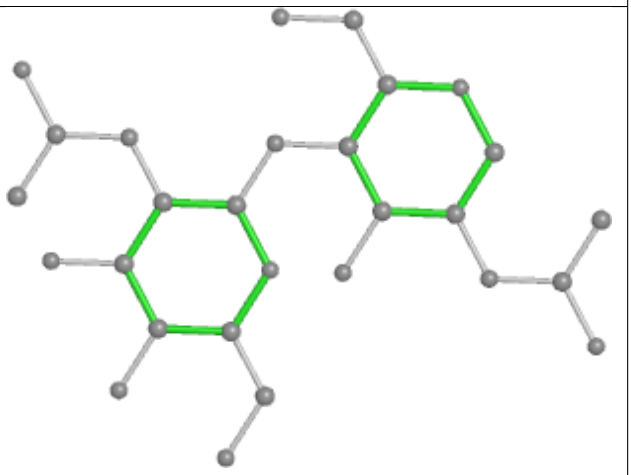
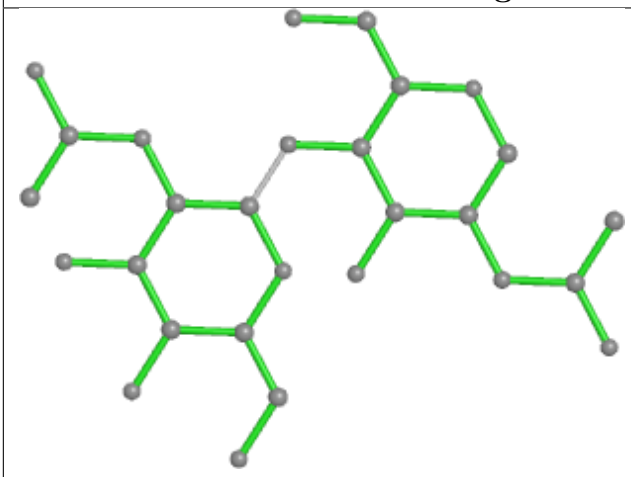


Rings

Oligosaccharide Chain R



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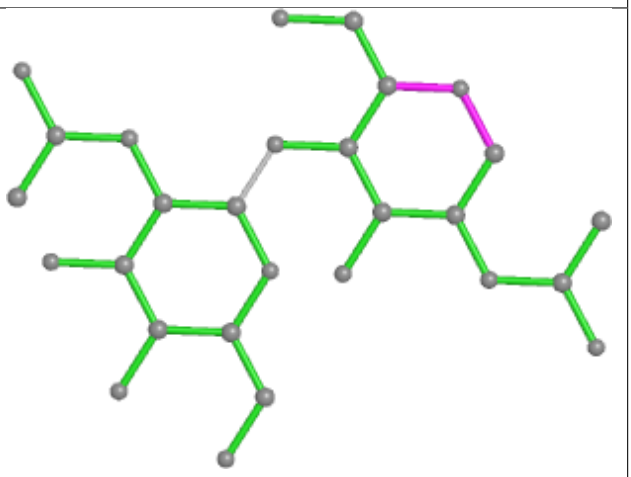
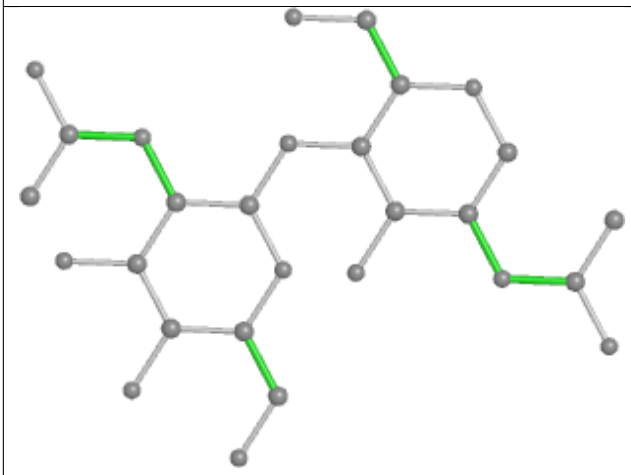


Bond angles



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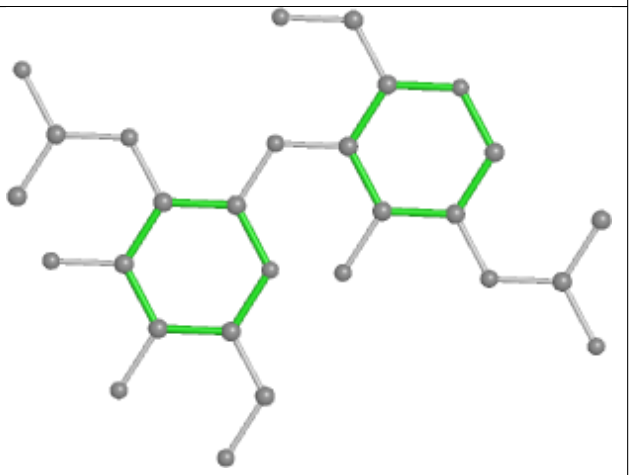
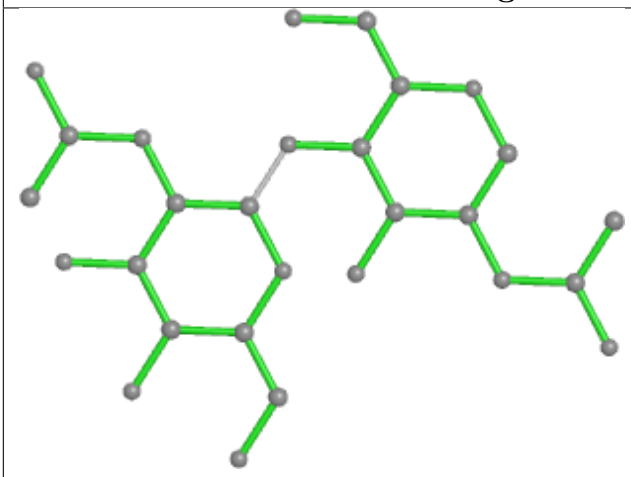


Rings

Oligosaccharide Chain S



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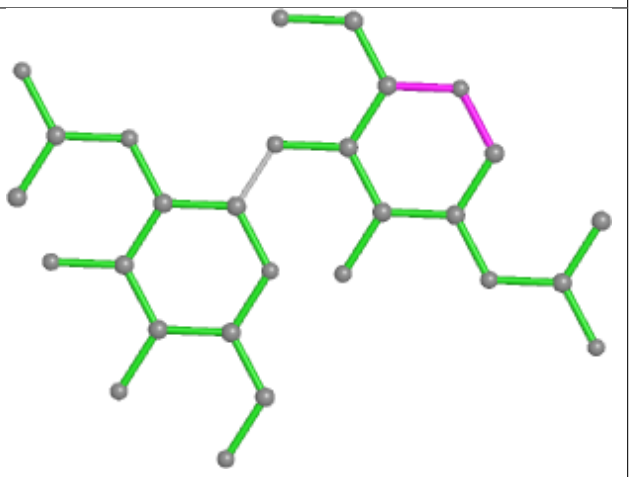
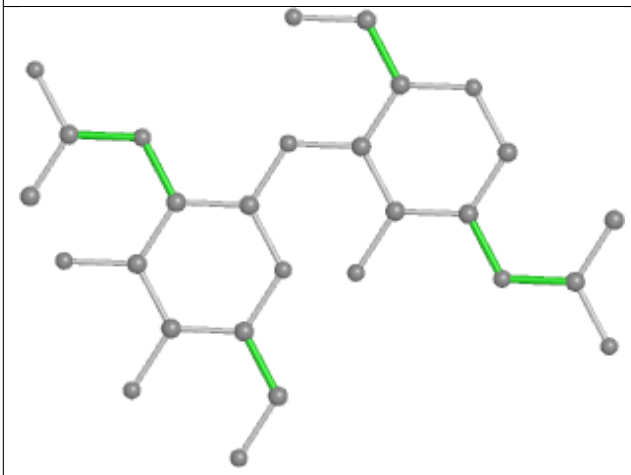


Bond angles



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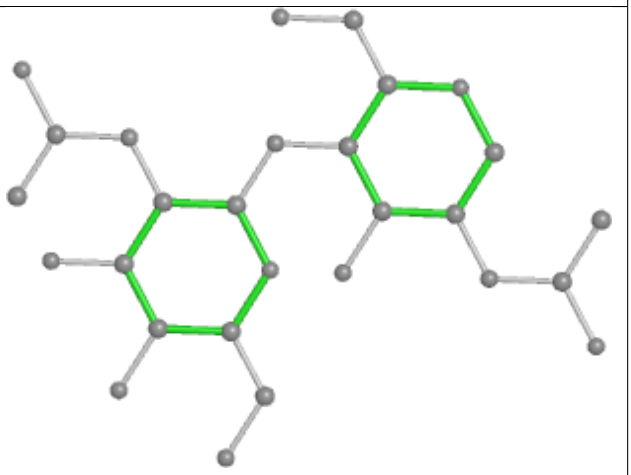
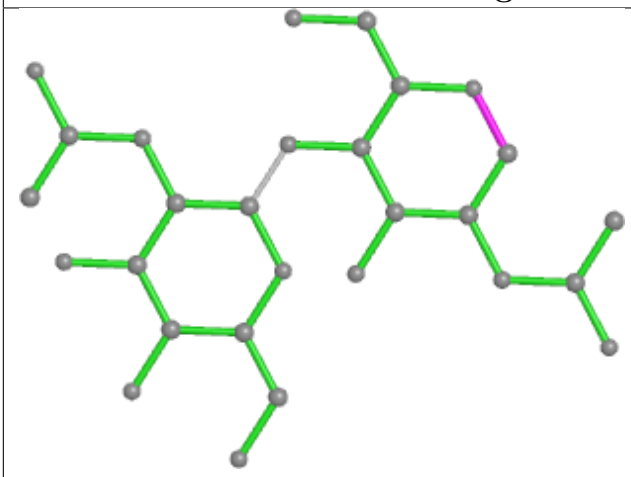


Rings

Oligosaccharide Chain T



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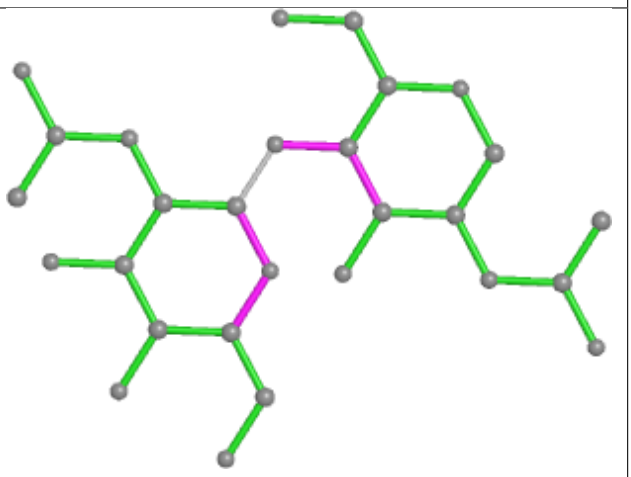

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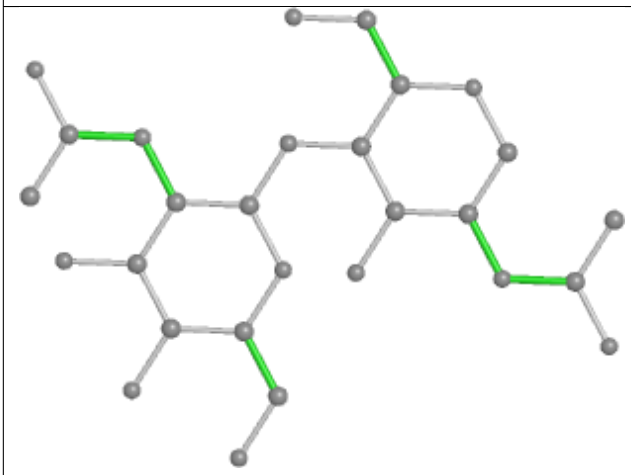

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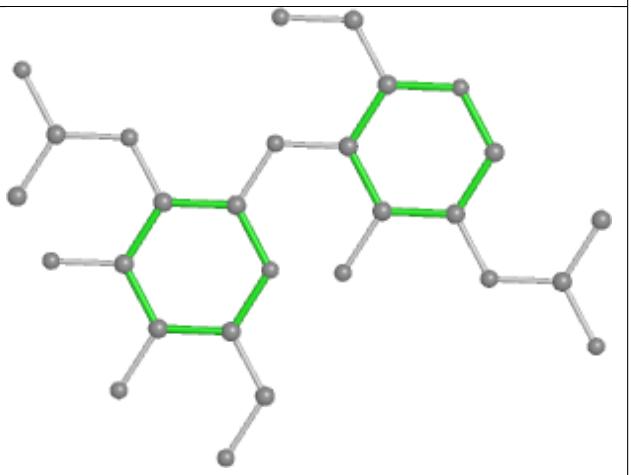
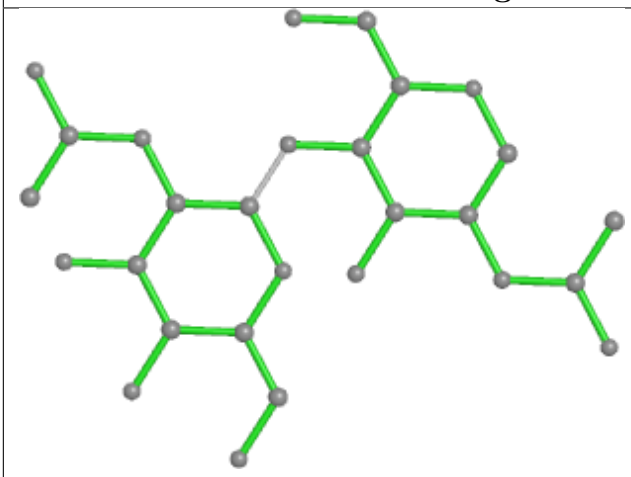


Rings

Oligosaccharide Chain U



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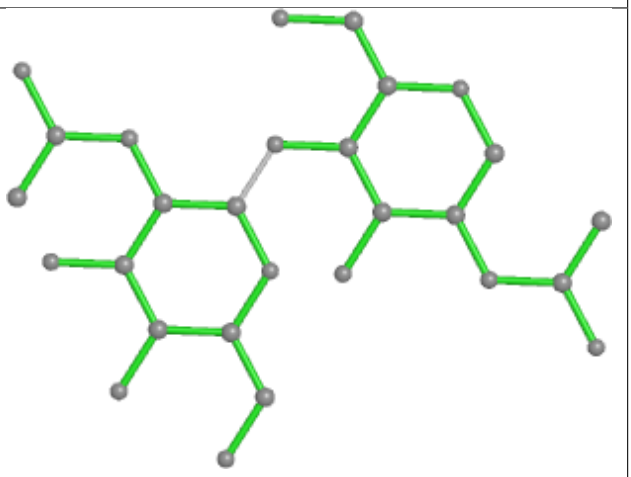

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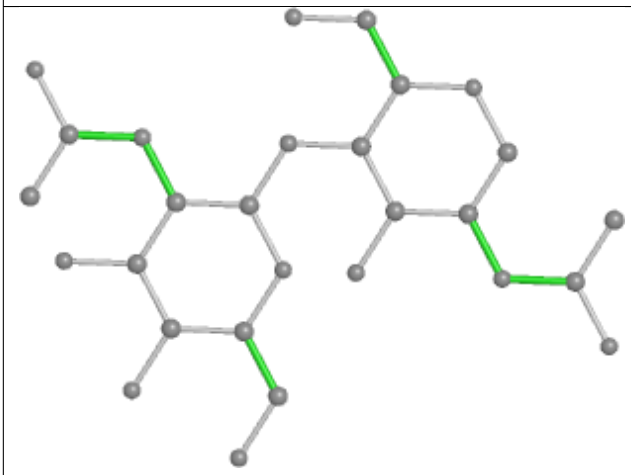

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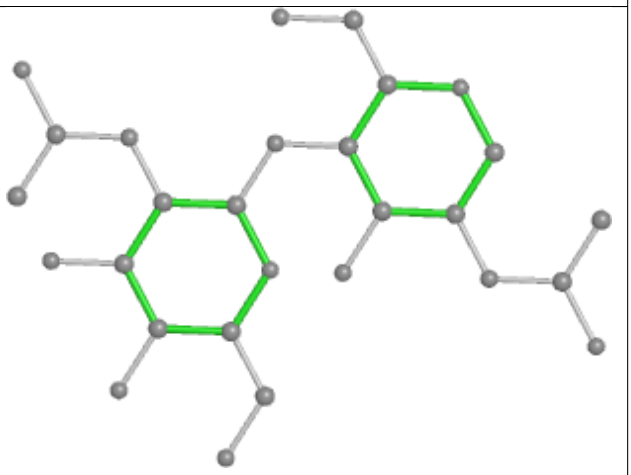
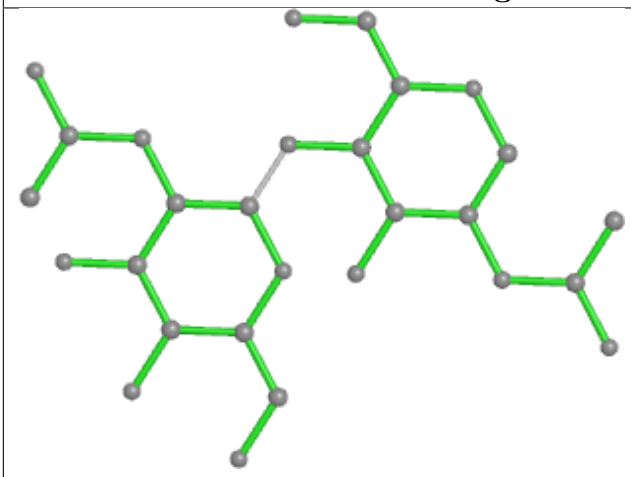


Rings

Oligosaccharide Chain V



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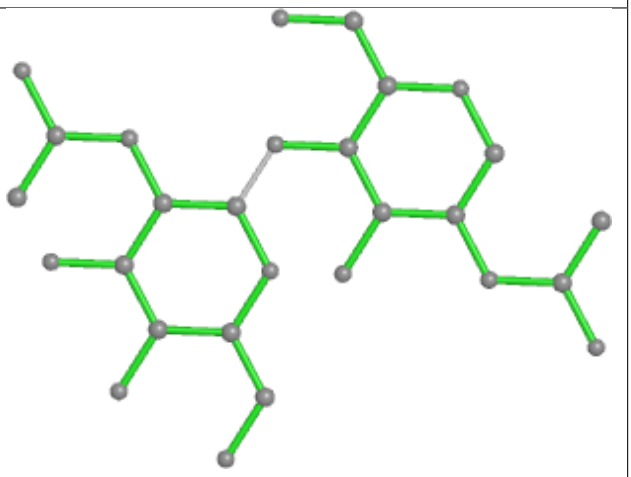
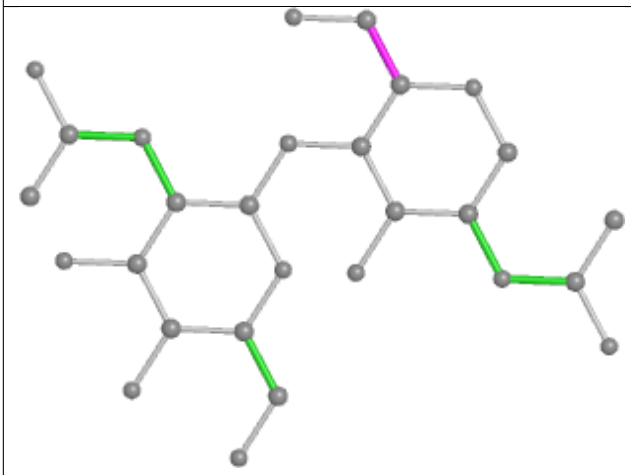


Bond angles



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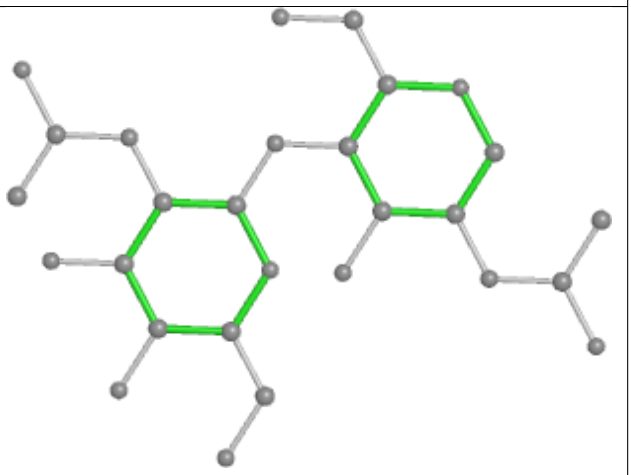
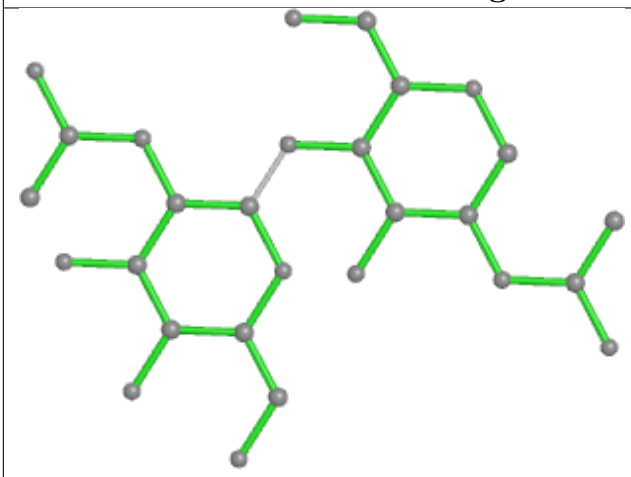


Rings

Oligosaccharide Chain W



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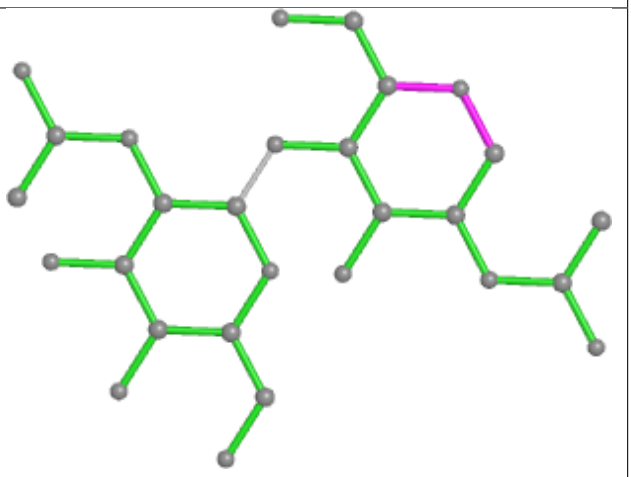
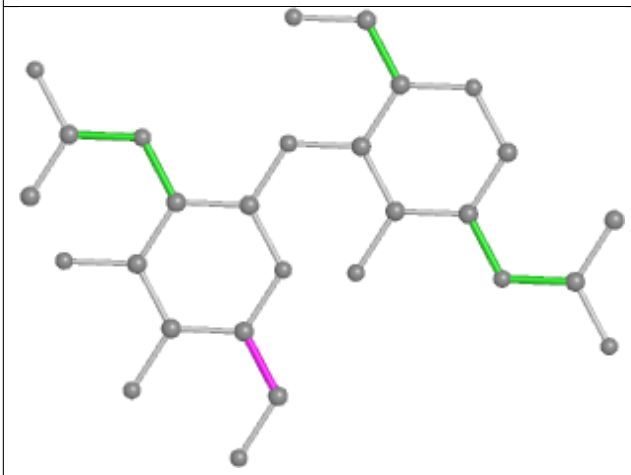


Bond angles



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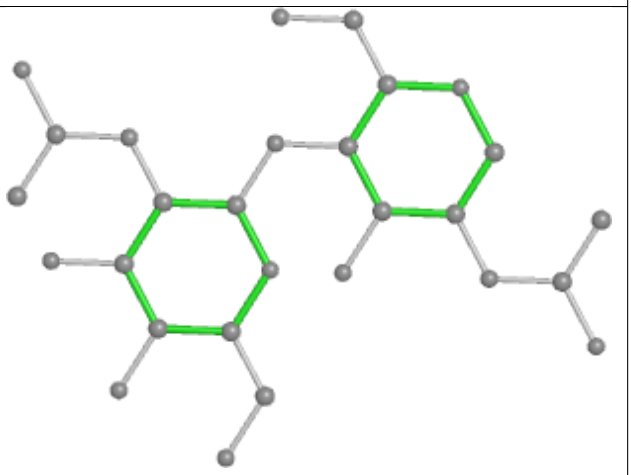
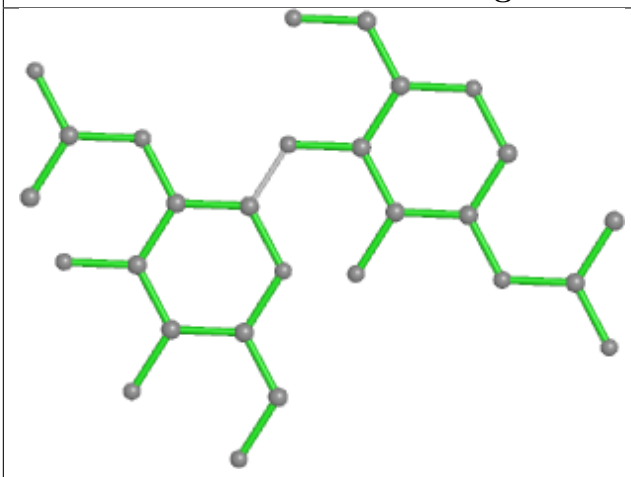
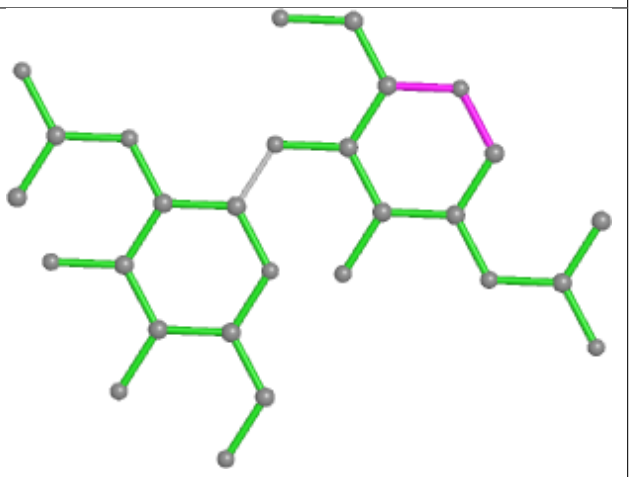


Rings

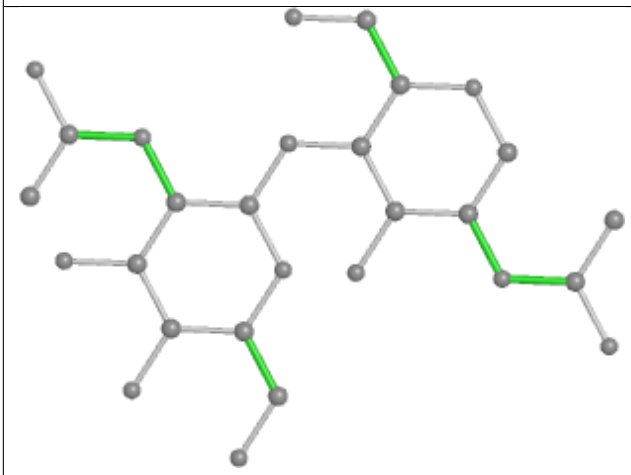
Oligosaccharide Chain X



Bond lengths



Bond angles



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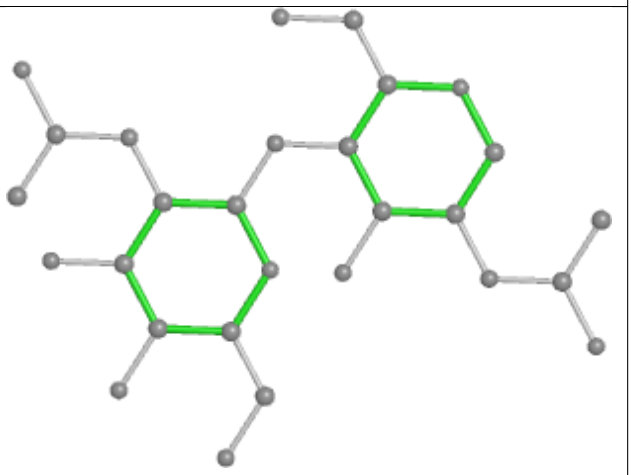
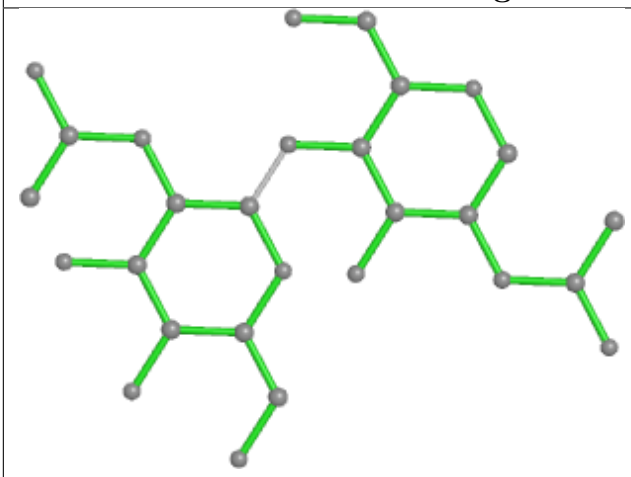
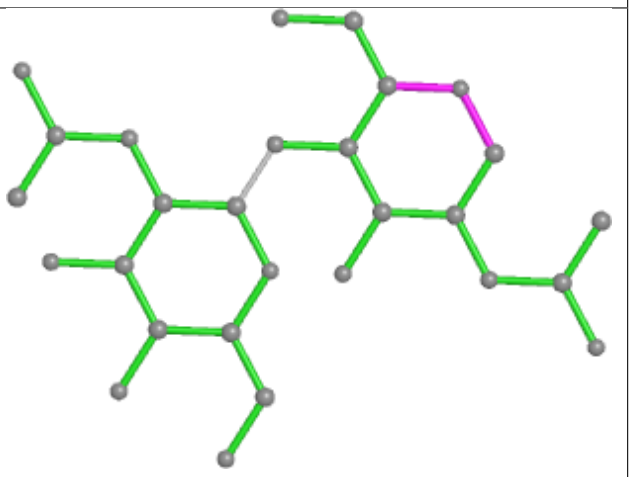


Rings

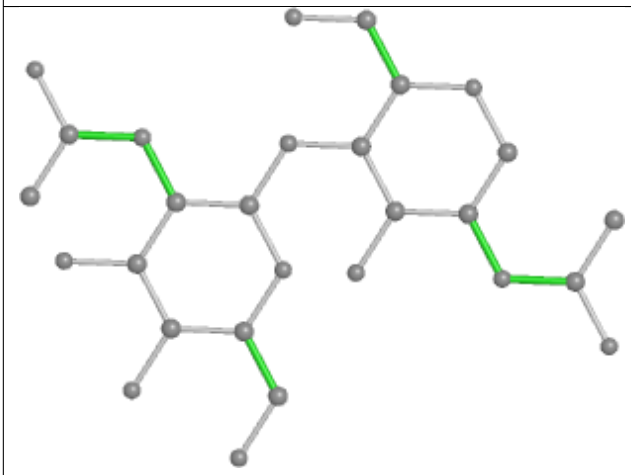
Oligosaccharide Chain Y



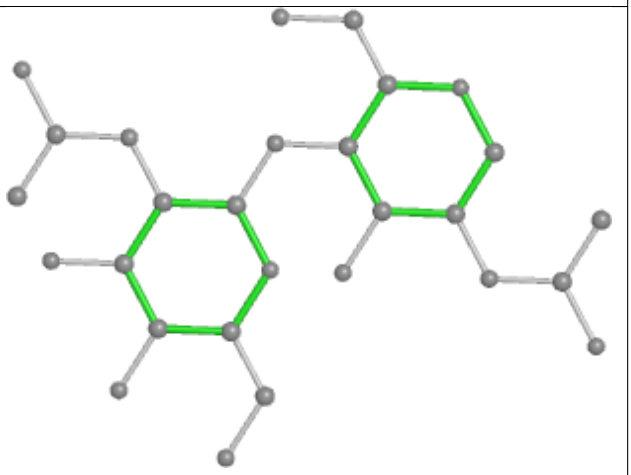
Bond lengths



Bond angles

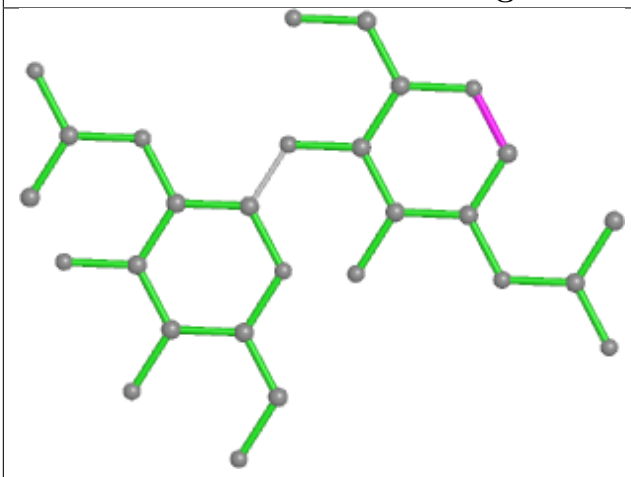


Torsions

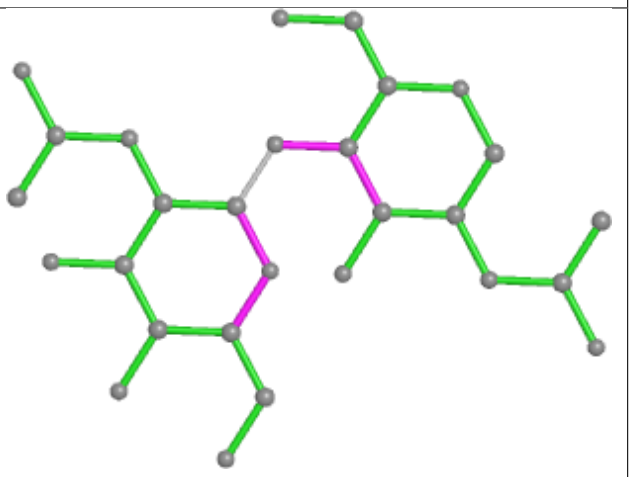


Rings

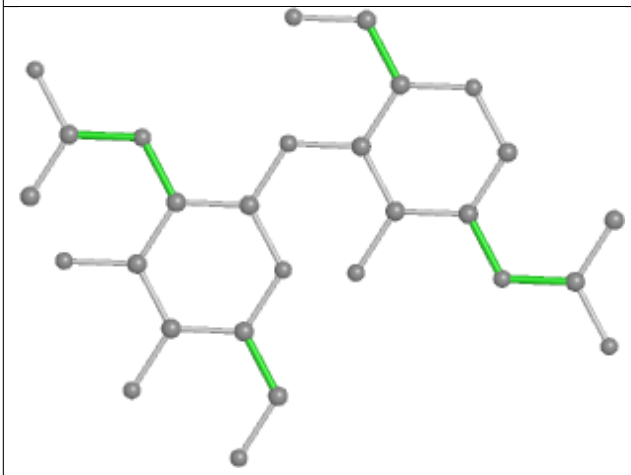
Oligosaccharide Chain Z



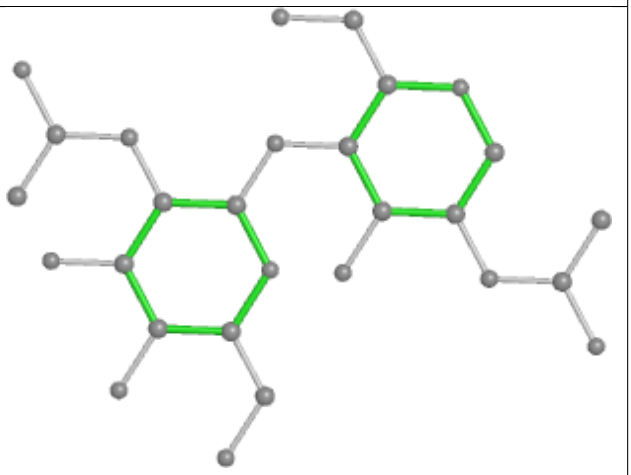
Bond lengths



Bond angles

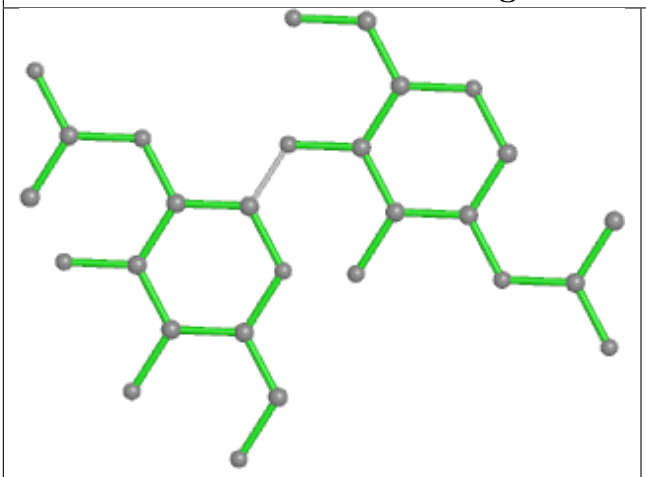


Torsions

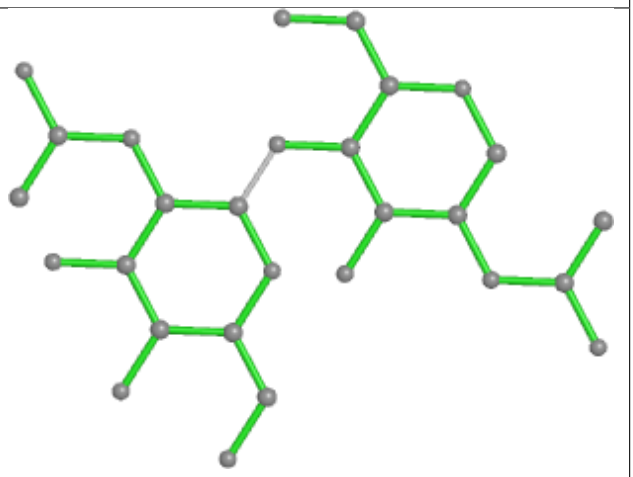


Rings

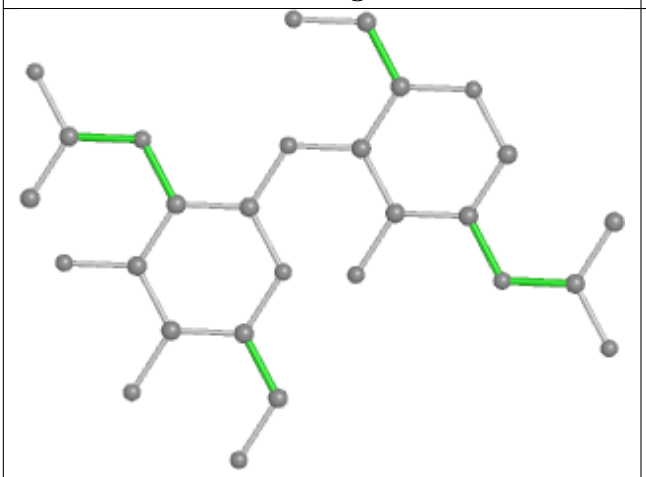
Oligosaccharide Chain a



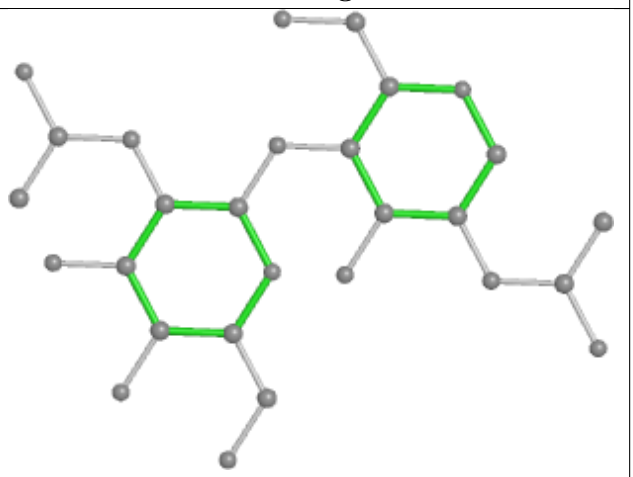
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	1401	1	14,14,15	0.25	0	17,19,21	0.54	0
5	NAG	C	1403	1	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	A	1409	1	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	A	1411	-	14,14,15	0.35	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	1404	1	14,14,15	0.23	0	17,19,21	0.58	0
5	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.50	0
5	NAG	B	1404	1	14,14,15	0.25	0	17,19,21	0.58	0
5	NAG	C	1410	1	14,14,15	0.42	0	17,19,21	1.14	2 (11%)
5	NAG	B	1401	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
5	NAG	C	1407	1	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	C	1406	1	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	B	1403	1	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.65	1 (5%)
5	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	A	1404	1	14,14,15	0.24	0	17,19,21	0.58	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.39	0
5	NAG	A	1410	1	14,14,15	0.42	0	17,19,21	1.14	2 (11%)
5	NAG	B	1409	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	B	1411	-	14,14,15	0.36	0	17,19,21	0.41	0
5	NAG	C	1411	-	14,14,15	0.36	0	17,19,21	0.41	0
5	NAG	A	1405	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	B	1410	1	14,14,15	0.41	0	17,19,21	1.14	2 (11%)
5	NAG	C	1409	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	B	1408	1	14,14,15	0.32	0	17,19,21	0.39	0
5	NAG	C	1408	1	14,14,15	0.32	0	17,19,21	0.40	0
5	NAG	A	1401	1	14,14,15	0.25	0	17,19,21	0.54	0
5	NAG	C	1405	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.65	1 (5%)
5	NAG	B	1405	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	A	1403	1	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	B	1406	1	14,14,15	0.27	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1402	NAG	C1-O5-C5	2.36	115.39	112.19
5	B	1402	NAG	C1-O5-C5	2.36	115.39	112.19
5	C	1402	NAG	C1-O5-C5	2.33	115.35	112.19
5	B	1410	NAG	C8-C7-N2	2.22	119.87	116.10
5	C	1410	NAG	C8-C7-N2	2.22	119.86	116.10
5	A	1410	NAG	C8-C7-N2	2.20	119.82	116.10
5	C	1410	NAG	C2-N2-C7	-2.08	119.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1410	NAG	C2-N2-C7	-2.07	119.96	122.90
5	B	1410	NAG	C2-N2-C7	-2.06	119.97	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1411	NAG	3	0
5	B	1404	NAG	2	0
5	C	1410	NAG	6	0
5	C	1402	NAG	1	0
5	B	1402	NAG	1	0

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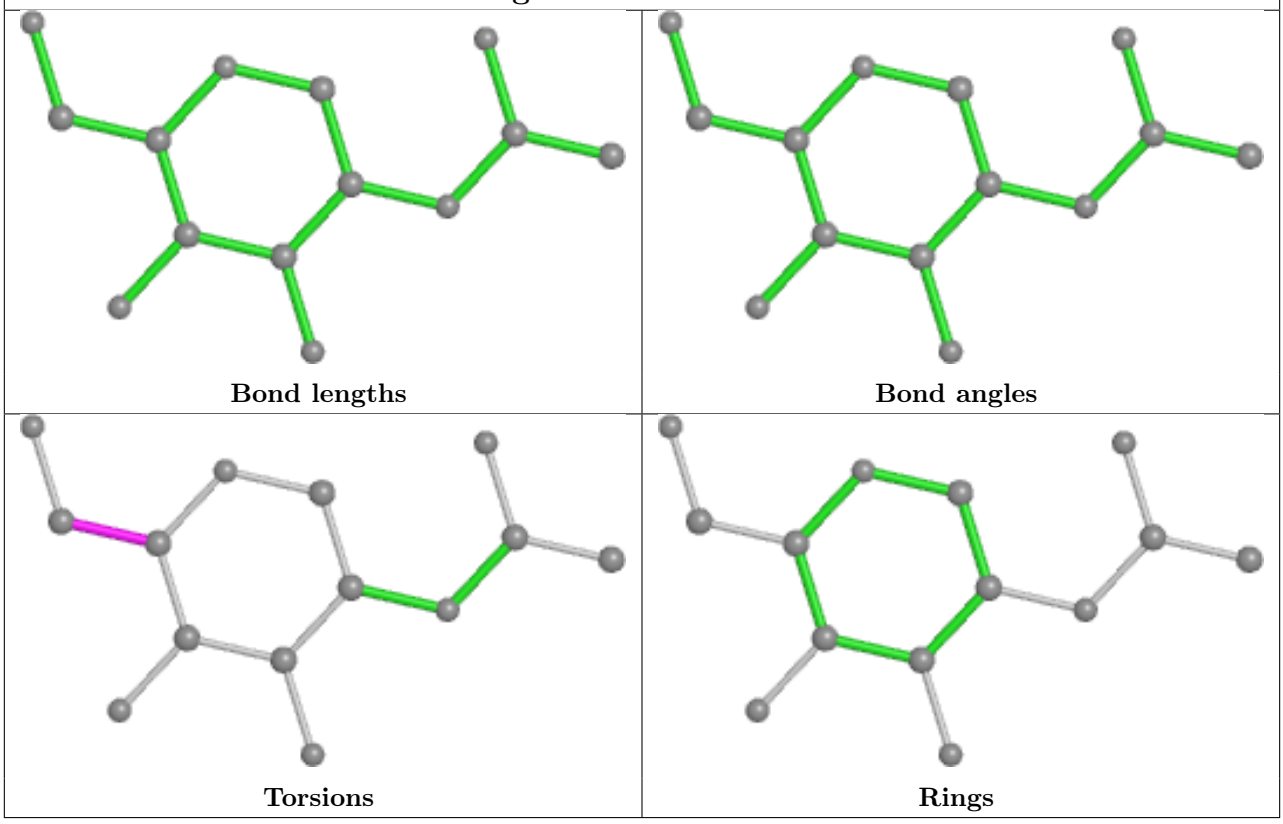
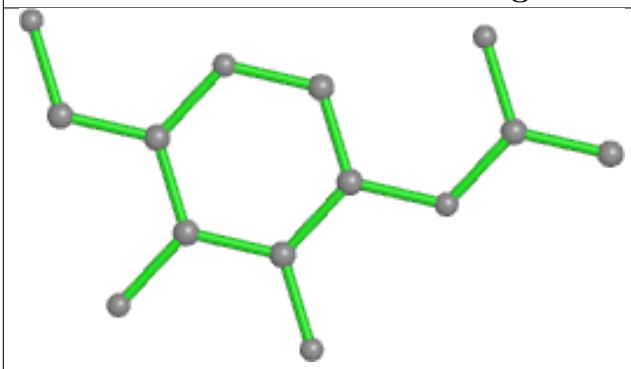
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1406	NAG	1	0
5	A	1410	NAG	5	0
5	B	1411	NAG	4	0
5	C	1411	NAG	4	0
5	B	1410	NAG	6	0
5	A	1402	NAG	1	0

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.

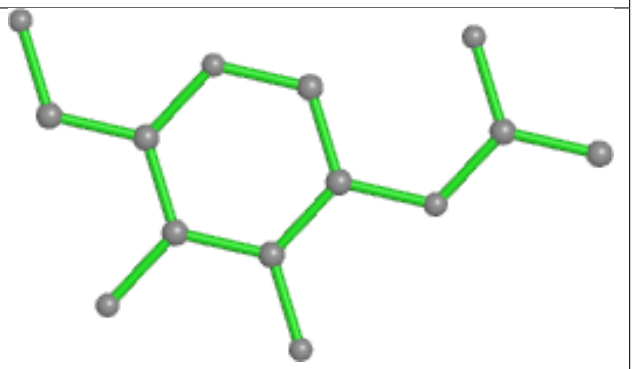
Ligand NAG C 1401



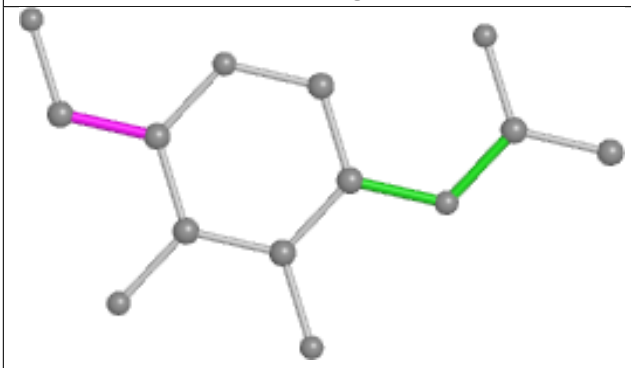
Ligand NAG C 1403



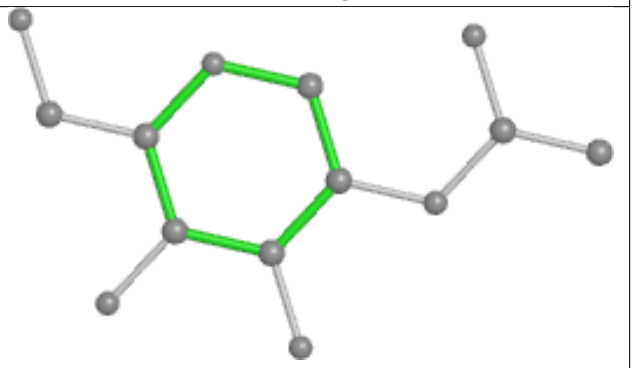
Bond lengths



Bond angles

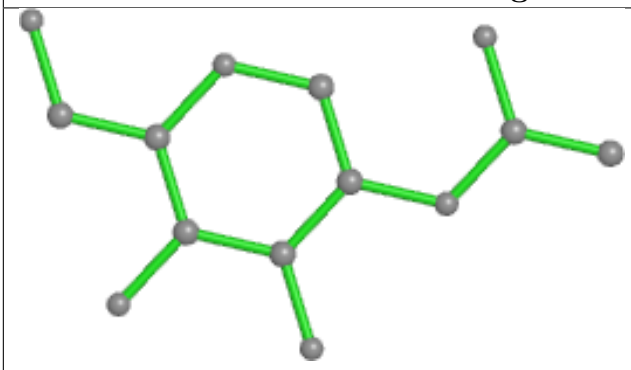


Torsions

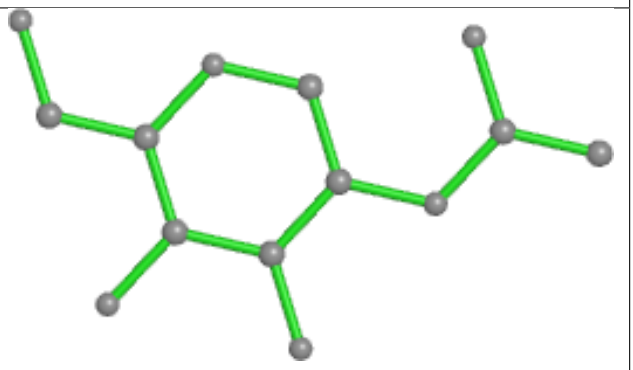


Rings

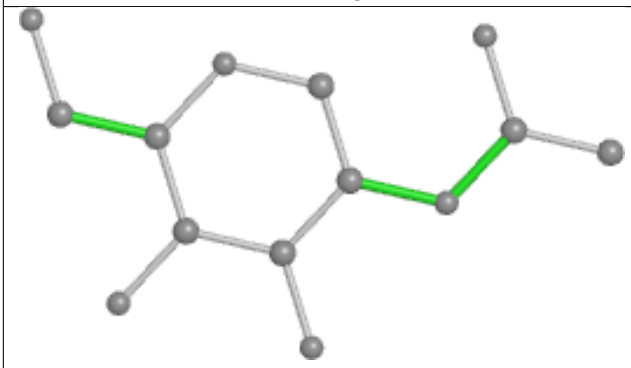
Ligand NAG A 1409



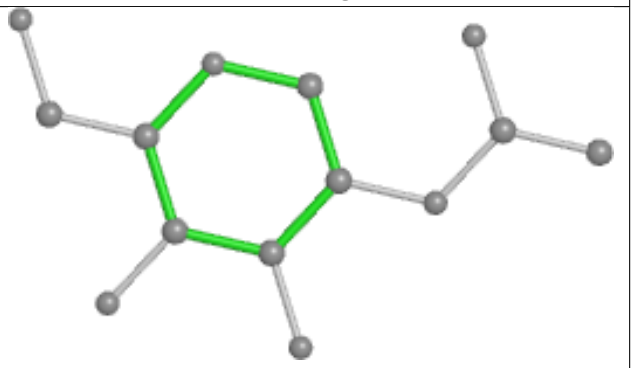
Bond lengths



Bond angles

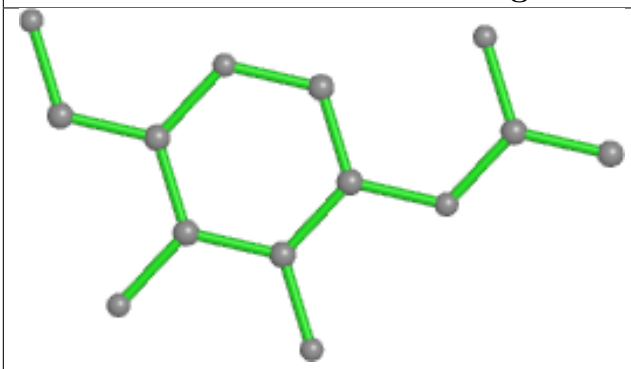


Torsions

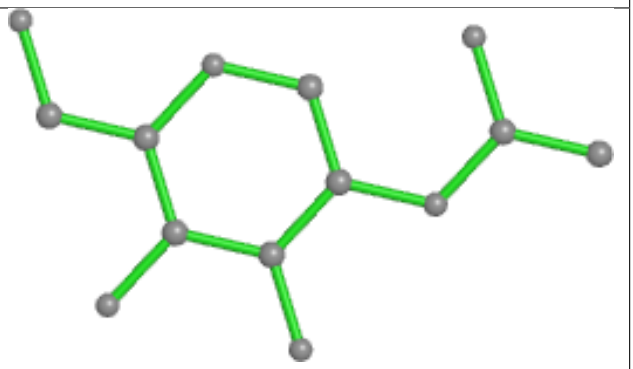


Rings

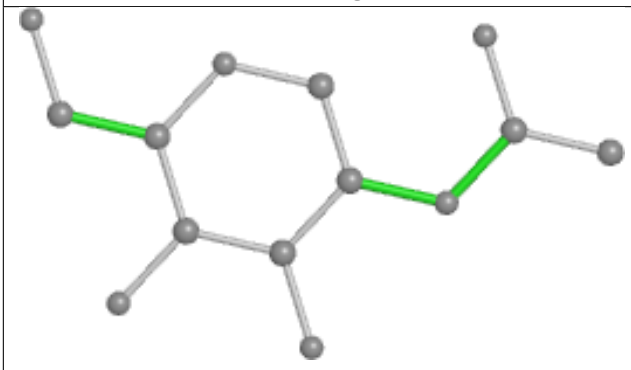
Ligand NAG A 1411



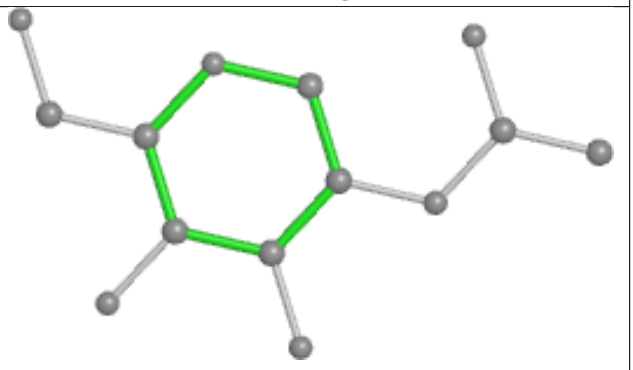
Bond lengths



Bond angles

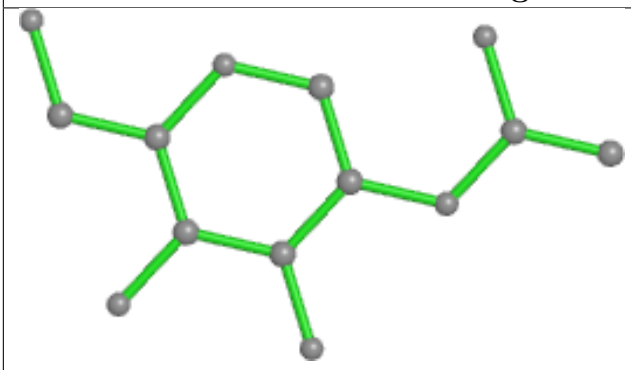


Torsions

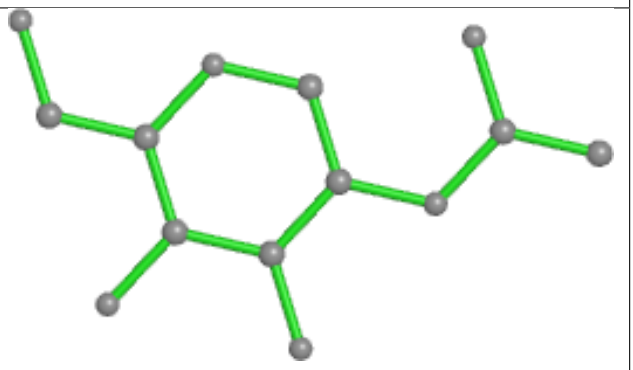


Rings

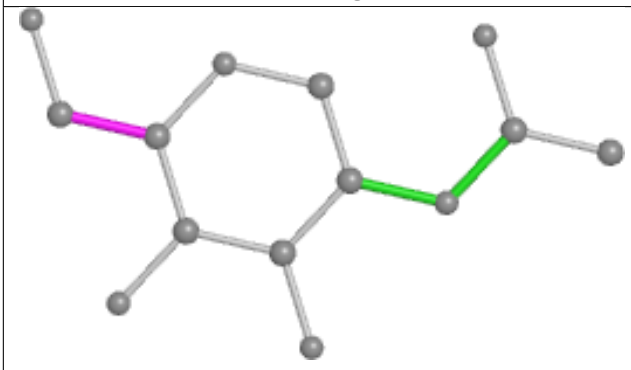
Ligand NAG C 1404



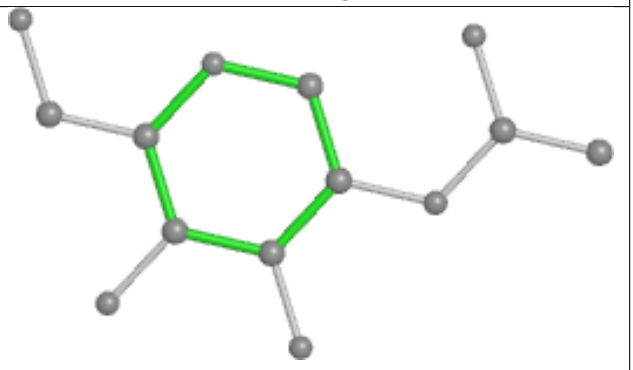
Bond lengths



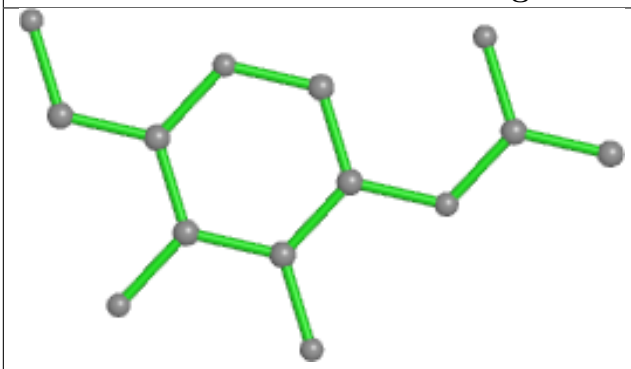
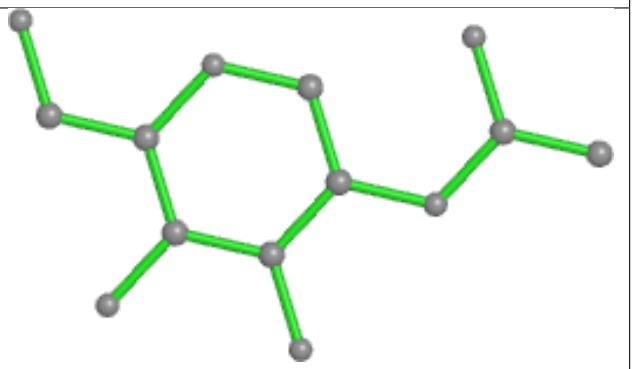
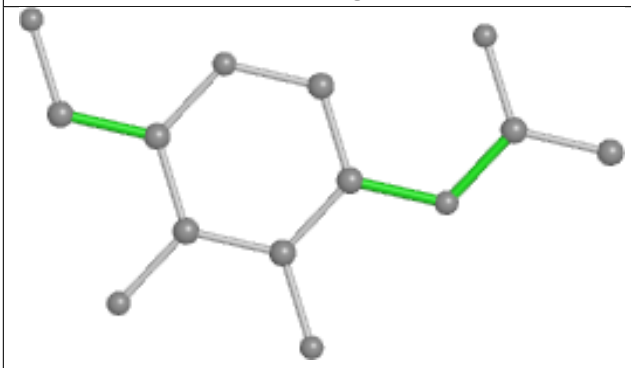
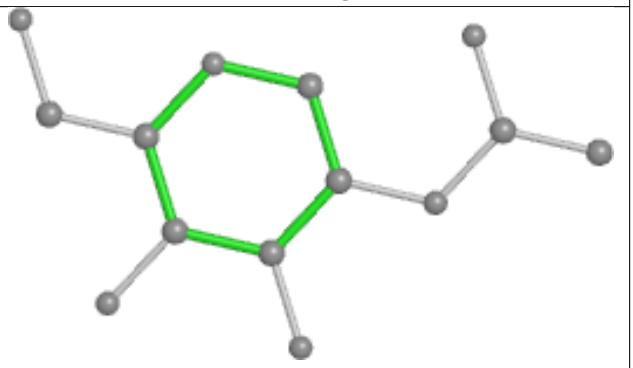
Bond angles

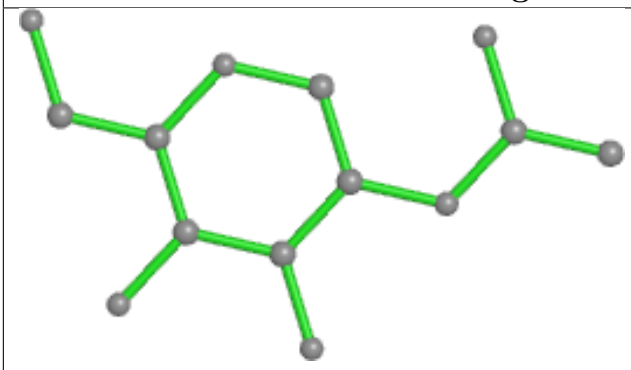
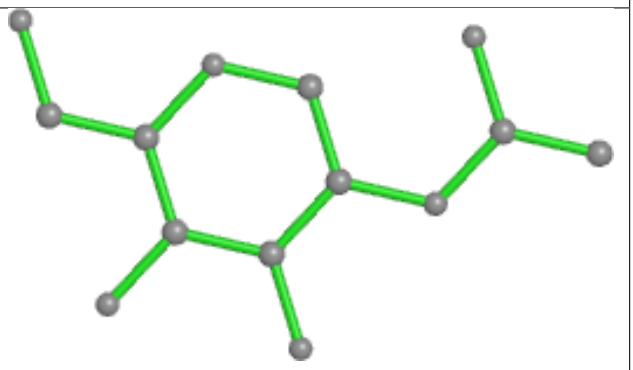
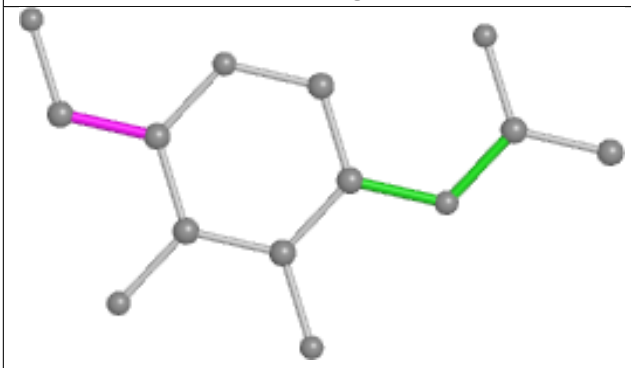
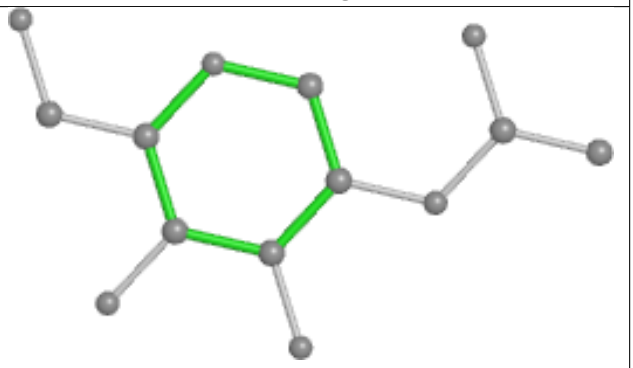


Torsions

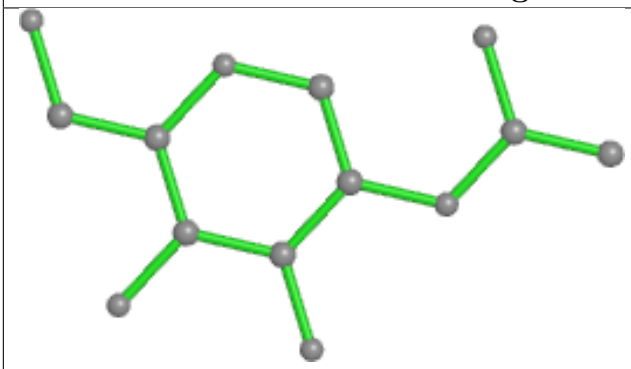


Rings

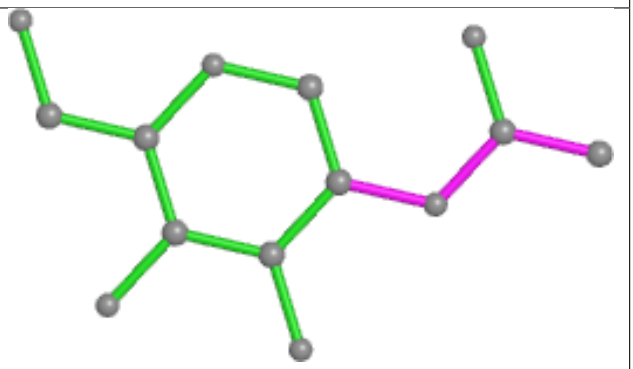
Ligand NAG B 1407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1404	
	
Bond lengths	Bond angles
	
Torsions	Rings

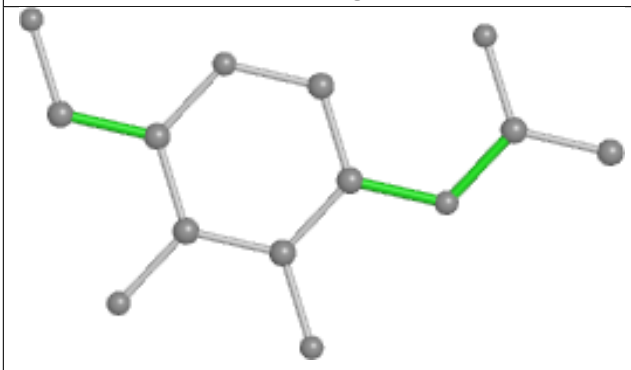
Ligand NAG C 1410



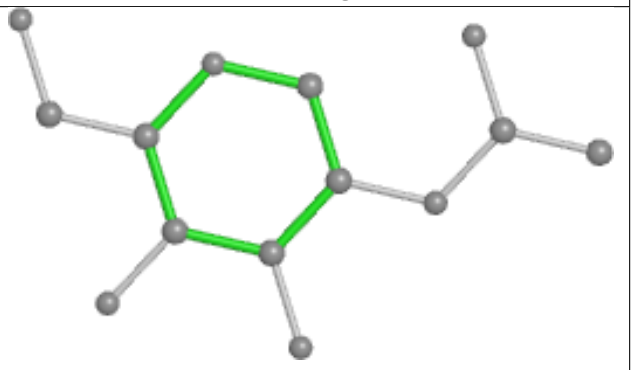
Bond lengths



Bond angles

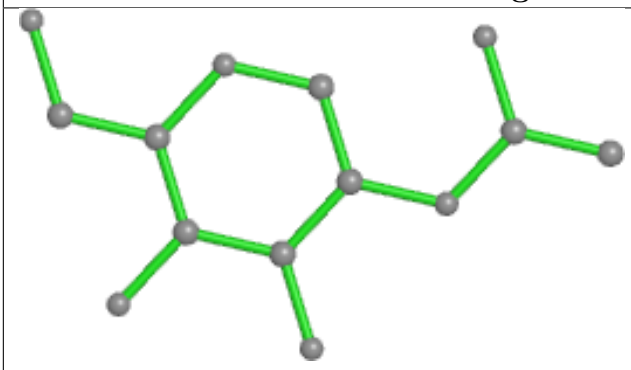


Torsions

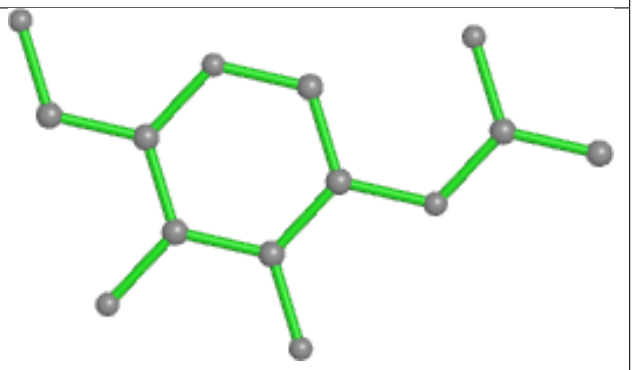


Rings

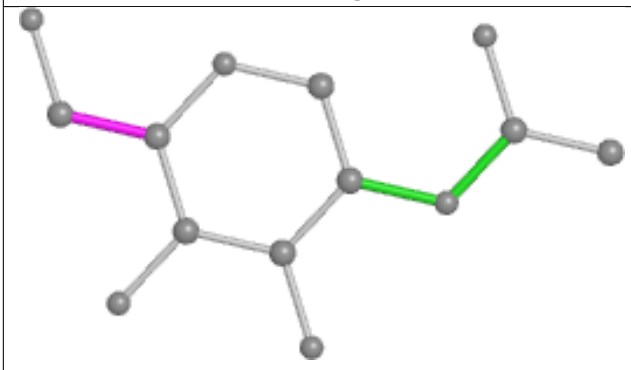
Ligand NAG B 1401



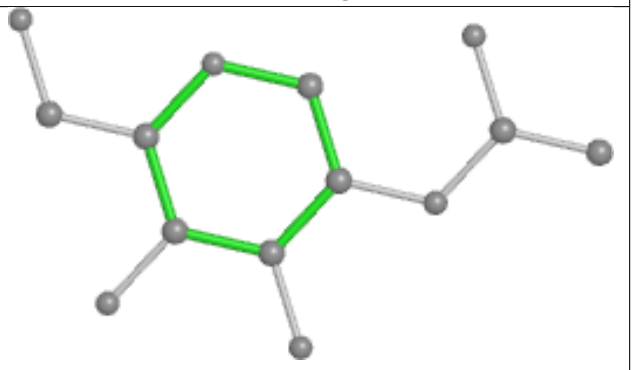
Bond lengths



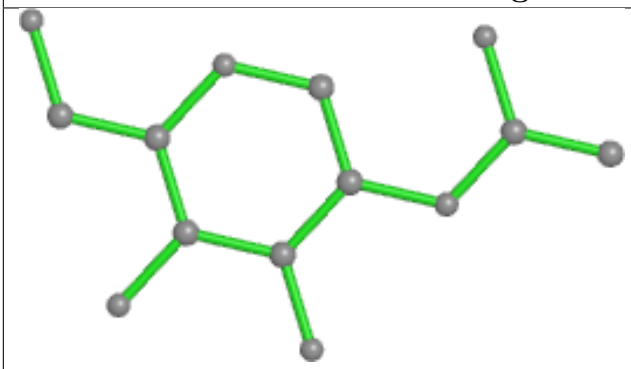
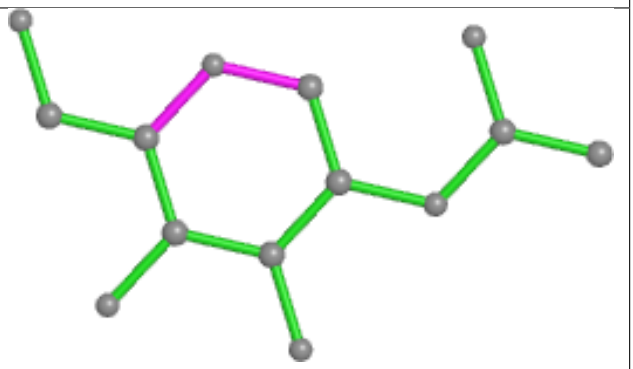
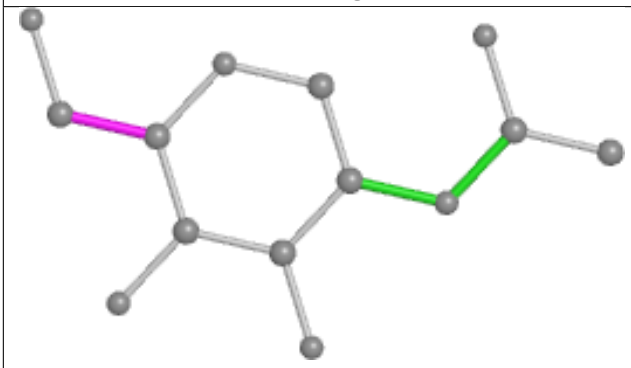
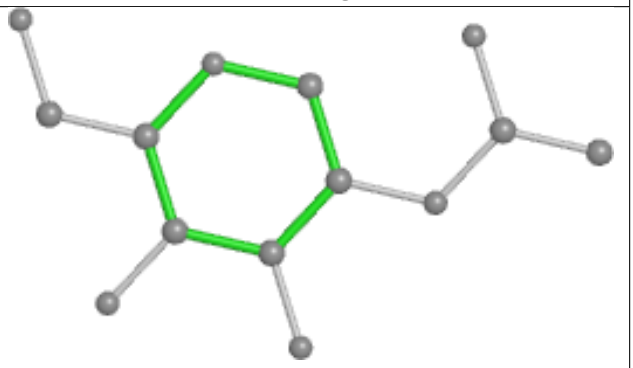
Bond angles

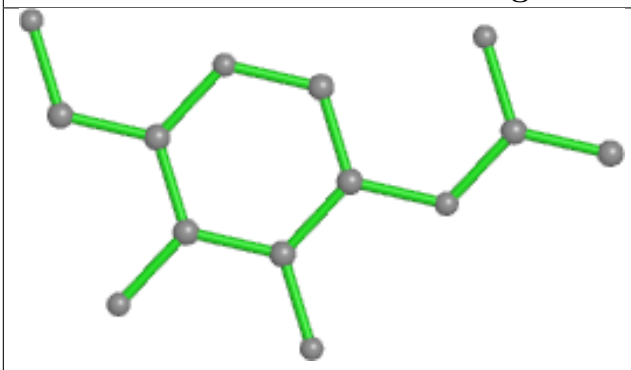
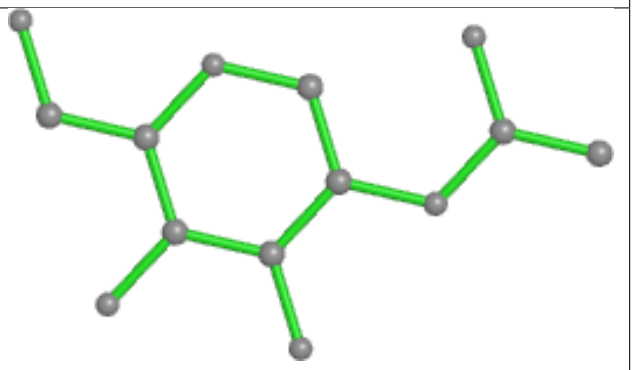
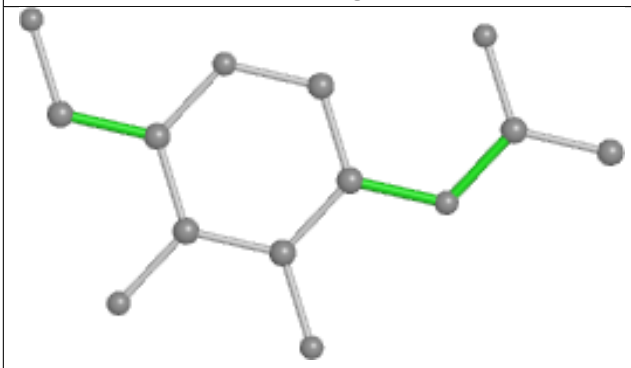
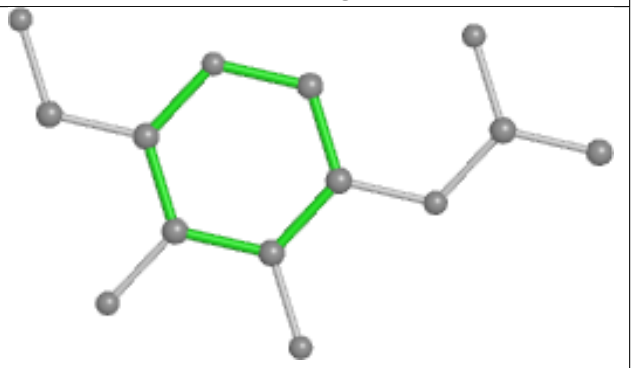


Torsions



Rings

Ligand NAG C 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

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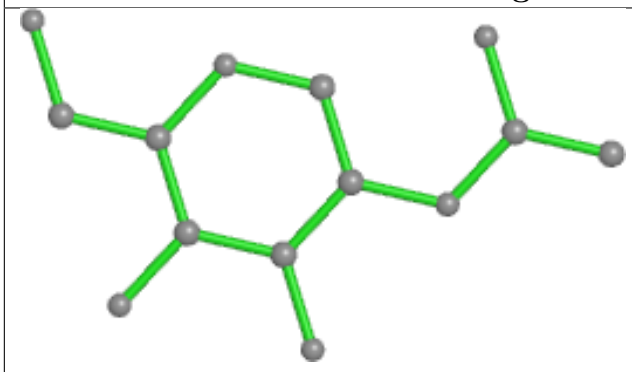
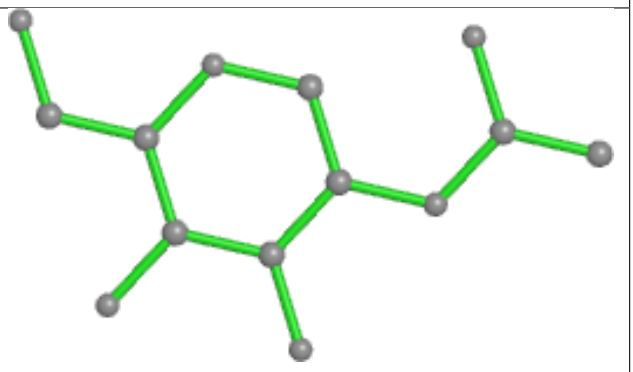
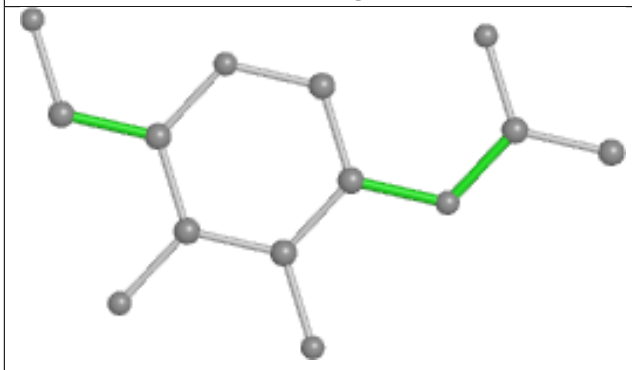


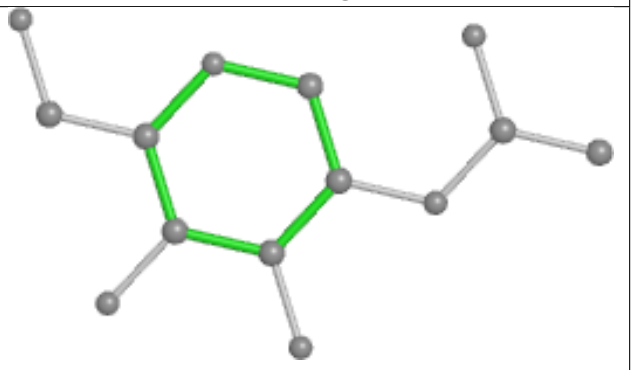
Bond lengths



Bond angles

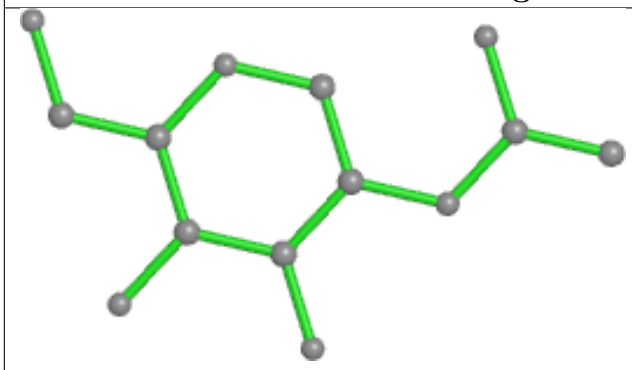


Torsions

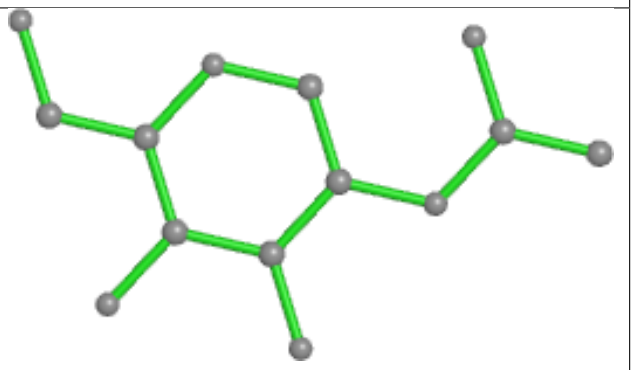


Rings

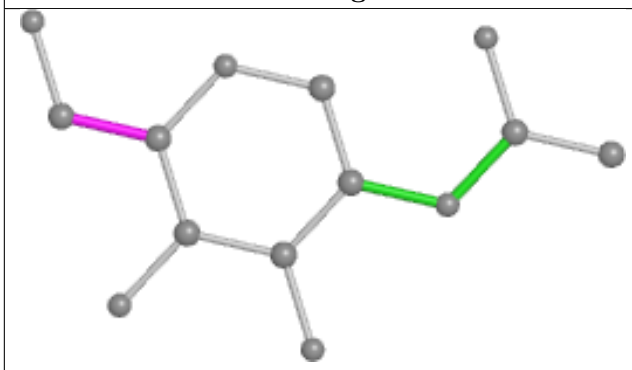
Ligand NAG B 1403



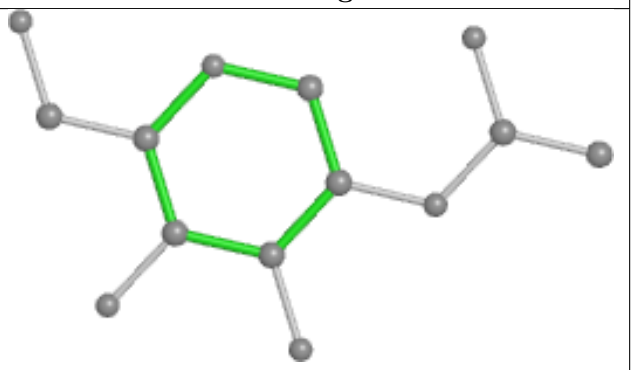
Bond lengths



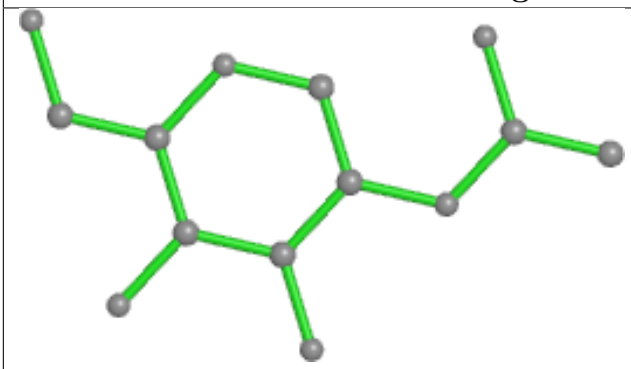
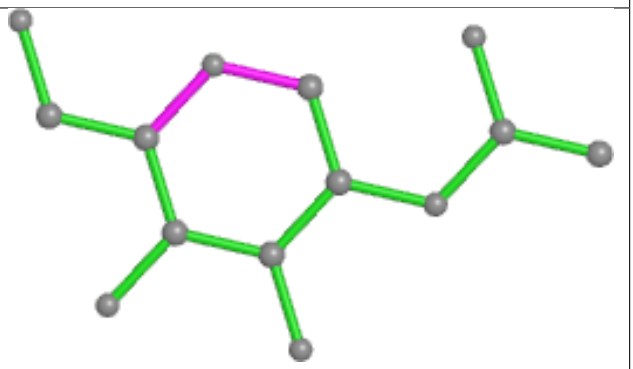
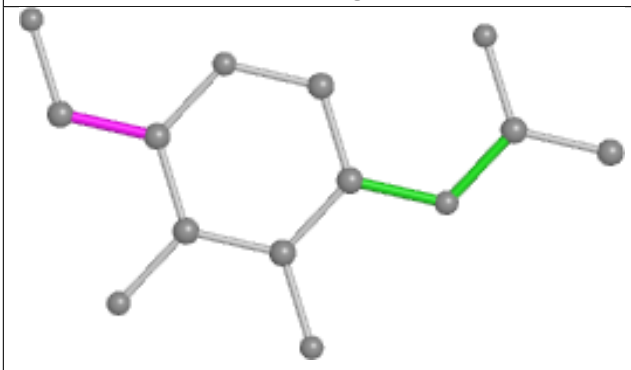
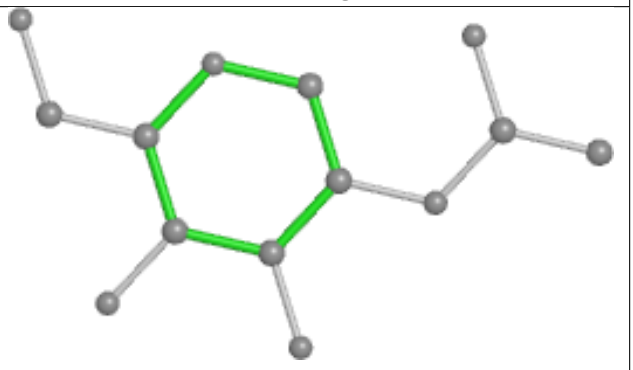
Bond angles

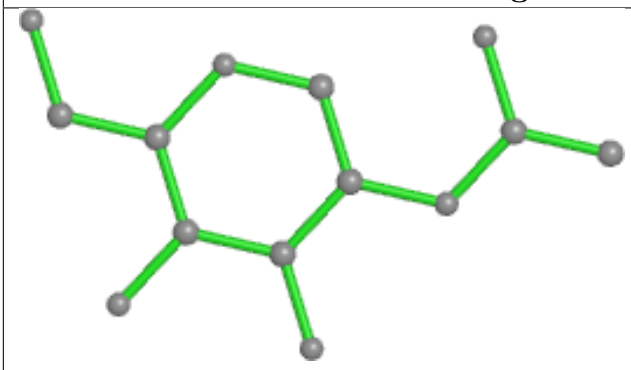
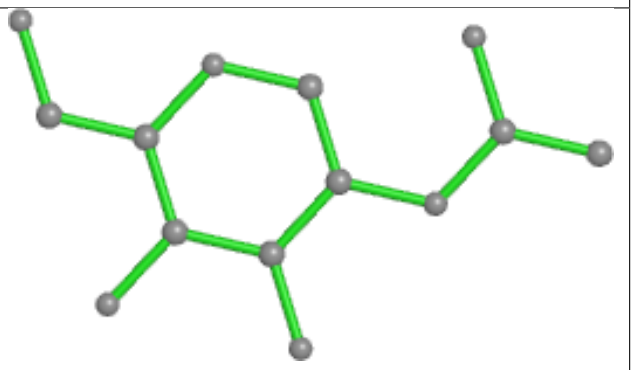
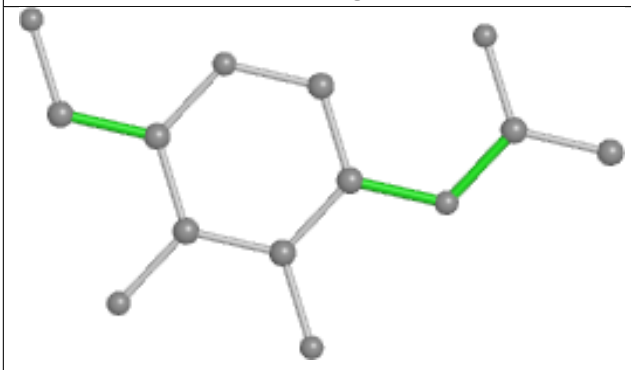
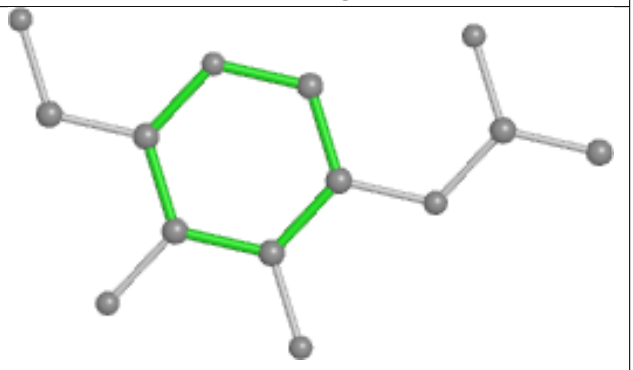


Torsions

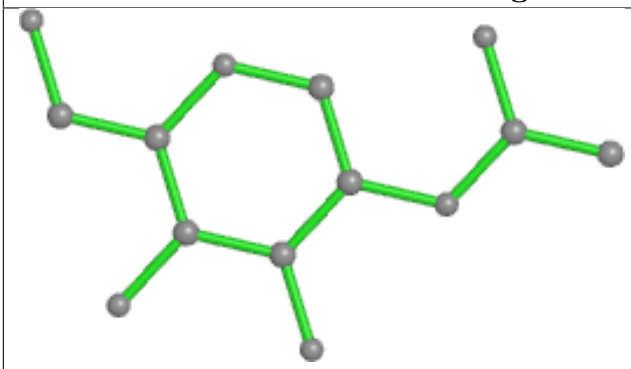


Rings

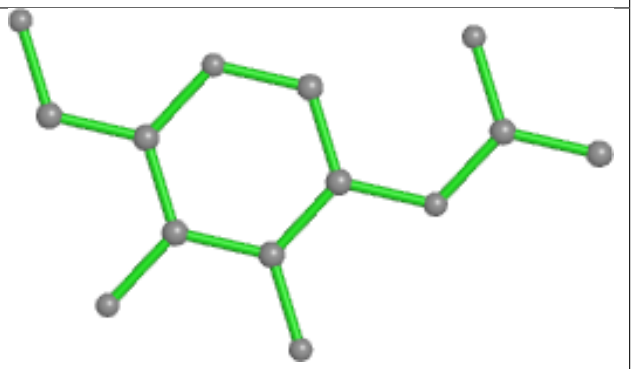
Ligand NAG B 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1408	
 Bond lengths	 Bond angles
 Torsions	 Rings

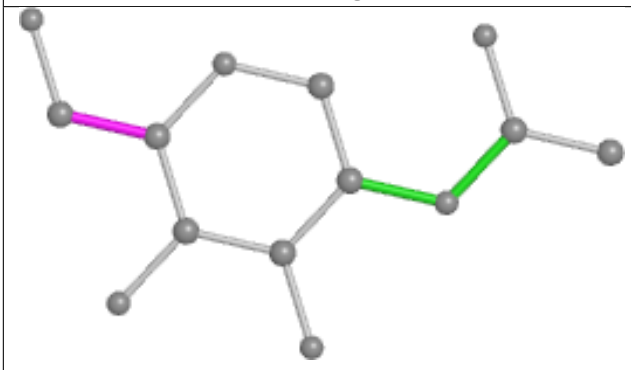
Ligand NAG A 1404



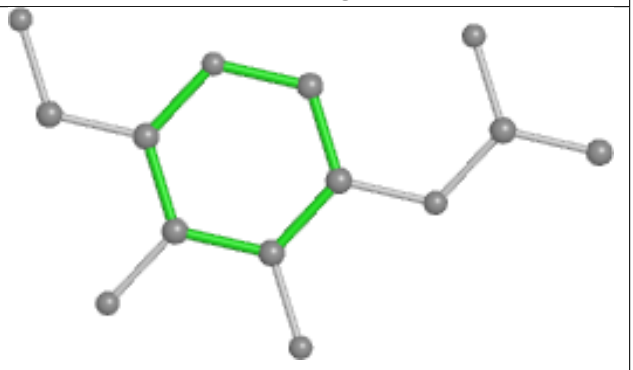
Bond lengths



Bond angles

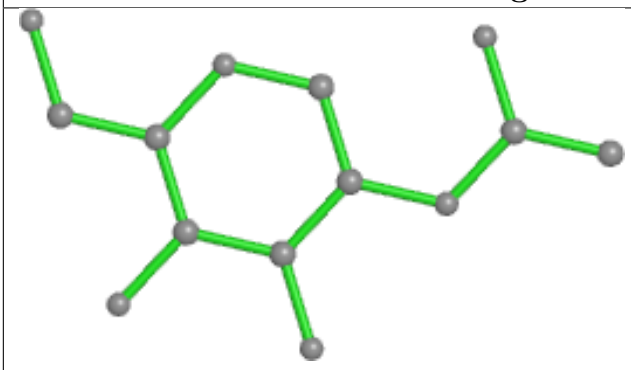


Torsions

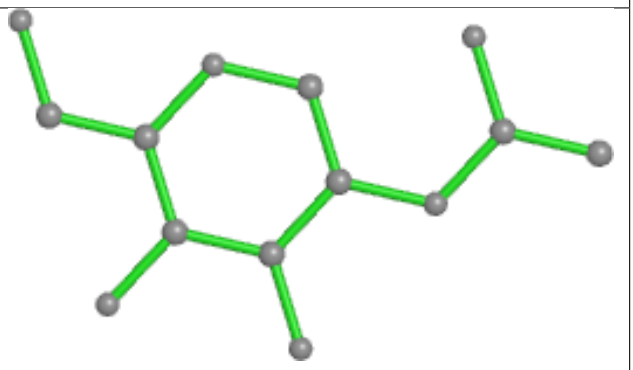


Rings

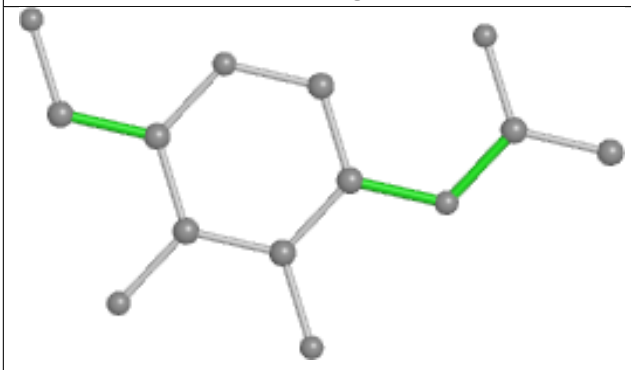
Ligand NAG A 1406



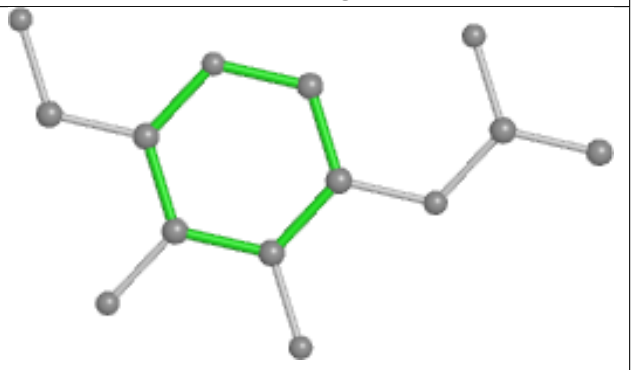
Bond lengths



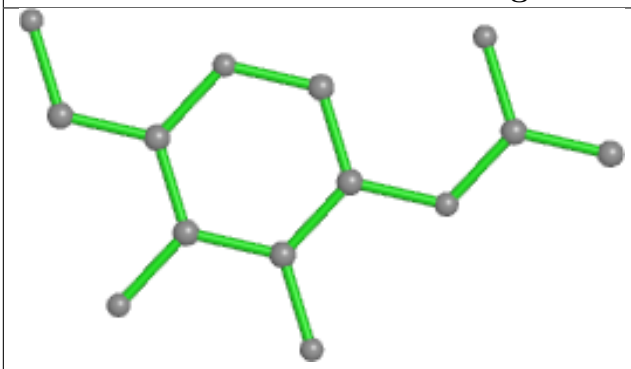
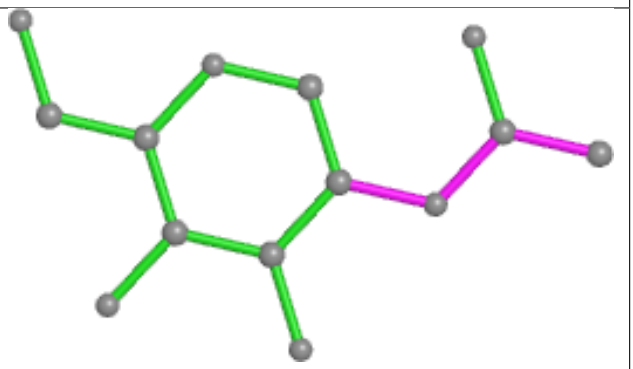
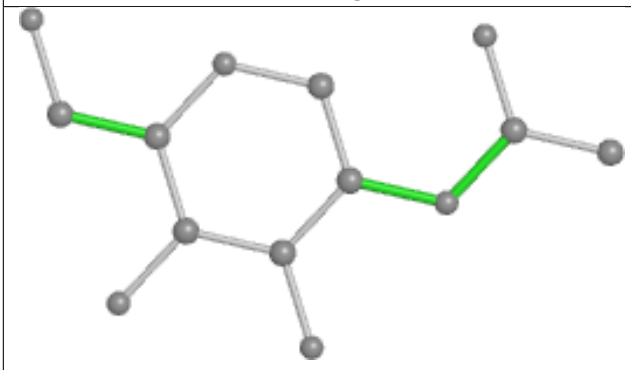
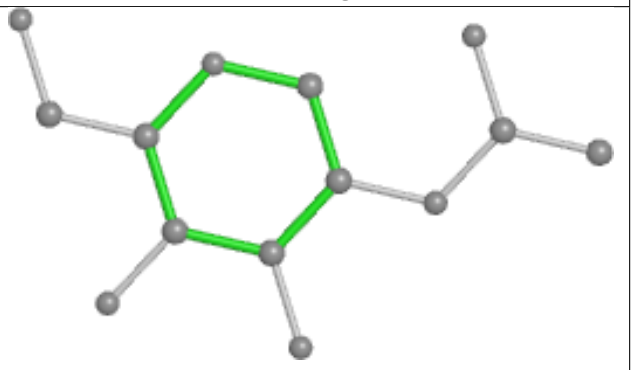
Bond angles

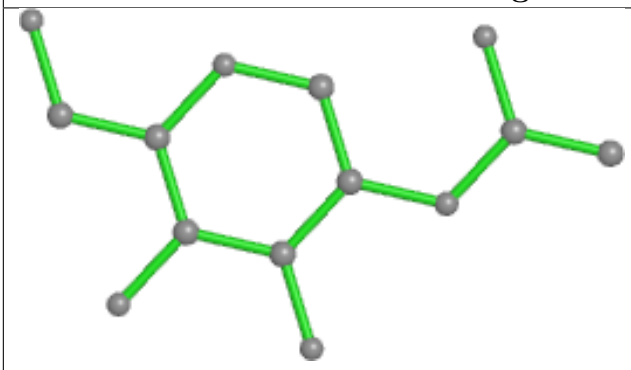
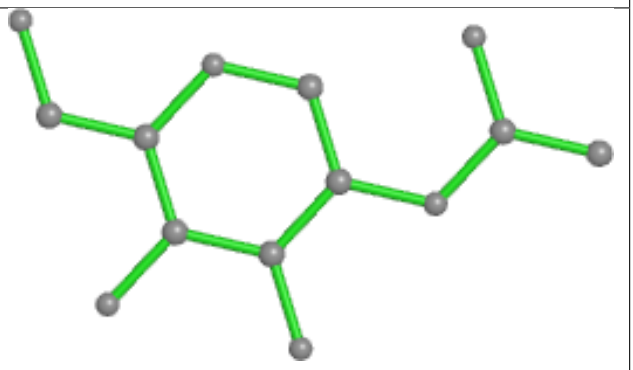
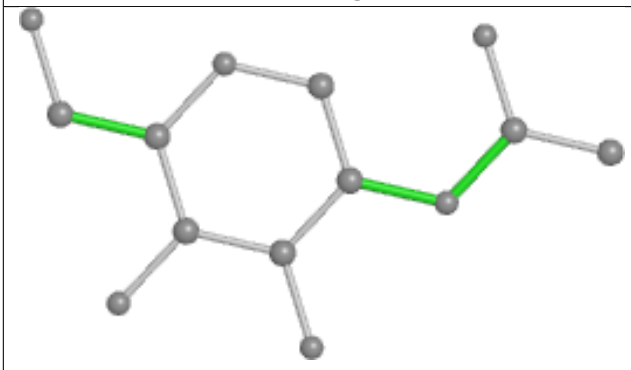
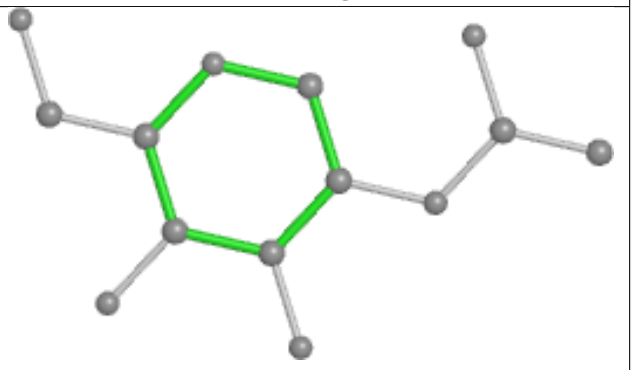


Torsions



Rings

Ligand NAG A 1410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1409	
 Bond lengths	 Bond angles
 Torsions	 Rings

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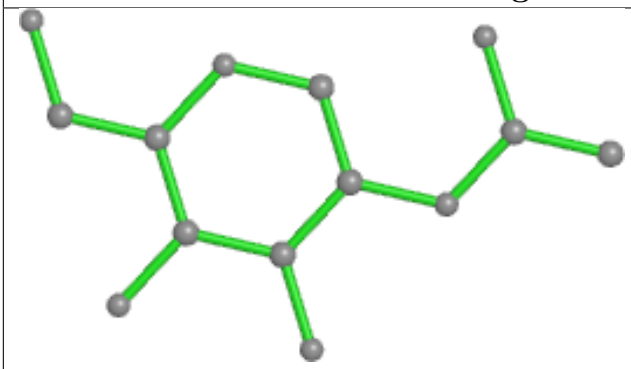
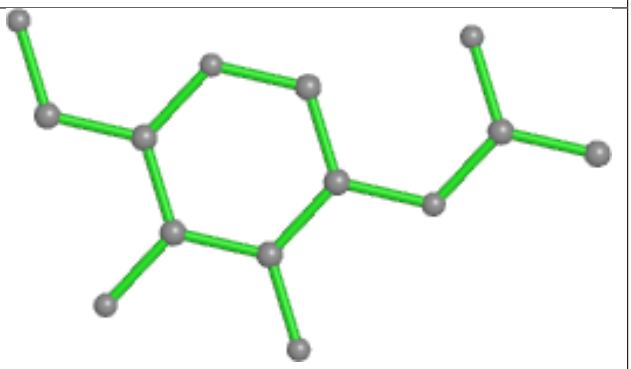
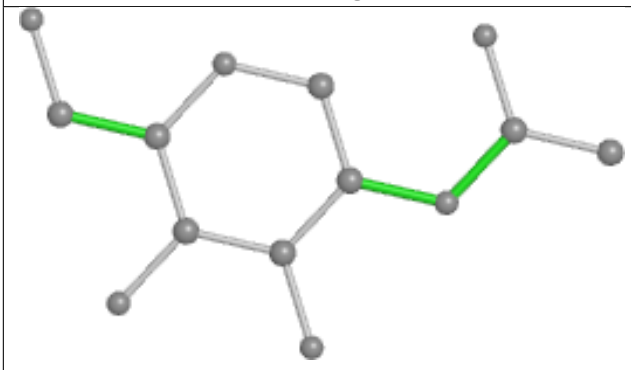
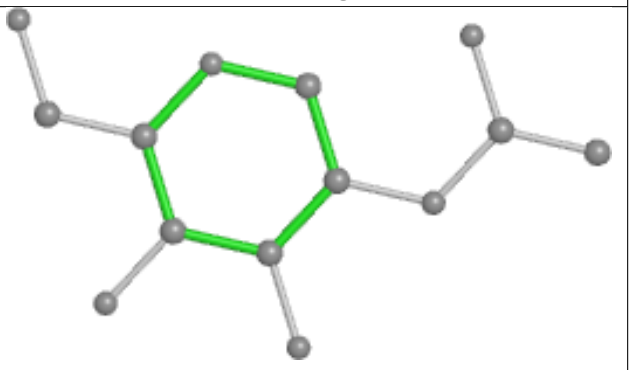
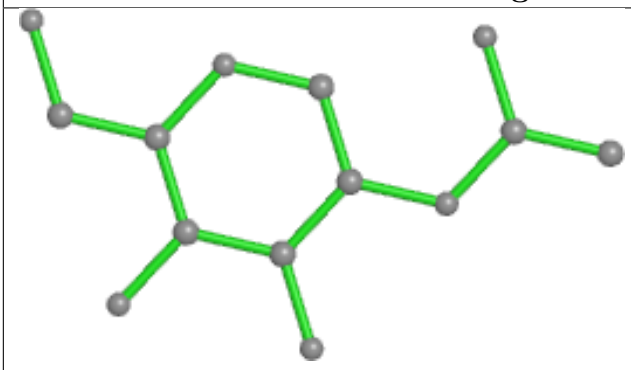
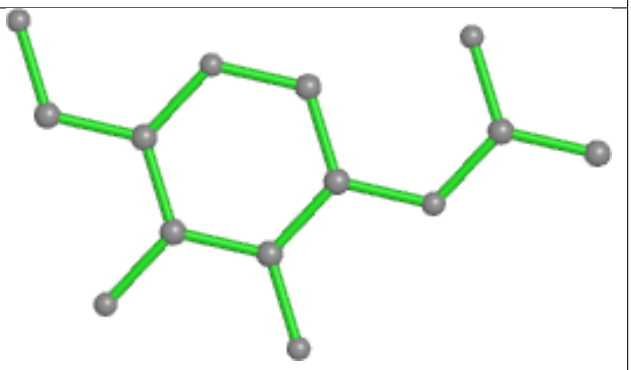
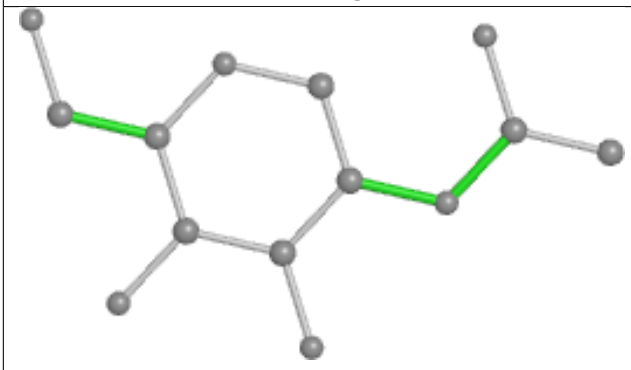
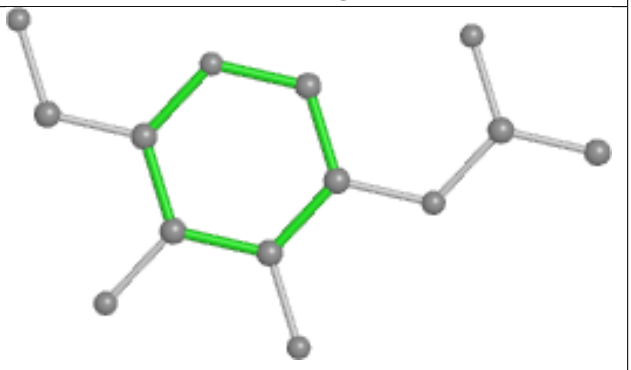
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1411	
 Bond lengths	 Bond angles
 Torsions	 Rings

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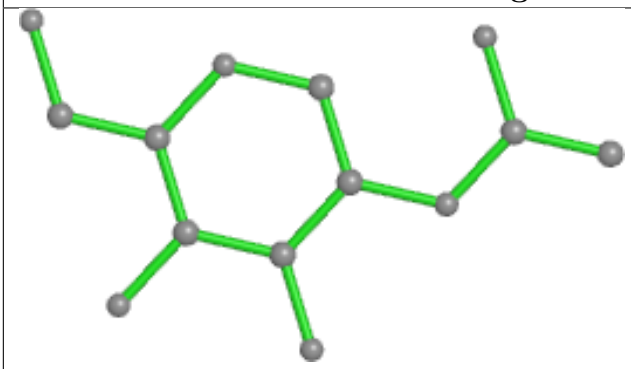
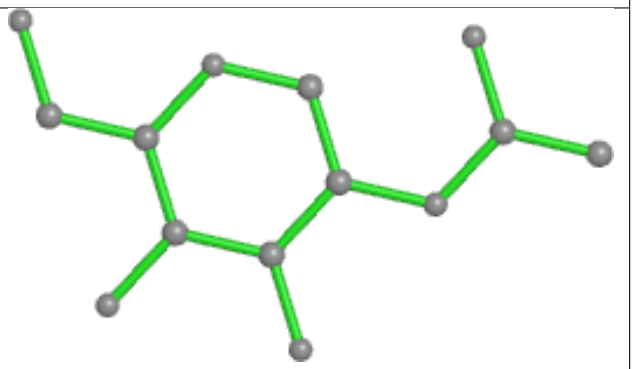
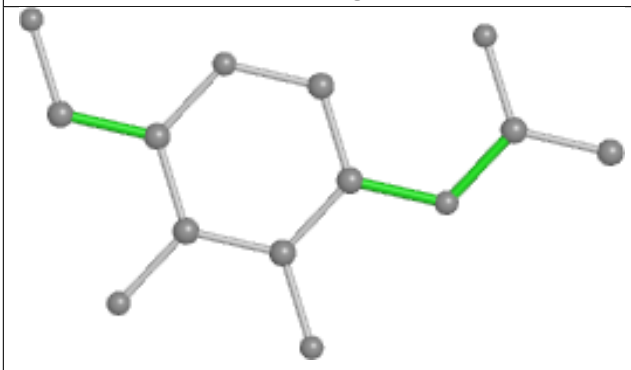
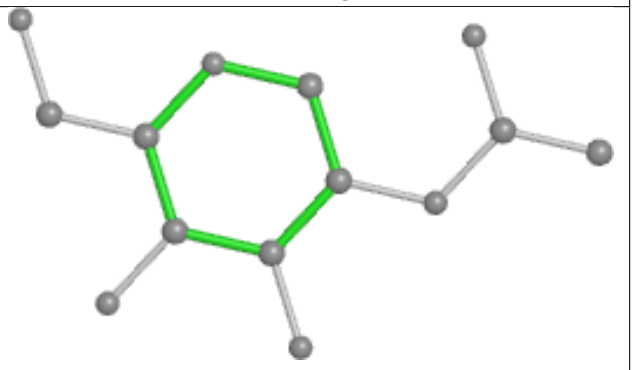
 Bond lengths	 Bond angles
 Torsions	 Rings

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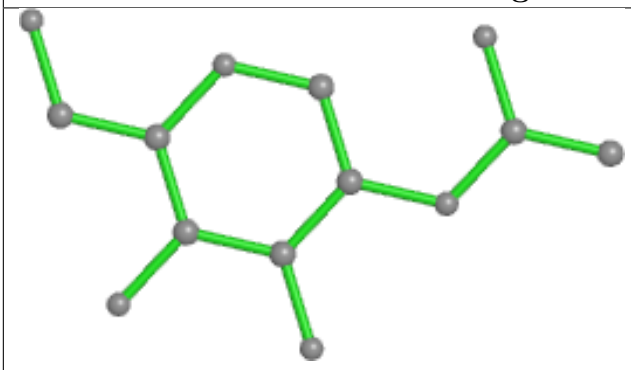
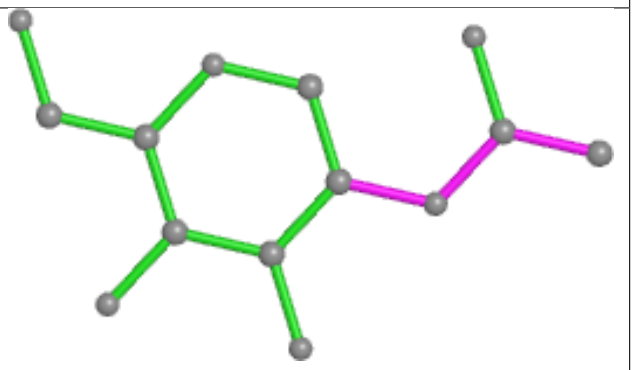
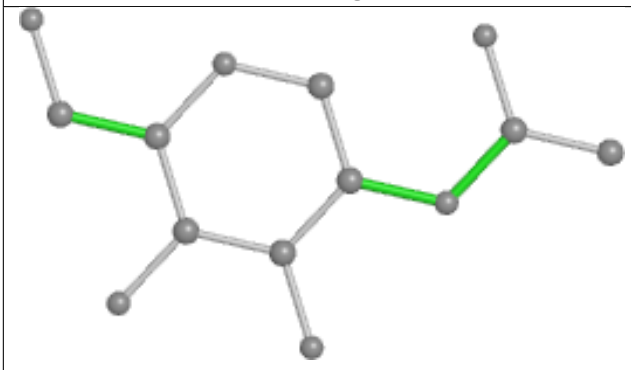
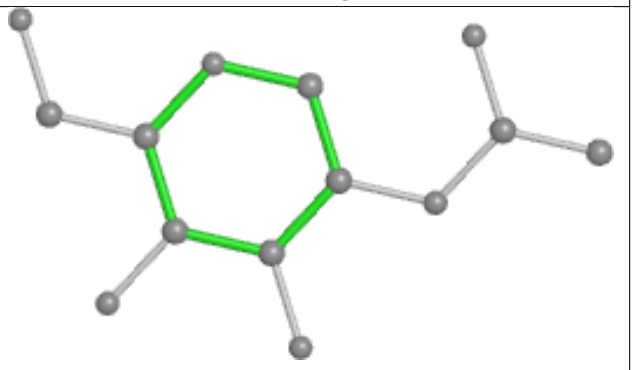
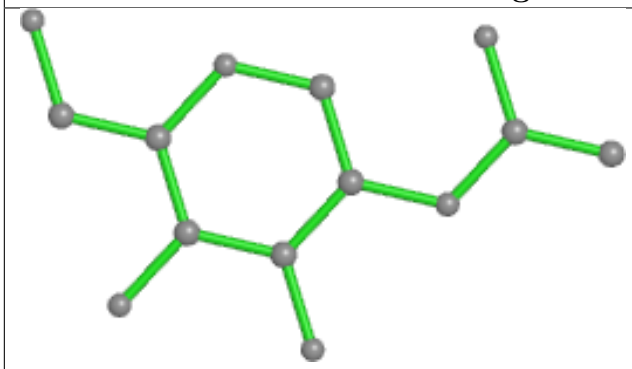
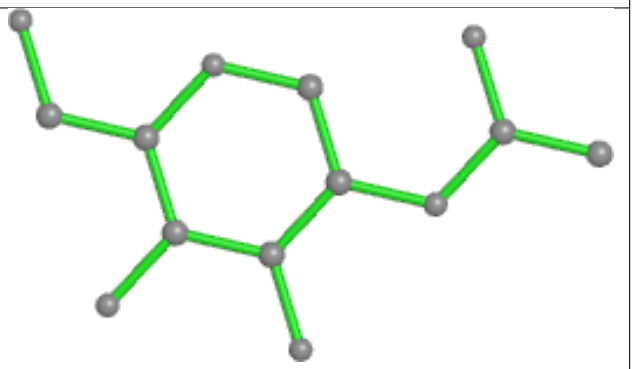
 Bond lengths	 Bond angles
 Torsions	 Rings

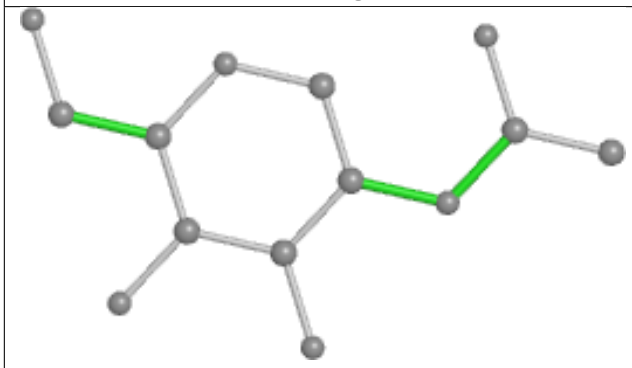
Ligand NAG C 1409



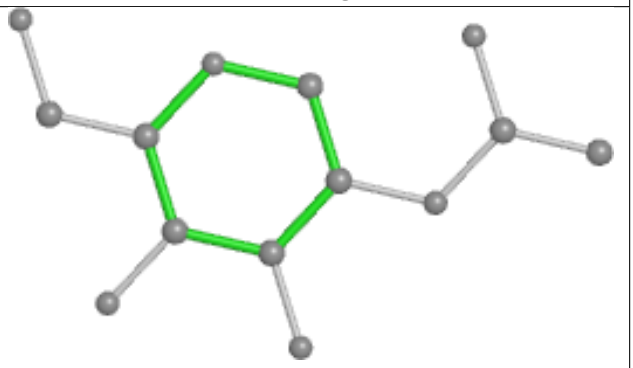
Bond lengths



Bond angles

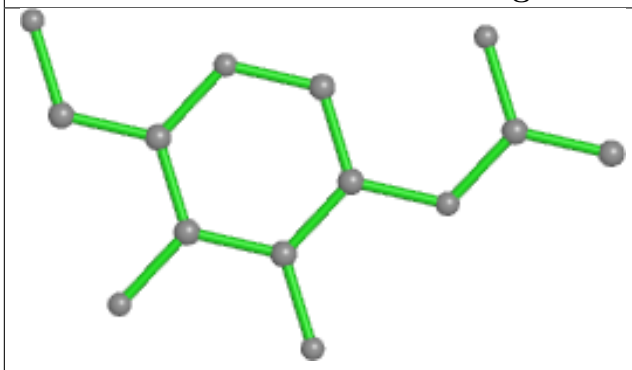


Torsions

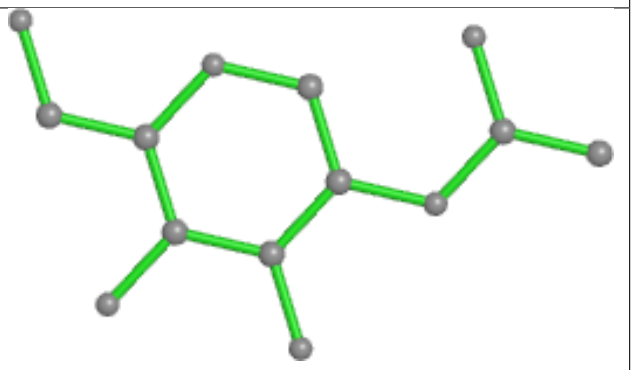


Rings

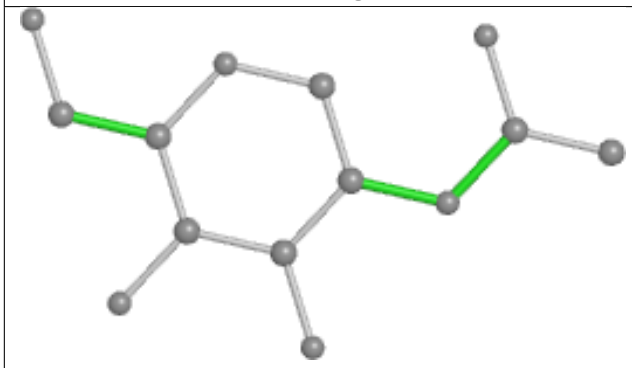
Ligand NAG B 1408



Bond lengths



Bond angles



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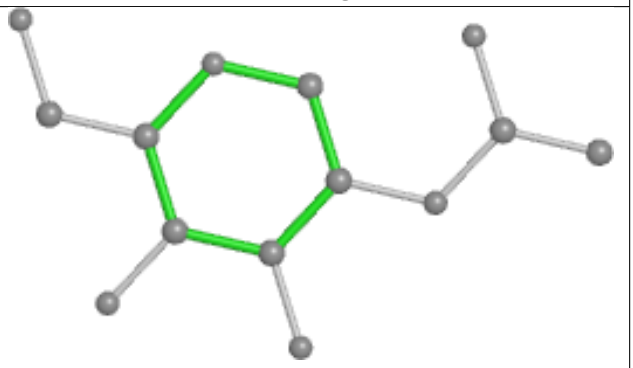
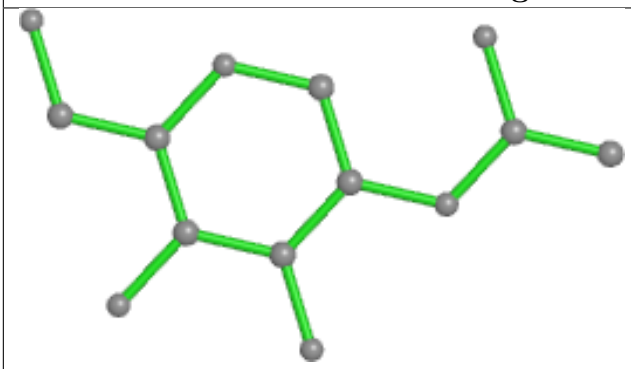
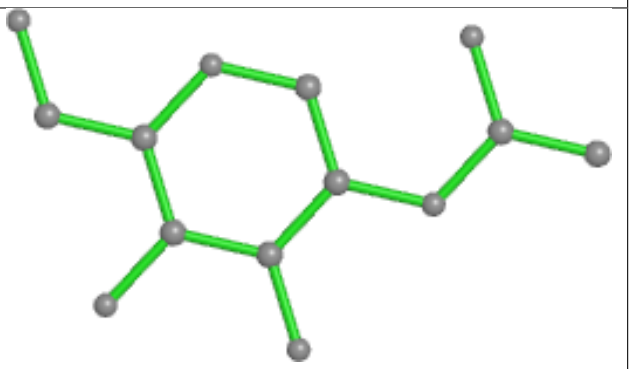
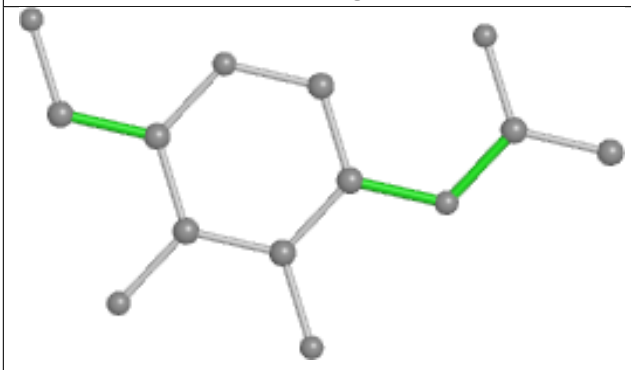
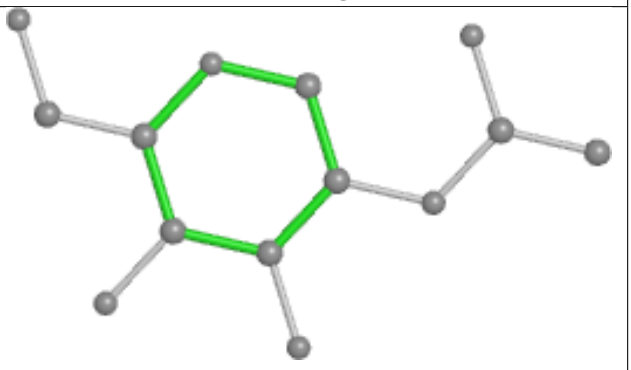
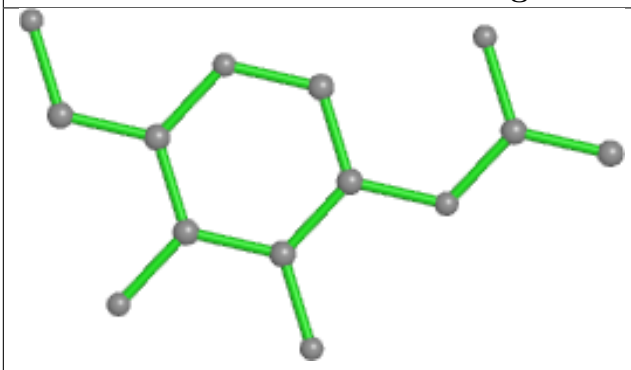
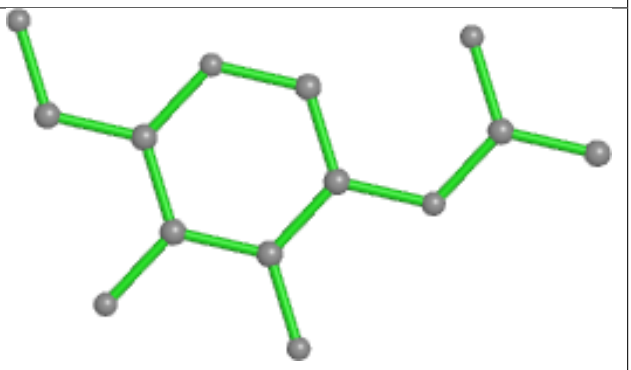
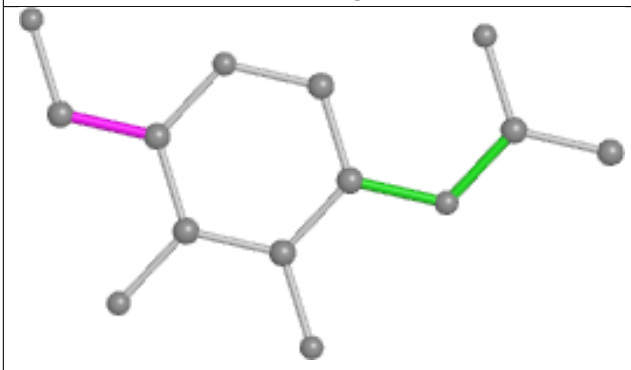
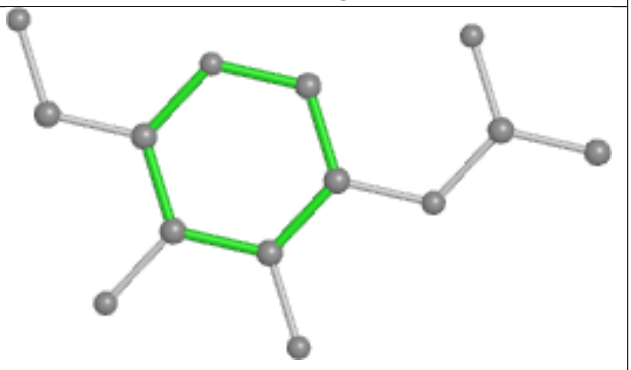
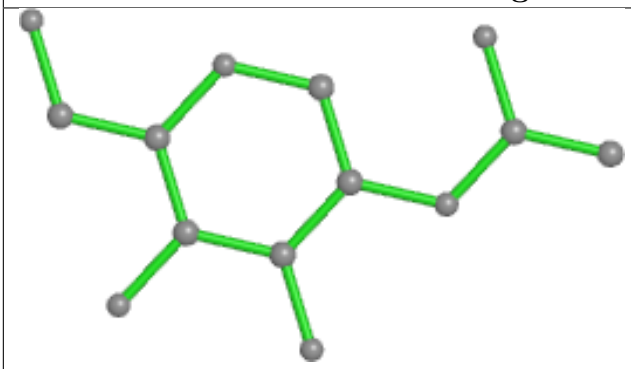


Rings

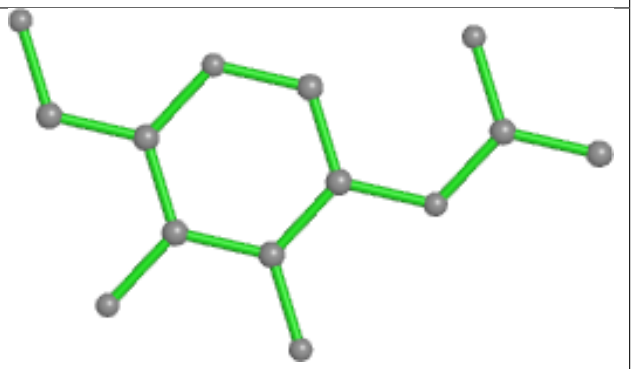
Ligand NAG C 1408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

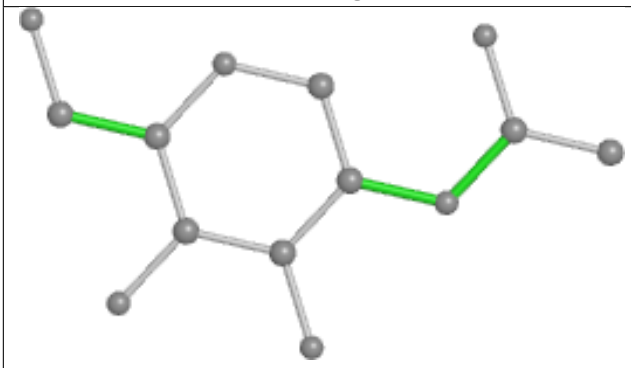
Ligand NAG C 1405



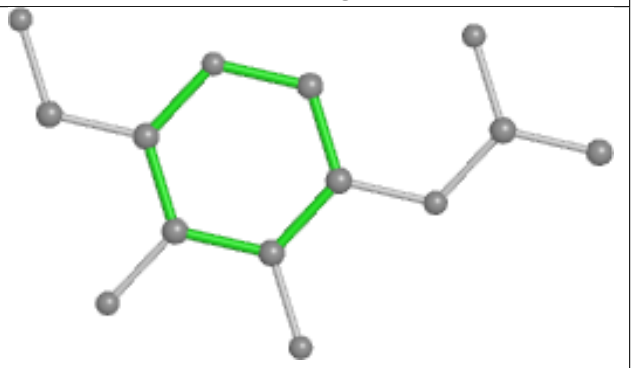
Bond lengths



Bond angles

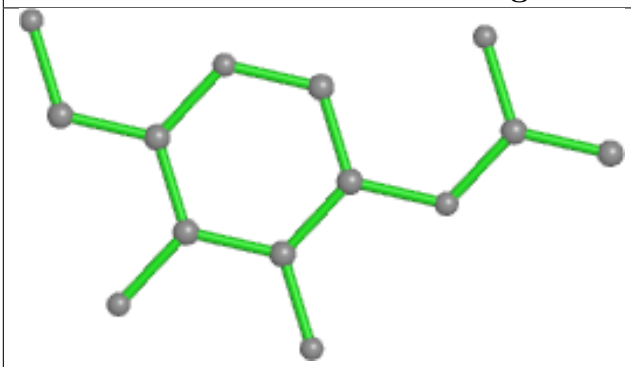


Torsions

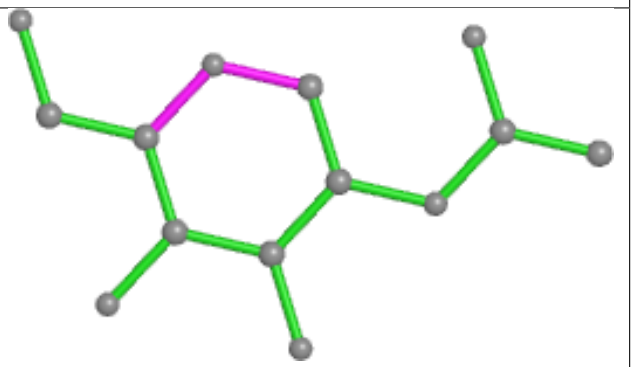


Rings

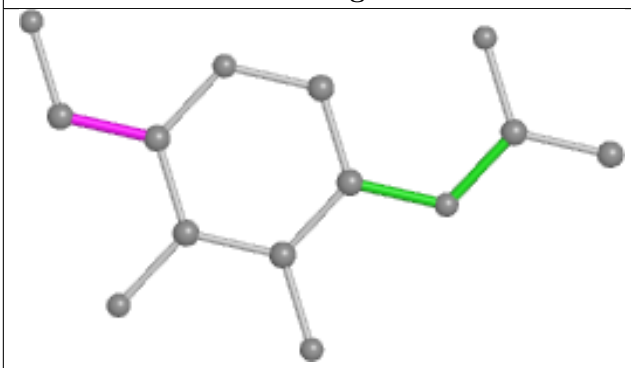
Ligand NAG A 1402



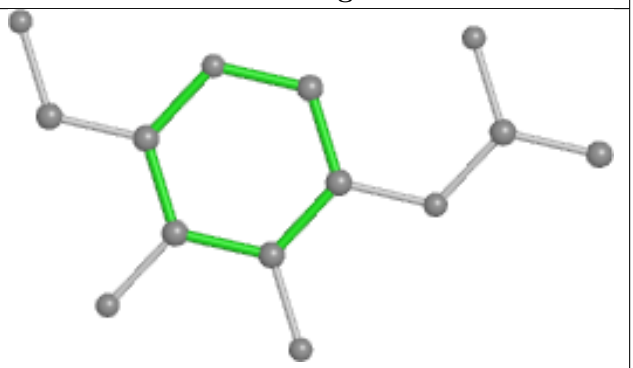
Bond lengths



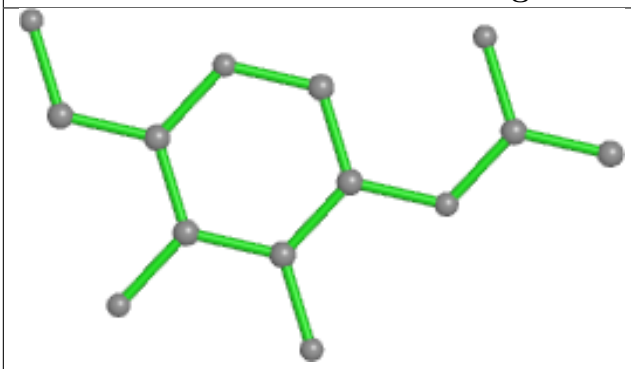
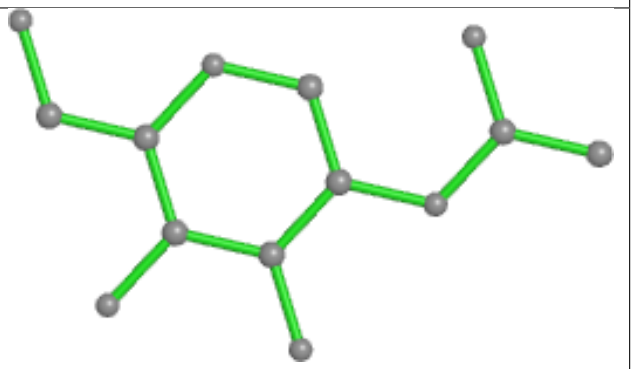
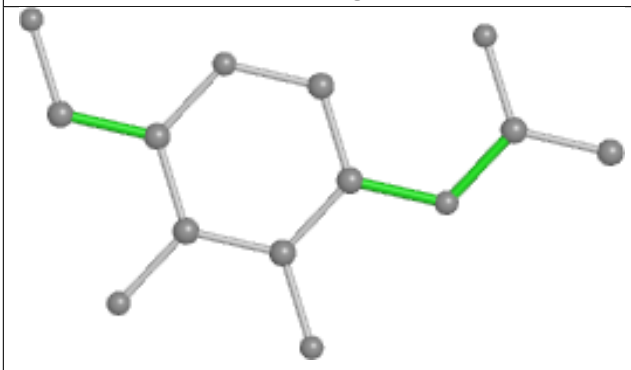
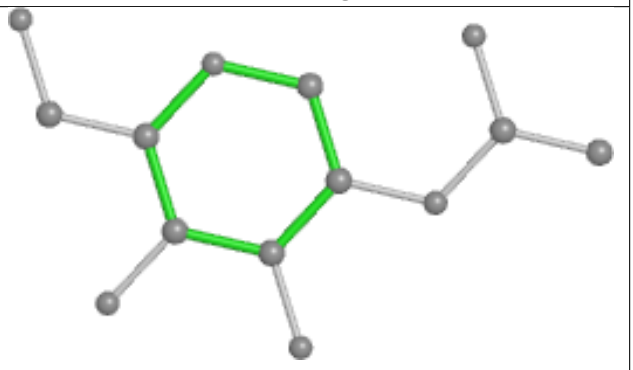
Bond angles

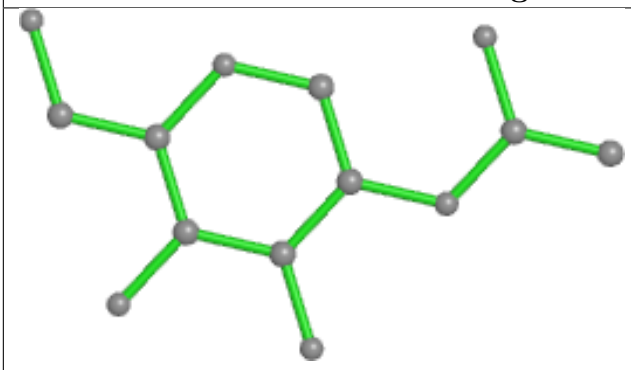
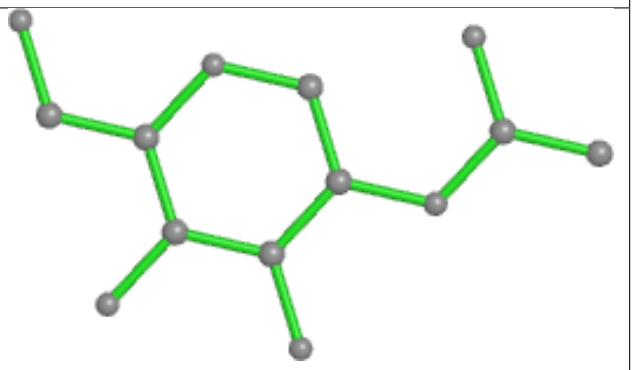
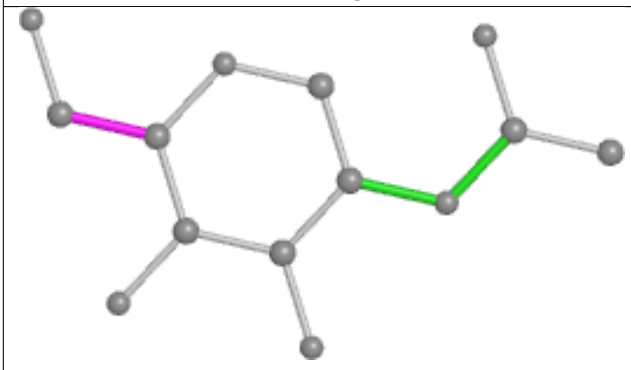
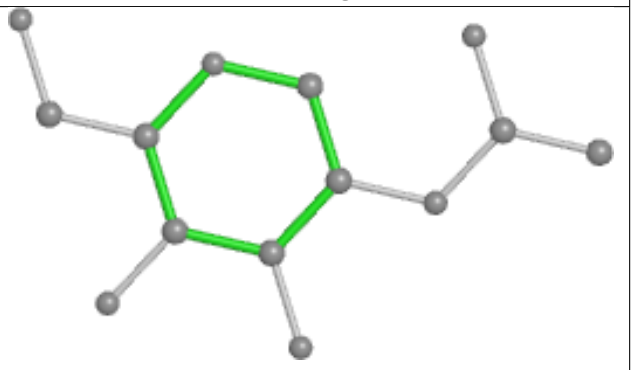


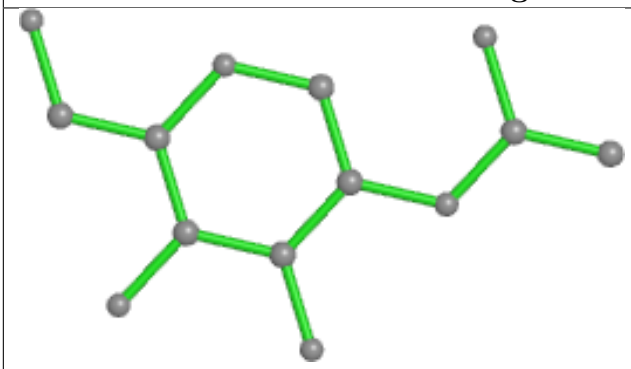
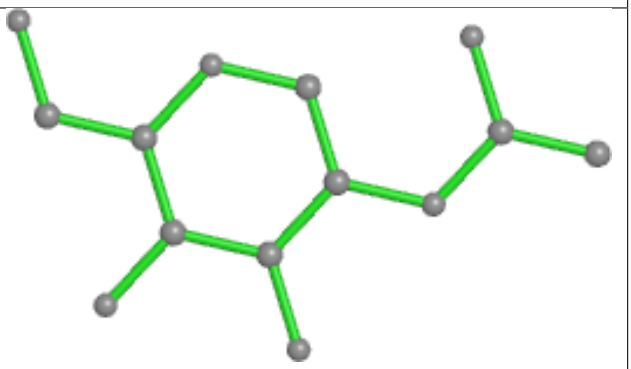
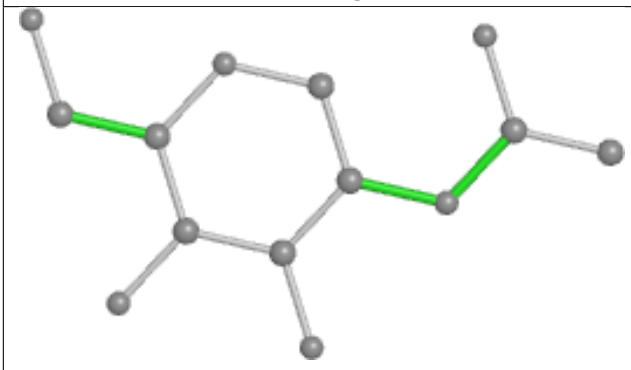
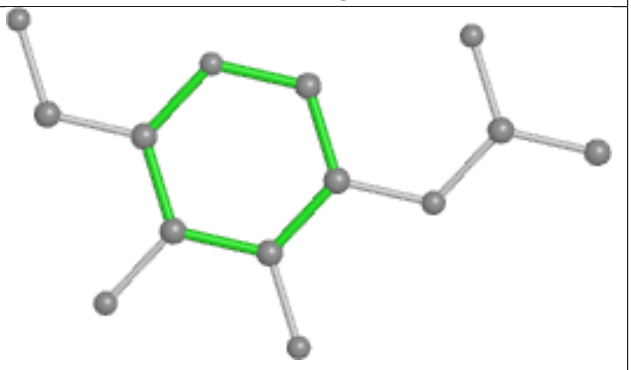
Torsions

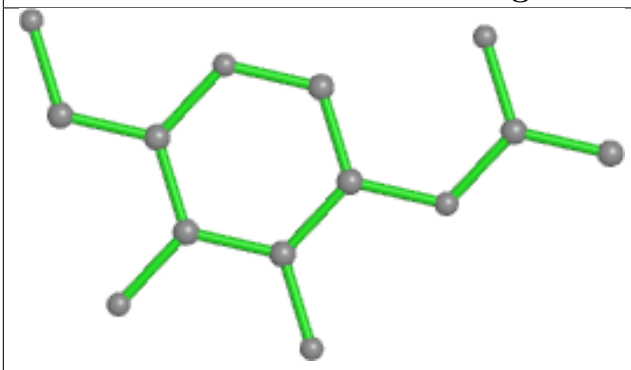
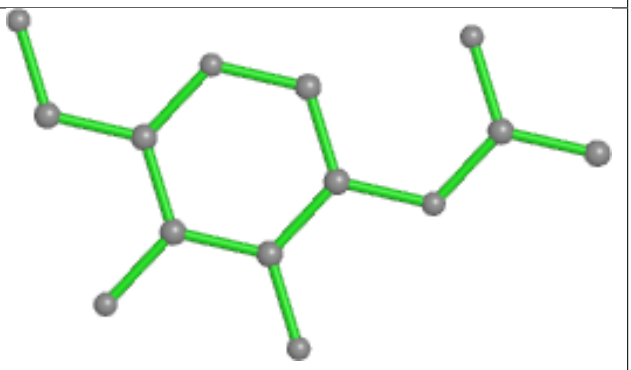
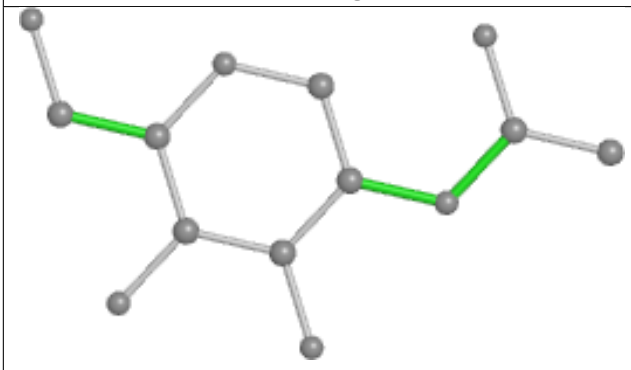
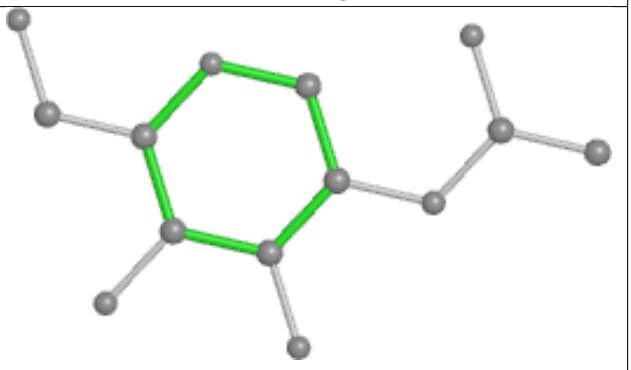


Rings

Ligand NAG B 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1406	
 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.

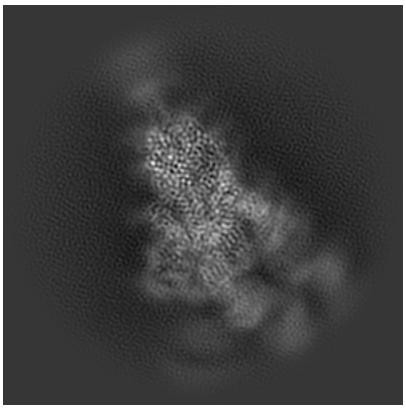
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34261. These allow visual inspection of the internal detail of the map and identification of artifacts.

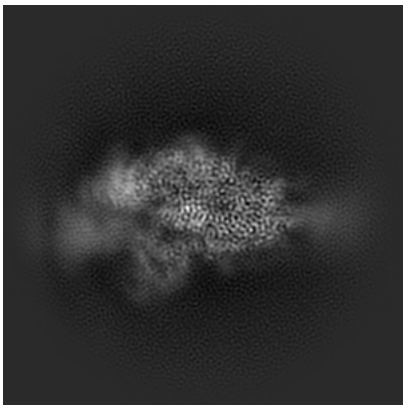
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

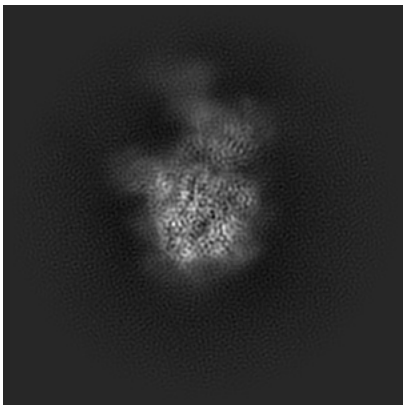
6.1.1 Primary map



X

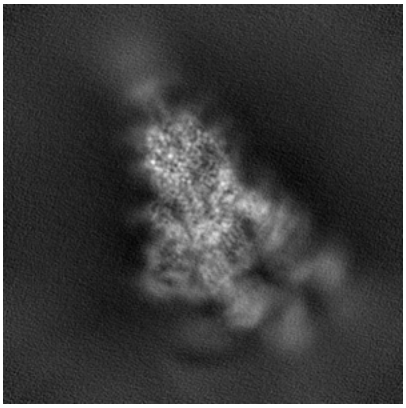


Y

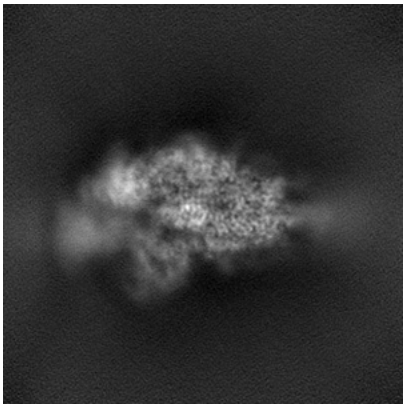


Z

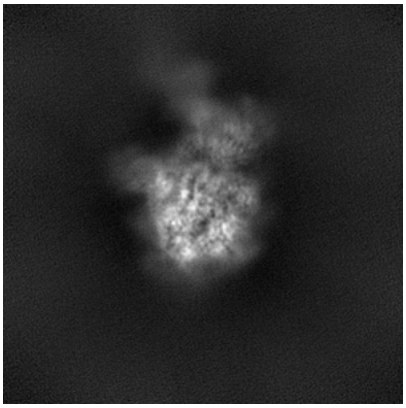
6.1.2 Raw map



X



Y

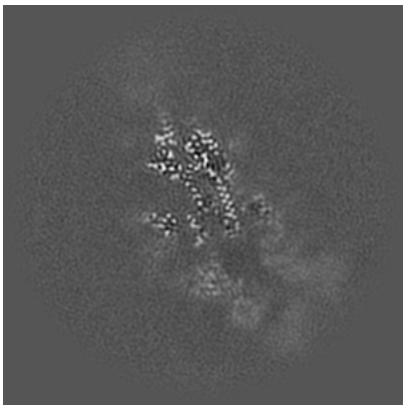


Z

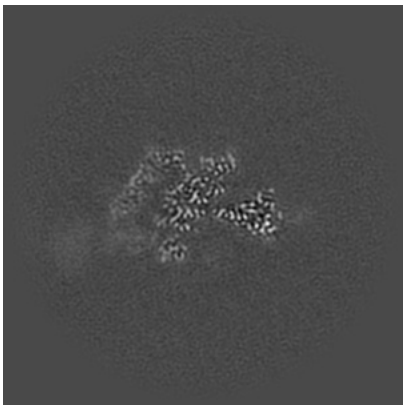
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

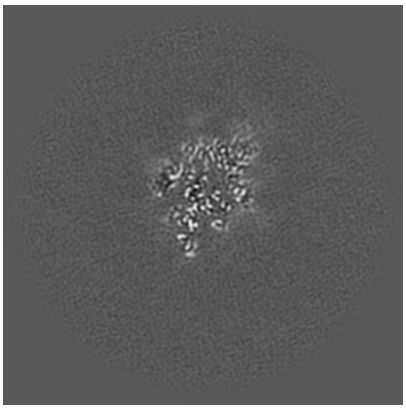
6.2.1 Primary map



X Index: 144

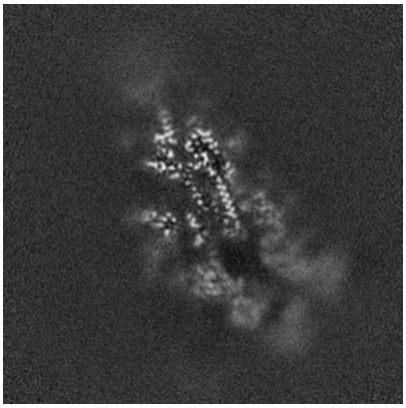


Y Index: 144

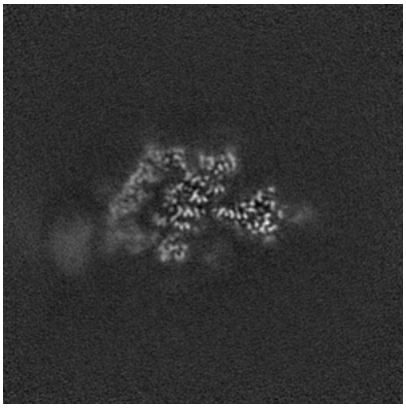


Z Index: 144

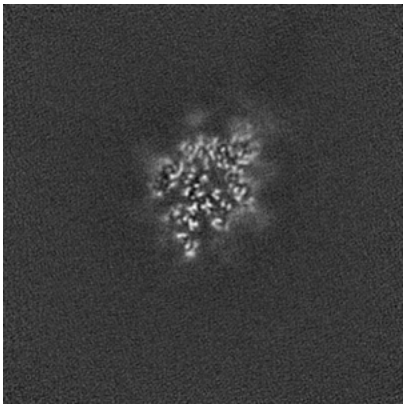
6.2.2 Raw map



X Index: 144



Y Index: 144

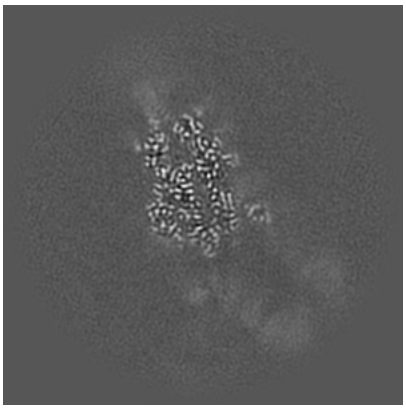


Z Index: 144

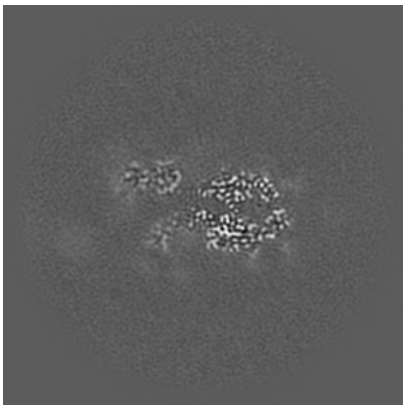
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

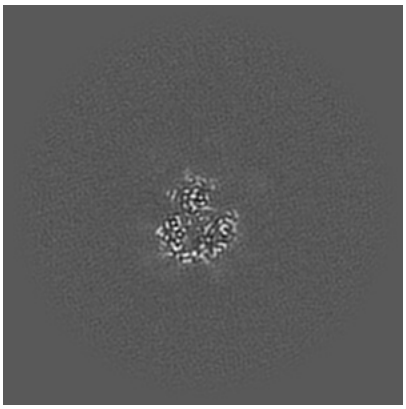
6.3.1 Primary map



X Index: 133

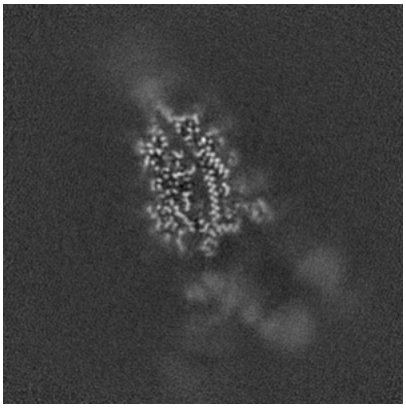


Y Index: 129

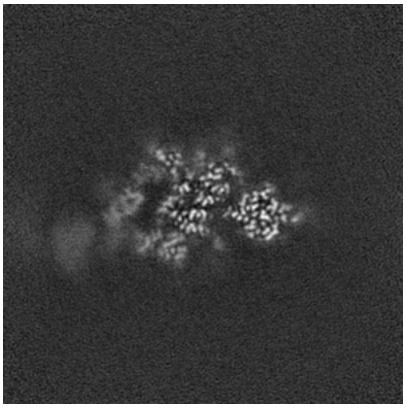


Z Index: 173

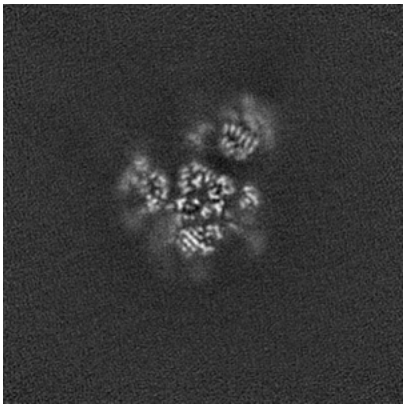
6.3.2 Raw map



X Index: 130



Y Index: 141

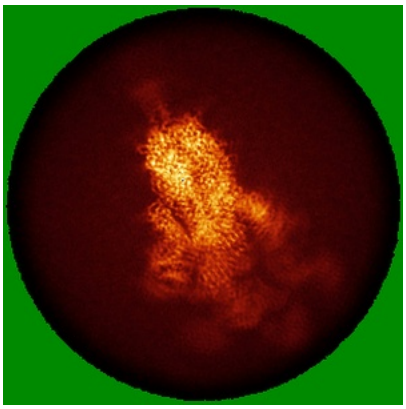


Z Index: 128

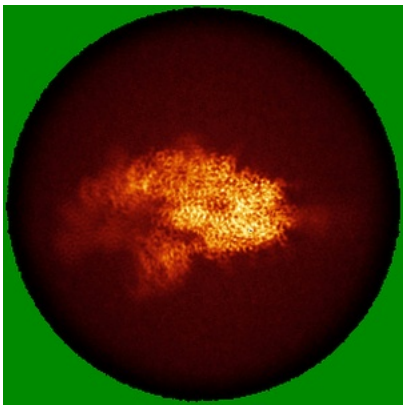
The images above show the largest variance slices of the map in three orthogonal directions.

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

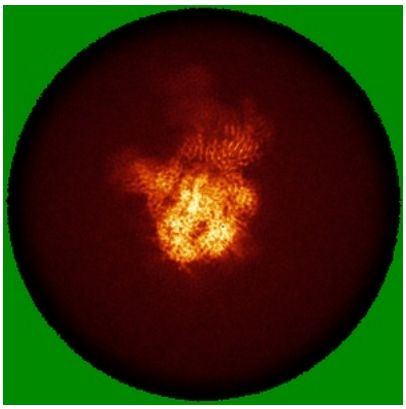
6.4.1 Primary map



X

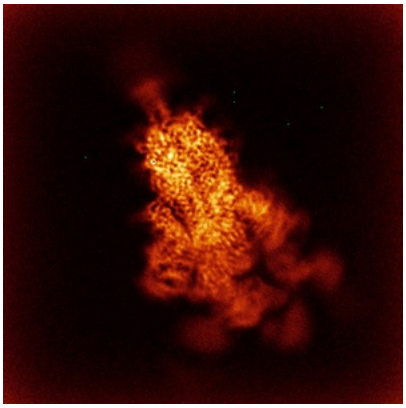


Y

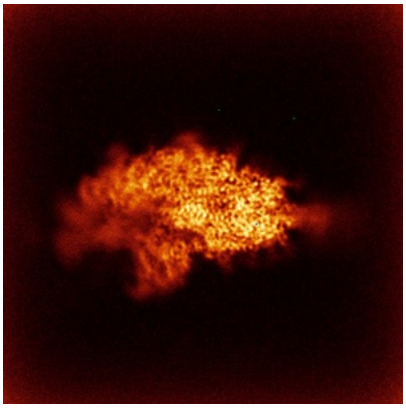


Z

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

6.5.2 Raw map

X Y Z

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

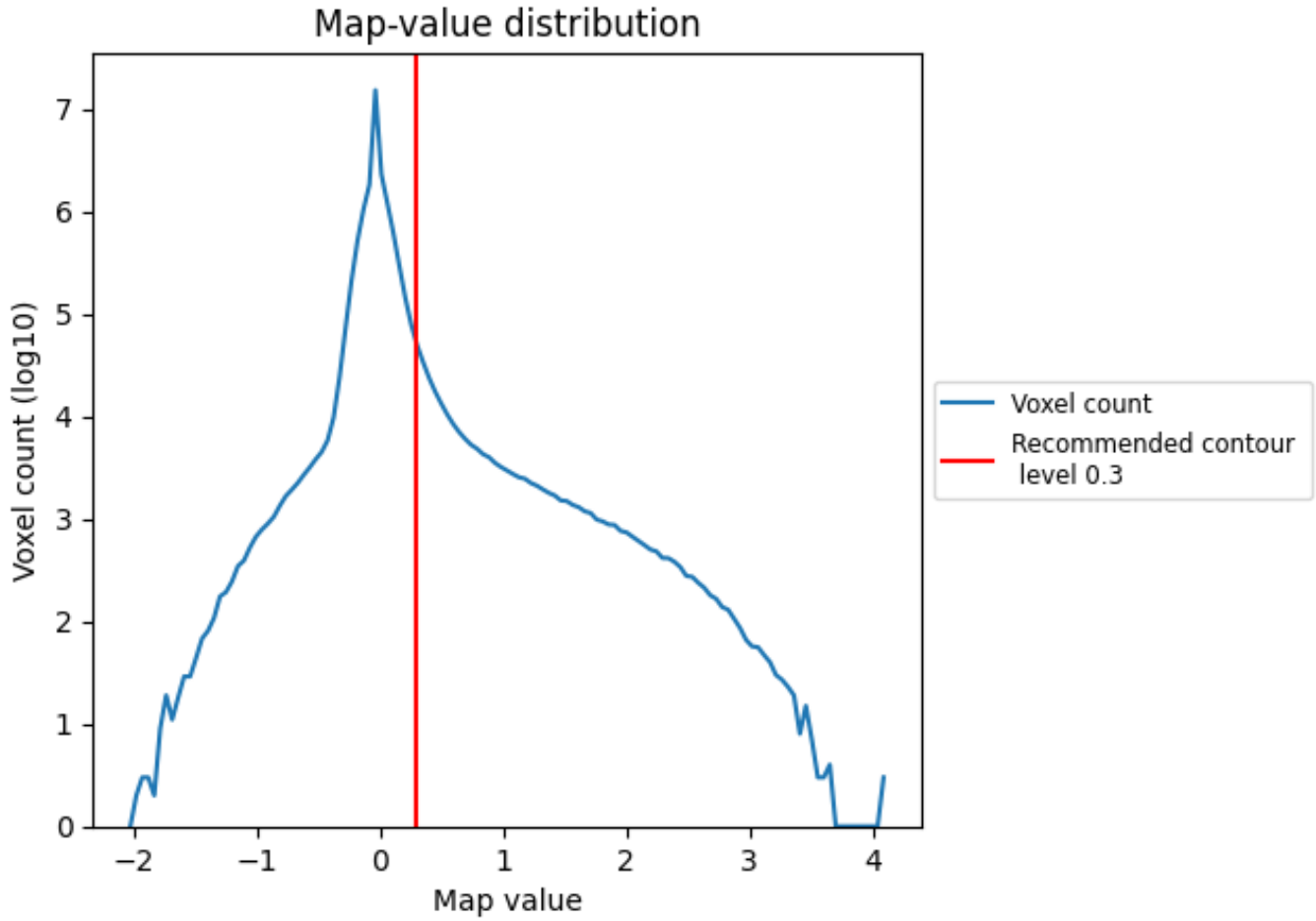
6.6 Mask visualisation (i)

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

7 Map analysis

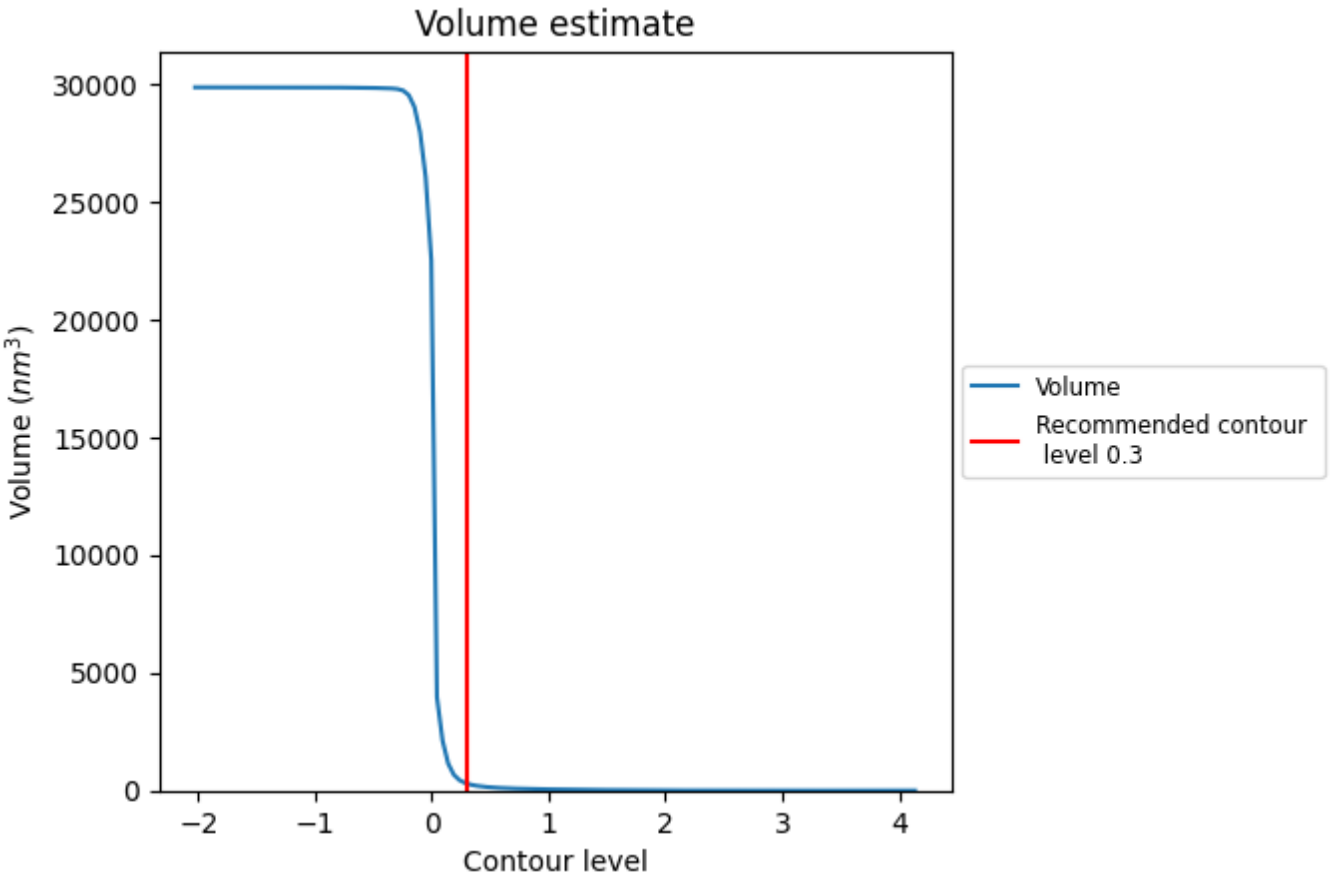
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

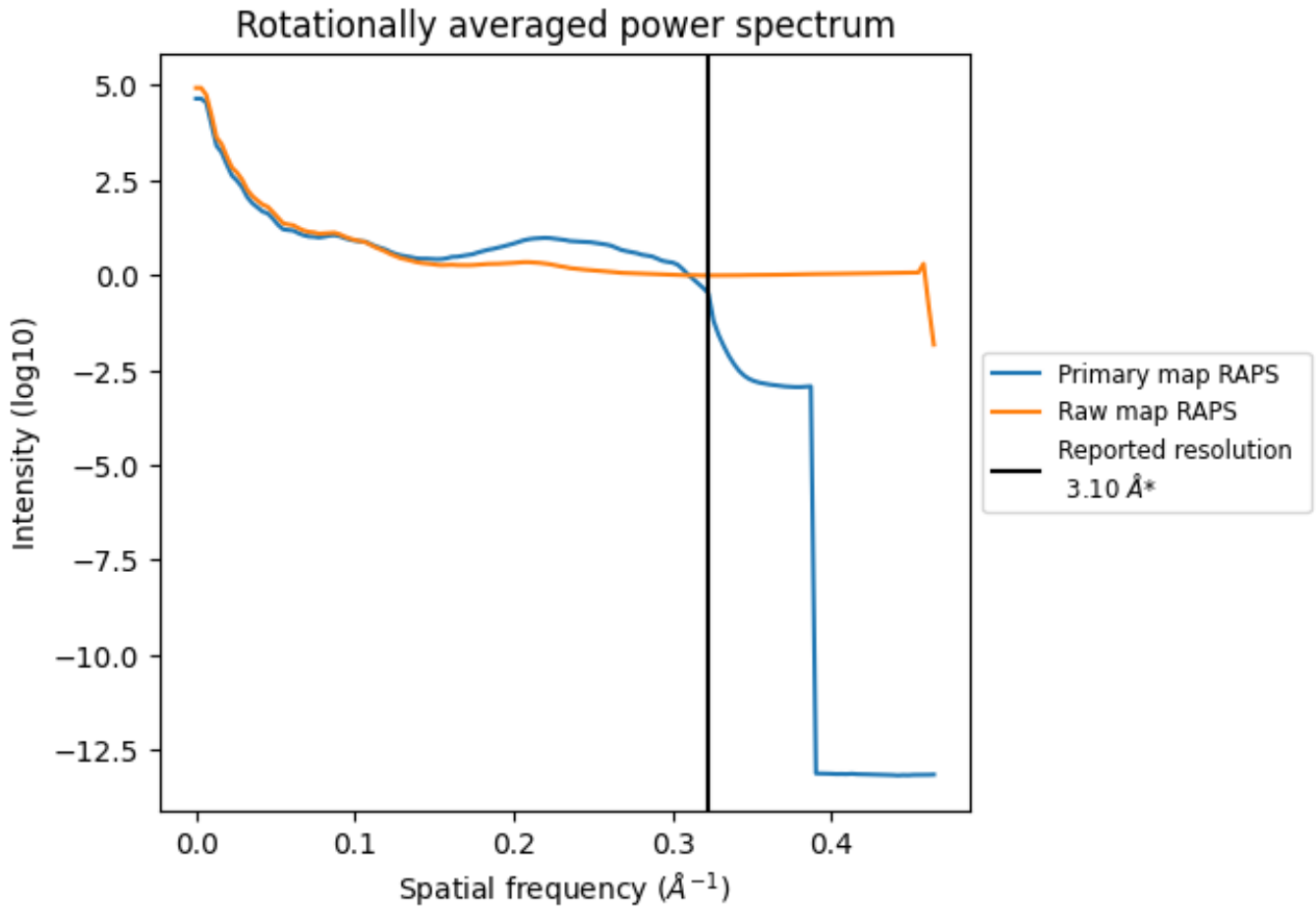
7.2 Volume estimate



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

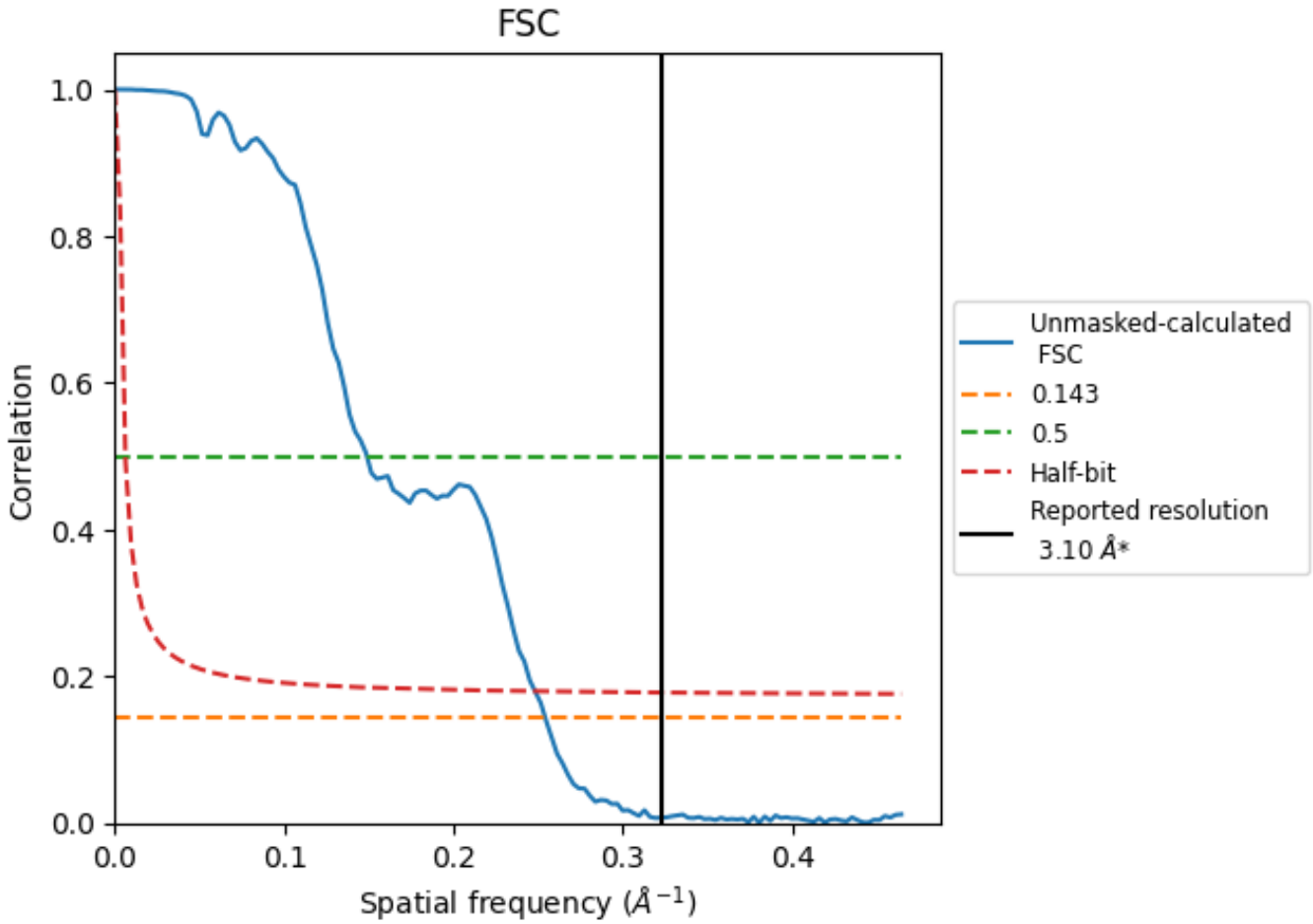


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

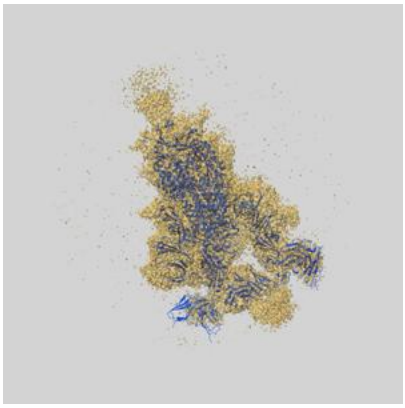
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.72	4.03

*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 3.94 differs from the reported value 3.1 by more than 10 %

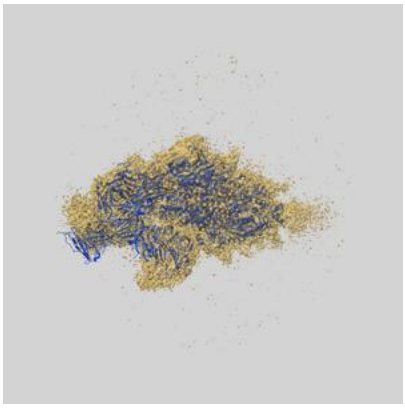
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34261 and PDB model 8GTP. Per-residue inclusion information can be found in section 3 on page 11.

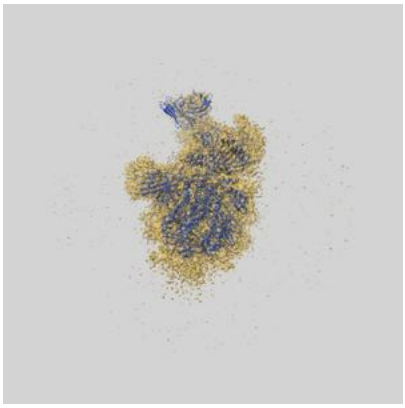
9.1 Map-model overlay



X



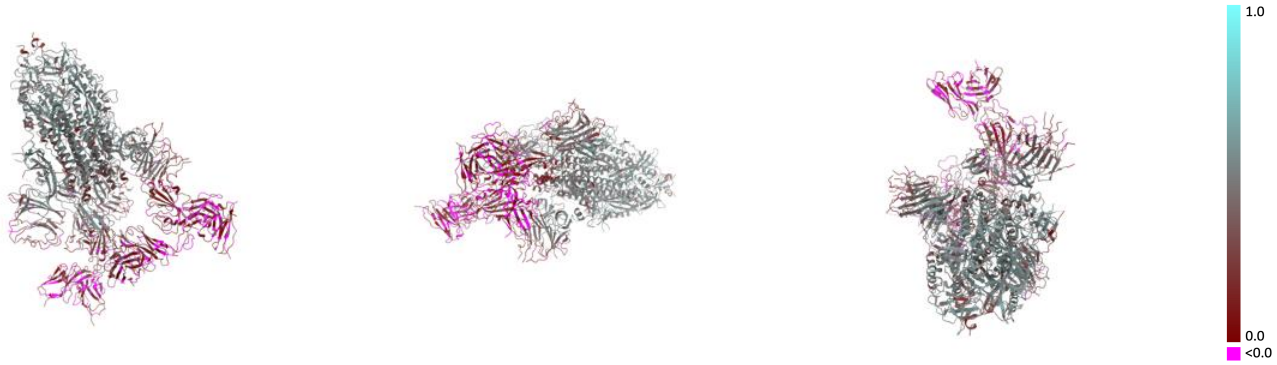
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

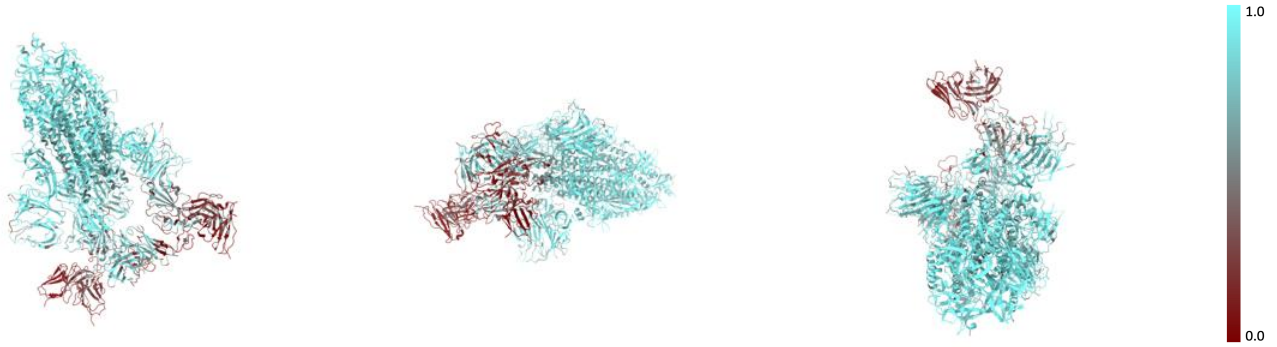
9.2 Q-score mapped to coordinate model (i)



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.

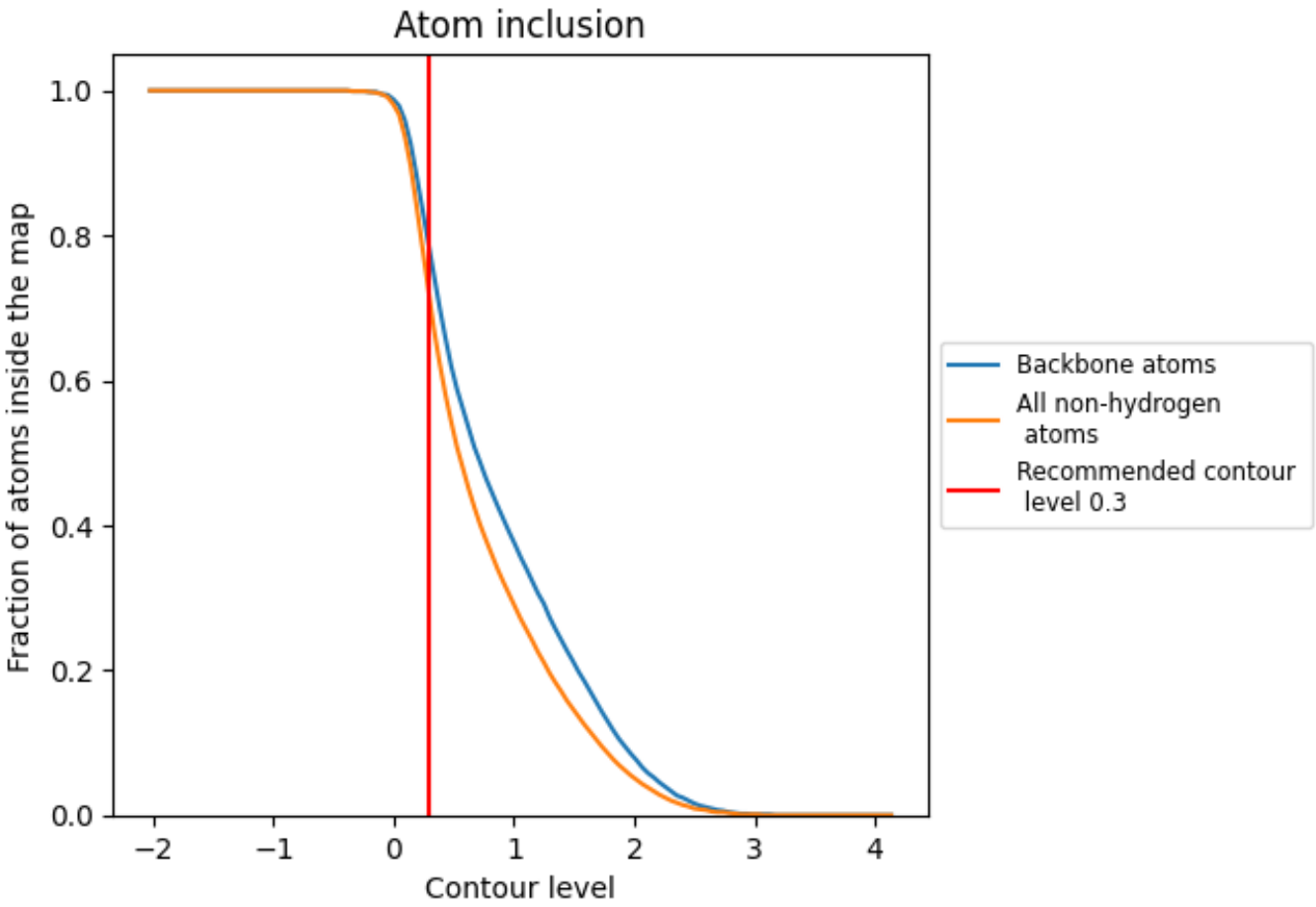
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.3350
A	0.8580	0.4320
B	0.7790	0.3780
C	0.7690	0.3650
D	0.4640	0.2470
E	0.5360	0.2650
F	0.7860	0.3230
G	0.7500	0.2850
H	0.6380	0.1410
I	0.0750	0.0370
J	0.1670	0.0680
K	0.8930	0.3770
L	0.5330	0.1310
M	0.0700	0.0280
N	0.0900	0.0250
O	0.7860	0.2960
P	0.4640	0.0480
Q	0.0360	0.0100
R	0.6790	0.2810
S	0.8210	0.3250
T	0.8570	0.3310
U	0.7860	0.3070
V	0.6790	0.1740
W	0.0000	0.0210
X	0.7140	0.3280
Y	0.7860	0.3280
Z	0.7500	0.2360
a	0.7860	0.2920