Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:21 AM JST

PDB ID	:	7DX8
EMDB ID	:	EMD-30899
Title	:	Trypsin-digested S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 2 (2 up RBD and 2 PD bound)
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on	:	2021-01-18
Resolution	:	2.90 Å(reported)

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

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

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

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

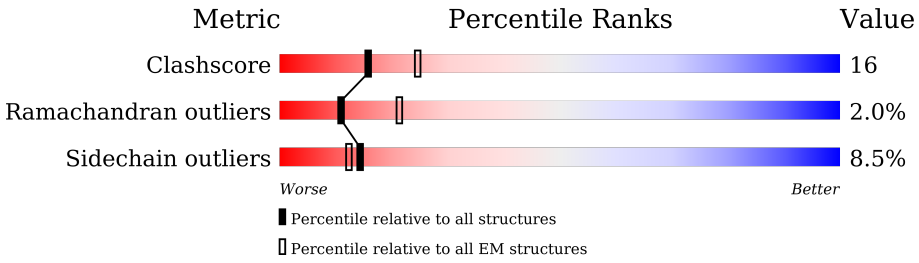
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 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	1283	13% 52% 21% • 22%
1	B	1283	9% 51% 20% • • 24%
1	C	1283	15% 54% 20% • • 22%
2	D	817	73% 65% 7% 27%
2	E	817	73% 65% 7% 27%
3	F	2	50% 100%
3	G	2	50% 50% 50%
3	H	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50%
3	J	2	50% 50%
3	K	2	50% 50%
3	L	2	50% 50%
3	M	2	50% 50%
3	N	2	100% 50% 50%
3	O	2	50% 100%
3	P	2	50% 50%
3	Q	2	50% 50%
3	R	2	100%
3	S	2	100%
3	T	2	50% 100%
3	U	2	100% 50% 50%
3	V	2	50% 50% 50%
3	W	2	50% 50%
3	X	2	100%
3	Y	2	50% 50% 50%
3	Z	2	100%
3	a	2	100%
3	b	2	100% 50% 50%
3	c	2	100% 50% 50%
3	d	2	100% 100%
3	e	2	100% 100%
3	f	2	100% 50% 50%
3	g	2	100% 50% 50%

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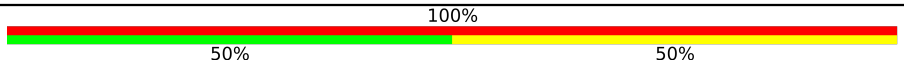
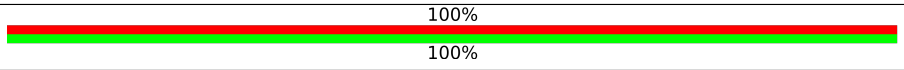
Mol	Chain	Length	Quality of chain
3	h	2	
3	i	2	
3	j	2	
3	k	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 34338 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	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
1	B	971	Total	C	N	O	S	0	0
			7584	4843	1262	1445	34		
1	C	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 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
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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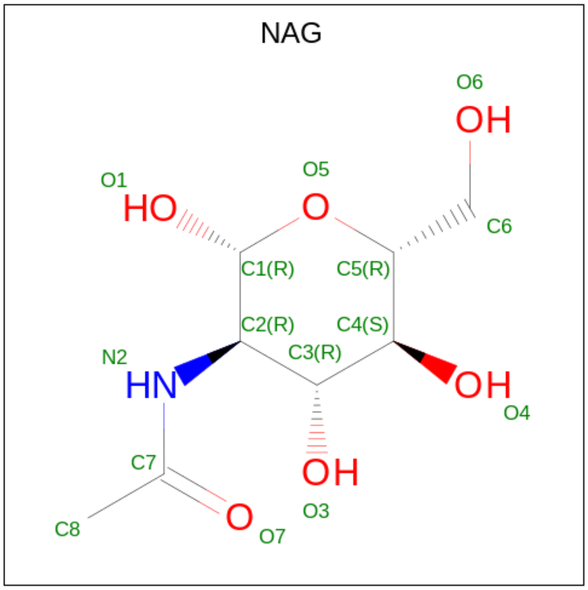
Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0

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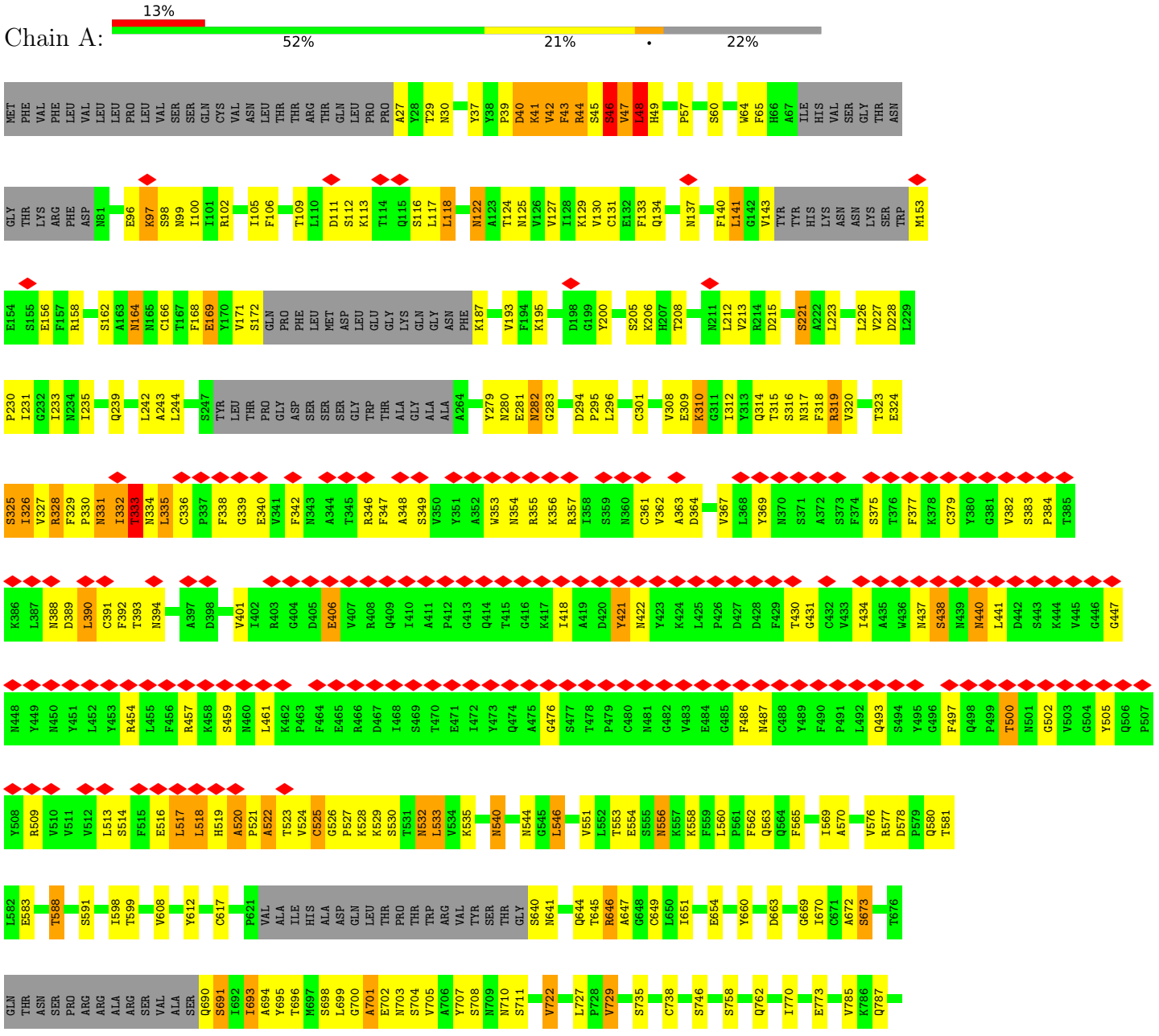
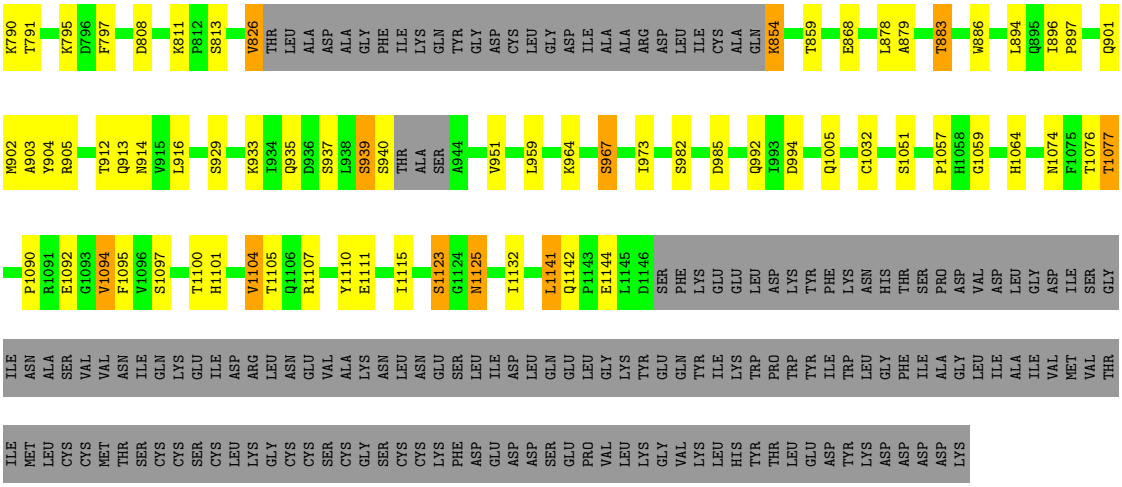
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	B	1	Total C N O 140 80 10 50	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	C	1	Total C N O 112 64 8 40	0
4	D	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0

3 Residue-property plots (i)

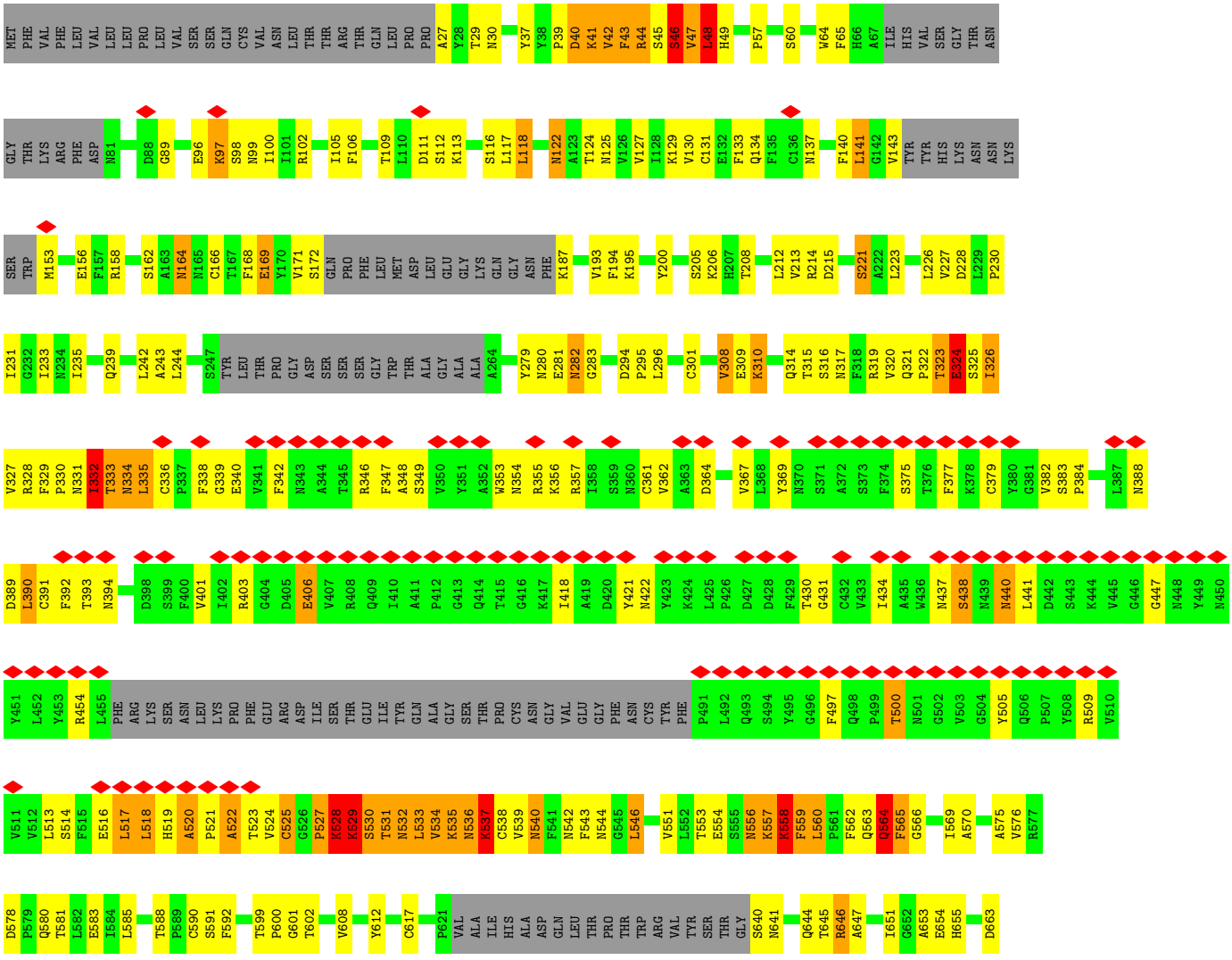
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

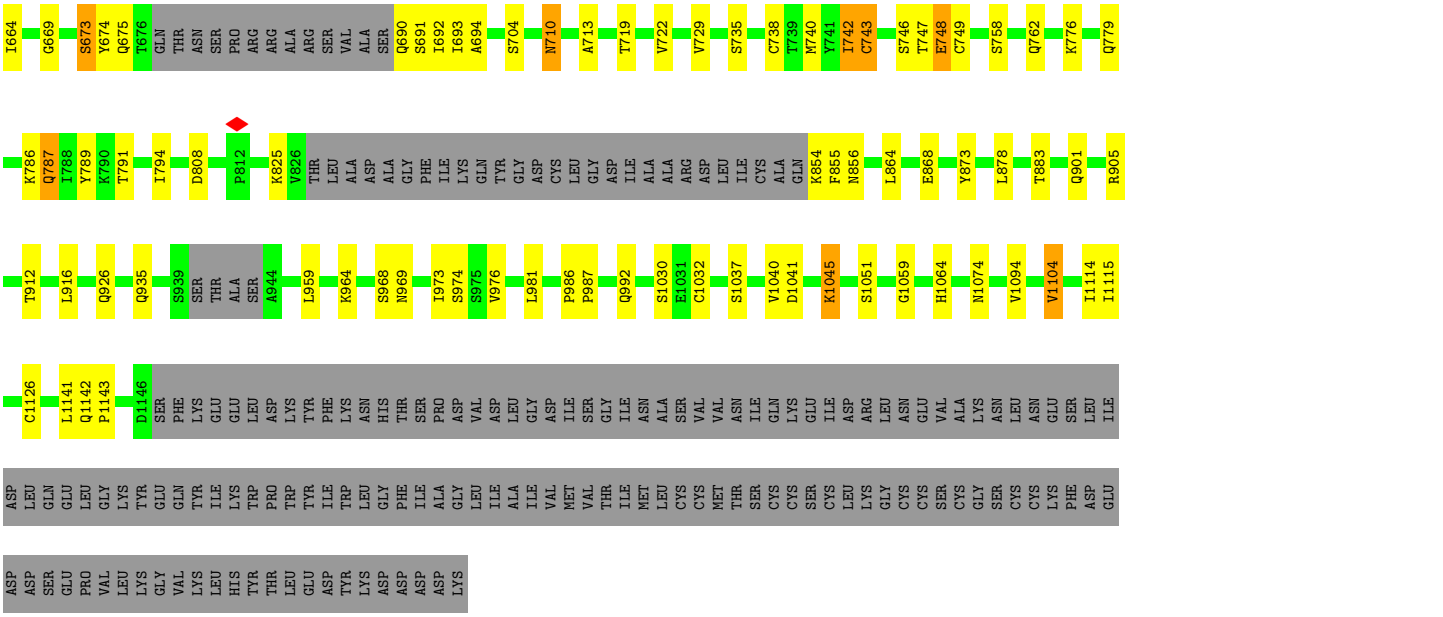
- Molecule 1: Spike glycoprotein





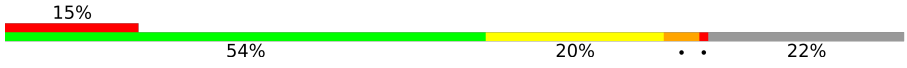
• Molecule 1: Spike glycoprotein

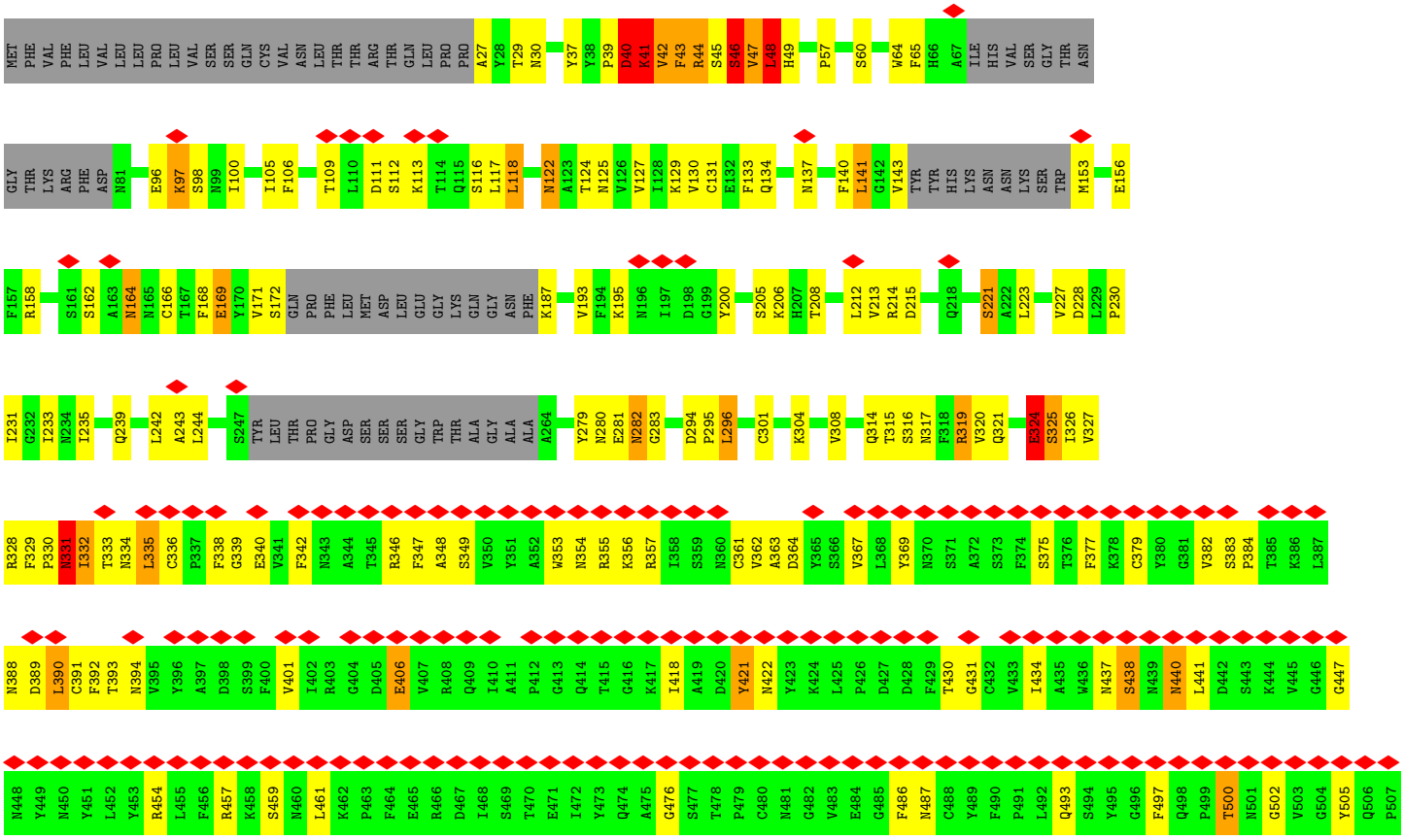


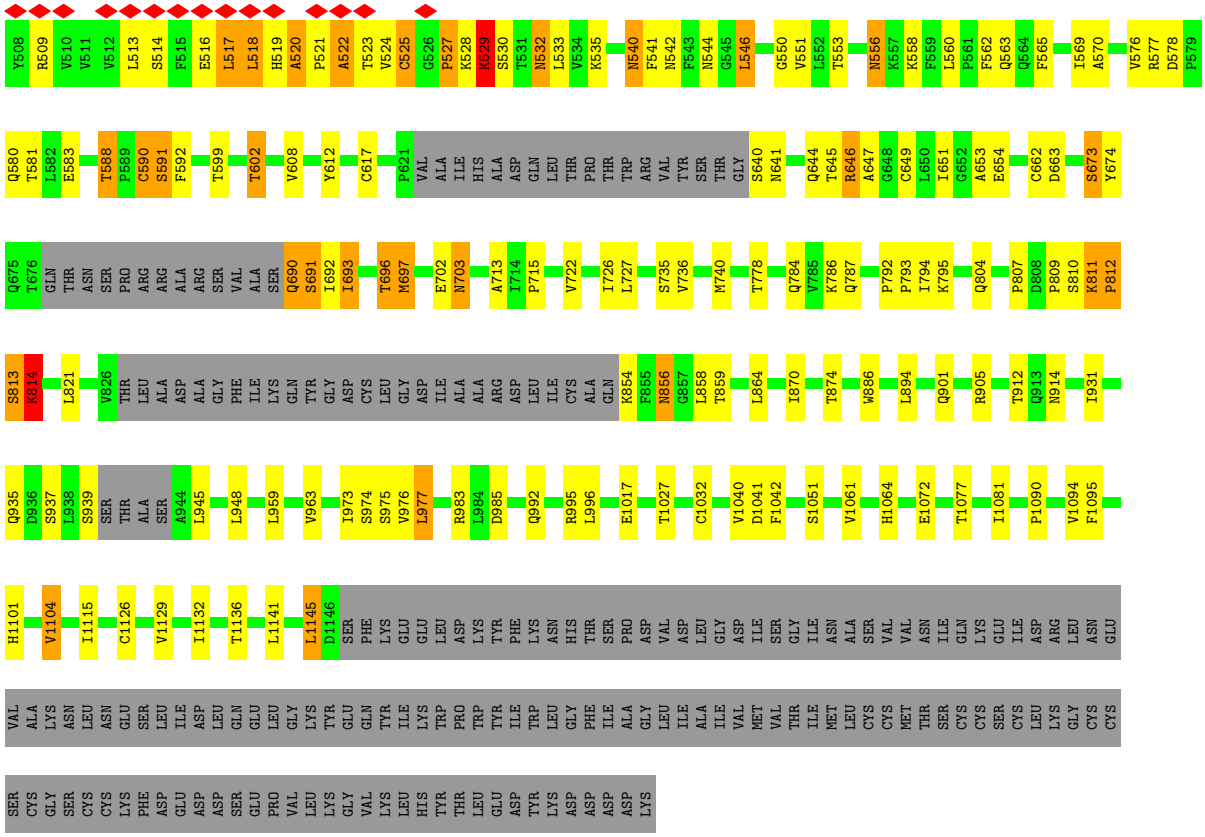


• Molecule 1: Spike glycoprotein

Chain C:

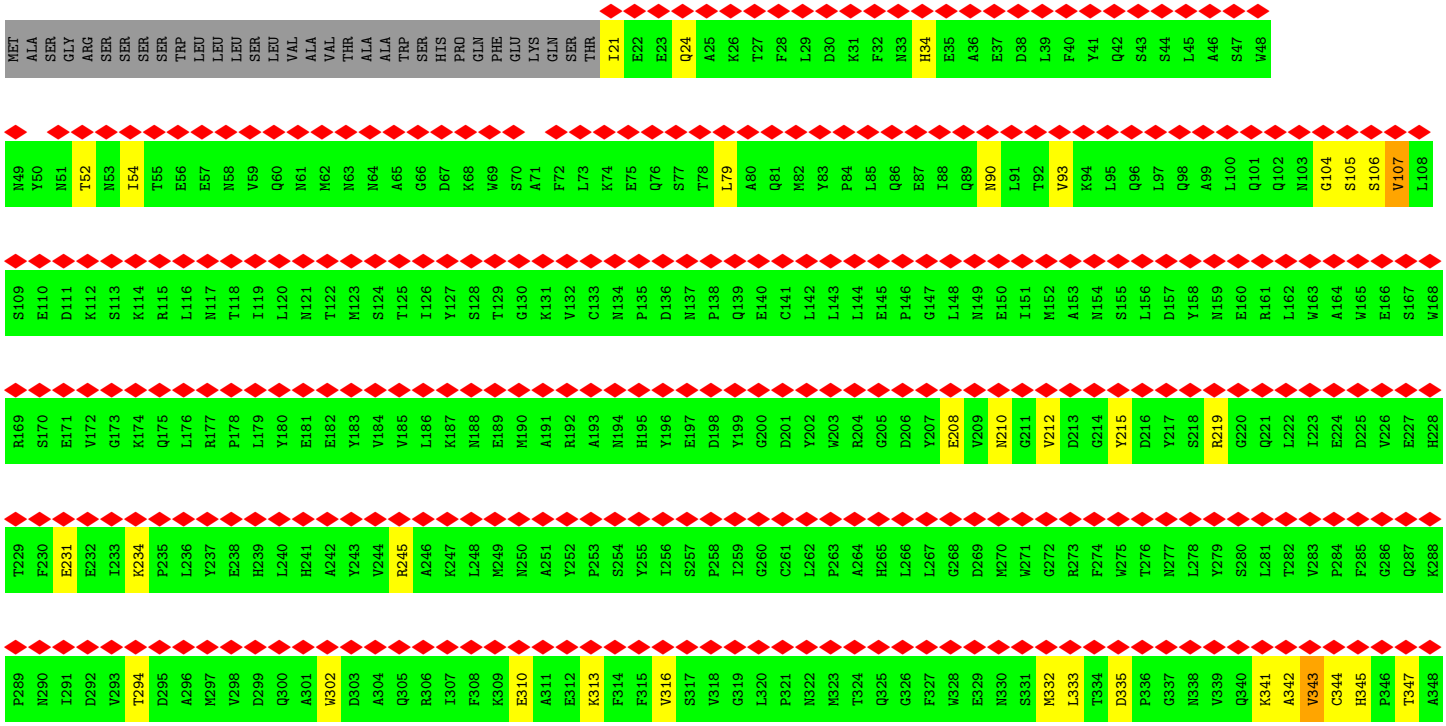


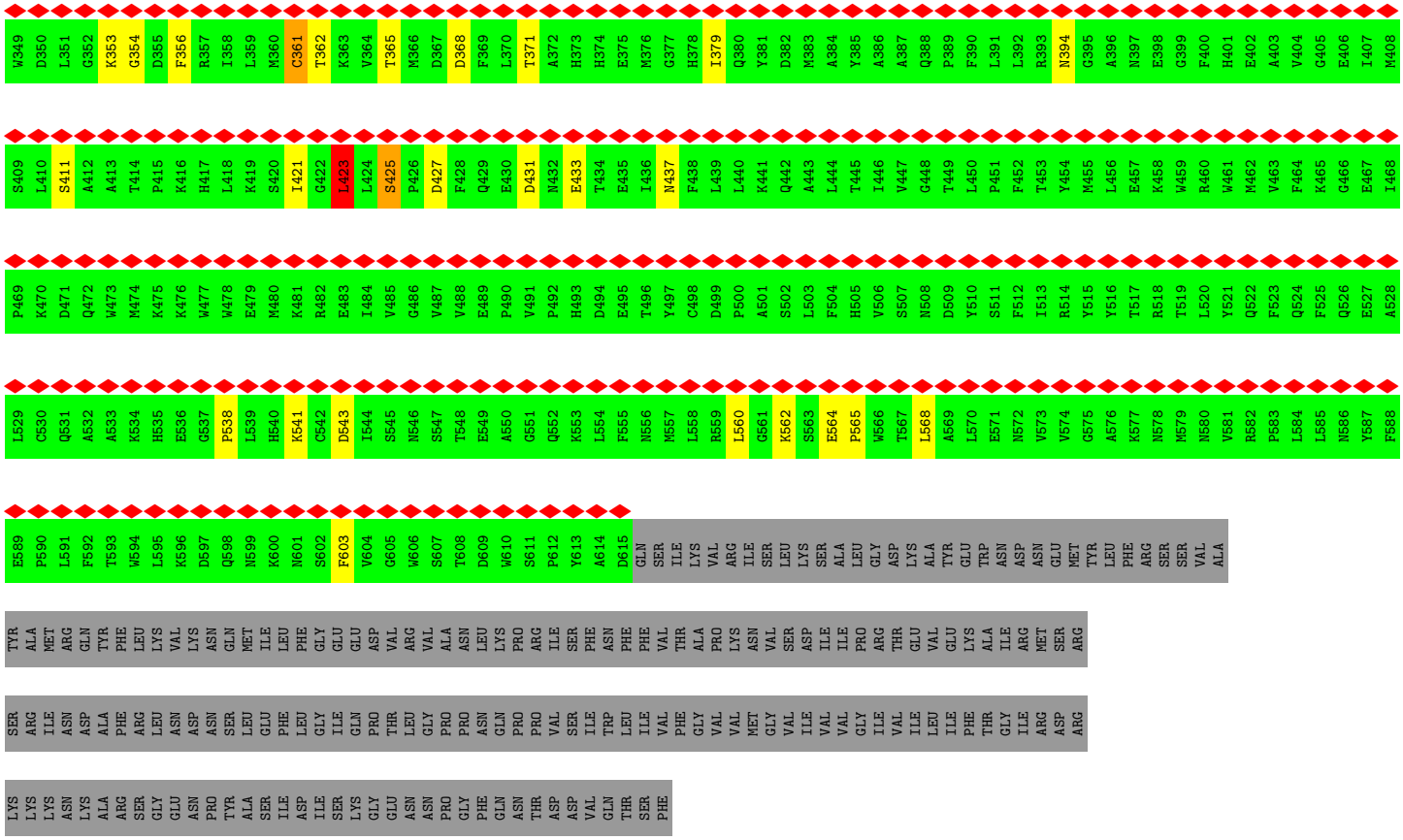




• Molecule 2: Angiotensin-converting enzyme 2

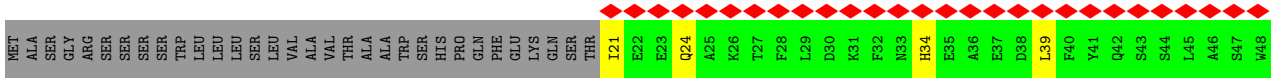
Chain D:

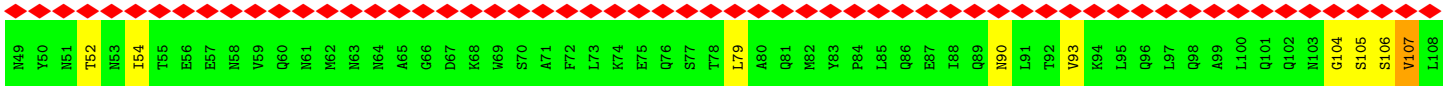


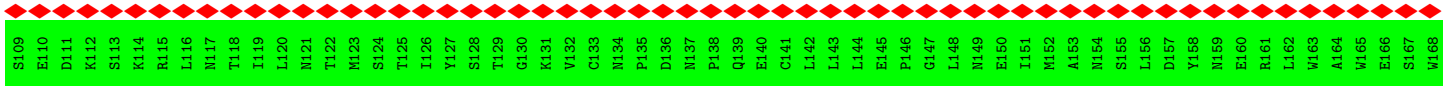


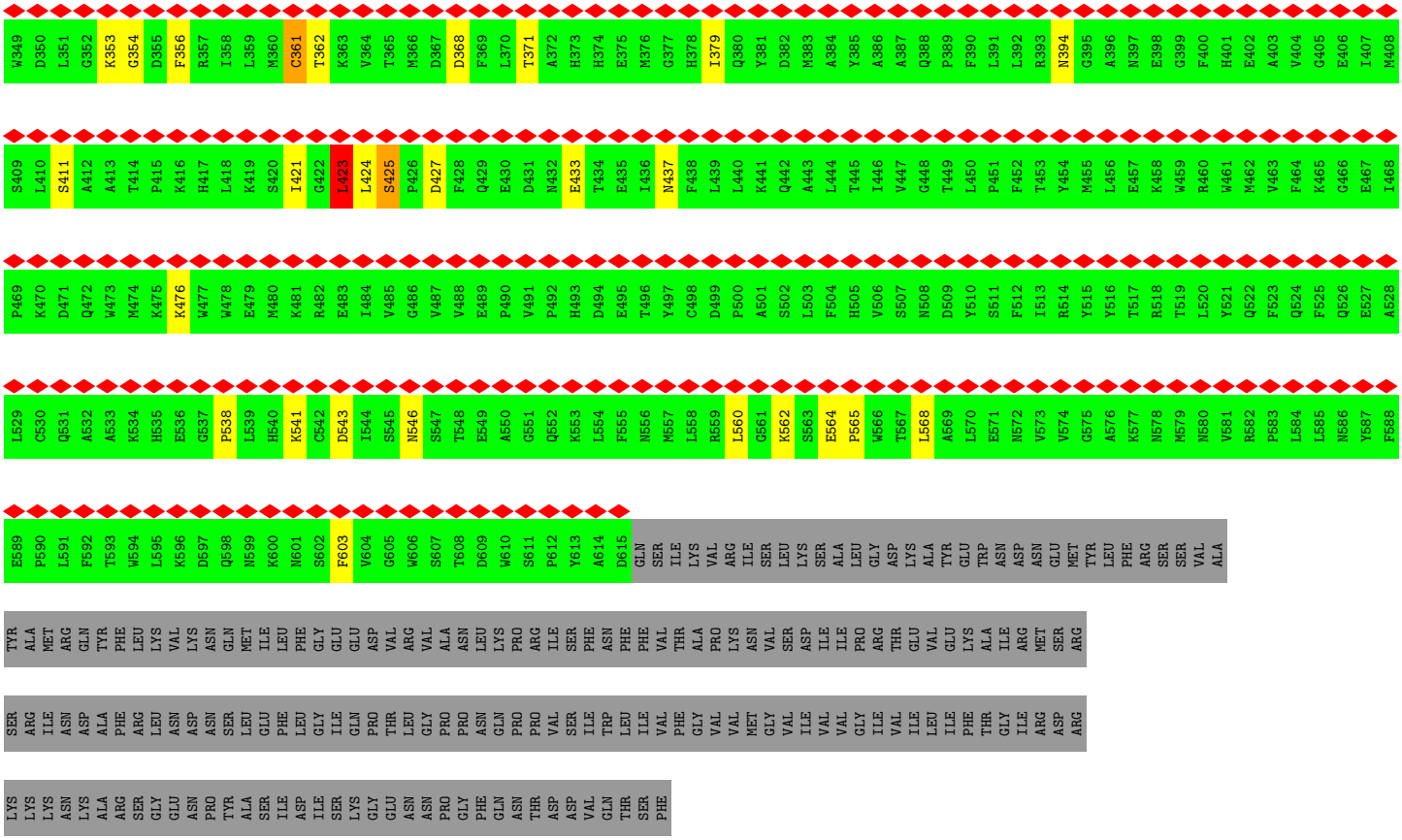
• Molecule 2: Angiotensin-converting enzyme 2

Chain E:



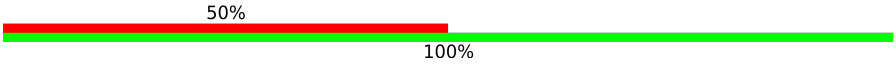






• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

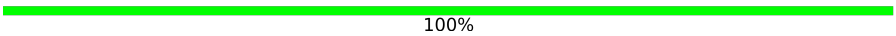


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

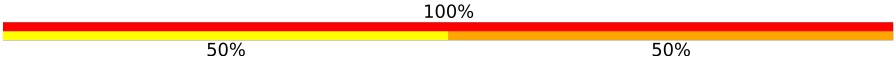
Chain L:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

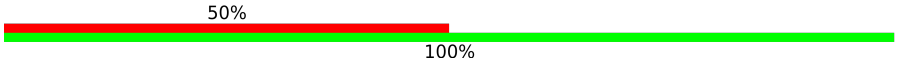
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

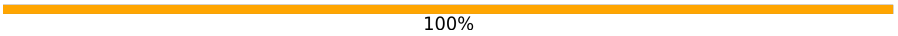
Chain P:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

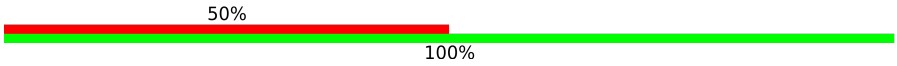


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

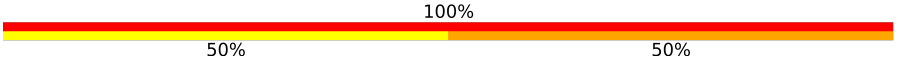
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

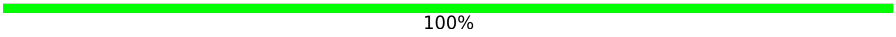
Chain V:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

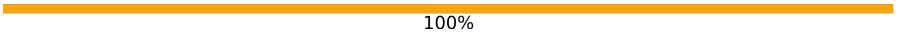


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

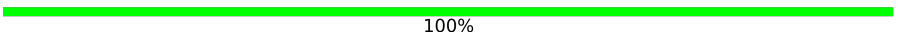
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



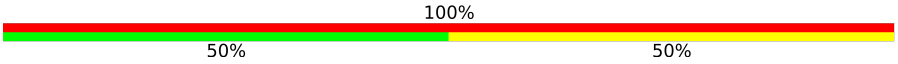
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



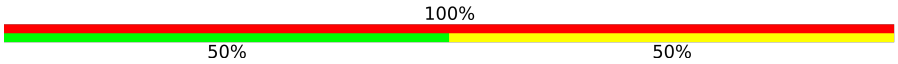
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



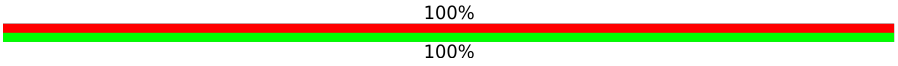
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

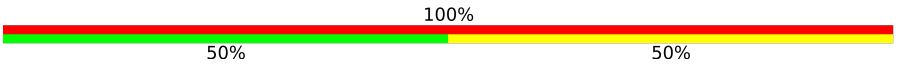


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

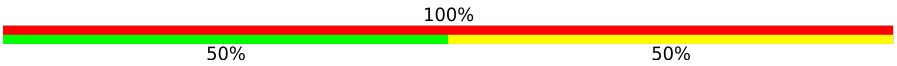
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



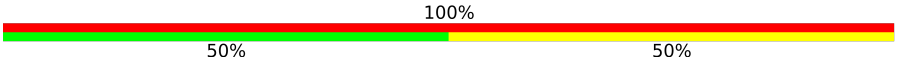
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

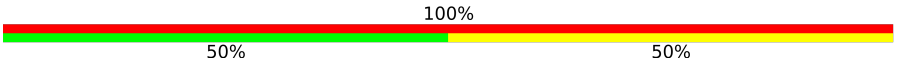
Chain i:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208455	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.58	0/8048	0.55	0/10947
1	B	0.57	0/7751	0.55	0/10544
1	C	0.58	0/8042	0.54	0/10939
2	D	0.35	0/4994	0.50	0/6785
2	E	0.35	0/4994	0.50	0/6785
All	All	0.52	0/33829	0.54	0/46000

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	7872	0	7668	335	0
1	B	7584	0	7402	364	0
1	C	7866	0	7663	373	0
2	D	4857	0	4624	66	0
2	E	4857	0	4624	67	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	6	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	2	0
3	N	28	0	25	3	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	4	0
3	V	28	0	25	1	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	1	0
3	Z	28	0	25	2	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	0	0
3	j	28	0	25	0	0
3	k	28	0	25	0	0
4	A	126	0	117	4	0
4	B	140	0	129	8	0
4	C	112	0	104	4	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
All	All	34338	0	33157	1090	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 16.

All (1090) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:GLU:HG3	1:C:693:ILE:CG2	1.37	1.50
4:B:1409:NAG:O4	4:B:1410:NAG:C1	1.63	1.46
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.47	1.44
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.28
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.21
1:C:486:PHE:CE1	2:E:79:LEU:HD22	1.75	1.20
1:B:320:VAL:HG23	1:B:591:SER:O	1.45	1.15
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:B:519:HIS:ND1	1:C:41:LYS:HD2	1.63	1.13
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.13
1:C:523:THR:HG22	1:C:524:VAL:H	0.98	1.12
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.15	1.12
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.11
1:C:654:GLU:CG	1:C:693:ILE:CG2	2.28	1.11
1:A:230:PRO:CA	1:C:521:PRO:CG	2.29	1.11
1:A:523:THR:HG22	1:A:524:VAL:H	0.98	1.10
1:B:748:GLU:HG3	1:B:981:LEU:HD21	1.32	1.10
1:B:392:PHE:HB3	1:B:517:LEU:HD21	1.35	1.09
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.35	1.09
1:B:523:THR:HG22	1:B:524:VAL:H	0.98	1.08
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.08
1:B:560:LEU:HD23	1:B:563:GLN:OE1	1.52	1.08
1:A:230:PRO:CA	1:C:521:PRO:HG3	1.84	1.08
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.07
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.35	1.07
1:A:230:PRO:HA	1:C:521:PRO:HG3	1.30	1.07
1:B:519:HIS:O	1:C:41:LYS:HD3	1.55	1.05
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.04
1:B:392:PHE:HB3	1:B:517:LEU:CD2	1.88	1.04
1:A:230:PRO:CB	1:C:521:PRO:CG	2.34	1.04
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.03
1:B:529:LYS:HA	1:B:529:LYS:HE3	1.40	1.03
1:C:674:TYR:HD1	1:C:691:SER:O	1.41	1.03
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.02
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.41	1.02
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
4:B:1409:NAG:C4	4:B:1410:NAG:C1	2.38	1.01
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.01
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	1.00
1:A:523:THR:HG22	1:A:524:VAL:N	1.73	1.00
1:C:44:ARG:O	1:C:283:GLY:HA2	1.61	1.00
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	0.99
1:B:523:THR:HG22	1:B:524:VAL:N	1.73	0.99
1:B:392:PHE:CB	1:B:517:LEU:HD21	1.91	0.99
1:C:654:GLU:O	1:C:693:ILE:HG22	1.62	0.99
1:B:748:GLU:CG	1:B:981:LEU:HD21	1.91	0.99
1:C:654:GLU:HG3	1:C:693:ILE:HG21	1.45	0.99
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:A:230:PRO:HB2	1:C:521:PRO:HG2	1.03	0.98
1:C:486:PHE:CE1	2:E:79:LEU:CD2	2.47	0.98
1:A:486:PHE:CE1	2:D:79:LEU:CD2	2.47	0.98
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.98
1:A:230:PRO:CA	1:C:521:PRO:HG2	1.92	0.97
1:C:523:THR:HG22	1:C:524:VAL:N	1.73	0.97
2:E:302:TRP:CH2	2:E:423:LEU:HD11	1.99	0.97
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.97
1:C:328:ARG:NE	1:C:533:LEU:HD23	1.80	0.96
1:B:523:THR:CG2	1:B:524:VAL:H	1.77	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.96
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.96
1:B:357:ARG:CZ	1:C:230:PRO:HB2	1.95	0.96
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.96
1:B:328:ARG:NH1	1:B:533:LEU:HD23	1.81	0.95
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.95
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.94
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.02	0.94
1:A:703:ASN:OD1	1:B:789:TYR:HE1	1.50	0.94
1:B:332:ILE:HD12	1:B:332:ILE:H	1.32	0.93
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.34	0.93
1:C:328:ARG:HE	1:C:533:LEU:HD23	1.34	0.92
1:A:505:TYR:CD2	2:D:353:LYS:O	2.23	0.92
2:E:302:TRP:HH2	2:E:423:LEU:HD11	1.34	0.92
1:C:505:TYR:CD2	2:E:353:LYS:O	2.23	0.91
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.91
1:B:529:LYS:HA	1:B:529:LYS:CE	1.99	0.91
1:C:486:PHE:HE1	2:E:79:LEU:CD2	1.84	0.90
1:C:319:ARG:HH21	1:C:319:ARG:HG3	1.35	0.89
1:A:486:PHE:HE1	2:D:79:LEU:CD2	1.84	0.89
1:A:476:GLY:CA	2:D:24:GLN:HE21	1.85	0.89
1:C:476:GLY:CA	2:E:24:GLN:HE21	1.85	0.88
1:B:519:HIS:CE1	1:C:40:ASP:HB2	2.08	0.88
1:C:674:TYR:CD1	1:C:691:SER:O	2.26	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HA	1:C:565:PHE:O	1.75	0.87
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.87
1:A:319:ARG:NH2	1:B:740:MET:SD	2.47	0.87
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.87
1:A:334:ASN:O	1:A:362:VAL:HB	1.74	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.86
1:C:654:GLU:CG	1:C:693:ILE:HG22	1.98	0.86
2:E:105:SER:O	2:E:106:SER:OG	1.93	0.86
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.57	0.86
1:A:565:PHE:O	1:B:42:VAL:HA	1.75	0.86
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.86
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.86
1:C:674:TYR:CZ	1:C:690:GLN:N	2.44	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.76	0.86
1:C:388:ASN:OD1	1:C:527:PRO:HD2	1.74	0.86
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.86
1:B:392:PHE:CD2	1:B:517:LEU:HD21	2.11	0.85
1:A:319:ARG:HH22	1:B:740:MET:CG	1.89	0.85
1:A:393:THR:O	1:A:523:THR:HG21	1.75	0.85
2:E:335:ASP:HB3	2:E:361:CYS:SG	2.16	0.85
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.59	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.85
1:B:559:PHE:O	1:B:560:LEU:O	1.95	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.85
1:B:560:LEU:HB3	1:B:562:PHE:CE2	2.12	0.85
1:C:46:SER:HA	1:C:279:TYR:O	1.76	0.85
1:B:393:THR:O	1:B:523:THR:HG21	1.75	0.84
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.06	0.84
1:B:519:HIS:O	1:C:41:LYS:CD	2.26	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.84
1:B:516:GLU:O	1:B:517:LEU:HD22	1.78	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:C:328:ARG:CZ	1:C:533:LEU:HD23	2.07	0.83
1:A:486:PHE:CZ	2:D:79:LEU:HD22	2.13	0.83
1:C:486:PHE:CZ	2:E:79:LEU:HD22	2.13	0.83
1:A:703:ASN:OD1	1:B:789:TYR:CE1	2.32	0.83
1:A:230:PRO:HB2	1:C:521:PRO:CG	2.00	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:HA	1:C:521:PRO:CG	2.01	0.82
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:B:519:HIS:CE1	1:C:41:LYS:HD2	2.15	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:B:519:HIS:ND1	1:C:41:LYS:CD	2.42	0.81
1:B:560:LEU:H	1:B:560:LEU:HD22	1.46	0.81
1:A:43:PHE:HD1	1:C:563:GLN:OE1	1.63	0.80
1:C:328:ARG:NH2	1:C:533:LEU:HD23	1.97	0.80
1:B:748:GLU:N	1:B:748:GLU:OE2	2.14	0.80
1:A:388:ASN:OD1	1:A:527:PRO:HD2	1.81	0.79
3:I:1:NAG:C3	3:I:2:NAG:HN2	4.90	0.79
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.65	0.79
1:A:230:PRO:C	1:C:521:PRO:CG	2.51	0.79
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.78
1:A:42:VAL:HG22	1:C:565:PHE:CE2	2.18	0.77
1:C:390:LEU:HD23	1:C:391:CYS:H	1.49	0.77
1:A:200:TYR:CE1	1:C:521:PRO:HB2	2.19	0.77
1:C:654:GLU:HG3	1:C:693:ILE:HG23	1.58	0.77
1:B:392:PHE:O	1:B:523:THR:HB	1.83	0.77
1:A:319:ARG:HH22	1:B:740:MET:HG3	1.47	0.77
1:C:335:LEU:HA	1:C:362:VAL:HB	1.67	0.76
1:C:476:GLY:HA3	2:E:24:GLN:HE21	1.50	0.76
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.66	0.76
2:E:302:TRP:HH2	2:E:423:LEU:CD1	1.98	0.76
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:C:476:GLY:HA2	2:E:24:GLN:HE21	1.50	0.76
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.76
1:B:335:LEU:HA	1:B:362:VAL:HB	1.67	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
1:A:476:GLY:HA2	2:D:24:GLN:HE21	1.50	0.76
1:B:675:GLN:O	1:B:690:GLN:HG3	1.86	0.76
1:A:476:GLY:HA3	2:D:24:GLN:HE21	1.50	0.75
1:B:361:CYS:SG	1:B:524:VAL:HG21	2.25	0.75
1:B:558:LYS:H	1:B:558:LYS:HD2	1.49	0.75
1:C:735:SER:OG	1:C:859:THR:CG2	2.34	0.75
1:A:390:LEU:HD23	1:A:391:CYS:H	1.49	0.75
1:B:357:ARG:HH12	1:B:394:ASN:ND2	1.84	0.75
1:B:390:LEU:HD23	1:B:391:CYS:H	1.49	0.75
1:B:559:PHE:HZ	1:B:566:GLY:N	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.75
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:C:361:CYS:SG	1:C:524:VAL:HG21	2.25	0.75
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.33	0.75
2:E:335:ASP:CB	2:E:361:CYS:SG	2.75	0.75
1:A:703:ASN:CB	1:B:787:GLN:OE1	2.23	0.74
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.74
1:C:332:ILE:HD12	1:C:332:ILE:N	2.02	0.74
1:C:320:VAL:HG23	1:C:591:SER:O	1.87	0.74
1:B:47:VAL:O	1:B:49:HIS:N	2.20	0.74
1:C:47:VAL:O	1:C:49:HIS:N	2.20	0.74
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.34	0.74
1:B:743:CYS:SG	1:B:749:CYS:C	2.67	0.74
1:A:43:PHE:N	1:C:565:PHE:O	2.21	0.74
1:B:382:VAL:HA	1:C:983:ARG:O	1.88	0.74
1:C:654:GLU:O	1:C:693:ILE:CG2	2.35	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.73
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.73
1:B:560:LEU:CD2	1:B:563:GLN:OE1	2.34	0.73
1:A:230:PRO:C	1:C:521:PRO:HG3	2.08	0.73
1:C:319:ARG:HG3	1:C:319:ARG:NH2	2.03	0.72
1:B:392:PHE:HD2	1:B:517:LEU:HD21	1.53	0.72
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.54	0.72
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.72
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.71	0.72
1:B:533:LEU:HD11	1:B:535:LYS:CE	2.19	0.72
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
1:C:674:TYR:CE1	1:C:691:SER:N	2.57	0.72
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.72
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
1:C:326:ILE:HD12	1:C:326:ILE:O	1.90	0.71
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.25	0.71
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.71
1:C:124:THR:HG21	4:C:1402:NAG:HN2	1.56	0.71
4:B:1409:NAG:H4	4:B:1410:NAG:C1	2.21	0.71
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.71
1:C:363:ALA:O	1:C:527:PRO:HD3	1.91	0.70
1:B:124:THR:HG21	4:B:1402:NAG:HN2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:O	1:A:580:GLN:HG2	1.91	0.70
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.70
1:B:530:SER:O	1:B:531:THR:HB	1.91	0.70
1:A:124:THR:HG21	4:A:1402:NAG:HN2	1.56	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
1:A:200:TYR:CZ	1:C:521:PRO:HB2	2.26	0.70
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.70
1:C:41:LYS:HD2	1:C:41:LYS:H	1.57	0.69
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.69
1:B:321:GLN:CD	1:B:322:PRO:HD2	2.13	0.69
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.69
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.75	0.69
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.74	0.69
1:A:42:VAL:CG2	1:C:565:PHE:CZ	2.74	0.69
1:C:44:ARG:O	1:C:283:GLY:CA	2.40	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.69
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.69
1:C:654:GLU:C	1:C:693:ILE:HG22	2.14	0.68
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.68
1:B:392:PHE:CG	1:B:517:LEU:HD21	2.29	0.68
1:B:560:LEU:HB2	1:B:563:GLN:OE1	1.93	0.68
1:C:654:GLU:CG	1:C:693:ILE:HG23	2.19	0.68
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.24	0.68
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.68
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.67
1:B:326:ILE:HD11	1:B:543:PHE:CE1	2.29	0.67
1:B:519:HIS:CE1	1:C:41:LYS:H	2.12	0.67
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.67
1:B:533:LEU:HD11	1:B:535:LYS:NZ	2.08	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:A:533:LEU:HD12	1:A:533:LEU:C	2.15	0.67
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.29	0.67
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:C:328:ARG:HH21	1:C:533:LEU:HD23	1.58	0.67
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.67
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.30	0.67
1:B:320:VAL:HG21	1:B:591:SER:HB2	1.77	0.67
1:B:320:VAL:CG2	1:B:591:SER:O	2.34	0.67
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASN:OD1	1:B:527:PRO:HD3	1.94	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.78	0.66
1:A:388:ASN:OD1	1:A:527:PRO:CD	2.43	0.66
1:B:535:LYS:O	1:B:536:ASN:HB2	1.95	0.66
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.66
1:A:334:ASN:O	1:A:362:VAL:CB	2.42	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.66
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.66
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.66
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.66
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.66
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.66
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.66
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.65
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.65
1:B:559:PHE:O	1:B:560:LEU:C	2.35	0.65
1:B:323:THR:O	1:B:539:VAL:HG23	1.97	0.65
1:B:357:ARG:NH2	1:C:230:PRO:HB2	2.11	0.65
1:B:560:LEU:HB3	1:B:562:PHE:CD2	2.32	0.65
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.65
1:C:493:GLN:OE1	2:E:34:HIS:CB	2.45	0.65
1:C:569:ILE:H	1:C:569:ILE:HD12	1.61	0.65
1:B:392:PHE:HD2	1:B:517:LEU:CD2	2.09	0.65
1:A:493:GLN:OE1	2:D:34:HIS:CB	2.45	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:B:332:ILE:HG12	1:B:362:VAL:HG22	1.79	0.65
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.65
2:E:310:GLU:OE1	2:E:421:ILE:HD11	1.97	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.64
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.64
1:A:533:LEU:HD11	1:A:535:LYS:HE3	1.78	0.64
1:B:535:LYS:HE2	1:B:585:LEU:CD2	2.27	0.64
1:B:569:ILE:CG1	1:C:47:VAL:HG11	2.27	0.64
1:B:326:ILE:HG22	1:B:534:VAL:HG22	1.79	0.64
1:C:321:GLN:HA	1:C:321:GLN:OE1	1.97	0.64
1:B:319:ARG:HB2	1:B:319:ARG:CZ	2.28	0.64
1:B:357:ARG:NH1	1:B:394:ASN:HD21	1.96	0.64
1:C:690:GLN:O	1:C:691:SER:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LYS:HD2	1:A:854:LYS:N	2.13	0.64
1:A:43:PHE:CE1	1:A:282:ASN:O	2.52	0.63
1:B:592:PHE:CZ	1:C:854:LYS:HE3	2.33	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
2:E:302:TRP:CZ3	2:E:423:LEU:HD11	2.34	0.63
1:A:700:GLY:O	1:A:701:ALA:O	2.17	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:C:388:ASN:OD1	1:C:527:PRO:CD	2.45	0.63
2:E:335:ASP:N	2:E:361:CYS:SG	2.72	0.63
1:B:326:ILE:HG21	1:B:534:VAL:HG23	1.79	0.63
1:B:326:ILE:HG22	1:B:534:VAL:CG2	2.28	0.63
1:B:527:PRO:O	1:B:528:LYS:HB3	1.98	0.63
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.63
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
3:I:1:NAG:H3	3:I:2:NAG:HN2	4.51	0.63
1:C:333:THR:OG1	1:C:334:ASN:N	2.32	0.62
1:A:43:PHE:HE1	1:A:282:ASN:O	1.83	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:A:326:ILE:O	1:A:326:ILE:HG13	2.00	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62
1:B:326:ILE:CG2	1:B:534:VAL:CG2	2.77	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.62
1:B:382:VAL:HB	1:C:983:ARG:HB2	1.81	0.62
1:C:43:PHE:CE1	1:C:282:ASN:O	2.52	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.82	0.62
1:B:592:PHE:CE1	1:C:854:LYS:HE3	2.35	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
1:A:327:VAL:O	1:A:328:ARG:HD3	1.99	0.62
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.62
1:B:325:SER:HA	1:B:540:ASN:O	1.99	0.62
1:B:522:ALA:O	1:B:523:THR:OG1	2.14	0.62
1:A:530:SER:CB	1:A:580:GLN:NE2	2.63	0.61
1:B:326:ILE:HD12	1:B:326:ILE:O	2.00	0.61
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.61
1:C:457:ARG:NH1	1:C:459:SER:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.61
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.61
1:C:662:CYS:HB2	1:C:697:MET:CE	2.26	0.61
1:B:521:PRO:O	1:B:522:ALA:HB2	2.01	0.61
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:C:43:PHE:HE1	1:C:282:ASN:O	1.82	0.60
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.83	0.60
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.83	0.60
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.60
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.60
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.60
1:C:327:VAL:HG12	1:C:328:ARG:N	2.16	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.60
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.83	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.60
1:B:332:ILE:HG12	1:B:362:VAL:CG2	2.32	0.60
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.60
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.60
1:C:328:ARG:HH21	1:C:533:LEU:CD2	2.15	0.59
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.59
1:C:533:LEU:O	1:C:533:LEU:HD12	2.02	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:B:565:PHE:O	1:C:42:VAL:HA	2.02	0.59
1:B:592:PHE:CE1	1:C:854:LYS:CE	2.85	0.59
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.59
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.35	0.59
1:B:516:GLU:O	1:B:517:LEU:CD2	2.48	0.59
1:C:674:TYR:CE1	1:C:690:GLN:N	2.71	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.59
1:C:556:ASN:HD22	1:C:556:ASN:H	1.50	0.59
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:B:738:CYS:O	1:B:742:ILE:HG13	2.03	0.59
1:C:328:ARG:NH1	1:C:580:GLN:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.58
1:B:392:PHE:CD2	1:B:517:LEU:CD2	2.85	0.58
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.58
4:B:1405:NAG:H83	4:B:1405:NAG:H3	1.86	0.58
1:C:391:CYS:SG	1:C:523:THR:O	2.61	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:B:334:ASN:N	1:B:334:ASN:OD1	2.36	0.58
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.58
1:A:476:GLY:HA3	2:D:24:GLN:NE2	2.17	0.58
1:A:532:ASN:N	1:A:532:ASN:OD1	2.35	0.58
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.58
1:B:338:PHE:O	1:B:340:GLU:N	2.37	0.58
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.58
1:B:565:PHE:O	1:B:565:PHE:HD1	1.86	0.58
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.58
1:C:476:GLY:HA3	2:E:24:GLN:NE2	2.18	0.58
2:E:212:VAL:HG21	2:E:565:PRO:HG3	1.84	0.58
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:A:318:PHE:CE2	1:A:320:VAL:CG2	2.86	0.58
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.58
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
3:Y:2:NAG:H3	3:Y:2:NAG:H83	1.86	0.58
1:C:328:ARG:NH2	1:C:533:LEU:CD2	2.65	0.58
1:C:361:CYS:SG	1:C:524:VAL:CG2	2.92	0.58
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.58
1:B:391:CYS:SG	1:B:523:THR:O	2.61	0.58
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.58
1:B:361:CYS:SG	1:B:524:VAL:CG2	2.92	0.58
1:B:392:PHE:HB3	1:B:517:LEU:HD22	1.82	0.58
1:B:519:HIS:CE1	1:C:41:LYS:N	2.72	0.58
1:B:560:LEU:HD22	1:B:560:LEU:N	2.16	0.58
1:C:338:PHE:O	1:C:340:GLU:N	2.37	0.58
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.58
1:A:332:ILE:HG22	1:A:333:THR:N	2.19	0.58
2:E:368:ASP:HA	2:E:371:THR:HG22	1.85	0.58
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.57
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.57
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.57
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1405:NAG:H3	4:A:1405:NAG:H83	1.86	0.57
1:B:41:LYS:O	1:B:42:VAL:HB	2.04	0.57
1:B:332:ILE:HD12	1:B:332:ILE:N	2.03	0.57
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.87	0.57
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:B:357:ARG:CZ	1:C:230:PRO:CB	2.77	0.57
1:A:391:CYS:SG	1:A:523:THR:O	2.61	0.57
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
1:A:318:PHE:CE2	1:A:320:VAL:HG23	2.39	0.57
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.57
1:A:335:LEU:HA	1:A:362:VAL:HB	1.86	0.57
1:A:530:SER:HB3	1:A:580:GLN:HE22	1.69	0.57
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:A:335:LEU:HD12	1:A:335:LEU:H	1.69	0.57
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.57
1:C:332:ILE:HD12	1:C:332:ILE:H	1.68	0.57
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.57
1:B:357:ARG:NH1	1:C:230:PRO:CB	2.68	0.57
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.57
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.57
1:B:533:LEU:O	1:B:533:LEU:HG	2.05	0.56
1:C:519:HIS:O	1:C:519:HIS:ND1	2.38	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.87	0.56
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.56
1:B:559:PHE:HE2	1:B:564:GLN:O	1.88	0.56
3:Z:2:NAG:H3	3:Z:2:NAG:H83	1.87	0.56
1:B:533:LEU:CD1	1:B:535:LYS:CE	2.83	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
1:C:654:GLU:O	1:C:693:ILE:CB	2.53	0.56
1:C:735:SER:OG	1:C:859:THR:HG23	2.04	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
1:B:560:LEU:O	1:B:562:PHE:N	2.36	0.56
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.32	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.56
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.45	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:41:LYS:O	1:A:42:VAL:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CZ	2:D:79:LEU:CD2	2.84	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:B:295:PRO:HB2	1:B:608:VAL:HG11	1.88	0.56
1:C:29:THR:HG22	1:C:30:ASN:H	1.70	0.56
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.56
4:C:1405:NAG:H3	4:C:1405:NAG:H83	1.86	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.56
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.40	0.56
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
2:E:54:ILE:HD12	2:E:341:LYS:HG3	1.87	0.56
2:E:425:SER:HB3	2:E:427:ASP:OD1	2.06	0.56
1:A:42:VAL:CA	1:C:565:PHE:O	2.50	0.56
1:C:45:SER:O	1:C:279:TYR:HB2	2.05	0.56
1:C:551:VAL:HB	1:C:588:THR:HG23	1.88	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.56
1:C:332:ILE:HG21	1:C:362:VAL:HG11	1.87	0.56
1:C:653:ALA:HB2	1:C:692:ILE:HG22	1.87	0.56
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.55
1:B:559:PHE:HZ	1:B:566:GLY:CA	2.19	0.55
1:C:342:PHE:HB3	3:U:1:NAG:H82	1.87	0.55
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.55
3:J:2:NAG:H83	3:J:2:NAG:H3	1.87	0.55
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.55
1:A:342:PHE:HB3	3:G:1:NAG:H82	1.87	0.55
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.55
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.88	0.55
1:B:535:LYS:HE2	1:B:585:LEU:HD22	1.89	0.55
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55
1:B:357:ARG:NH1	1:B:394:ASN:ND2	2.54	0.55
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.55
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55
1:A:476:GLY:CA	2:D:24:GLN:NE2	2.65	0.55
1:B:328:ARG:HH22	1:B:580:GLN:HB2	1.70	0.55
1:B:342:PHE:HB3	3:N:1:NAG:H82	1.87	0.55
1:B:558:LYS:O	1:C:43:PHE:CE1	2.59	0.55
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:CE1	1:C:43:PHE:CB	2.89	0.55
1:C:45:SER:HA	1:C:280:ASN:O	2.06	0.55
1:C:326:ILE:HD12	1:C:541:PHE:HA	1.88	0.55
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.55
2:E:538:PRO:HD2	2:E:541:LYS:HD2	1.88	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.55
1:B:546:LEU:HD11	1:B:565:PHE:CD2	2.42	0.55
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.55
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.55
2:E:335:ASP:N	2:E:335:ASP:OD1	2.39	0.55
1:A:329:PHE:O	1:A:580:GLN:CG	2.55	0.55
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
3:N:1:NAG:H61	3:N:2:NAG:HN2	1.71	0.55
1:A:563:GLN:CD	1:B:43:PHE:HA	2.27	0.54
1:B:551:VAL:HB	1:B:588:THR:CG2	2.37	0.54
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:B:392:PHE:HA	1:B:517:LEU:HD11	1.89	0.54
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54
1:A:530:SER:HB3	1:A:580:GLN:NE2	2.21	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
1:C:486:PHE:CZ	2:E:79:LEU:CD2	2.84	0.54
3:G:1:NAG:H61	3:G:2:NAG:HN2	1.71	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.42	0.54
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.54
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.54
1:C:653:ALA:HA	1:C:692:ILE:O	2.08	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:C:421:TYR:HA	1:C:461:LEU:HG	1.89	0.54
1:A:43:PHE:CD1	1:C:563:GLN:OE1	2.52	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.86	0.54
1:B:557:LYS:HE3	1:B:575:ALA:HB2	1.90	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.54
2:E:231:GLU:HA	2:E:234:LYS:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:VAL:HB	1:B:588:THR:HG22	1.89	0.54
1:B:560:LEU:C	1:B:562:PHE:H	2.11	0.54
3:U:1:NAG:H61	3:U:2:NAG:HN2	1.71	0.54
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.54
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.90	0.54
1:B:559:PHE:CZ	1:B:566:GLY:N	2.73	0.54
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.53
1:A:327:VAL:O	1:A:328:ARG:CD	2.56	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:B:530:SER:O	1:B:531:THR:CB	2.56	0.53
1:B:570:ALA:HB1	1:C:963:VAL:CG1	2.39	0.53
2:E:52:THR:OG1	2:E:332:MET:SD	2.66	0.53
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.53
1:B:748:GLU:HG3	1:B:981:LEU:CD2	2.23	0.53
1:C:41:LYS:O	1:C:42:VAL:HB	2.08	0.53
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.53
1:A:505:TYR:CG	2:D:353:LYS:O	2.62	0.53
1:C:476:GLY:H	1:C:487:ASN:HB3	1.74	0.53
1:C:532:ASN:N	1:C:532:ASN:OD1	2.40	0.53
1:A:334:ASN:C	1:A:362:VAL:HB	2.28	0.53
1:A:690:GLN:O	1:A:691:SER:HB3	2.09	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.53
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.53
3:I:2:NAG:H3	3:I:2:NAG:H83	1.90	0.53
1:A:325:SER:HA	1:A:540:ASN:O	2.09	0.53
1:A:363:ALA:O	1:A:527:PRO:HD3	2.08	0.53
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.44	0.53
1:B:328:ARG:HH11	1:B:533:LEU:HD23	1.66	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.53
1:B:328:ARG:HH21	1:B:580:GLN:HG3	1.73	0.53
1:C:325:SER:HB3	1:C:540:ASN:HB3	1.90	0.53
1:A:310:LYS:HB3	1:A:310:LYS:HZ2	1.74	0.53
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.52
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.52
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.52
2:E:245:ARG:NH1	2:E:603:PHE:O	2.42	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.72	0.52
3:I:1:NAG:H3	3:I:2:NAG:N2	4.61	0.52
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
1:C:324:GLU:CG	1:C:325:SER:N	2.73	0.52
1:C:505:TYR:CG	2:E:353:LYS:O	2.62	0.52
1:A:334:ASN:O	1:A:362:VAL:CG2	2.58	0.52
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.52
1:C:326:ILE:HD11	1:C:541:PHE:CB	2.40	0.52
1:C:1101:HIS:CD2	3:Z:1:NAG:H5	2.45	0.52
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
2:E:90:ASN:HB3	2:E:93:VAL:HG12	1.91	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.39	0.52
2:E:394:ASN:HB2	2:E:562:LYS:HD2	1.92	0.52
1:A:530:SER:OG	1:A:580:GLN:NE2	2.42	0.52
1:A:563:GLN:OE1	1:B:43:PHE:CD1	2.56	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52
1:B:748:GLU:HG2	1:B:981:LEU:HD21	1.83	0.52
1:C:327:VAL:CG1	1:C:328:ARG:N	2.73	0.52
1:B:559:PHE:CE1	1:C:43:PHE:HB2	2.45	0.52
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.51
1:A:318:PHE:CZ	1:A:320:VAL:HG22	2.46	0.51
1:A:493:GLN:OE1	2:D:34:HIS:HB3	2.10	0.51
1:A:565:PHE:CZ	1:B:42:VAL:CG2	2.93	0.51
1:A:854:LYS:N	1:A:854:LYS:CD	2.73	0.51
1:B:580:GLN:HB3	3:M:1:NAG:H5	1.91	0.51
1:C:338:PHE:C	1:C:340:GLU:H	2.13	0.51
1:C:493:GLN:OE1	2:E:34:HIS:HB3	2.10	0.51
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.51
1:A:505:TYR:CE2	2:D:354:GLY:HA3	2.45	0.51
1:C:529:LYS:HE2	1:C:530:SER:H	1.75	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:565:PHE:O	1:B:42:VAL:CA	2.55	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:B:569:ILE:HG12	1:C:47:VAL:CG1	2.41	0.51
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HB3	1:A:310:LYS:NZ	2.25	0.51
1:B:320:VAL:CG2	1:B:591:SER:HB2	2.39	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.51
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.51
1:A:319:ARG:NH2	1:B:740:MET:HG3	2.23	0.51
1:B:516:GLU:OE2	1:C:200:TYR:HE2	1.94	0.51
2:E:104:GLY:O	2:E:107:VAL:HG22	2.10	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.37	0.51
1:B:324:GLU:HG2	1:B:325:SER:N	2.24	0.51
1:B:338:PHE:C	1:B:340:GLU:H	2.13	0.51
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.51
2:E:433:GLU:O	2:E:437:ASN:ND2	2.44	0.51
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.85	0.50
1:C:505:TYR:CE2	2:E:354:GLY:HA3	2.45	0.50
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.50
1:A:41:LYS:N	1:A:41:LYS:CD	2.73	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:A:705:VAL:HB	1:B:883:THR:HG21	1.93	0.50
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.50
1:C:327:VAL:O	1:C:328:ARG:HG2	2.11	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.77	0.50
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.50
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.50
1:B:565:PHE:HD1	1:B:565:PHE:C	2.15	0.50
1:C:326:ILE:HD11	1:C:541:PHE:HB3	1.94	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.11	0.50
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.93	0.50
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.50
1:B:560:LEU:CB	1:B:562:PHE:CE2	2.92	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
2:E:208:GLU:OE2	2:E:219:ARG:NH1	2.44	0.50
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.50
1:A:310:LYS:HE2	1:A:663:ASP:OD1	2.12	0.50
1:A:502:GLY:O	1:A:505:TYR:HB2	2.12	0.50
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.50
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.49
1:A:328:ARG:HB3	1:A:328:ARG:HH21	1.77	0.49
1:A:335:LEU:HD12	1:A:335:LEU:N	2.26	0.49
2:E:342:ALA:O	2:E:343:VAL:C	2.50	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.49
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.49
2:E:302:TRP:CH2	2:E:423:LEU:CD1	2.78	0.49
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
3:R:1:NAG:H62	3:R:2:NAG:H2	1.93	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:C:331:ASN:OD1	1:C:331:ASN:N	2.40	0.49
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.49
1:C:502:GLY:O	1:C:505:TYR:HB2	2.12	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.49
1:C:122:ASN:OD1	1:C:122:ASN:N	2.46	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:B:521:PRO:HA	1:B:564:GLN:HG3	1.94	0.49
2:E:335:ASP:CA	2:E:361:CYS:SG	3.00	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
1:C:654:GLU:CA	1:C:693:ILE:HG22	2.43	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.48
1:B:308:VAL:O	1:B:601:GLY:HA2	2.13	0.48
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.48
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.48
1:C:361:CYS:O	1:C:524:VAL:HG23	2.13	0.48
2:E:564:GLU:HB3	2:E:568:LEU:HD23	1.94	0.48
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.48
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.48
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.48
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.48
1:A:524:VAL:HG22	1:A:525:CYS:N	2.27	0.48
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.28	0.48
1:B:357:ARG:NH1	1:C:230:PRO:HB2	2.27	0.48
1:B:533:LEU:CD1	1:B:535:LYS:NZ	2.77	0.48
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.48
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.77	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:C:332:ILE:HG23	1:C:362:VAL:HG21	1.94	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
1:C:505:TYR:CE2	2:E:353:LYS:C	2.87	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.94	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:B:361:CYS:O	1:B:524:VAL:HG23	2.13	0.48
1:B:516:GLU:C	1:B:517:LEU:CD2	2.82	0.48
1:C:319:ARG:NH2	1:C:319:ARG:CG	2.73	0.48
1:A:42:VAL:HG22	1:C:565:PHE:CE1	2.47	0.48
1:A:328:ARG:HH21	1:A:328:ARG:CG	2.27	0.48
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.48
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.48
1:A:672:ALA:HA	1:A:693:ILE:O	2.14	0.48
1:B:535:LYS:HE2	1:B:585:LEU:HD21	1.96	0.48
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.48
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.48
1:C:653:ALA:CB	1:C:692:ILE:HG22	2.44	0.48
1:B:524:VAL:HG22	1:B:525:CYS:N	2.28	0.48
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.47
1:A:505:TYR:CE2	2:D:353:LYS:C	2.87	0.47
1:C:476:GLY:HA2	2:E:24:GLN:NE2	2.26	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:B:533:LEU:HD11	1:B:535:LYS:HE2	1.95	0.47
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.76	0.47
1:B:569:ILE:CG1	1:C:47:VAL:CG1	2.92	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
2:D:421:ILE:HG13	2:D:421:ILE:O	2.14	0.47
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.47
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.95	0.47
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.47
1:C:326:ILE:HD12	1:C:326:ILE:C	2.34	0.47
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.47
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.47
1:B:565:PHE:C	1:B:565:PHE:CD1	2.85	0.47
2:E:254:SER:O	2:E:254:SER:OG	2.31	0.47
3:I:2:NAG:H83	3:I:2:NAG:C3	2.67	0.47
1:A:669:GLY:N	1:B:864:LEU:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.47
1:C:486:PHE:HE1	2:E:79:LEU:CD1	2.27	0.47
1:A:486:PHE:HE1	2:D:79:LEU:CD1	2.27	0.47
1:B:332:ILE:O	1:B:333:THR:OG1	2.30	0.47
1:B:570:ALA:HB1	1:C:963:VAL:HG12	1.96	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.47
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.47
1:A:316:SER:OG	1:A:317:ASN:N	2.48	0.47
1:A:524:VAL:C	1:A:525:CYS:SG	2.93	0.47
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.98	0.46
1:C:476:GLY:CA	2:E:24:GLN:NE2	2.65	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.46
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.46
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.46
1:C:393:THR:HA	1:C:523:THR:HB	1.98	0.46
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.46
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.98	0.46
1:B:113:LYS:O	1:B:113:LYS:NZ	2.31	0.46
2:E:333:LEU:O	2:E:362:THR:HG22	2.15	0.46
2:E:421:ILE:O	2:E:421:ILE:HG13	2.14	0.46
2:E:560:LEU:HD22	2:E:564:GLU:HG3	1.98	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.46
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.46
1:C:316:SER:OG	1:C:317:ASN:N	2.48	0.46
2:E:317:SER:HG	2:E:546:ASN:H	1.58	0.46
1:B:528:LYS:O	1:B:529:LYS:HG2	2.15	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.46
1:B:500:THR:O	1:B:500:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:A:41:LYS:N	1:A:41:LYS:HD3	2.31	0.46
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:A:565:PHE:O	1:B:43:PHE:N	2.49	0.46
1:B:393:THR:HA	1:B:523:THR:HB	1.97	0.46
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:A:985:ASP:OD1	1:A:985:ASP:N	2.45	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.46
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.46
2:E:425:SER:C	2:E:427:ASP:H	2.19	0.46
1:B:316:SER:OG	1:B:317:ASN:N	2.48	0.46
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.46
1:C:45:SER:O	1:C:279:TYR:CB	2.64	0.46
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.46
1:A:127:VAL:HG11	4:A:1402:NAG:H61	1.98	0.45
1:A:328:ARG:NH2	1:A:578:ASP:OD1	2.50	0.45
1:B:560:LEU:HD23	1:B:563:GLN:CD	2.29	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.45
1:A:388:ASN:CG	1:A:527:PRO:HD2	2.36	0.45
1:B:570:ALA:CB	1:C:963:VAL:CG1	2.94	0.45
2:E:52:THR:HA	2:E:342:ALA:HB1	1.98	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.45
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.99	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.45
2:D:431:ASP:OD1	2:D:431:ASP:N	2.44	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.45
1:A:318:PHE:CE2	1:A:320:VAL:HG22	2.52	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:C:388:ASN:CG	1:C:527:PRO:HD2	2.37	0.45
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:565:PHE:HE1	1:C:42:VAL:HG22	1.81	0.45
1:B:655:HIS:HD2	1:B:694:ALA:O	2.00	0.45
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.45
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:B:127:VAL:HG11	4:B:1402:NAG:H61	1.98	0.45
1:B:324:GLU:CG	1:B:325:SER:N	2.79	0.45
1:C:493:GLN:OE1	2:E:34:HIS:CG	2.70	0.45
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:A:646:ARG:HG3	1:A:646:ARG:O	2.17	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:C:127:VAL:HG11	4:C:1402:NAG:H61	1.98	0.45
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.45
1:A:486:PHE:CE1	2:D:79:LEU:HD21	2.48	0.44
1:A:940:SER:O	1:A:940:SER:OG	2.33	0.44
2:E:356:PHE:HB3	2:E:379:ILE:HD12	1.98	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.44
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.44
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.44
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.44
1:A:551:VAL:HB	1:A:588:THR:HG23	2.00	0.44
1:B:335:LEU:C	1:B:362:VAL:O	2.56	0.44
1:C:691:SER:OG	1:C:692:ILE:N	2.50	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.16	0.44
1:B:328:ARG:HD3	1:B:531:THR:O	2.17	0.44
1:B:519:HIS:O	1:C:41:LYS:CE	2.65	0.44
1:B:521:PRO:O	1:B:522:ALA:CB	2.66	0.44
1:C:646:ARG:HG3	1:C:646:ARG:O	2.17	0.44
1:A:323:THR:O	1:A:323:THR:OG1	2.30	0.44
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:C	1:B:525:CYS:SG	2.95	0.44
1:B:569:ILE:HG13	1:C:47:VAL:HG11	1.99	0.44
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:B:393:THR:O	1:B:523:THR:CG2	2.58	0.44
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.44
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.44
1:B:321:GLN:NE2	1:B:322:PRO:HD2	2.32	0.44
1:B:560:LEU:HD23	1:C:43:PHE:HD1	1.82	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.44
1:A:476:GLY:HA2	2:D:24:GLN:NE2	2.26	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:C:335:LEU:C	1:C:362:VAL:O	2.56	0.44
2:E:208:GLU:OE1	2:E:210:ASN:ND2	2.50	0.44
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.43
1:A:493:GLN:OE1	2:D:34:HIS:CG	2.70	0.43
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.43
1:A:660:TYR:O	1:A:698:SER:HB2	2.17	0.43
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.01	0.43
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:C:533:LEU:HD12	1:C:533:LEU:C	2.38	0.43
1:B:319:ARG:HG3	1:B:319:ARG:HH21	1.84	0.43
1:B:332:ILE:HB	1:B:333:THR:H	1.55	0.43
1:B:519:HIS:HE1	1:C:41:LYS:N	2.14	0.43
1:B:559:PHE:CE2	1:B:564:GLN:O	2.70	0.43
1:B:669:GLY:N	1:C:864:LEU:O	2.49	0.43
1:C:127:VAL:HG21	4:C:1402:NAG:H5	2.01	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:B:327:VAL:O	1:B:530:SER:O	2.36	0.43
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.43
1:A:312:ILE:HG13	1:A:598:ILE:HG13	2.00	0.43
1:A:335:LEU:C	1:A:362:VAL:O	2.57	0.43
1:A:390:LEU:O	1:A:525:CYS:HB3	2.18	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.43
1:B:127:VAL:HG21	4:B:1402:NAG:H5	2.00	0.43
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.43
1:C:486:PHE:CE1	2:E:79:LEU:HD21	2.47	0.43
3:I:1:NAG:C3	3:I:2:NAG:N2	4.88	0.43
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.43
1:B:520:ALA:CB	1:B:521:PRO:CD	2.79	0.43
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
3:G:1:NAG:H61	3:G:2:NAG:N2	2.33	0.43
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.71	0.43
1:B:332:ILE:HD13	1:B:362:VAL:HG21	2.00	0.43
1:B:558:LYS:HD2	1:B:558:LYS:N	2.27	0.43
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.43
1:C:486:PHE:HE1	2:E:79:LEU:HD21	1.77	0.43
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.43
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.43
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.43
3:N:1:NAG:H61	3:N:2:NAG:N2	2.33	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.43
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.43
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.43
3:U:1:NAG:H61	3:U:2:NAG:N2	2.33	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.42
1:C:296:LEU:HD11	1:C:602:THR:HG22	2.01	0.42
1:C:326:ILE:C	1:C:326:ILE:CD1	2.87	0.42
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.42
1:A:48:LEU:H	1:A:48:LEU:CD1	2.32	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
1:B:986:PRO:CB	1:B:987:PRO:HD3	2.45	0.42
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.42
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.42
1:C:304:LYS:HE3	1:C:304:LYS:HB3	1.78	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:C	1:B:517:LEU:HD23	2.39	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:B:533:LEU:HD11	1:B:535:LYS:HZ3	1.80	0.42
1:A:316:SER:C	1:A:317:ASN:ND2	2.73	0.42
1:B:580:GLN:O	3:M:1:NAG:O4	2.38	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:C:735:SER:OG	1:C:859:THR:HG22	2.17	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.42
1:A:565:PHE:CE1	1:B:42:VAL:HG22	2.54	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:B:327:VAL:O	1:B:531:THR:HB	2.19	0.42
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.42
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.42
1:C:674:TYR:HE1	1:C:691:SER:N	2.12	0.42
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.52	0.42
2:E:212:VAL:HG23	2:E:215:TYR:HB2	2.02	0.42
2:E:313:LYS:HA	2:E:316:VAL:HG12	2.00	0.42
1:A:127:VAL:HG21	4:A:1402:NAG:H5	2.01	0.42
1:A:670:ILE:HA	1:A:695:TYR:O	2.20	0.42
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.42
1:C:696:THR:O	1:C:697:MET:C	2.56	0.42
1:A:325:SER:HB3	1:A:540:ASN:O	2.19	0.42
1:A:524:VAL:CG2	1:A:525:CYS:N	2.83	0.42
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.42
1:C:332:ILE:N	1:C:332:ILE:CD1	2.73	0.42
1:A:500:THR:O	1:A:500:THR:OG1	2.31	0.42
1:A:502:GLY:HA3	2:D:354:GLY:O	2.20	0.42
1:B:748:GLU:CG	1:B:981:LEU:CD2	2.81	0.42
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.42
1:C:280:ASN:OD1	1:C:281:GLU:N	2.50	0.42
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.42
2:E:425:SER:C	2:E:427:ASP:N	2.73	0.42
3:V:1:NAG:H3	3:V:1:NAG:H83	2.02	0.42
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.42
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:316:SER:C	1:B:317:ASN:ND2	2.73	0.42
1:B:653:ALA:CB	1:B:692:ILE:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:ILE:H	1:B:794:ILE:HG13	1.69	0.42
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.41
1:A:328:ARG:CG	1:A:328:ARG:NH2	2.83	0.41
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.41
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.41
1:B:322:PRO:HA	1:B:538:CYS:HB3	2.02	0.41
1:B:560:LEU:CD2	1:B:560:LEU:N	2.83	0.41
1:C:48:LEU:H	1:C:48:LEU:CD1	2.32	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41
1:B:310:LYS:CG	1:B:664:ILE:HD11	2.50	0.41
1:B:537:LYS:O	1:B:538:CYS:C	2.58	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
2:E:39:LEU:HD23	2:E:39:LEU:HA	1.93	0.41
1:A:964:LYS:HE3	1:C:570:ALA:HA	2.01	0.41
1:B:569:ILE:HG12	1:C:47:VAL:HG12	2.02	0.41
4:B:1409:NAG:O4	4:B:1410:NAG:O5	2.28	0.41
1:C:502:GLY:HA3	2:E:354:GLY:O	2.20	0.41
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.41
1:B:556:ASN:C	1:B:556:ASN:ND2	2.73	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.93	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:770:ILE:HG21	1:A:770:ILE:HD13	1.76	0.41
1:B:390:LEU:O	1:B:525:CYS:HB3	2.19	0.41
1:B:523:THR:O	1:B:525:CYS:SG	2.79	0.41
1:C:592:PHE:CD1	1:C:592:PHE:C	2.92	0.41
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.41
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.41
1:B:406:GLU:CG	1:B:418:ILE:HG13	2.50	0.41
1:B:516:GLU:OE2	1:C:200:TYR:CE2	2.73	0.41
1:B:557:LYS:HE3	1:B:575:ALA:CB	2.50	0.41
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.41
1:C:393:THR:O	1:C:523:THR:CG2	2.58	0.41
2:D:21:ILE:HD12	2:D:21:ILE:HA	1.97	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:226:LEU:HB3	1:A:227:VAL:HG23	2.03	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:A:505:TYR:CD2	2:D:353:LYS:C	2.93	0.41
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:654:GLU:HG3	1:B:693:ILE:HG22	2.03	0.41
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.41
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.41
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.41
2:E:21:ILE:HD12	2:E:21:ILE:HA	1.97	0.41
1:A:486:PHE:CE1	2:D:79:LEU:HD13	2.56	0.41
1:A:1123:SER:O	1:A:1123:SER:OG	2.39	0.41
1:B:532:ASN:OD1	1:B:532:ASN:N	2.53	0.41
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.90	0.41
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.41
1:C:406:GLU:CG	1:C:418:ILE:HG13	2.50	0.41
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.41
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.40
1:A:694:ALA:O	1:A:695:TYR:HB3	2.22	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.40
1:B:226:LEU:HB3	1:B:227:VAL:HG23	2.03	0.40
1:B:310:LYS:CD	1:B:664:ILE:HD11	2.51	0.40
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.40
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.40
1:A:45:SER:O	1:A:47:VAL:N	2.54	0.40
1:A:45:SER:OG	1:A:281:GLU:HA	2.21	0.40
1:A:318:PHE:HE2	1:A:320:VAL:CG2	2.32	0.40
1:B:89:GLY:HA2	1:B:194:PHE:O	2.22	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40
1:C:166:CYS:HB3	1:C:169:GLU:OE1	2.21	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:486:PHE:CE1	2:E:79:LEU:HD13	2.56	0.40
1:C:654:GLU:HG2	1:C:693:ILE:HG23	2.02	0.40
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.40
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.40
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.56	0.40
1:A:347:PHE:CD1	1:A:509:ARG:HD3	2.56	0.40
1:A:708:SER:OG	1:A:711:SER:HB2	2.22	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.40
1:B:227:VAL:CG1	1:B:228:ASP:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:H	1:B:309:GLU:HG2	1.71	0.40
1:B:338:PHE:C	1:B:340:GLU:N	2.75	0.40
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.21	0.40
1:C:127:VAL:HG22	1:C:171:VAL:HG13	2.04	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
1:B:200:TYR:CE1	1:B:230:PRO:HB3	2.56	0.40
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.04	0.40
1:B:692:ILE:HD13	1:B:692:ILE:HG21	1.93	0.40
1:C:45:SER:O	1:C:47:VAL:N	2.54	0.40
1:C:100:ILE:HG22	1:C:242:LEU:HD23	2.04	0.40
1:C:342:PHE:CB	3:U:1:NAG:H82	2.52	0.40
2:E:476:LYS:HB3	2:E:476:LYS:HE3	1.92	0.40
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.40
1:A:334:ASN:O	1:A:362:VAL:HG21	2.21	0.40
1:A:486:PHE:HE1	2:D:79:LEU:HD21	1.77	0.40
1:A:505:TYR:CE2	2:D:353:LYS:O	2.73	0.40
1:A:879:ALA:O	1:A:883:THR:HB	2.22	0.40
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.51	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:369:TYR:CZ	1:B:384:PRO:HB2	2.57	0.40
1:B:524:VAL:CG2	1:B:525:CYS:N	2.83	0.40
2:E:411:SER:OG	2:E:543:ASP:OD1	2.38	0.40
2:E:424:LEU:HD23	2:E:424:LEU:HA	1.87	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	989/1283 (77%)	876 (89%)	91 (9%)	22 (2%)	6 24
1	B	951/1283 (74%)	823 (86%)	98 (10%)	30 (3%)	4 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	988/1283 (77%)	866 (88%)	96 (10%)	26 (3%)	5 20
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
2	E	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
All	All	4114/5483 (75%)	3691 (90%)	341 (8%)	82 (2%)	11 27

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	A	518	LEU
1	A	701	ALA
1	B	48	LEU
1	B	518	LEU
1	B	529	LYS
1	B	537	LYS
1	B	560	LEU
1	B	564	GLN
1	C	48	LEU
1	C	518	LEU
1	C	691	SER
1	C	814	LYS
1	A	41	LYS
1	A	46	SER
1	A	339	GLY
1	B	41	LYS
1	B	46	SER
1	B	333	THR
1	B	339	GLY
1	B	527	PRO
1	B	528	LYS
1	B	742	ILE
1	B	743	CYS
1	C	41	LYS
1	C	46	SER
1	C	324	GLU
1	C	339	GLY
1	C	528	LYS
1	C	529	LYS

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Mol	Chain	Res	Type
1	C	697	MET
1	C	810	SER
2	D	343	VAL
2	E	343	VAL
1	A	43	PHE
1	A	336	CYS
1	A	522	ALA
1	A	710	ASN
1	B	43	PHE
1	B	324	GLU
1	B	336	CYS
1	B	522	ALA
1	B	558	LYS
1	C	43	PHE
1	C	331	ASN
1	C	336	CYS
1	C	522	ALA
1	C	527	PRO
2	D	423	LEU
2	E	423	LEU
1	A	44	ARG
1	A	349	SER
1	A	520	ALA
1	A	691	SER
1	B	44	ARG
1	B	349	SER
1	B	520	ALA
1	B	531	THR
1	B	536	ASN
1	B	746	SER
1	C	44	ARG
1	C	349	SER
1	C	520	ALA
1	C	813	SER
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	B	40	ASP
1	B	42	VAL
1	B	47	VAL
1	C	40	ASP
1	C	42	VAL

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Mol	Chain	Res	Type
1	C	47	VAL
1	C	812	PRO
1	C	811	LYS
1	B	332	ILE
1	B	326	ILE
1	A	326	ILE
1	A	526	GLY

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	882/1122 (79%)	776 (88%)	106 (12%)	5 15
1	B	850/1122 (76%)	746 (88%)	104 (12%)	5 15
1	C	881/1122 (78%)	792 (90%)	89 (10%)	7 23
2	D	525/721 (73%)	518 (99%)	7 (1%)	69 90
2	E	525/721 (73%)	518 (99%)	7 (1%)	69 90
All	All	3663/4808 (76%)	3350 (92%)	313 (8%)	14 31

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	48	LEU
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	282	ASN
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	310	LYS
1	A	314	GLN
1	A	315	THR
1	A	319	ARG
1	A	324	GLU
1	A	325	SER
1	A	328	ARG
1	A	331	ASN
1	A	333	THR
1	A	335	LEU
1	A	353	TRP
1	A	355	ARG
1	A	375	SER
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	406	GLU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	440	ASN
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	532	ASN
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU

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Mol	Chain	Res	Type
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR
1	A	591	SER
1	A	599	THR
1	A	646	ARG
1	A	673	SER
1	A	693	ILE
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	854	LYS
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	982	SER
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR

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Mol	Chain	Res	Type
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	310	LYS
1	B	314	GLN
1	B	315	THR
1	B	323	THR
1	B	324	GLU
1	B	331	ASN
1	B	332	ILE
1	B	334	ASN
1	B	335	LEU
1	B	353	TRP

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Mol	Chain	Res	Type
1	B	355	ARG
1	B	375	SER
1	B	383	SER
1	B	389	ASP
1	B	390	LEU
1	B	406	GLU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	440	ASN
1	B	500	THR
1	B	514	SER
1	B	517	LEU
1	B	518	LEU
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	530	SER
1	B	532	ASN
1	B	533	LEU
1	B	534	VAL
1	B	535	LYS
1	B	537	LYS
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	557	LYS
1	B	558	LYS
1	B	559	PHE
1	B	564	GLN
1	B	565	PHE
1	B	576	VAL
1	B	583	GLU
1	B	590	CYS
1	B	599	THR
1	B	602	THR
1	B	646	ARG
1	B	673	SER
1	B	704	SER
1	B	710	ASN

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Mol	Chain	Res	Type
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	40	ASP
1	C	41	LYS
1	C	46	SER
1	C	48	LEU
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	137	ASN
1	C	141	LEU
1	C	143	VAL

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Mol	Chain	Res	Type
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	282	ASN
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	319	ARG
1	C	324	GLU
1	C	325	SER
1	C	331	ASN
1	C	332	ILE
1	C	335	LEU
1	C	353	TRP
1	C	355	ARG
1	C	375	SER
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	406	GLU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	440	ASN
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	529	LYS
1	C	532	ASN
1	C	535	LYS
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	556	ASN

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Mol	Chain	Res	Type
1	C	558	LYS
1	C	576	VAL
1	C	583	GLU
1	C	588	THR
1	C	590	CYS
1	C	591	SER
1	C	599	THR
1	C	602	THR
1	C	646	ARG
1	C	673	SER
1	C	690	GLN
1	C	693	ILE
1	C	696	THR
1	C	703	ASN
1	C	727	LEU
1	C	740	MET
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	D	107	VAL
2	D	344	CYS
2	D	345	HIS
2	D	347	THR
2	D	361	CYS
2	D	423	LEU
2	D	425	SER

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Mol	Chain	Res	Type
2	E	107	VAL
2	E	344	CYS
2	E	345	HIS
2	E	347	THR
2	E	361	CYS
2	E	423	LEU
2	E	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	317	ASN
1	A	354	ASN
1	A	360	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	498	GLN
1	A	540	ASN
1	A	556	ASN
1	A	580	GLN
1	A	644	GLN
1	A	658	ASN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	856	ASN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	134	GLN
1	B	137	ASN

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Mol	Chain	Res	Type
1	B	188	ASN
1	B	239	GLN
1	B	317	ASN
1	B	321	GLN
1	B	354	ASN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	498	GLN
1	B	540	ASN
1	B	556	ASN
1	B	644	GLN
1	B	655	HIS
1	B	658	ASN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	239	GLN
1	C	317	ASN
1	C	360	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	498	GLN
1	C	540	ASN
1	C	556	ASN
1	C	580	GLN
1	C	644	GLN
1	C	658	ASN
1	C	690	GLN
1	C	703	ASN
1	C	784	GLN

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Mol	Chain	Res	Type
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	D	24	GLN
2	D	58	ASN
2	D	96	GLN
2	D	175	GLN
2	D	239	HIS
2	D	277	ASN
2	D	505	HIS
2	D	586	ASN
2	E	24	GLN
2	E	58	ASN
2	E	96	GLN
2	E	175	GLN
2	E	239	HIS
2	E	277	ASN
2	E	472	GLN
2	E	505	HIS
2	E	586	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

64 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	$\#\|Z\| > 2$
3	NAG	F	1	1,3	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	G	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	0.48	0
3	NAG	I	1	1,3	14,14,15	0.37	0	17,19,21	0.73	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	J	2	3	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	L	1	1,3	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	M	1	1,3	14,14,15	0.56	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	N	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	O	1	1,3	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	O	2	3	14,14,15	0.37	0	17,19,21	0.35	0
3	NAG	P	1	1,3	14,14,15	0.35	0	17,19,21	1.14	1 (5%)
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	R	1	1,3	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	R	2	3	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	U	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	V	1	1,3	14,14,15	0.23	0	17,19,21	1.36	1 (5%)
3	NAG	V	2	3	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	W	1	1,3	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
3	NAG	W	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	X	1	1,3	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.74	0
3	NAG	Y	1	1,3	14,14,15	0.36	0	17,19,21	0.48	0
3	NAG	Y	2	3	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
3	NAG	Z	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
3	NAG	a	1	1,3	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	b	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	b	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	c	1	2,3	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	c	2	3	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	d	2	3	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	e	1	2,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	e	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	f	1	2,3	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	f	2	3	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	g	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	h	1	2,3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	h	2	3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	j	1	2,3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	j	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	k	1	2,3	14,14,15	0.22	0	17,19,21	0.62	0
3	NAG	k	2	3	14,14,15	0.32	0	17,19,21	0.59	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	4/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	4/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.68	1.39	1.43
3	K	1	NAG	O5-C1	-2.55	1.39	1.43
3	J	1	NAG	O5-C1	-2.33	1.40	1.43
3	b	1	NAG	O5-C1	-2.19	1.40	1.43
3	g	1	NAG	O5-C1	-2.17	1.40	1.43
3	Z	1	NAG	O5-C1	-2.10	1.40	1.43
3	G	1	NAG	O5-C1	-2.05	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	-2.04	1.40	1.43
3	N	1	NAG	O5-C1	-2.02	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1	NAG	C2-N2-C7	4.64	129.52	122.90
3	J	2	NAG	C2-N2-C7	4.43	129.21	122.90
3	Z	2	NAG	C2-N2-C7	4.35	129.10	122.90
3	I	2	NAG	C2-N2-C7	4.29	129.00	122.90
3	Y	2	NAG	C2-N2-C7	4.28	128.99	122.90
3	P	1	NAG	C1-O5-C5	3.35	116.73	112.19
3	h	2	NAG	C1-O5-C5	2.50	115.58	112.19
3	c	2	NAG	C1-O5-C5	2.47	115.54	112.19
3	J	2	NAG	C1-C2-N2	2.40	114.59	110.49
3	I	2	NAG	C1-C2-N2	2.37	114.53	110.49
3	R	1	NAG	O4-C4-C3	-2.36	104.89	110.35
3	Q	1	NAG	C1-O5-C5	2.28	115.29	112.19
3	W	1	NAG	C1-O5-C5	2.26	115.26	112.19
3	Z	2	NAG	C1-C2-N2	2.22	114.27	110.49
3	L	1	NAG	C1-O5-C5	2.09	115.03	112.19
3	J	2	NAG	C1-O5-C5	2.08	115.02	112.19
3	R	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	f	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	k	2	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	i	1	NAG	C8-C7-N2-C2
3	i	1	NAG	O7-C7-N2-C2
3	i	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C8-C7-N2-C2
3	i	2	NAG	O7-C7-N2-C2
3	V	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	W	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	Y	2	NAG	O7-C7-N2-C2
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
3	f	2	NAG	C4-C5-C6-O6
3	k	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	d	2	NAG	C1-C2-N2-C7
3	i	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	N	2	NAG	C1-C2-N2-C7
3	U	2	NAG	C1-C2-N2-C7
3	Z	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	O	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	R	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C4-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C1-C2-N2-C7
3	N	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
3	V	1	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7
3	U	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	NAG	2	0
3	G	1	NAG	3	0
3	I	1	NAG	4	0
3	R	2	NAG	1	0
3	Z	1	NAG	1	0
3	Z	2	NAG	1	0
3	V	1	NAG	1	0
3	M	1	NAG	2	0
3	J	2	NAG	1	0
3	G	2	NAG	2	0
3	U	1	NAG	4	0
3	R	1	NAG	1	0
3	U	2	NAG	2	0

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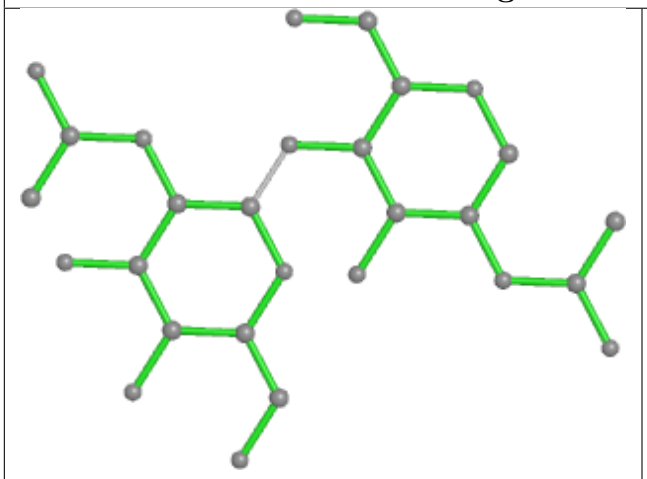
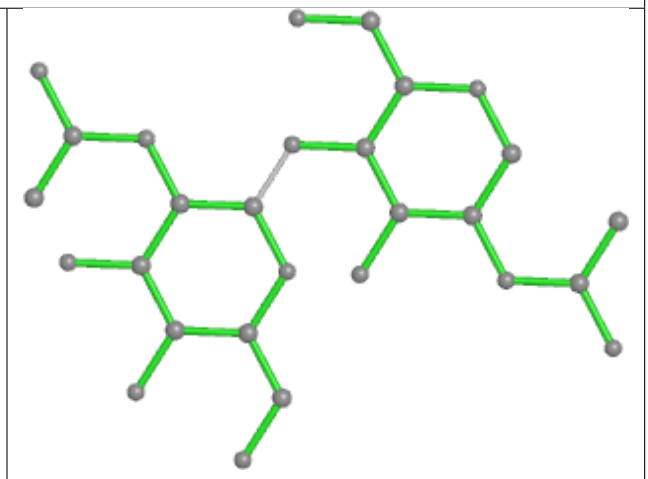
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	6	0
3	Y	2	NAG	1	0
3	N	1	NAG	3	0

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

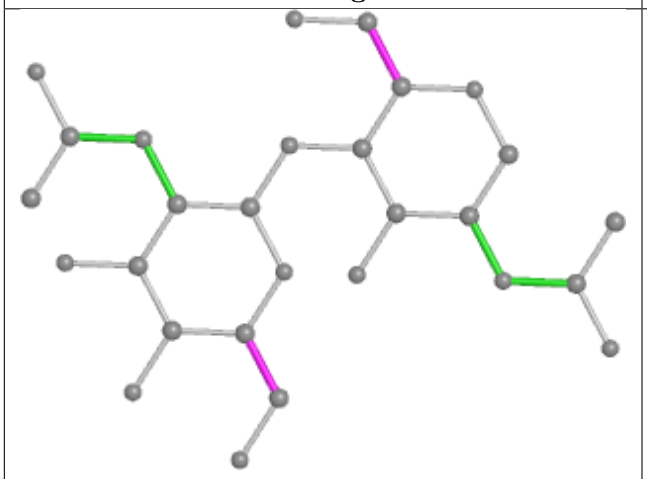
Oligosaccharide Chain F



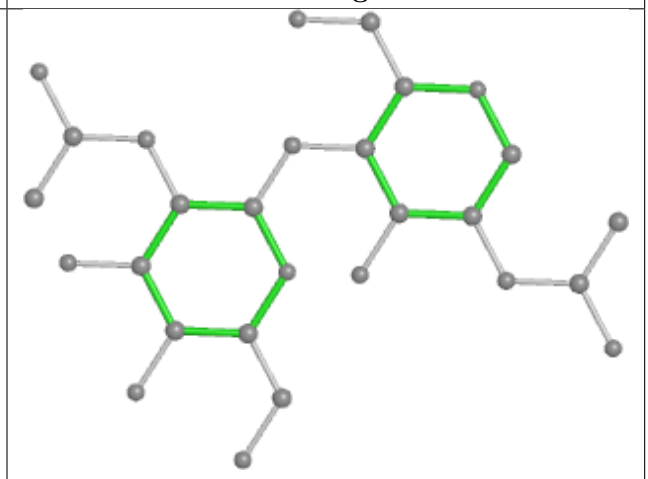
Bond lengths



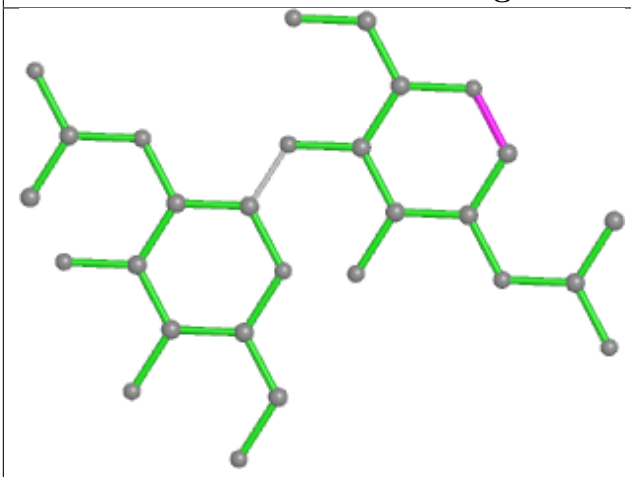
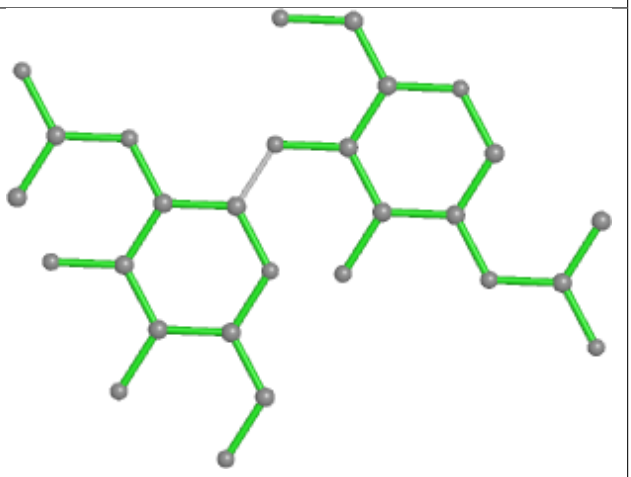
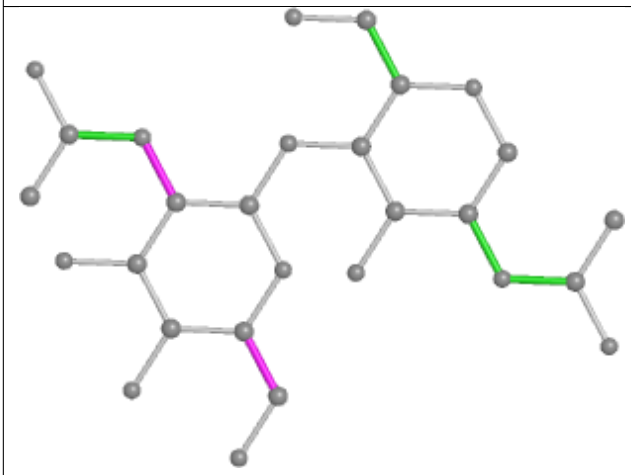
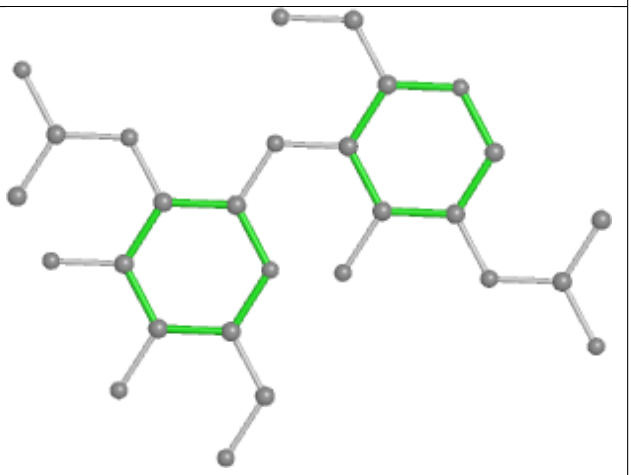
Bond angles



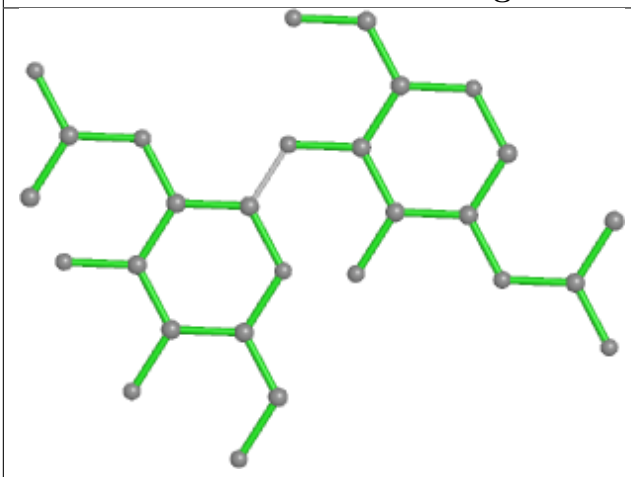
Torsions



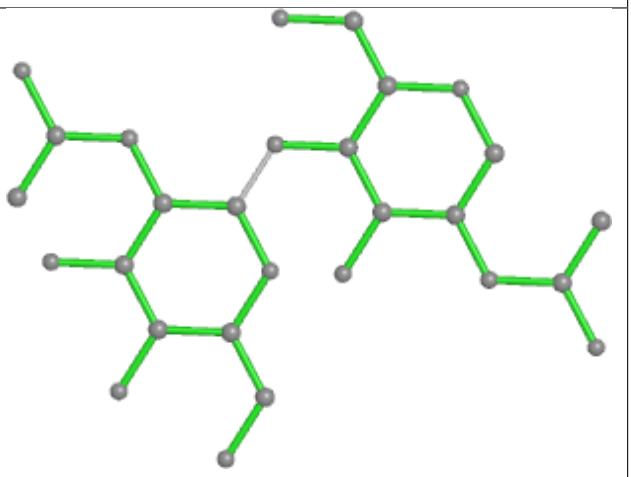
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

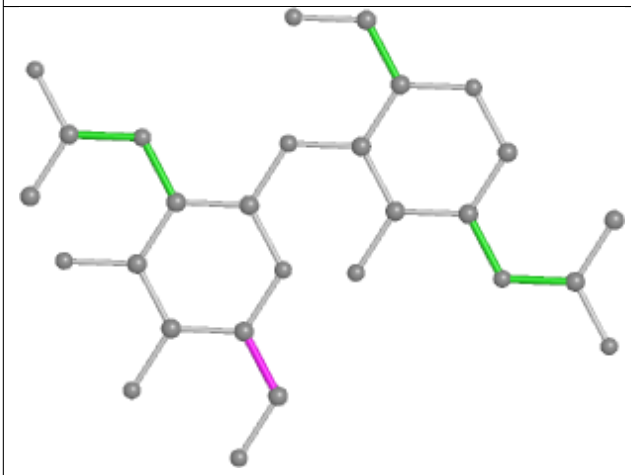
Oligosaccharide Chain H



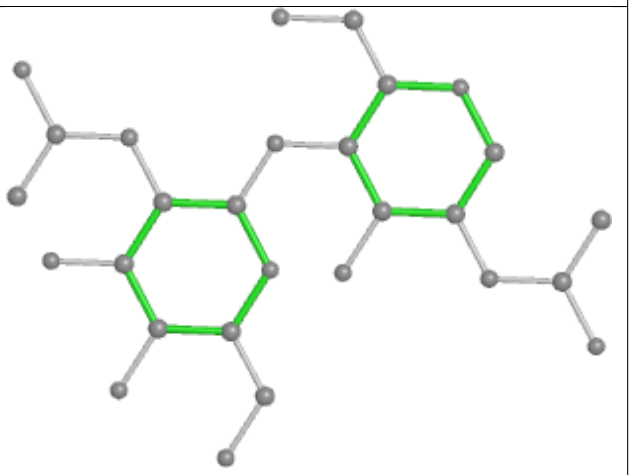
Bond lengths



Bond angles

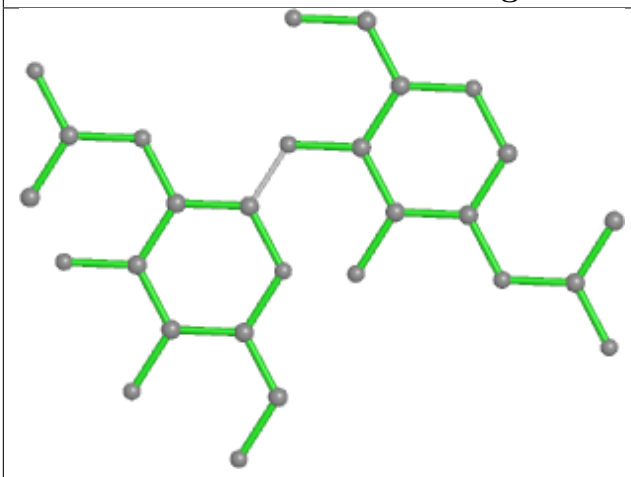


Torsions



Rings

Oligosaccharide Chain I



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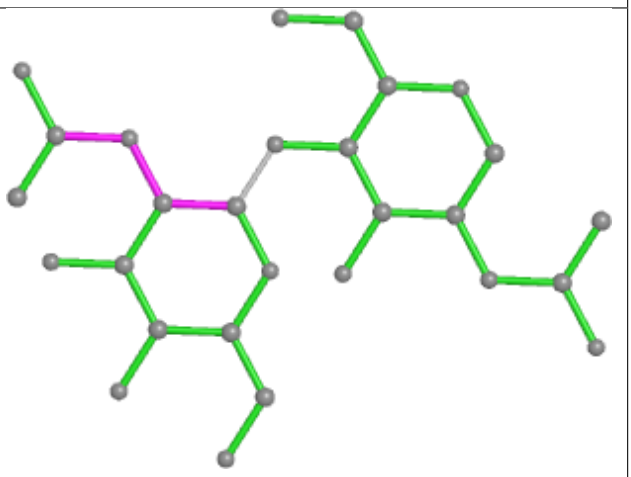
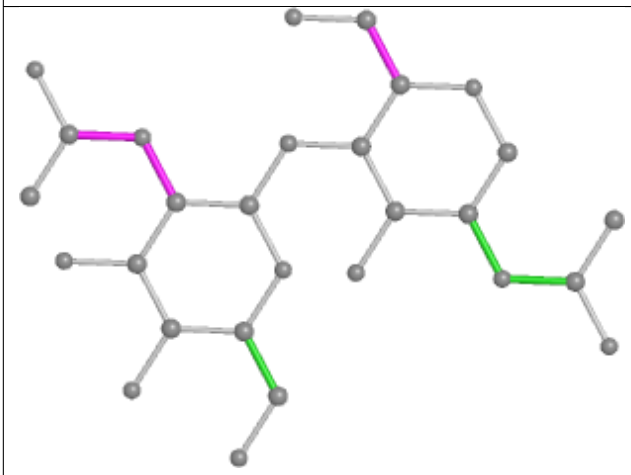


Bond angles



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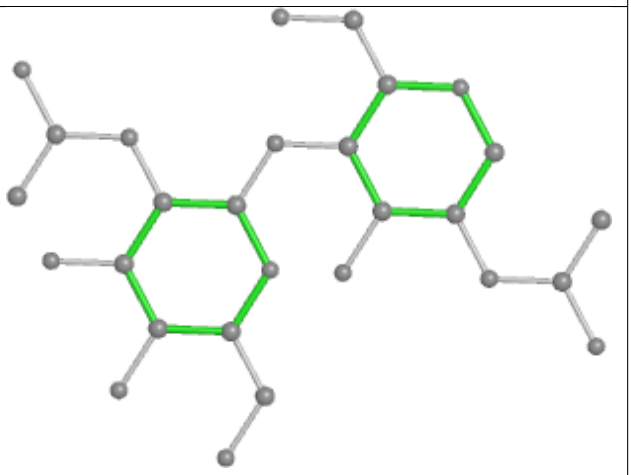
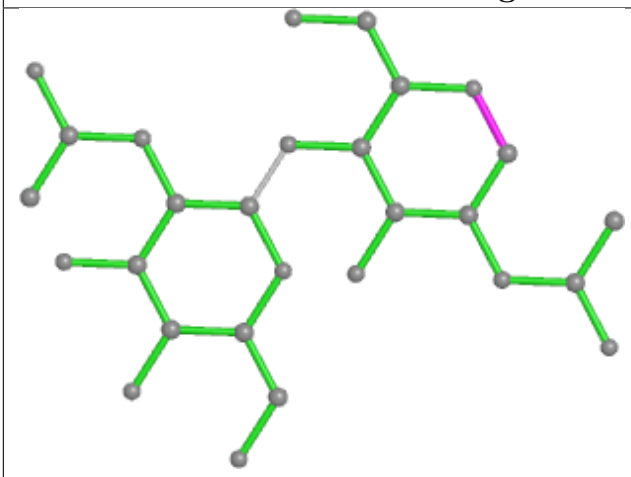


Rings

Oligosaccharide Chain J



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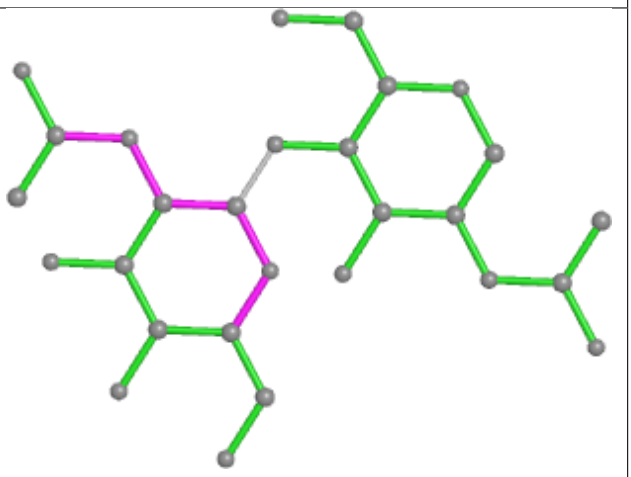
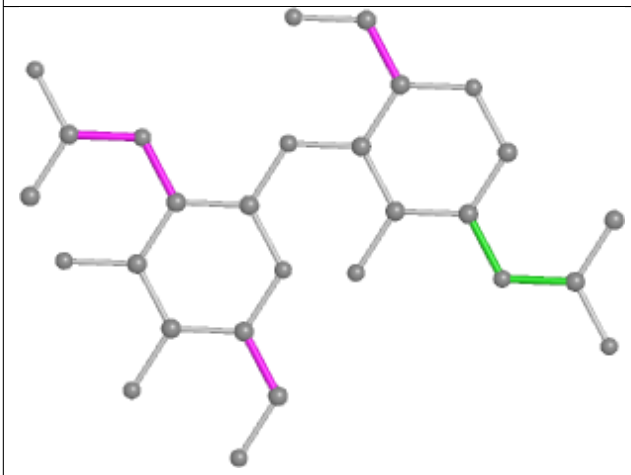


Bond angles



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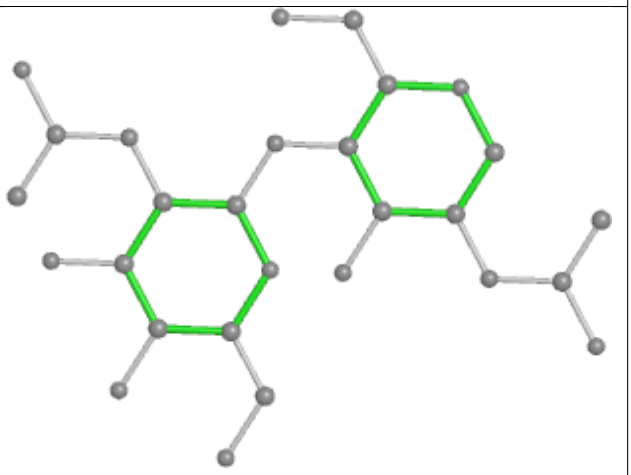
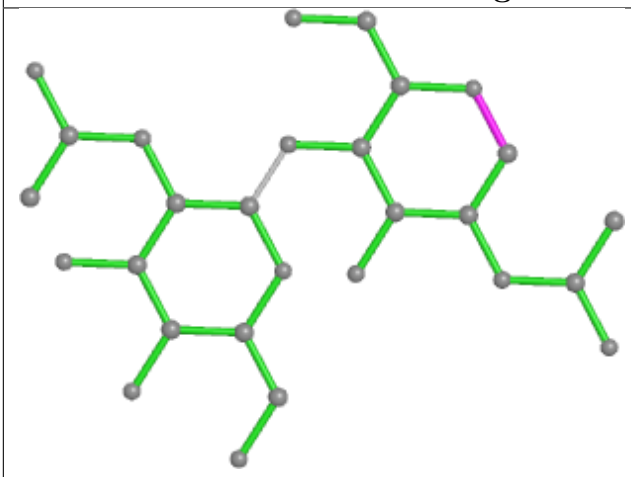


Rings

Oligosaccharide Chain K



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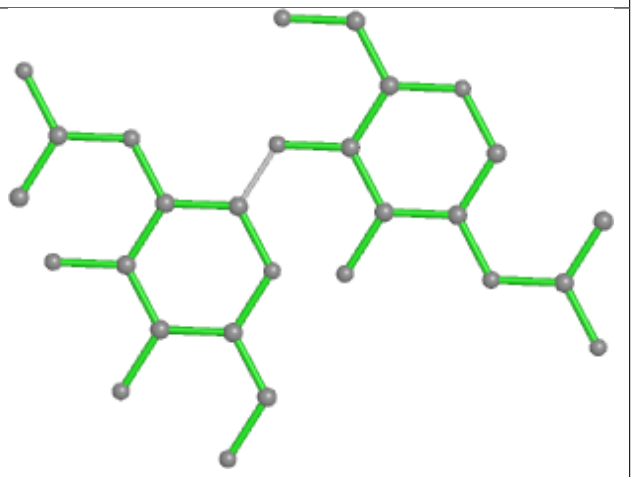
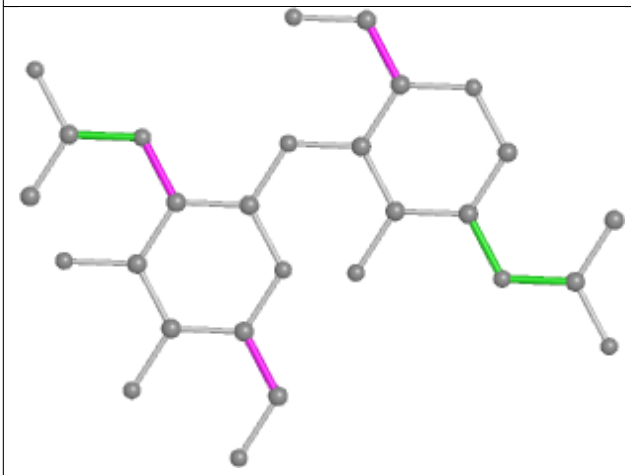
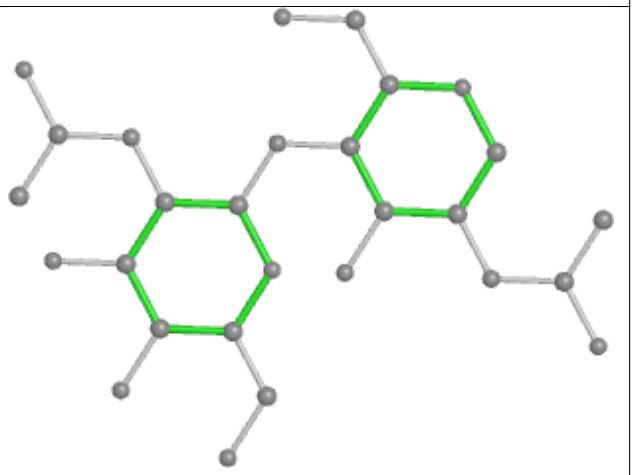


Bond angles

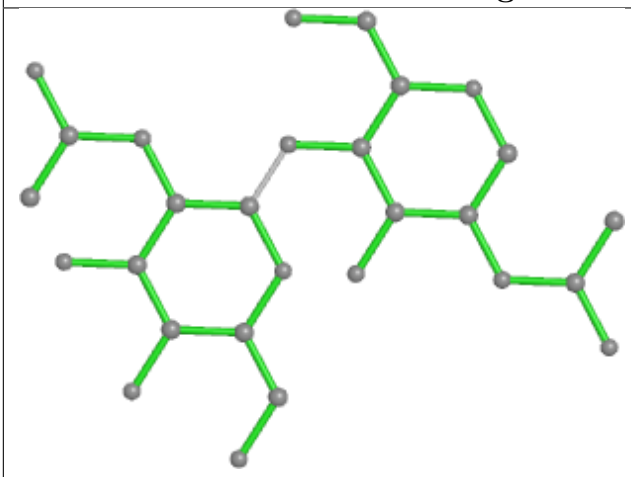


Torsions



Rings

Oligosaccharide Chain L



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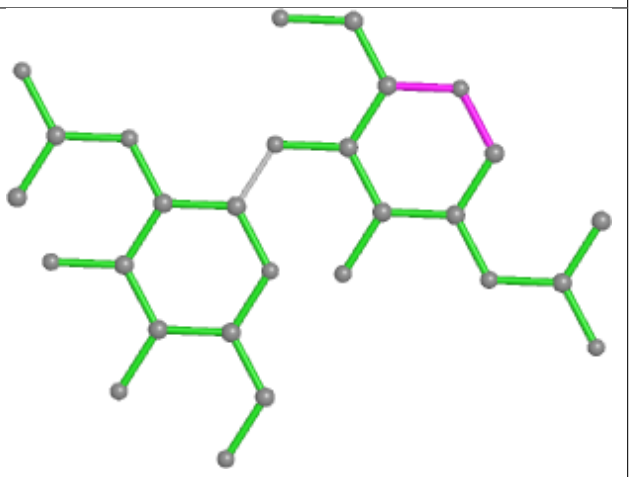
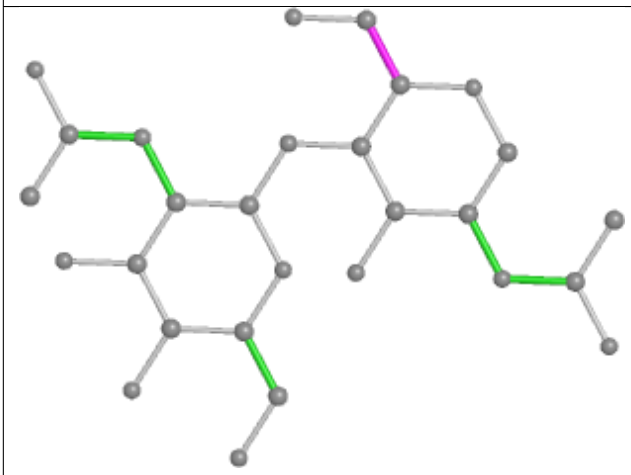


Bond angles



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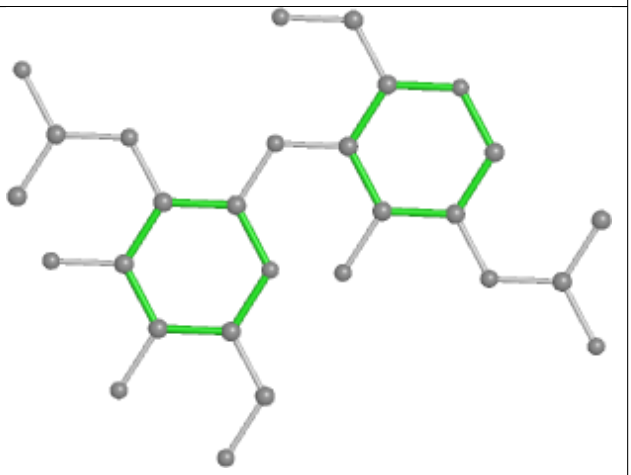
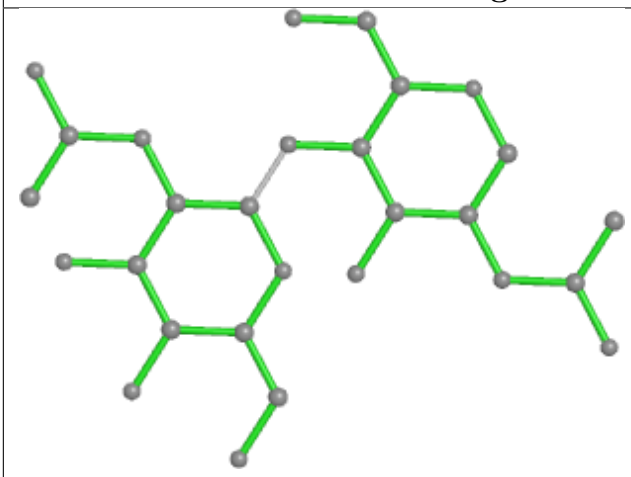


Rings

Oligosaccharide Chain M



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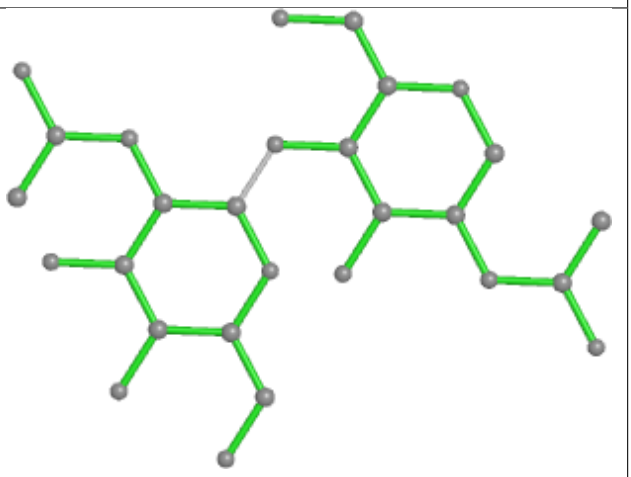
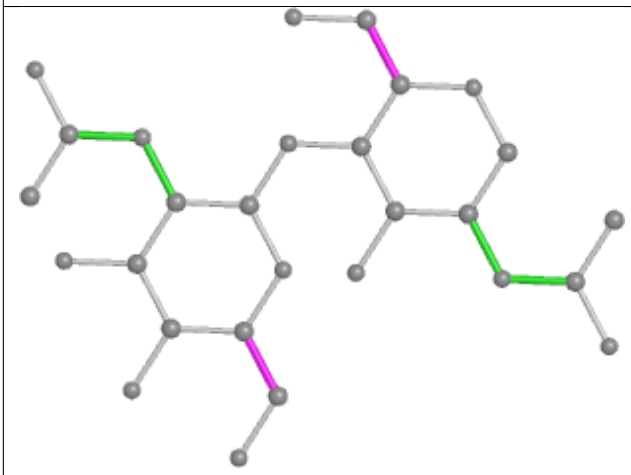


Bond angles



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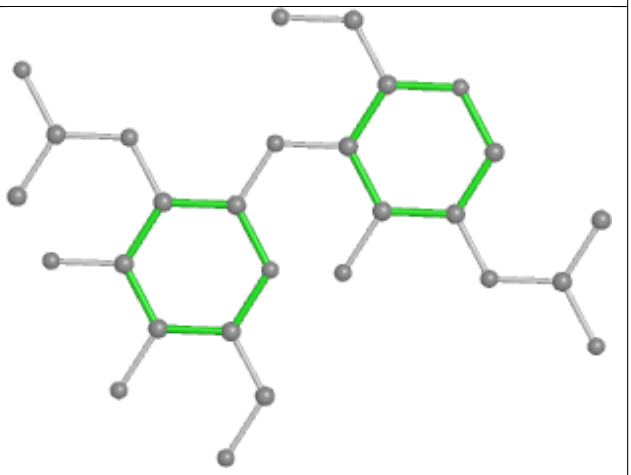
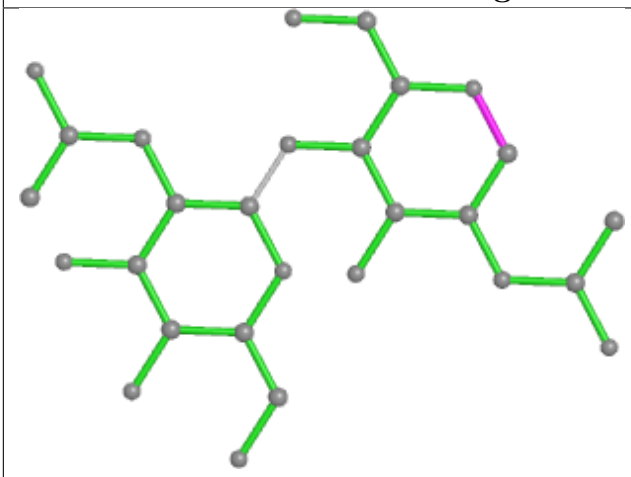


Rings

Oligosaccharide Chain N



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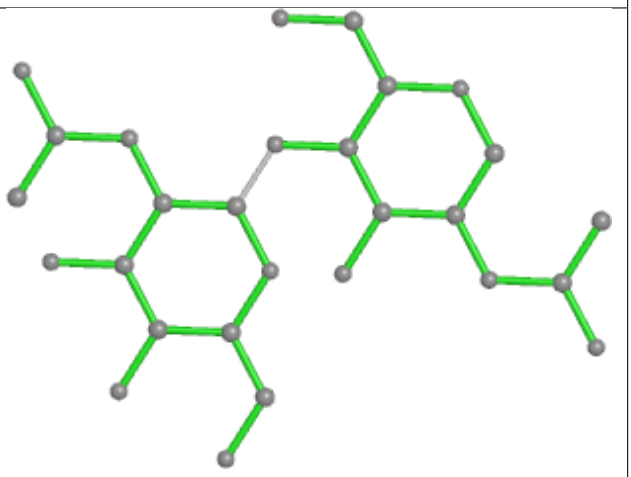
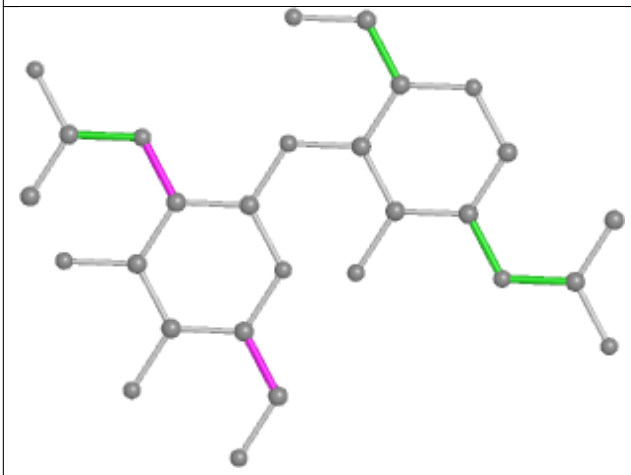


Bond angles



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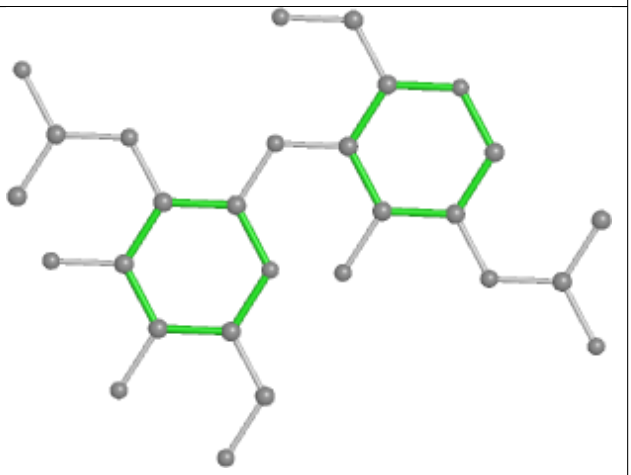
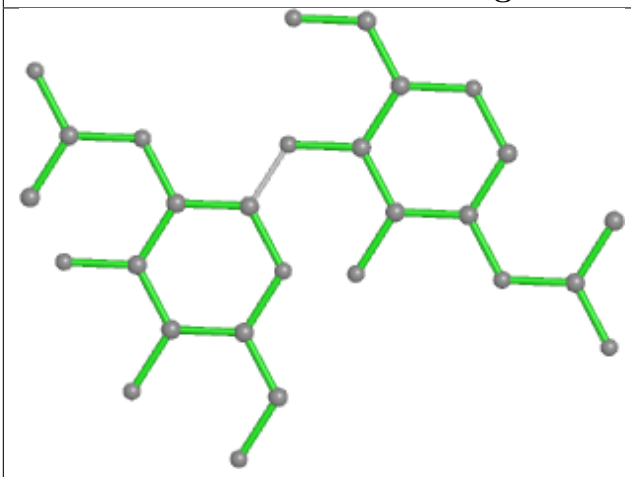


Rings

Oligosaccharide Chain O



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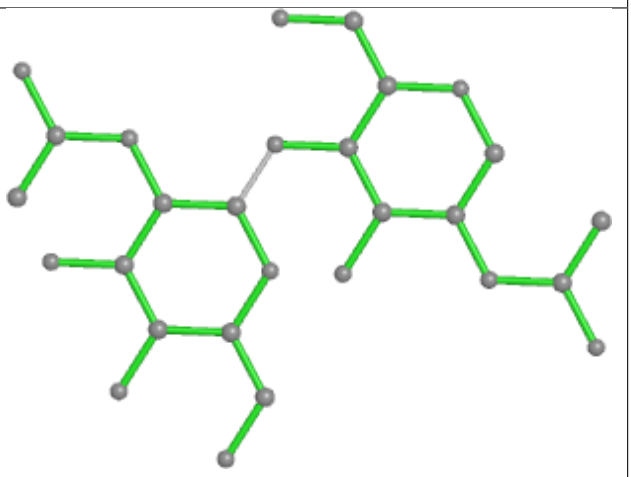
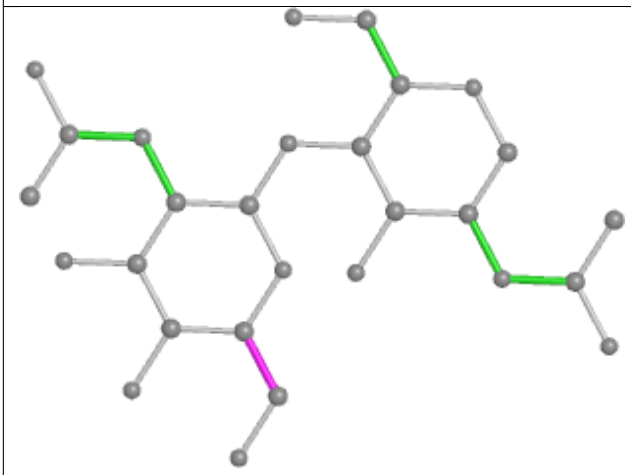


Bond angles



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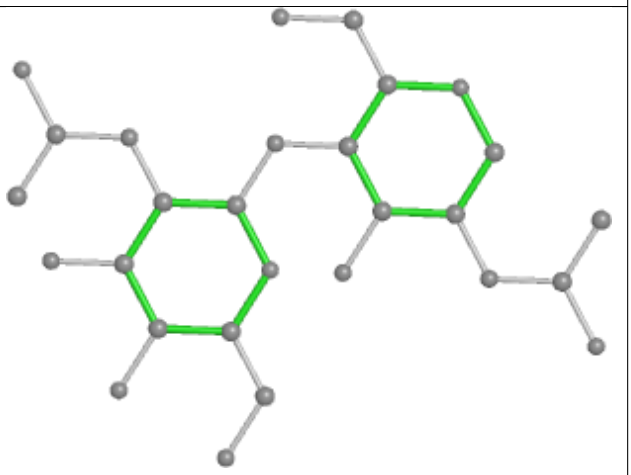
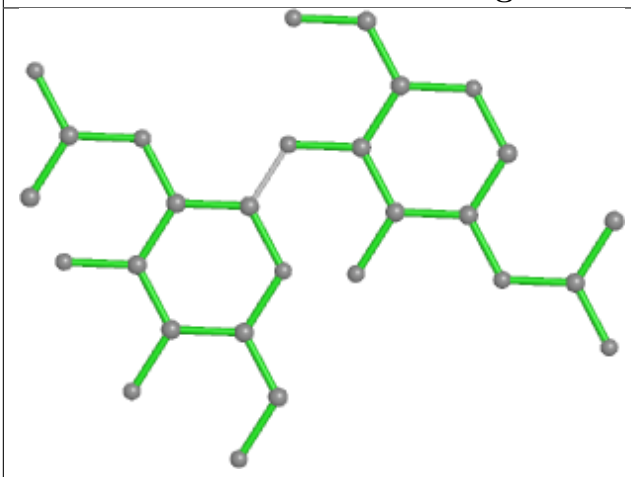


Rings

Oligosaccharide Chain P



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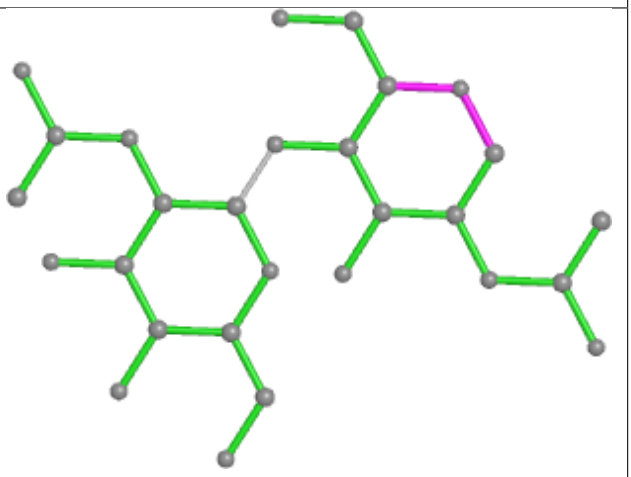
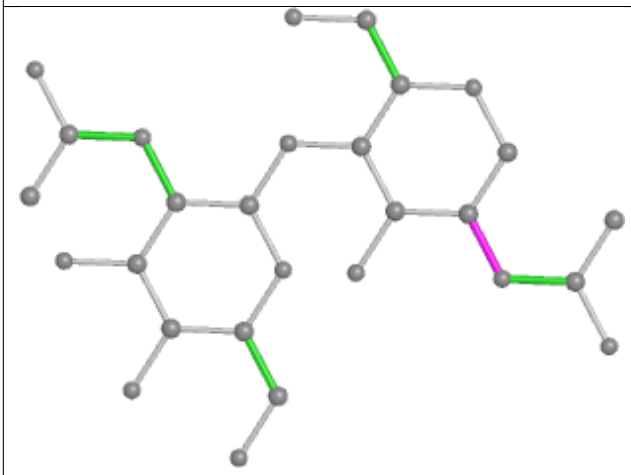


Bond angles



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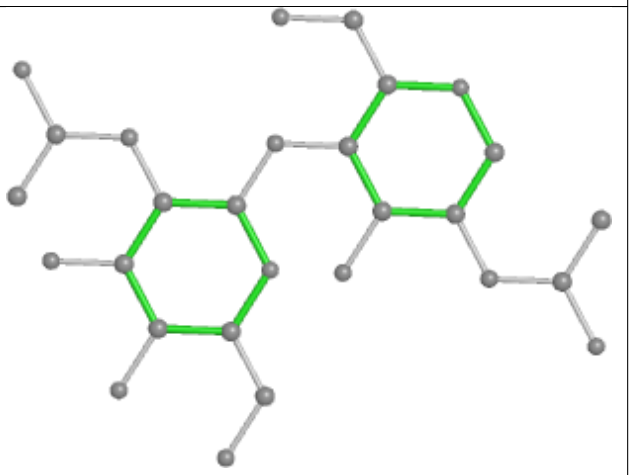
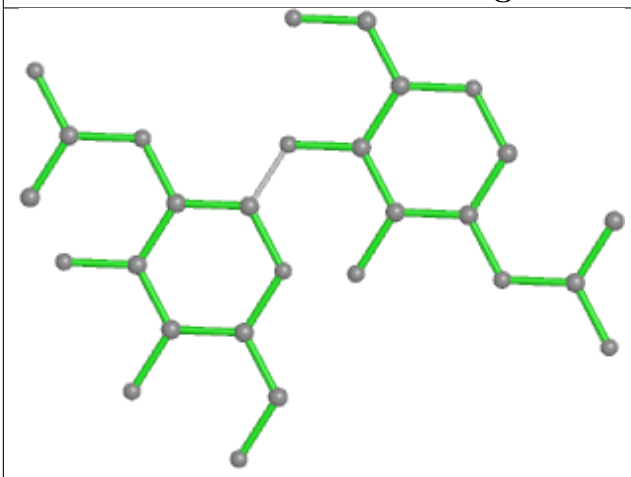


Rings

Oligosaccharide Chain Q



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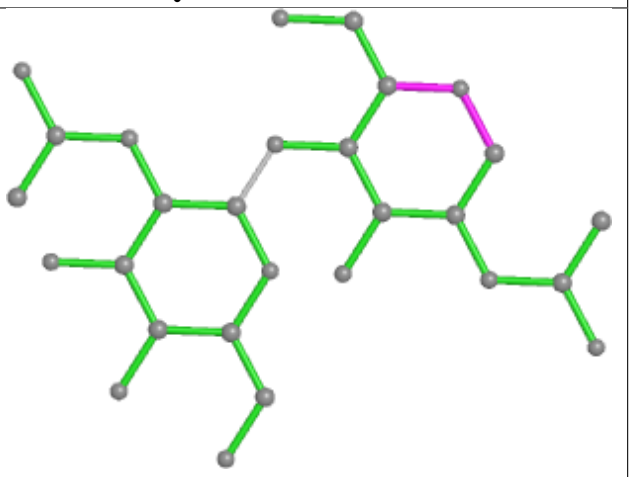
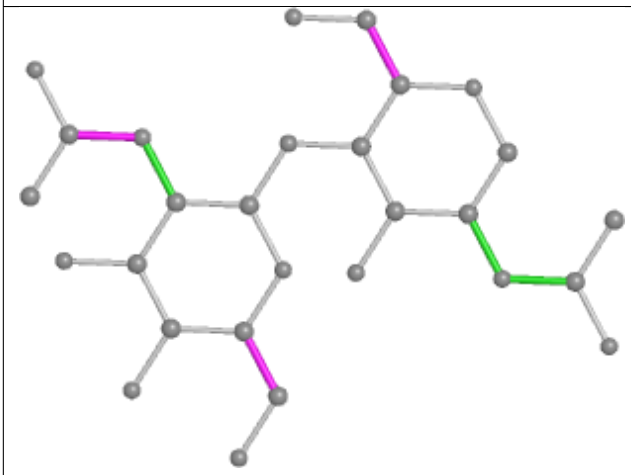
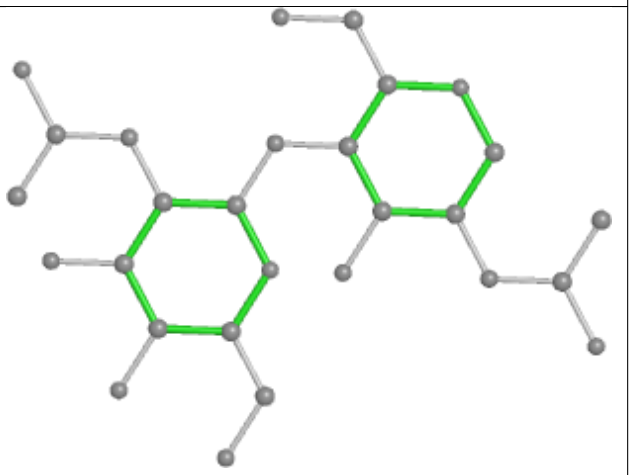


Bond angles

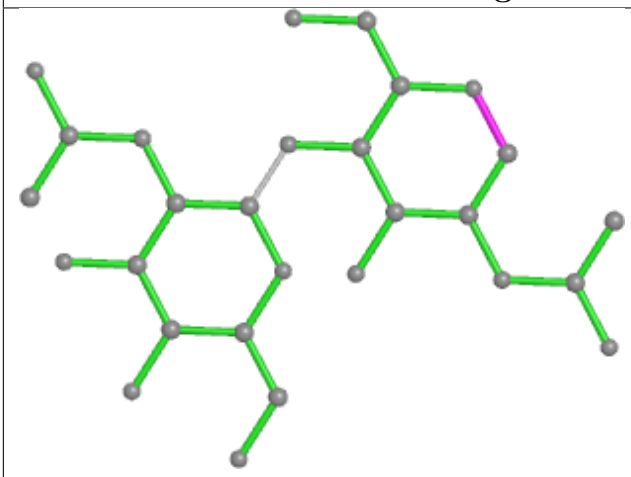


Torsions



Rings

Oligosaccharide Chain R



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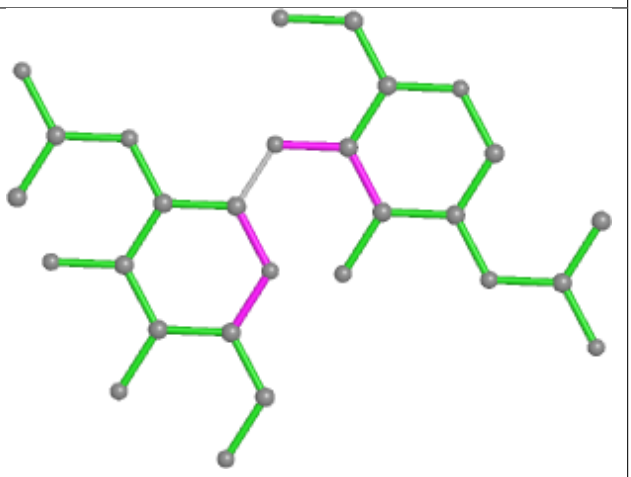
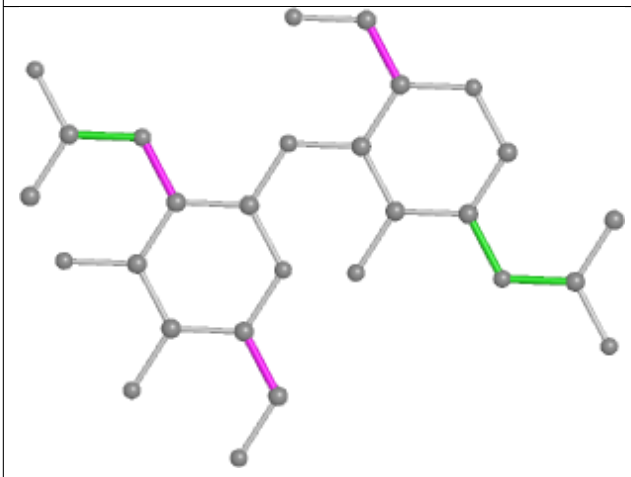


Bond angles



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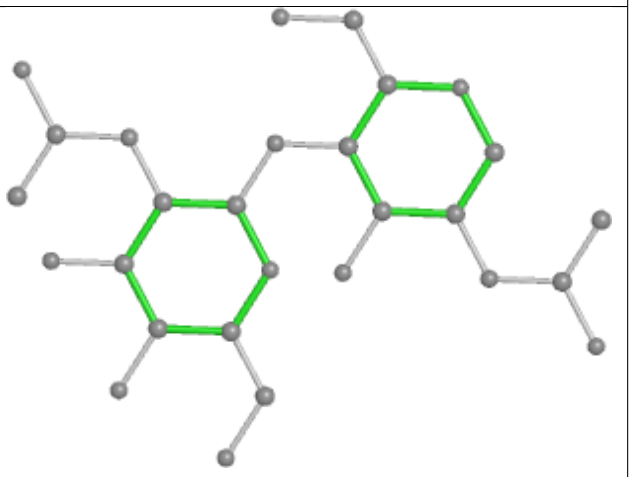
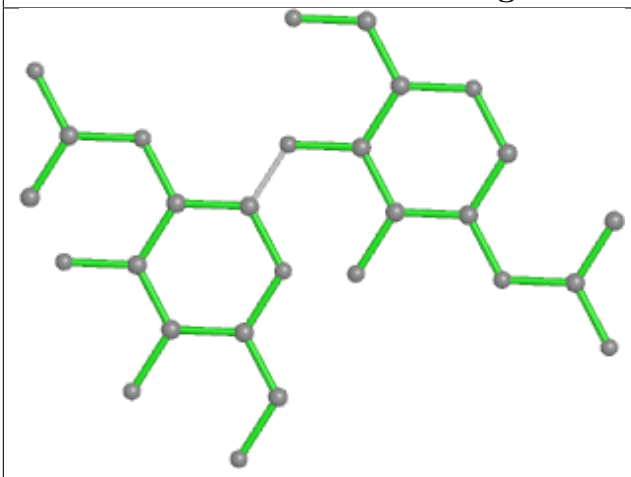


Rings

Oligosaccharide Chain S



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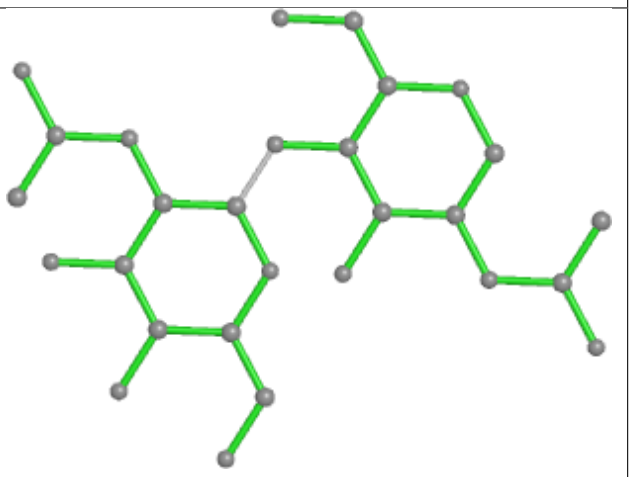
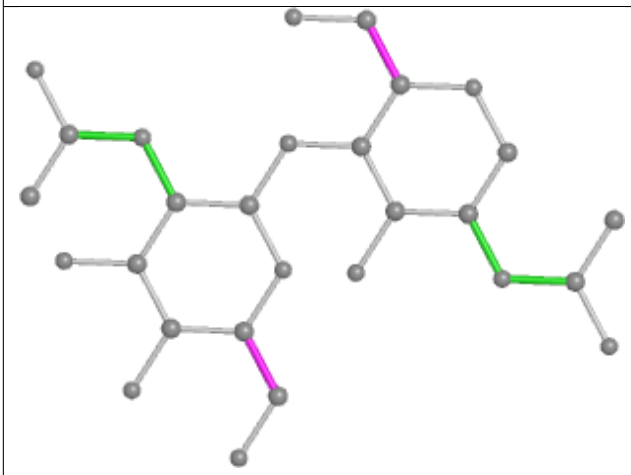
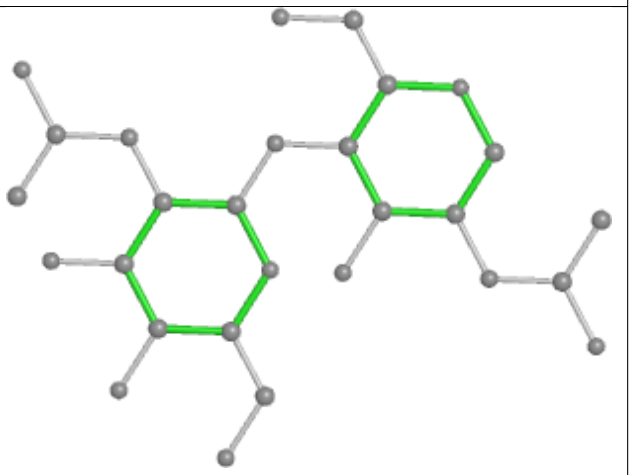


Bond angles

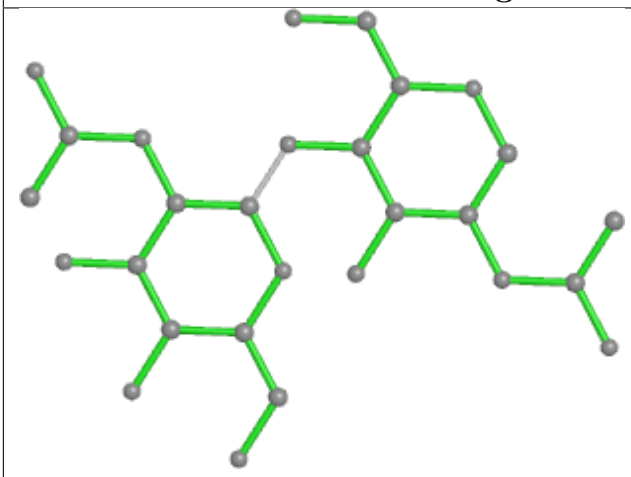


Torsions



Rings

Oligosaccharide Chain T



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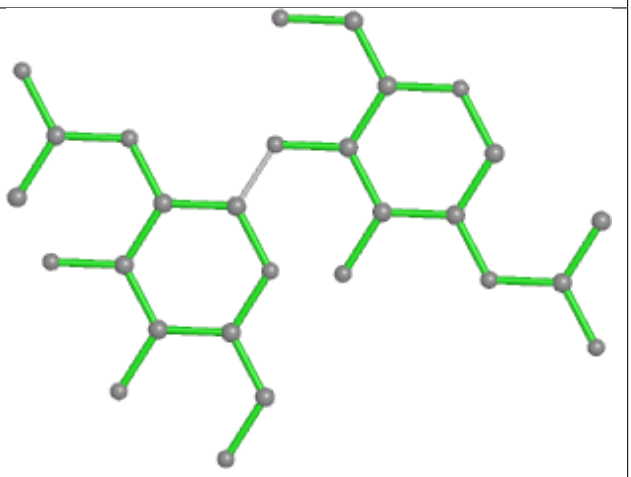
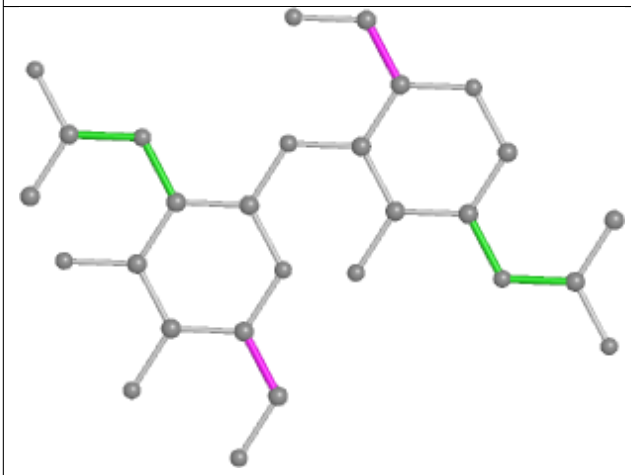
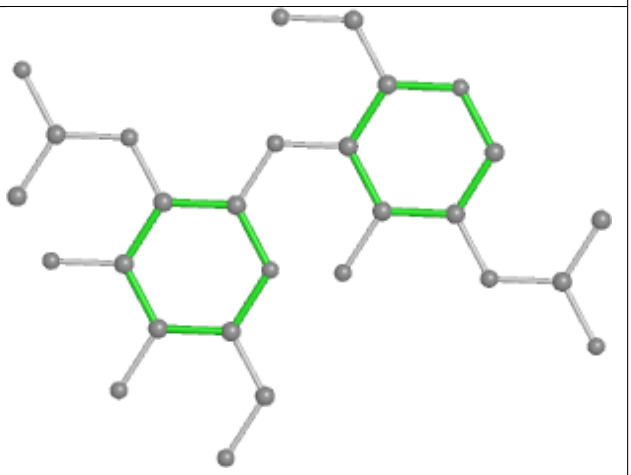


Bond angles

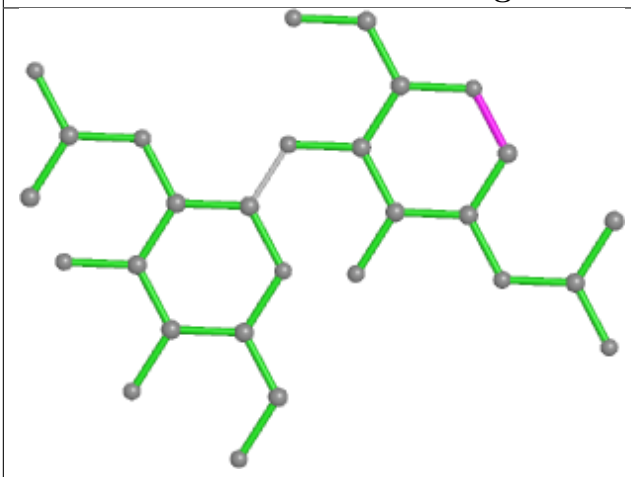


Torsions

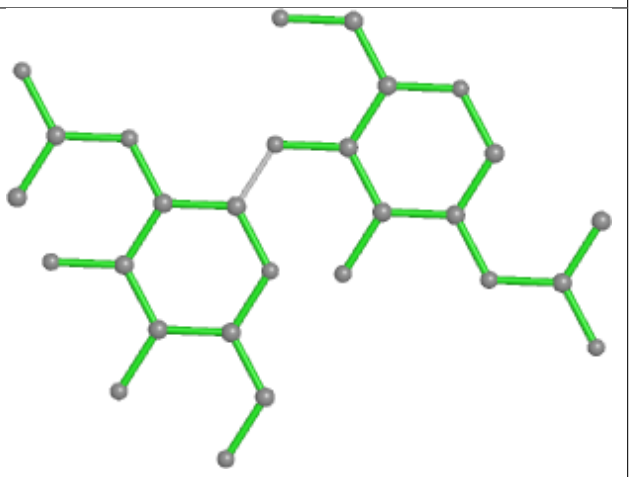


Rings

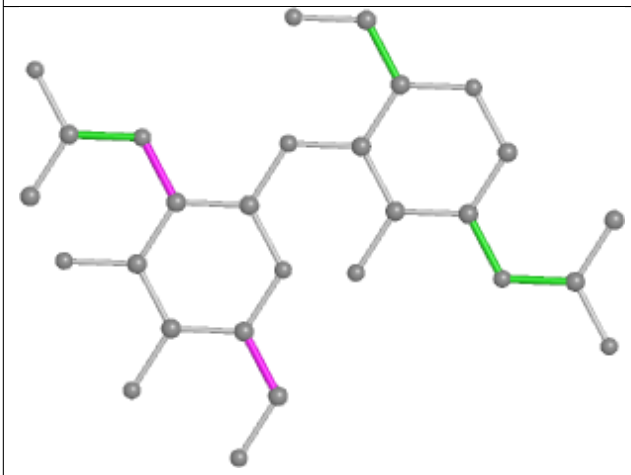
Oligosaccharide Chain U



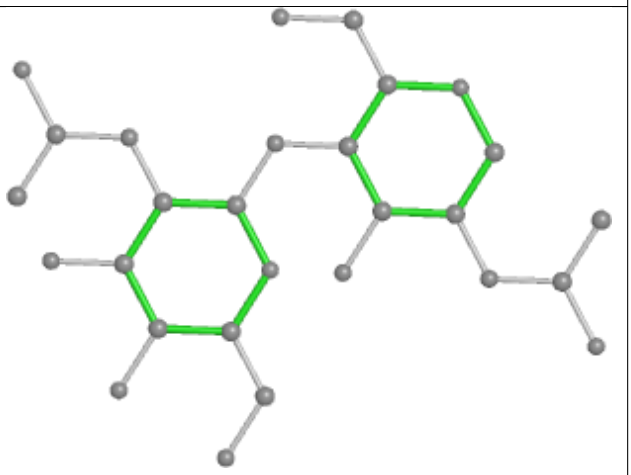
Bond lengths



Bond angles

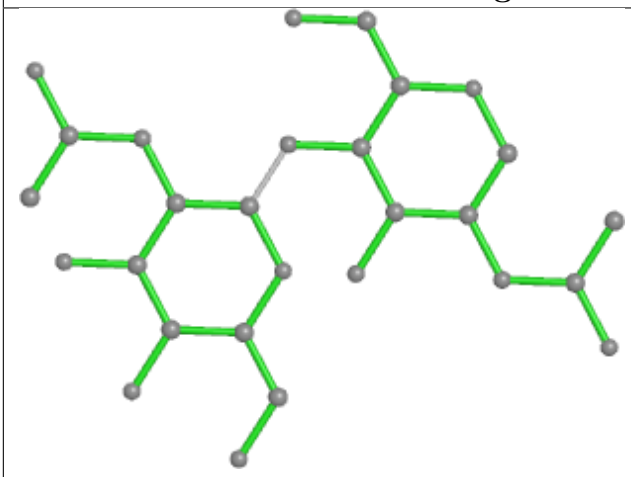


Torsions

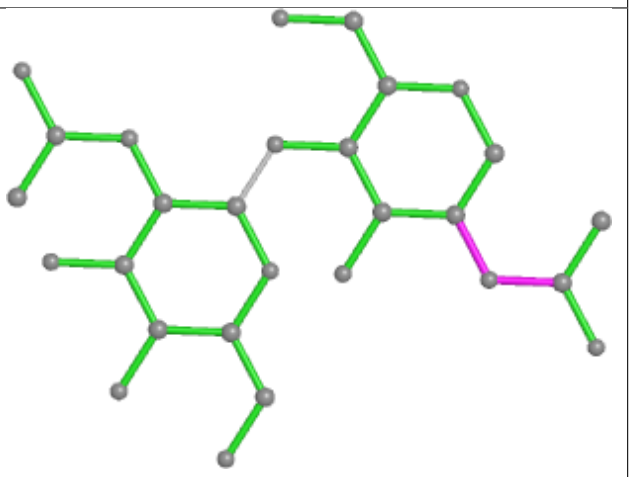


Rings

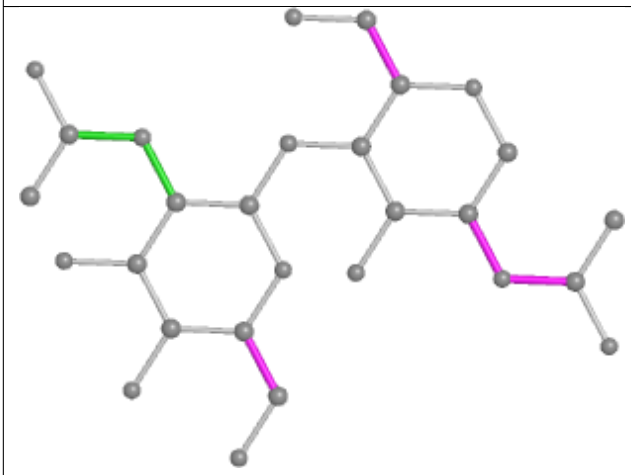
Oligosaccharide Chain V



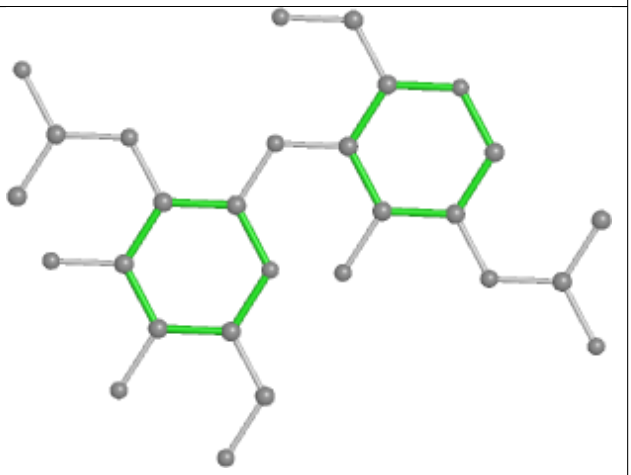
Bond lengths



Bond angles

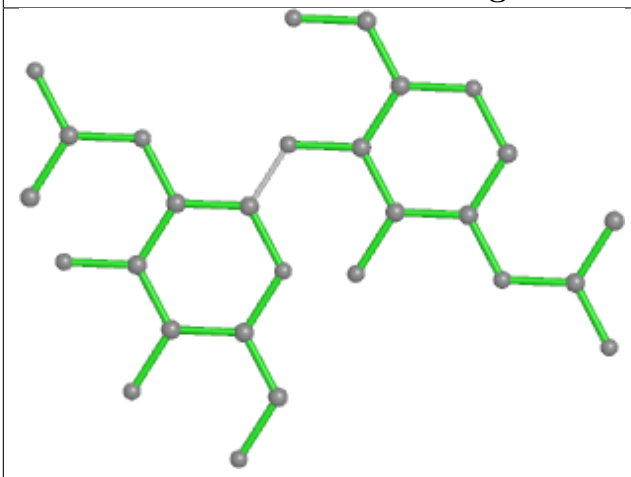


Torsions

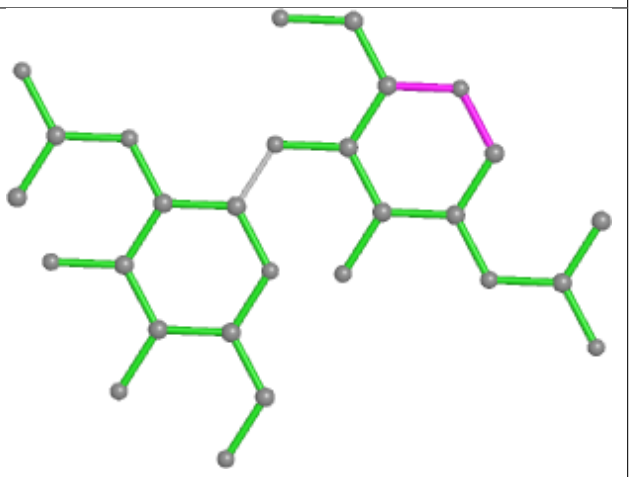


Rings

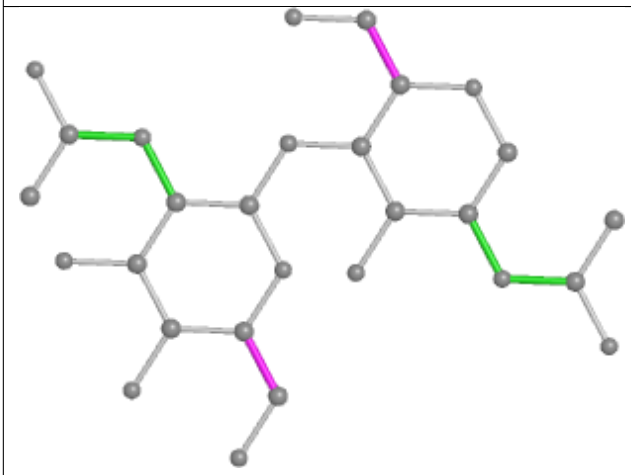
Oligosaccharide Chain W



Bond lengths



Bond angles



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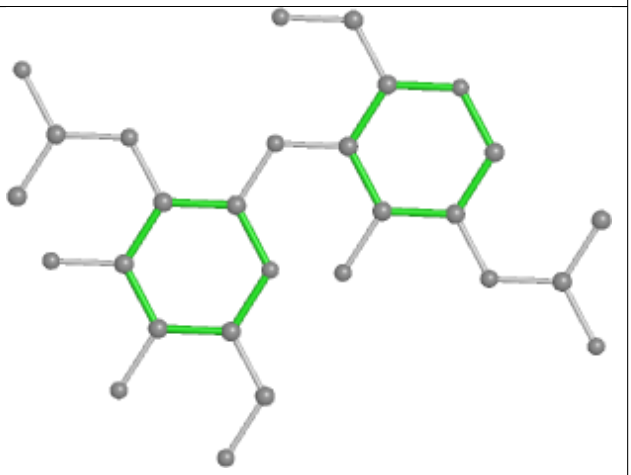
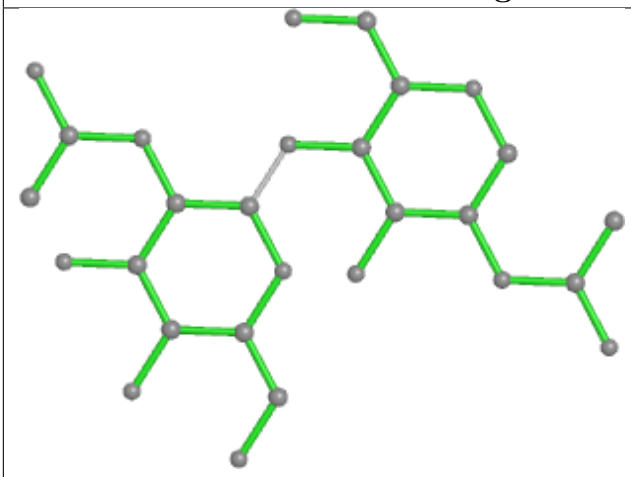


Rings

Oligosaccharide Chain X



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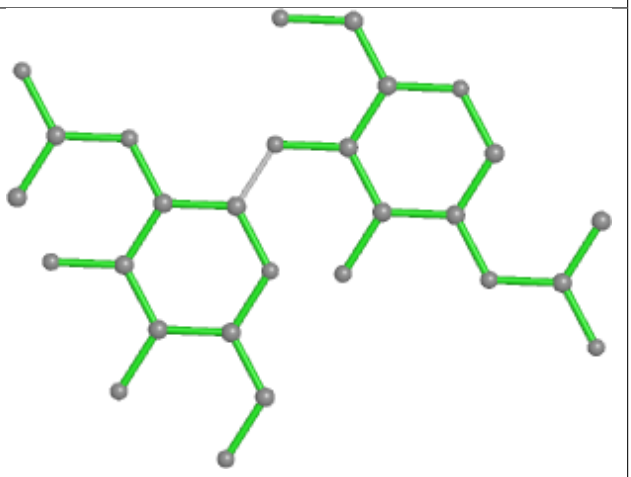
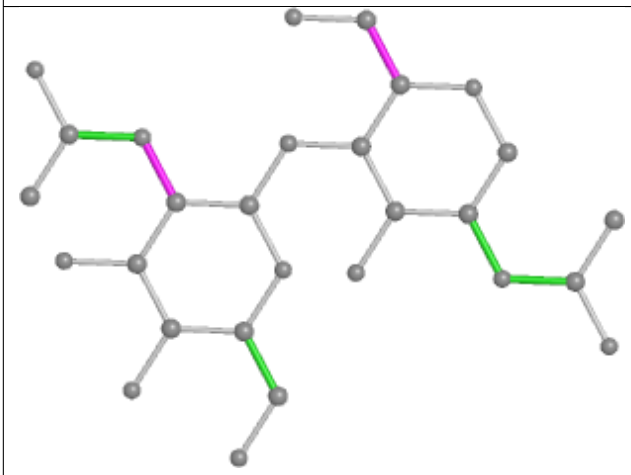


Bond angles



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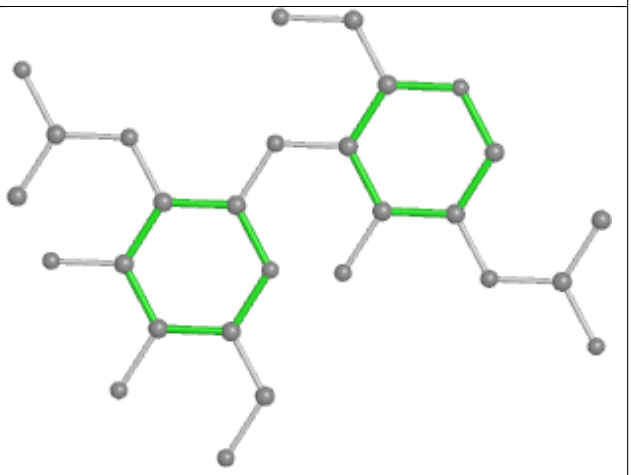
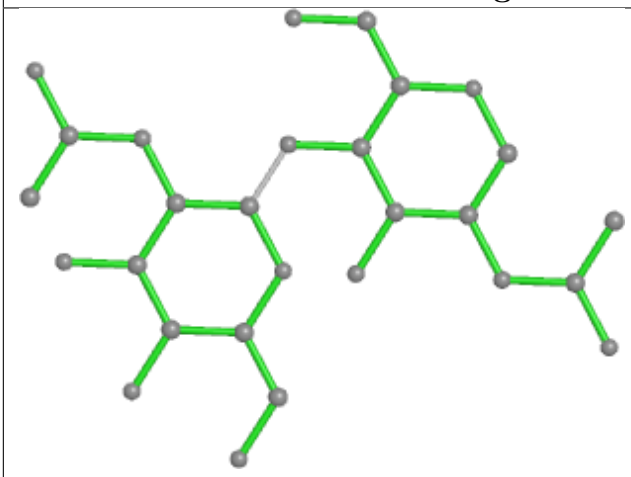


Rings

Oligosaccharide Chain Y



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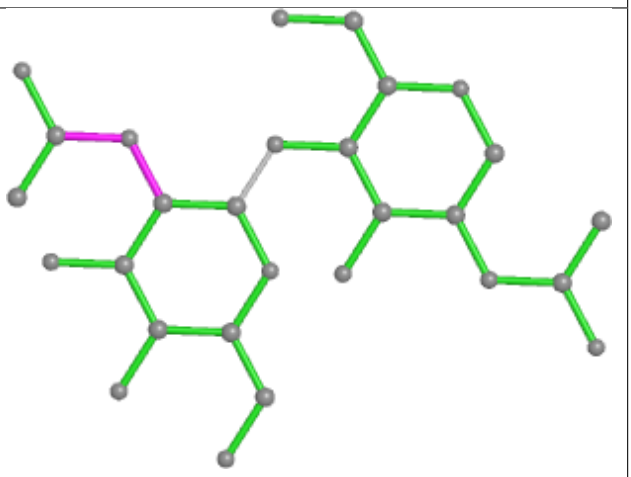

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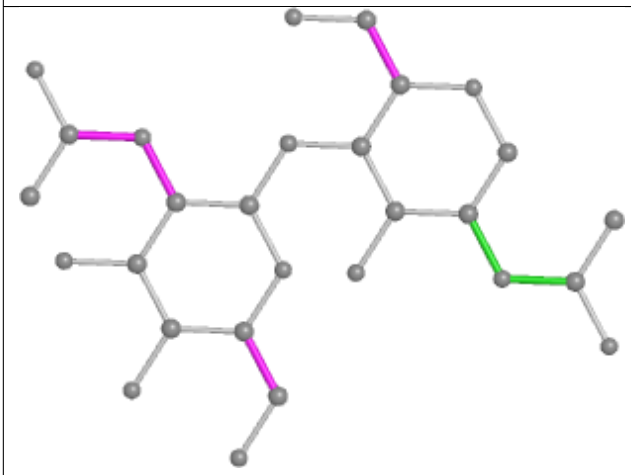

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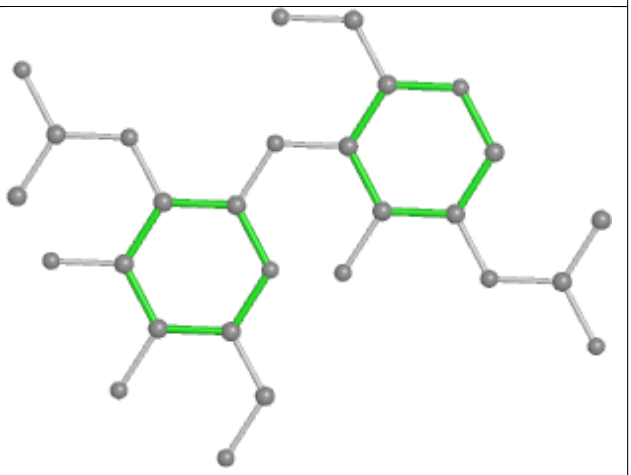
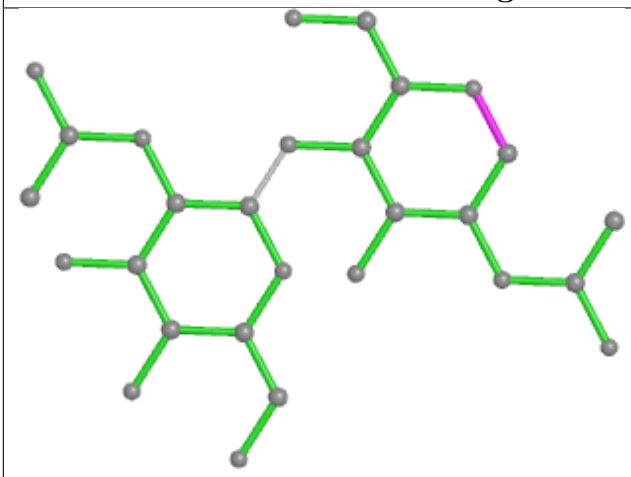


Rings

Oligosaccharide Chain Z



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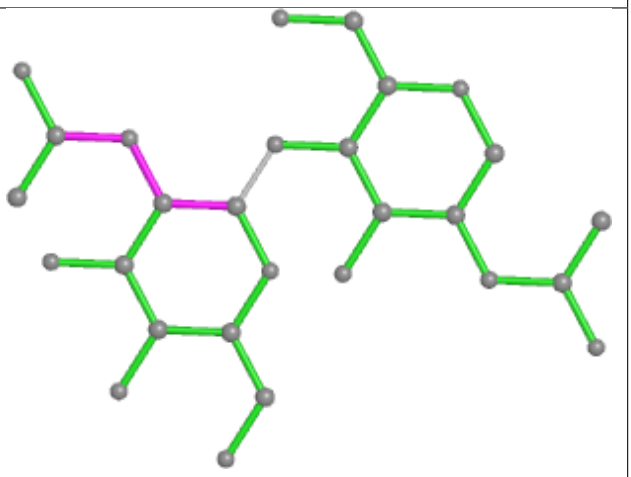
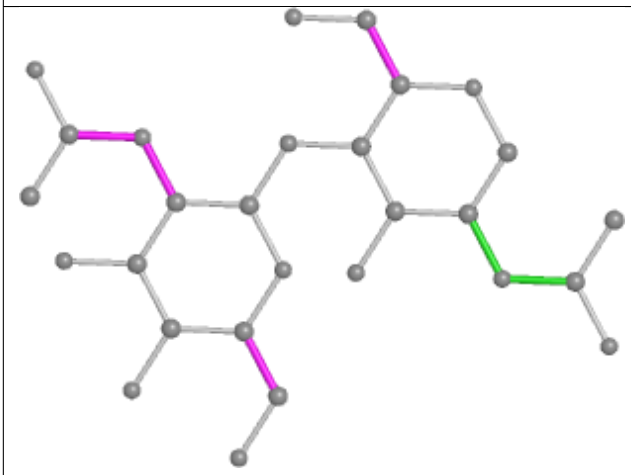


Bond angles



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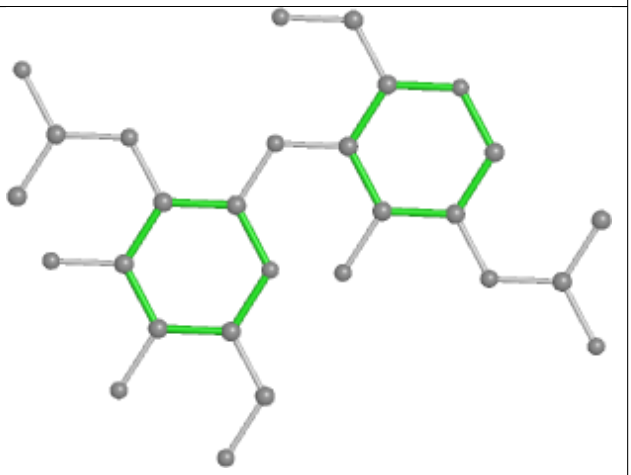
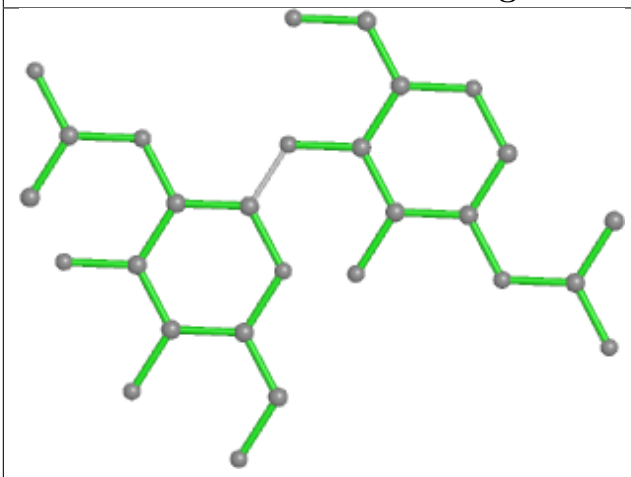


Rings

Oligosaccharide Chain a



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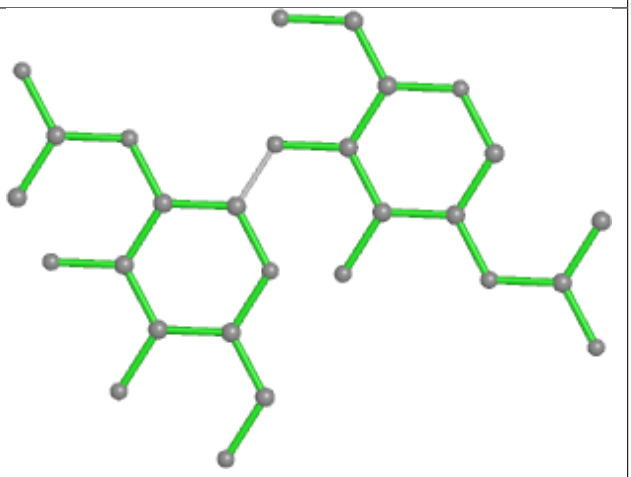

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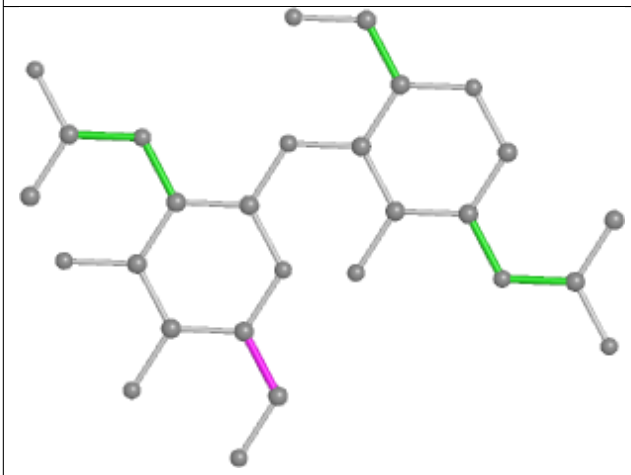

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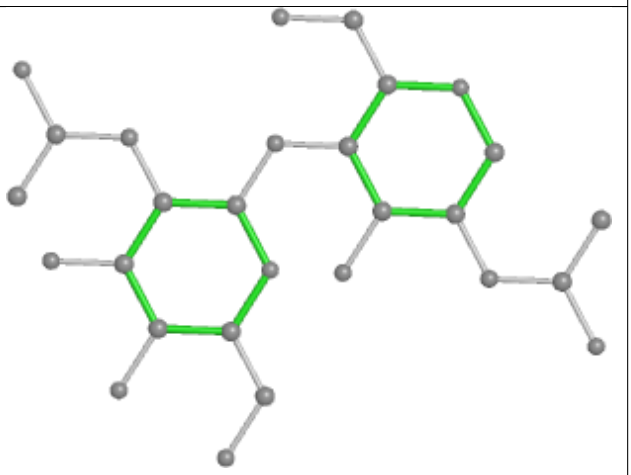
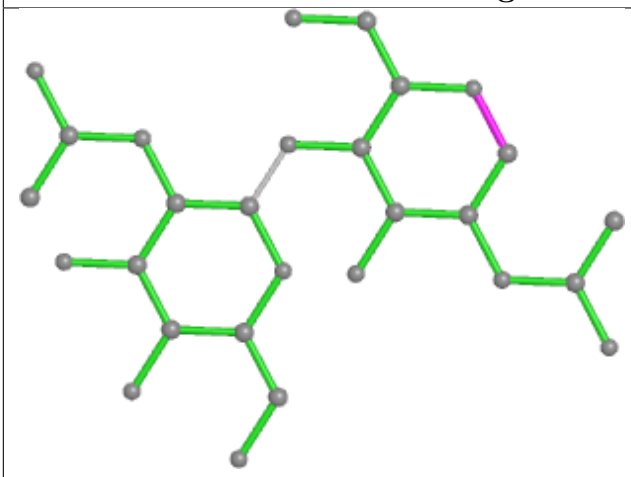


Rings

Oligosaccharide Chain b



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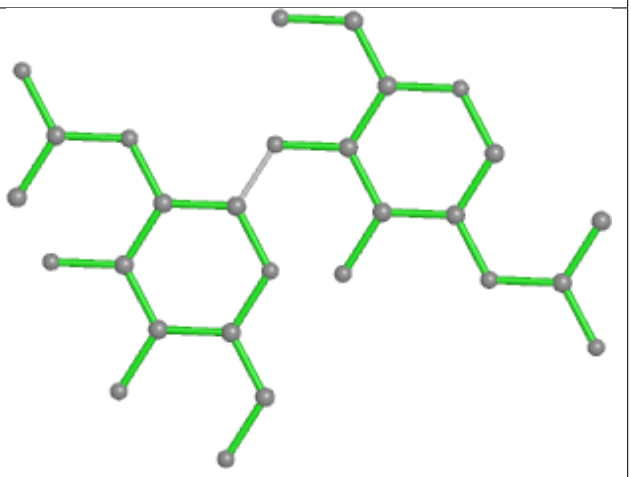

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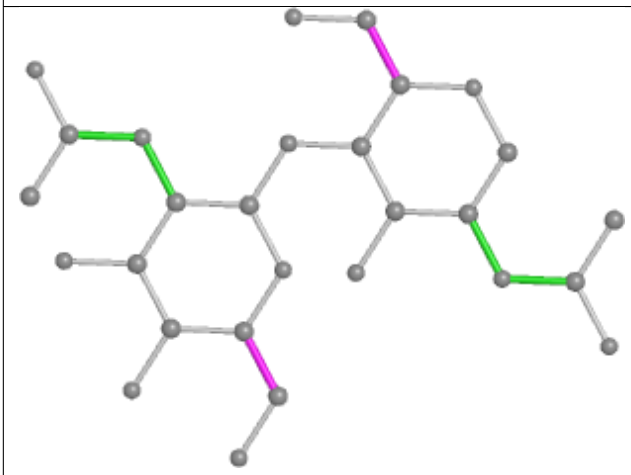

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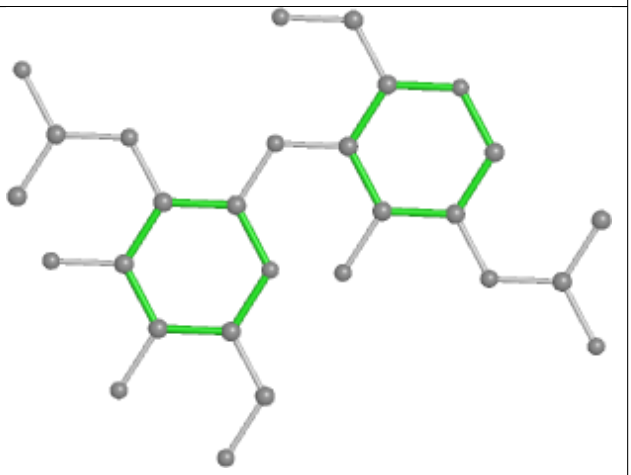
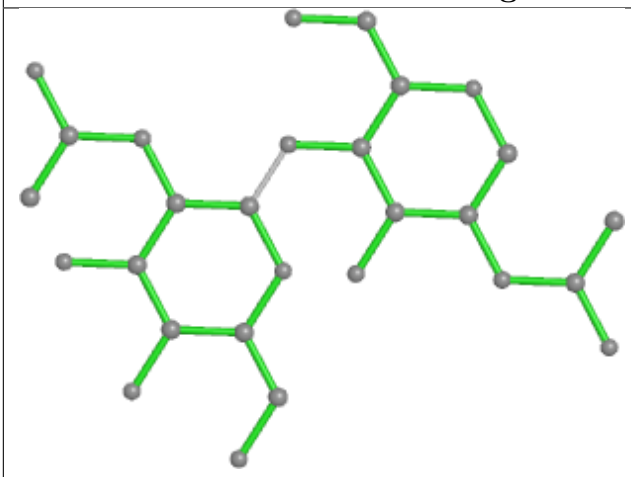


Rings

Oligosaccharide Chain c



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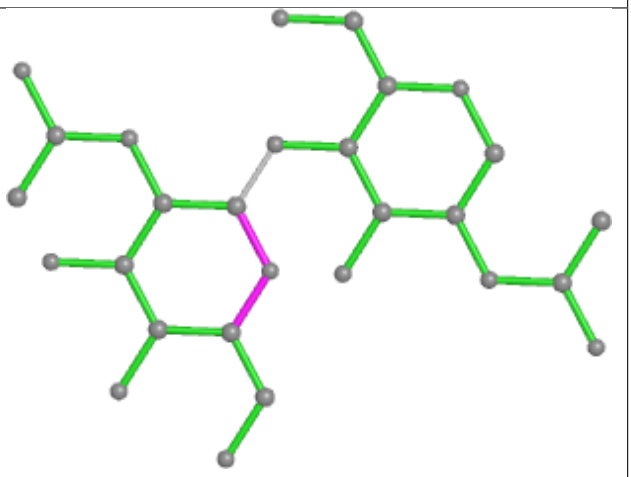

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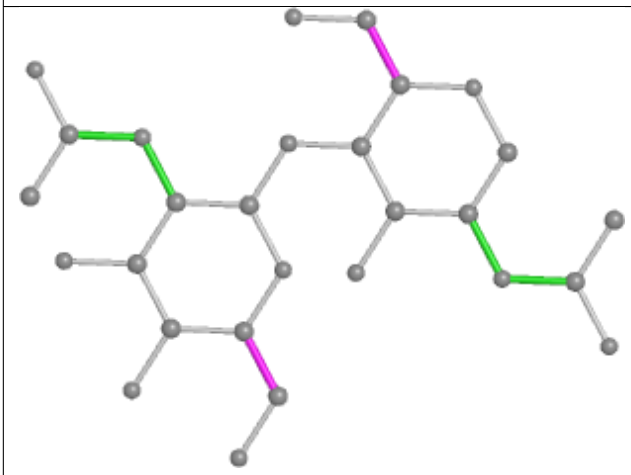

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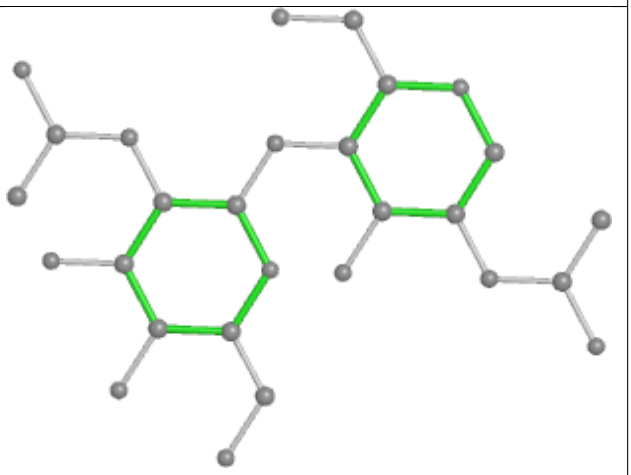
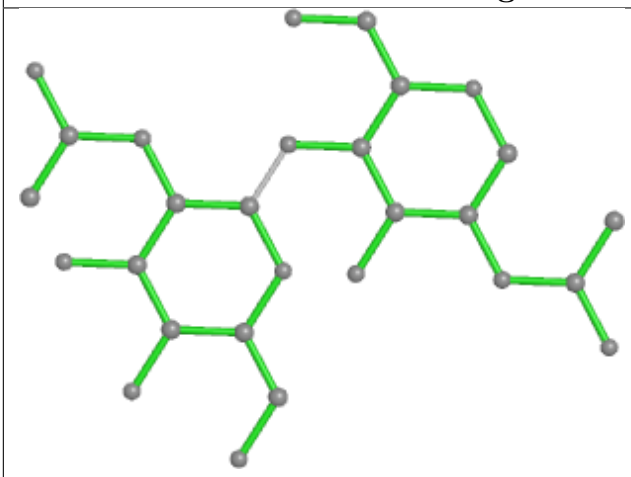


Rings

Oligosaccharide Chain d



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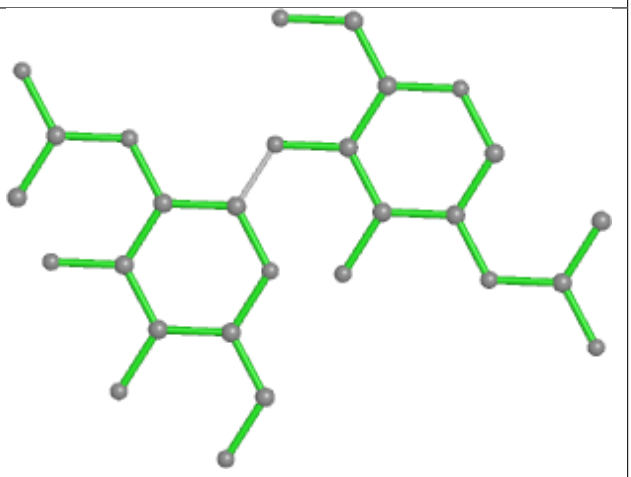

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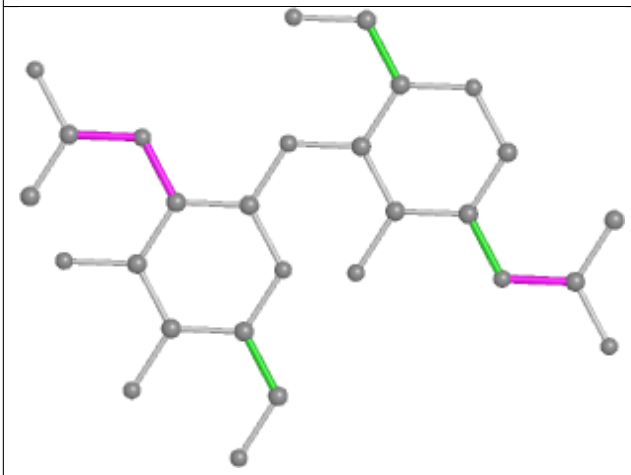

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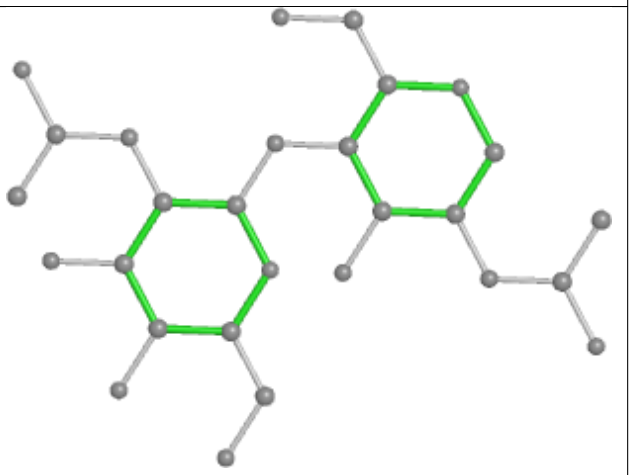
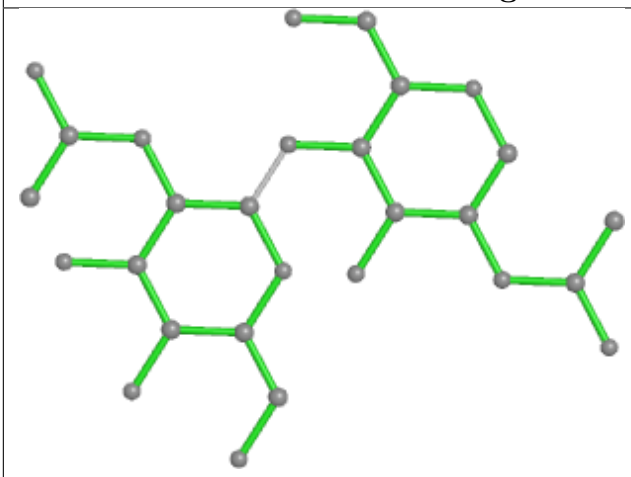


Rings

Oligosaccharide Chain e



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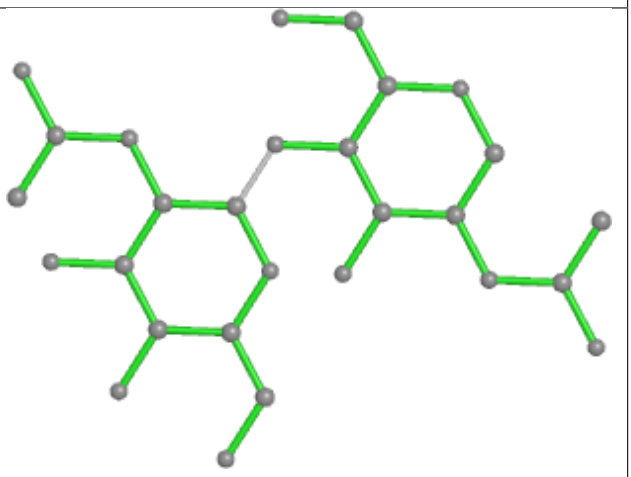

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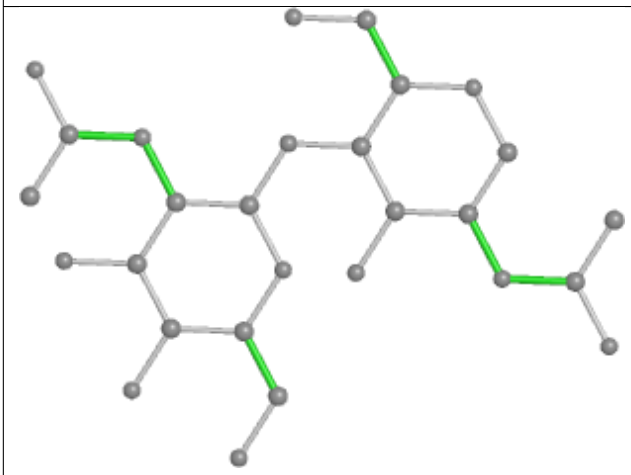

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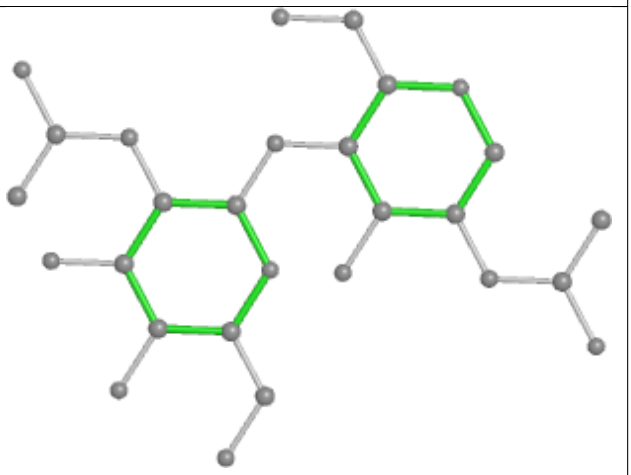
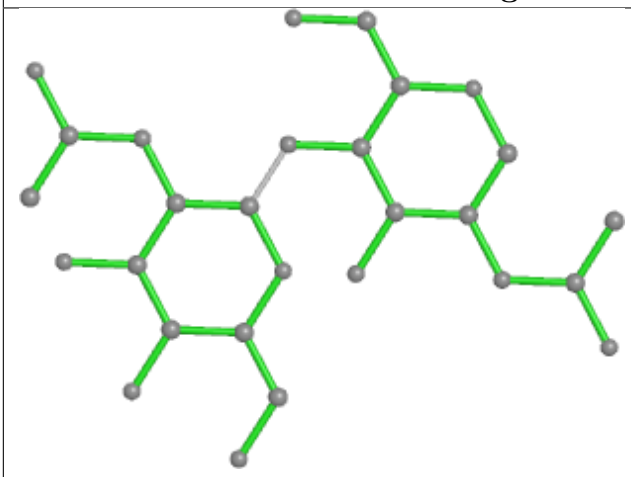


Rings

Oligosaccharide Chain f



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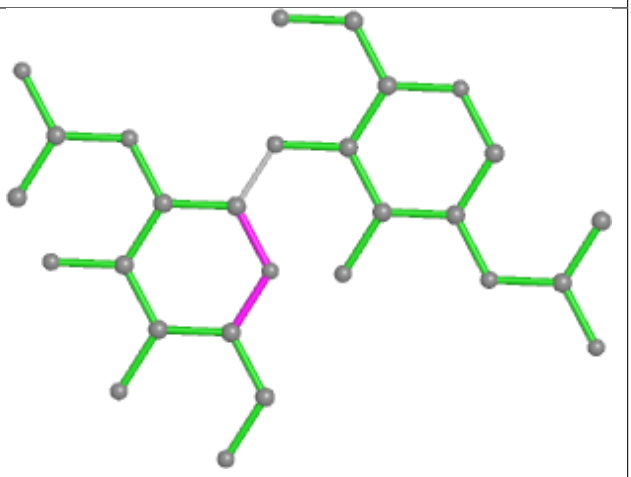

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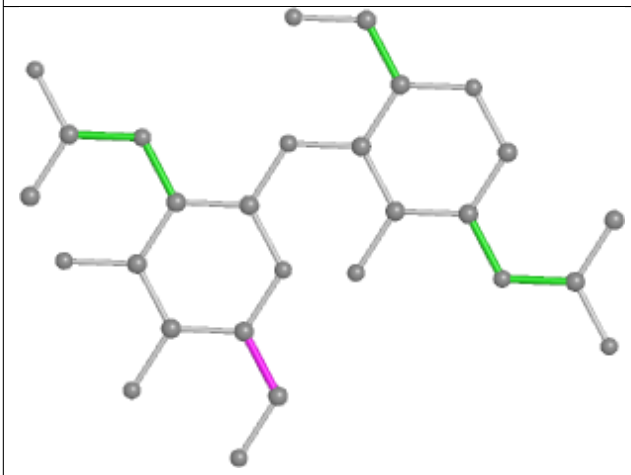

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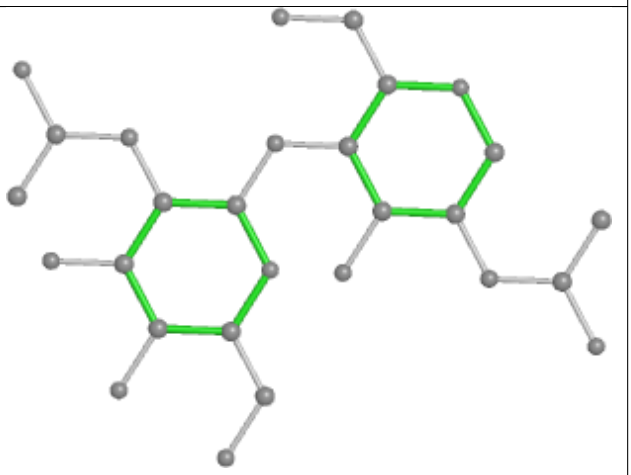
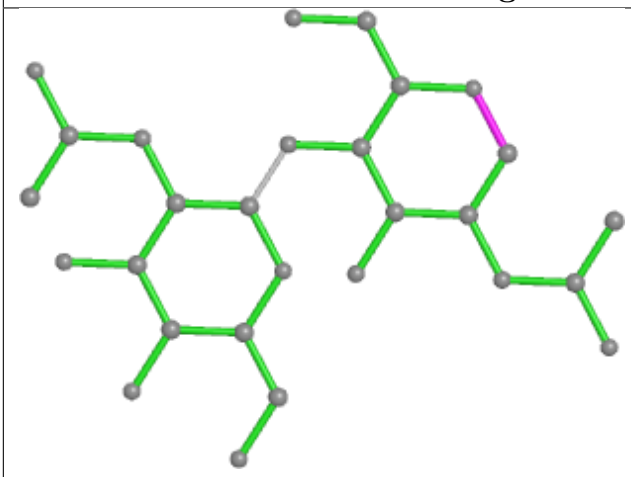


Rings

Oligosaccharide Chain g



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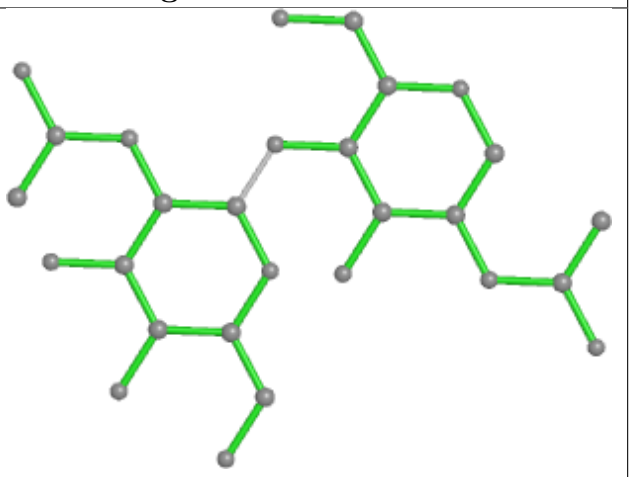
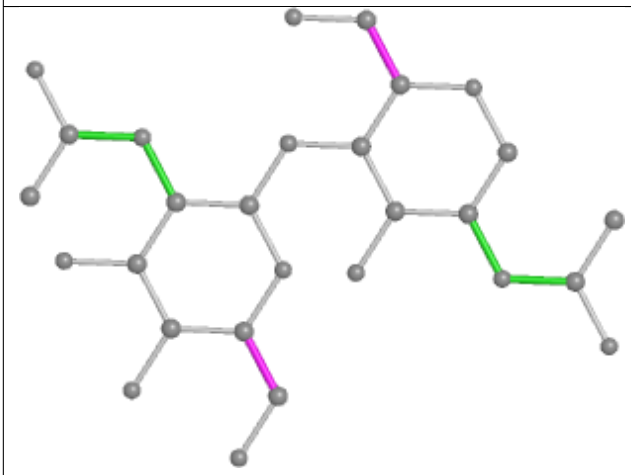


Bond angles



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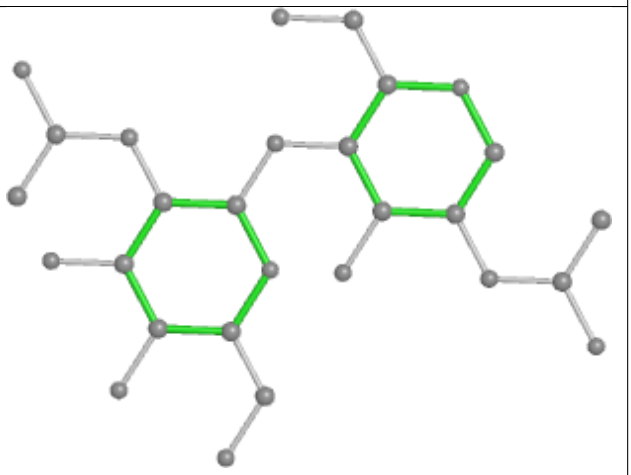
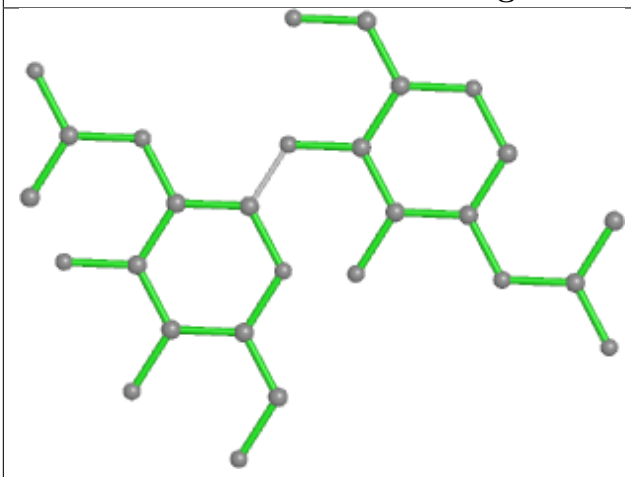


Rings

Oligosaccharide Chain h



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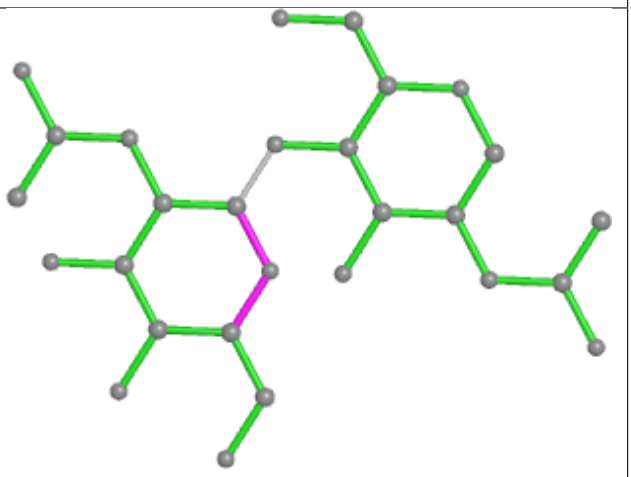

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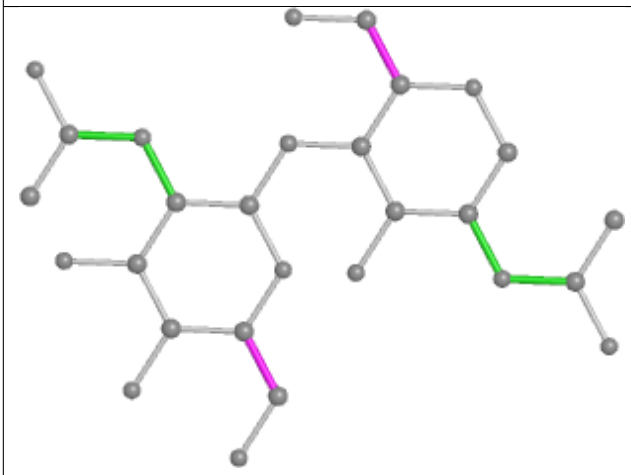

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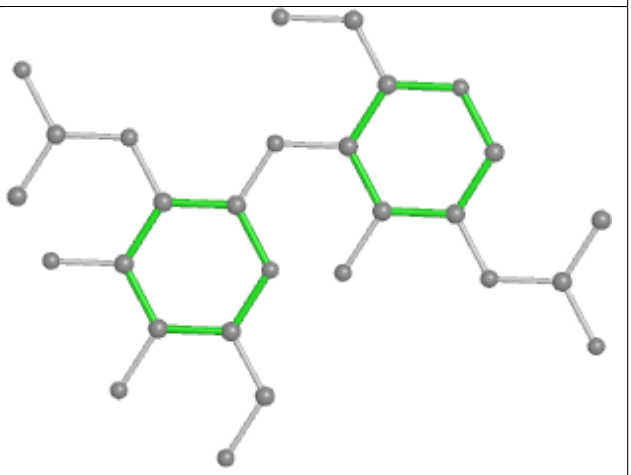
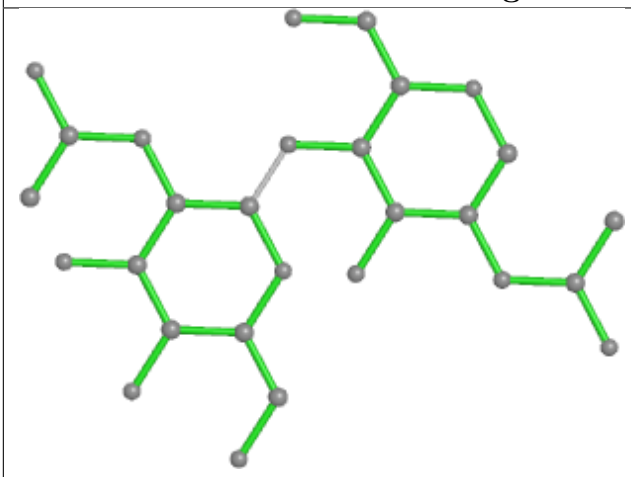


Rings

Oligosaccharide Chain i



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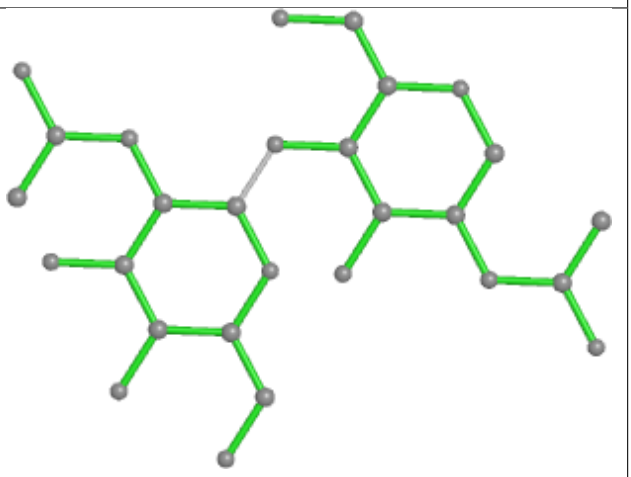
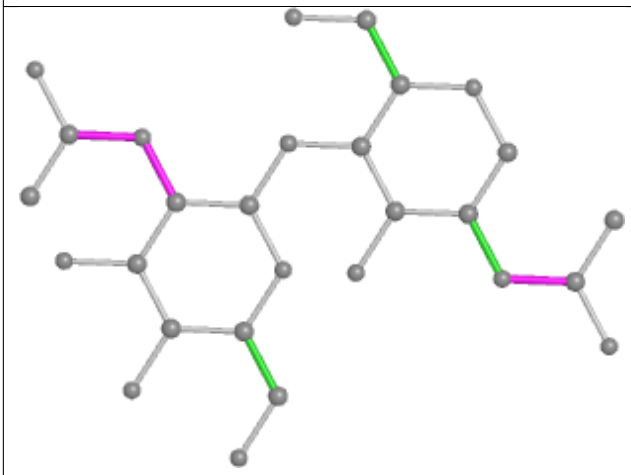


Bond angles



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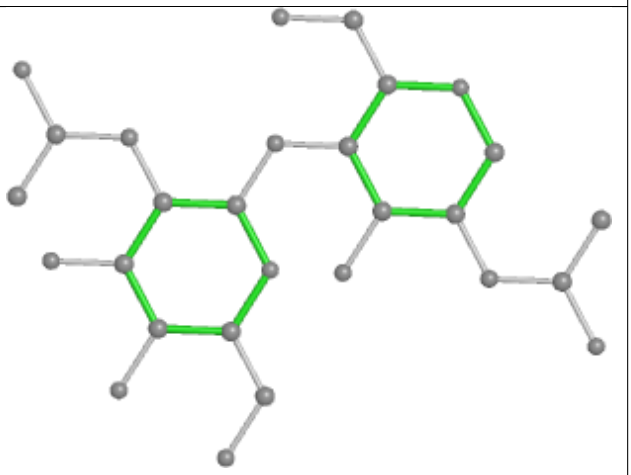
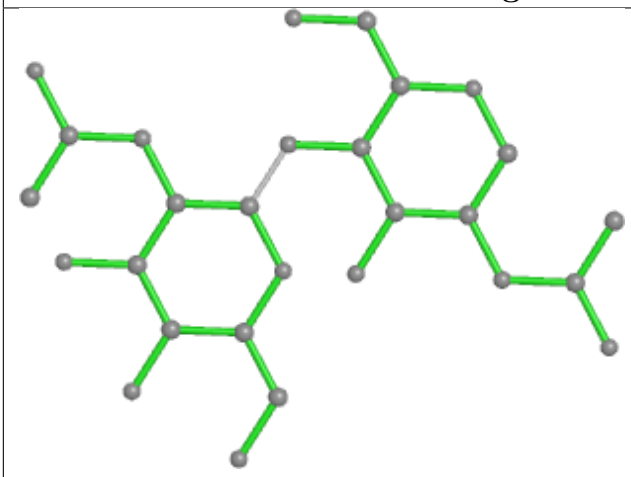


Rings

Oligosaccharide Chain j



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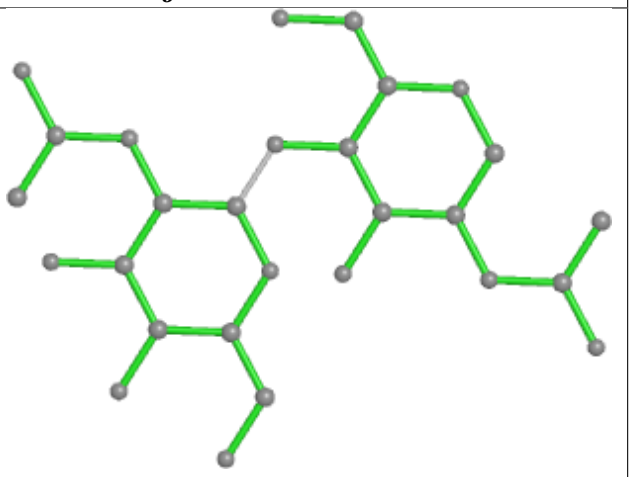
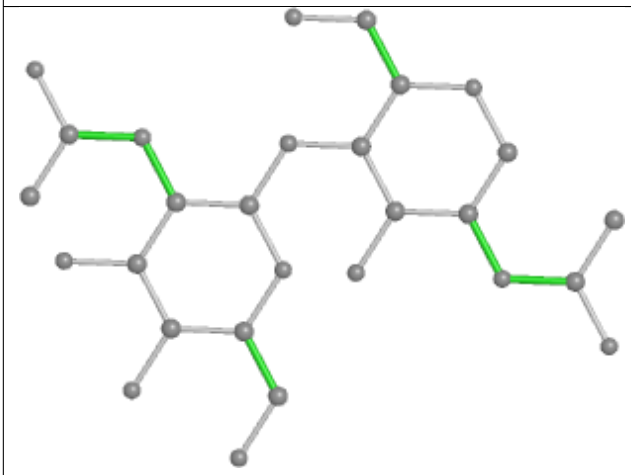


Bond angles



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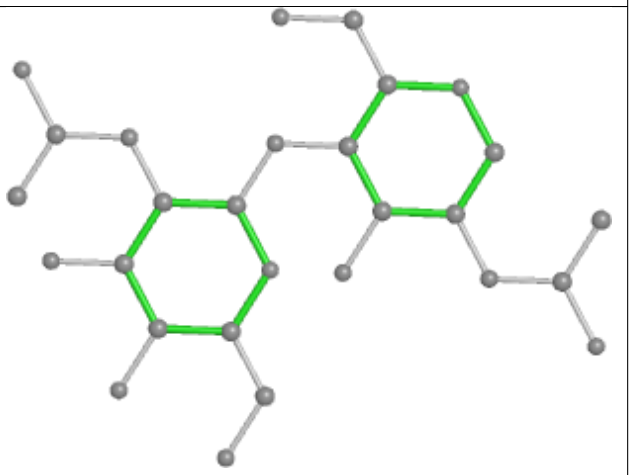
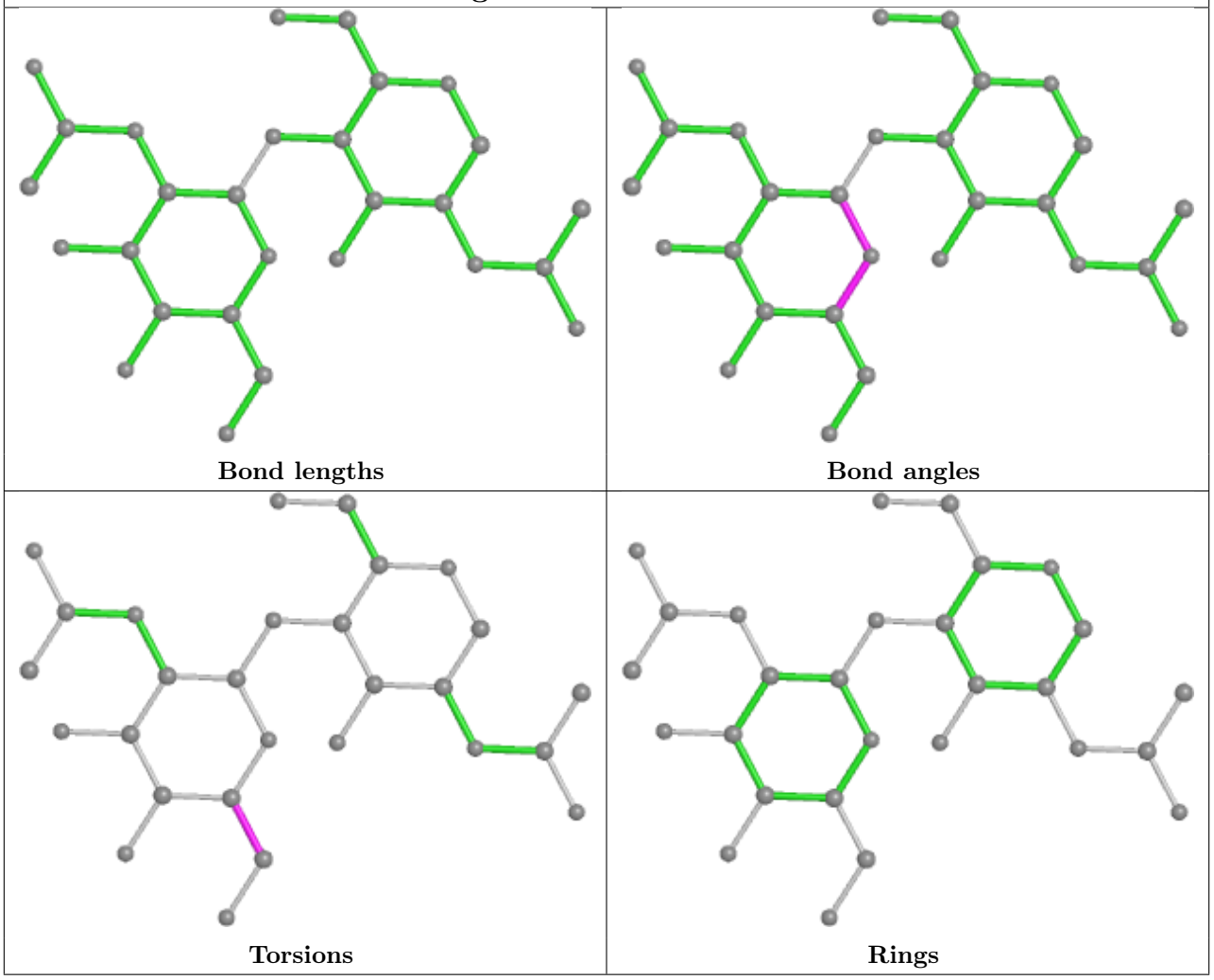


Rings

Oligosaccharide Chain k



5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
4	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.36	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	C	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	E	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1410	-	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.64	0
4	NAG	C	1401	1	14,14,15	0.30	0	17,19,21	0.34	0
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	C	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.54	0
4	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.64	0
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.42	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	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1405	NAG	C2-N2-C7	4.34	129.08	122.90
4	A	1405	NAG	C2-N2-C7	4.32	129.05	122.90
4	B	1405	NAG	C2-N2-C7	4.29	129.02	122.90
4	B	1409	NAG	C8-C7-N2	2.29	119.97	116.10
4	E	901	NAG	C1-O5-C5	2.09	115.02	112.19
4	D	901	NAG	C1-O5-C5	2.07	114.99	112.19
4	B	1409	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	E	901	NAG	C4-C5-C6-O6
4	C	1407	NAG	C1-C2-N2-C7
4	A	1407	NAG	C1-C2-N2-C7
4	B	1407	NAG	C1-C2-N2-C7
4	A	1405	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

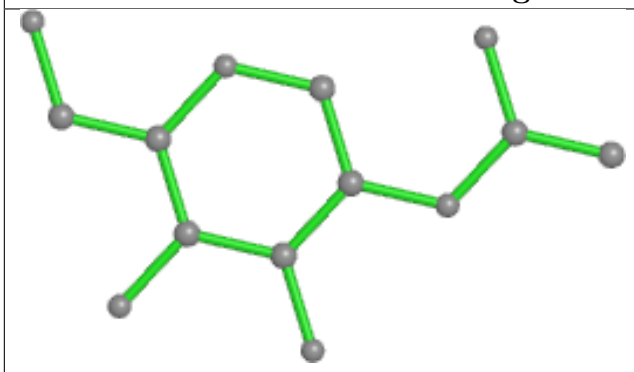
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1402	NAG	3	0
4	C	1405	NAG	1	0
4	B	1410	NAG	4	0
4	B	1402	NAG	3	0
4	A	1405	NAG	1	0
4	B	1409	NAG	4	0
4	B	1405	NAG	1	0
4	A	1402	NAG	3	0

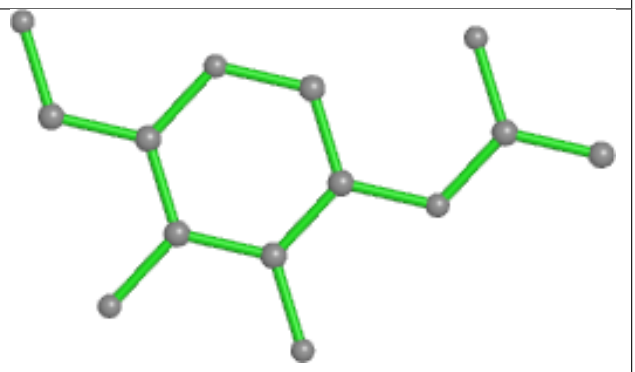
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

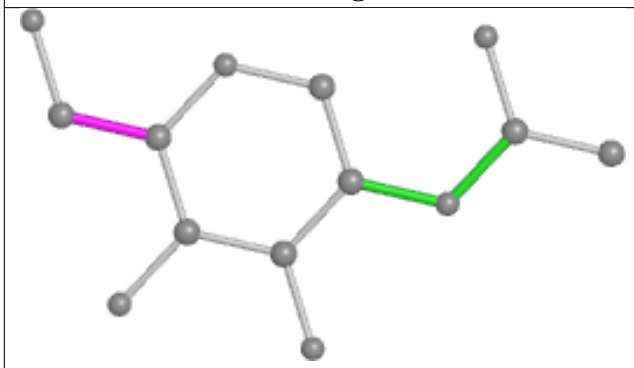
Ligand NAG B 1406



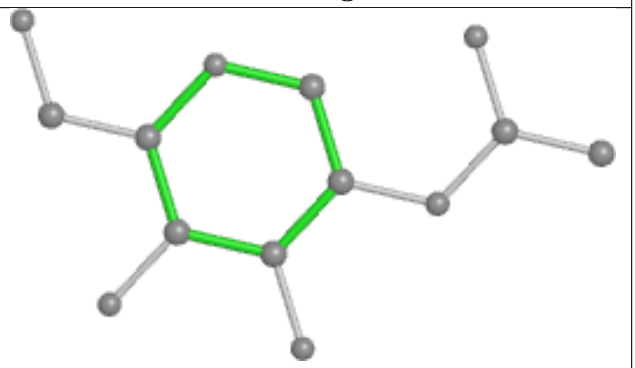
Bond lengths



Bond angles

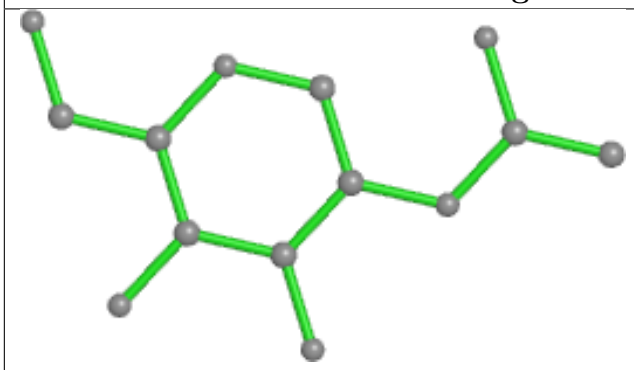


Torsions

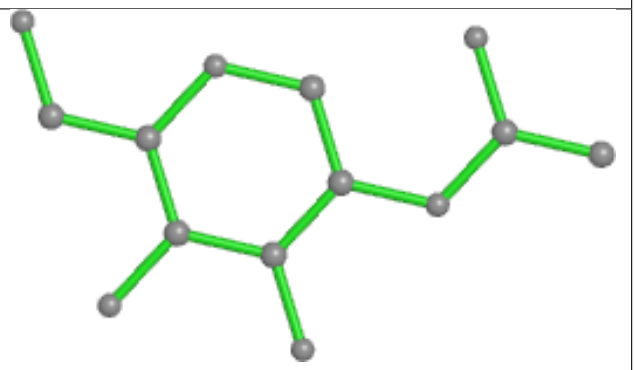


Rings

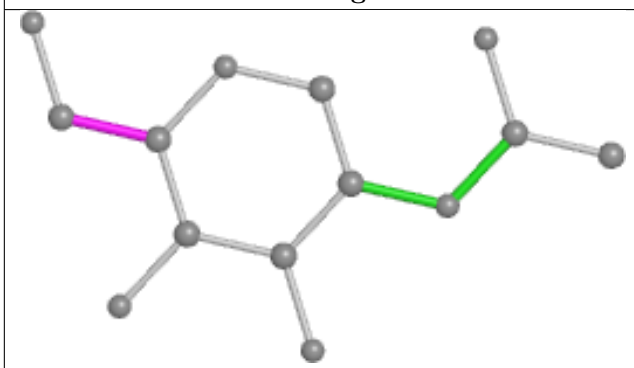
Ligand NAG A 1408



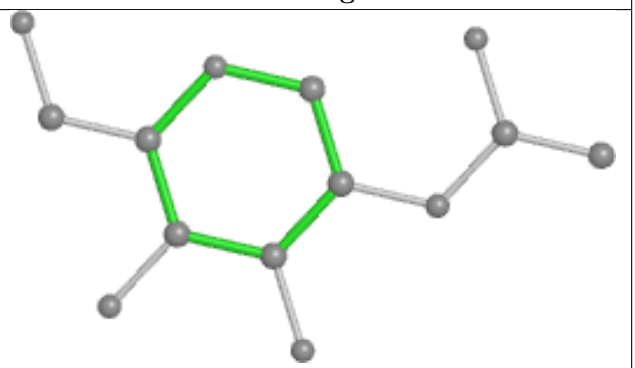
Bond lengths



Bond angles

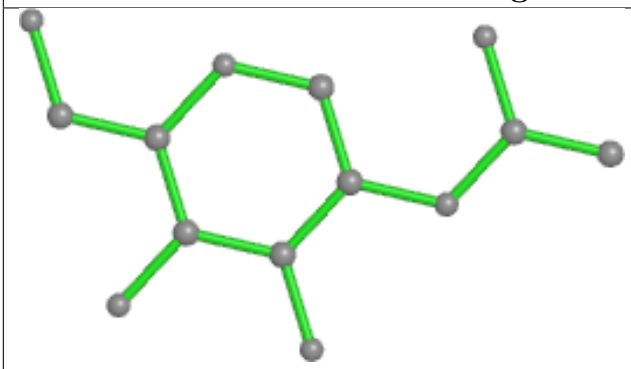


Torsions

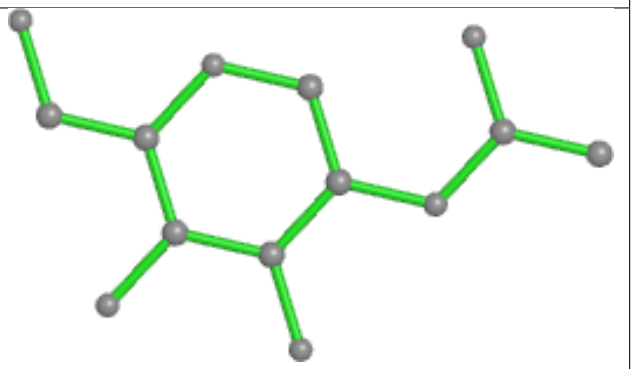


Rings

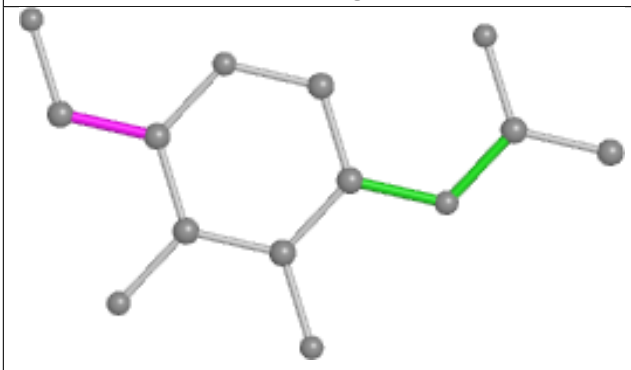
Ligand NAG A 1409



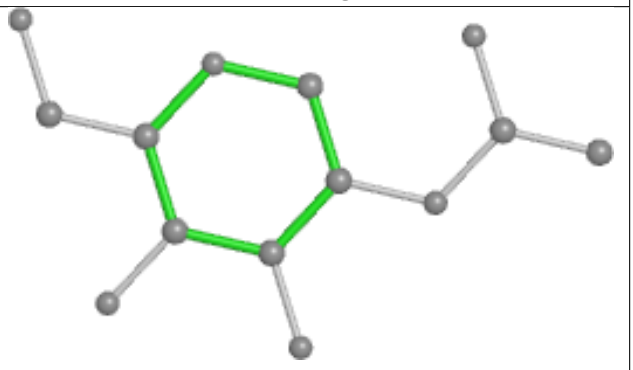
Bond lengths



Bond angles

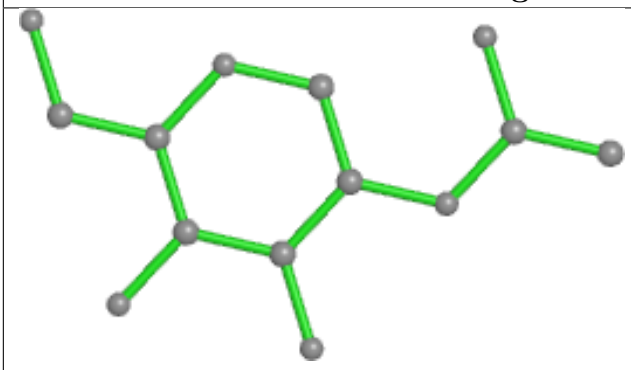


Torsions

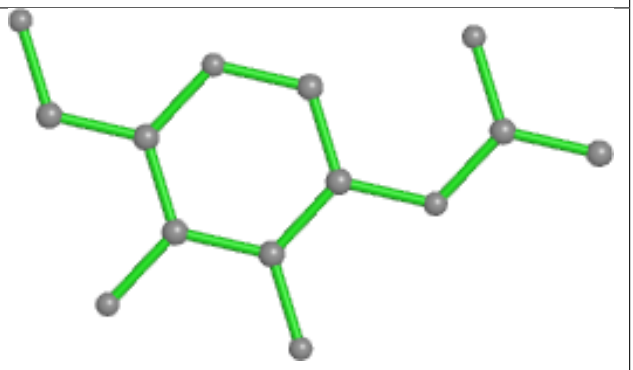


Rings

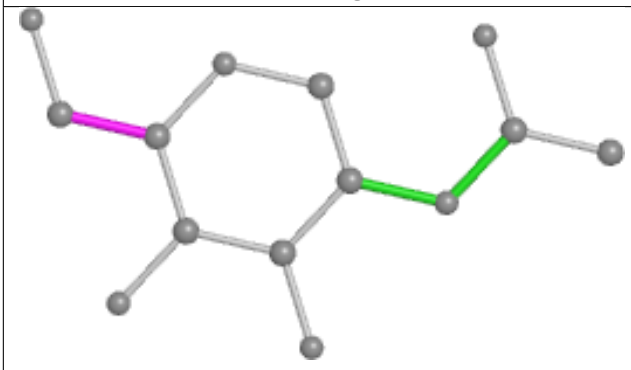
Ligand NAG C 1402



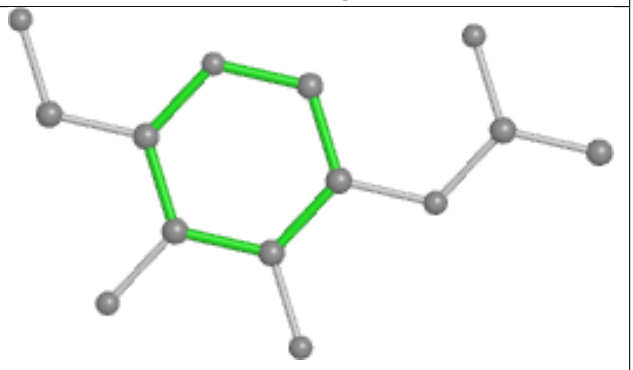
Bond lengths



Bond angles

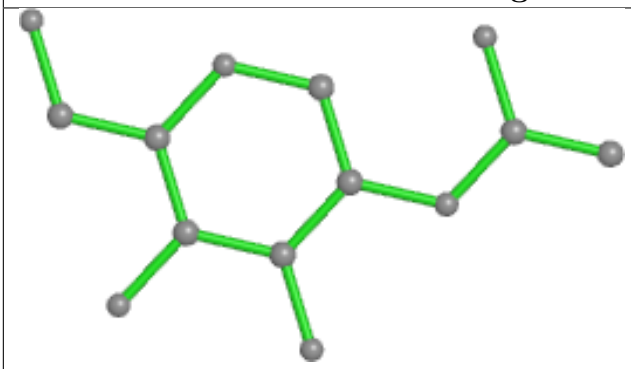


Torsions

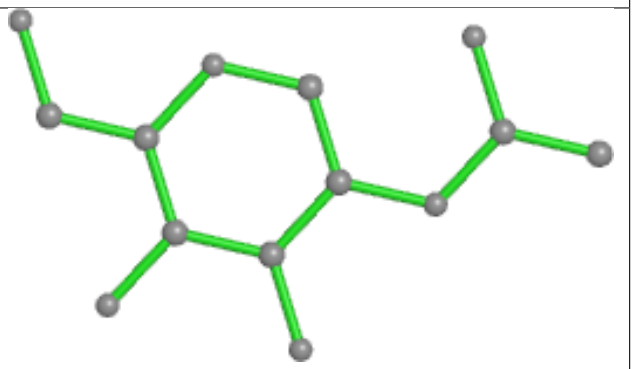


Rings

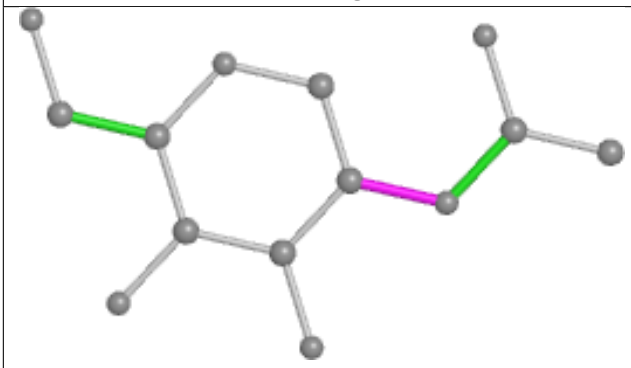
Ligand NAG A 1407



Bond lengths



Bond angles



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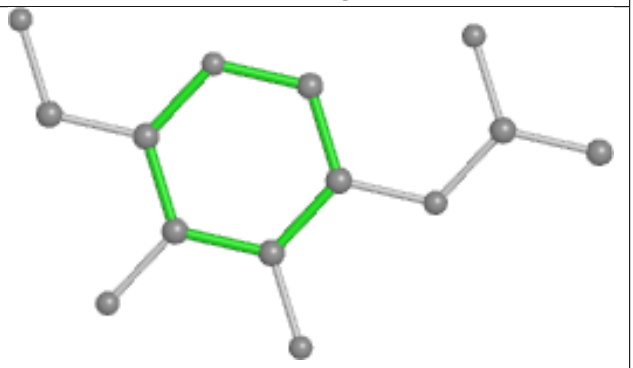
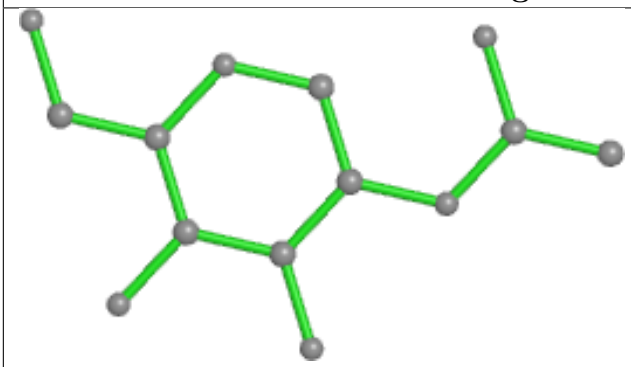
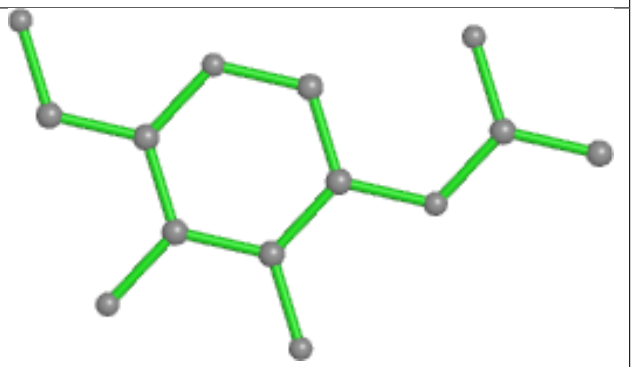


Rings

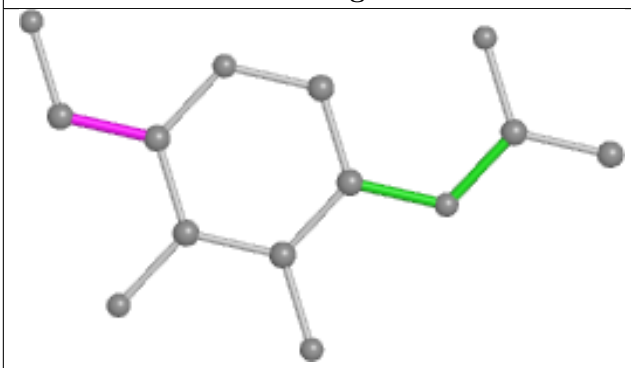
Ligand NAG B 1403



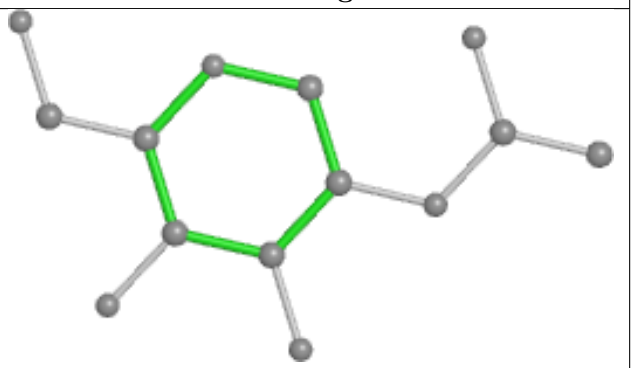
Bond lengths



Bond angles

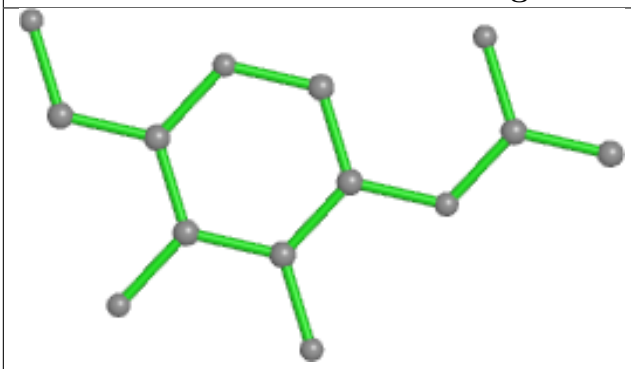


Torsions

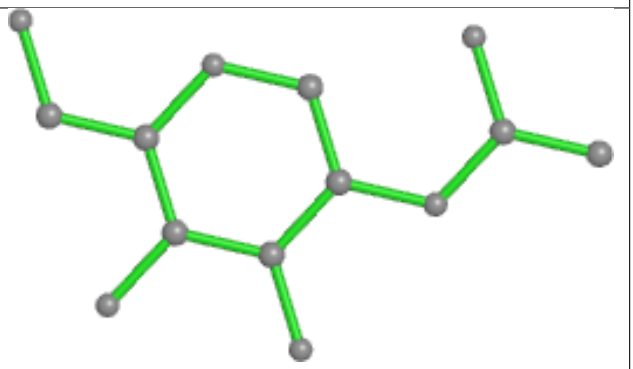


Rings

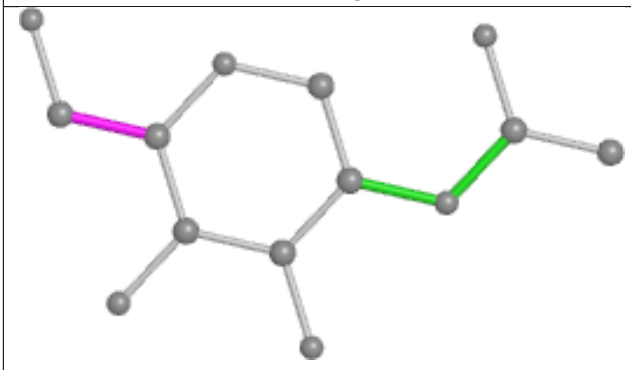
Ligand NAG A 1401



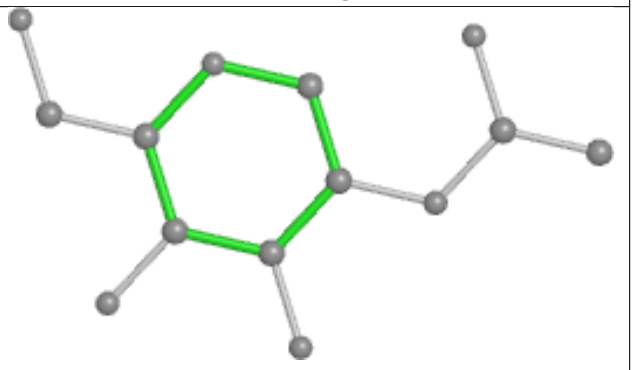
Bond lengths



Bond angles

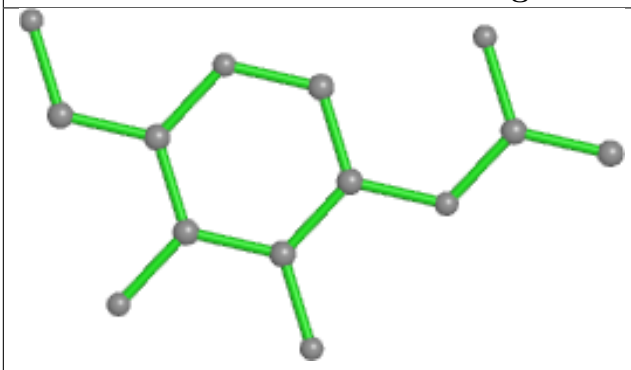


Torsions



Rings

Ligand NAG C 1405



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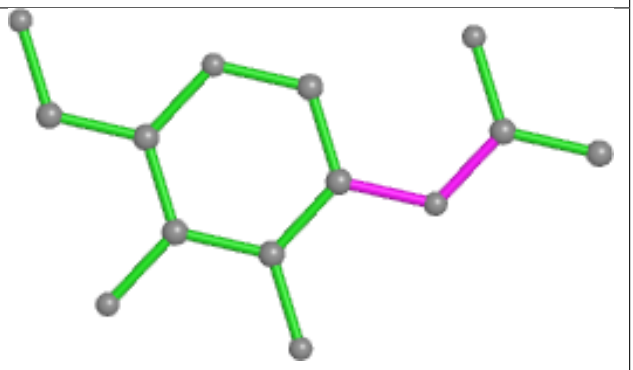
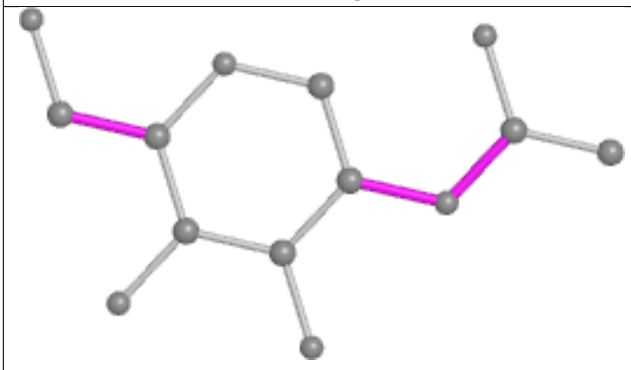
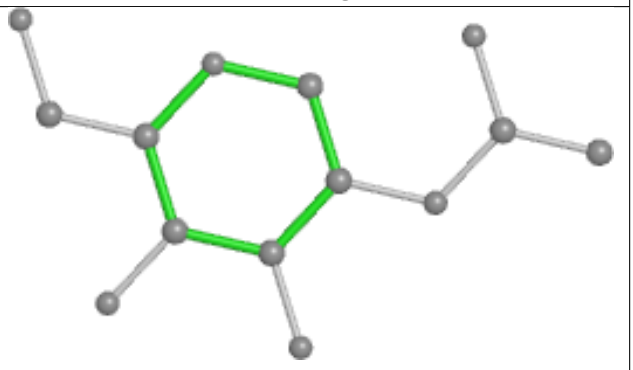


Bond angles

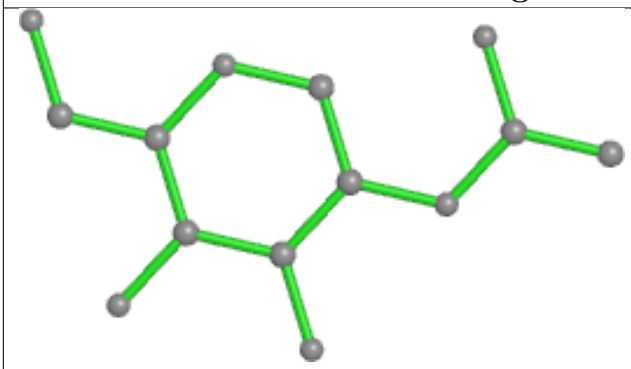


Torsions

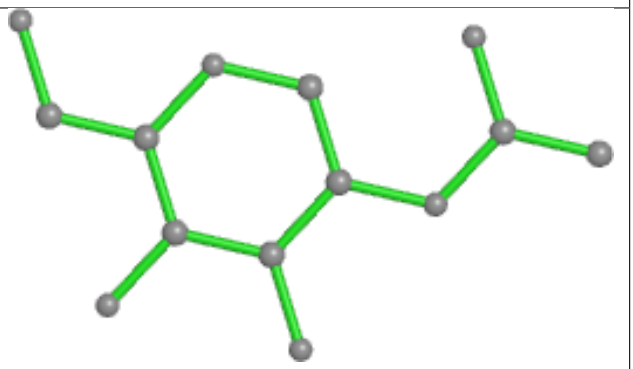


Rings

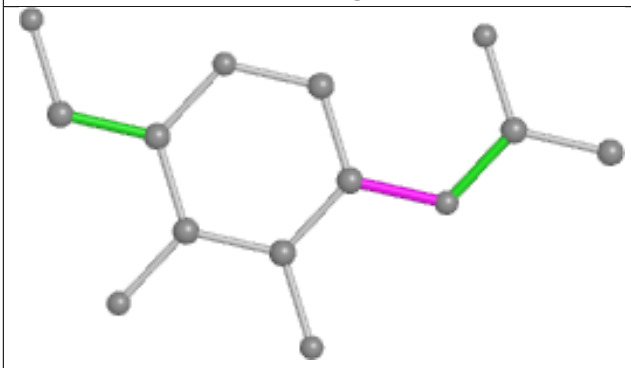
Ligand NAG C 1407



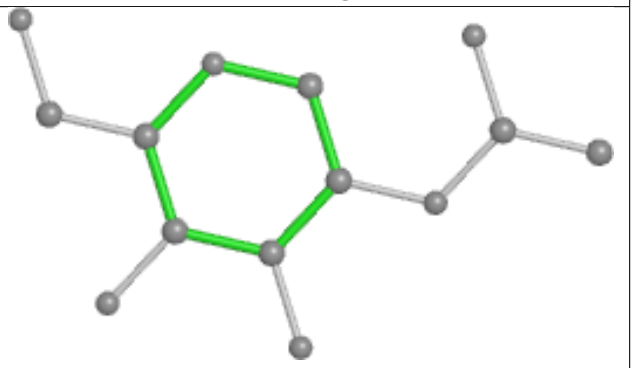
Bond lengths



Bond angles

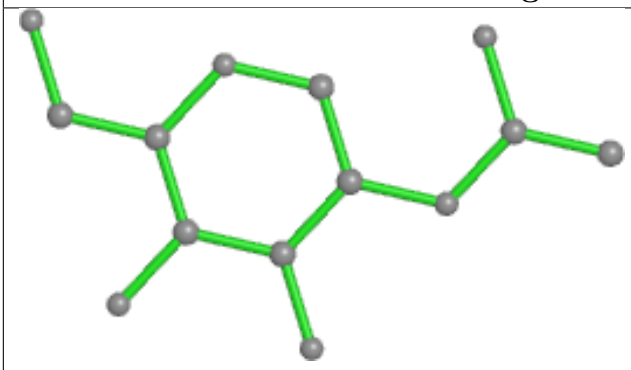


Torsions



Rings

Ligand NAG E 901



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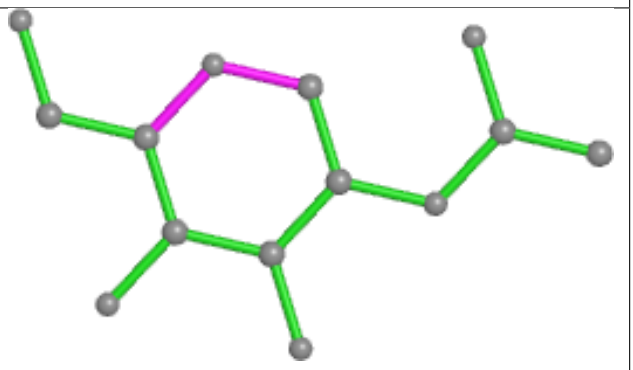
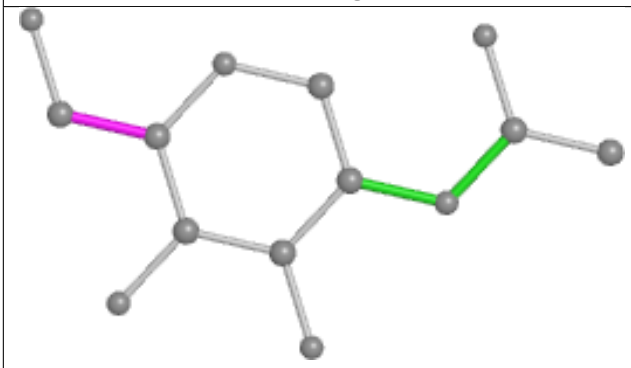


Bond angles



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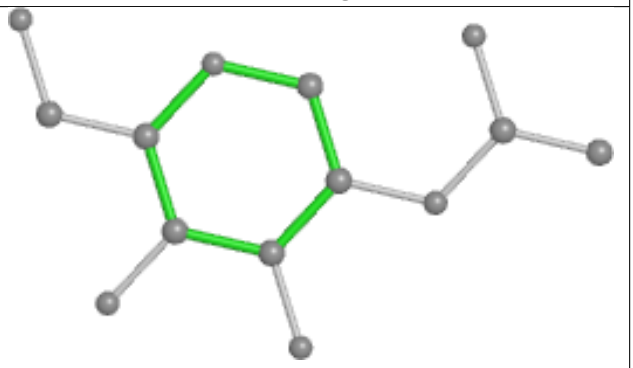
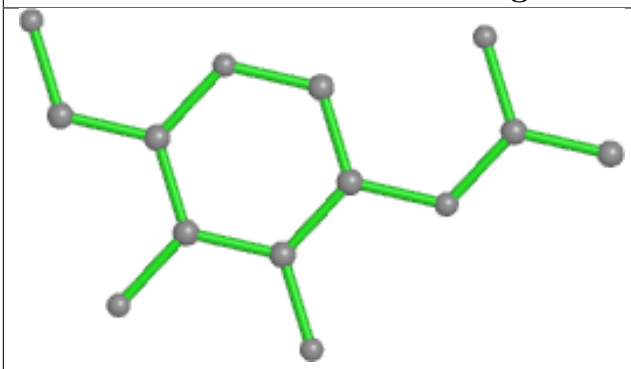
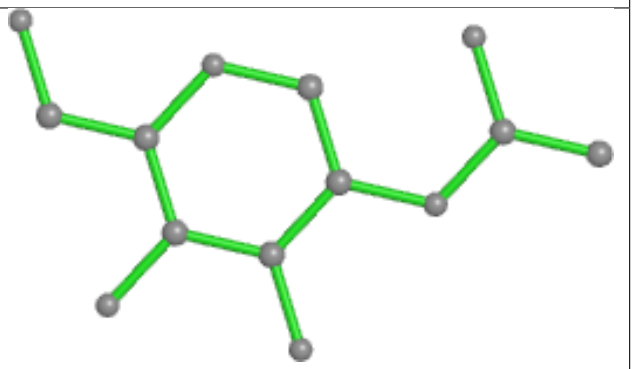


Rings

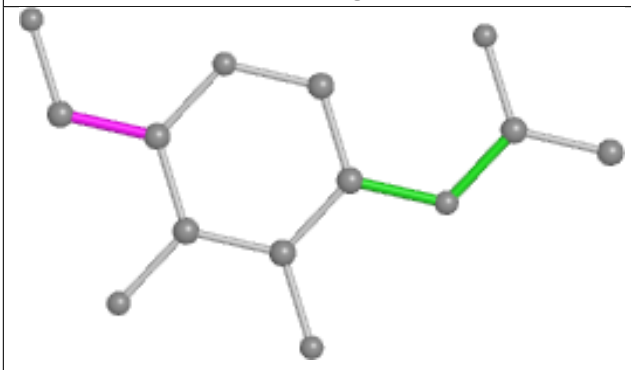
Ligand NAG A 1403



Bond lengths



Bond angles



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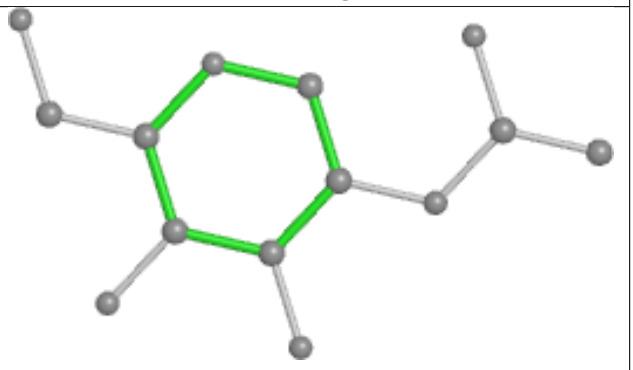
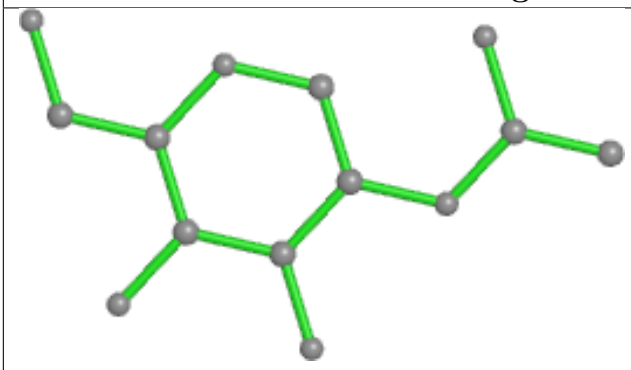


Rings

Ligand NAG B 1410



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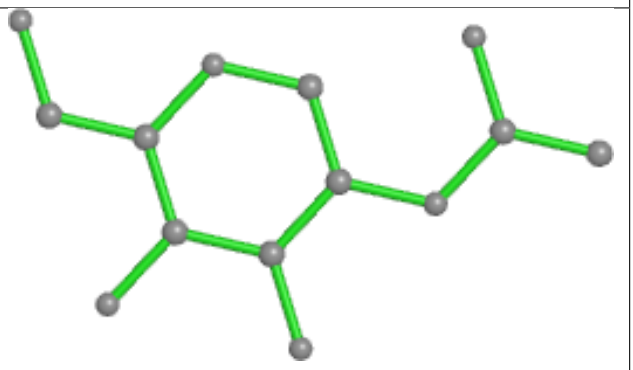
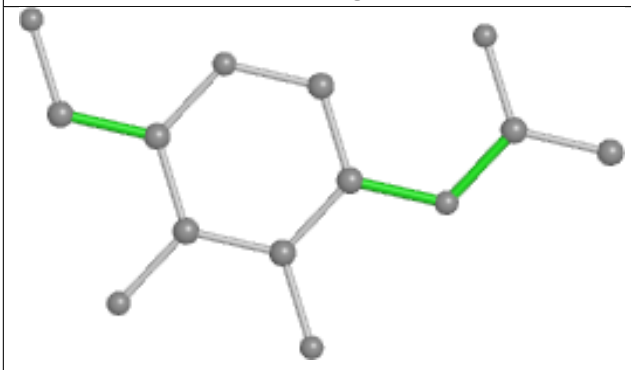
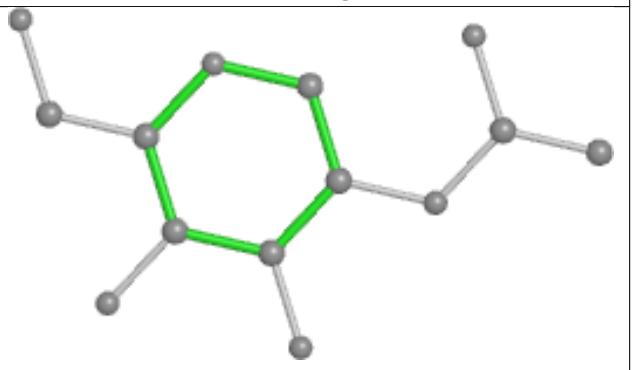


Bond angles

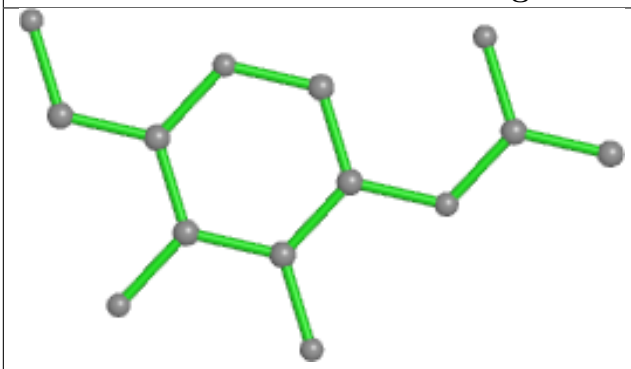


Torsions

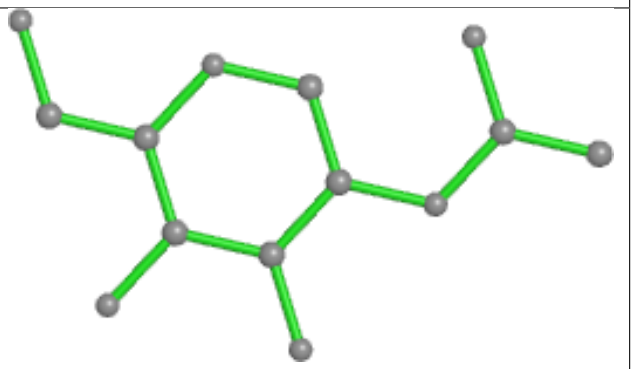


Rings

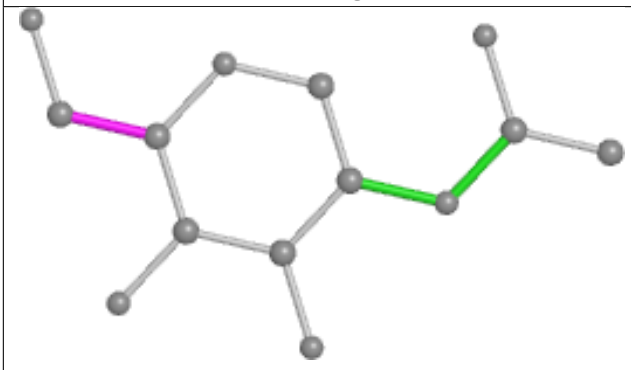
Ligand NAG B 1402



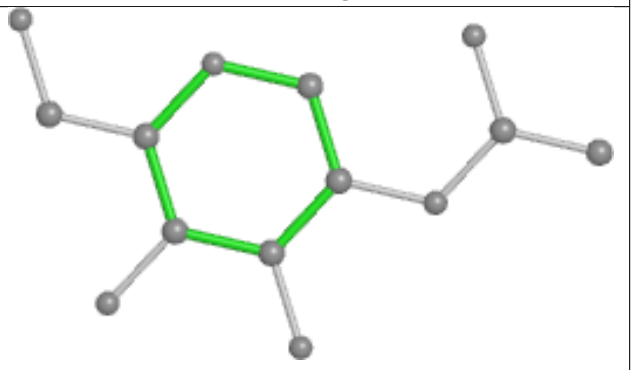
Bond lengths



Bond angles

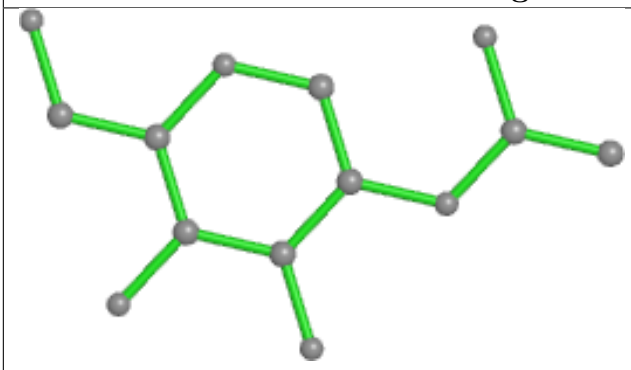


Torsions

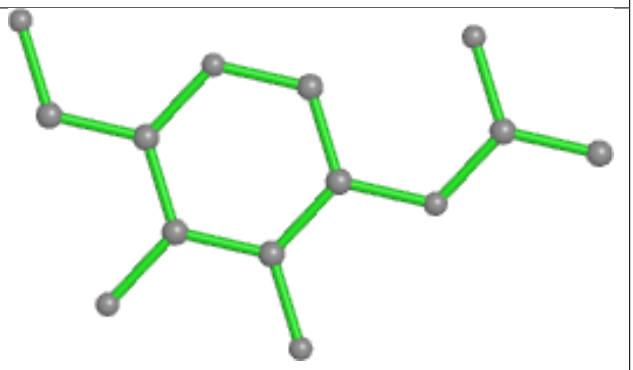


Rings

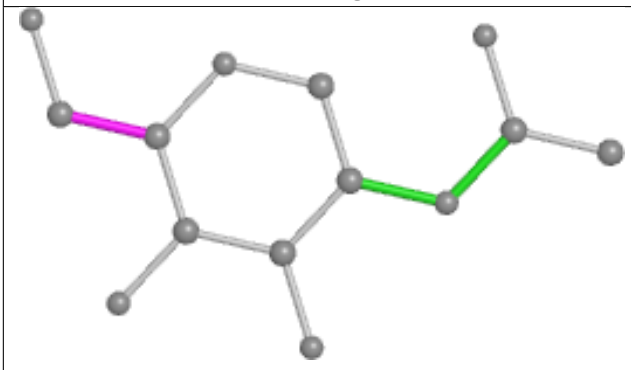
Ligand NAG C 1401



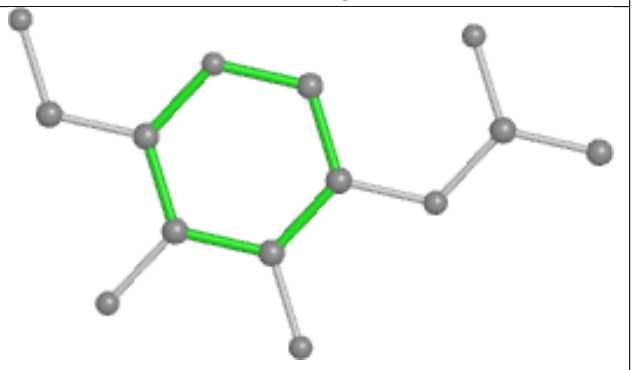
Bond lengths



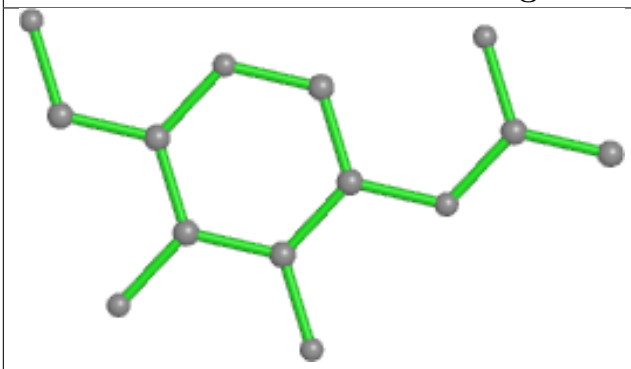
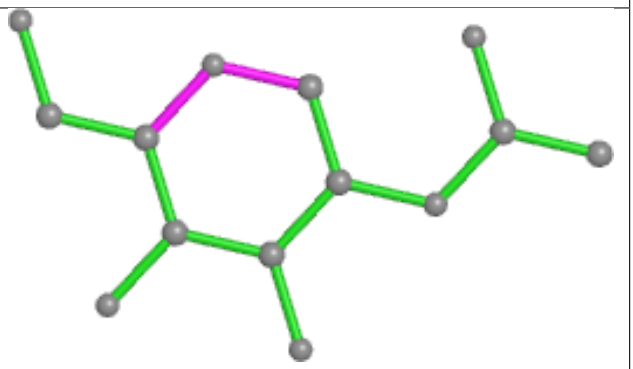
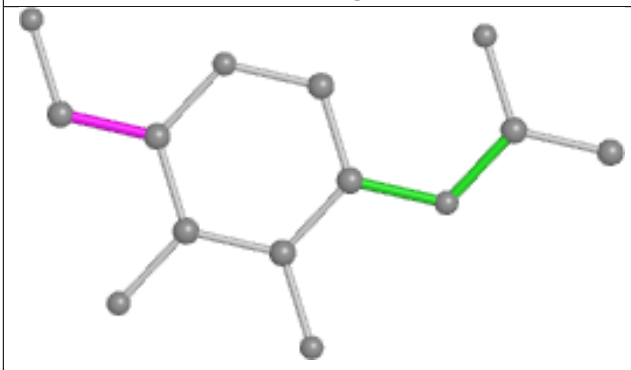
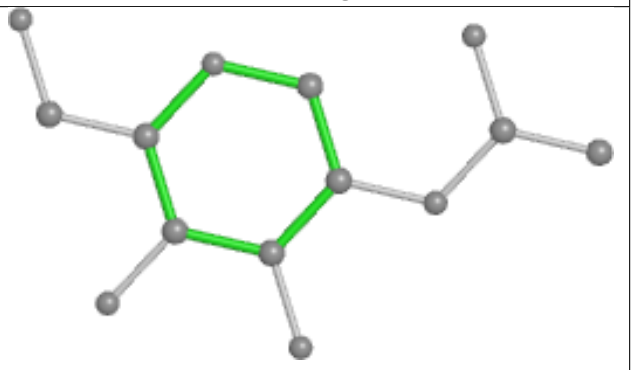
Bond angles

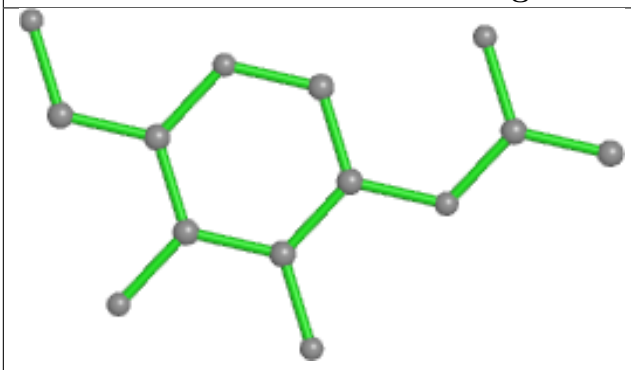
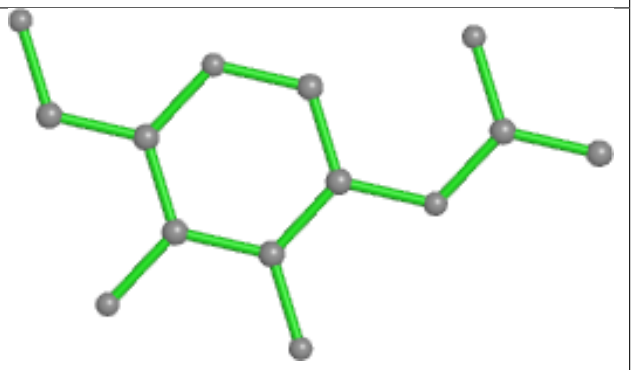
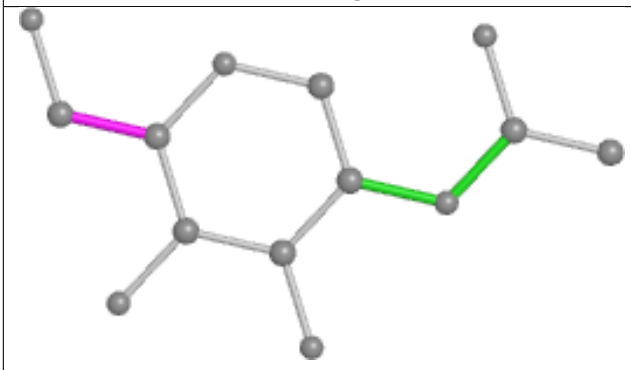
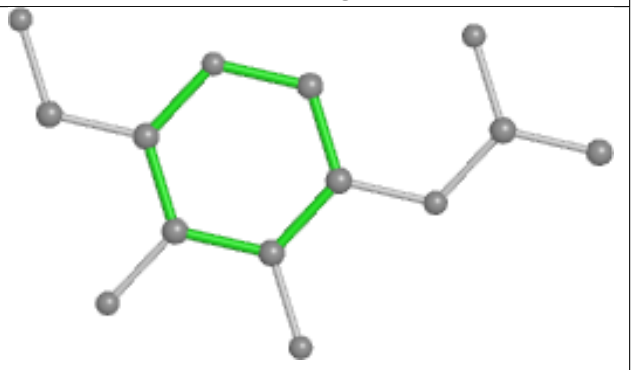


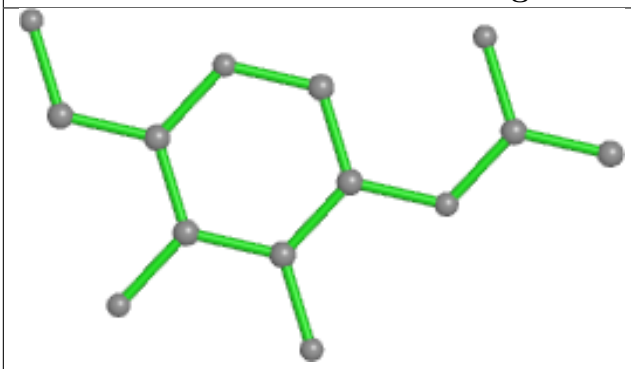
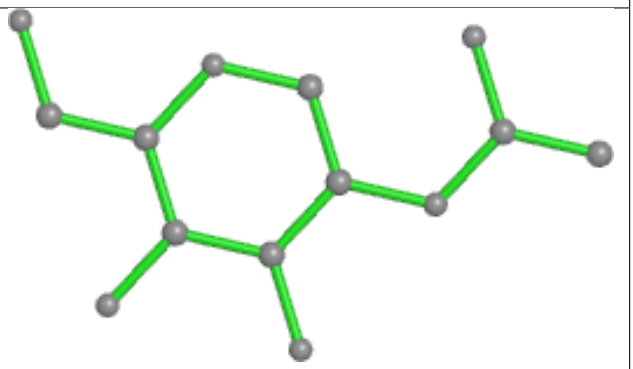
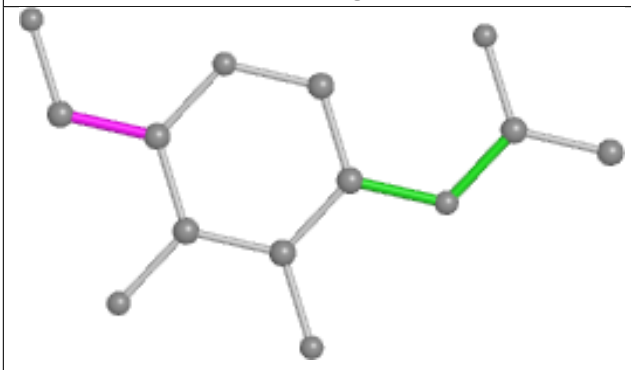
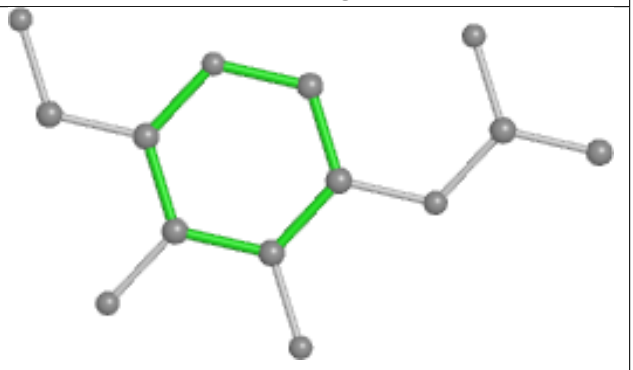
Torsions

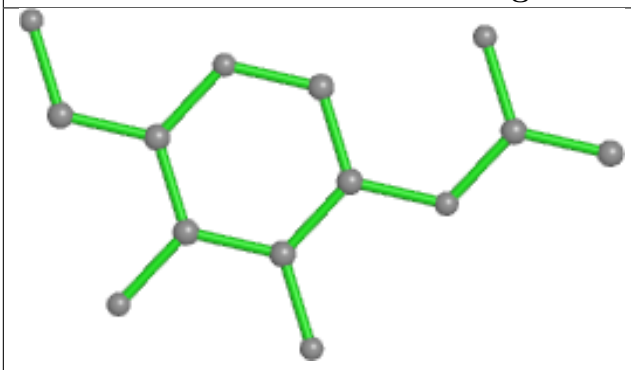
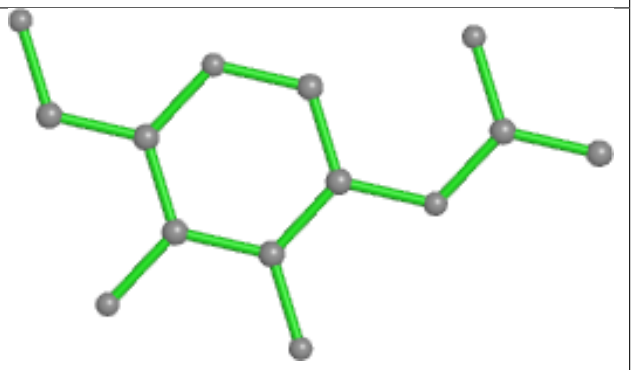
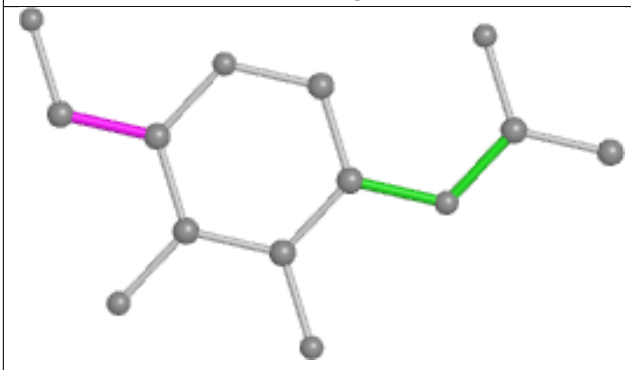
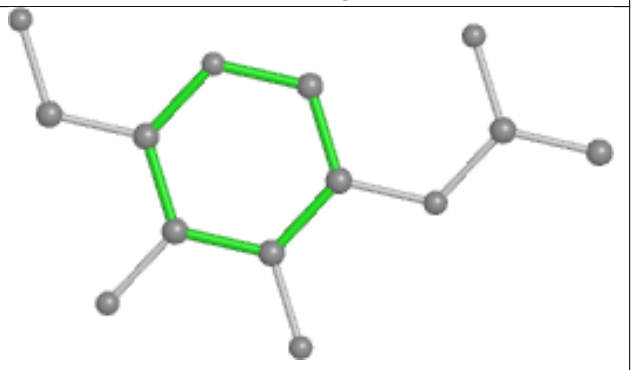


Rings

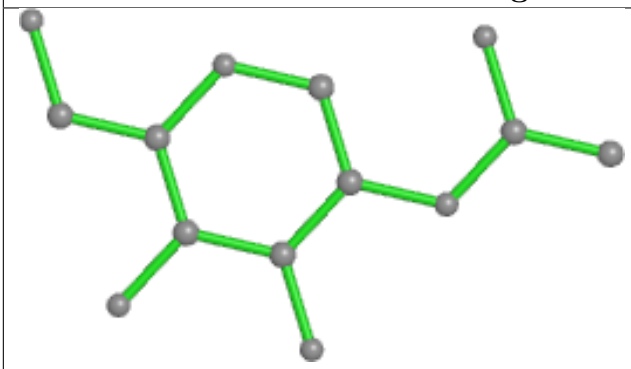
Ligand NAG D 901	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1404	
	
Bond lengths	Bond angles
	
Torsions	Rings

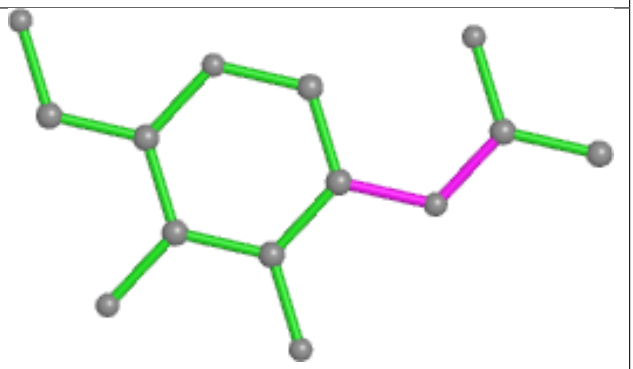
Ligand NAG C 1406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

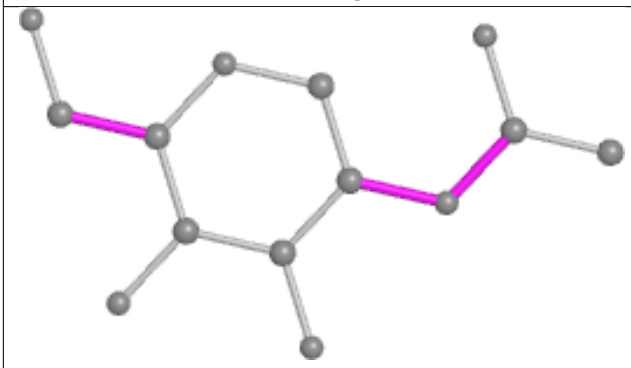
Ligand NAG A 1405



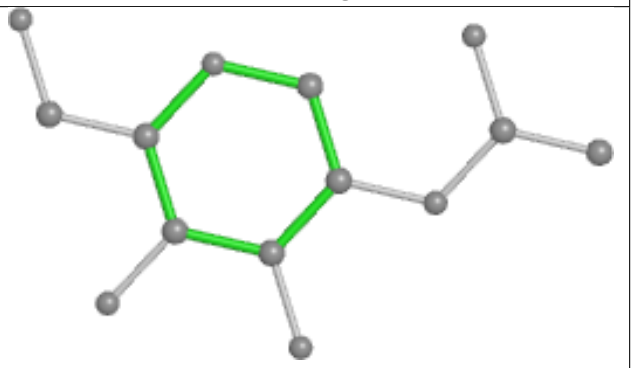
Bond lengths



Bond angles

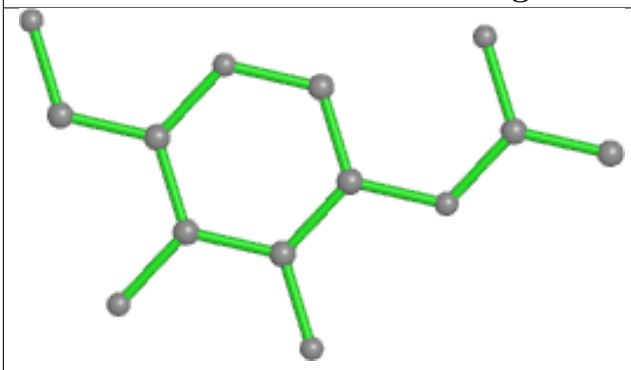


Torsions

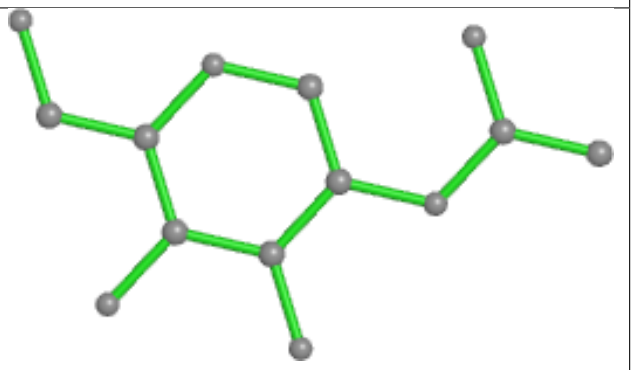


Rings

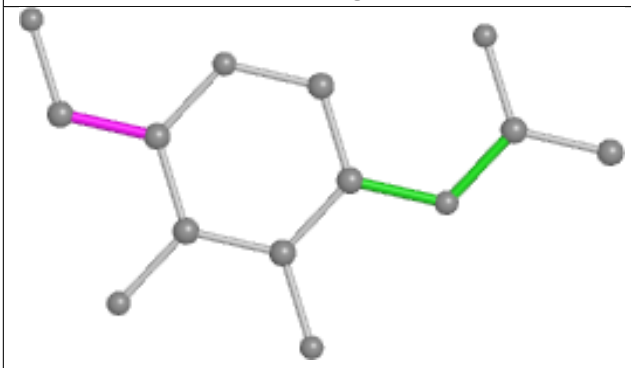
Ligand NAG B 1408



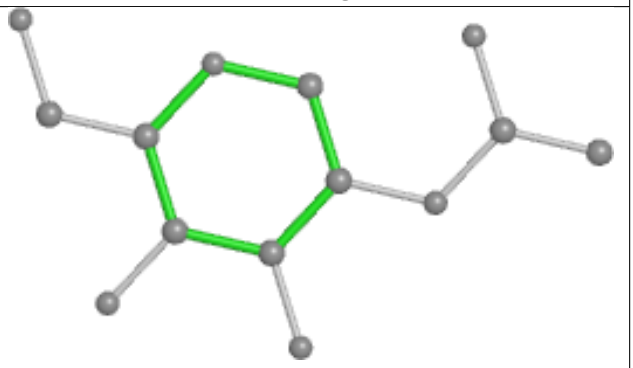
Bond lengths



Bond angles

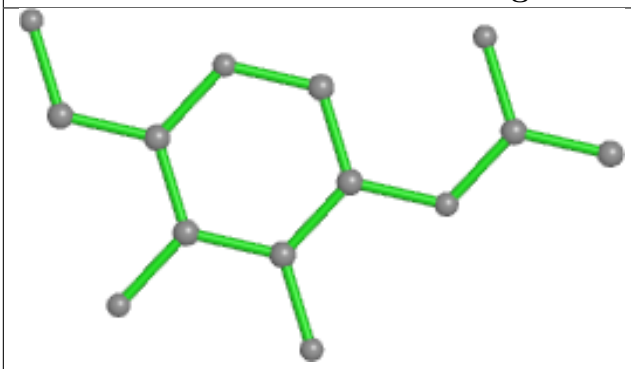


Torsions

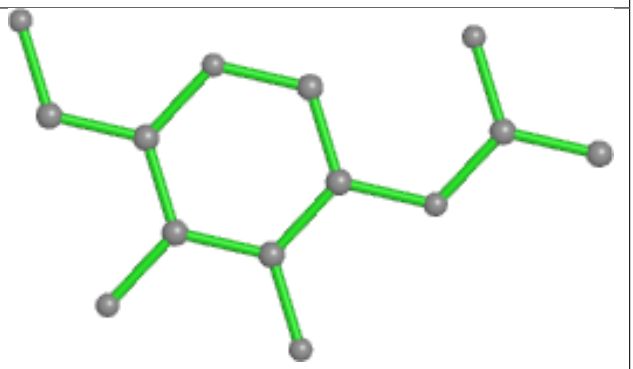


Rings

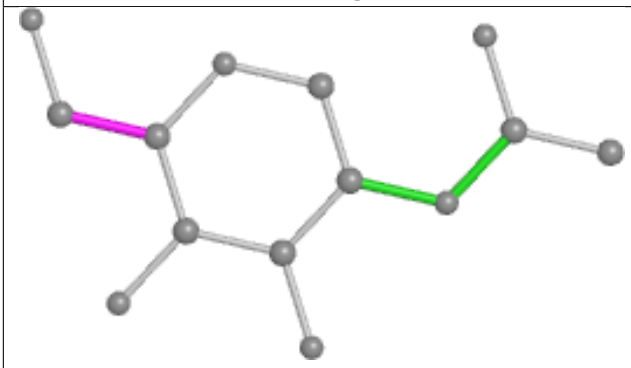
Ligand NAG C 1404



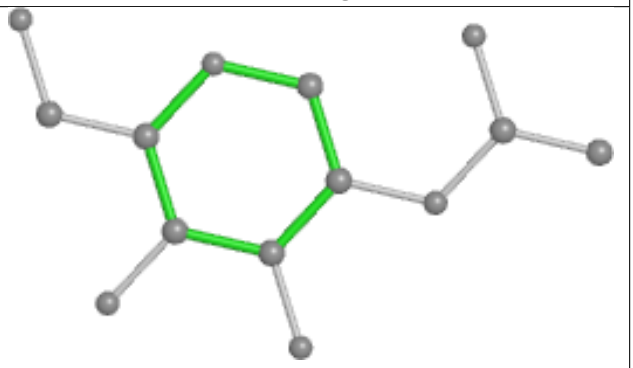
Bond lengths



Bond angles

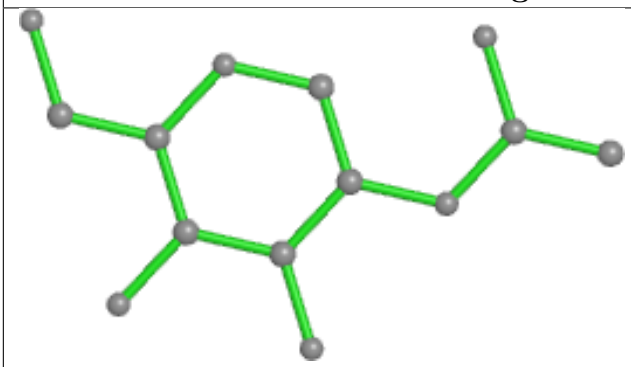


Torsions

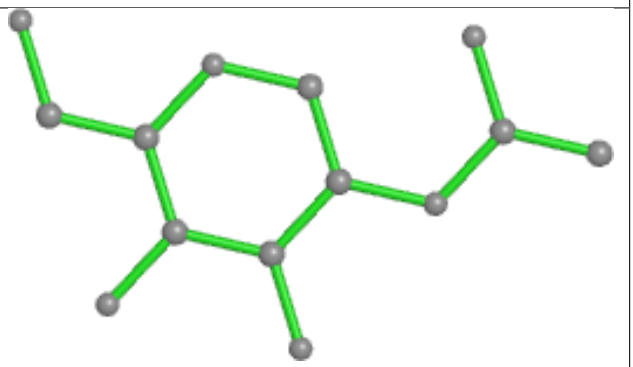


Rings

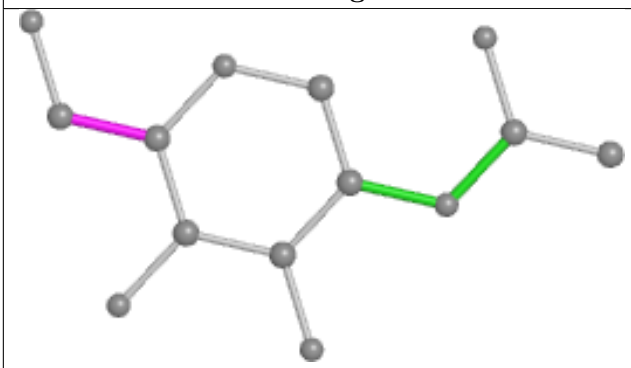
Ligand NAG C 1408



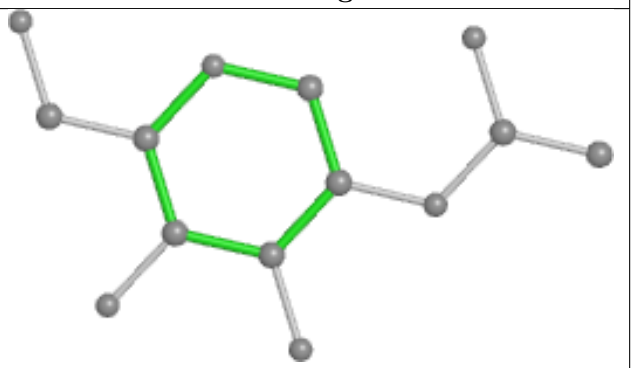
Bond lengths



Bond angles

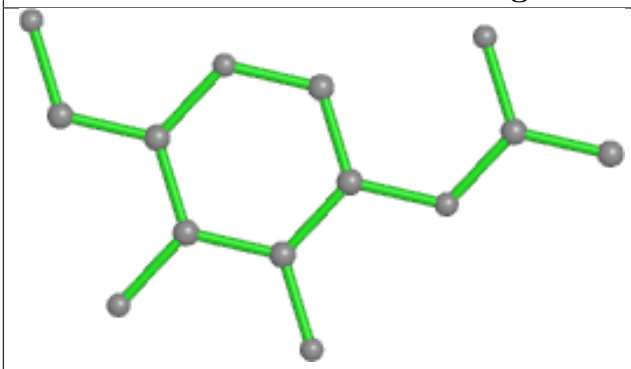


Torsions

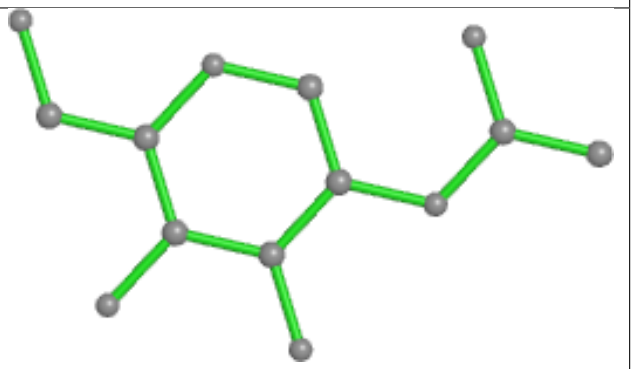


Rings

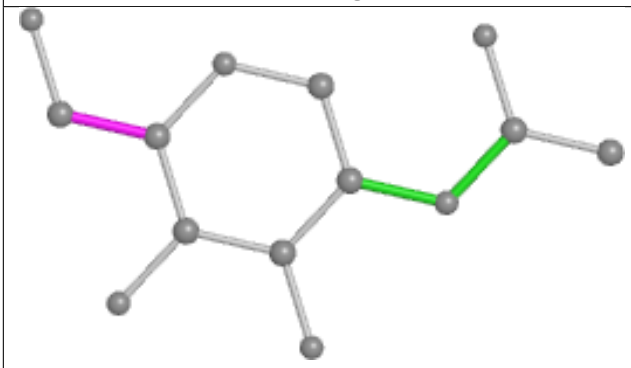
Ligand NAG A 1404



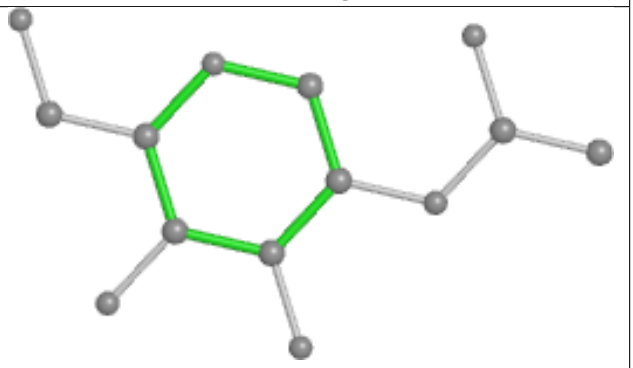
Bond lengths



Bond angles

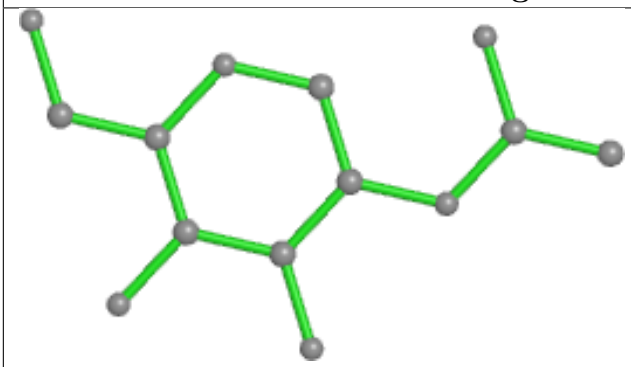


Torsions

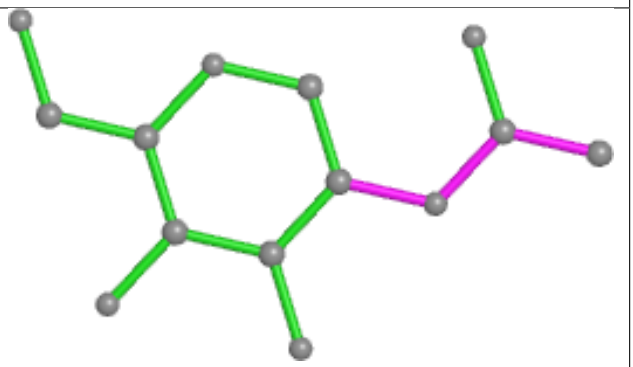


Rings

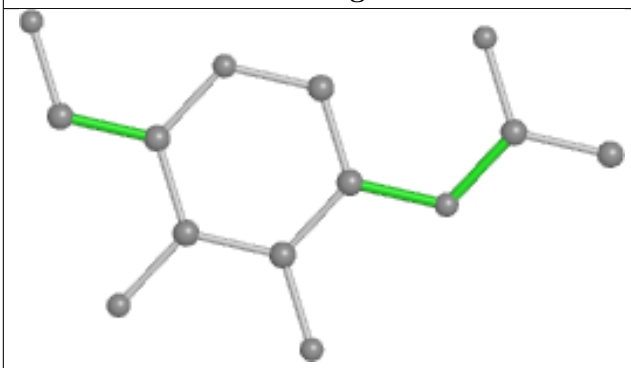
Ligand NAG B 1409



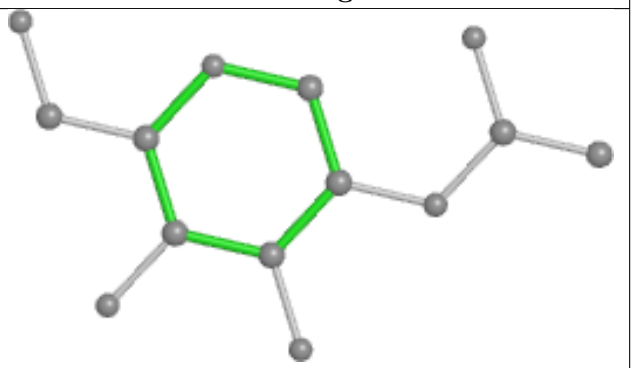
Bond lengths



Bond angles

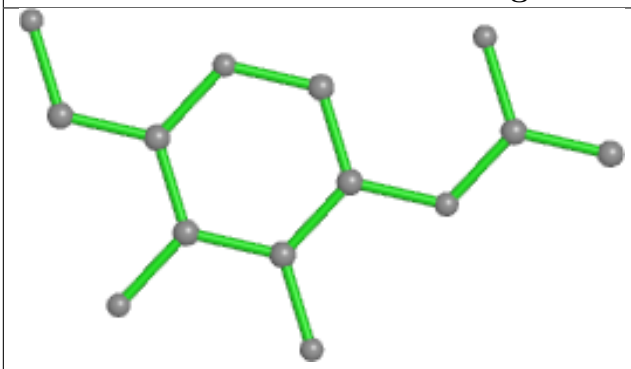


Torsions

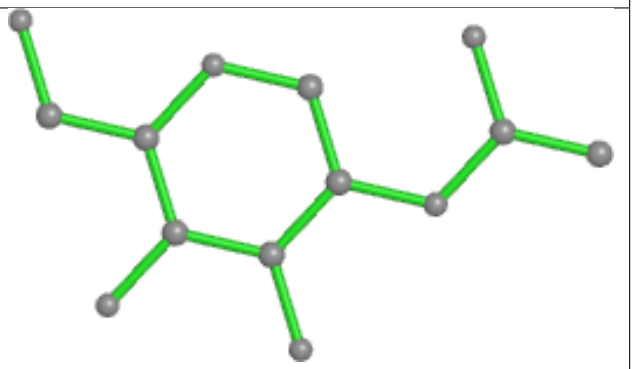


Rings

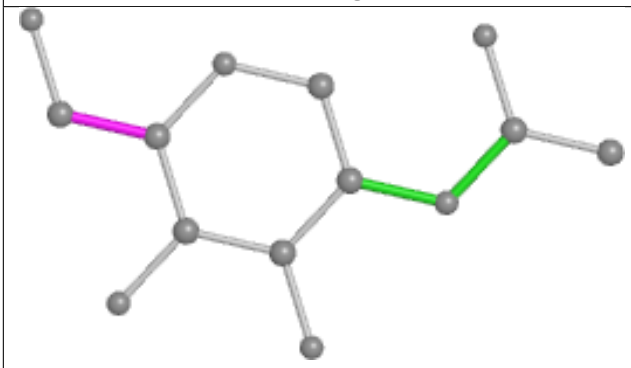
Ligand NAG A 1406



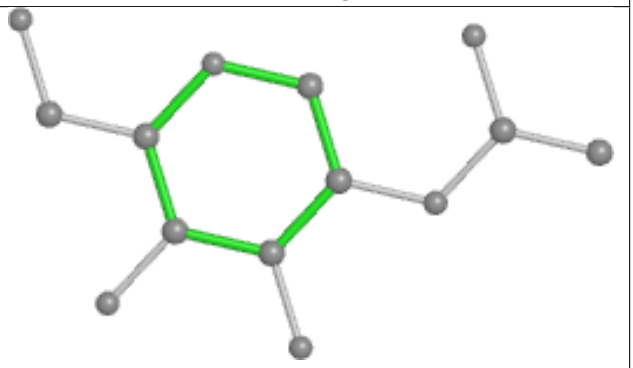
Bond lengths



Bond angles

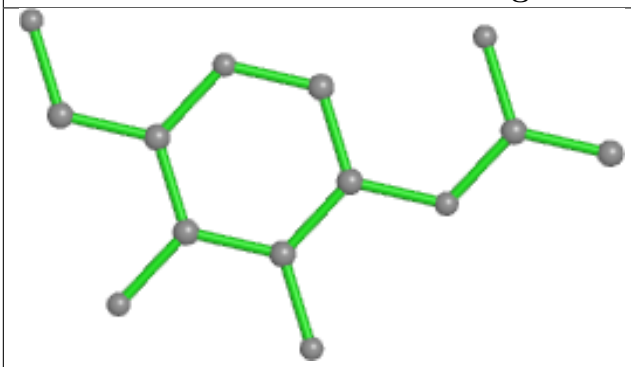


Torsions

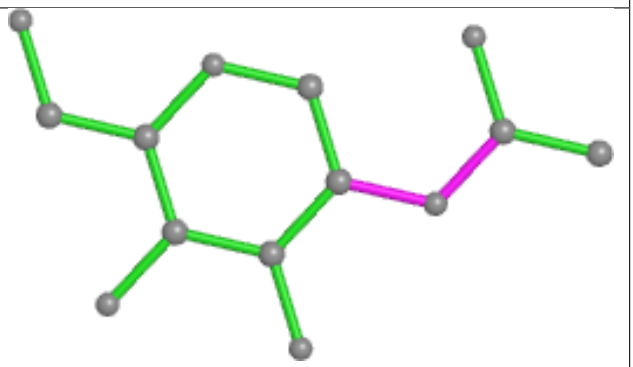


Rings

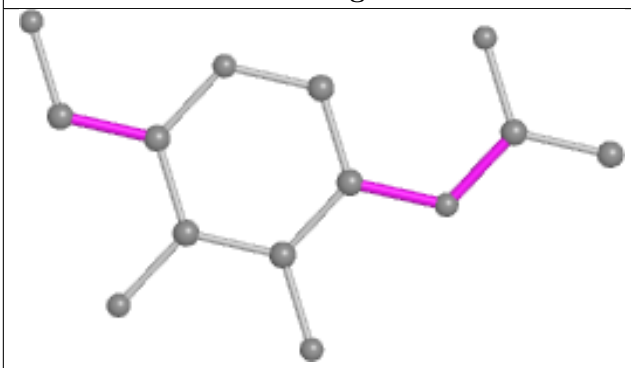
Ligand NAG B 1405



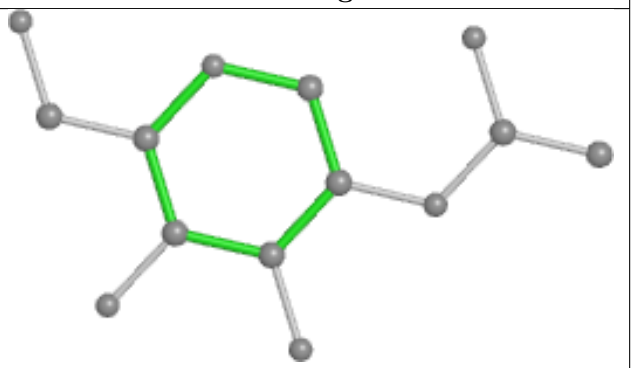
Bond lengths



Bond angles

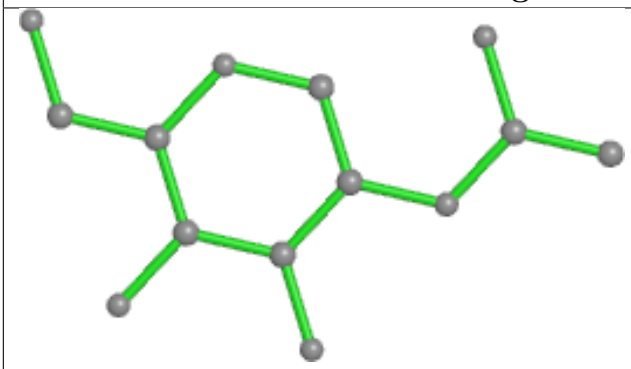


Torsions

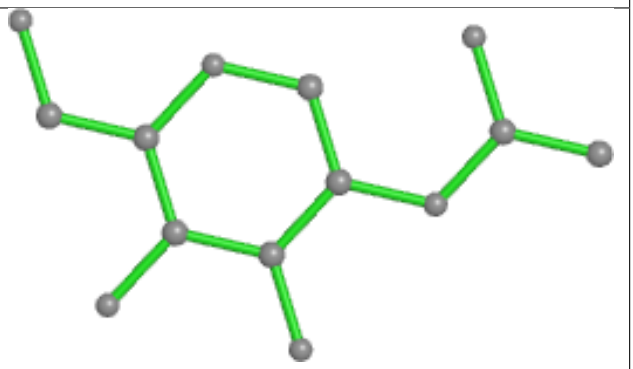


Rings

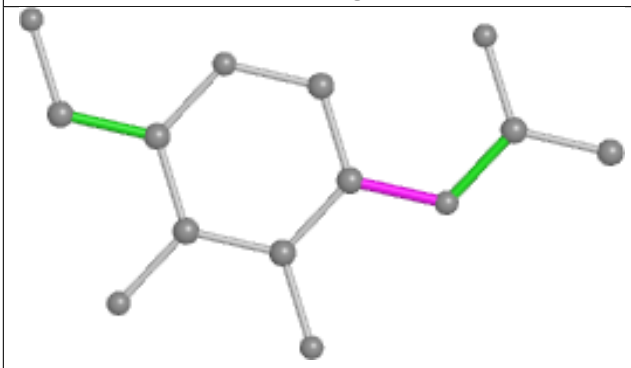
Ligand NAG B 1407



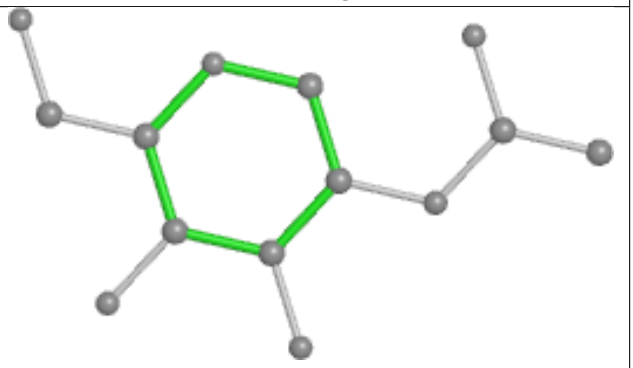
Bond lengths



Bond angles

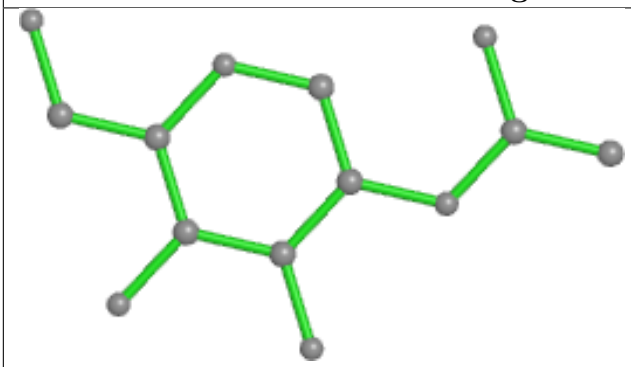


Torsions

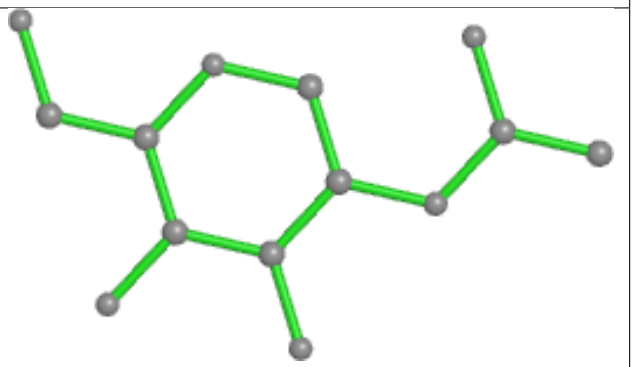


Rings

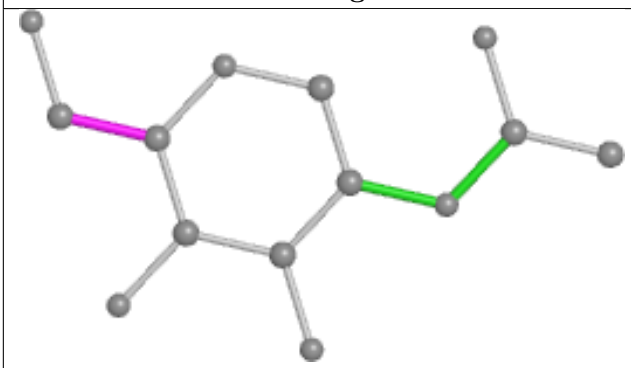
Ligand NAG A 1402



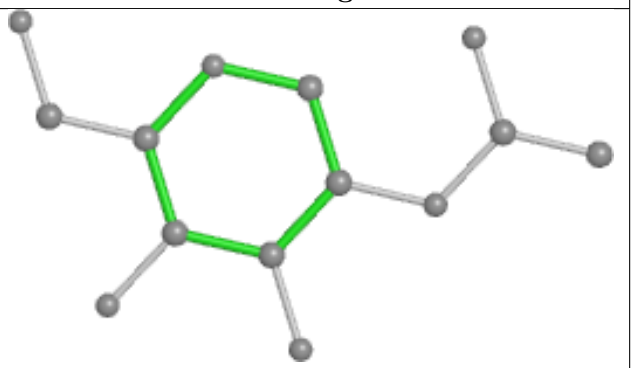
Bond lengths



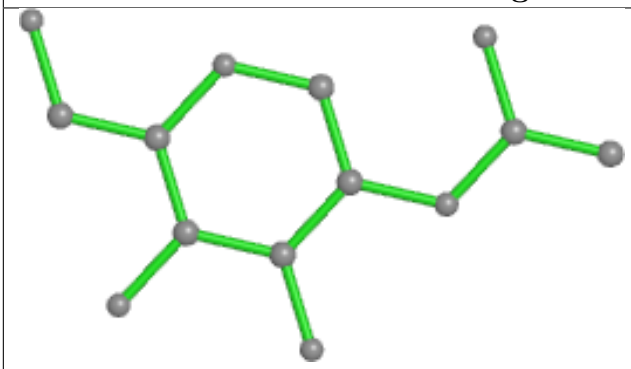
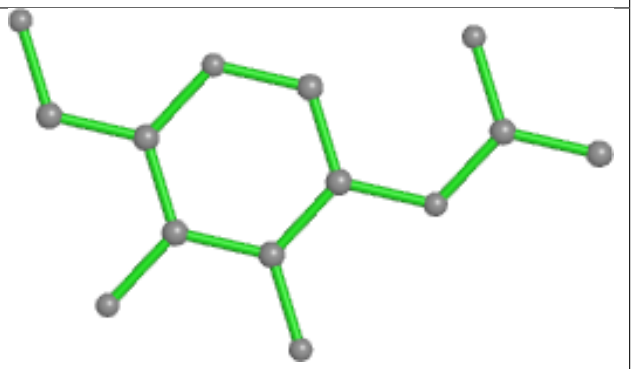
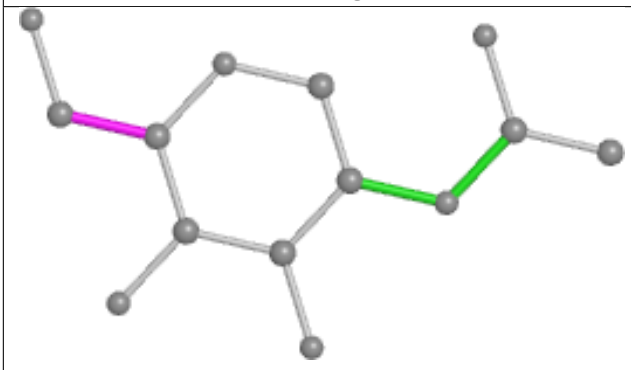
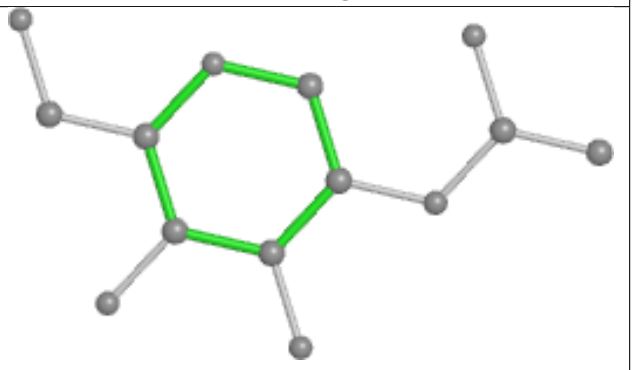
Bond angles



Torsions



Rings

Ligand NAG C 1403	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

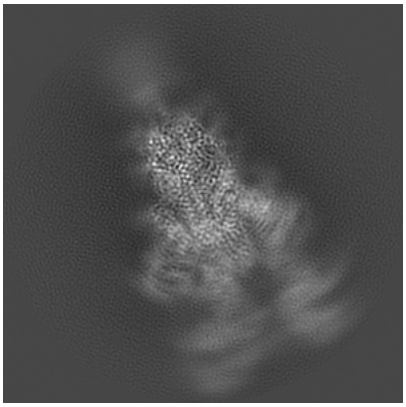
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30899. These allow visual inspection of the internal detail of the map and identification of artifacts.

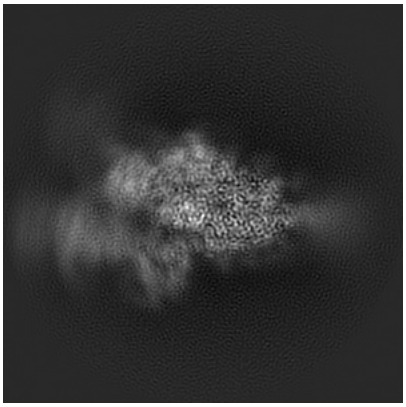
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

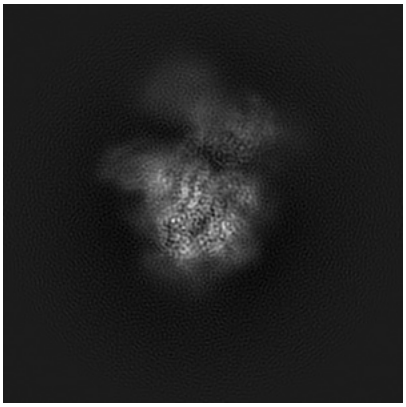
6.1.1 Primary map



X



Y

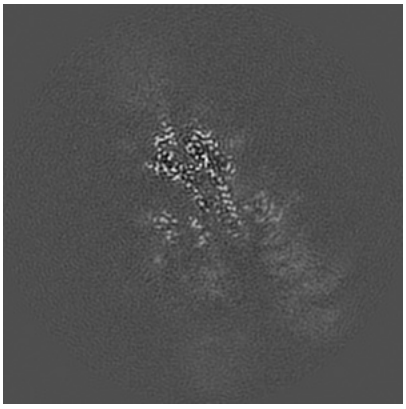


Z

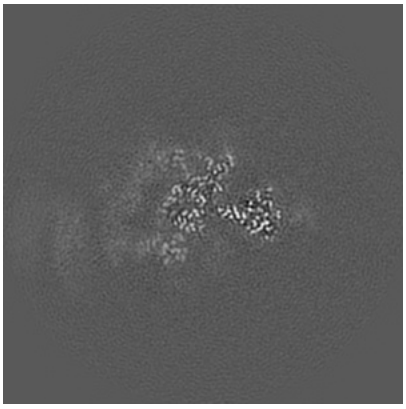
The images above show the map projected in three orthogonal directions.

6.2 Central slices

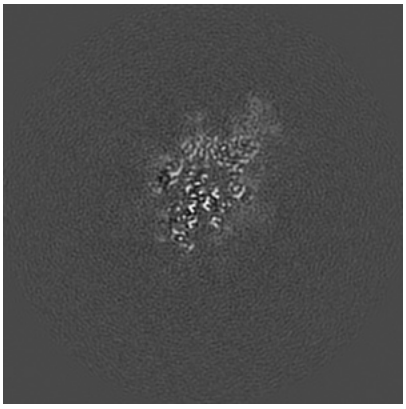
6.2.1 Primary map



X Index: 144



Y Index: 144

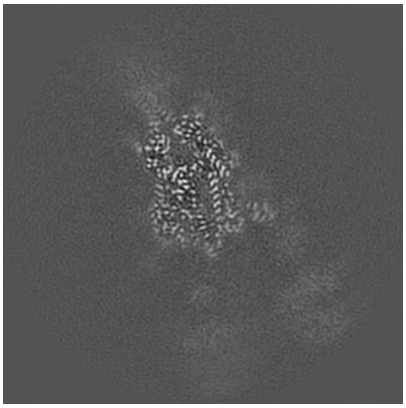


Z Index: 144

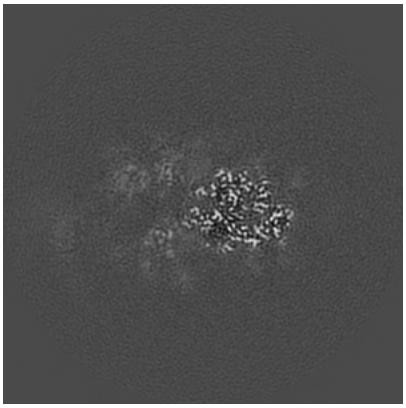
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

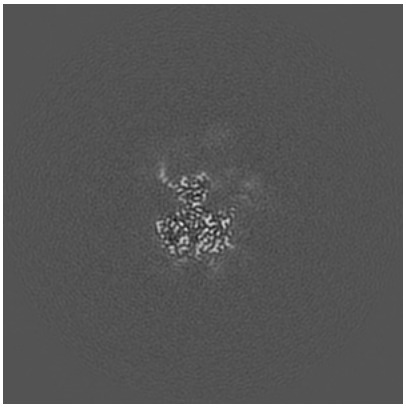
6.3.1 Primary map



X Index: 132



Y Index: 133

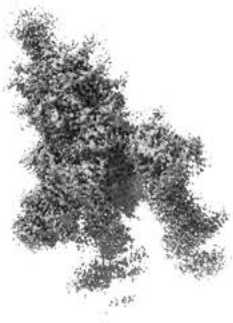


Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

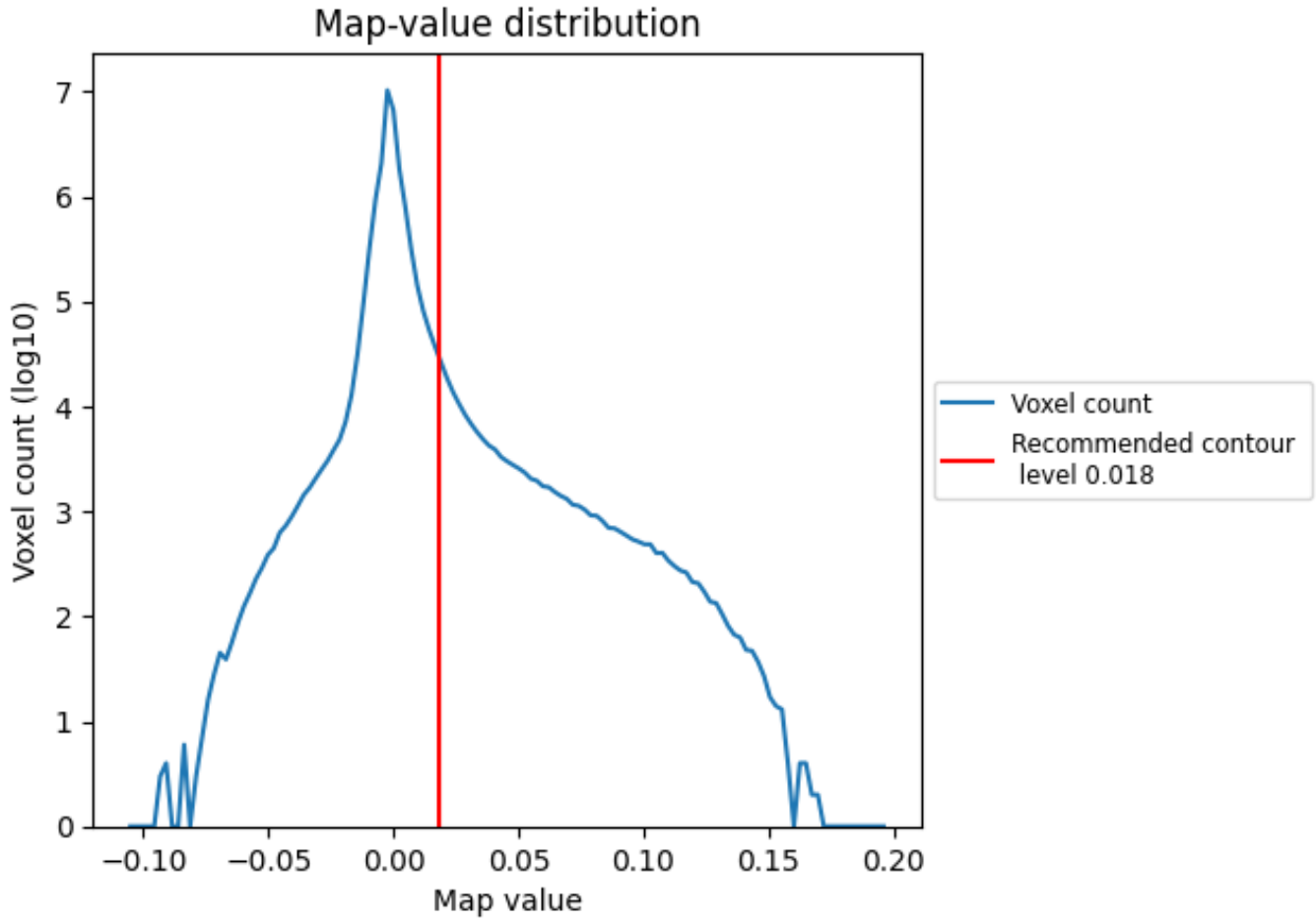
6.5 Mask visualisation (i)

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

7 Map analysis

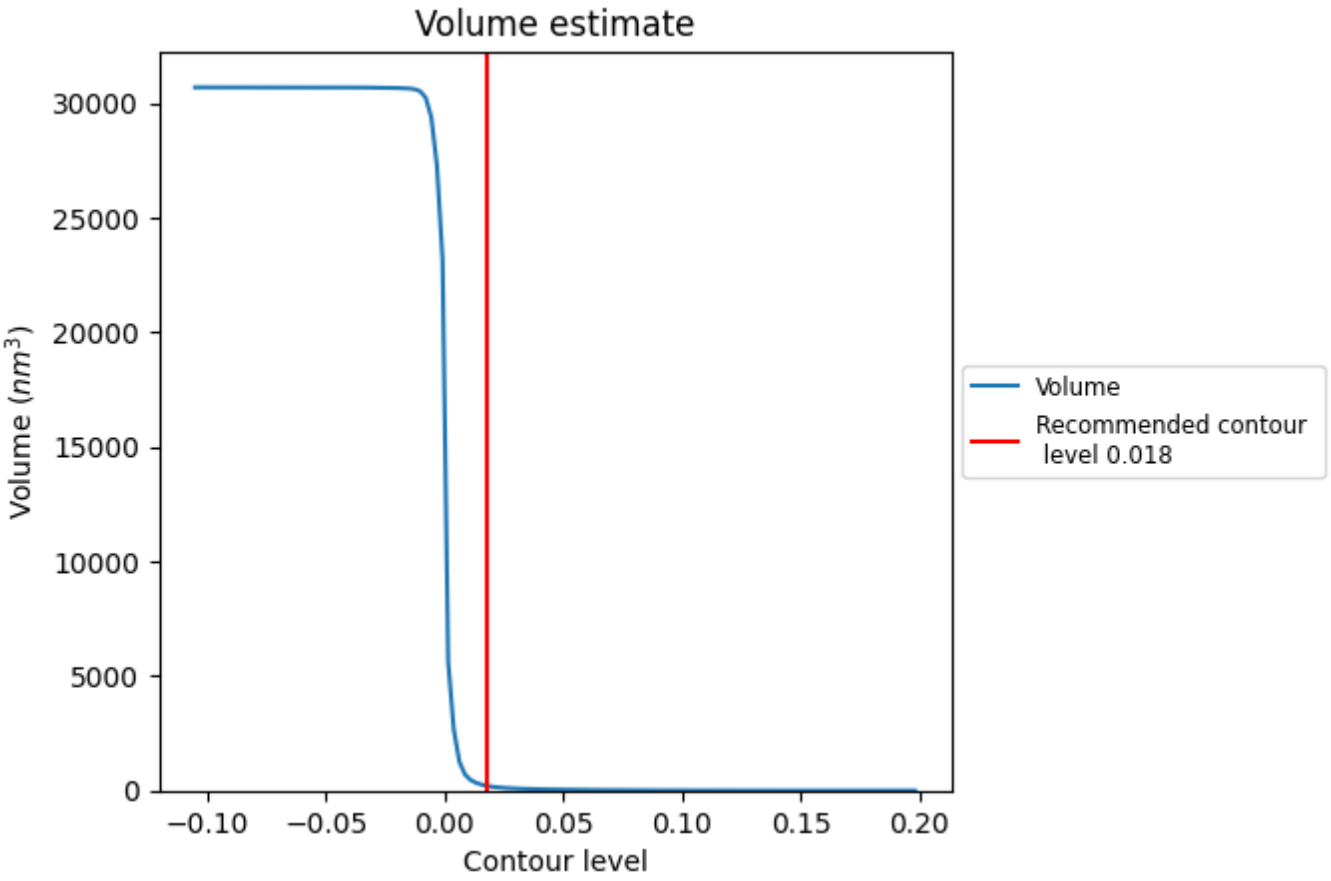
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

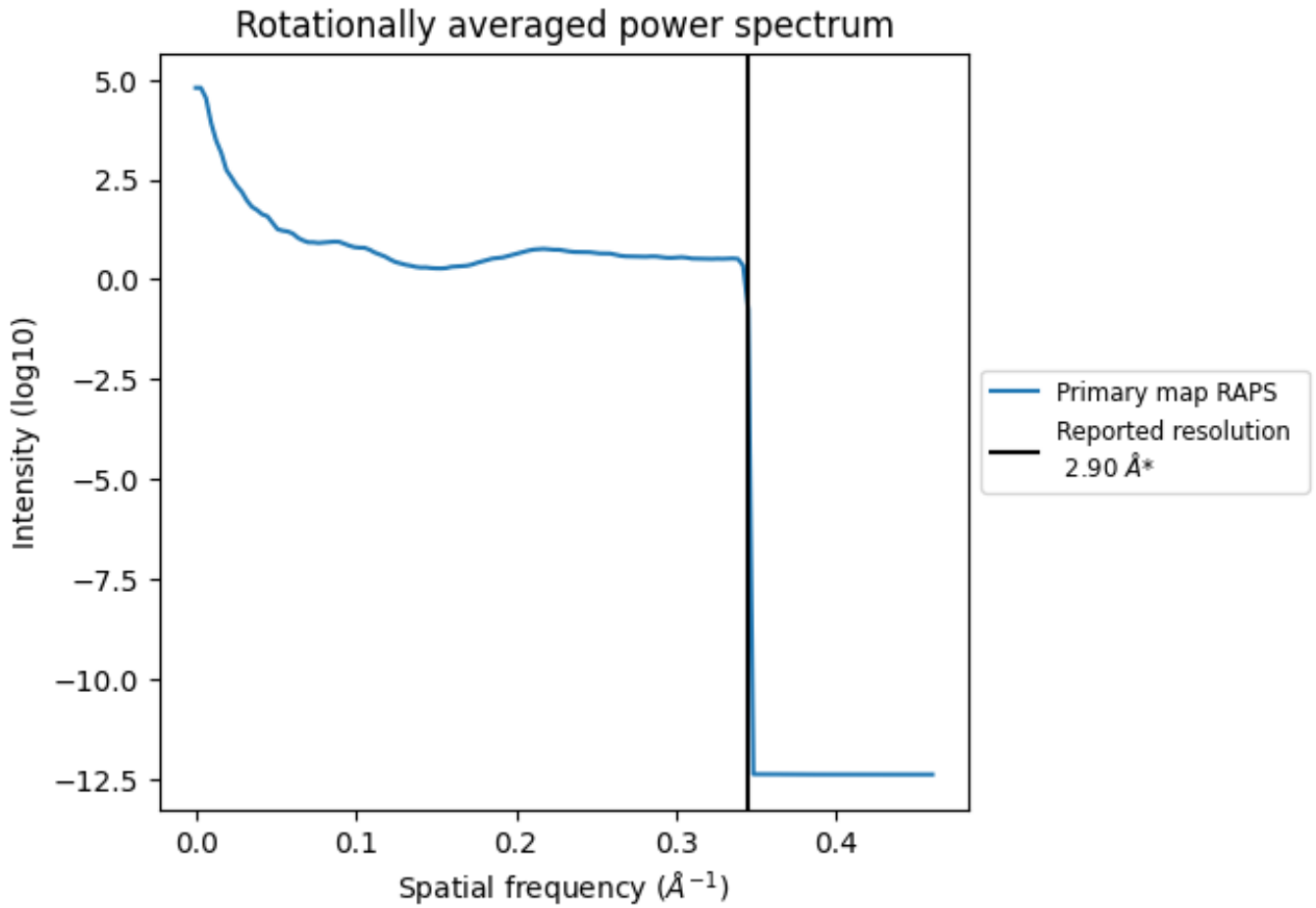
7.2 Volume estimate



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 184 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 0.345 $Å^{-1}$

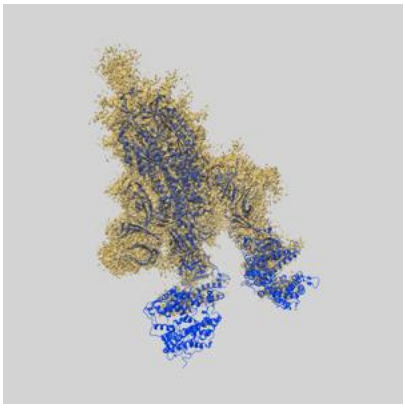
8 Fourier-Shell correlation (i)

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

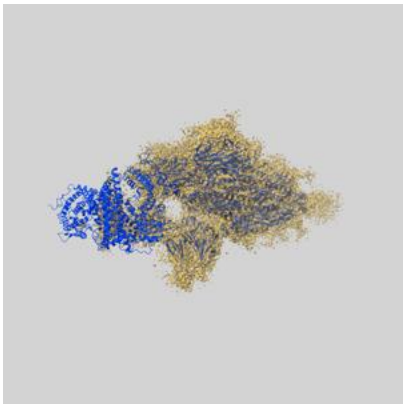
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30899 and PDB model 7DX8. Per-residue inclusion information can be found in section 3 on page 11.

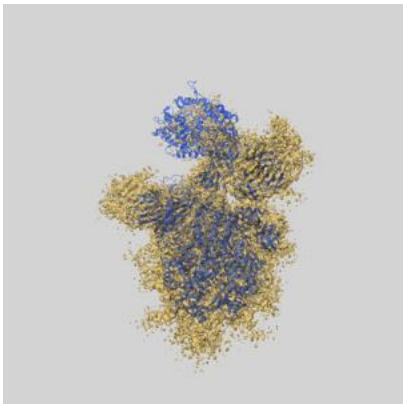
9.1 Map-model overlay



X



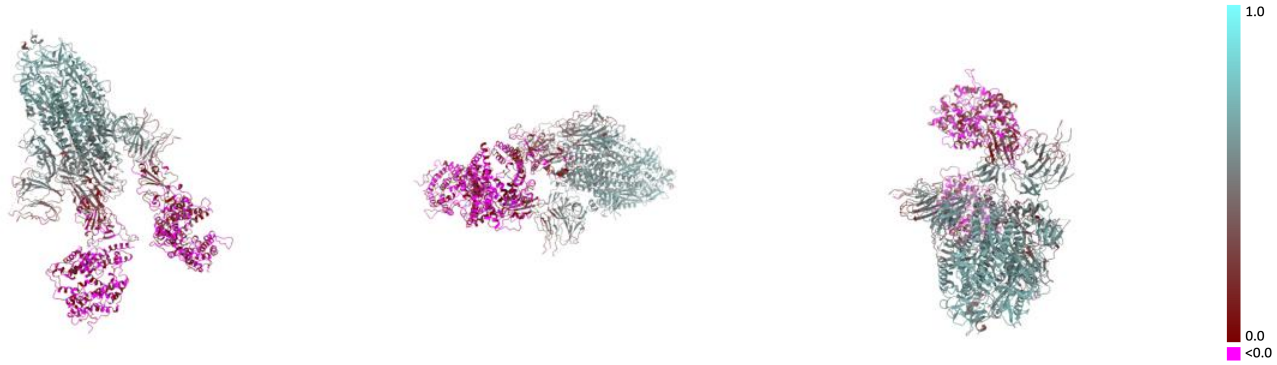
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

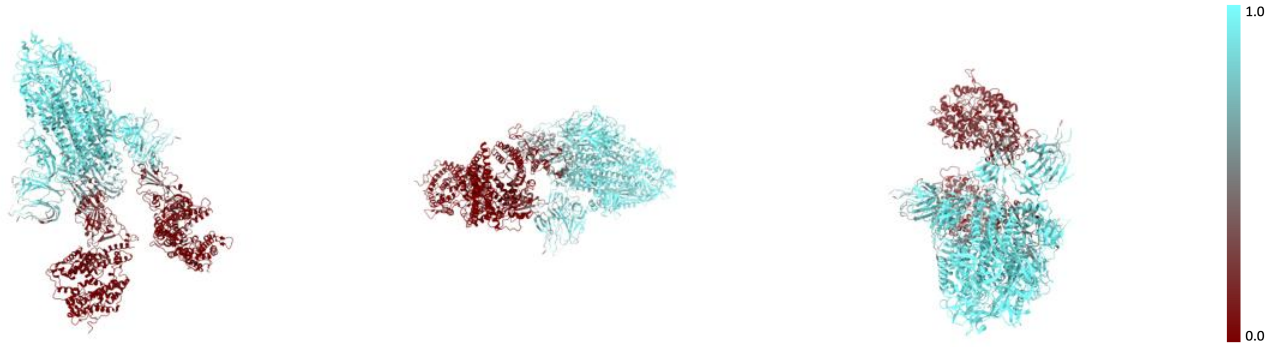
9.2 Q-score mapped to coordinate model (i)



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.

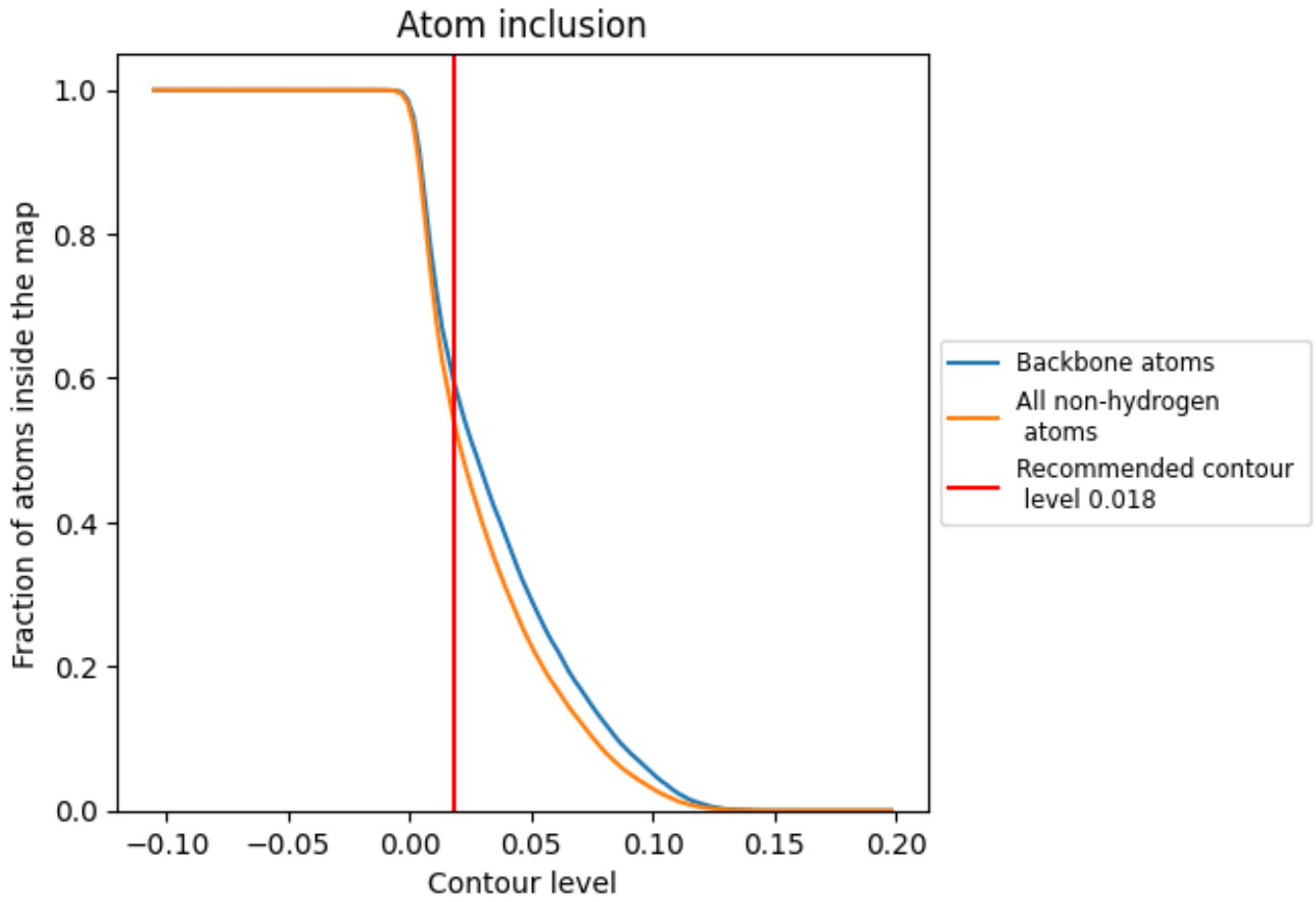
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 54% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5440	0.3260
A	0.7549	0.4550
B	0.7953	0.4820
C	0.7388	0.4400
D	0.0272	0.0150
E	0.0130	0.0070
F	0.5000	0.2070
G	0.2857	0.2920
H	0.9286	0.5270
I	0.8214	0.3920
J	0.6786	0.4650
K	0.8571	0.4920
L	0.7857	0.3800
M	0.4286	0.1450
N	0.1071	0.0750
O	0.6429	0.2710
P	0.8929	0.4990
Q	0.7857	0.3950
R	0.7500	0.4590
S	0.7500	0.3730
T	0.4286	0.2830
U	0.0714	-0.0220
V	0.6429	0.3330
W	0.8571	0.5040
X	0.7500	0.4480
Y	0.6429	0.3680
Z	0.8214	0.4550
a	0.7500	0.4460
b	0.0357	0.0860
c	0.0000	-0.0140
d	0.0000	0.0290
e	0.0000	0.0820
f	0.0000	-0.0280
g	0.0000	-0.0920
h	0.0000	0.0400

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Chain	Atom inclusion	Q-score
i	0.0000	0.1070
j	0.0000	-0.0520
k	0.0000	0.0290