Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID	:	7DX5 / pdb_00007dx5
EMDB ID	:	EMD-30896
Title	:	S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 2 (1 up RBD and 1 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	:	3.30 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:

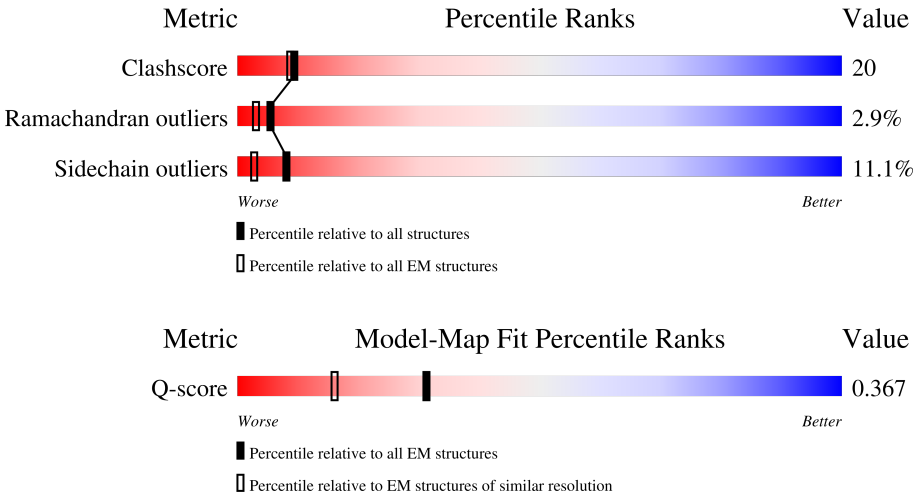
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	12% 50% 23% 5% 22%
1	B	1283	8% 51% 19% 5% • 24%
1	C	1283	13% 49% 21% 5% • 24%
2	D	817	71% 65% 7% • 27%

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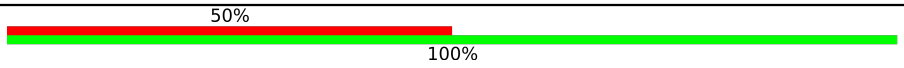
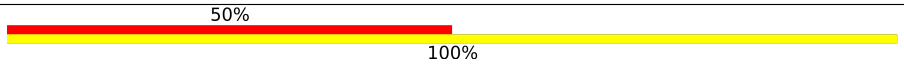
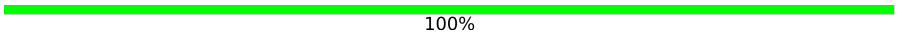
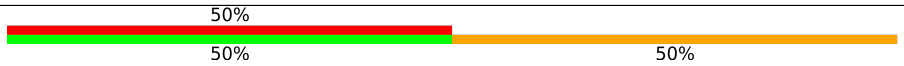
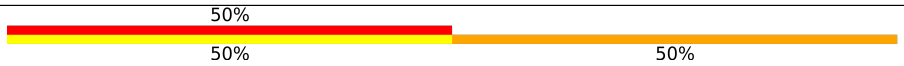
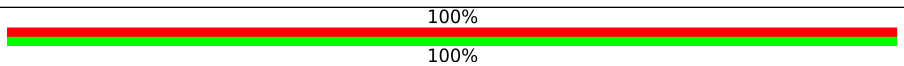
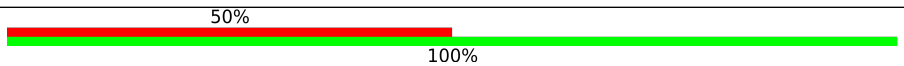
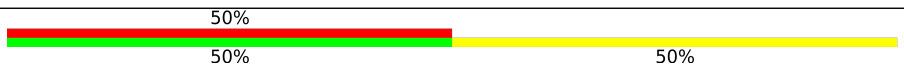
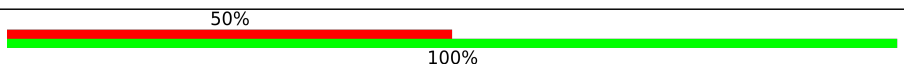
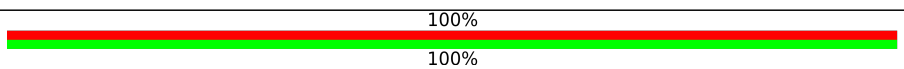
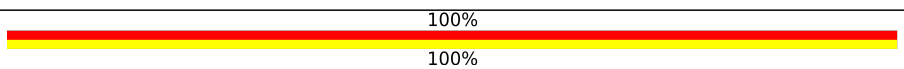
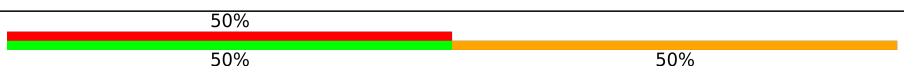
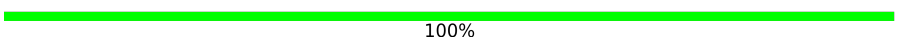
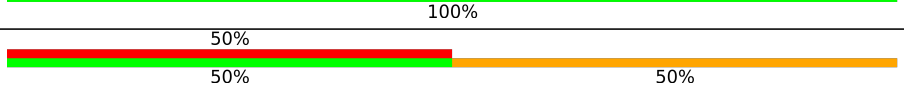
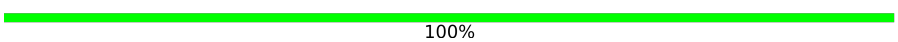
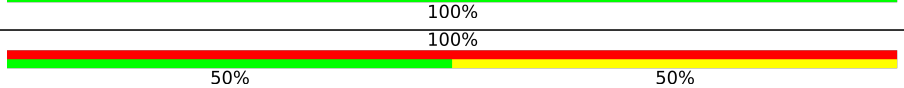
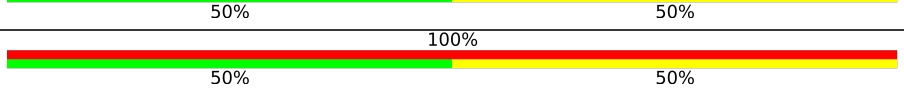
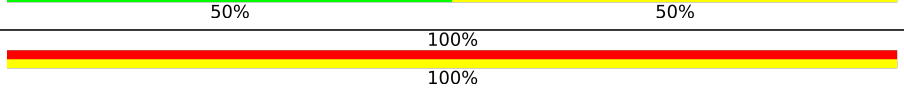
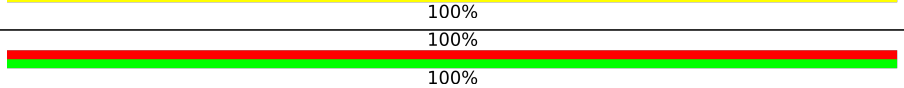
Mol	Chain	Length	Quality of chain
3	E	2	
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	

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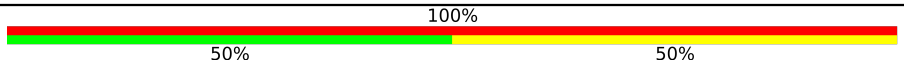
Mol	Chain	Length	Quality of chain
3	d	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1407	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29045 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	971	Total	C	N	O	S	0	0
			7584	4843	1262	1445	34		

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		

There are 13 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

- 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	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		
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		
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		

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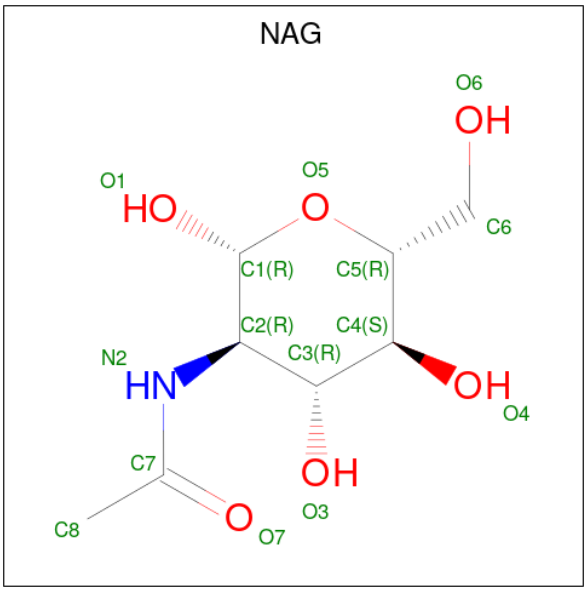
Mol	Chain	Residues	Atoms	AltConf	Trace
3	a	2	Total C N O 28 16 2 10	0	0
3	b	2	Total C N O 28 16 2 10	0	0
3	c	2	Total C N O 28 16 2 10	0	0
3	d	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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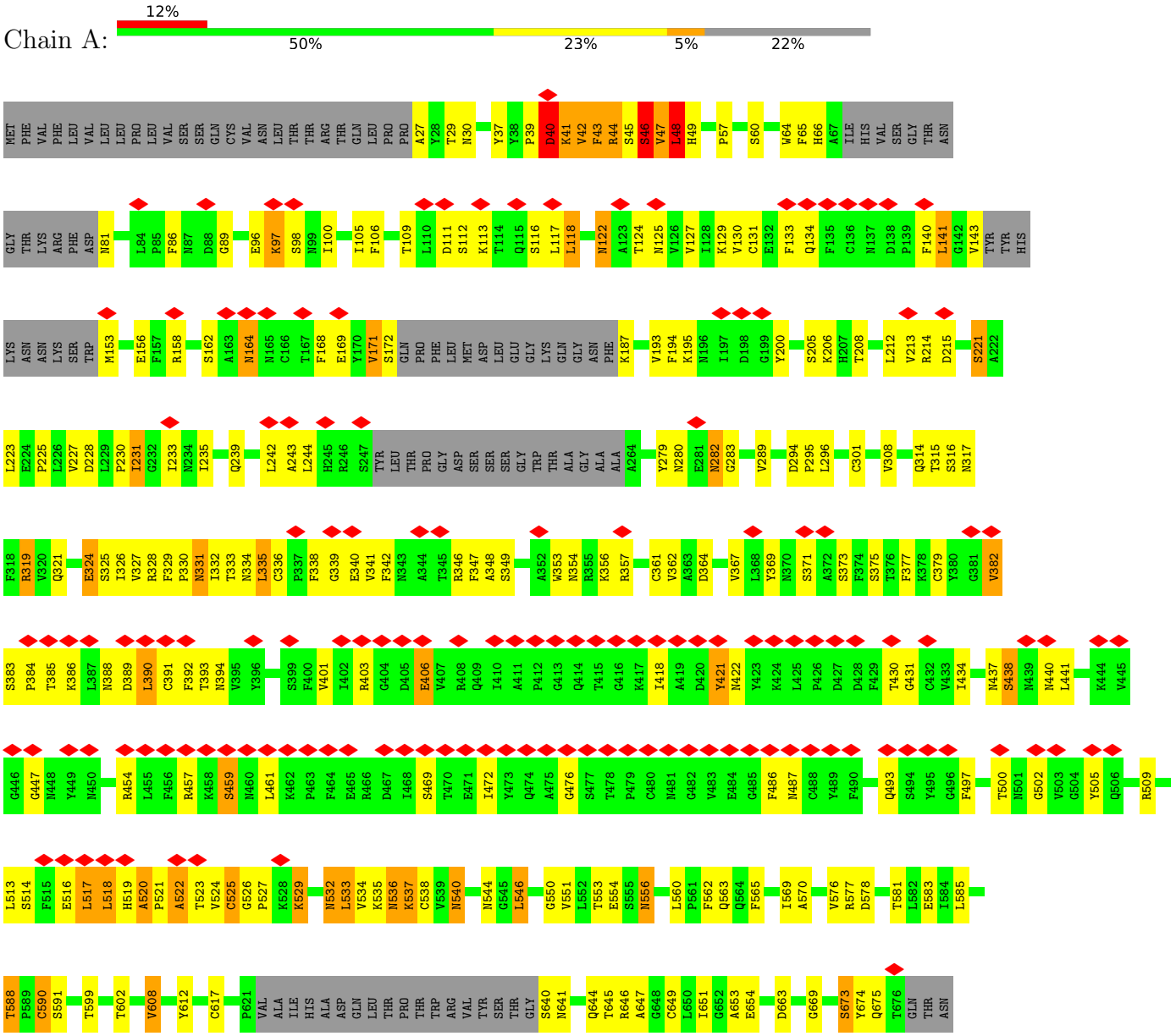
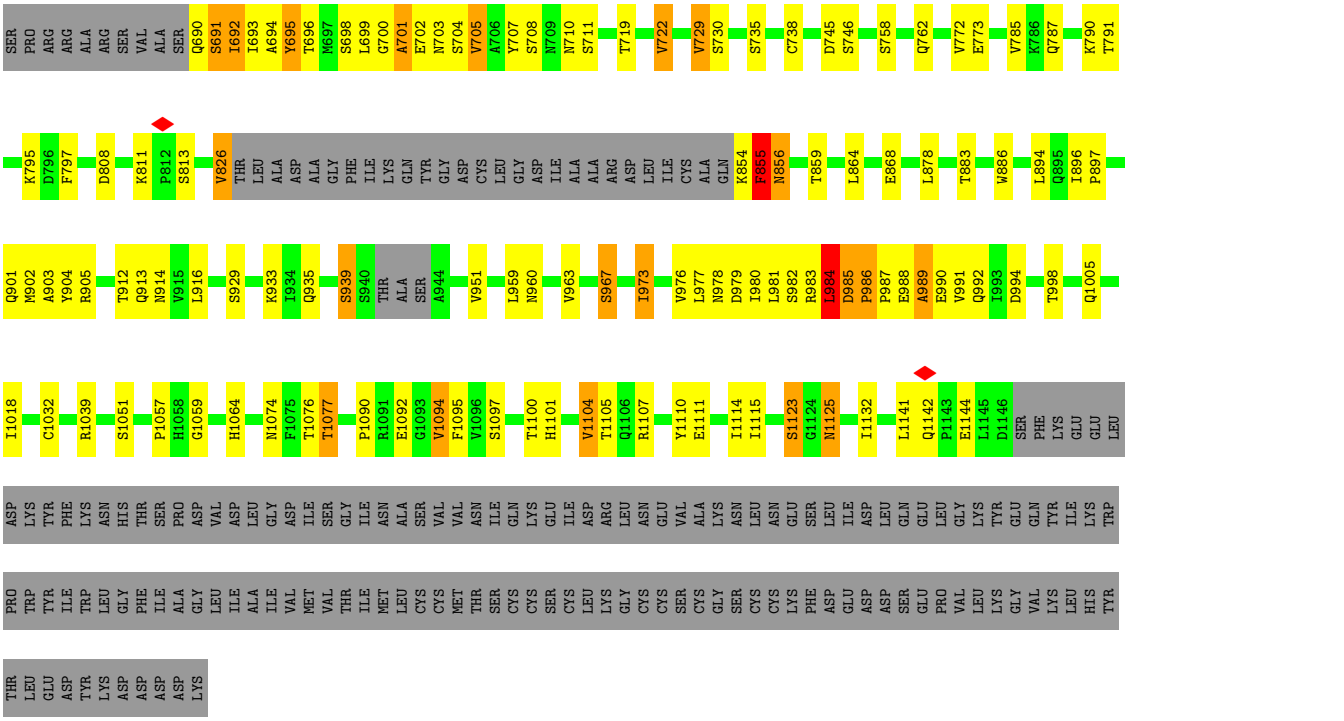
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

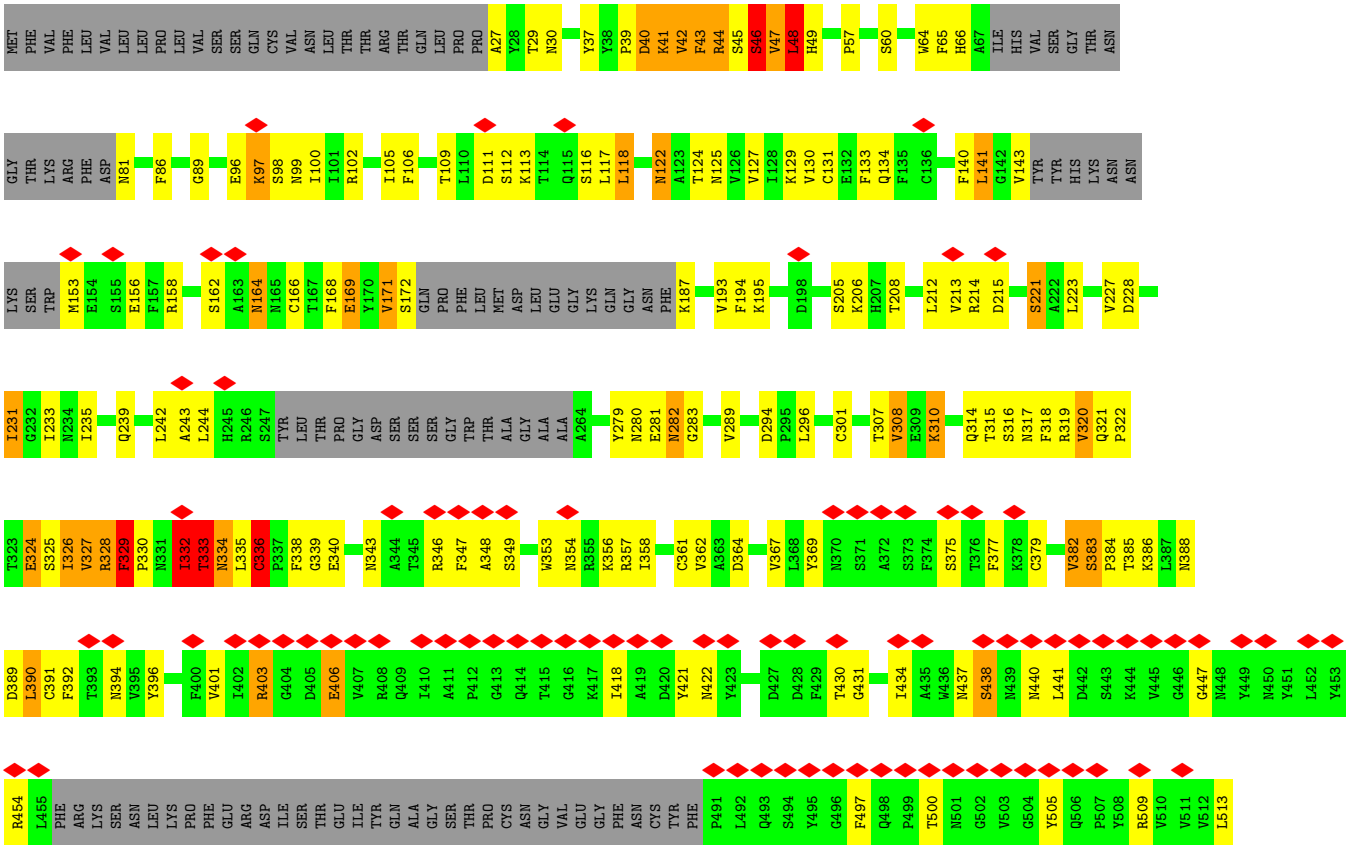


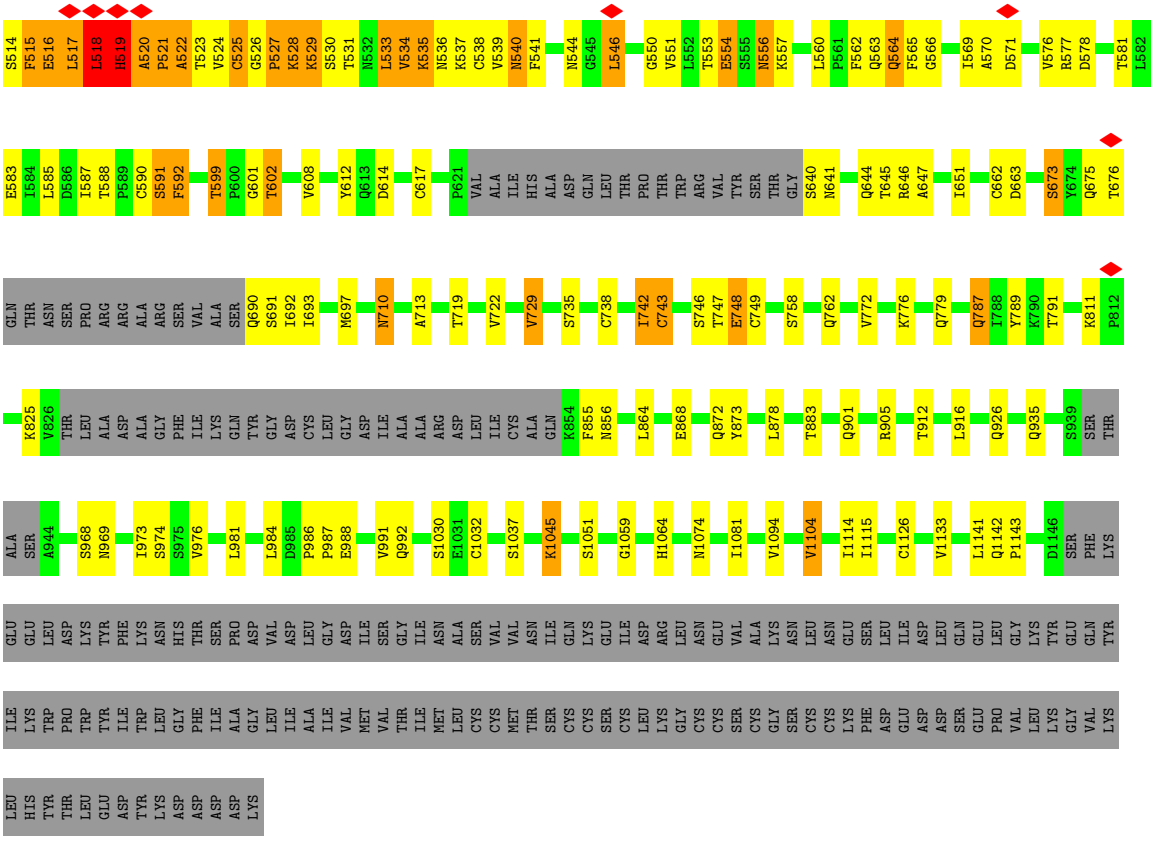


• Molecule 1: Spike glycoprotein

Chain B:



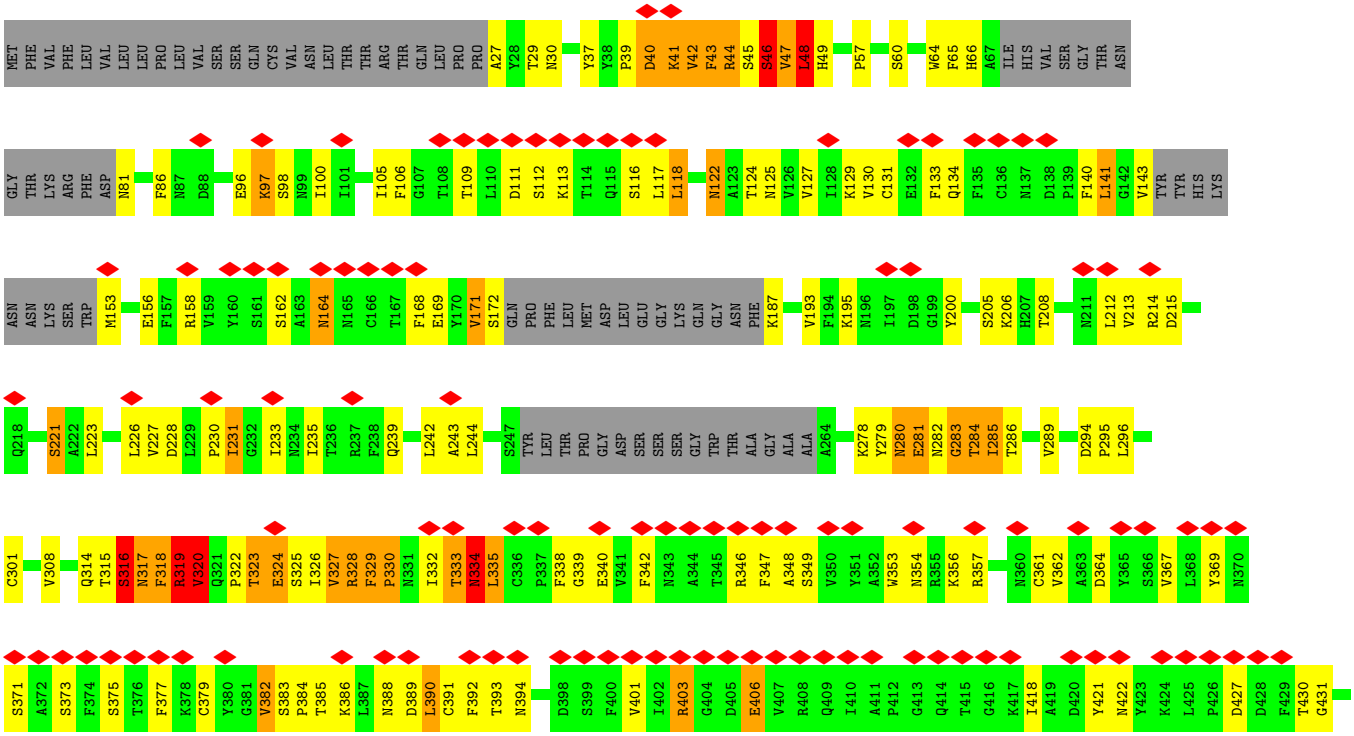


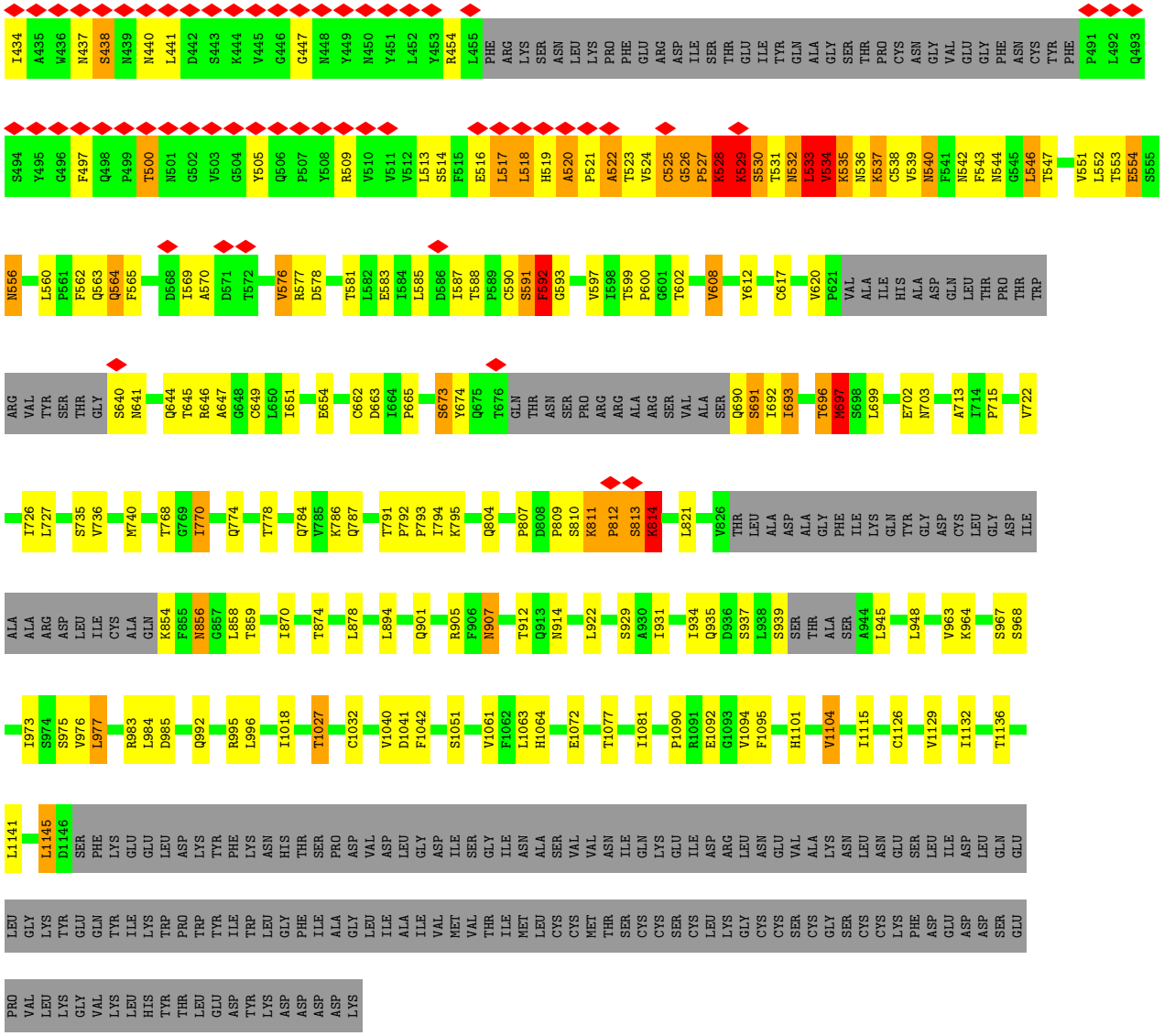


• Molecule 1: Spike glycoprotein

Chain C:



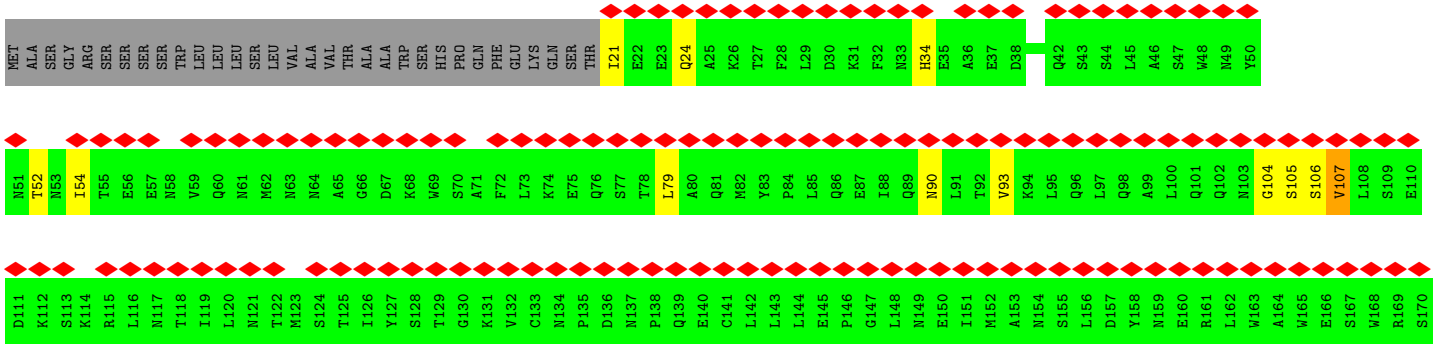


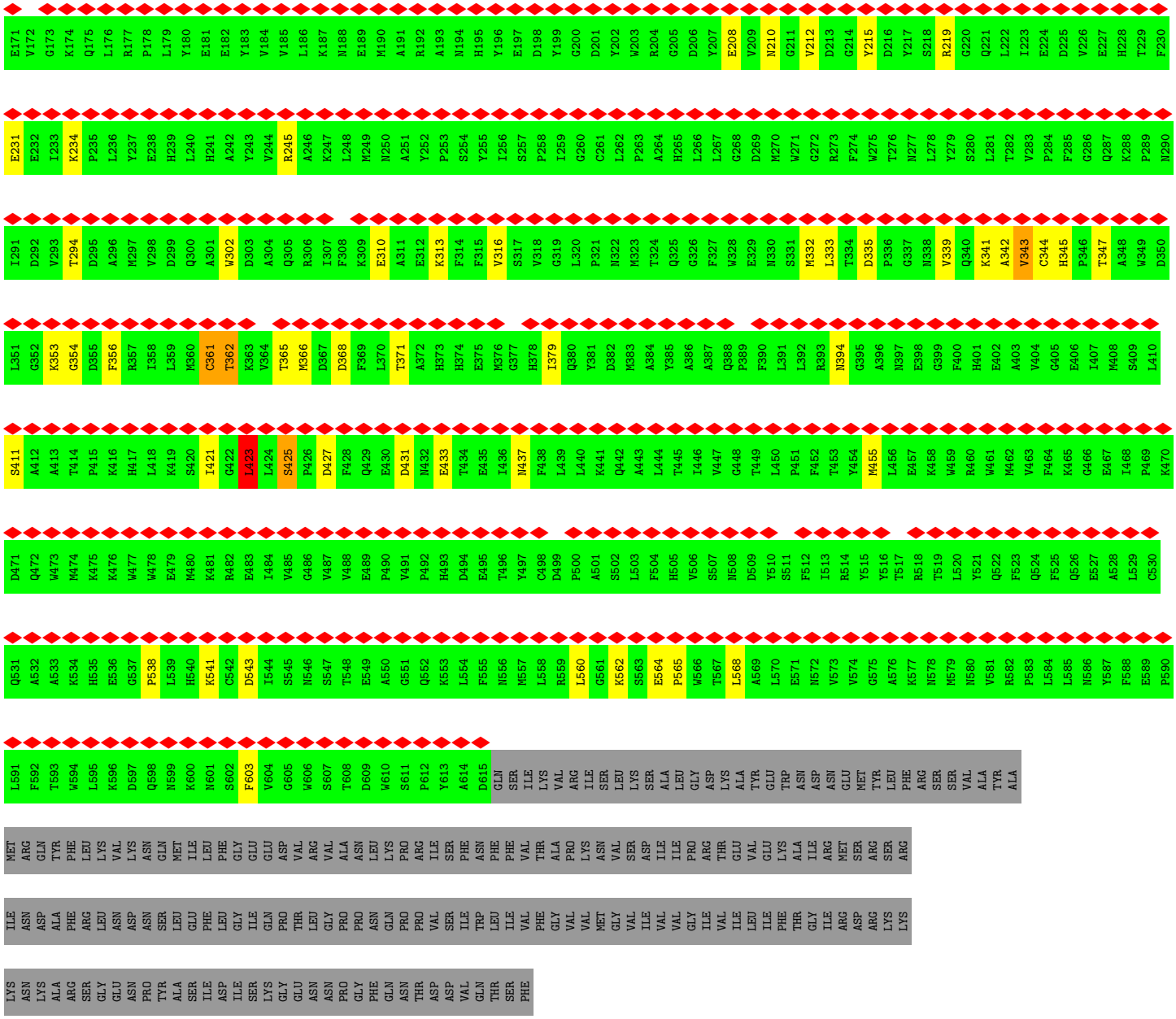


• Molecule 2: Angiotensin-converting enzyme 2

Chain D:

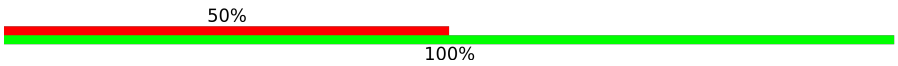






• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





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

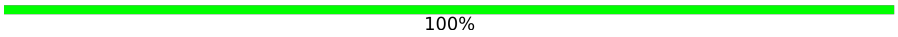
Chain F:





• 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

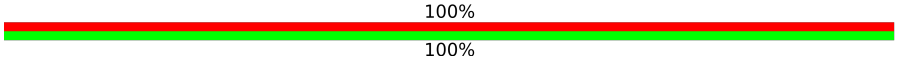
Chain K:





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

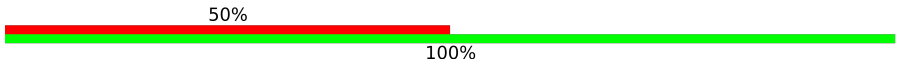
Chain L:





• 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

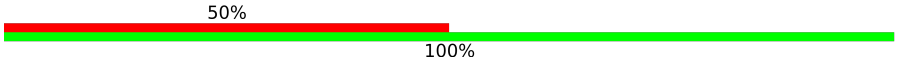
Chain P:





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

Chain Q:





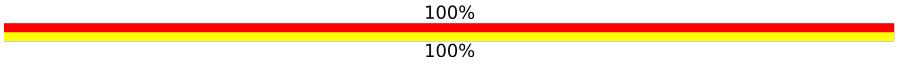
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:





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





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



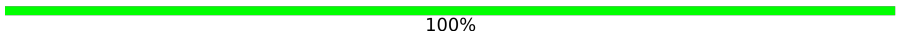


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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





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





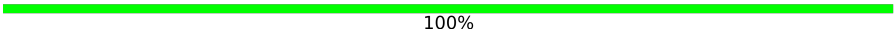
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

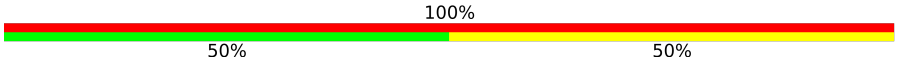
Chain Y:





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

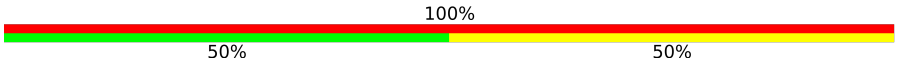
Chain Z:





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

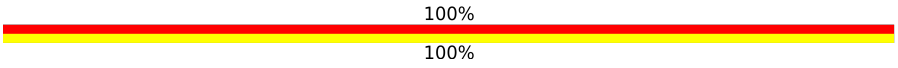
Chain a:





• 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

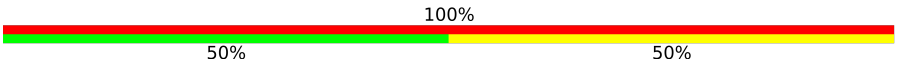
Chain c:





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

Chain d:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98516	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	0.141	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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	0.53	2/8048 (0.0%)	0.63	6/10947 (0.1%)
1	B	0.51	0/7751	0.63	2/10544 (0.0%)
1	C	0.51	0/7751	0.61	2/10544 (0.0%)
2	D	0.30	0/4994	0.54	1/6785 (0.0%)
All	All	0.49	2/28544 (0.0%)	0.61	11/38820 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	SER	CA-C	-6.63	1.44	1.52
1	A	985	ASP	C-N	5.20	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	985	ASP	CA-C-N	-6.19	114.01	120.38
1	A	985	ASP	C-N-CA	-6.19	114.01	120.38
2	D	362	THR	N-CA-C	6.01	119.32	109.76
1	A	86	PHE	CA-C-N	5.90	132.81	121.54
1	A	86	PHE	C-N-CA	5.90	132.81	121.54
1	C	86	PHE	CA-C-N	5.89	132.79	121.54
1	C	86	PHE	C-N-CA	5.89	132.79	121.54
1	B	86	PHE	CA-C-N	5.88	132.77	121.54
1	B	86	PHE	C-N-CA	5.88	132.77	121.54
1	A	986	PRO	CA-C-N	-5.11	113.93	119.24
1	A	986	PRO	C-N-CA	-5.11	113.93	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7872	0	7671	380	0
1	B	7584	0	7403	363	0
1	C	7584	0	7404	459	0
2	D	4857	0	4624	69	0
3	E	28	0	25	0	0
3	F	28	0	25	3	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	3	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	1	0
3	X	28	0	25	2	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	6	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
4	A	126	0	117	4	0
4	B	168	0	154	15	0
4	C	112	0	104	4	0
4	D	14	0	13	0	0
All	All	29045	0	28140	1150	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 20.

All (1150) 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:333:THR:HG21	1:C:361:CYS:C	1.36	1.49
1:A:41:LYS:HD2	1:C:562:PHE:CD2	1.46	1.48
4:B:1411:NAG:O4	4:B:1412:NAG:C1	1.63	1.45
1:C:329:PHE:CE2	1:C:528:LYS:HG2	1.56	1.39
1:C:329:PHE:CZ	1:C:528:LYS:HG2	1.60	1.36
1:B:431:GLY:HA2	1:B:515:PHE:CE1	1.59	1.34
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.31
1:A:536:ASN:O	1:A:537:LYS:CG	1.81	1.26
1:C:333:THR:CG2	1:C:362:VAL:HG23	1.66	1.25
1:B:367:VAL:CG2	4:B:1407:NAG:H83	1.65	1.24
1:A:41:LYS:CD	1:C:562:PHE:HD2	1.50	1.23
1:C:329:PHE:CE2	1:C:528:LYS:CG	2.22	1.22
1:A:536:ASN:O	1:A:537:LYS:HG2	1.11	1.22
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.20
1:C:536:ASN:HA	1:C:551:VAL:CG1	1.72	1.19
1:C:536:ASN:HA	1:C:551:VAL:HG13	1.20	1.16
1:B:367:VAL:HG21	4:B:1407:NAG:H83	1.21	1.16
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:A:565:PHE:O	1:B:42:VAL:HA	1.48	1.13
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.17	1.12
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.12
1:C:280:ASN:OD1	1:C:286:THR:HG21	1.48	1.12
1:A:41:LYS:HG2	1:C:519:HIS:HD1	1.10	1.12
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.20	1.11
1:A:41:LYS:CD	1:C:562:PHE:CD2	2.29	1.11
1:C:333:THR:CG2	1:C:361:CYS:C	2.24	1.11
1:B:392:PHE:HE2	1:B:517:LEU:HB2	1.13	1.10
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.10
1:C:333:THR:HG22	1:C:362:VAL:HG23	1.29	1.10
1:C:523:THR:HG22	1:C:524:VAL:H	0.98	1.09
1:B:748:GLU:HG3	1:B:981:LEU:HD21	1.32	1.09
1:A:523:THR:HG22	1:A:524:VAL:H	0.98	1.08
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.08
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.08
1:B:332:ILE:HG22	1:B:362:VAL:HG22	1.35	1.08
1:A:533:LEU:CD2	1:A:535:LYS:HE3	1.84	1.08
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.07
1:B:523:THR:HG22	1:B:524:VAL:H	1.20	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.30	1.07
1:A:41:LYS:HG2	1:C:519:HIS:ND1	1.71	1.05
1:B:392:PHE:CE2	1:B:517:LEU:HD12	1.91	1.05
1:B:367:VAL:HG21	4:B:1407:NAG:C8	1.87	1.04
1:C:329:PHE:CD2	1:C:528:LYS:HG2	1.92	1.04
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.04
1:C:329:PHE:CZ	1:C:528:LYS:CG	2.38	1.04
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.34	1.04
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.03
1:B:392:PHE:HD2	1:B:517:LEU:HA	1.23	1.03
1:C:333:THR:HG22	1:C:362:VAL:CG2	1.88	1.03
1:C:333:THR:HG21	1:C:361:CYS:O	1.55	1.03
1:C:536:ASN:CA	1:C:551:VAL:HG13	1.88	1.02
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.41	1.02
1:B:328:ARG:HG2	1:B:578:ASP:OD1	1.58	1.02
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
1:C:403:ARG:NH1	1:C:505:TYR:HE1	1.58	1.01
1:B:517:LEU:HD22	1:C:983:ARG:NE	1.76	1.01
1:C:280:ASN:CG	1:C:286:THR:HG21	1.85	1.01
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.00
4:B:1411:NAG:C4	4:B:1412:NAG:C1	2.38	1.00
1:A:41:LYS:HD2	1:C:562:PHE:CE2	1.96	1.00
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	0.99
1:B:332:ILE:HG22	1:B:362:VAL:CG2	1.92	0.99
1:B:748:GLU:CG	1:B:981:LEU:HD21	1.91	0.99
1:C:333:THR:HG23	1:C:334:ASN:H	1.23	0.99
1:B:357:ARG:NH2	1:C:230:PRO:HG3	1.77	0.98
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.44	0.98
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.91	0.98
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	0.98
1:C:329:PHE:CE1	1:C:528:LYS:HG2	1.99	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:C:654:GLU:HG3	1:C:693:ILE:CG2	1.94	0.98
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.43	0.97
1:B:523:THR:HG22	1:B:524:VAL:N	1.74	0.97
1:C:329:PHE:CE2	1:C:528:LYS:CB	2.48	0.97
1:C:329:PHE:CE2	1:C:528:LYS:HB2	1.98	0.97
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.44	0.97
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.97
1:A:41:LYS:HB3	1:C:563:GLN:HA	1.44	0.96
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.96
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.96
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.96
1:C:328:ARG:HG2	1:C:578:ASP:OD1	1.66	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.95
1:C:403:ARG:NH1	1:C:505:TYR:CE1	2.33	0.95
1:B:392:PHE:CE2	1:B:517:LEU:HB2	2.01	0.95
1:C:523:THR:HG22	1:C:524:VAL:N	1.73	0.95
1:B:392:PHE:CD2	1:B:517:LEU:HA	2.01	0.95
1:A:980:ILE:O	1:A:984:LEU:HB2	1.67	0.95
1:A:985:ASP:HB2	1:A:987:PRO:HD2	1.49	0.95
1:C:528:LYS:O	1:C:529:LYS:HE3	1.67	0.94
1:A:703:ASN:OD1	1:B:789:TYR:HE1	1.50	0.94
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.34	0.93
1:B:329:PHE:CE1	1:B:544:ASN:HA	2.03	0.92
1:A:533:LEU:HD21	1:A:535:LYS:HG3	1.52	0.92
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.92
1:A:505:TYR:CD2	2:D:353:LYS:O	2.23	0.92
1:C:333:THR:HG23	1:C:362:VAL:HG23	1.50	0.92
1:B:392:PHE:HE2	1:B:517:LEU:CB	1.83	0.91
1:B:327:VAL:O	1:B:530:SER:HB2	1.70	0.91
1:C:333:THR:HG21	1:C:362:VAL:N	1.85	0.91
1:C:329:PHE:CD2	1:C:528:LYS:CB	2.54	0.91
1:B:386:LYS:HZ2	1:C:985:ASP:HB3	1.35	0.91
1:A:319:ARG:HH21	1:A:319:ARG:HG3	1.35	0.90
1:B:326:ILE:HD13	1:B:327:VAL:N	1.86	0.90
1:C:327:VAL:O	1:C:530:SER:HA	1.70	0.90
1:B:431:GLY:CA	1:B:515:PHE:CE1	2.53	0.89
1:A:476:GLY:CA	2:D:24:GLN:HE21	1.85	0.89
1:A:486:PHE:HE1	2:D:79:LEU:CD2	1.84	0.89
1:C:538:CYS:HB2	1:C:590:CYS:SG	2.13	0.89
1:A:533:LEU:HD21	1:A:535:LYS:HE3	1.54	0.89
1:C:333:THR:CG2	1:C:362:VAL:CG2	2.47	0.89
1:B:570:ALA:HB2	1:C:963:VAL:HG12	1.54	0.89
1:B:551:VAL:HB	1:B:588:THR:HG23	1.56	0.88
1:B:390:LEU:CD1	1:B:517:LEU:HD11	2.03	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.87
1:A:41:LYS:CE	1:C:562:PHE:HD2	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:O	1:C:523:THR:HG21	1.75	0.86
1:B:517:LEU:CD2	1:C:983:ARG:NE	2.39	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:B:569:ILE:HG22	1:C:964:LYS:HE2	1.58	0.86
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.85
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.85
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:B:569:ILE:HG13	1:C:47:VAL:HG11	1.58	0.85
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.84
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.84
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
1:A:393:THR:O	1:A:523:THR:HG21	1.76	0.84
1:B:390:LEU:HD11	1:B:517:LEU:HD11	1.57	0.84
1:C:324:GLU:OE1	1:C:324:GLU:N	2.09	0.84
1:A:41:LYS:C	1:C:563:GLN:HG2	2.03	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.84
1:C:329:PHE:CZ	1:C:528:LYS:HD3	2.13	0.83
1:A:230:PRO:HB2	1:C:357:ARG:CZ	2.09	0.83
1:B:517:LEU:HD22	1:C:983:ARG:CZ	2.08	0.83
1:C:329:PHE:CD2	1:C:528:LYS:CG	2.57	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:B:431:GLY:HA2	1:B:515:PHE:HE1	1.04	0.83
1:C:538:CYS:CB	1:C:590:CYS:SG	2.67	0.83
1:A:486:PHE:CZ	2:D:79:LEU:HD22	2.13	0.83
1:A:703:ASN:OD1	1:B:789:TYR:CE1	2.32	0.83
1:B:357:ARG:HH22	1:C:230:PRO:HG3	1.40	0.83
1:B:523:THR:CG2	1:B:524:VAL:H	1.90	0.83
1:C:662:CYS:HB2	1:C:697:MET:CE	2.09	0.83
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:C:328:ARG:NE	1:C:533:LEU:HD22	1.94	0.82
1:C:322:PRO:HA	1:C:538:CYS:O	1.79	0.82
1:A:983:ARG:O	1:A:984:LEU:HD23	1.80	0.82
1:B:571:ASP:HB2	1:C:967:SER:CB	2.09	0.82
1:A:42:VAL:N	1:C:563:GLN:HG2	1.95	0.82
1:C:280:ASN:HB2	1:C:284:THR:O	1.80	0.81
1:A:529:LYS:HZ3	1:A:529:LYS:HA	1.45	0.81
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:A:654:GLU:HG3	1:A:693:ILE:CG2	2.09	0.81
1:B:396:TYR:HE2	1:C:200:TYR:HH	0.82	0.81
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.08	0.81
1:C:329:PHE:CZ	1:C:528:LYS:CD	2.64	0.80
1:A:334:ASN:O	1:A:362:VAL:HB	1.81	0.80
1:B:319:ARG:NH2	1:C:740:MET:SD	2.55	0.80
1:C:318:PHE:CZ	1:C:620:VAL:O	2.35	0.80
3:b:1:NAG:C3	3:b:2:NAG:HN2	1.95	0.80
1:B:748:GLU:N	1:B:748:GLU:OE2	2.14	0.79
1:B:521:PRO:O	1:B:564:GLN:HG3	1.82	0.79
1:B:328:ARG:CG	1:B:578:ASP:OD1	2.31	0.79
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.65	0.79
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.79
1:C:532:ASN:O	1:C:533:LEU:HD23	1.82	0.79
1:B:743:CYS:SG	1:B:749:CYS:C	2.66	0.78
1:C:280:ASN:CG	1:C:286:THR:CG2	2.56	0.78
1:B:325:SER:HA	1:B:540:ASN:O	1.83	0.78
1:B:396:TYR:HE2	1:C:200:TYR:OH	1.63	0.78
1:B:390:LEU:HD23	1:B:391:CYS:H	1.48	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
1:B:332:ILE:CG2	1:B:362:VAL:HG22	2.13	0.78
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.13	0.78
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.14	0.78
1:C:531:THR:HG22	1:C:532:ASN:H	1.48	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.49	0.77
1:A:335:LEU:HA	1:A:362:VAL:HB	1.67	0.77
1:A:529:LYS:HA	1:A:529:LYS:NZ	1.98	0.77
1:A:979:ASP:O	1:A:983:ARG:HG3	1.84	0.77
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.77
1:B:361:CYS:SG	1:B:524:VAL:HG21	2.25	0.77
1:B:310:LYS:HB2	1:B:310:LYS:HZ2	1.50	0.77
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.77
1:B:396:TYR:OH	1:C:230:PRO:HB3	1.85	0.77
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:B:332:ILE:CG2	1:B:362:VAL:CG2	2.63	0.76
1:A:476:GLY:HA2	2:D:24:GLN:HE21	1.50	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
1:A:703:ASN:CB	1:B:787:GLN:OE1	2.23	0.76
1:A:390:LEU:HD23	1:A:391:CYS:H	1.49	0.76
1:A:41:LYS:HG2	1:C:519:HIS:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:CD2	1:A:535:LYS:HG3	2.15	0.76
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.76
1:A:529:LYS:HA	1:A:529:LYS:CE	2.16	0.76
1:A:963:VAL:HG12	1:C:570:ALA:HB1	1.67	0.76
1:B:571:ASP:HB2	1:C:967:SER:HB3	1.66	0.76
1:A:476:GLY:HA3	2:D:24:GLN:HE21	1.50	0.76
1:A:565:PHE:O	1:B:42:VAL:CA	2.32	0.76
1:A:533:LEU:HD22	1:A:535:LYS:HE3	1.66	0.75
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:B:392:PHE:CE2	1:B:517:LEU:CD1	2.68	0.75
1:C:329:PHE:CD2	1:C:528:LYS:HB2	2.19	0.75
1:C:361:CYS:SG	1:C:524:VAL:HG21	2.25	0.75
1:C:735:SER:OG	1:C:859:THR:CG2	2.34	0.75
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.75
1:A:536:ASN:C	1:A:537:LYS:HG2	2.09	0.75
1:A:980:ILE:O	1:A:984:LEU:CB	2.35	0.75
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.75
1:B:392:PHE:CZ	1:B:517:LEU:HD12	2.22	0.75
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:C:403:ARG:HH11	1:C:505:TYR:HE1	1.33	0.74
1:B:329:PHE:HE1	1:B:544:ASN:HA	1.49	0.74
1:C:536:ASN:HA	1:C:551:VAL:HG11	1.66	0.74
1:A:326:ILE:HD12	1:A:533:LEU:HA	1.69	0.74
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.74
1:B:392:PHE:CE2	1:B:517:LEU:CB	2.65	0.74
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.74
1:B:335:LEU:HA	1:B:362:VAL:HB	1.69	0.74
1:C:532:ASN:C	1:C:533:LEU:HD23	2.13	0.74
1:B:324:GLU:O	1:B:539:VAL:HG22	1.86	0.73
1:A:987:PRO:HB2	1:A:988:GLU:OE2	1.88	0.73
1:B:569:ILE:CG1	1:C:47:VAL:CG1	2.67	0.73
1:A:319:ARG:HG3	1:A:319:ARG:NH2	2.03	0.73
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.71	0.73
1:C:328:ARG:NH2	1:C:543:PHE:CZ	2.55	0.73
1:C:531:THR:HG22	1:C:532:ASN:N	2.04	0.73
1:B:357:ARG:NH2	1:C:230:PRO:CG	2.52	0.73
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.73
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.32	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ALA:CB	1:C:963:VAL:HG12	2.18	0.72
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
1:C:328:ARG:CZ	1:C:543:PHE:CZ	2.73	0.72
1:B:388:ASN:OD1	1:B:527:PRO:CD	2.37	0.72
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.72
1:B:533:LEU:HD12	1:B:533:LEU:C	2.15	0.72
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.71	0.72
1:A:41:LYS:CE	1:C:562:PHE:CD2	2.69	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
1:B:569:ILE:HG12	1:C:47:VAL:HG12	1.70	0.71
1:A:536:ASN:C	1:A:537:LYS:CG	2.59	0.71
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.71
1:A:41:LYS:H	1:C:519:HIS:CE1	2.09	0.71
1:A:536:ASN:O	1:A:537:LYS:HG3	1.87	0.71
4:B:1411:NAG:H4	4:B:1412:NAG:C1	2.21	0.71
1:C:333:THR:HG23	1:C:334:ASN:N	2.04	0.71
1:B:335:LEU:O	1:B:335:LEU:HD12	1.90	0.71
1:B:390:LEU:CD1	1:B:517:LEU:CD1	2.68	0.70
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.70
1:A:124:THR:HG21	4:A:1402:NAG:HN2	1.56	0.70
1:C:329:PHE:CB	1:C:330:PRO:CD	2.69	0.70
1:C:329:PHE:CG	1:C:528:LYS:HG2	2.26	0.70
1:C:124:THR:HG21	4:C:1402:NAG:HN2	1.56	0.70
1:B:390:LEU:HD13	1:B:517:LEU:CD1	2.21	0.70
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.70
1:A:41:LYS:CA	1:C:563:GLN:HG2	2.21	0.70
1:A:988:GLU:O	1:A:990:GLU:N	2.25	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.69
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.69
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69
1:B:124:THR:HG21	4:B:1402:NAG:HN2	1.56	0.69
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.69
1:C:333:THR:OG1	1:C:334:ASN:ND2	2.25	0.69
1:C:329:PHE:CD1	1:C:528:LYS:HG2	2.28	0.69
1:B:431:GLY:CA	1:B:515:PHE:HE1	1.94	0.69
1:C:335:LEU:HD12	1:C:335:LEU:N	2.07	0.69
1:B:324:GLU:O	1:B:539:VAL:CG2	2.40	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.74	0.69
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:HA	1:A:540:ASN:O	1.93	0.69
1:B:569:ILE:CG2	1:C:964:LYS:HE2	2.21	0.69
1:A:551:VAL:HB	1:A:588:THR:HG23	1.75	0.68
1:A:41:LYS:N	1:C:519:HIS:CE1	2.62	0.68
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.21	0.68
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.68
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.68
1:B:321:GLN:OE1	1:B:321:GLN:HA	1.93	0.68
1:B:551:VAL:HB	1:B:588:THR:CG2	2.22	0.68
1:B:388:ASN:OD1	1:B:527:PRO:HD2	1.94	0.67
1:B:571:ASP:HB2	1:C:967:SER:HB2	1.77	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.67
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.67
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.67
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.22	0.67
1:C:333:THR:OG1	1:C:361:CYS:CA	2.43	0.67
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.67
1:B:396:TYR:OH	1:C:230:PRO:CB	2.43	0.67
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.67
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.67
1:A:41:LYS:HE3	1:C:562:PHE:CD2	2.30	0.66
1:C:335:LEU:HA	1:C:362:VAL:HB	1.77	0.66
1:A:988:GLU:C	1:A:990:GLU:H	2.02	0.66
1:B:431:GLY:HA2	1:B:515:PHE:CD1	2.27	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:A:325:SER:CB	1:A:540:ASN:HB3	2.26	0.66
1:B:332:ILE:O	1:B:333:THR:HG23	1.96	0.66
1:B:390:LEU:HD12	1:C:983:ARG:HB3	1.75	0.66
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.66
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.66
1:A:529:LYS:HA	1:A:529:LYS:HE2	1.76	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:C:280:ASN:CB	1:C:286:THR:CG2	2.73	0.66
1:A:963:VAL:CG1	1:C:570:ALA:HB1	2.26	0.65
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.65
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.65
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.78	0.65
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:OD1	1:A:527:PRO:CD	2.43	0.65
1:C:535:LYS:HD3	1:C:554:GLU:OE2	1.97	0.65
1:A:533:LEU:HD21	1:A:535:LYS:CG	2.26	0.65
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:B:569:ILE:CG1	1:C:47:VAL:HG12	2.26	0.65
1:A:388:ASN:OD1	1:A:527:PRO:HD2	1.97	0.65
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.65
1:B:390:LEU:CD1	1:C:983:ARG:HB3	2.26	0.65
1:B:392:PHE:CD2	1:B:517:LEU:CA	2.78	0.65
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:A:745:ASP:HB2	1:C:319:ARG:NH1	2.12	0.65
1:C:316:SER:OG	1:C:317:ASN:N	2.30	0.65
1:C:569:ILE:H	1:C:569:ILE:HD12	1.60	0.65
1:C:690:GLN:O	1:C:691:SER:HB3	1.97	0.65
1:C:333:THR:CG2	1:C:362:VAL:N	2.54	0.64
1:C:335:LEU:O	1:C:361:CYS:HB2	1.97	0.64
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.64
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.64
1:A:493:GLN:OE1	2:D:34:HIS:CB	2.45	0.64
1:A:41:LYS:CB	1:C:519:HIS:HE1	2.11	0.64
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.64
1:A:533:LEU:CD2	1:A:535:LYS:CE	2.70	0.64
1:B:544:ASN:HD21	1:B:564:GLN:NE2	1.95	0.64
1:A:325:SER:HB2	1:A:540:ASN:HB3	1.79	0.64
1:A:985:ASP:OD1	1:A:988:GLU:HB2	1.97	0.64
1:A:385:THR:HG1	1:A:386:LYS:HZ3	1.46	0.64
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.64
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.64
3:b:1:NAG:H3	3:b:2:NAG:HN2	1.63	0.64
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.63
1:A:43:PHE:CE1	1:A:282:ASN:O	2.52	0.63
1:A:985:ASP:CB	1:A:987:PRO:HD2	2.26	0.63
1:A:669:GLY:N	1:B:864:LEU:O	2.30	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
1:A:326:ILE:CD1	1:A:533:LEU:HA	2.28	0.63
1:C:333:THR:OG1	1:C:361:CYS:N	2.31	0.63
1:C:591:SER:C	1:C:592:PHE:HD1	2.07	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.63
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLN:HA	1:A:321:GLN:OE1	1.97	0.63
1:B:396:TYR:OH	1:C:230:PRO:HG3	1.98	0.63
1:B:571:ASP:CB	1:C:967:SER:HB2	2.29	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.63
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.62
1:A:654:GLU:CG	1:A:693:ILE:HG22	2.14	0.62
1:A:700:GLY:O	1:A:701:ALA:O	2.17	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62
1:C:323:THR:N	1:C:538:CYS:O	2.32	0.62
1:A:43:PHE:HE1	1:A:282:ASN:O	1.83	0.62
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.83	0.62
1:B:520:ALA:CB	1:B:521:PRO:HD2	2.23	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:B:329:PHE:CD1	1:B:544:ASN:HA	2.35	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.62
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.62
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.24	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.62
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.62
1:C:318:PHE:HB3	1:C:592:PHE:O	1.98	0.62
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:B:334:ASN:H	1:B:334:ASN:ND2	1.96	0.62
1:A:534:VAL:HG23	1:A:534:VAL:O	2.00	0.61
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:B:327:VAL:O	1:B:530:SER:CB	2.46	0.61
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.61
1:A:988:GLU:C	1:A:990:GLU:N	2.57	0.61
1:C:295:PRO:HB3	1:C:597:VAL:HG22	1.82	0.61
1:C:281:GLU:OE2	1:C:281:GLU:N	2.33	0.61
1:C:328:ARG:CZ	1:C:543:PHE:HZ	2.13	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:B:310:LYS:HZ2	1:B:310:LYS:CB	2.13	0.61
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:CG	1:C:319:ARG:HH21	2.14	0.61
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.83	0.61
1:C:556:ASN:HD22	1:C:556:ASN:H	1.49	0.61
1:A:327:VAL:O	1:A:328:ARG:HG2	2.01	0.60
1:B:569:ILE:CG1	1:C:47:VAL:HG11	2.24	0.60
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.60
1:B:320:VAL:HG23	1:B:591:SER:O	2.00	0.60
1:C:576:VAL:HG22	1:C:587:ILE:HD11	1.84	0.60
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.60
1:B:529:LYS:C	1:B:529:LYS:HE3	2.27	0.60
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.60
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.83	0.60
1:C:525:CYS:O	1:C:526:GLY:O	2.18	0.60
1:B:308:VAL:O	1:B:601:GLY:HA2	2.02	0.60
1:B:320:VAL:HG21	1:B:591:SER:HB2	1.84	0.60
1:B:388:ASN:OD1	1:B:527:PRO:HD3	2.00	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.60
1:A:40:ASP:HB2	1:C:519:HIS:CE1	2.36	0.60
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.60
1:B:556:ASN:H	1:B:556:ASN:HD22	1.49	0.60
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.60
1:C:280:ASN:HB2	1:C:286:THR:CG2	2.32	0.60
1:C:319:ARG:HH21	1:C:319:ARG:HG2	1.66	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.60
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.60
1:A:532:ASN:N	1:A:532:ASN:OD1	2.32	0.59
1:C:319:ARG:O	1:C:320:VAL:HG13	2.02	0.59
1:C:322:PRO:CA	1:C:538:CYS:O	2.50	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.37	0.59
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:B:325:SER:CA	1:B:540:ASN:O	2.49	0.59
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.59
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.59
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.59
1:B:529:LYS:HE3	1:B:529:LYS:O	2.01	0.59
1:C:333:THR:HG22	1:C:362:VAL:HG22	1.80	0.59
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:C:587:ILE:HG22	1:C:587:ILE:O	2.02	0.59
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.59
1:A:41:LYS:CB	1:C:519:HIS:CE1	2.86	0.59
1:A:230:PRO:CB	1:C:357:ARG:CZ	2.81	0.59
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.59
1:B:738:CYS:O	1:B:742:ILE:HG13	2.03	0.59
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.59
1:C:333:THR:OG1	1:C:361:CYS:HA	2.02	0.59
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.59
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.38	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:A:325:SER:CA	1:A:540:ASN:O	2.52	0.58
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.58
1:C:280:ASN:HB2	1:C:286:THR:HG23	1.84	0.58
1:A:978:ASN:O	1:A:982:SER:HB3	2.03	0.58
1:A:325:SER:HB2	1:A:540:ASN:O	2.03	0.58
1:A:983:ARG:HB2	1:C:382:VAL:HB	1.85	0.58
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:C:391:CYS:SG	1:C:523:THR:O	2.61	0.58
1:A:476:GLY:HA3	2:D:24:GLN:NE2	2.17	0.58
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.58
4:B:1405:NAG:H83	4:B:1405:NAG:H3	1.86	0.58
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.58
1:C:338:PHE:O	1:C:340:GLU:N	2.37	0.58
3:W:2:NAG:H3	3:W:2:NAG:H83	1.86	0.58
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.58
4:A:1405:NAG:H3	4:A:1405:NAG:H83	1.86	0.58
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.58
1:B:570:ALA:CB	1:C:963:VAL:CG1	2.82	0.58
1:C:537:LYS:O	1:C:538:CYS:C	2.47	0.58
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.58
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
4:C:1405:NAG:H3	4:C:1405:NAG:H83	1.86	0.57
1:A:230:PRO:HB2	1:C:357:ARG:NH2	2.20	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.57
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.86	0.57
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.57
1:B:361:CYS:SG	1:B:524:VAL:CG2	2.92	0.57
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.57
1:C:654:GLU:CG	1:C:693:ILE:CG2	2.77	0.57
1:C:735:SER:OG	1:C:859:THR:HG23	2.04	0.57
1:A:391:CYS:SG	1:A:523:THR:O	2.61	0.57
1:B:336:CYS:SG	1:B:358:ILE:CG2	2.93	0.57
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.57
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
1:C:338:PHE:C	1:C:340:GLU:H	2.13	0.57
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.57
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.57
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.40	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:C:361:CYS:SG	1:C:524:VAL:CG2	2.92	0.57
1:C:388:ASN:O	1:C:527:PRO:HD2	2.05	0.57
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.57
1:B:41:LYS:O	1:B:42:VAL:HB	2.04	0.57
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.57
1:B:675:GLN:HB3	1:B:693:ILE:HD11	1.87	0.57
1:C:41:LYS:O	1:C:42:VAL:HB	2.05	0.57
1:C:342:PHE:HB3	3:S:1:NAG:H82	1.87	0.57
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.57
3:X:2:NAG:H83	3:X:2:NAG:H3	1.87	0.57
1:B:338:PHE:O	1:B:340:GLU:N	2.37	0.57
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.57
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:B:591:SER:O	1:B:592:PHE:HB3	2.05	0.56
1:C:43:PHE:HE1	1:C:283:GLY:HA3	1.70	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.56
1:B:357:ARG:HH21	1:C:230:PRO:HG3	1.69	0.56
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.56
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.56
1:C:690:GLN:O	1:C:690:GLN:HG3	2.04	0.56
1:A:41:LYS:O	1:A:42:VAL:HB	2.05	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.56
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.56
1:B:338:PHE:C	1:B:340:GLU:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:HIS:ND1	1:C:519:HIS:O	2.38	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.88	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
1:B:515:PHE:CD1	1:B:515:PHE:N	2.73	0.56
1:C:318:PHE:O	1:C:319:ARG:CB	2.53	0.56
1:A:295:PRO:CB	1:A:608:VAL:HG11	2.28	0.56
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.56
1:B:533:LEU:HD12	1:B:534:VAL:O	2.06	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:A:654:GLU:O	1:A:693:ILE:HA	2.05	0.56
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.40	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.89	0.56
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.41	0.56
1:B:563:GLN:O	1:B:577:ARG:NH1	2.38	0.56
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.87	0.56
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.56
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.56
1:B:329:PHE:CE2	1:B:528:LYS:HG3	2.41	0.56
1:B:521:PRO:O	1:B:522:ALA:HB2	2.05	0.56
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.56
1:A:978:ASN:ND2	1:C:547:THR:HG22	2.21	0.56
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.55
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.55
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.55
1:C:530:SER:O	1:C:531:THR:OG1	2.21	0.55
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.88	0.55
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.55
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.55
1:B:318:PHE:O	1:B:592:PHE:HA	2.07	0.55
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:B:517:LEU:HD23	1:B:517:LEU:O	2.06	0.55
1:C:674:TYR:HA	1:C:691:SER:O	2.06	0.55
3:I:2:NAG:H3	3:I:2:NAG:H83	1.87	0.55
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.55
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:A:486:PHE:CZ	2:D:79:LEU:CD2	2.84	0.55
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.55
1:C:531:THR:CG2	1:C:532:ASN:H	2.19	0.55
1:B:357:ARG:HH21	1:C:230:PRO:CG	2.19	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.85	0.55
3:F:1:NAG:H61	3:F:2:NAG:HN2	1.71	0.55
1:A:342:PHE:HB3	3:F:1:NAG:H82	1.87	0.55
1:C:29:THR:HG22	1:C:30:ASN:H	1.71	0.55
1:C:295:PRO:HB3	1:C:597:VAL:CG2	2.35	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.55
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.55
1:B:535:LYS:HE2	1:B:554:GLU:CD	2.31	0.55
1:B:676:THR:HB	1:B:693:ILE:HG21	1.88	0.55
3:S:1:NAG:H61	3:S:2:NAG:HN2	1.72	0.55
1:A:41:LYS:HB2	1:C:519:HIS:HE1	1.71	0.54
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54
1:A:388:ASN:OD1	1:A:527:PRO:HD3	2.08	0.54
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:B:326:ILE:HD11	1:B:328:ARG:HD2	1.89	0.54
1:A:41:LYS:CG	1:C:519:HIS:CE1	2.90	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:A:476:GLY:CA	2:D:24:GLN:NE2	2.65	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.42	0.54
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.54
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.54
1:B:390:LEU:HD11	1:C:983:ARG:HD3	1.89	0.54
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.54
1:C:591:SER:C	1:C:592:PHE:CD1	2.86	0.54
1:B:353:TRP:H	1:B:353:TRP:CD1	2.23	0.53
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.53
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.53
1:B:310:LYS:HA	1:B:599:THR:O	2.08	0.53
1:A:538:CYS:HG	1:A:590:CYS:HG	0.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLU:HG2	1:B:981:LEU:HD21	1.83	0.53
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.53
1:B:748:GLU:HG3	1:B:981:LEU:CD2	2.23	0.53
1:C:385:THR:HG1	1:C:386:LYS:HZ3	1.50	0.53
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.53
1:A:505:TYR:CG	2:D:353:LYS:O	2.62	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.53
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.53
1:B:556:ASN:HD22	1:B:556:ASN:N	2.05	0.53
1:B:592:PHE:CD1	1:B:592:PHE:C	2.87	0.53
1:C:280:ASN:CB	1:C:286:THR:HG23	2.39	0.53
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.53
1:C:592:PHE:CD1	1:C:592:PHE:N	2.76	0.53
1:B:388:ASN:CG	1:B:527:PRO:HD2	2.34	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
1:C:528:LYS:O	1:C:529:LYS:CE	2.49	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:B:326:ILE:HD13	1:B:327:VAL:H	1.72	0.53
1:B:396:TYR:OH	1:C:230:PRO:CG	2.57	0.53
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.53
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.53
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.53
3:H:2:NAG:H3	3:H:2:NAG:H83	1.90	0.53
3:b:1:NAG:H3	3:b:2:NAG:N2	2.24	0.53
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.52
1:A:529:LYS:CE	1:A:529:LYS:CA	2.86	0.52
1:A:505:TYR:CE2	2:D:353:LYS:C	2.87	0.52
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.52
1:B:675:GLN:O	1:B:690:GLN:HG3	2.08	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.52
1:C:318:PHE:O	1:C:319:ARG:HG2	2.10	0.52
1:A:328:ARG:HD3	1:A:578:ASP:OD1	2.09	0.52
1:A:524:VAL:C	1:A:525:CYS:SG	2.93	0.52
1:C:1101:HIS:CD2	3:X:1:NAG:H5	2.45	0.52
1:B:536:ASN:O	1:B:537:LYS:HG2	2.09	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
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
1:B:310:LYS:CB	1:B:310:LYS:NZ	2.73	0.52
1:A:694:ALA:O	1:A:695:TYR:HB3	2.10	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:B:390:LEU:HD22	1:B:517:LEU:HD12	1.92	0.52
1:C:403:ARG:NH1	1:C:505:TYR:CD1	2.78	0.52
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.52
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:A:319:ARG:NH2	1:A:319:ARG:CG	2.73	0.51
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.51
1:A:493:GLN:OE1	2:D:34:HIS:HB3	2.10	0.51
1:A:745:ASP:HB2	1:C:319:ARG:HH12	1.75	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:B:524:VAL:C	1:B:525:CYS:SG	2.93	0.51
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.51
1:C:319:ARG:CG	1:C:319:ARG:NH2	2.73	0.51
1:C:324:GLU:O	1:C:539:VAL:HG23	2.11	0.51
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
1:A:505:TYR:CE2	2:D:354:GLY:HA3	2.45	0.51
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.51
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.51
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	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
1:C:325:SER:HB2	1:C:540:ASN:HB3	1.93	0.51
1:A:41:LYS:CD	1:A:41:LYS:N	2.73	0.51
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51
1:A:854:LYS:O	1:A:854:LYS:HG2	2.11	0.51
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.51
1:C:285:ILE:HG22	1:C:286:THR:N	2.25	0.51
1:B:328:ARG:HH11	1:B:533:LEU:HD22	1.75	0.51
1:C:335:LEU:N	1:C:335:LEU:CD1	2.73	0.51
1:A:41:LYS:CA	1:C:519:HIS:HE1	2.24	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.51
1:A:705:VAL:HB	1:B:883:THR:HG21	1.93	0.51
1:B:321:GLN:OE1	1:B:322:PRO:HD2	2.10	0.51
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.76	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.50
1:B:326:ILE:CG2	1:B:541:PHE:CB	2.90	0.50
1:B:550:GLY:HA2	1:B:590:CYS:SG	2.52	0.50
1:B:367:VAL:CG2	4:B:1407:NAG:C8	2.55	0.50
1:A:41:LYS:HA	1:C:563:GLN:HG2	1.90	0.50
1:C:327:VAL:HG11	1:C:528:LYS:HE2	1.94	0.50
1:C:329:PHE:CE2	1:C:528:LYS:CD	2.91	0.50
1:C:674:TYR:CD1	1:C:691:SER:O	2.64	0.50
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.11	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.50
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.50
3:P:1:NAG:H62	3:P:2:NAG:H2	1.93	0.50
1:A:502:GLY:O	1:A:505:TYR:HB2	2.12	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.50
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.49
1:B:316:SER:OG	1:B:317:ASN:N	2.44	0.49
1:B:329:PHE:HE2	1:B:528:LYS:HG3	1.76	0.49
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.49
1:A:977:LEU:O	1:A:981:LEU:HG	2.12	0.49
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:517:LEU:HD22	1:C:983:ARG:CD	2.41	0.49
1:B:520:ALA:CB	1:B:521:PRO:CD	2.85	0.49
1:C:535:LYS:CD	1:C:554:GLU:OE2	2.60	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
1:C:318:PHE:O	1:C:319:ARG:HB2	2.12	0.49
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LYS:C	1:B:529:LYS:CE	2.85	0.49
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
1:B:367:VAL:HG21	4:B:1407:NAG:H81	1.90	0.49
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.49
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.49
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.76	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:C:122:ASN:OD1	1:C:122:ASN:N	2.46	0.49
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
1:A:334:ASN:O	1:A:362:VAL:CB	2.56	0.49
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:B:335:LEU:C	1:B:362:VAL:O	2.55	0.49
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.49
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.49
1:A:335:LEU:C	1:A:362:VAL:O	2.56	0.48
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:B:524:VAL:HG22	1:B:525:CYS:N	2.27	0.48
1:B:675:GLN:HB3	1:B:693:ILE:CD1	2.42	0.48
1:C:41:LYS:N	1:C:41:LYS:CD	2.73	0.48
1:A:41:LYS:CD	1:C:562:PHE:CE2	2.78	0.48
1:A:41:LYS:HB2	1:C:519:HIS:CE1	2.47	0.48
1:C:552:LEU:HD23	1:C:587:ILE:HG12	1.96	0.48
1:B:517:LEU:HD21	1:C:983:ARG:NE	2.24	0.48
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.76	0.48
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.48
1:A:978:ASN:HD22	1:C:547:THR:HG22	1.77	0.48
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.48
1:C:328:ARG:NH2	1:C:543:PHE:HZ	2.03	0.48
1:A:335:LEU:HD12	1:A:335:LEU:H	1.78	0.48
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:A:533:LEU:HD21	1:A:535:LYS:CE	2.34	0.48
1:A:538:CYS:HG	1:A:590:CYS:CB	2.20	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:C:576:VAL:CG2	1:C:587:ILE:HD11	2.43	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLN:O	1:A:690:GLN:NE2	2.35	0.48
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.48
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.48
1:A:563:GLN:CD	1:B:43:PHE:HA	2.39	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.48
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.48
1:B:557:LYS:HD2	1:C:43:PHE:HE2	1.78	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
1:B:544:ASN:HD21	1:B:564:GLN:HE22	1.61	0.48
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.48
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.47
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.47
1:C:361:CYS:O	1:C:524:VAL:HG23	2.13	0.47
1:A:524:VAL:HG22	1:A:525:CYS:N	2.27	0.47
1:B:560:LEU:O	1:B:562:PHE:N	2.47	0.47
1:C:318:PHE:CG	1:C:319:ARG:N	2.70	0.47
1:B:361:CYS:O	1:B:524:VAL:HG23	2.13	0.47
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.47
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.47
1:B:325:SER:O	1:B:325:SER:OG	2.29	0.47
1:B:326:ILE:CG2	1:B:541:PHE:HB3	2.45	0.47
1:B:392:PHE:HE2	1:B:517:LEU:CD1	2.16	0.47
1:B:566:GLY:HA2	1:C:43:PHE:HB3	1.96	0.47
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.47
1:A:486:PHE:HE1	2:D:79:LEU:CD1	2.27	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:B:367:VAL:HG22	4:B:1407:NAG:H83	1.82	0.47
1:C:328:ARG:NE	1:C:578:ASP:OD1	2.47	0.47
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	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:HD23	2.39	0.47
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.55	0.47
1:B:328:ARG:HA	1:B:530:SER:HB2	1.97	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:C:538:CYS:CB	1:C:590:CYS:HG	2.23	0.47
1:A:316:SER:C	1:A:317:ASN:ND2	2.73	0.47
1:A:653:ALA:HA	1:A:692:ILE:O	2.14	0.47
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HG13	1:C:47:VAL:CG1	2.28	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
3:b:2:NAG:C3	3:b:2:NAG:H83	2.45	0.47
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.47
1:B:327:VAL:O	1:B:530:SER:HA	2.14	0.47
1:B:517:LEU:CD1	1:C:983:ARG:HD3	2.45	0.47
1:B:562:PHE:CE2	1:C:41:LYS:HD2	2.50	0.47
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.47
1:C:535:LYS:O	1:C:536:ASN:HB2	2.15	0.47
1:C:696:THR:O	1:C:697:MET:C	2.56	0.47
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.47
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.47
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.46
1:B:562:PHE:HE2	1:C:41:LYS:HD2	1.79	0.46
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.50	0.46
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.46
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.98	0.46
1:C:281:GLU:N	1:C:281:GLU:CD	2.73	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.97	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:529:LYS:C	1:B:529:LYS:NZ	2.73	0.46
1:C:534:VAL:HG11	1:C:537:LYS:HZ2	1.81	0.46
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.46
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.46
1:A:388:ASN:CG	1:A:527:PRO:HD2	2.41	0.46
1:B:326:ILE:HD11	1:B:328:ARG:CD	2.45	0.46
1:B:367:VAL:HG23	4:B:1407:NAG:H83	1.82	0.46
1:B:385:THR:HG1	1:B:386:LYS:HZ3	1.59	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
1:B:328:ARG:O	1:B:329:PHE:CD1	2.69	0.46
1:A:983:ARG:O	1:A:984:LEU:CD2	2.60	0.46
1:B:327:VAL:O	1:B:530:SER:CA	2.64	0.46
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.46
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:B:390:LEU:CD2	1:B:517:LEU:HD11	2.45	0.46
1:C:41:LYS:N	1:C:41:LYS:HD3	2.31	0.46
1:C:531:THR:CG2	1:C:532:ASN:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:N	1:A:41:LYS:HD3	2.31	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.46
1:C:393:THR:HA	1:C:523:THR:HB	1.98	0.46
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.46
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.46
1:A:535:LYS:O	1:A:536:ASN:HB2	2.16	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.46
1:B:127:VAL:HG11	4:B:1402:NAG:H61	1.98	0.46
1:B:517:LEU:CD2	1:C:983:ARG:CD	2.93	0.46
1:C:322:PRO:O	1:C:324:GLU:N	2.49	0.46
1:C:326:ILE:C	1:C:327:VAL:HG23	2.41	0.46
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.46
1:B:390:LEU:CD2	1:B:517:LEU:CD1	2.94	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.45
2:D:105:SER:C	2:D:106:SER:HG	2.02	0.45
1:A:225:PRO:CG	1:C:562:PHE:CZ	3.00	0.45
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.45
1:A:505:TYR:CD2	2:D:353:LYS:C	2.93	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
1:B:338:PHE:C	1:B:340:GLU:N	2.75	0.45
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.45
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.45
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:325:SER:CB	1:C:540:ASN:HB3	2.47	0.45
1:C:590:CYS:O	1:C:592:PHE:HD1	2.00	0.45
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.45
1:A:127:VAL:HG11	4:A:1402:NAG:H61	1.98	0.45
1:A:325:SER:HB3	1:A:540:ASN:HB3	1.98	0.45
1:A:329:PHE:CD1	1:A:544:ASN:HA	2.52	0.45
1:A:338:PHE:C	1:A:340:GLU:N	2.75	0.45
1:A:476:GLY:HA2	2:D:24:GLN:NE2	2.26	0.45
1:A:486:PHE:CE1	2:D:79:LEU:HD21	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.45
1:B:587:ILE:O	1:B:587:ILE:HG22	2.17	0.45
1:C:646:ARG:HG3	1:C:646:ARG:O	2.17	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:C:328:ARG:HE	1:C:533:LEU:HD22	1.78	0.45
1:C:527:PRO:HG2	1:C:528:LYS:H	1.82	0.45
1:A:316:SER:OG	1:A:317:ASN:N	2.48	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:B:614:ASP:OD2	1:C:854:LYS:HD2	2.16	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
1:A:854:LYS:O	1:A:855:PHE:CD1	2.70	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
1:C:127:VAL:HG11	4:C:1402:NAG:H61	1.98	0.45
1:C:323:THR:HG21	1:C:537:LYS:HE2	1.99	0.45
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:A:529:LYS:NZ	1:A:529:LYS:CA	2.73	0.44
1:A:565:PHE:CZ	1:B:42:VAL:CG2	2.99	0.44
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.44
1:A:984:LEU:HD22	1:A:984:LEU:HA	1.80	0.44
1:C:279:TYR:HA	1:C:285:ILE:HA	1.98	0.44
1:C:317:ASN:N	1:C:317:ASN:ND2	2.65	0.44
1:C:333:THR:CG2	1:C:334:ASN:H	2.06	0.44
1:C:537:LYS:NZ	1:C:537:LYS:CB	2.80	0.44
2:D:431:ASP:OD1	2:D:431:ASP:N	2.44	0.44
1:B:326:ILE:HG22	1:B:541:PHE:HB3	1.98	0.44
1:B:326:ILE:C	1:B:327:VAL:HG23	2.43	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:C:535:LYS:HG3	1:C:552:LEU:O	2.17	0.44
1:A:225:PRO:HG2	1:C:562:PHE:CE1	2.52	0.44
1:B:328:ARG:NH1	1:B:533:LEU:HD22	2.32	0.44
1:B:518:LEU:O	1:B:519:HIS:CG	2.71	0.44
1:C:43:PHE:HZ	1:C:282:ASN:O	2.00	0.44
1:C:333:THR:C	1:C:334:ASN:HD22	2.25	0.44
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HA	1:C:563:GLN:CG	2.47	0.44
1:A:538:CYS:SG	1:A:590:CYS:CB	3.05	0.44
1:A:856:ASN:OD1	1:A:856:ASN:N	2.50	0.44
1:B:322:PRO:HB3	1:B:538:CYS:SG	2.57	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.44
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.44
1:C:334:ASN:ND2	1:C:361:CYS:HA	2.33	0.44
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.44
1:B:383:SER:OG	1:C:985:ASP:OD2	2.32	0.44
1:B:392:PHE:CE2	1:B:517:LEU:CA	3.01	0.44
1:C:536:ASN:C	1:C:551:VAL:HG13	2.40	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.44
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:C:322:PRO:HA	1:C:538:CYS:C	2.41	0.44
1:C:527:PRO:O	1:C:528:LYS:HB2	2.16	0.44
1:A:493:GLN:OE1	2:D:34:HIS:CG	2.70	0.43
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.43
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.00	0.43
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.43
1:B:127:VAL:HG21	4:B:1402:NAG:H5	2.01	0.43
1:B:592:PHE:CD1	1:B:592:PHE:O	2.71	0.43
4:B:1411:NAG:O4	4:B:1412:NAG:O5	2.28	0.43
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
1:A:979:ASP:O	1:A:983:ARG:CG	2.60	0.43
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.43
1:B:334:ASN:ND2	1:B:334:ASN:N	2.60	0.43
1:C:316:SER:C	1:C:317:ASN:CG	2.86	0.43
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.43
3:S:1:NAG:H61	3:S:2:NAG:N2	2.33	0.43
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:B:986:PRO:CB	1:B:987:PRO:HD3	2.45	0.43
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.43
1:C:323:THR:HG22	1:C:324:GLU:HG2	2.01	0.43
1:C:393:THR:O	1:C:523:THR:CG2	2.58	0.43
1:C:590:CYS:O	1:C:592:PHE:CD1	2.70	0.43
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.43
1:A:325:SER:CB	1:A:540:ASN:O	2.65	0.43
1:A:390:LEU:O	1:A:525:CYS:HB3	2.18	0.43
1:A:535:LYS:O	1:A:536:ASN:CB	2.66	0.43
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.99	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:B:324:GLU:O	1:B:539:VAL:HG23	2.16	0.43
1:B:987:PRO:HG3	1:C:427:ASP:OD2	2.18	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:C:552:LEU:CD2	1:C:587:ILE:HG12	2.48	0.43
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.43
1:A:703:ASN:HB2	1:B:787:GLN:CD	2.26	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.43
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.78	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.43
1:B:557:LYS:HD2	1:C:43:PHE:CE2	2.53	0.43
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.43
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.43
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.43
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.43
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.43
3:F:1:NAG:H61	3:F:2:NAG:N2	2.33	0.43
1:B:546:LEU:HD11	1:B:565:PHE:CG	2.53	0.43
1:C:285:ILE:CG2	1:C:286:THR:N	2.81	0.43
1:C:333:THR:CG2	1:C:361:CYS:O	2.45	0.43
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.43
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.42
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.42
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42
1:B:332:ILE:CG2	1:B:362:VAL:HG21	2.48	0.42
1:B:517:LEU:HD11	1:C:983:ARG:HD3	1.99	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:502:GLY:HA3	2:D:354:GLY:O	2.20	0.42
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.42
1:A:41:LYS:HA	1:C:562:PHE:CE2	2.54	0.42
1:B:524:VAL:CG2	1:B:525:CYS:N	2.83	0.42
1:B:662:CYS:HB2	1:B:697:MET:CE	2.48	0.42
1:C:317:ASN:HB3	1:C:593:GLY:O	2.20	0.42
1:A:565:PHE:O	1:B:43:PHE:N	2.53	0.42
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.42
1:B:390:LEU:O	1:B:525:CYS:HB3	2.18	0.42
1:B:392:PHE:HD2	1:B:517:LEU:CA	2.08	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:C:127:VAL:HG21	4:C:1402:NAG:H5	2.01	0.42
1:C:529:LYS:HD3	1:C:529:LYS:HA	1.80	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.42
1:A:982:SER:OG	1:A:983:ARG:N	2.53	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:C:654:GLU:CG	1:C:693:ILE:HG22	2.12	0.42
3:T:1:NAG:H3	3:T:1:NAG:H83	2.02	0.42
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.42
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.42
1:A:690:GLN:HB2	1:A:691:SER:H	1.69	0.42
1:B:516:GLU:C	1:B:518:LEU:H	2.27	0.42
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.42
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.42
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:319:ARG:HH22	1:C:740:MET:CG	2.33	0.42
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.42
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.42
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.42
3:b:2:NAG:H83	3:b:2:NAG:H3	2.02	0.42
1:A:326:ILE:HD13	1:A:534:VAL:H	1.85	0.41
1:A:524:VAL:CG2	1:A:525:CYS:N	2.83	0.41
1:A:529:LYS:HE2	1:A:529:LYS:CA	2.45	0.41
1:A:674:TYR:CD1	1:A:691:SER:O	2.73	0.41
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.41
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.55	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ASN:OD1	1:C:564:GLN:NE2	2.44	0.41
1:C:735:SER:OG	1:C:859:THR:HG22	2.17	0.41
1:A:699:LEU:HD12	1:B:872:GLN:CD	2.45	0.41
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.41
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.41
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.41
1:B:325:SER:O	1:B:327:VAL:HG23	2.19	0.41
1:B:517:LEU:HD13	1:C:983:ARG:HD2	2.00	0.41
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.41
1:C:325:SER:HB2	1:C:540:ASN:O	2.20	0.41
1:C:392:PHE:CA	1:C:517:LEU:HD21	2.49	0.41
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.41
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:864:LEU:HD13	1:C:665:PRO:CB	2.50	0.41
1:B:307:THR:HA	1:B:602:THR:OG1	2.20	0.41
1:C:406:GLU:CG	1:C:418:ILE:HG13	2.50	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.41
1:B:48:LEU:H	1:B:48:LEU:CD1	2.32	0.41
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.41
1:C:521:PRO:O	1:C:522:ALA:CB	2.66	0.41
1:A:127:VAL:HG21	4:A:1402:NAG:H5	2.01	0.41
1:A:654:GLU:O	1:A:693:ILE:CA	2.69	0.41
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:B:535:LYS:O	1:B:537:LYS:HG3	2.20	0.41
1:B:536:ASN:C	1:B:537:LYS:HG2	2.45	0.41
1:C:740:MET:HE2	1:C:740:MET:HB2	1.91	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
3:b:1:NAG:C3	3:b:2:NAG:N2	2.74	0.41
1:A:1123:SER:O	1:A:1123:SER:OG	2.39	0.41
1:B:386:LYS:NZ	1:C:985:ASP:HB3	2.20	0.41
1:C:45:SER:O	1:C:47:VAL:N	2.54	0.41
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
1:A:330:PRO:O	1:A:331:ASN:O	2.39	0.41
1:A:486:PHE:HE1	2:D:79:LEU:HD21	1.77	0.41
1:A:855:PHE:HB3	1:A:856:ASN:H	1.69	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.41
1:C:907:ASN:HD22	1:C:907:ASN:HA	1.64	0.41
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.91	0.41
1:A:371:SER:C	1:A:373:SER:H	2.29	0.41
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.41
2:D:21:ILE:HD12	2:D:21:ILE:HA	1.97	0.41
2:D:366:MET:HE3	2:D:366:MET:HB2	2.01	0.41
1:B:89:GLY:HA2	1:B:194:PHE:O	2.21	0.40
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.40
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.40
1:A:46:SER:C	1:A:47:VAL:HG13	2.46	0.40
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.40
1:A:864:LEU:HD13	1:C:665:PRO:HB2	2.04	0.40
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:392:PHE:CE2	1:B:517:LEU:CG	3.03	0.40
1:B:984:LEU:HD23	1:B:988:GLU:HB3	2.03	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:324:GLU:N	1:C:324:GLU:CD	2.73	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
1:A:89:GLY:HA2	1:A:194:PHE:O	2.22	0.40
1:A:213:VAL:HG23	1:A:214:ARG:N	2.36	0.40
1:A:505:TYR:CE2	2:D:353:LYS:O	2.73	0.40
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
1:C:46:SER:C	1:C:47:VAL:HG13	2.46	0.40
1:C:371:SER:C	1:C:373:SER:H	2.30	0.40
1:C:516:GLU:C	1:C:517:LEU:HD22	2.43	0.40
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.40
2:D:455:MET:HE3	2:D:455:MET:HB3	1.80	0.40
1:A:187:LYS:N	1:A:187:LYS:HE2	2.37	0.40
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.78	0.40
1:A:340:GLU:HG3	1:A:341:VAL:N	2.37	0.40
1:A:486:PHE:CE1	2:D:79:LEU:HD13	2.56	0.40
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40
1:B:187:LYS:N	1:B:187:LYS:HE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:O	1:A:47:VAL:N	2.54	0.40
1:A:708:SER:OG	1:A:711:SER:HB2	2.22	0.40
1:C:226:LEU:HB3	1:C:227:VAL:HG23	2.03	0.40
1:C:693:ILE:H	1:C:693:ILE:HG13	1.82	0.40
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	989/1283 (77%)	871 (88%)	92 (9%)	26 (3%)	4 23
1	B	951/1283 (74%)	826 (87%)	96 (10%)	29 (3%)	3 20
1	C	951/1283 (74%)	807 (85%)	101 (11%)	43 (4%)	2 13
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	36 65
All	All	3484/4666 (75%)	3067 (88%)	317 (9%)	100 (3%)	5 21

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	518	LEU
1	A	691	SER
1	A	701	ALA
1	A	855	PHE
1	B	48	LEU
1	B	333	THR
1	B	518	LEU
1	B	519	HIS

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Mol	Chain	Res	Type
1	B	520	ALA
1	C	48	LEU
1	C	323	THR
1	C	333	THR
1	C	334	ASN
1	C	518	LEU
1	C	526	GLY
1	C	532	ASN
1	C	814	LYS
1	A	41	LYS
1	A	46	SER
1	A	339	GLY
1	A	536	ASN
1	A	537	LYS
1	A	989	ALA
1	B	41	LYS
1	B	46	SER
1	B	339	GLY
1	B	526	GLY
1	B	534	VAL
1	B	742	ILE
1	B	743	CYS
1	C	41	LYS
1	C	46	SER
1	C	280	ASN
1	C	318	PHE
1	C	319	ARG
1	C	332	ILE
1	C	339	GLY
1	C	527	PRO
1	C	592	PHE
1	C	697	MET
1	C	810	SER
2	D	343	VAL
1	A	43	PHE
1	A	324	GLU
1	A	336	CYS
1	A	522	ALA
1	A	695	TYR
1	A	710	ASN
1	A	984	LEU
1	B	43	PHE

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Mol	Chain	Res	Type
1	B	521	PRO
1	C	43	PHE
1	C	316	SER
1	C	522	ALA
1	C	528	LYS
1	C	691	SER
2	D	423	LEU
1	A	44	ARG
1	A	349	SER
1	A	520	ALA
1	B	44	ARG
1	B	349	SER
1	B	517	LEU
1	B	522	ALA
1	B	592	PHE
1	B	746	SER
1	C	44	ARG
1	C	329	PHE
1	C	349	SER
1	C	520	ALA
1	C	529	LYS
1	C	533	LEU
1	C	591	SER
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	B	329	PHE
1	B	531	THR
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL
1	C	283	GLY
1	C	330	PRO
1	C	812	PRO
1	B	527	PRO
1	C	285	ILE
1	C	320	VAL
1	C	811	LYS

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Mol	Chain	Res	Type
1	B	332	ILE
1	B	336	CYS
1	B	327	VAL
1	C	327	VAL
1	C	534	VAL
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%)	762 (86%)	120 (14%)	3 16
1	B	850/1122 (76%)	743 (87%)	107 (13%)	4 18
1	C	850/1122 (76%)	740 (87%)	110 (13%)	4 17
2	D	525/721 (73%)	517 (98%)	8 (2%)	57 72
All	All	3107/4087 (76%)	2762 (89%)	345 (11%)	8 22

All (345) 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	66	HIS
1	A	81	ASN
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	171	VAL
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	231	ILE
1	A	282	ASN
1	A	289	VAL
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	319	ARG
1	A	324	GLU
1	A	332	ILE
1	A	333	THR
1	A	335	LEU
1	A	375	SER
1	A	382	VAL
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	403	ARG
1	A	406	GLU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	459	SER
1	A	469	SER
1	A	472	ILE
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	529	LYS
1	A	532	ASN
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR

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Mol	Chain	Res	Type
1	A	554	GLU
1	A	556	ASN
1	A	576	VAL
1	A	583	GLU
1	A	585	LEU
1	A	588	THR
1	A	590	CYS
1	A	591	SER
1	A	599	THR
1	A	602	THR
1	A	608	VAL
1	A	673	SER
1	A	692	ILE
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	705	VAL
1	A	719	THR
1	A	722	VAL
1	A	729	VAL
1	A	730	SER
1	A	738	CYS
1	A	746	SER
1	A	772	VAL
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	855	PHE
1	A	856	ASN
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	939	SER
1	A	951	VAL
1	A	960	ASN
1	A	967	SER
1	A	973	ILE

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Mol	Chain	Res	Type
1	A	976	VAL
1	A	984	LEU
1	A	991	VAL
1	A	994	ASP
1	A	998	THR
1	A	1005	GLN
1	A	1018	ILE
1	A	1039	ARG
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1114	ILE
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1142	GLN
1	A	1144	GLU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	66	HIS
1	B	81	ASN
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	171	VAL
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	231	ILE

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	289	VAL
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	320	VAL
1	B	324	GLU
1	B	326	ILE
1	B	328	ARG
1	B	329	PHE
1	B	332	ILE
1	B	333	THR
1	B	334	ASN
1	B	336	CYS
1	B	343	ASN
1	B	375	SER
1	B	382	VAL
1	B	383	SER
1	B	389	ASP
1	B	390	LEU
1	B	403	ARG
1	B	406	GLU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	500	THR
1	B	514	SER
1	B	515	PHE
1	B	516	GLU
1	B	518	LEU
1	B	519	HIS
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	533	LEU
1	B	535	LYS
1	B	540	ASN
1	B	546	LEU
1	B	553	THR

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Mol	Chain	Res	Type
1	B	554	GLU
1	B	556	ASN
1	B	564	GLN
1	B	576	VAL
1	B	583	GLU
1	B	585	LEU
1	B	591	SER
1	B	599	THR
1	B	602	THR
1	B	608	VAL
1	B	673	SER
1	B	710	ASN
1	B	729	VAL
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	772	VAL
1	B	779	GLN
1	B	787	GLN
1	B	791	THR
1	B	811	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	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	991	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1081	ILE
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS

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Mol	Chain	Res	Type
1	B	1133	VAL
1	B	1141	LEU
1	C	40	ASP
1	C	46	SER
1	C	48	LEU
1	C	66	HIS
1	C	81	ASN
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	141	LEU
1	C	143	VAL
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	171	VAL
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	231	ILE
1	C	278	LYS
1	C	281	GLU
1	C	284	THR
1	C	289	VAL
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	316	SER
1	C	317	ASN
1	C	319	ARG
1	C	320	VAL
1	C	324	GLU
1	C	328	ARG
1	C	334	ASN
1	C	335	LEU
1	C	375	SER
1	C	382	VAL

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Mol	Chain	Res	Type
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	403	ARG
1	C	406	GLU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	528	LYS
1	C	529	LYS
1	C	530	SER
1	C	533	LEU
1	C	534	VAL
1	C	535	LYS
1	C	537	LYS
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	564	GLN
1	C	576	VAL
1	C	583	GLU
1	C	585	LEU
1	C	588	THR
1	C	592	PHE
1	C	599	THR
1	C	602	THR
1	C	608	VAL
1	C	673	SER
1	C	693	ILE
1	C	696	THR
1	C	697	MET
1	C	699	LEU
1	C	727	LEU
1	C	768	THR
1	C	770	ILE

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Mol	Chain	Res	Type
1	C	778	THR
1	C	787	GLN
1	C	791	THR
1	C	814	LYS
1	C	856	ASN
1	C	878	LEU
1	C	907	ASN
1	C	922	LEU
1	C	929	SER
1	C	931	ILE
1	C	934	ILE
1	C	937	SER
1	C	968	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1018	ILE
1	C	1027	THR
1	C	1063	LEU
1	C	1077	THR
1	C	1092	GLU
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	339	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	317	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	450	ASN
1	A	487	ASN
1	A	498	GLN
1	A	556	ASN
1	A	580	GLN
1	A	613	GLN
1	A	644	GLN
1	A	658	ASN
1	A	675	GLN
1	A	703	ASN
1	A	755	GLN
1	A	762	GLN
1	A	787	GLN
1	A	901	GLN
1	A	914	ASN
1	A	926	GLN
1	A	949	GLN
1	A	969	ASN
1	A	978	ASN
1	A	992	GLN
1	A	1010	GLN
1	A	1054	GLN
1	A	1125	ASN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	317	ASN
1	B	334	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	450	ASN
1	B	498	GLN
1	B	542	ASN
1	B	556	ASN
1	B	564	GLN
1	B	613	GLN

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Mol	Chain	Res	Type
1	B	644	GLN
1	B	658	ASN
1	B	675	GLN
1	B	690	GLN
1	B	703	ASN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	920	GLN
1	B	926	GLN
1	B	949	GLN
1	B	957	GLN
1	B	960	ASN
1	B	992	GLN
1	B	1011	GLN
1	B	1083	HIS
1	B	1101	HIS
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	317	ASN
1	C	334	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	450	ASN
1	C	498	GLN
1	C	519	HIS
1	C	556	ASN
1	C	644	GLN
1	C	658	ASN
1	C	675	GLN
1	C	690	GLN
1	C	703	ASN
1	C	764	ASN
1	C	779	GLN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN

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Mol	Chain	Res	Type
1	C	926	GLN
1	C	935	GLN
1	C	992	GLN
1	C	1010	GLN
1	C	1011	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1125	ASN
2	D	24	GLN
2	D	58	ASN
2	D	63	ASN
2	D	89	GLN
2	D	96	GLN
2	D	117	ASN
2	D	121	ASN
2	D	175	GLN
2	D	277	ASN
2	D	300	GLN
2	D	417	HIS
2	D	472	GLN
2	D	508	ASN
2	D	572	ASN
2	D	586	ASN
2	D	599	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

52 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	E	1	1,3	14,14,15	0.53	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.61	0
3	NAG	F	1	1,3	14,14,15	0.56	0	17,19,21	0.58	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.47	0
3	NAG	G	1	1,3	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.48	0
3	NAG	H	1	1,3	14,14,15	0.37	0	17,19,21	0.74	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	1.40	2 (11%)
3	NAG	I	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	1.49	3 (17%)
3	NAG	J	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
3	NAG	J	2	3	14,14,15	0.29	0	17,19,21	0.68	0
3	NAG	K	1	1,3	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
3	NAG	K	2	3	14,14,15	0.16	0	17,19,21	0.50	0
3	NAG	L	1	1,3	14,14,15	0.52	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.61	0
3	NAG	M	1	1,3	14,14,15	0.31	0	17,19,21	0.42	0
3	NAG	M	2	3	14,14,15	0.39	0	17,19,21	0.38	0
3	NAG	N	1	1,3	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	O	1	1,3	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	P	1	1,3	14,14,15	0.71	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	P	2	3	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
3	NAG	Q	1	1,3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	Q	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	R	1	1,3	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	R	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	S	1	1,3	14,14,15	0.56	0	17,19,21	0.58	0
3	NAG	S	2	3	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	T	1	1,3	14,14,15	0.23	0	17,19,21	1.44	2 (11%)
3	NAG	T	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	U	1	1,3	14,14,15	0.51	0	17,19,21	0.73	1 (5%)
3	NAG	U	2	3	14,14,15	0.38	0	17,19,21	0.49	0
3	NAG	V	1	1,3	14,14,15	0.39	0	17,19,21	0.41	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.77	0
3	NAG	W	1	1,3	14,14,15	0.38	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	W	2	3	14,14,15	0.58	0	17,19,21	1.37	2 (11%)
3	NAG	X	1	1,3	14,14,15	0.60	0	17,19,21	0.45	0
3	NAG	X	2	3	14,14,15	0.35	0	17,19,21	1.44	2 (11%)
3	NAG	Y	1	1,3	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	Y	2	3	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	Z	1	3,2	14,14,15	0.59	1 (7%)	17,19,21	0.75	0
3	NAG	Z	2	3	14,14,15	0.55	0	17,19,21	0.38	0
3	NAG	a	1	3,2	14,14,15	0.41	0	17,19,21	0.67	0
3	NAG	a	2	3	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
3	NAG	b	1	3,2	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	b	2	3	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	c	1	3,2	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	c	2	3	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	d	1	3,2	14,14,15	0.23	0	17,19,21	0.63	0
3	NAG	d	2	3	14,14,15	0.36	0	17,19,21	0.60	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	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	6/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	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	-	6/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	3/6/23/26	0/1/1/1
3	NAG	c	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	NAG	d	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	-2.55	1.39	1.43
3	J	1	NAG	O5-C1	-2.42	1.39	1.43
3	I	1	NAG	O5-C1	-2.19	1.40	1.43
3	Z	1	NAG	O5-C1	-2.05	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	1	NAG	C2-N2-C7	4.98	129.57	122.90
3	I	2	NAG	C2-N2-C7	4.70	129.20	122.90
3	X	2	NAG	C2-N2-C7	4.65	129.13	122.90
3	H	2	NAG	C2-N2-C7	4.56	129.01	122.90
3	W	2	NAG	C2-N2-C7	4.51	128.95	122.90
3	N	1	NAG	C1-O5-C5	3.36	116.69	112.19
3	I	2	NAG	C1-C2-N2	2.64	114.60	110.43
3	H	2	NAG	C1-C2-N2	2.59	114.52	110.43
3	a	2	NAG	C1-O5-C5	2.49	115.52	112.19
3	X	2	NAG	C1-C2-N2	2.45	114.29	110.43
3	O	1	NAG	C1-O5-C5	2.35	115.33	112.19
3	U	1	NAG	C1-O5-C5	2.32	115.29	112.19
3	P	1	NAG	O4-C4-C3	-2.31	104.93	110.38
3	T	1	NAG	C1-C2-N2	2.16	113.84	110.43
3	K	1	NAG	C1-O5-C5	2.13	115.04	112.19
3	I	2	NAG	C1-O5-C5	2.09	114.99	112.19
3	P	2	NAG	C1-O5-C5	2.06	114.95	112.19
3	d	2	NAG	C1-O5-C5	2.06	114.95	112.19
3	W	2	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	b	2	NAG	C3-C2-N2-C7
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	T	2	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	a	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C1-C2-N2-C7
3	E	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7
3	P	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C1-C2-N2-C7
3	V	2	NAG	C1-C2-N2-C7
3	W	2	NAG	C1-C2-N2-C7
3	X	2	NAG	C1-C2-N2-C7
3	S	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	S	2	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

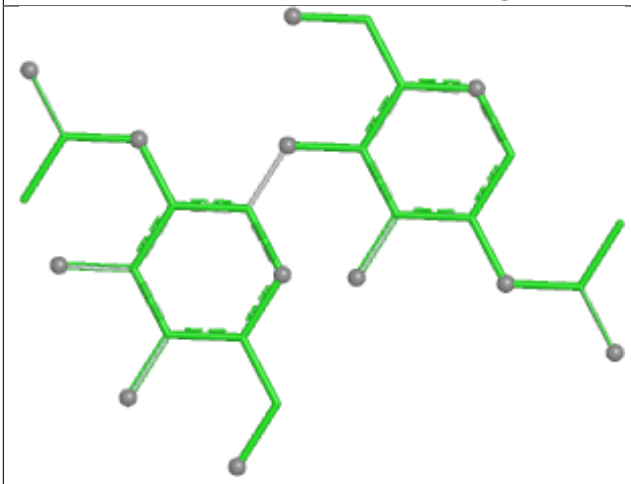
There are no ring outliers.

14 monomers are involved in 19 short contacts:

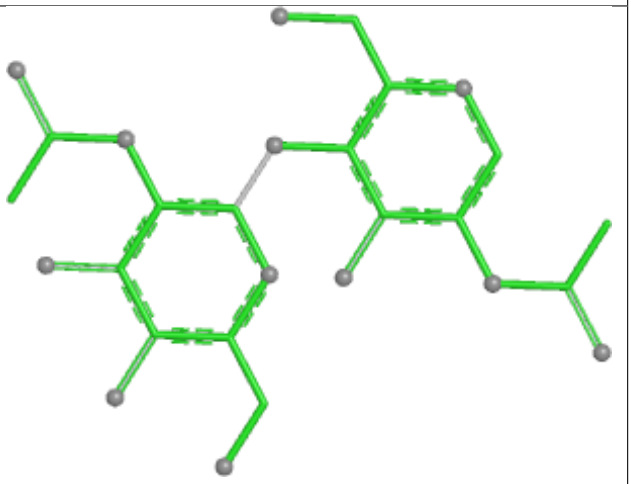
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
3	X	2	NAG	1	0
3	S	2	NAG	2	0
3	F	1	NAG	3	0
3	W	2	NAG	1	0
3	X	1	NAG	1	0
3	I	2	NAG	1	0
3	P	2	NAG	1	0
3	F	2	NAG	2	0
3	T	1	NAG	1	0
3	S	1	NAG	3	0
3	H	2	NAG	1	0
3	b	1	NAG	4	0
3	b	2	NAG	6	0

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

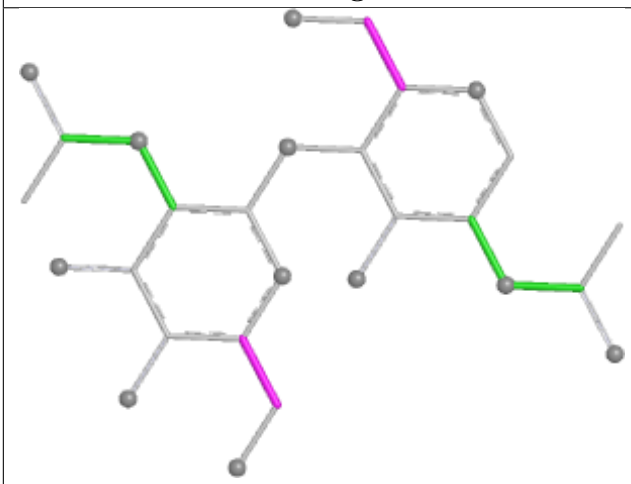
Oligosaccharide Chain E



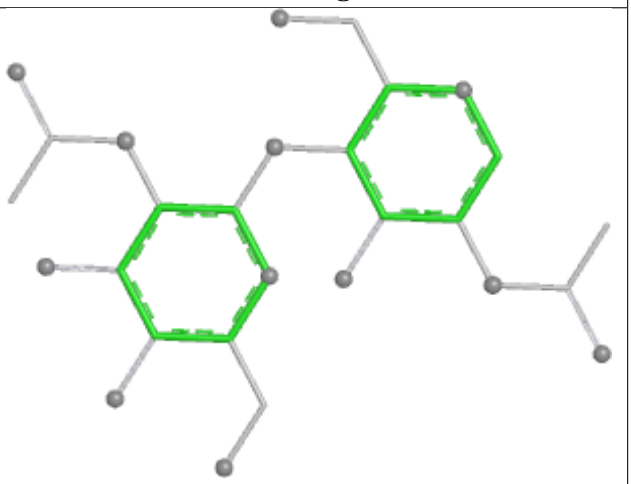
Bond lengths



Bond angles

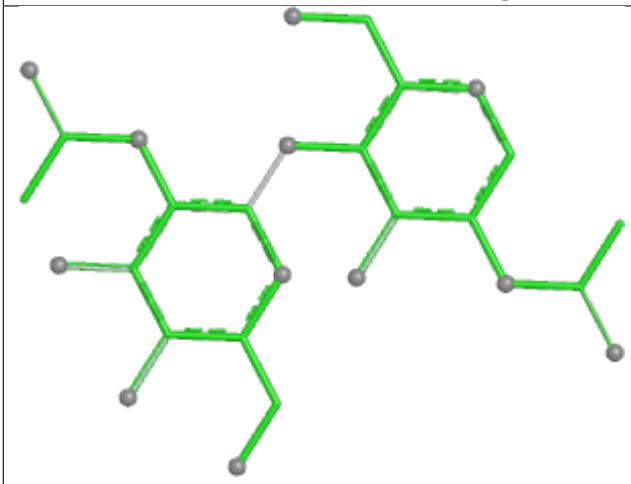


Torsions

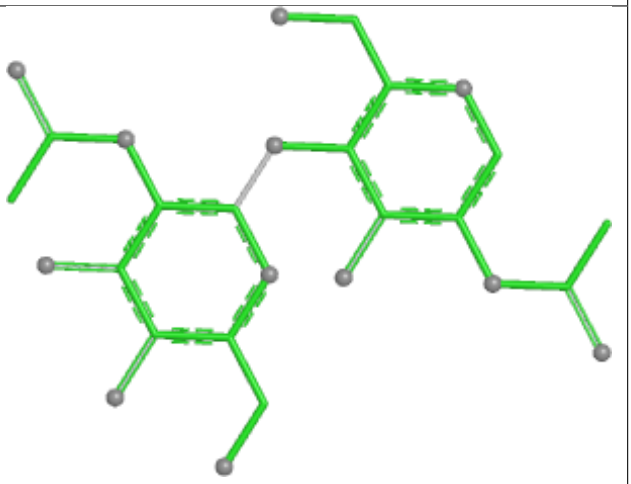


Rings

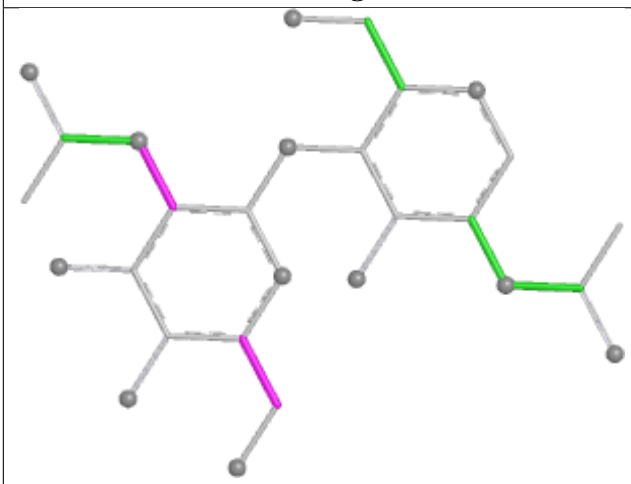
Oligosaccharide Chain F



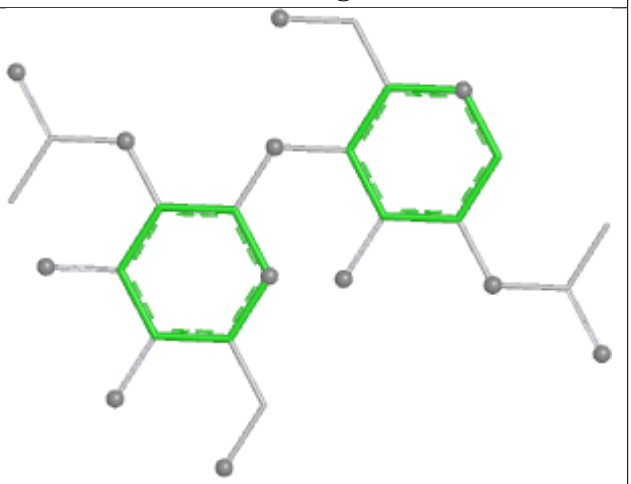
Bond lengths



Bond angles

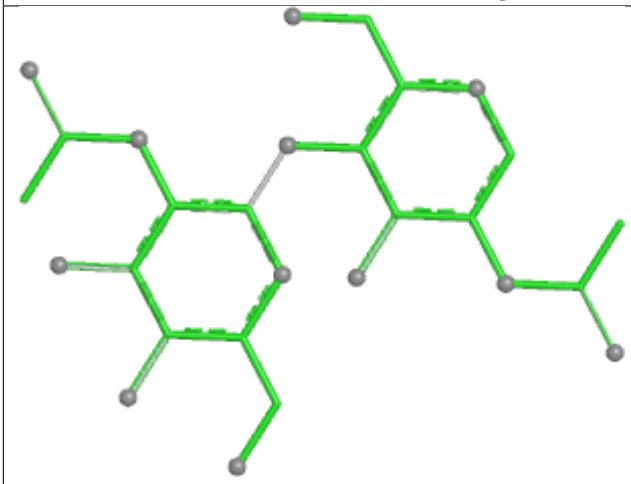


Torsions

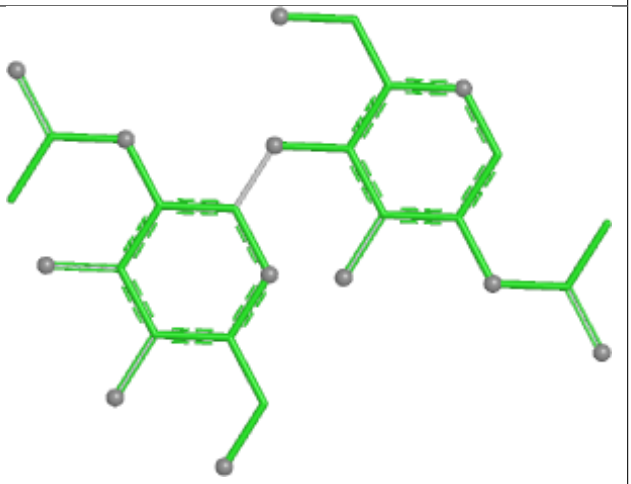


Rings

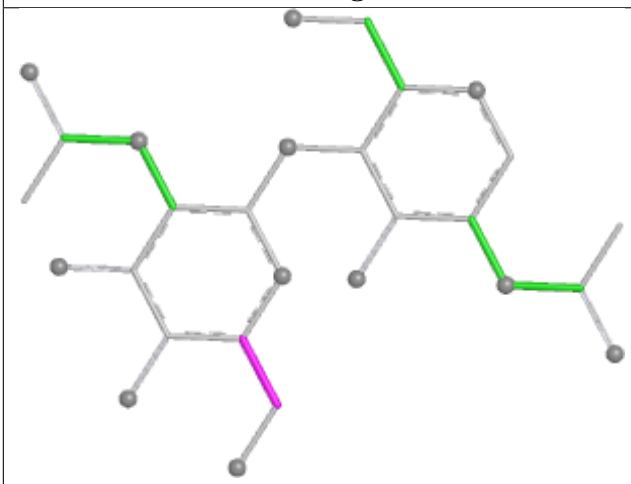
Oligosaccharide Chain G



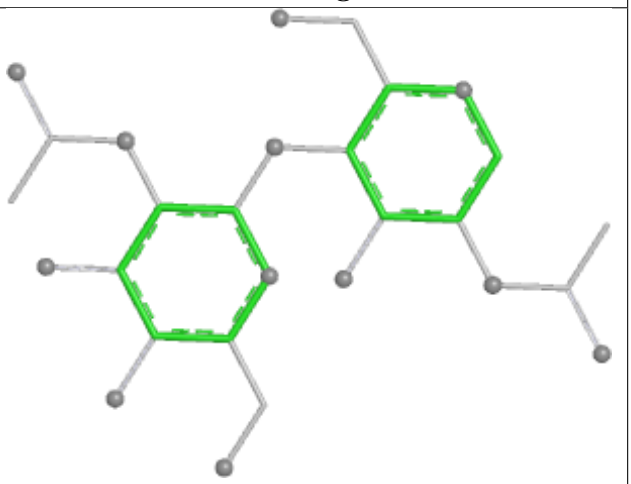
Bond lengths



Bond angles

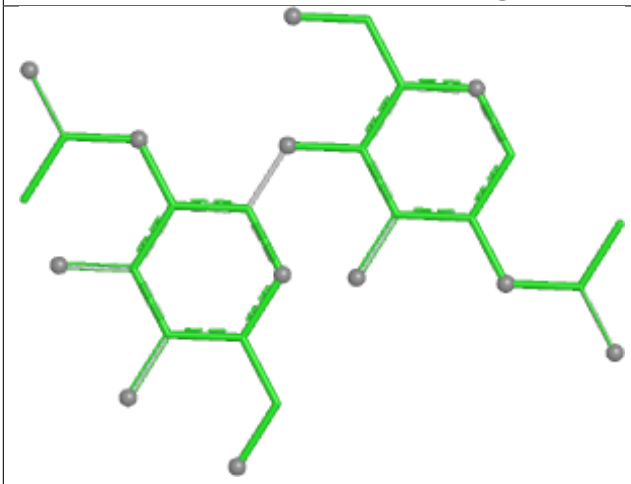


Torsions

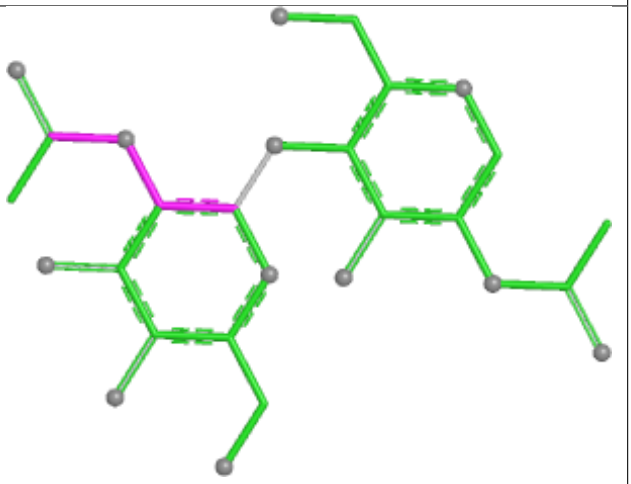


Rings

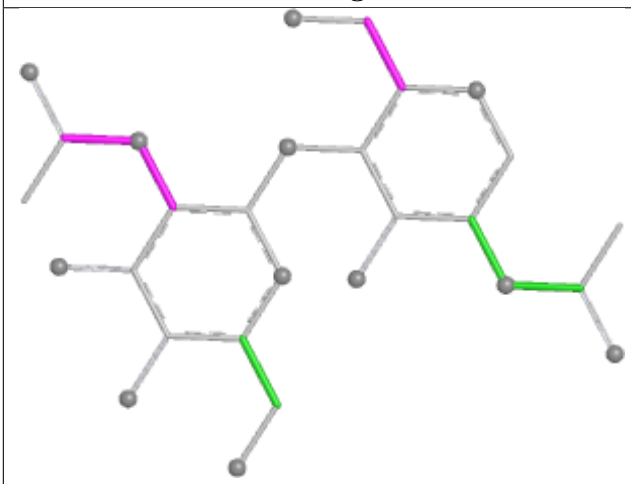
Oligosaccharide Chain H



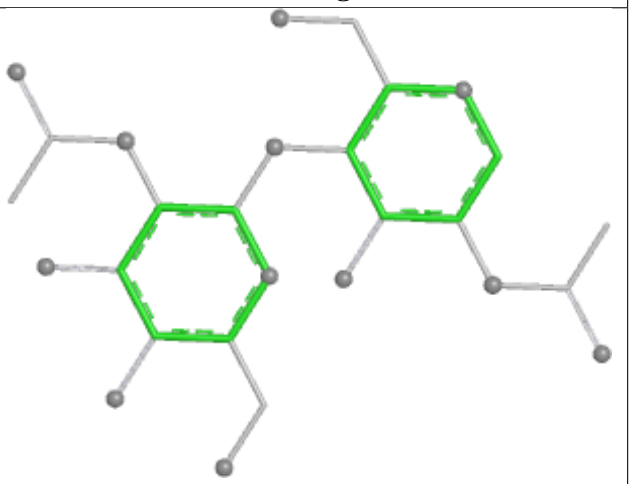
Bond lengths



Bond angles

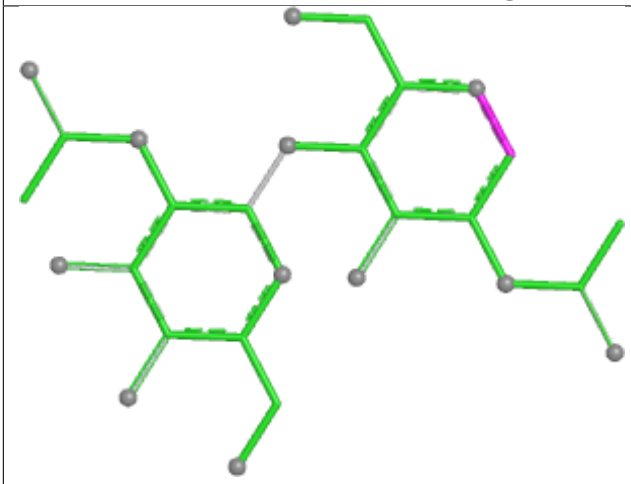


Torsions

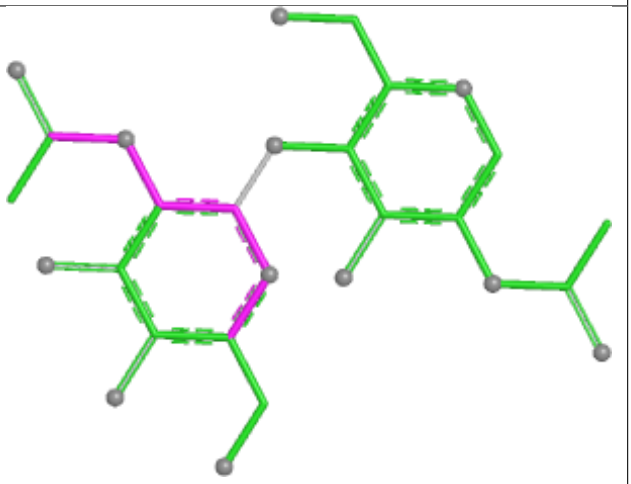


Rings

Oligosaccharide Chain I



Bond lengths



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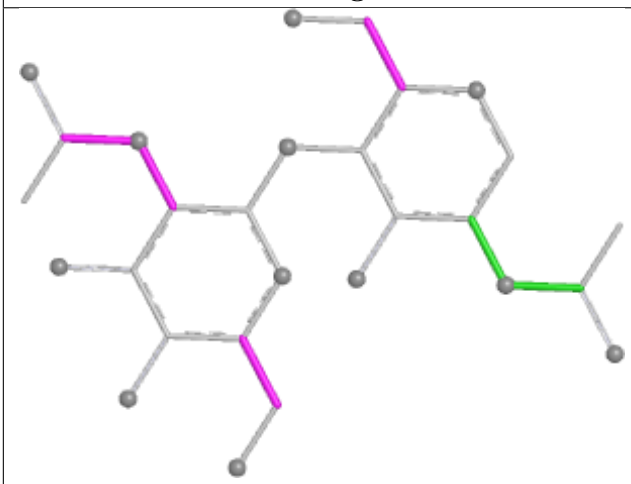
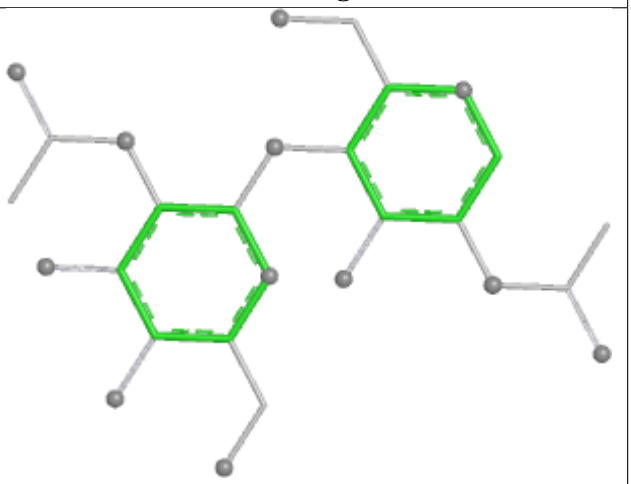
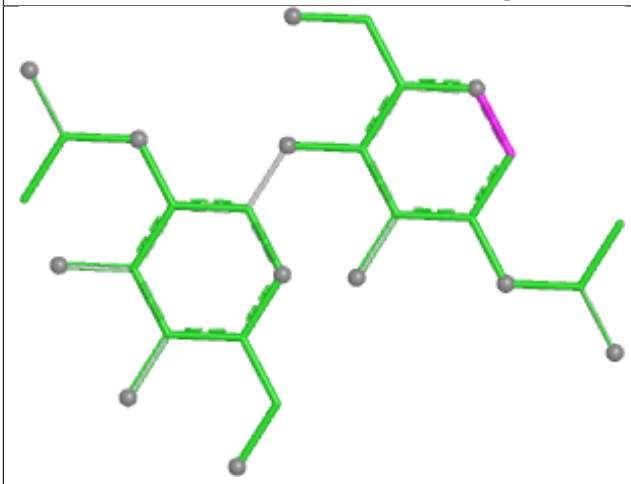


Torsions



Rings

Oligosaccharide Chain J



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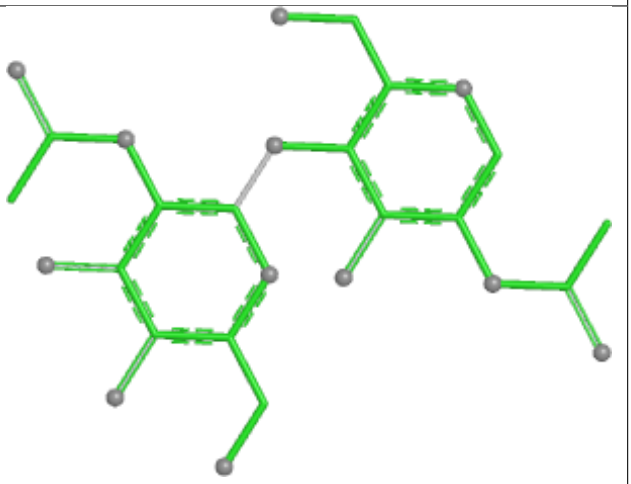

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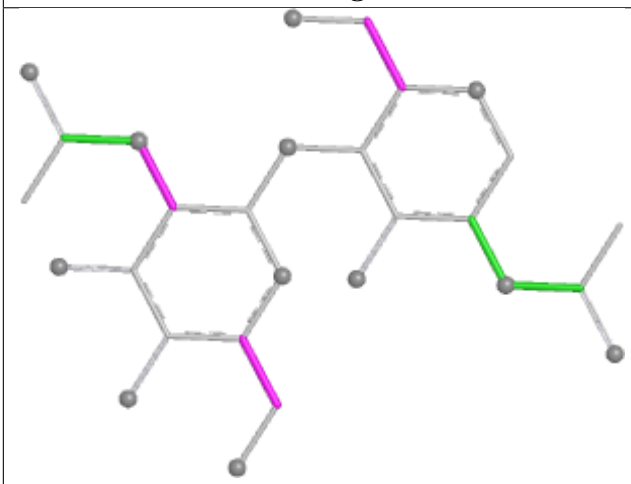

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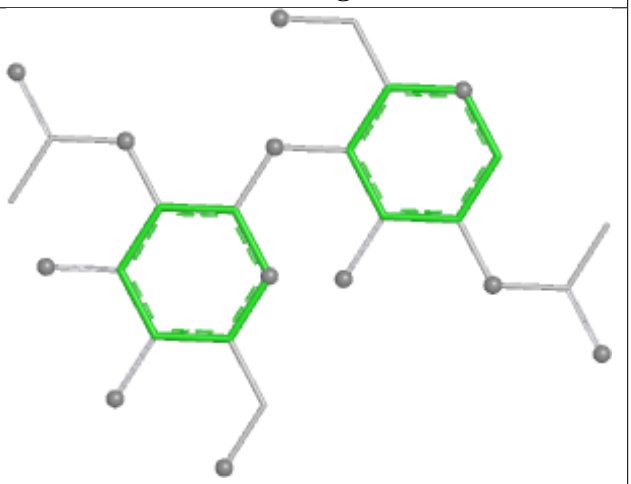
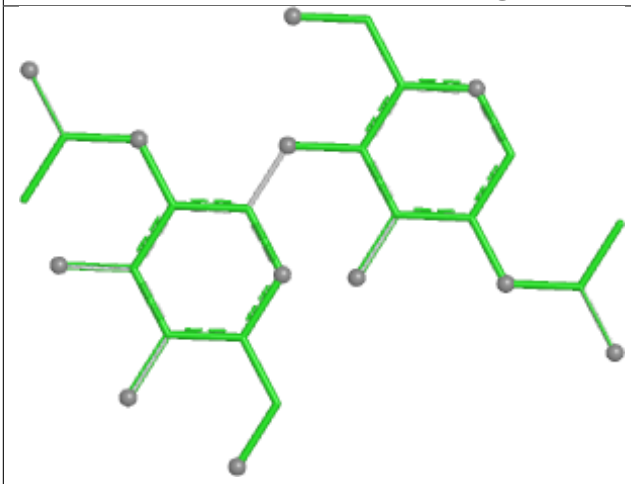


Rings

Oligosaccharide Chain K



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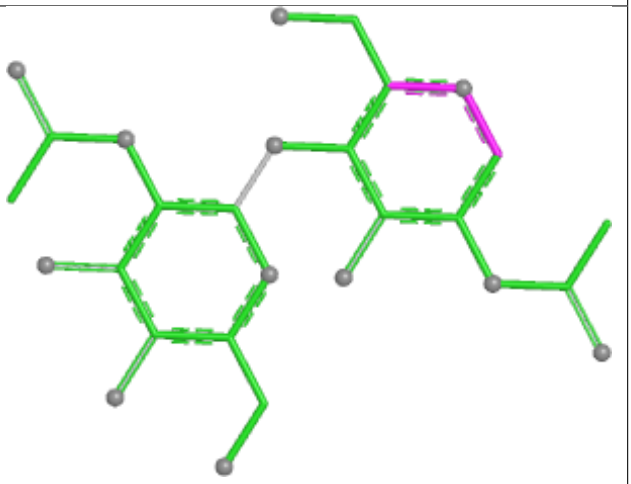
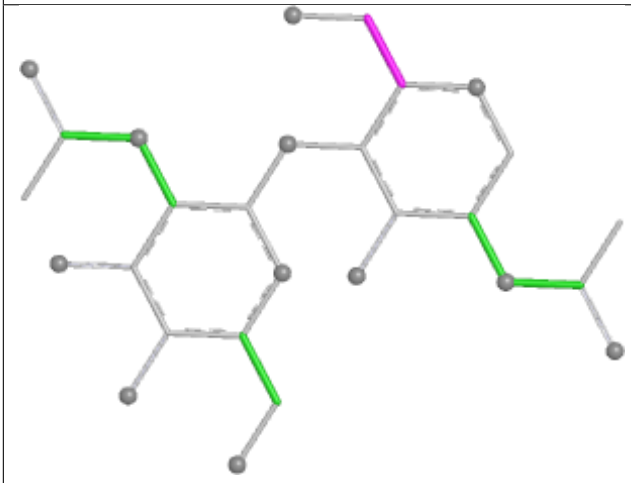


Bond angles



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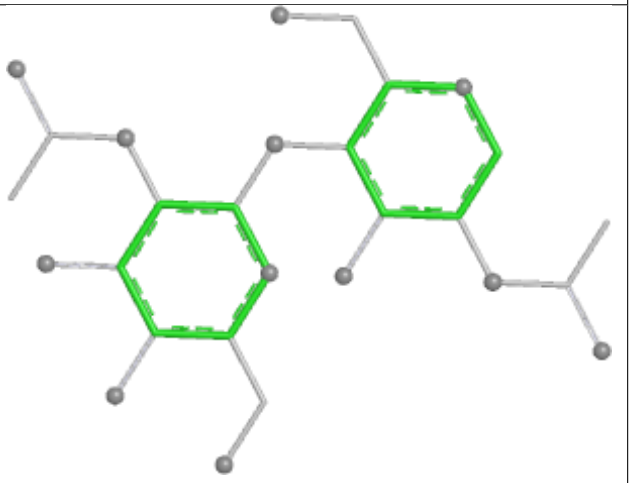
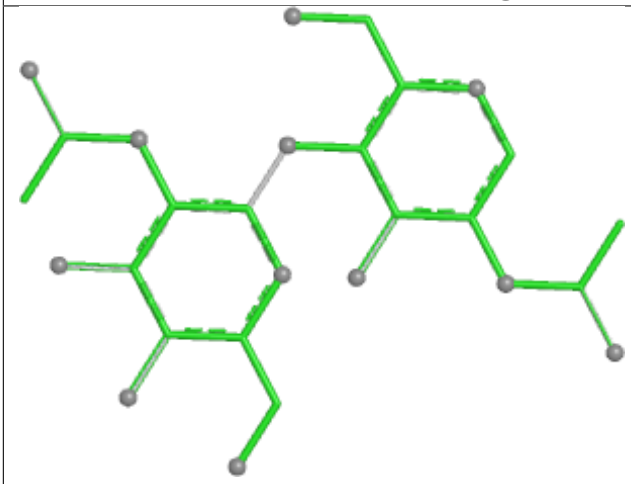


Rings

Oligosaccharide Chain L



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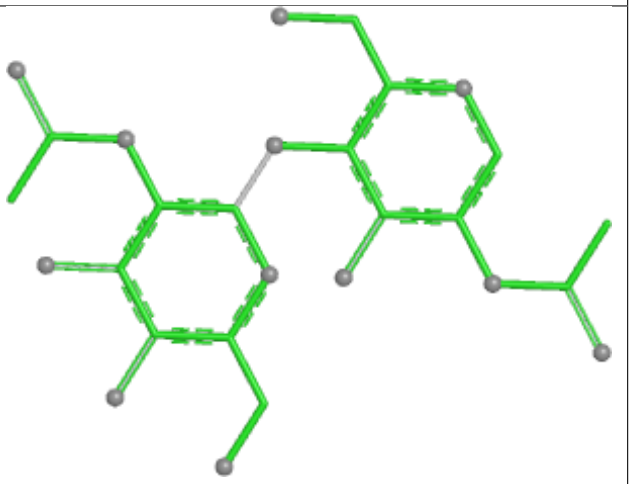
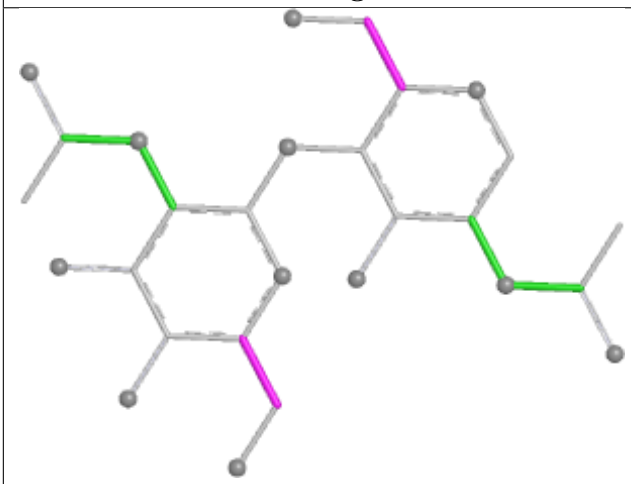


Bond angles



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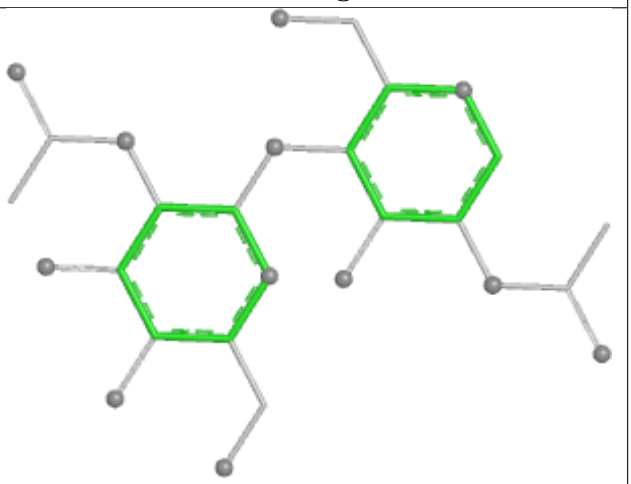
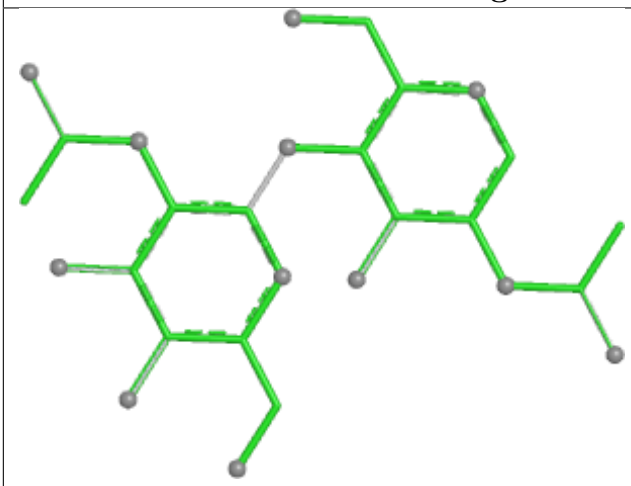


Rings

Oligosaccharide Chain M



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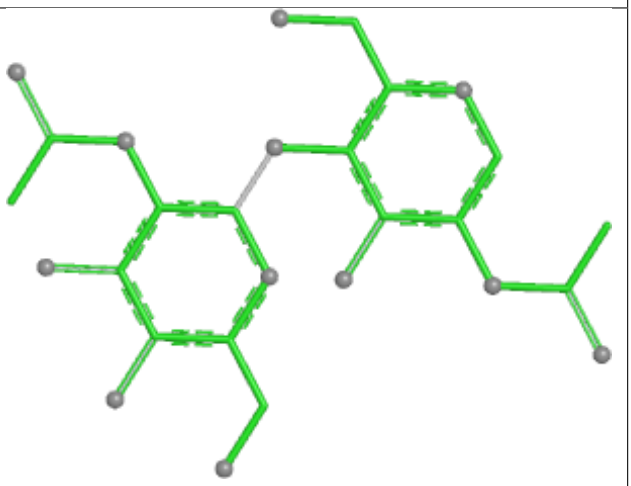
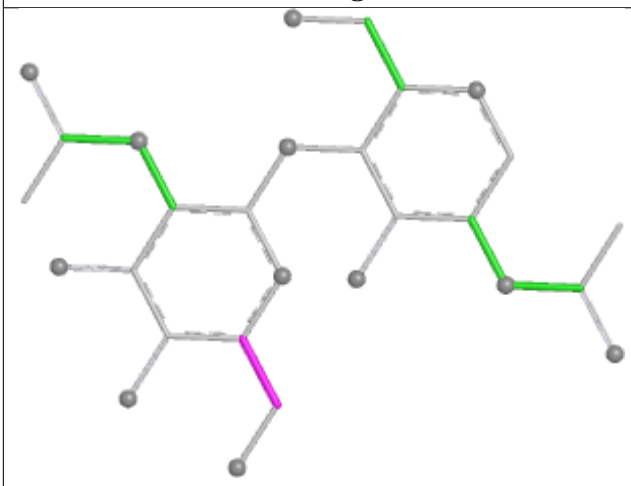
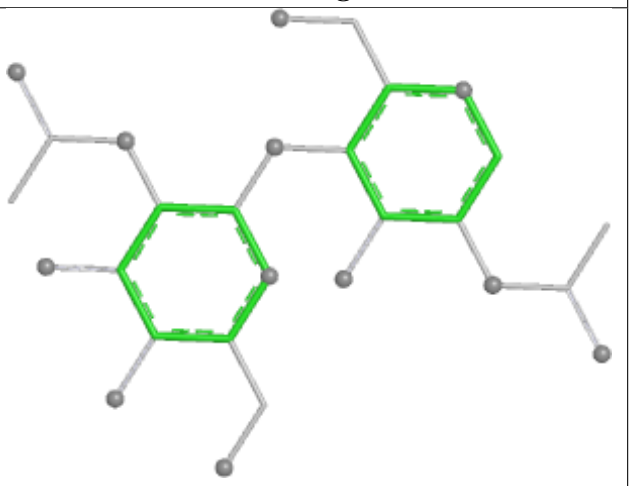


Bond angles

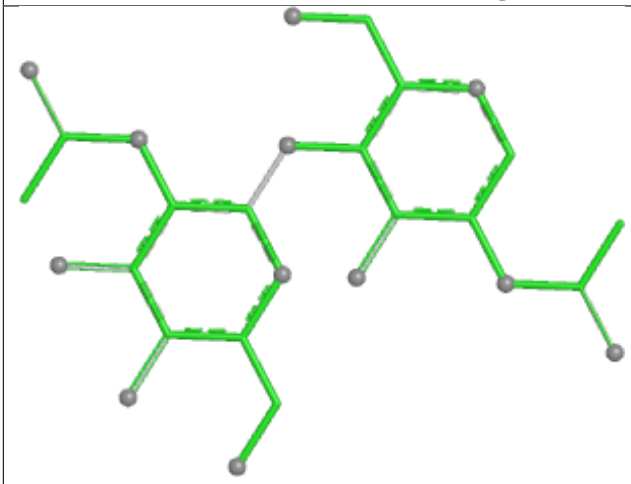


Torsions



Rings

Oligosaccharide Chain N



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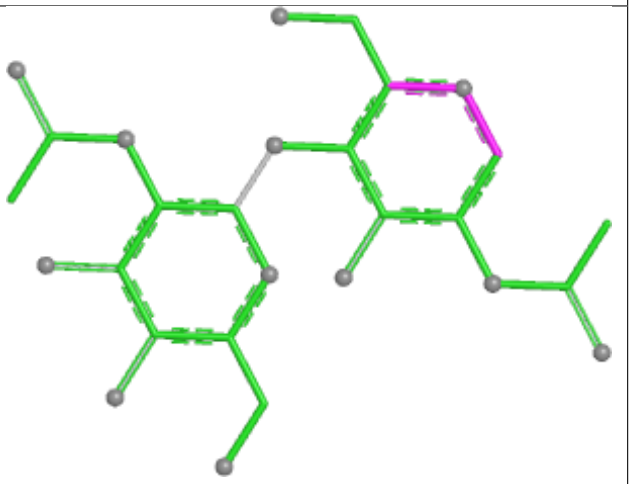

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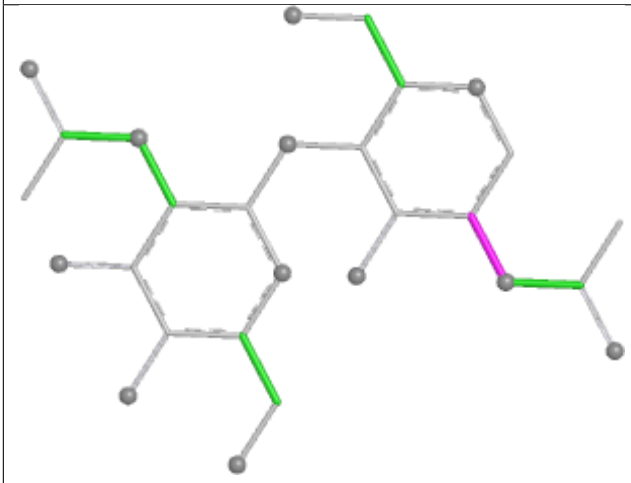

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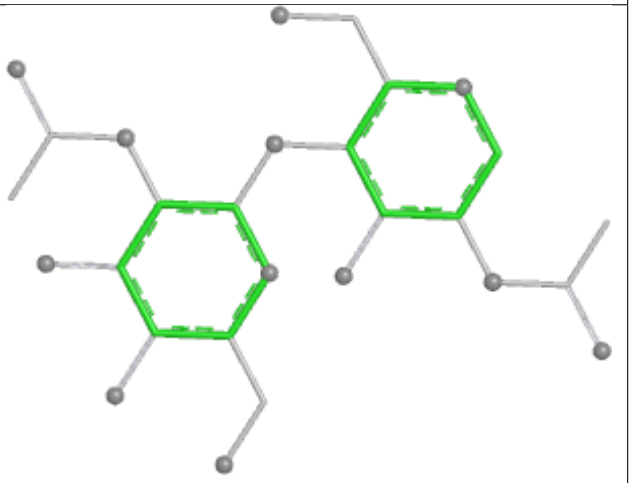
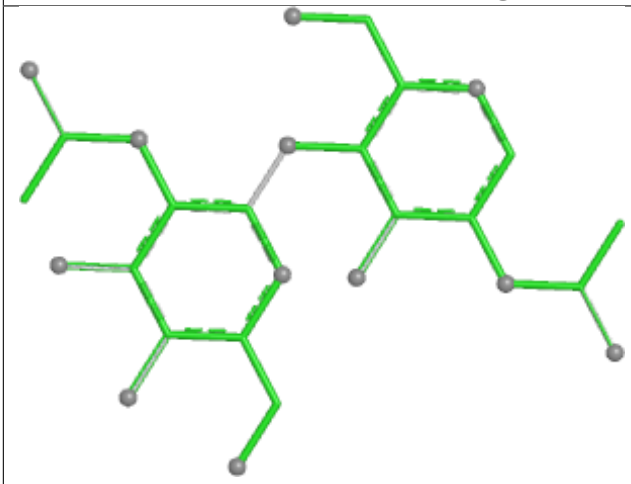


Rings

Oligosaccharide Chain O



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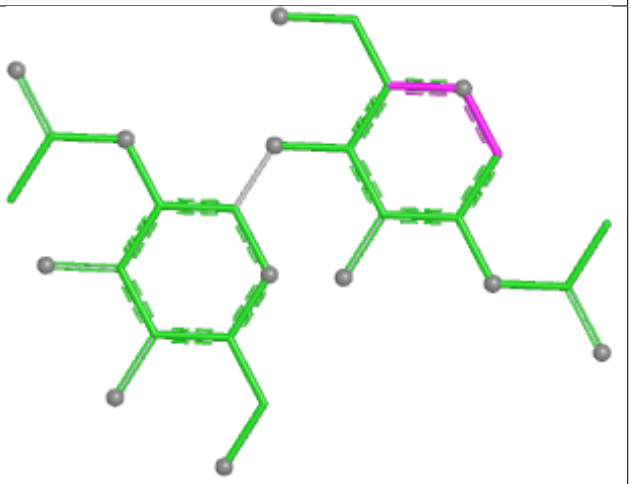

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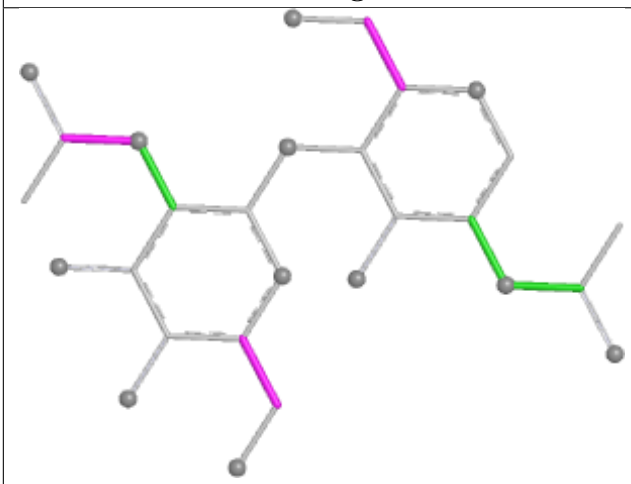

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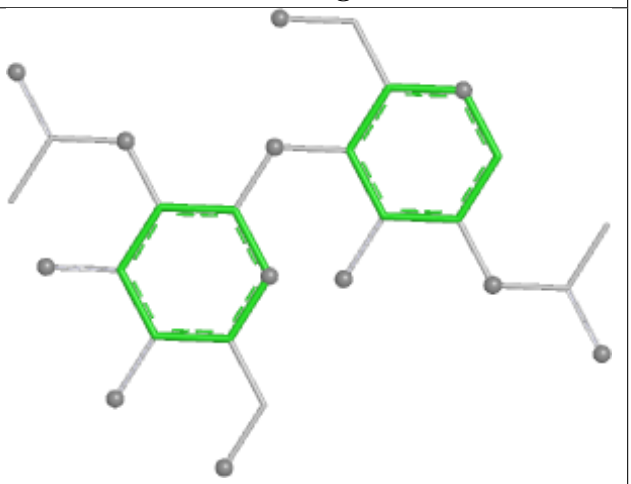
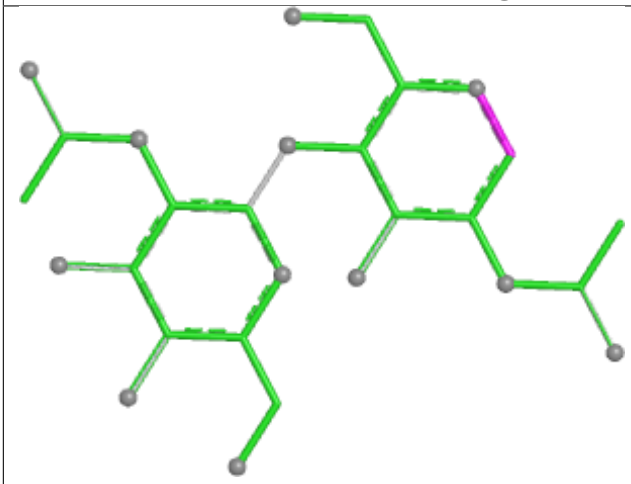


Rings

Oligosaccharide Chain P



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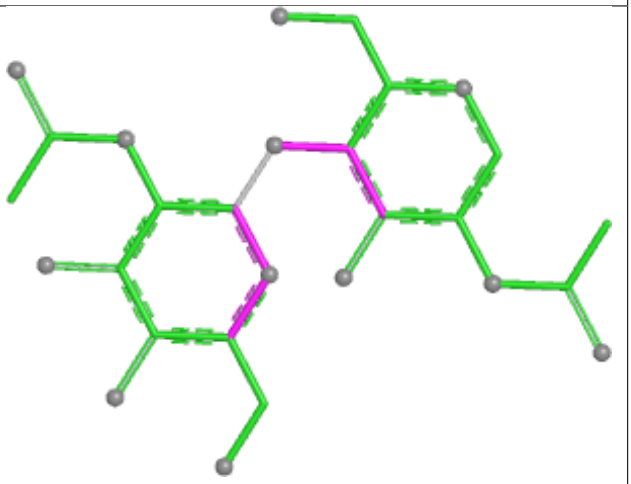
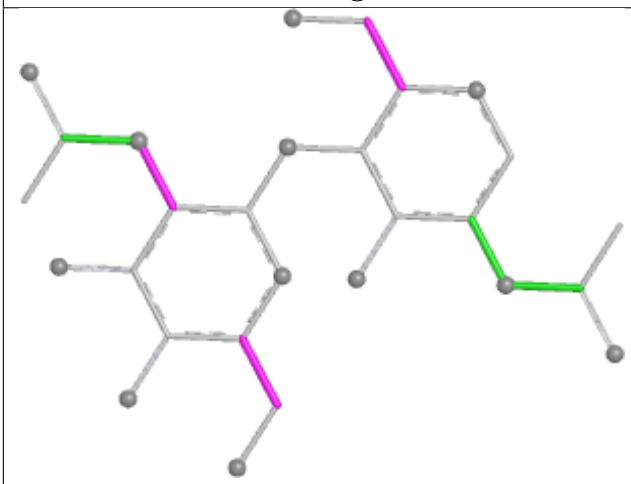


Bond angles



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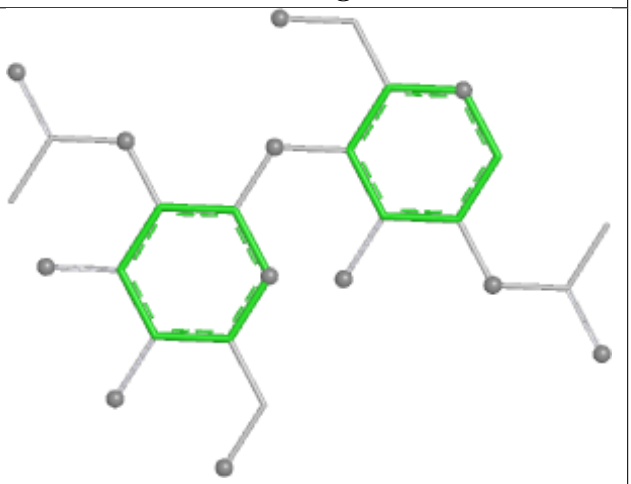
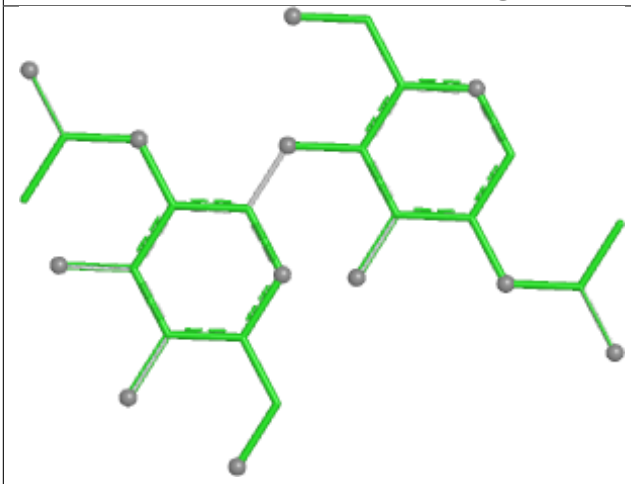
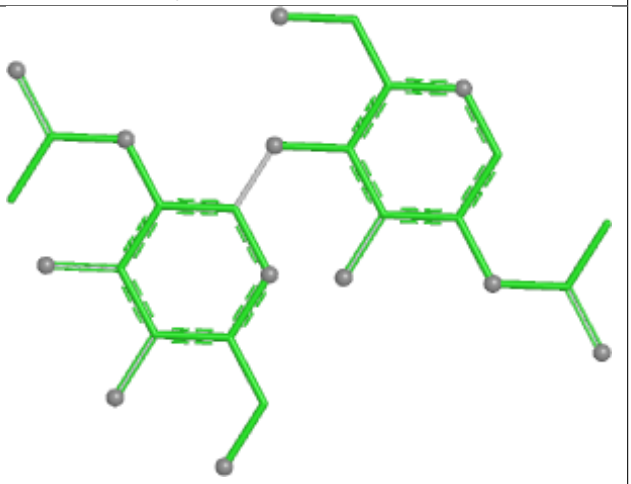


Rings

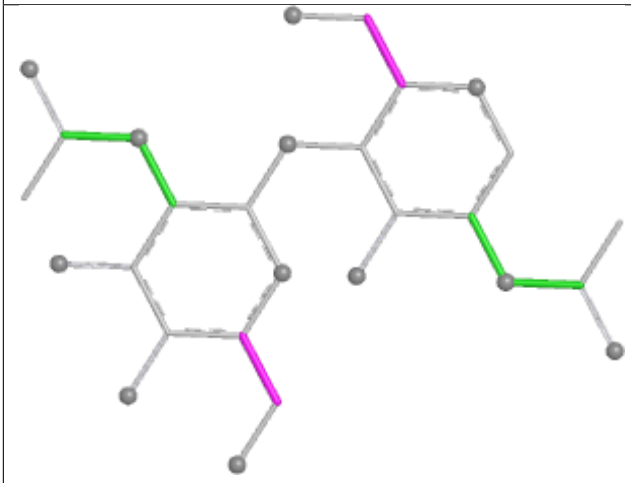
Oligosaccharide Chain Q



Bond lengths



Bond angles



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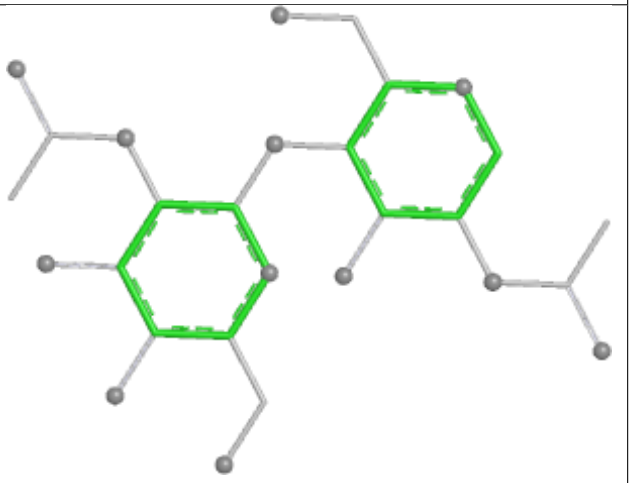
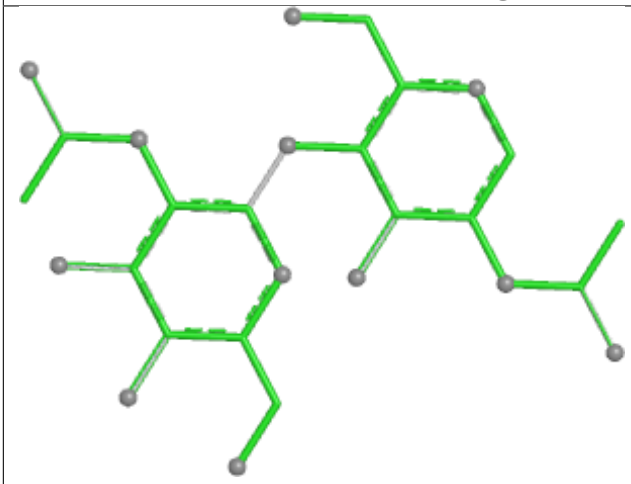
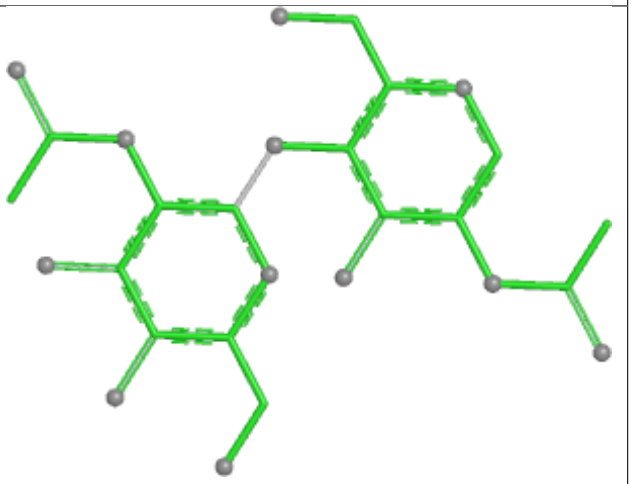


Rings

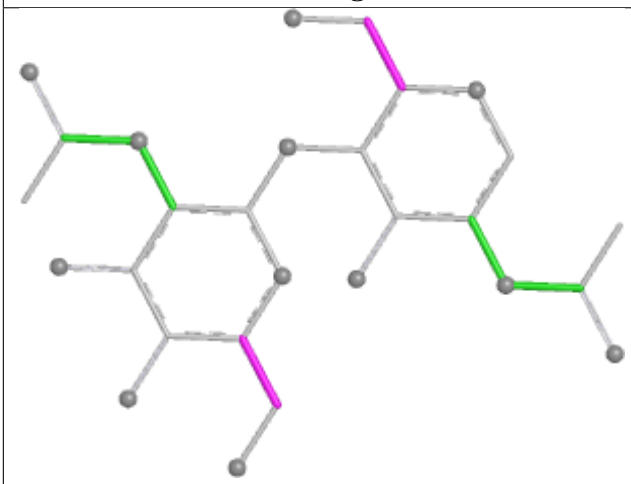
Oligosaccharide Chain R



Bond lengths



Bond angles



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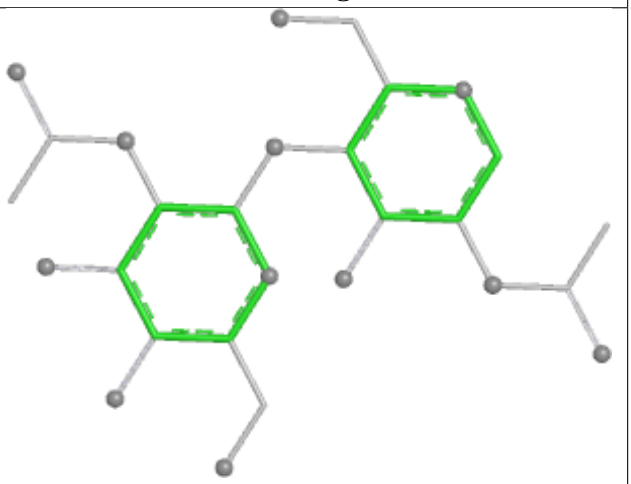
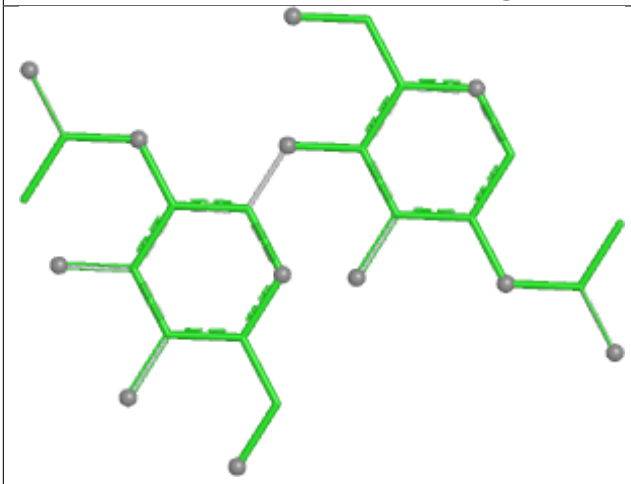
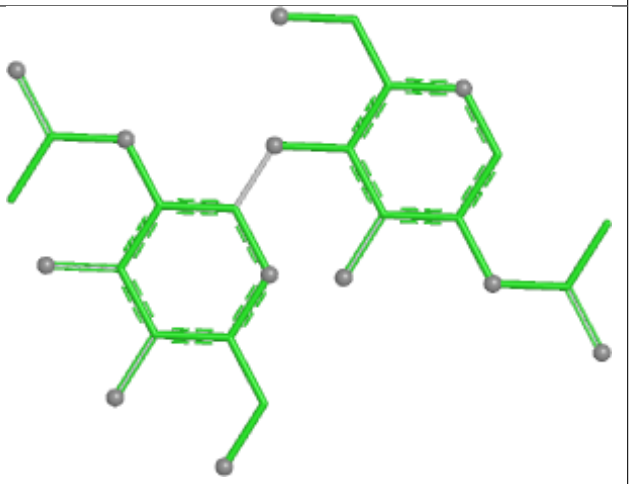


Rings

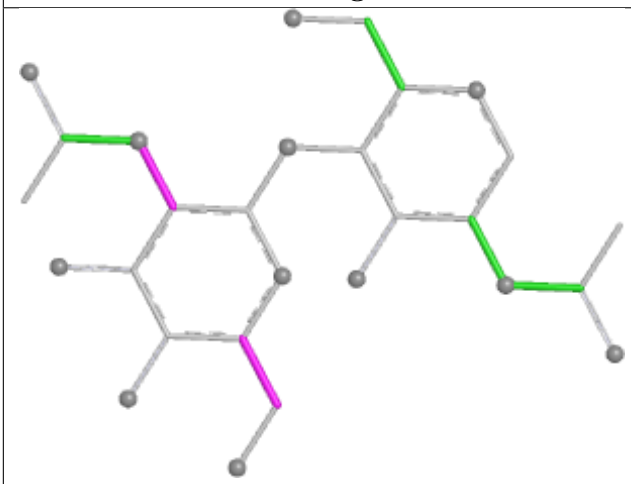
Oligosaccharide Chain S



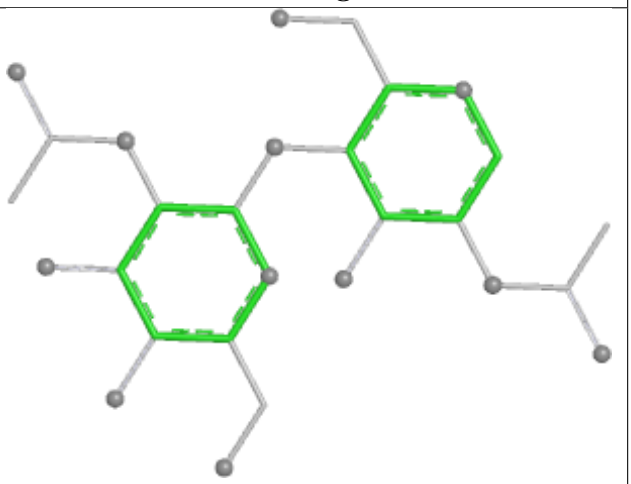
Bond lengths



Bond angles

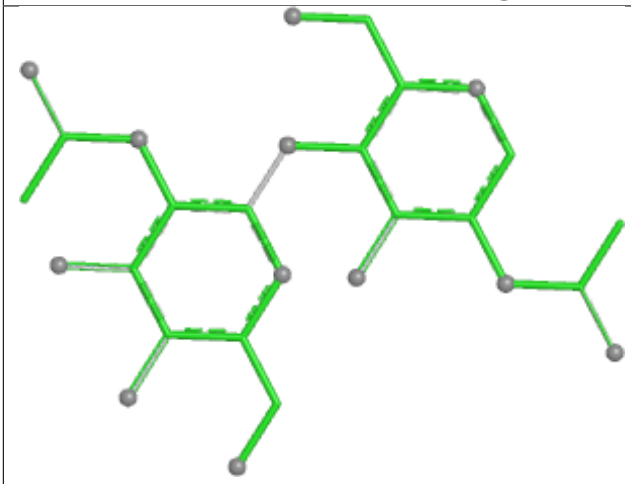


Torsions

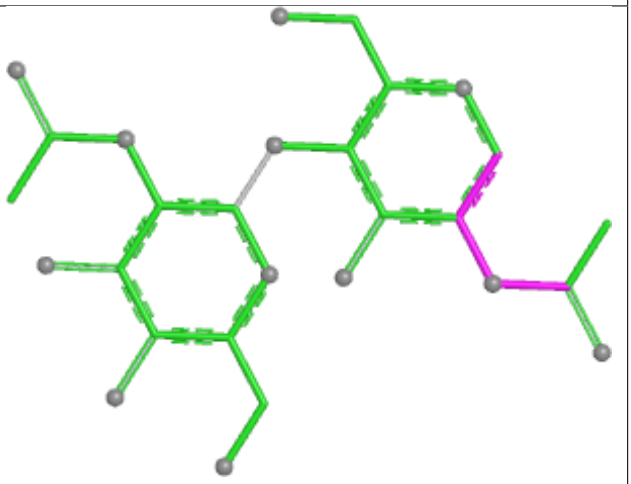


Rings

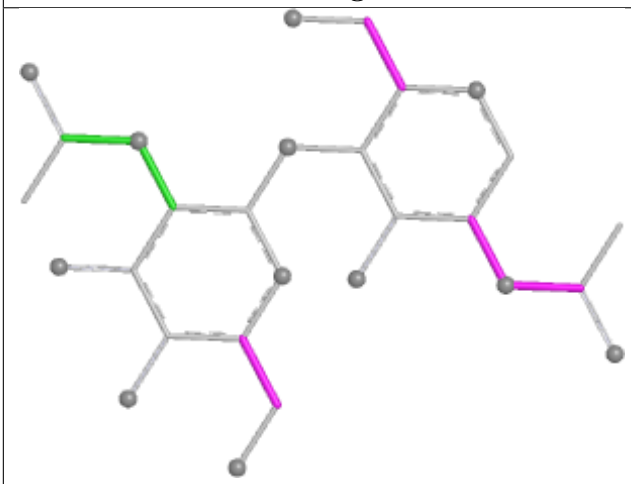
Oligosaccharide Chain T



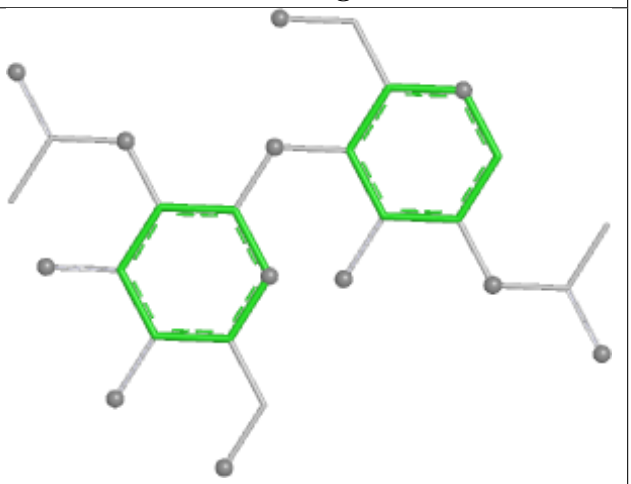
Bond lengths



Bond angles

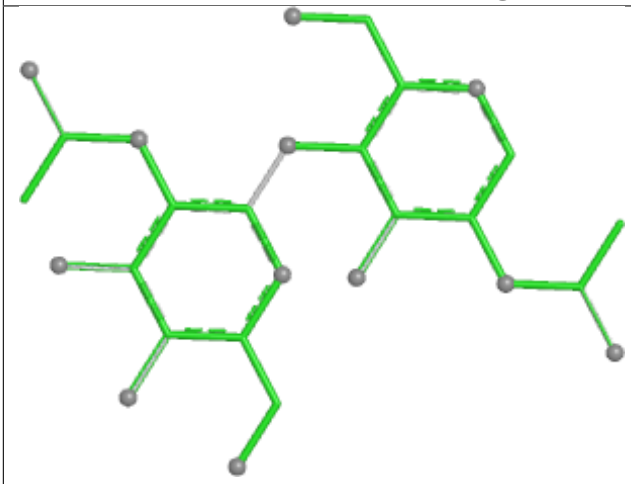


Torsions

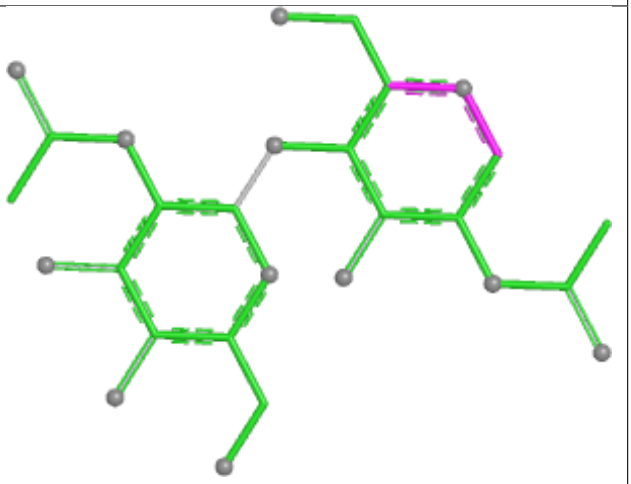


Rings

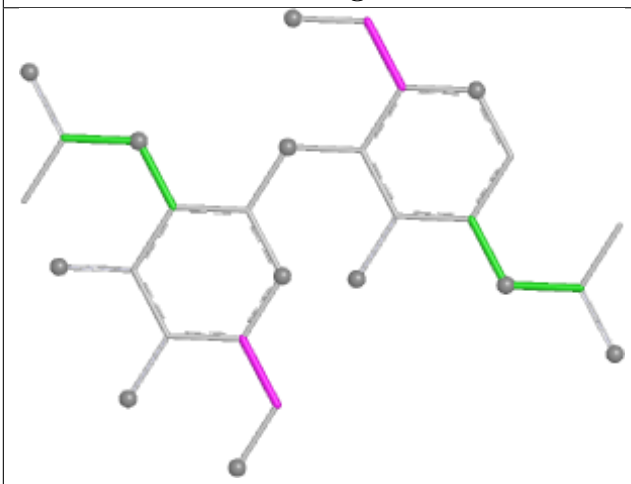
Oligosaccharide Chain U



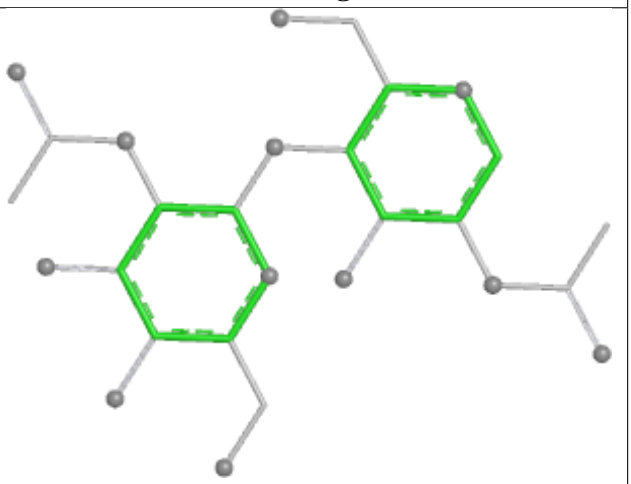
Bond lengths



Bond angles

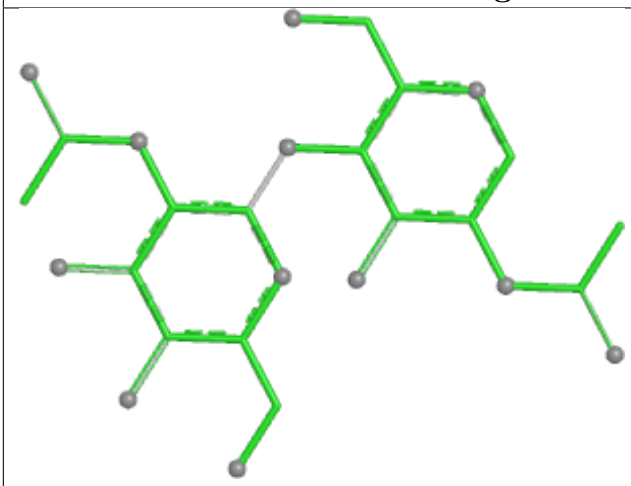


Torsions

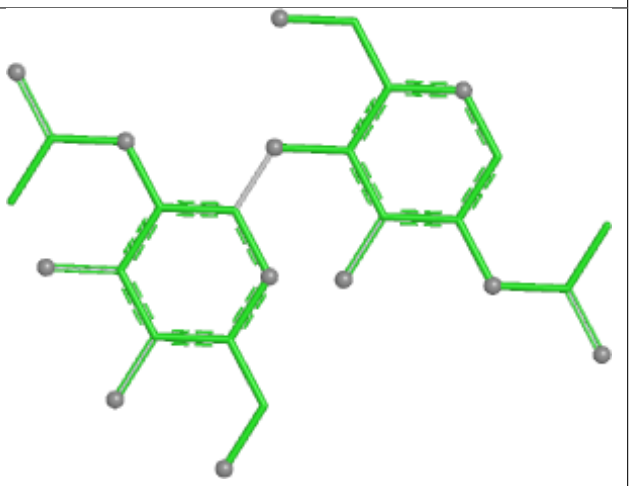


Rings

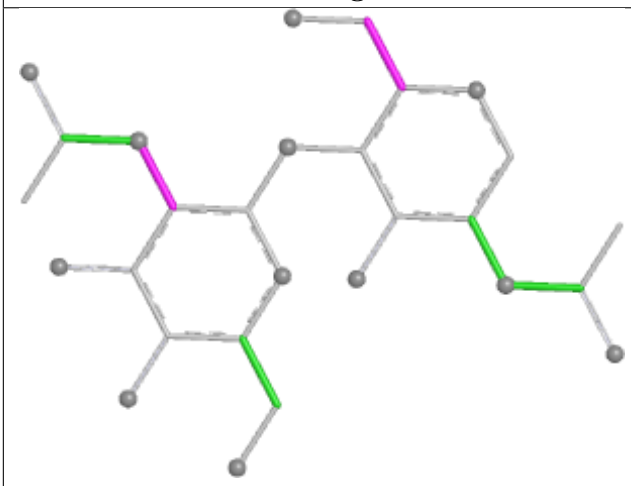
Oligosaccharide Chain V



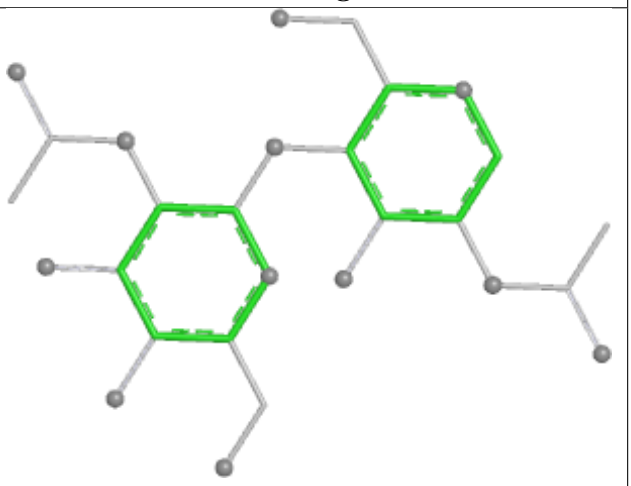
Bond lengths



Bond angles

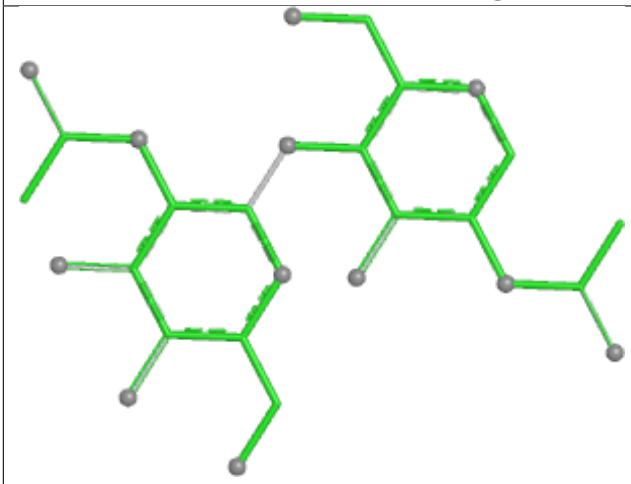


Torsions

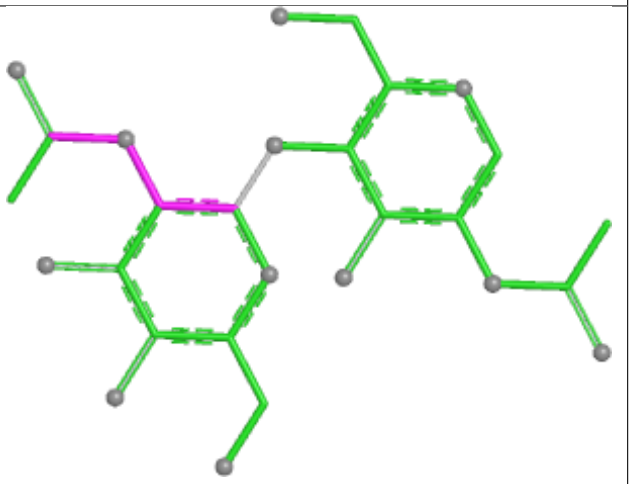


Rings

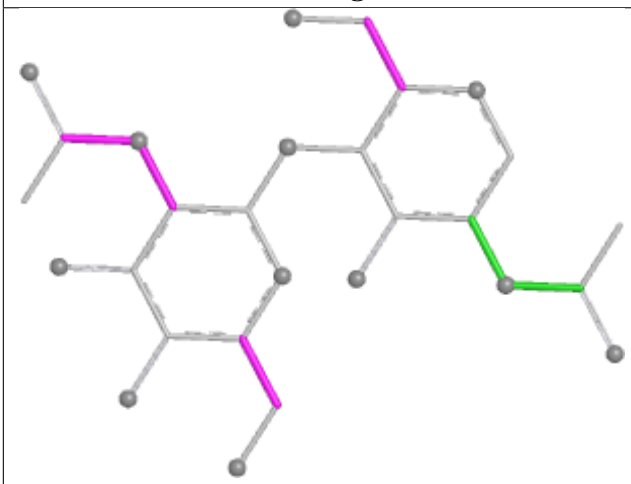
Oligosaccharide Chain W



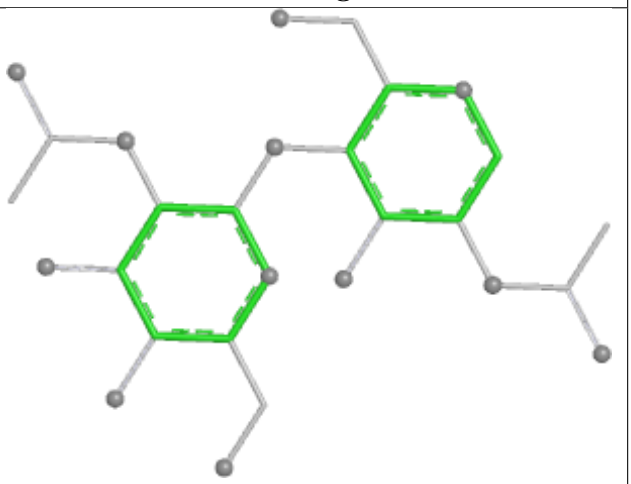
Bond lengths



Bond angles

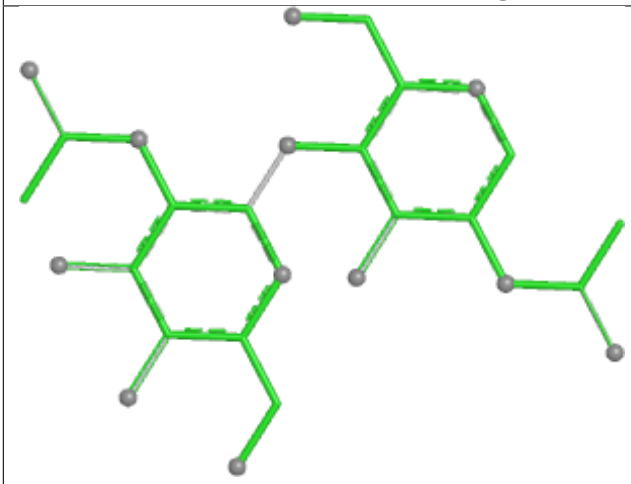


Torsions

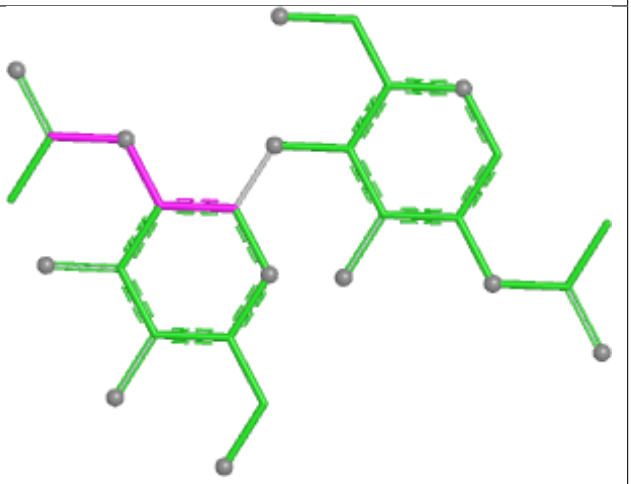


Rings

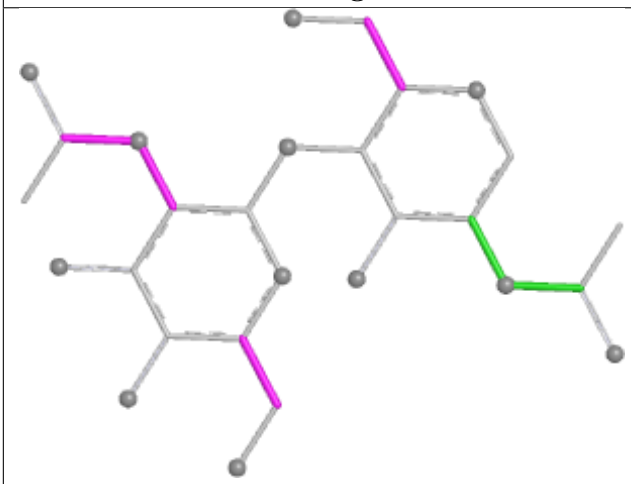
Oligosaccharide Chain X



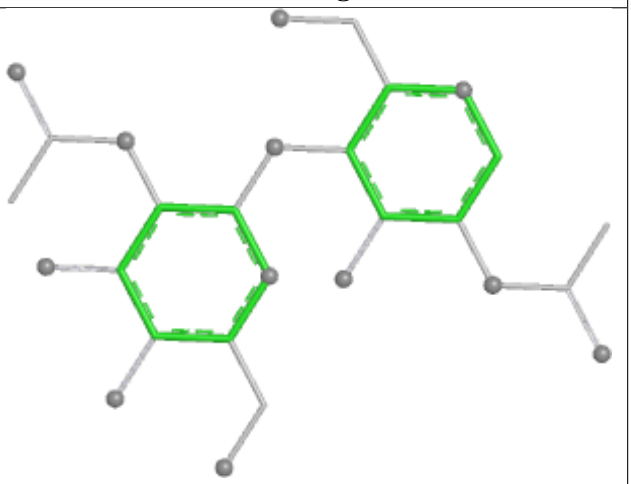
Bond lengths



Bond angles

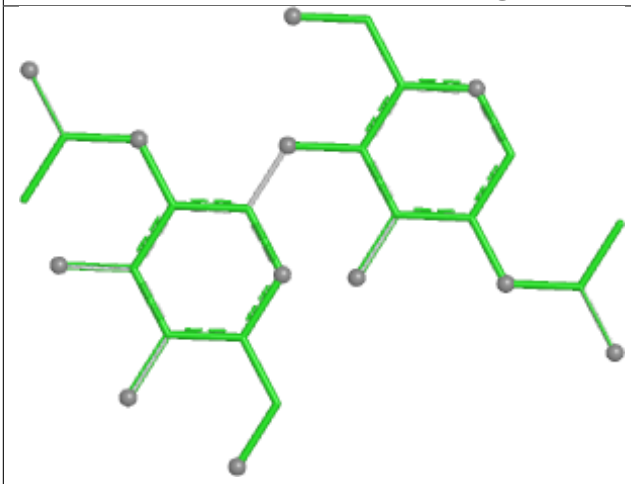


Torsions

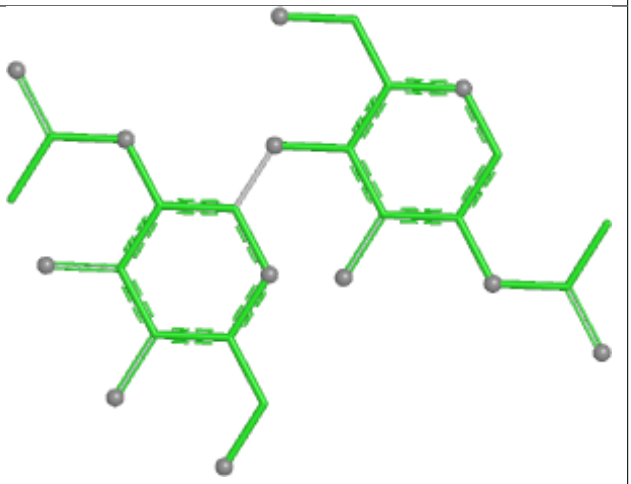


Rings

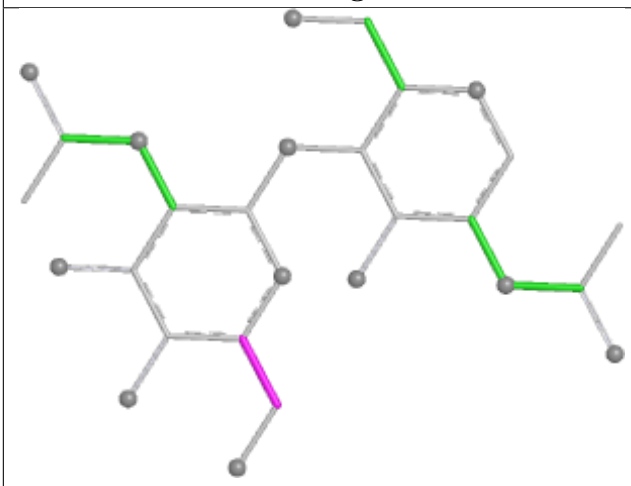
Oligosaccharide Chain Y



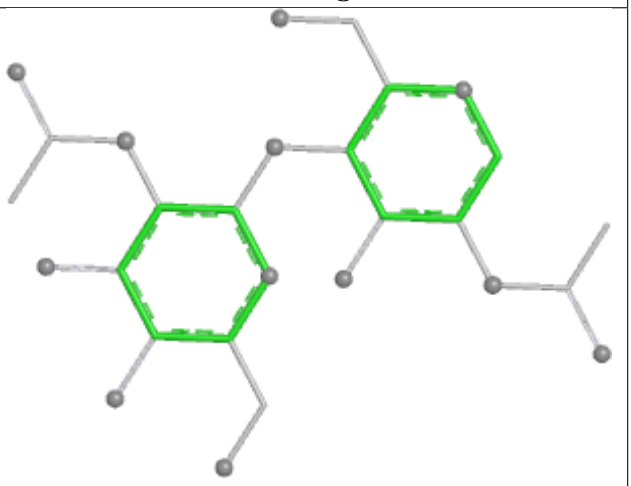
Bond lengths



Bond angles

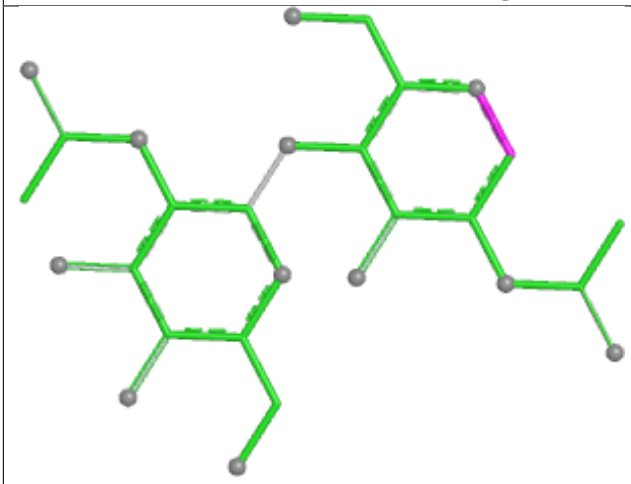


Torsions

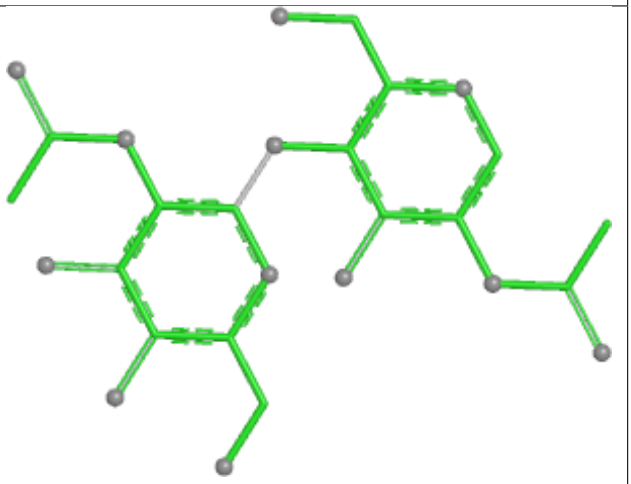


Rings

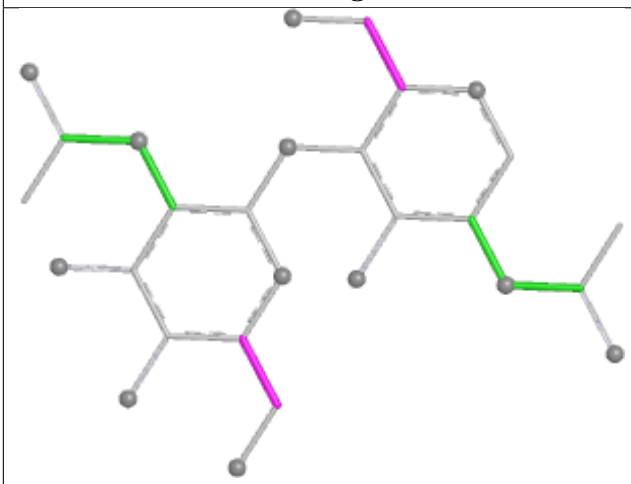
Oligosaccharide Chain Z



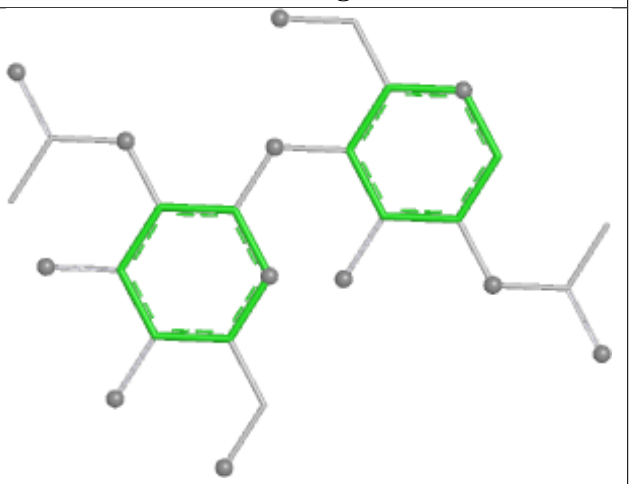
Bond lengths



Bond angles

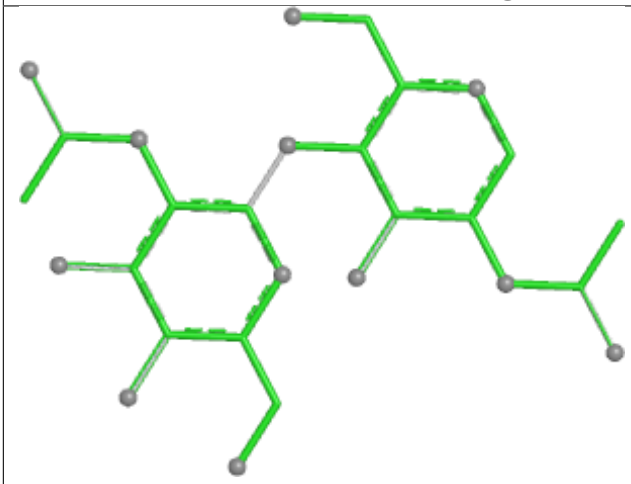


Torsions

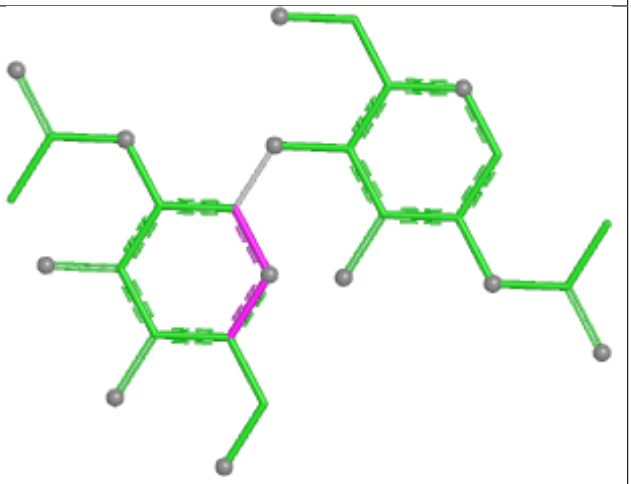


Rings

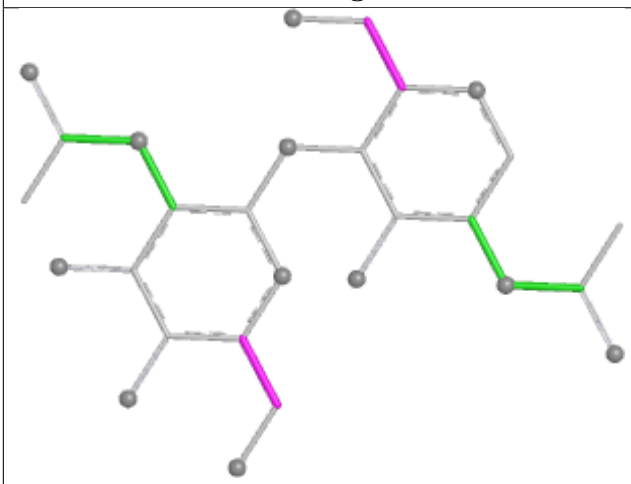
Oligosaccharide Chain a



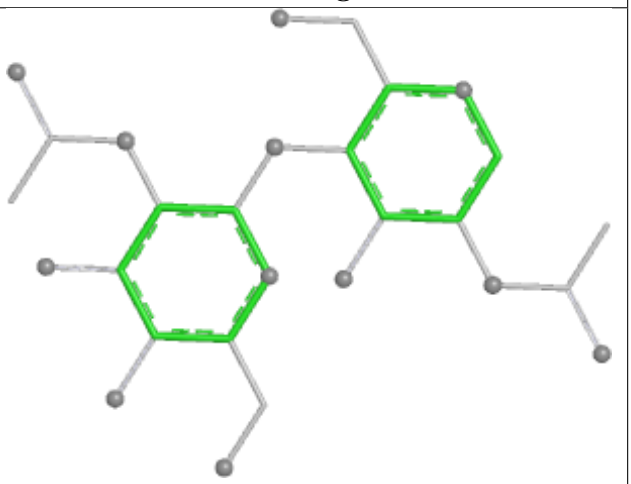
Bond lengths



Bond angles

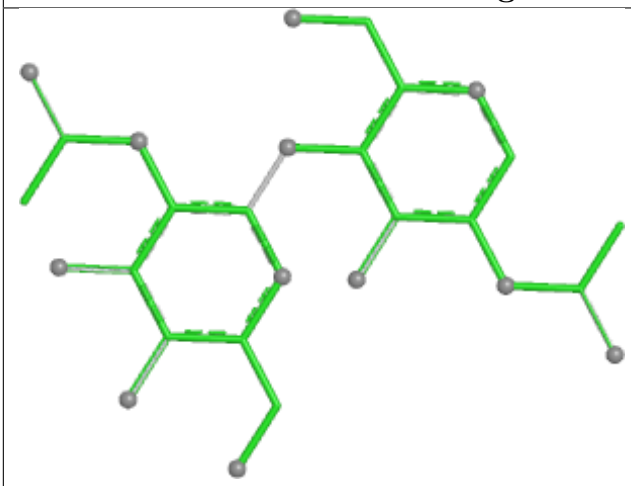


Torsions

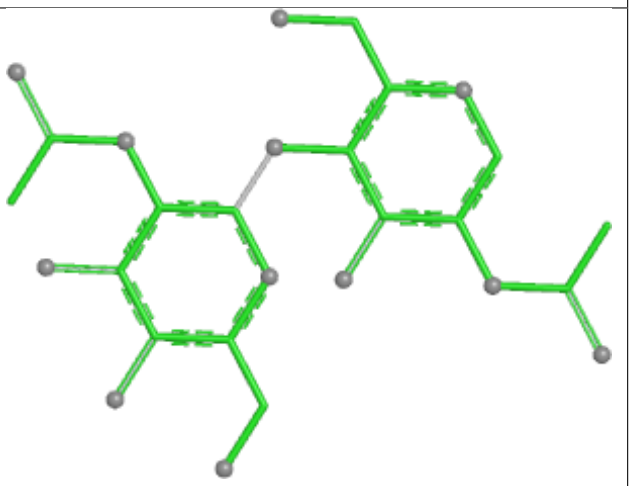


Rings

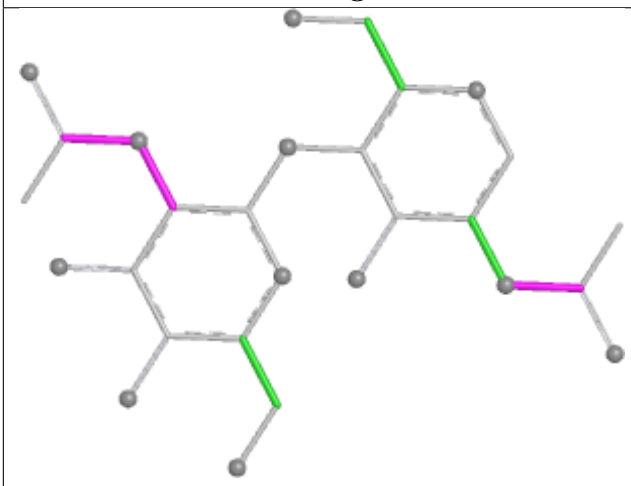
Oligosaccharide Chain b



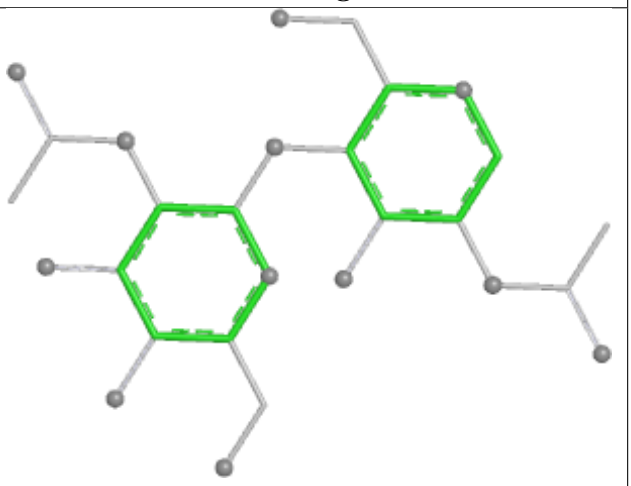
Bond lengths



Bond angles

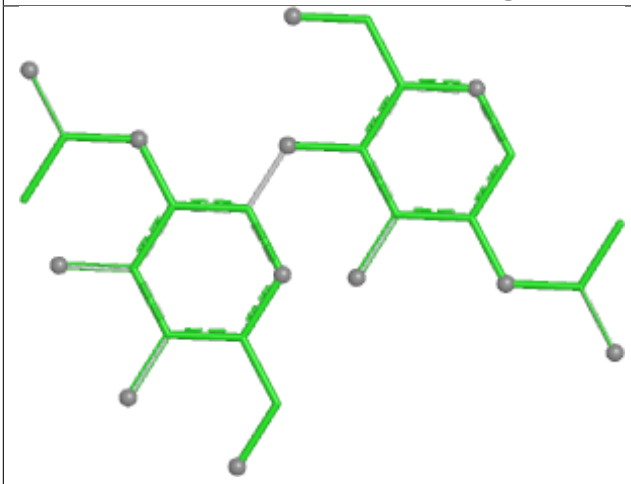


Torsions

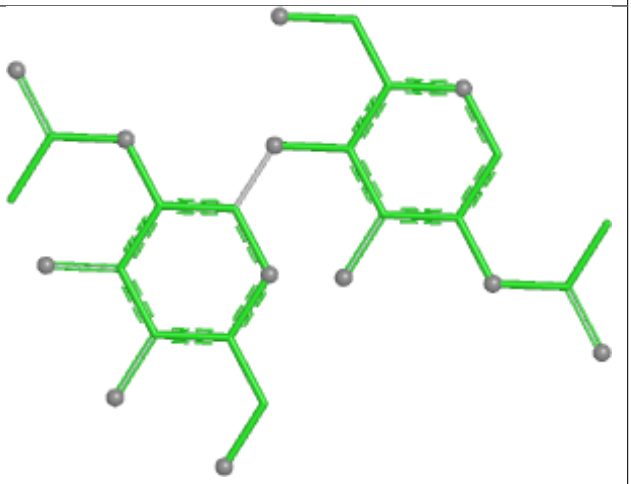


Rings

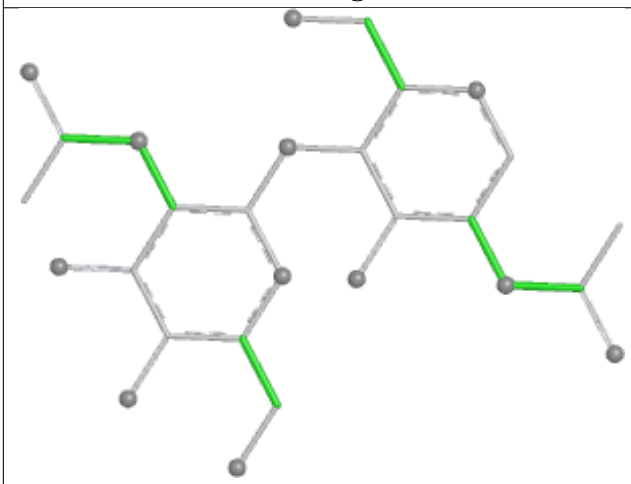
Oligosaccharide Chain c



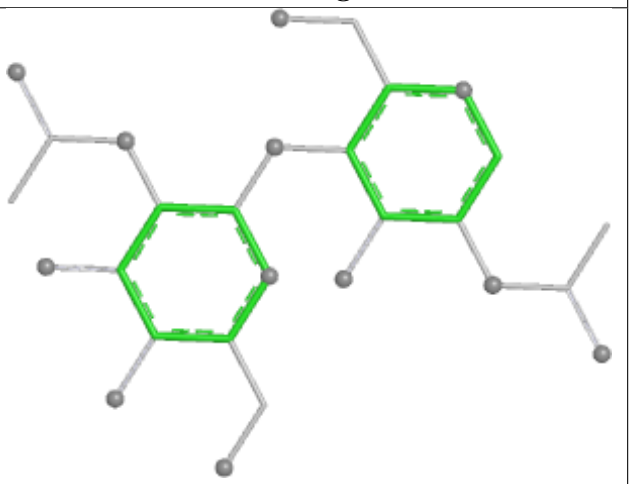
Bond lengths



Bond angles

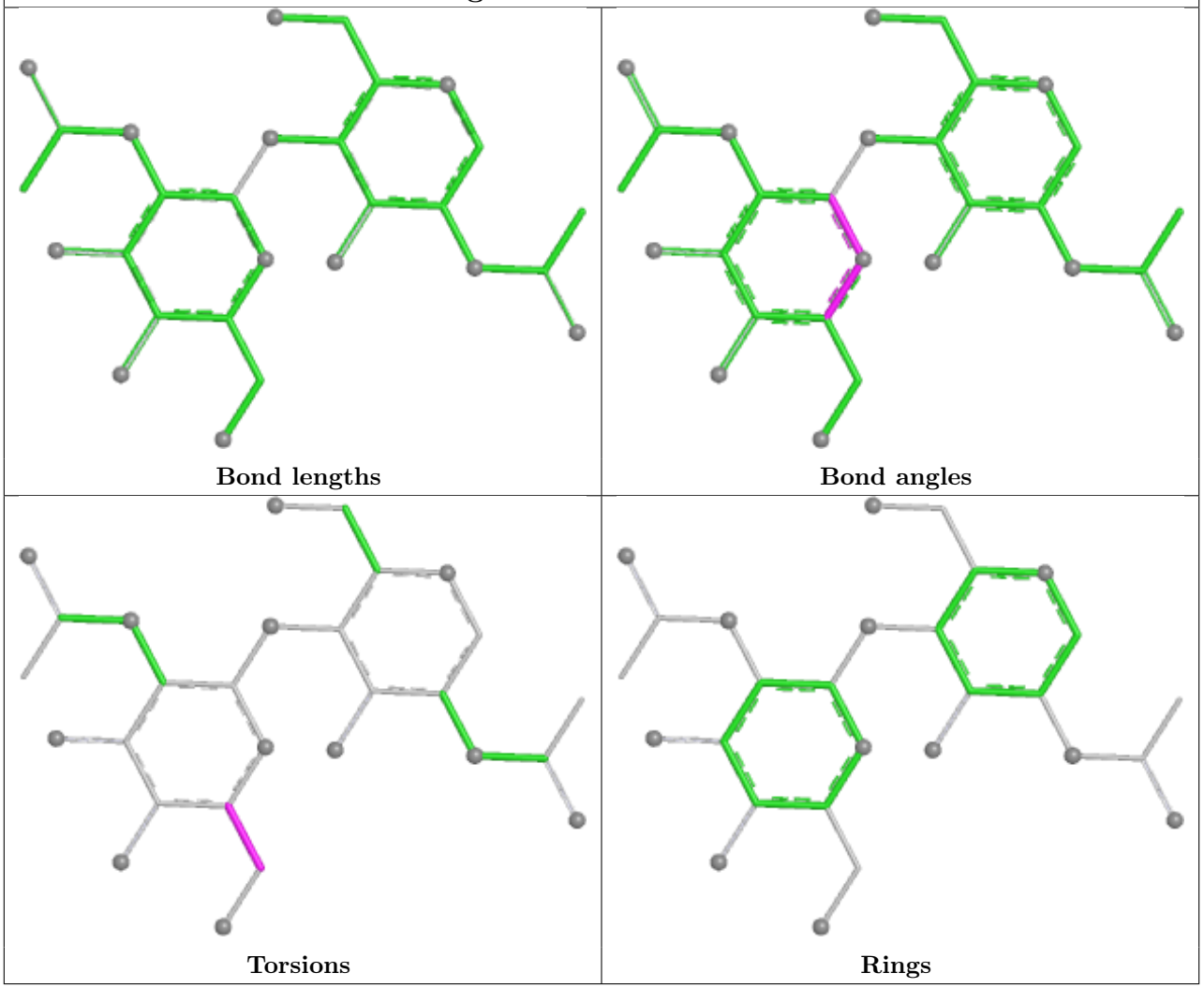


Torsions



Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

30 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	1412	-	14,14,15	0.37	0	17,19,21	0.42	0
4	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.67	0
4	NAG	B	1406	-	14,14,15	0.42	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1407	-	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	C	1407	1	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	B	1403	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	A	1409	1	14,14,15	0.50	0	17,19,21	0.36	0
4	NAG	C	1404	1	14,14,15	0.50	0	17,19,21	0.54	0
4	NAG	C	1408	1	14,14,15	0.34	0	17,19,21	0.40	0
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.40	0
4	NAG	C	1401	1	14,14,15	0.33	0	17,19,21	0.35	0
4	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	C	1405	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
4	NAG	A	1407	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	A	1405	1	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
4	NAG	C	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	A	1401	1	14,14,15	0.30	0	17,19,21	0.35	0
4	NAG	A	1408	1	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	A	1404	1	14,14,15	0.49	0	17,19,21	0.54	0
4	NAG	B	1408	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.62	1 (5%)
4	NAG	B	1410	1	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	B	1409	1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.66	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	B	1411	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.44	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	1412	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1405	NAG	C2-N2-C7	4.59	129.06	122.90
4	A	1405	NAG	C2-N2-C7	4.58	129.03	122.90
4	C	1405	NAG	C2-N2-C7	4.57	129.02	122.90
4	B	1406	NAG	C8-C7-N2	2.36	120.03	116.12
4	B	1411	NAG	C8-C7-N2	2.29	119.92	116.12
4	B	1411	NAG	C2-N2-C7	-2.19	119.97	122.90
4	C	1405	NAG	C1-C2-N2	2.16	113.83	110.43
4	B	1406	NAG	C2-N2-C7	-2.15	120.02	122.90
4	A	1405	NAG	C1-C2-N2	2.10	113.74	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1405	NAG	C1-C2-N2	2.09	113.73	110.43
4	D	901	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-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	B	1405	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	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	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-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	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	B	1410	NAG	O5-C5-C6-O6
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1406	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

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Mol	Chain	Res	Type	Atoms
4	A	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
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	1403	NAG	O5-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	B	1410	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	B	1407	NAG	C4-C5-C6-O6
4	A	1405	NAG	C1-C2-N2-C7
4	B	1405	NAG	C1-C2-N2-C7
4	C	1405	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.

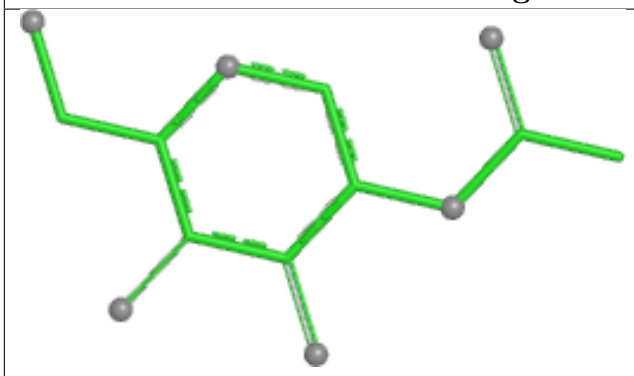
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1412	NAG	4	0
4	A	1402	NAG	3	0
4	B	1407	NAG	7	0
4	B	1405	NAG	1	0
4	C	1405	NAG	1	0
4	A	1405	NAG	1	0
4	B	1402	NAG	3	0
4	C	1402	NAG	3	0
4	B	1411	NAG	4	0

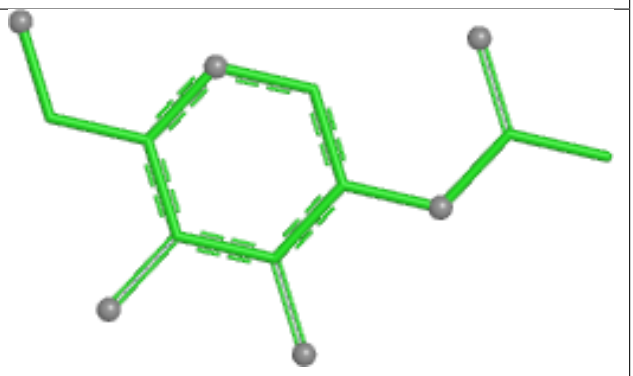
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

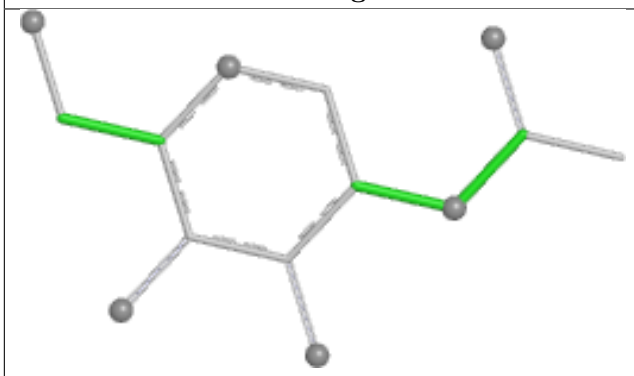
Ligand NAG B 1412



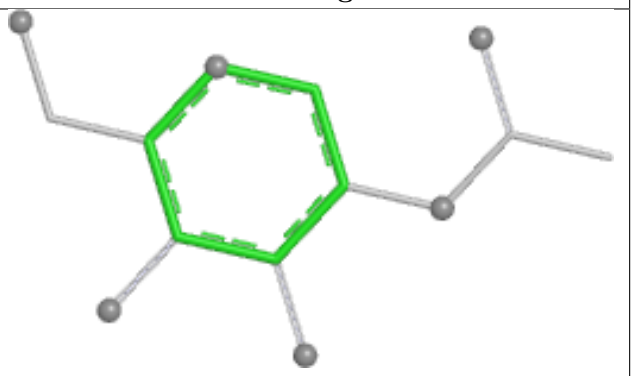
Bond lengths



Bond angles

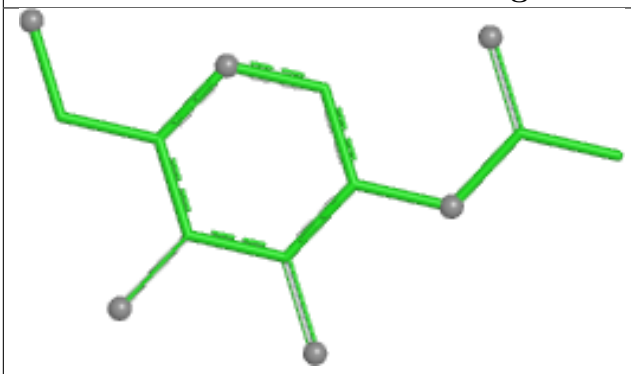


Torsions

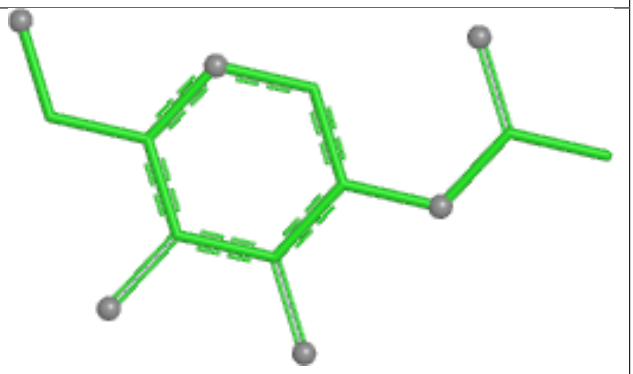


Rings

Ligand NAG A 1402



Bond lengths



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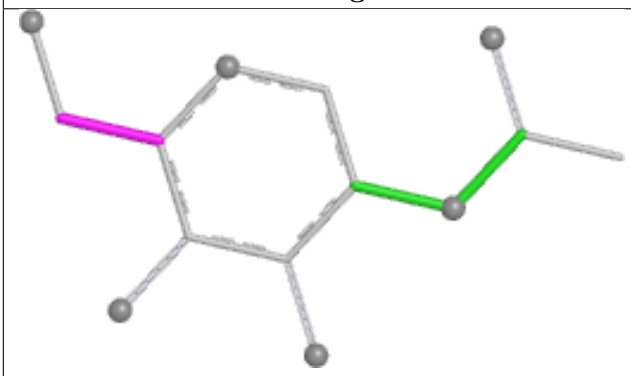

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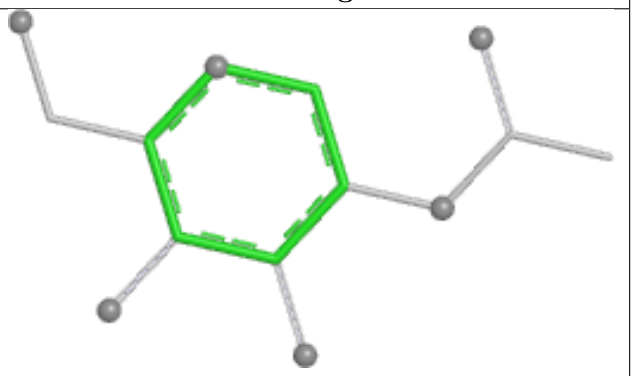
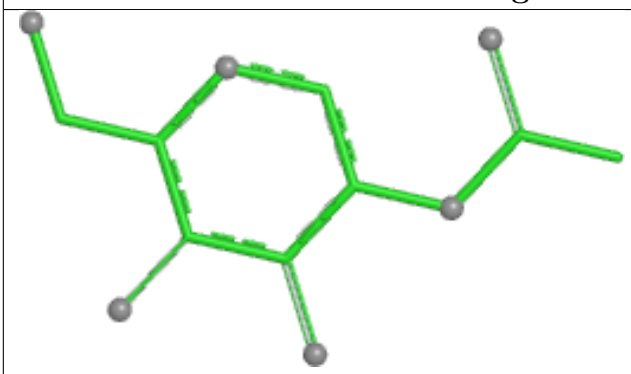


Rings

Ligand NAG B 1406



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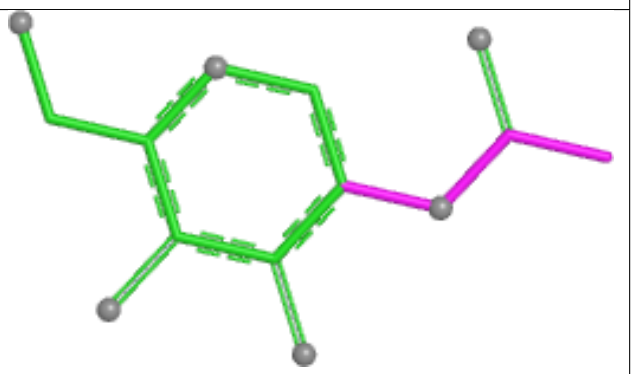
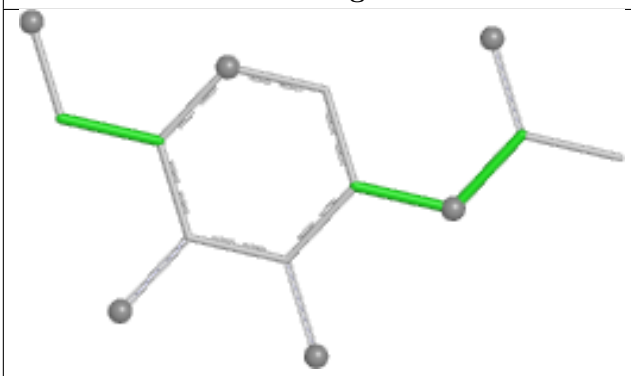


Bond angles



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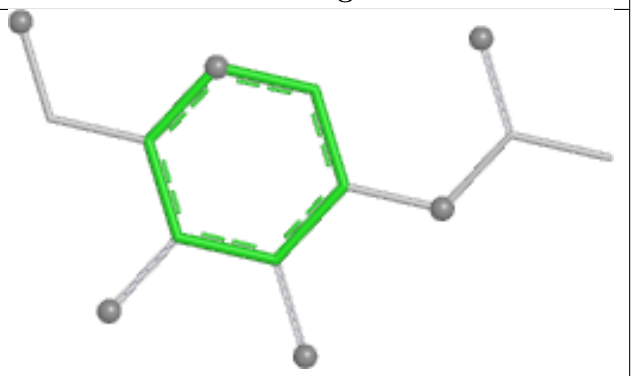
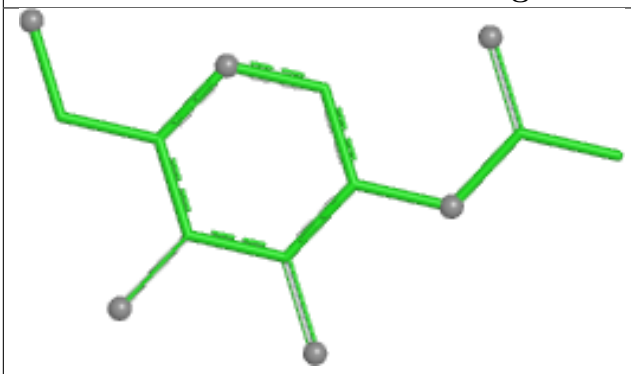


Rings

Ligand NAG B 1407



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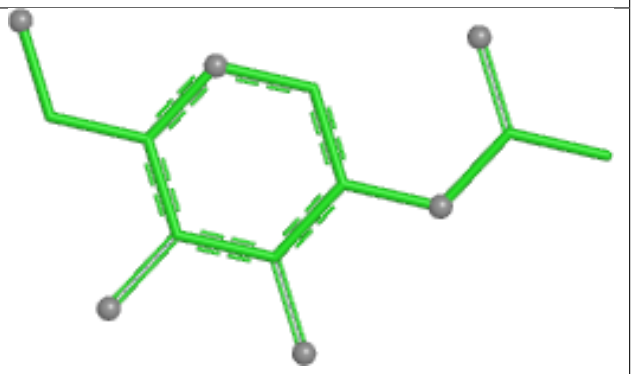
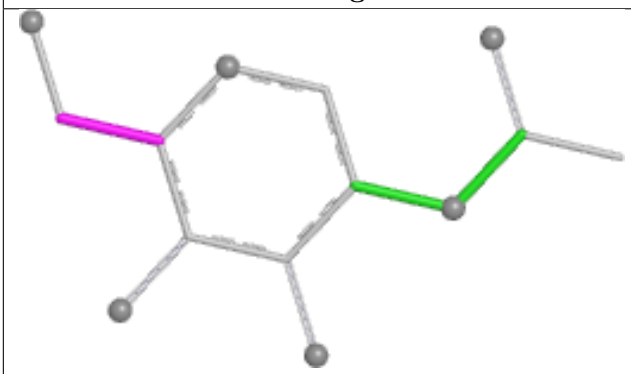


Bond angles



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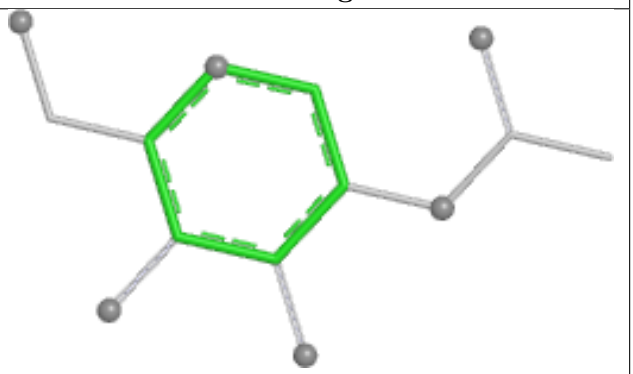
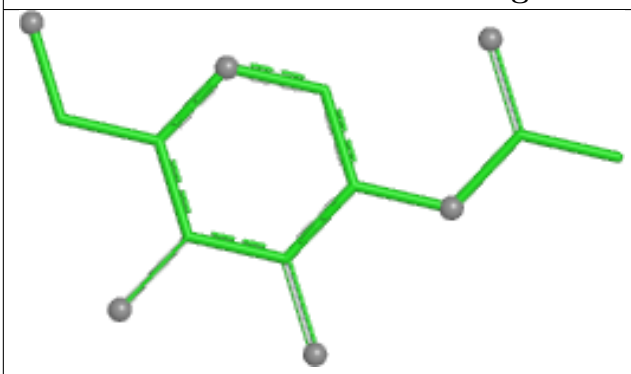


Rings

Ligand NAG C 1407



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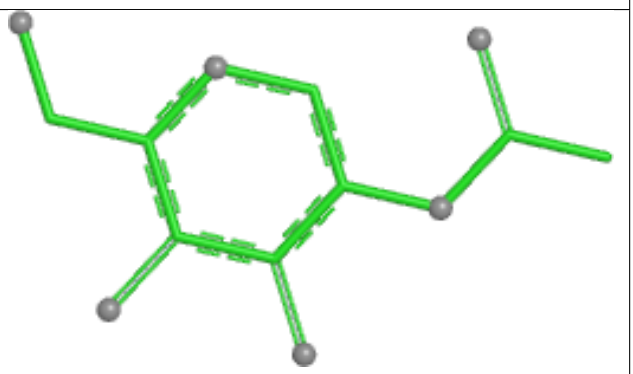

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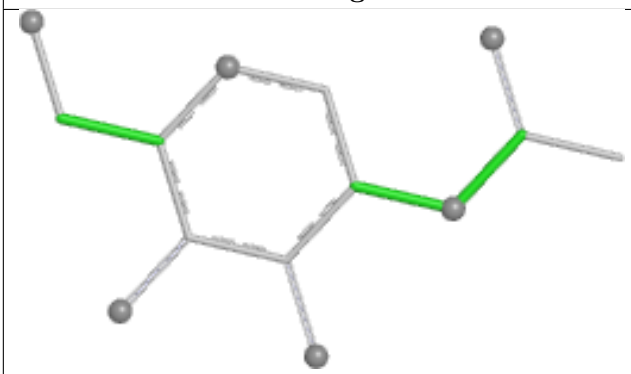

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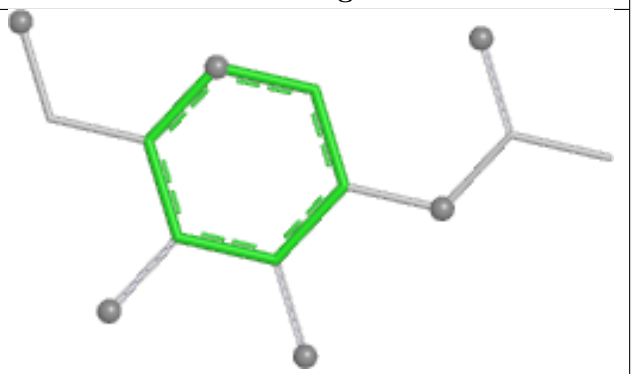
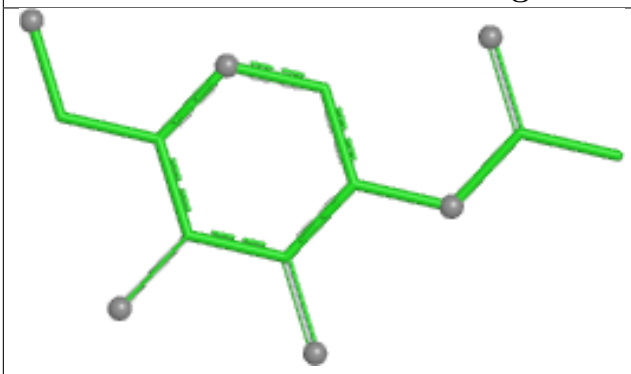


Rings

Ligand NAG B 1403



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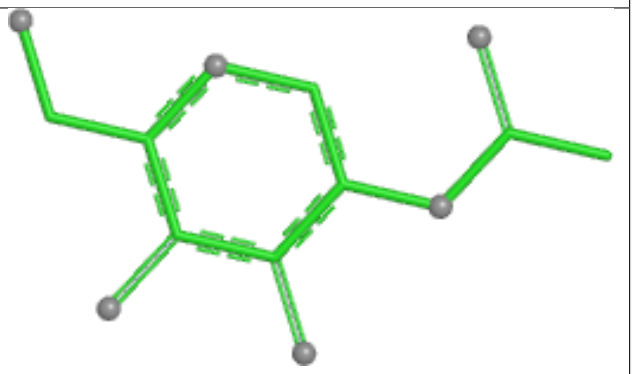

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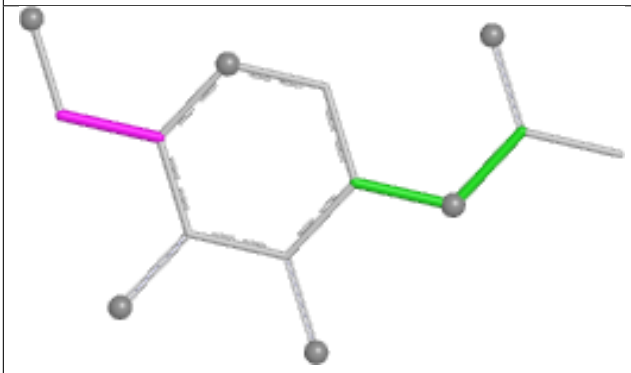

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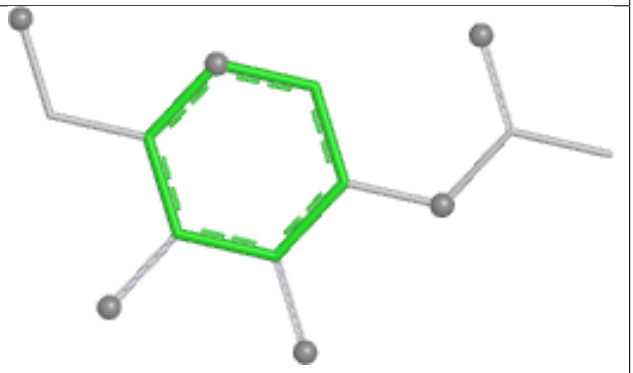
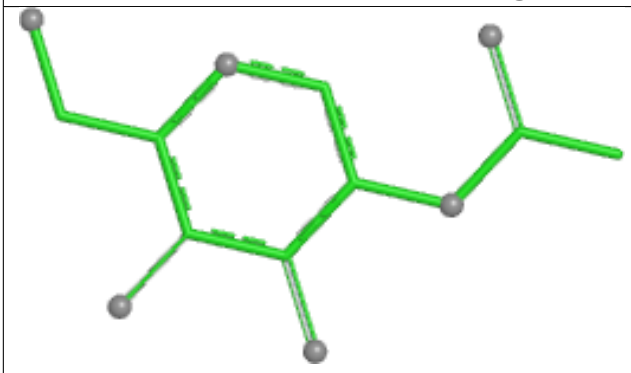


Rings

Ligand NAG A 1409



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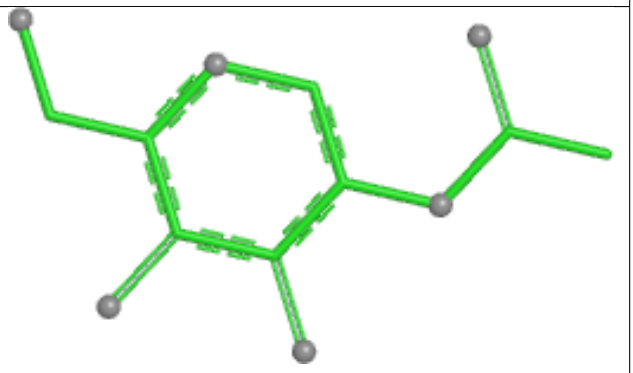

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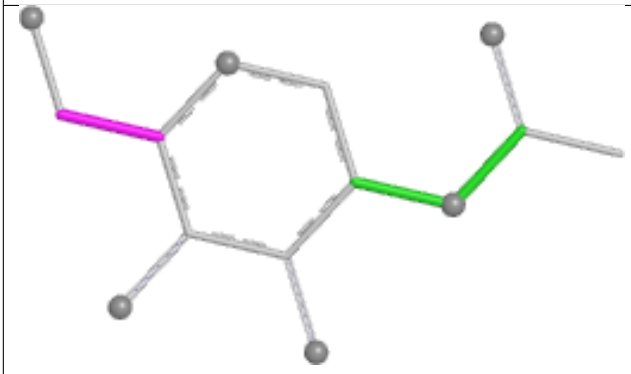

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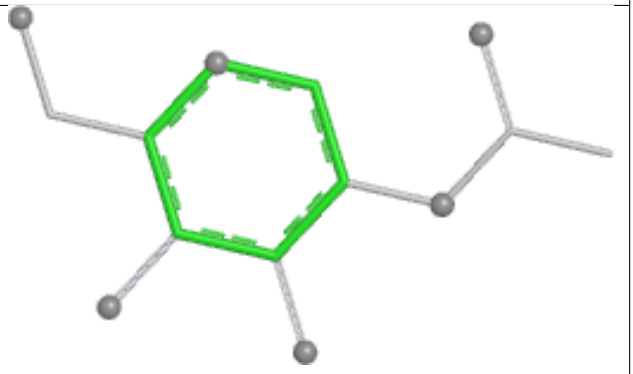
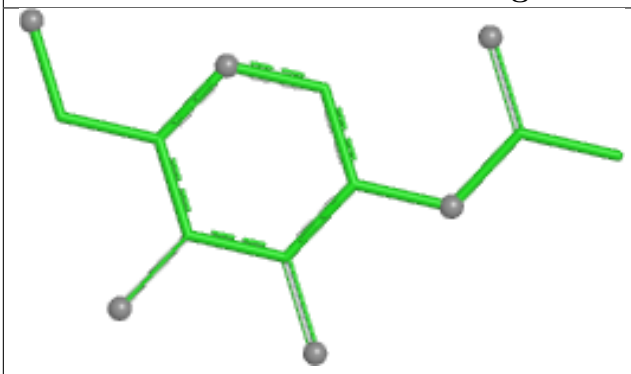


Rings

Ligand NAG C 1404



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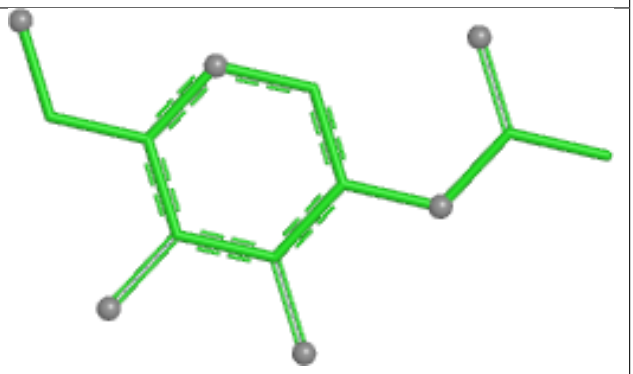

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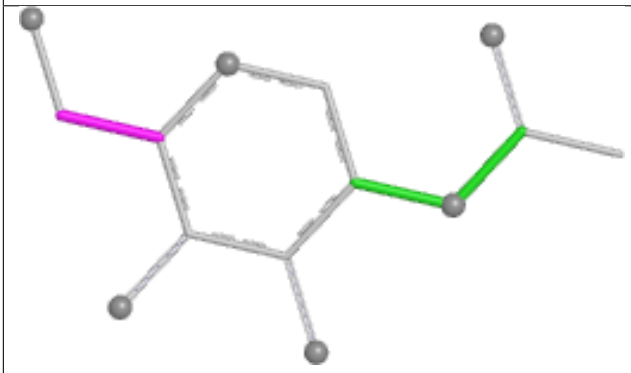

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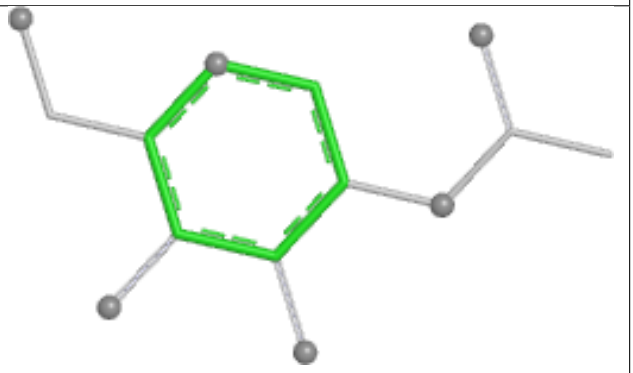
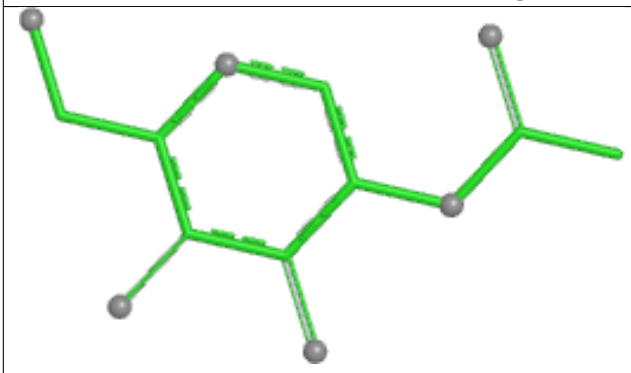


Rings

Ligand NAG C 1408



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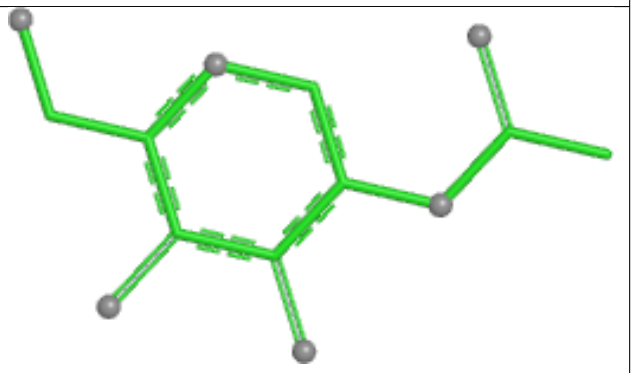
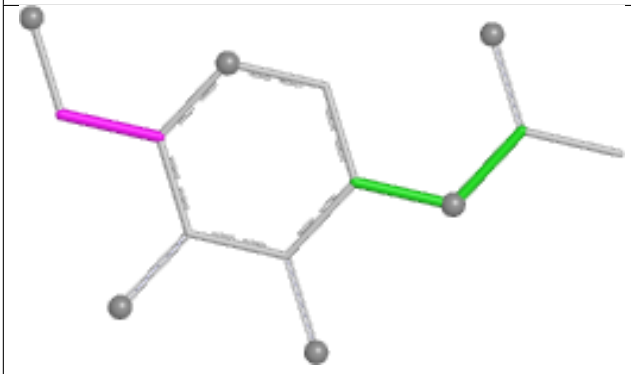


Bond angles



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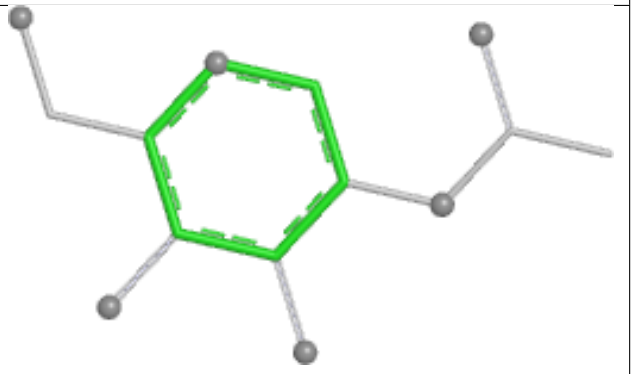
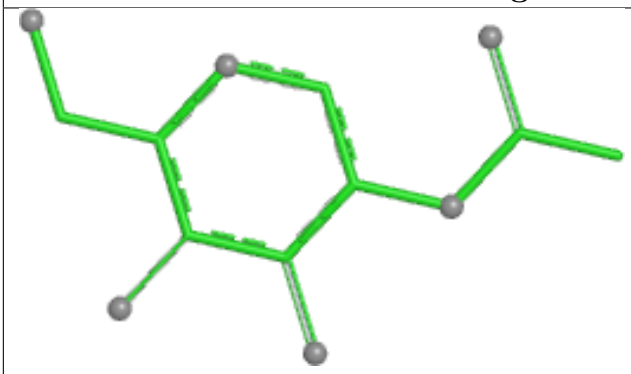
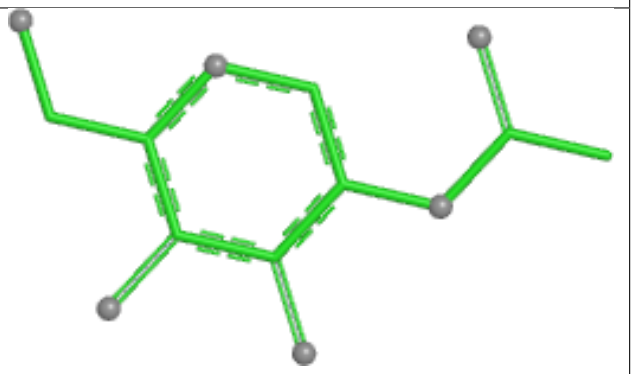


Rings

Ligand NAG A 1406



Bond lengths



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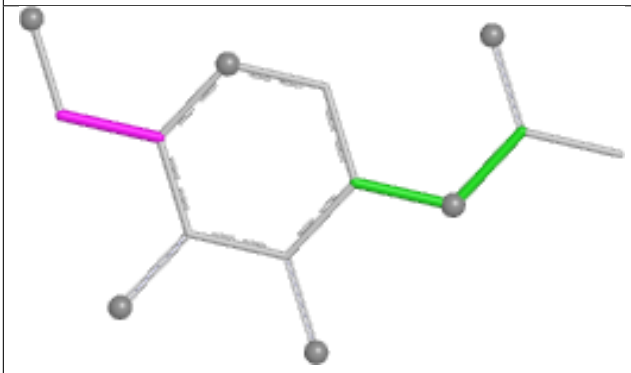
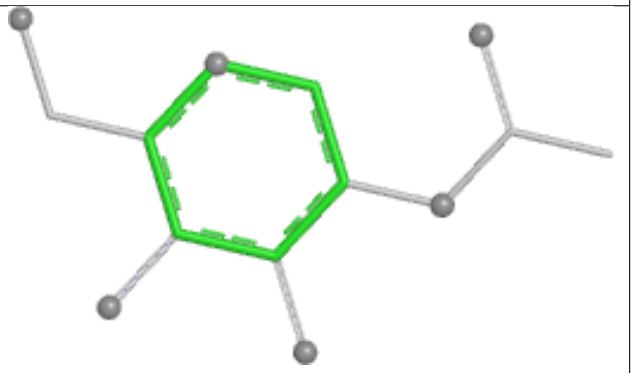
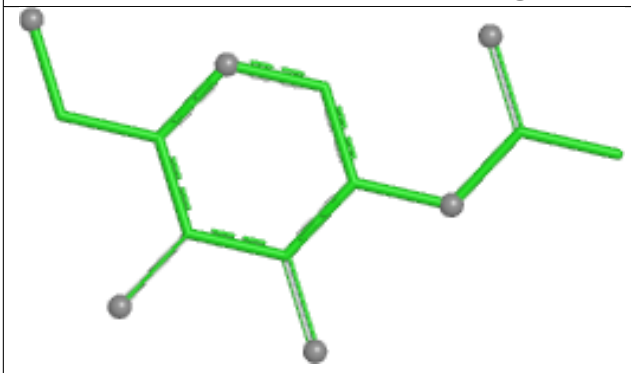


Torsions

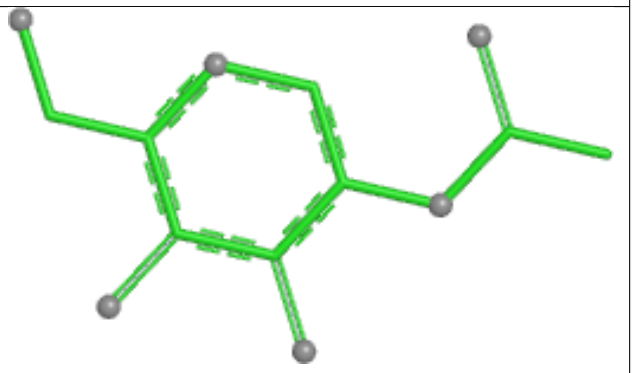


Rings

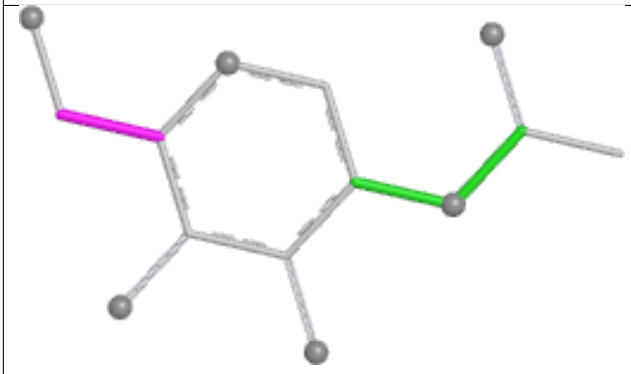
Ligand NAG C 1401



Bond lengths



Bond angles



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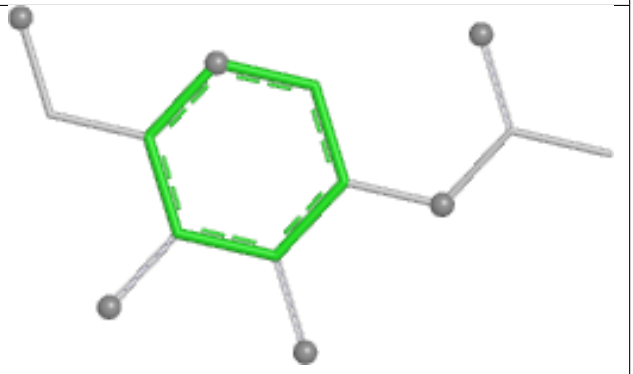
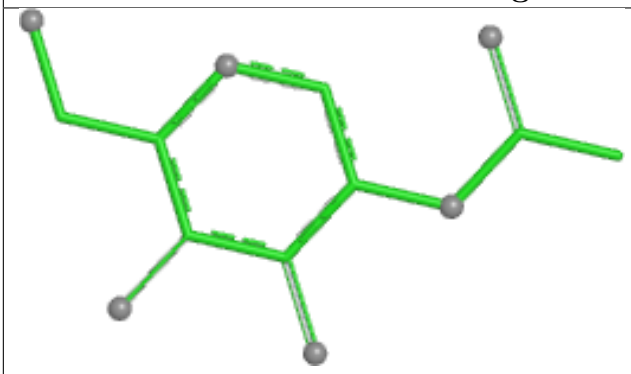


Rings

Ligand NAG B 1405



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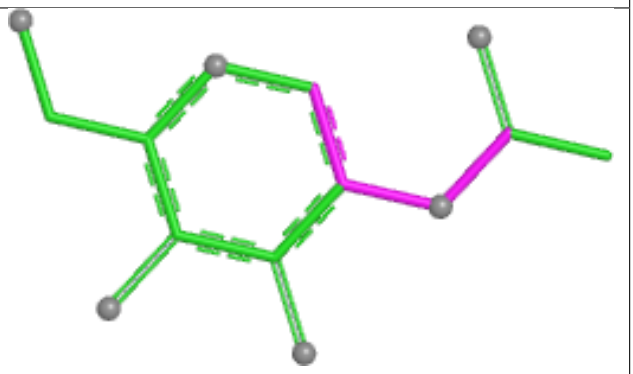

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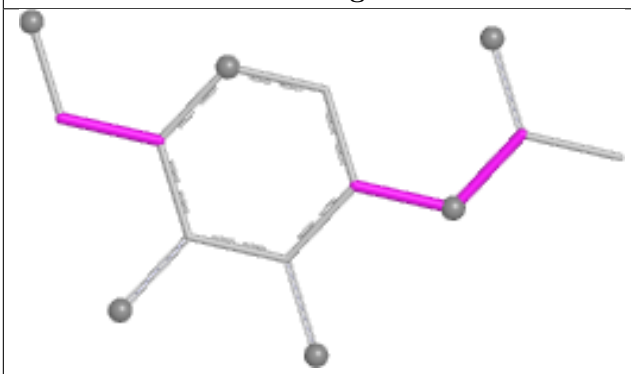

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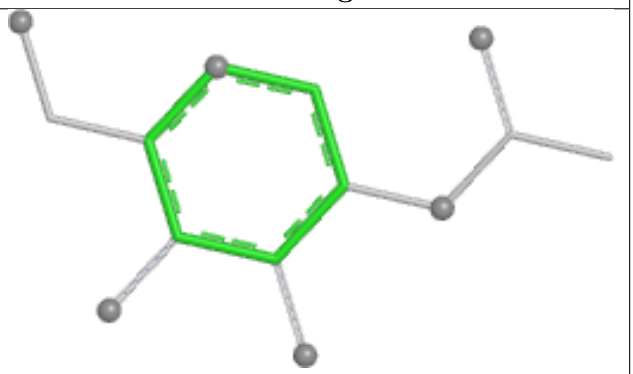
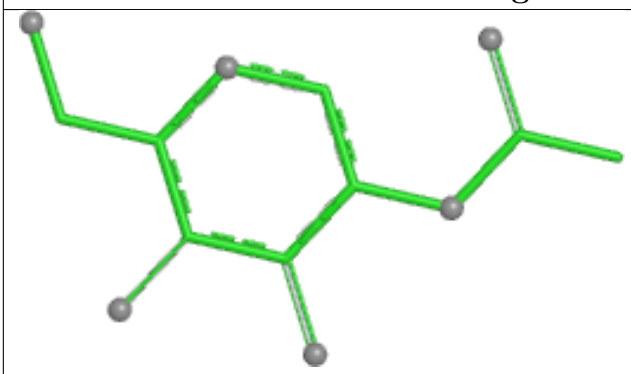


Rings

Ligand NAG B 1401



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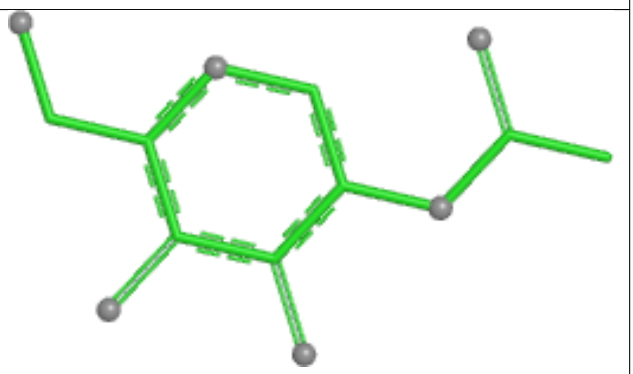

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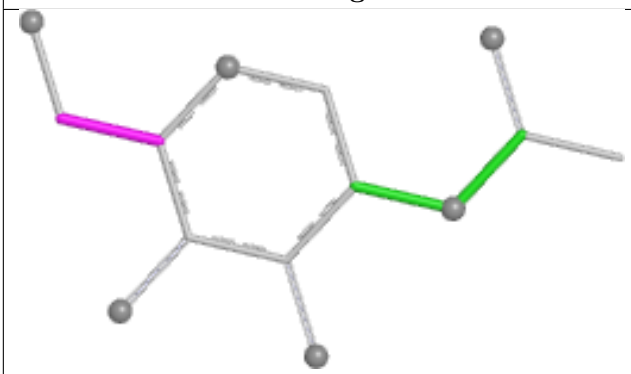

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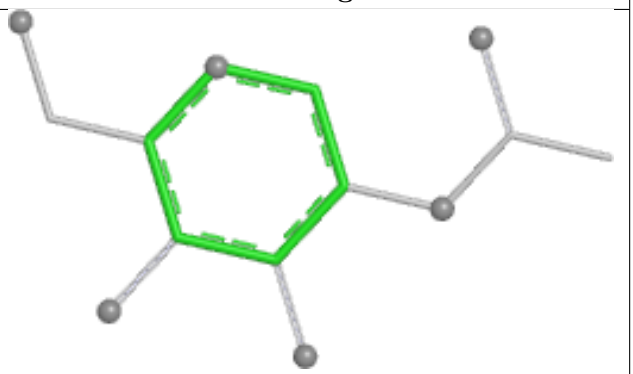
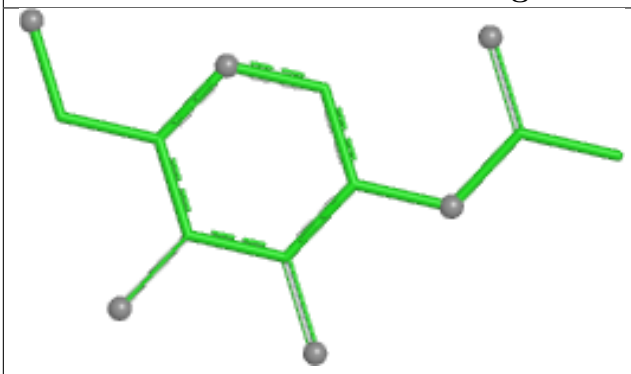


Rings

Ligand NAG C 1405



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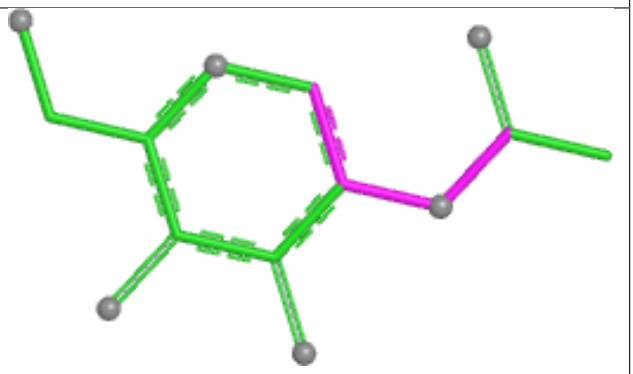
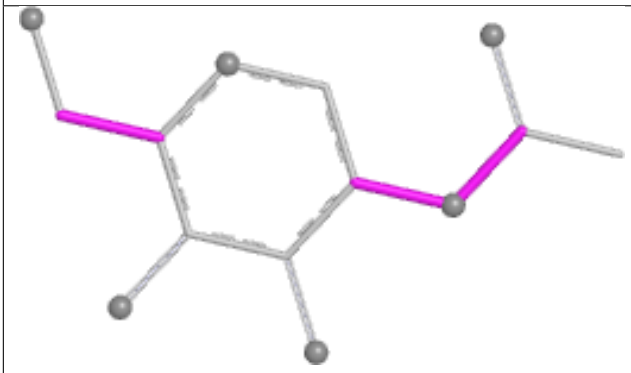


Bond angles



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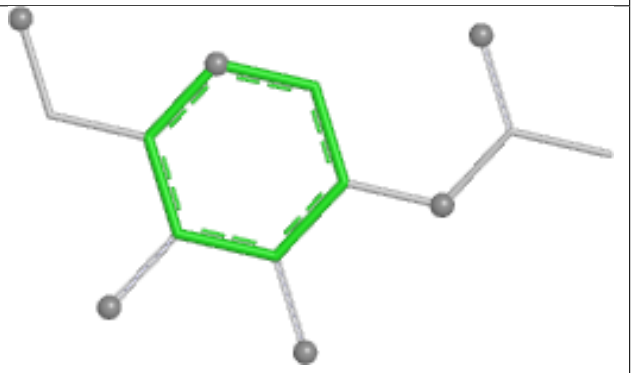
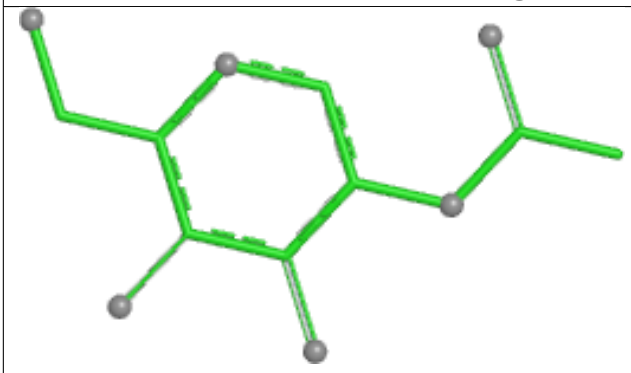


Rings

Ligand NAG A 1407



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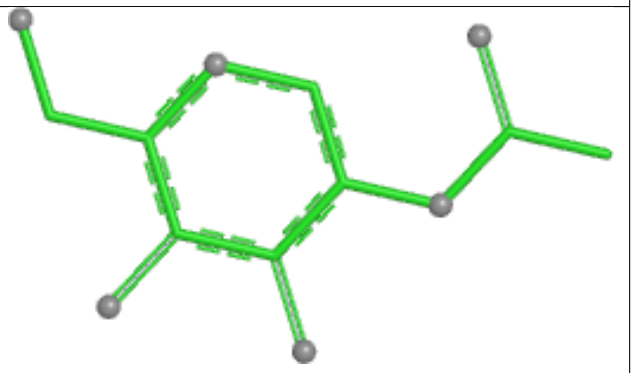

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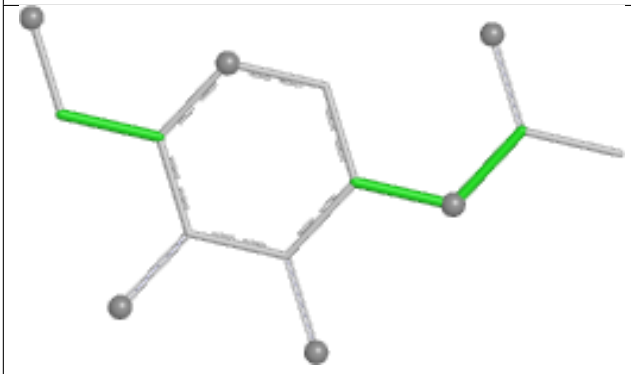

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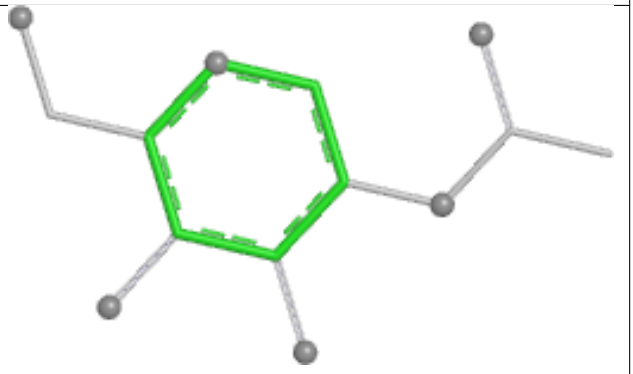
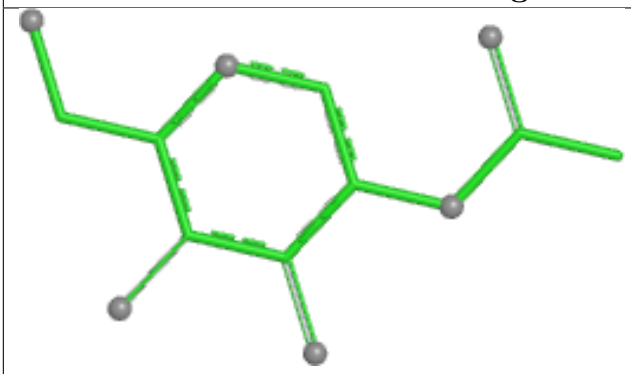


Rings

Ligand NAG A 1403



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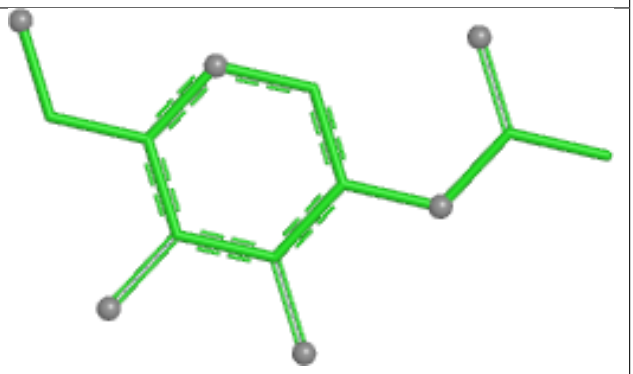
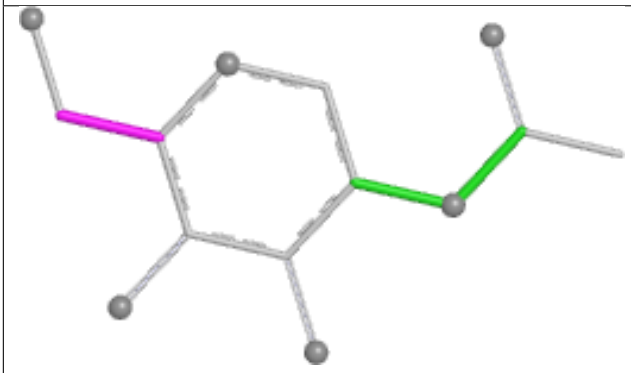


Bond angles



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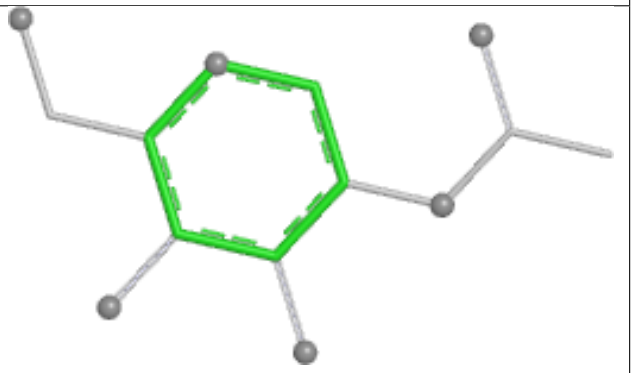
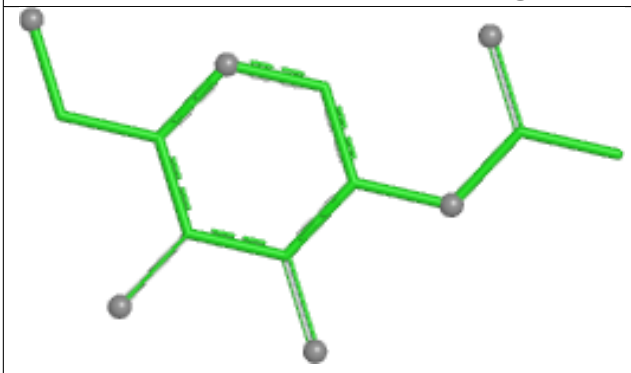


Rings

Ligand NAG B 1404



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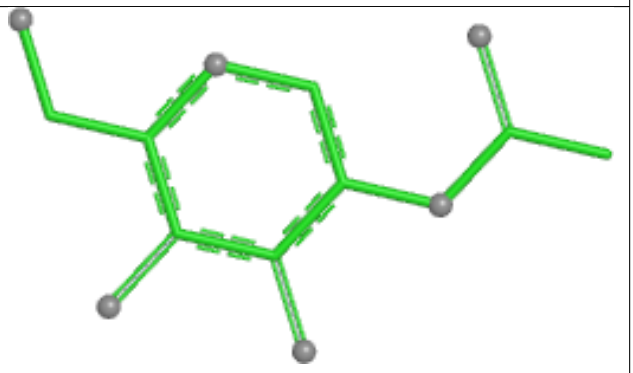

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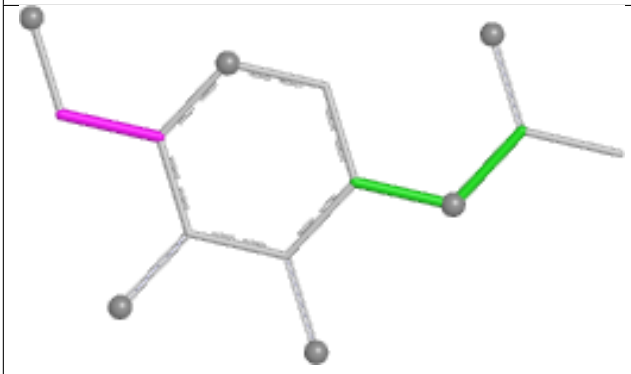

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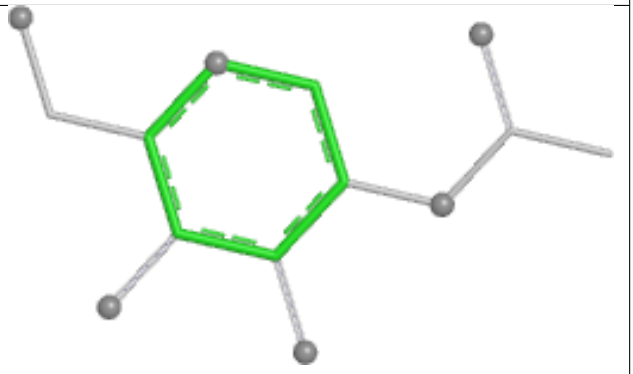
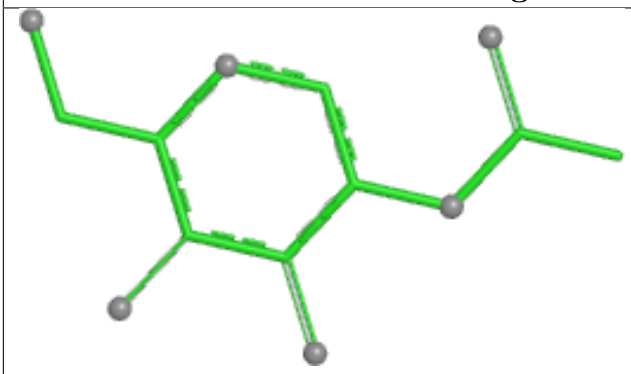


Rings

Ligand NAG A 1405



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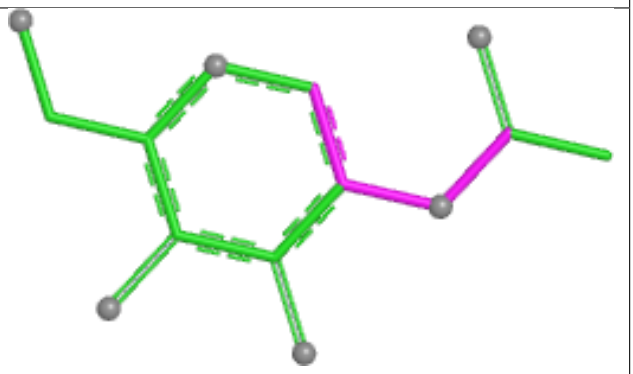
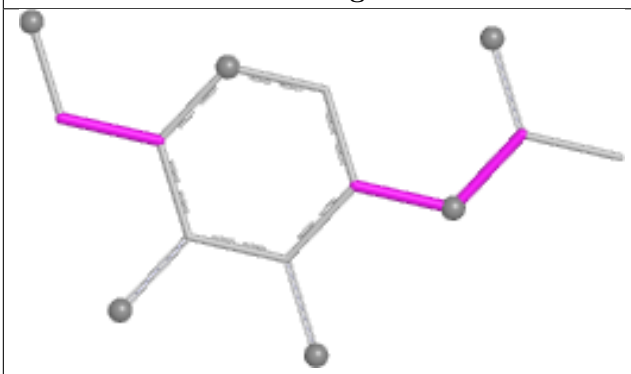


Bond angles



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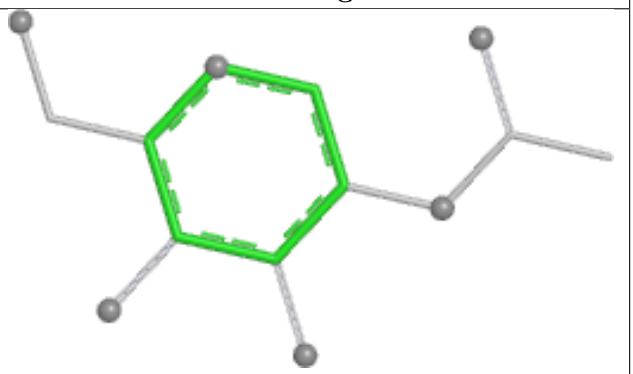
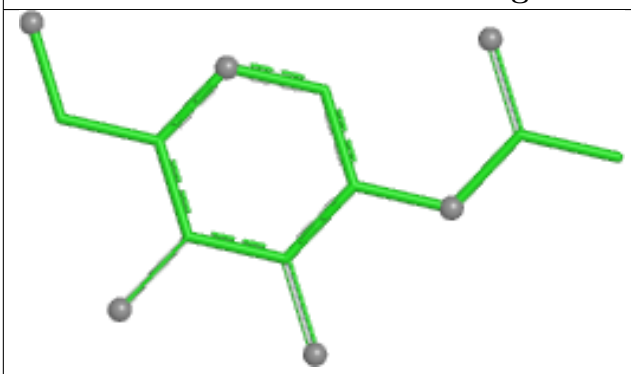


Rings

Ligand NAG C 1406



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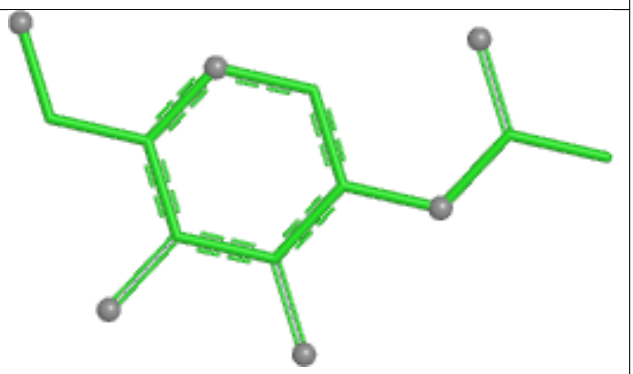
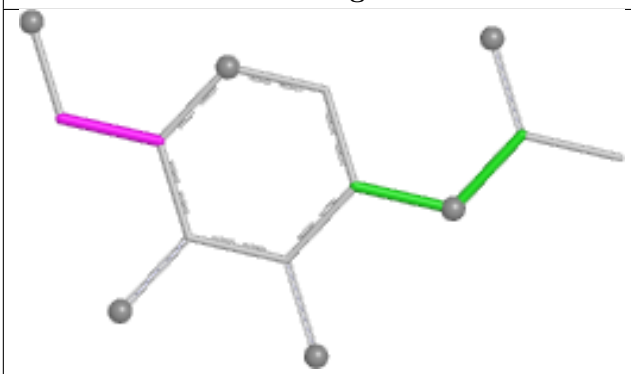


Bond angles



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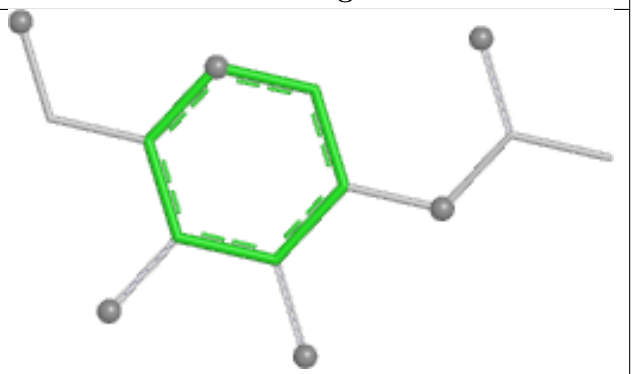
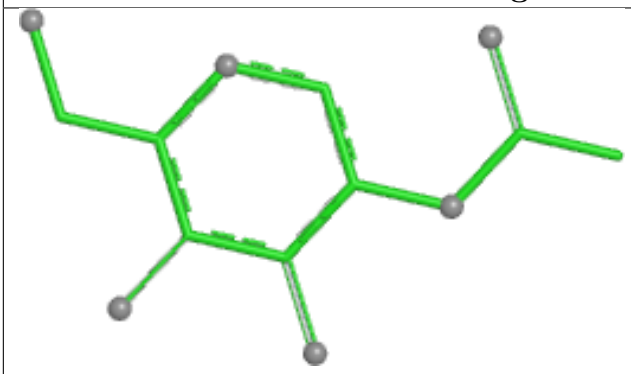


Rings

Ligand NAG A 1401



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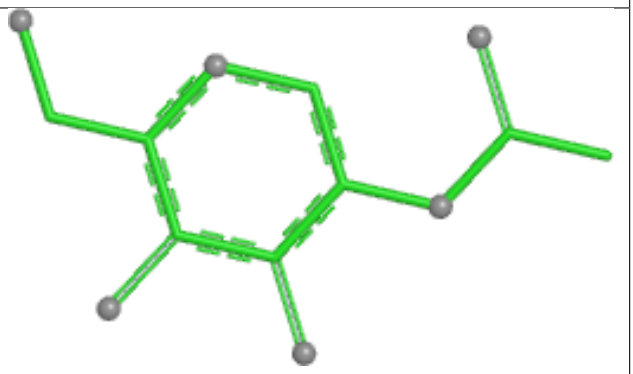

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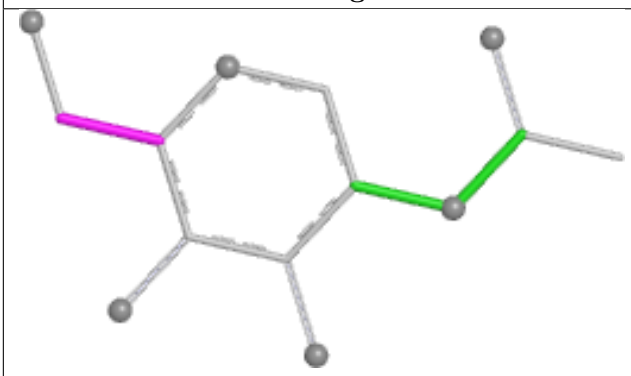

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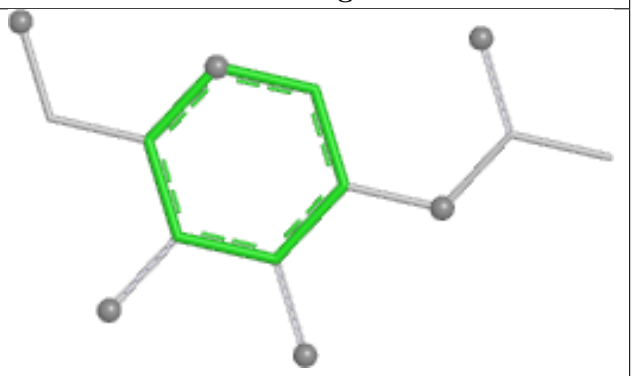
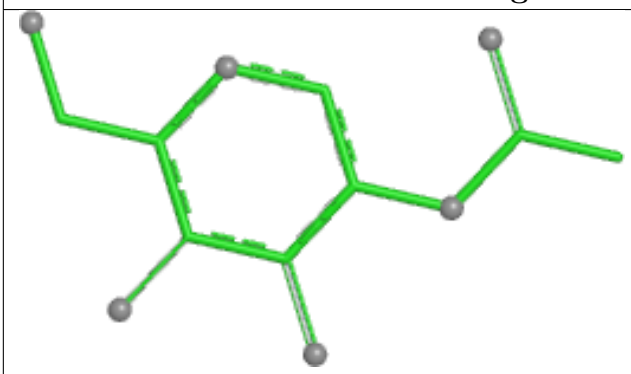


Rings

Ligand NAG A 1408



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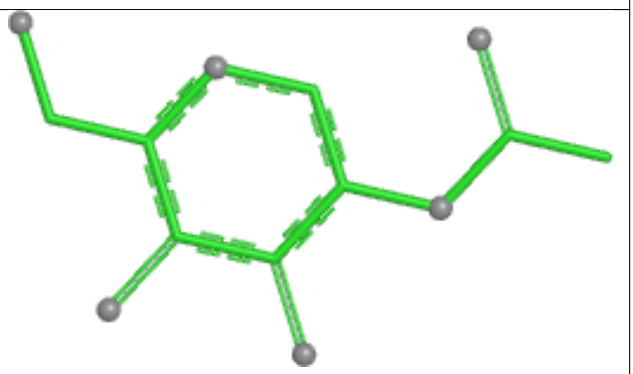
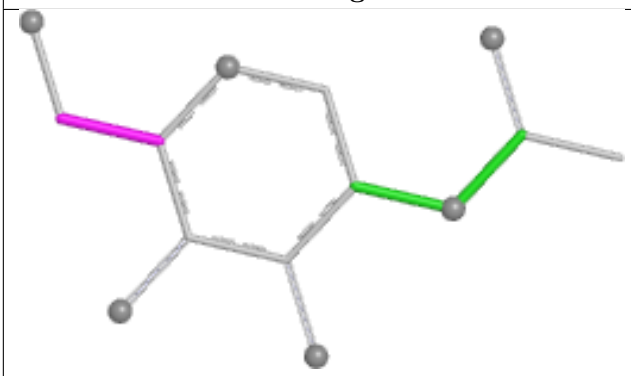


Bond angles



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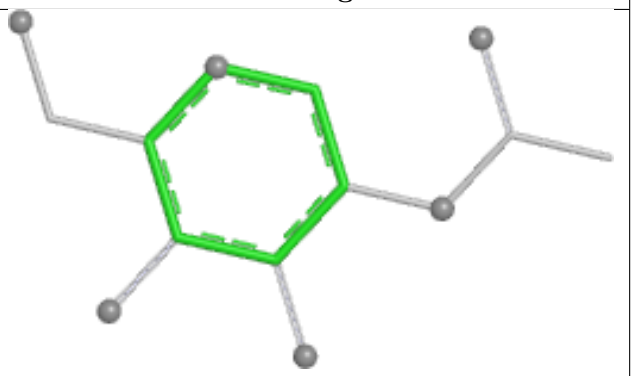
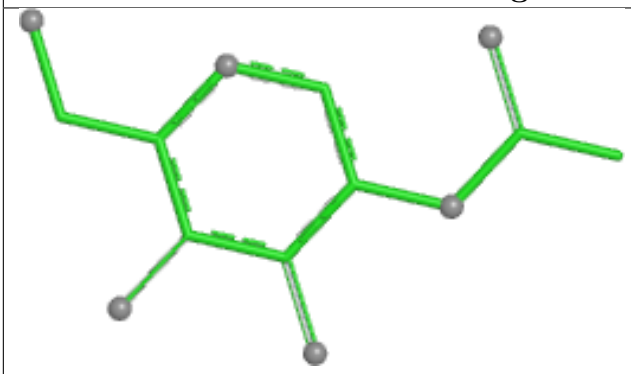


Rings

Ligand NAG A 1404



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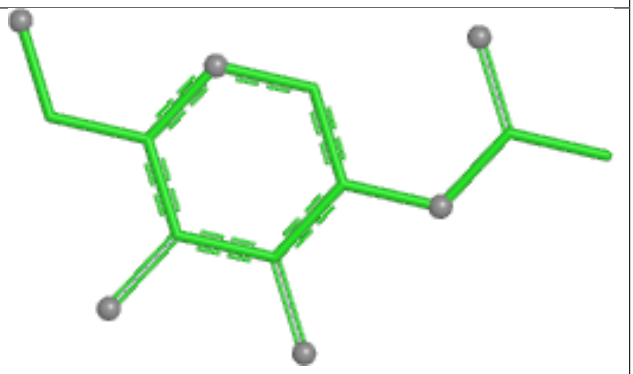
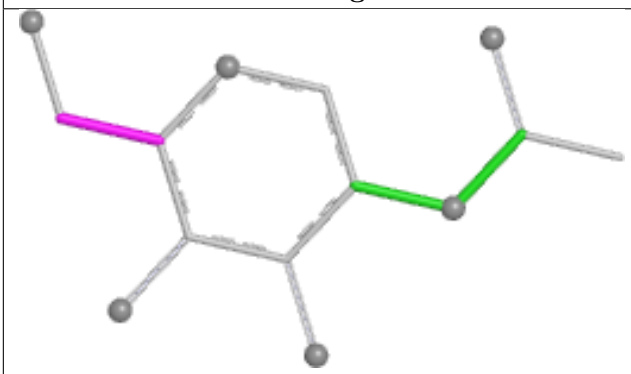


Bond angles



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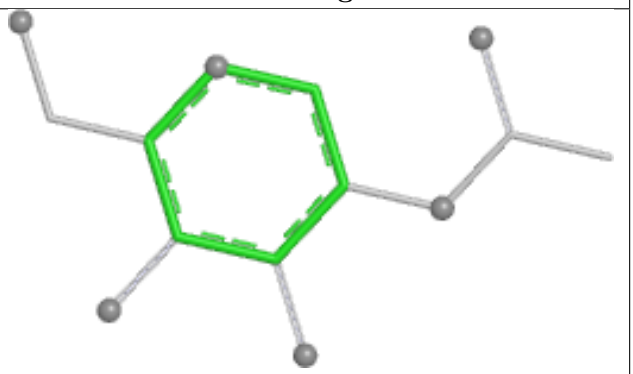
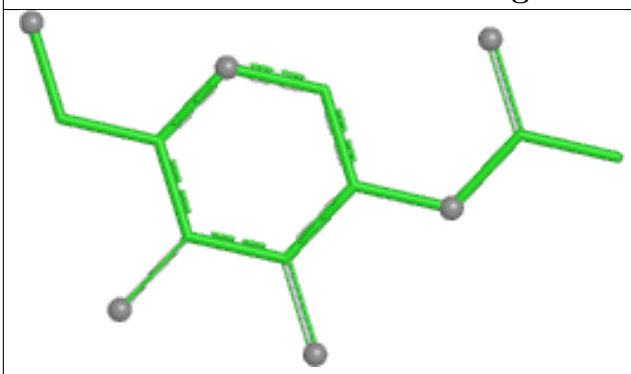
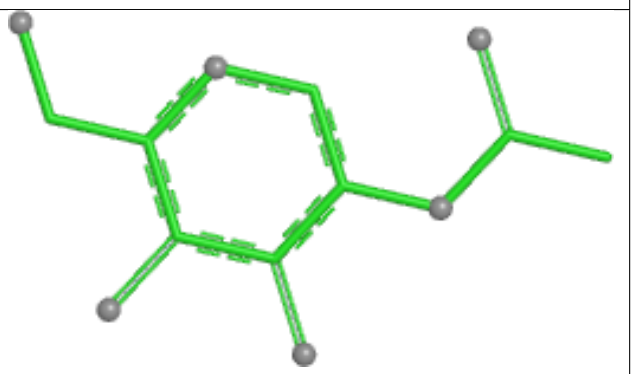


Rings

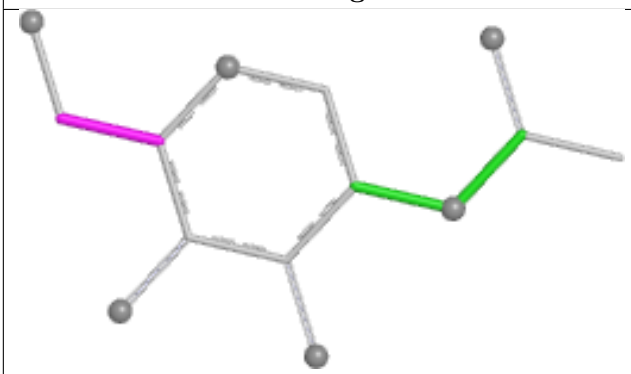
Ligand NAG B 1408



Bond lengths



Bond angles



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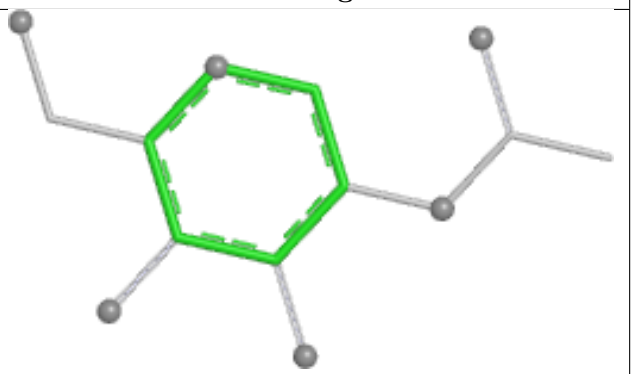
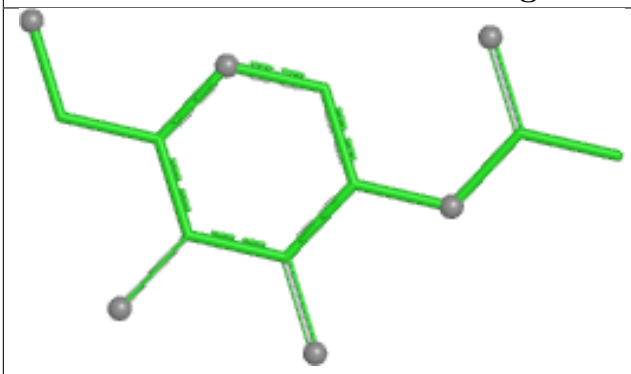


Rings

Ligand NAG D 901



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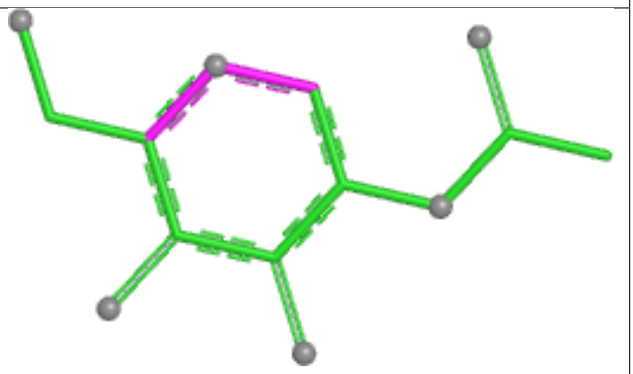
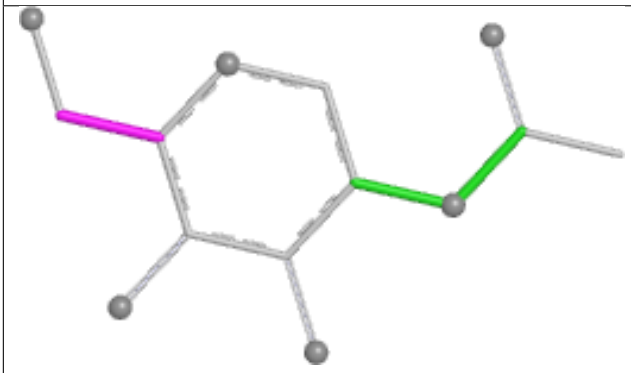


Bond angles



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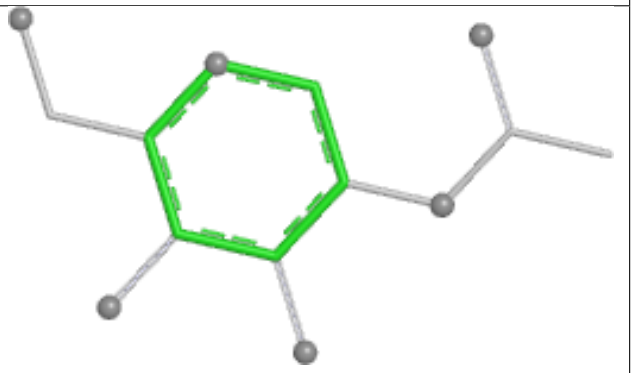
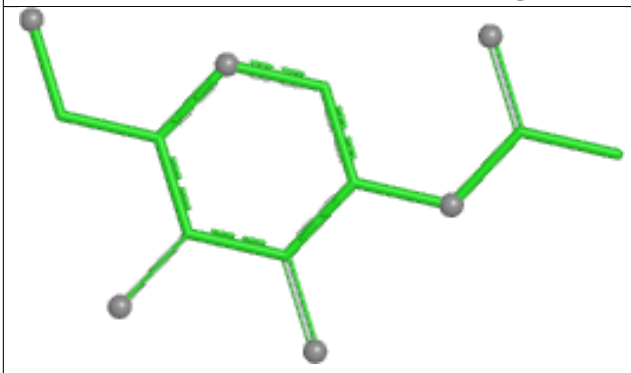
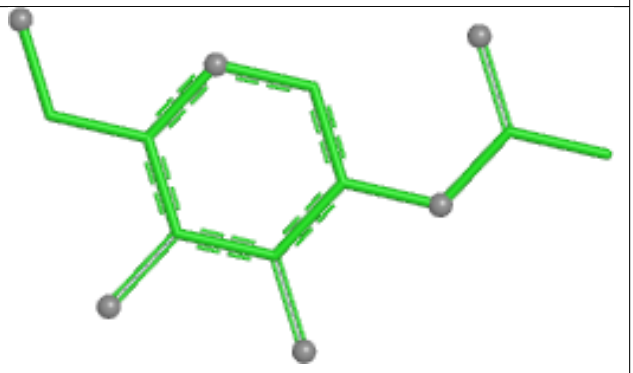


Rings

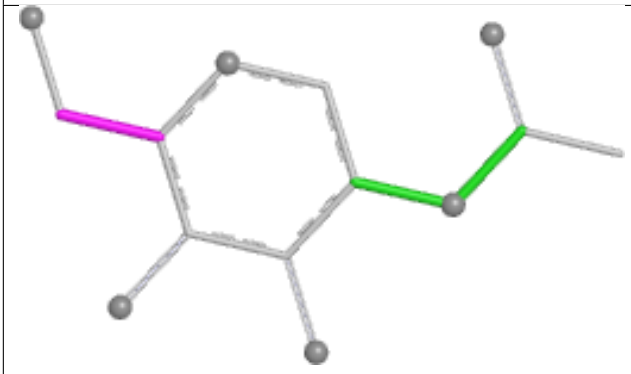
Ligand NAG B 1410



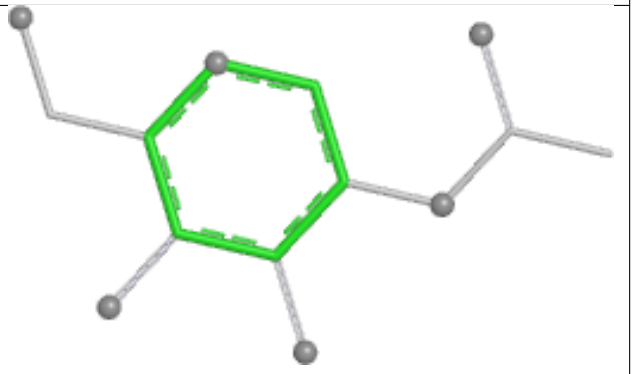
Bond lengths



Bond angles

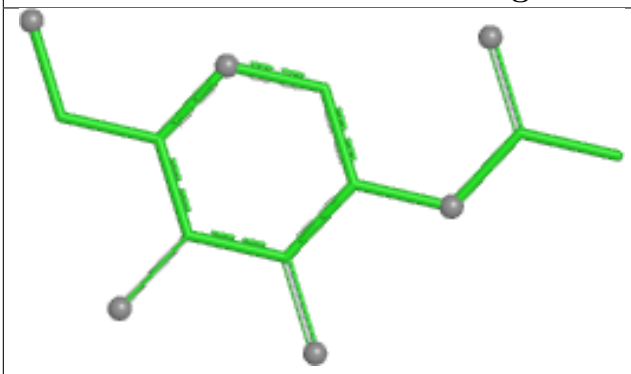


Torsions

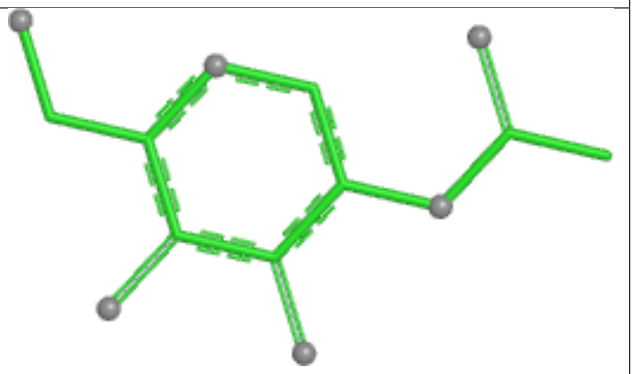


Rings

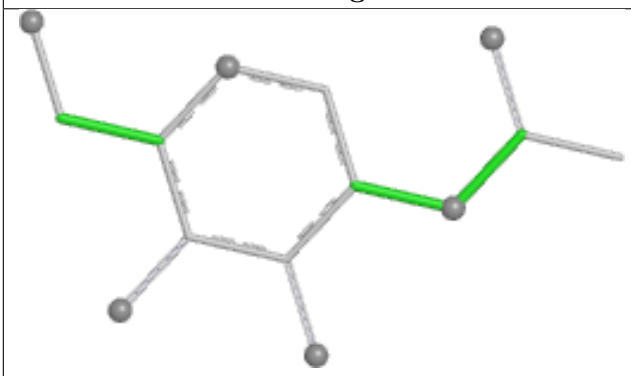
Ligand NAG B 1409



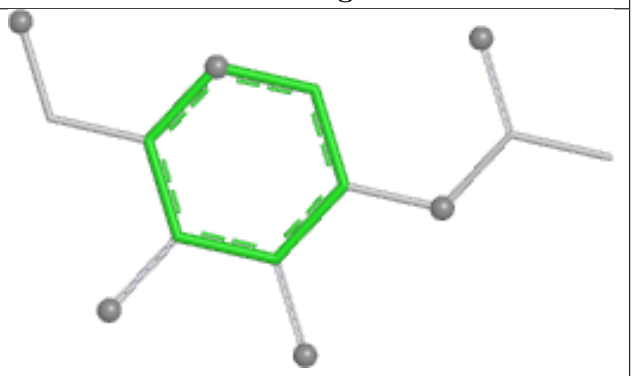
Bond lengths



Bond angles

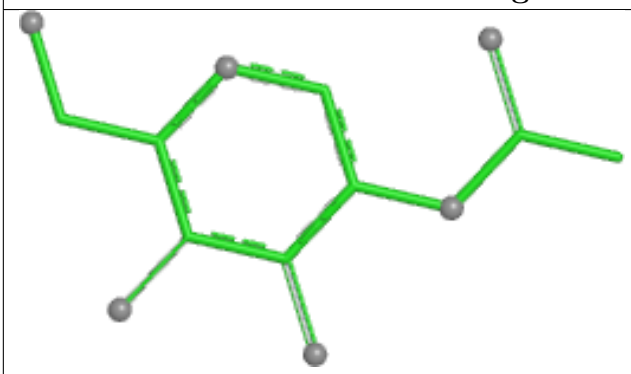


Torsions

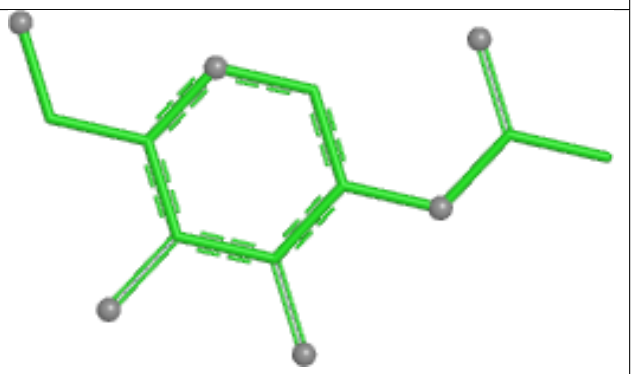


Rings

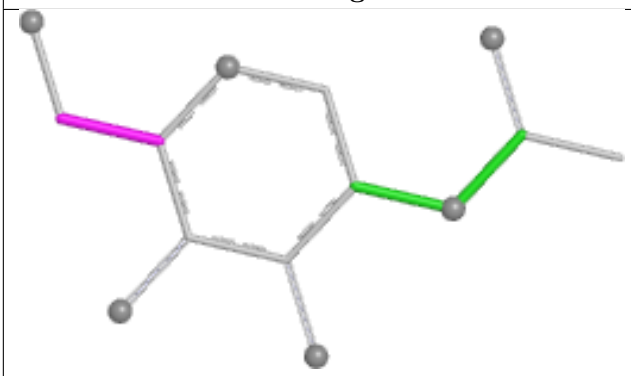
Ligand NAG B 1402



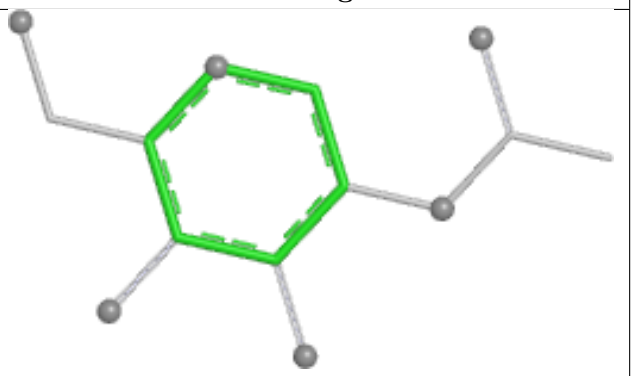
Bond lengths



Bond angles

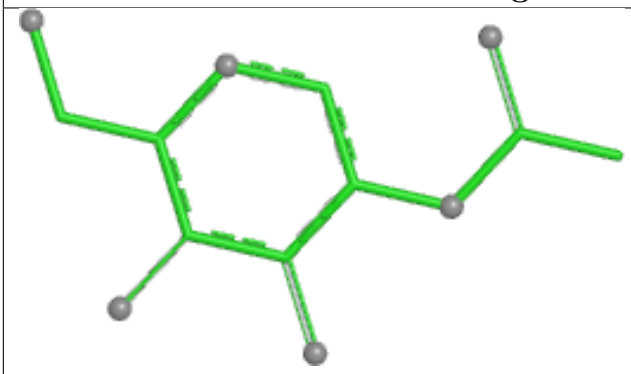


Torsions

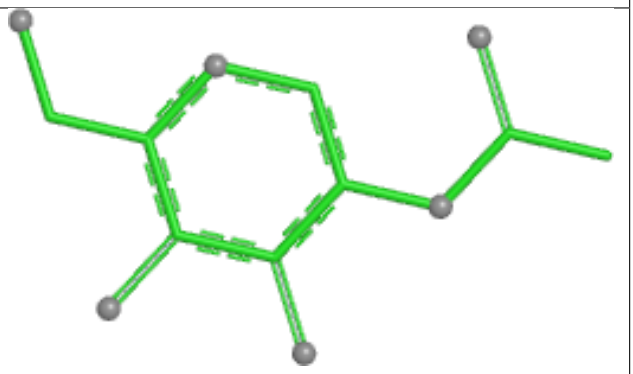


Rings

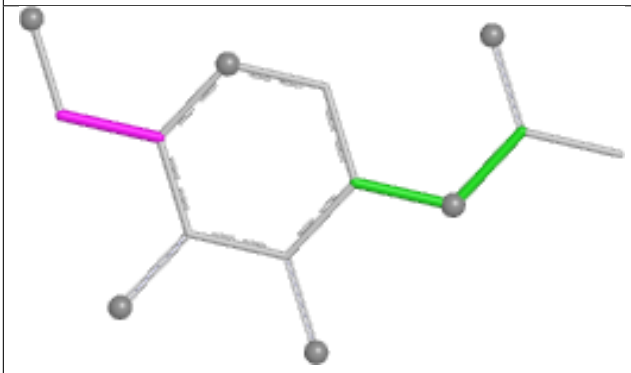
Ligand NAG C 1402



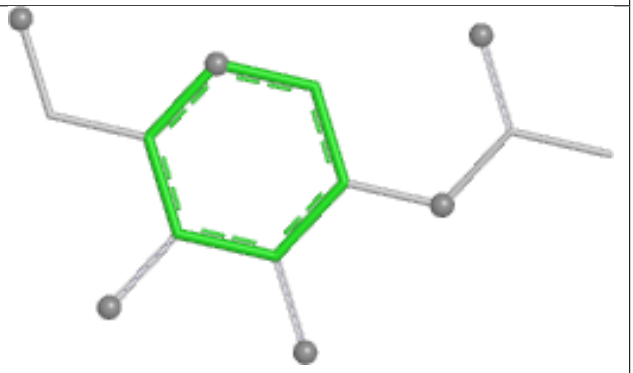
Bond lengths



Bond angles

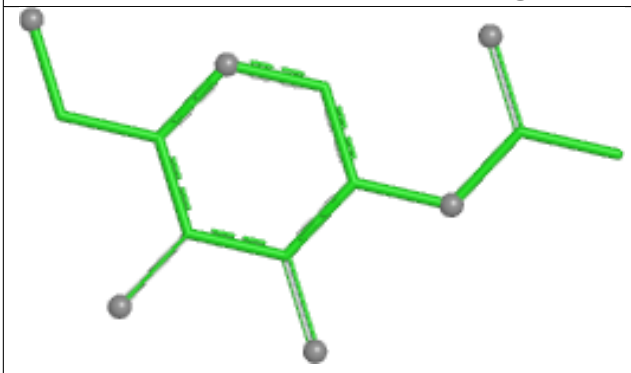


Torsions

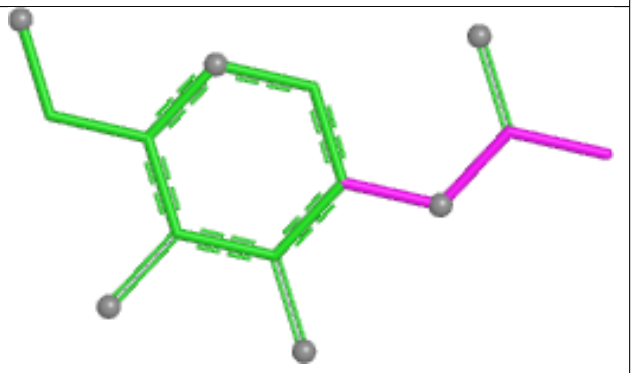


Rings

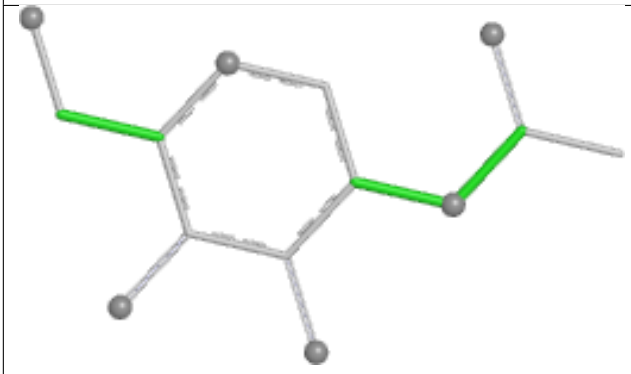
Ligand NAG B 1411



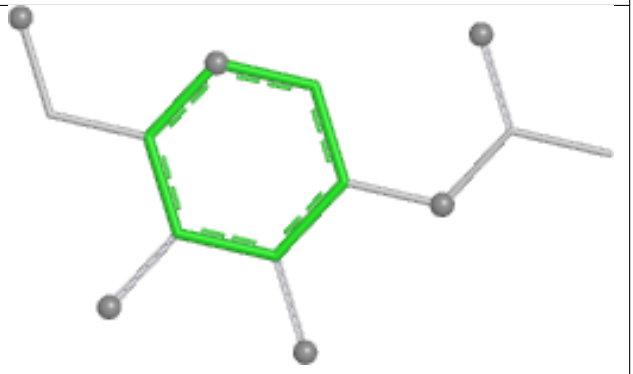
Bond lengths



Bond angles

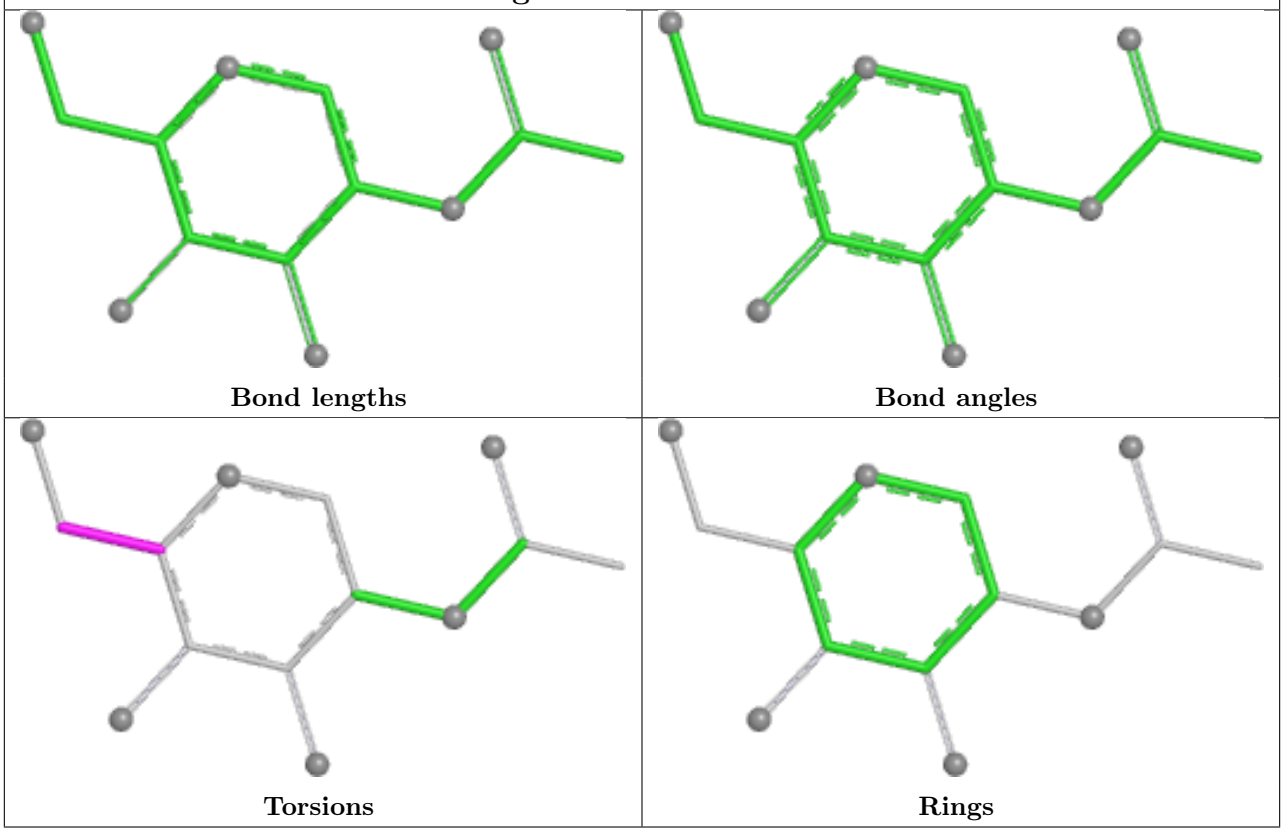


Torsions



Rings

Ligand NAG C 1403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

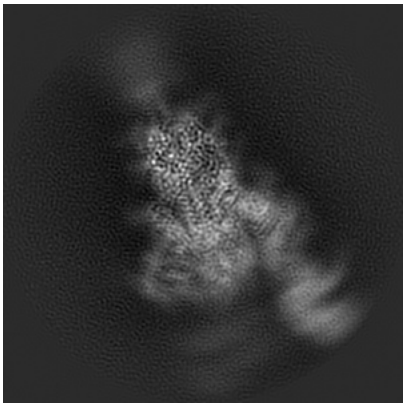
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30896. These allow visual inspection of the internal detail of the map and identification of artifacts.

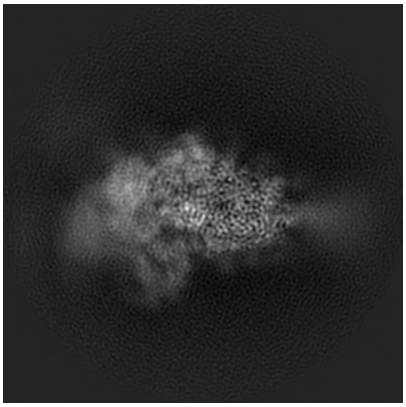
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

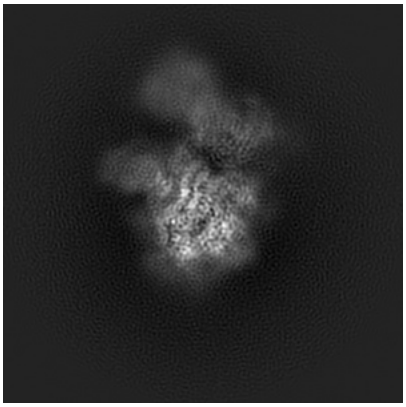
6.1.1 Primary map



X



Y

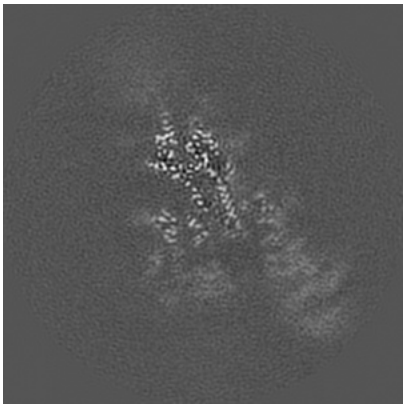


Z

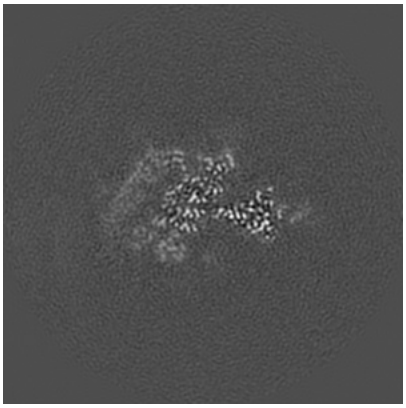
The images above show the map projected in three orthogonal directions.

6.2 Central slices

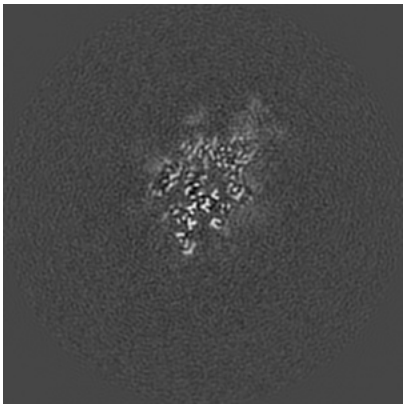
6.2.1 Primary map



X Index: 144



Y Index: 144

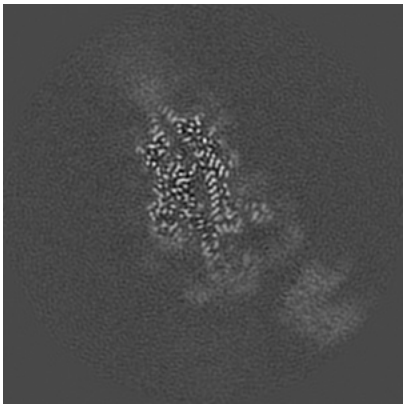


Z Index: 144

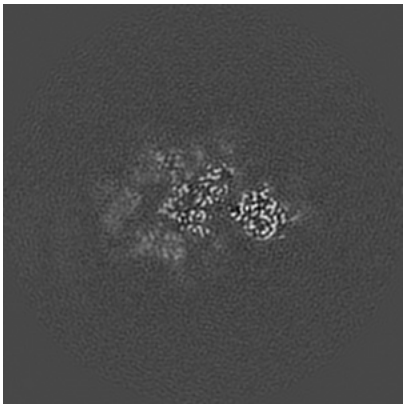
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

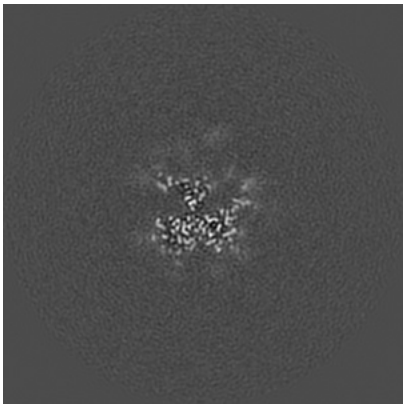
6.3.1 Primary map



X Index: 131



Y Index: 141

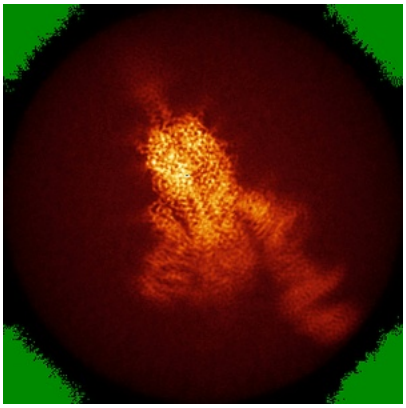


Z Index: 164

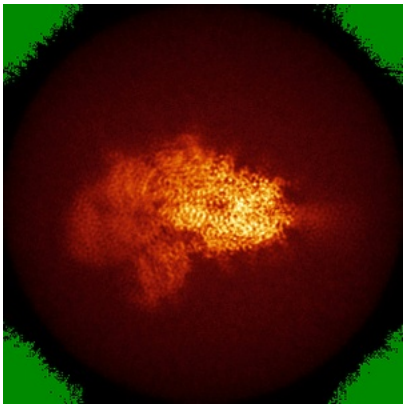
The images above show the largest variance slices of the map in three orthogonal directions.

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

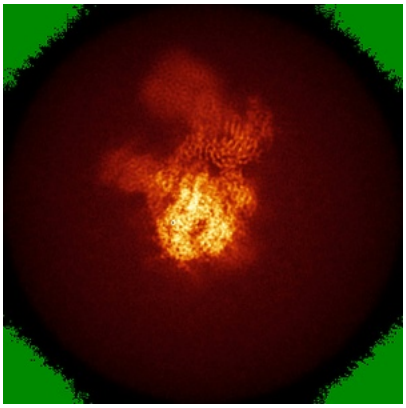
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

This section was not generated.

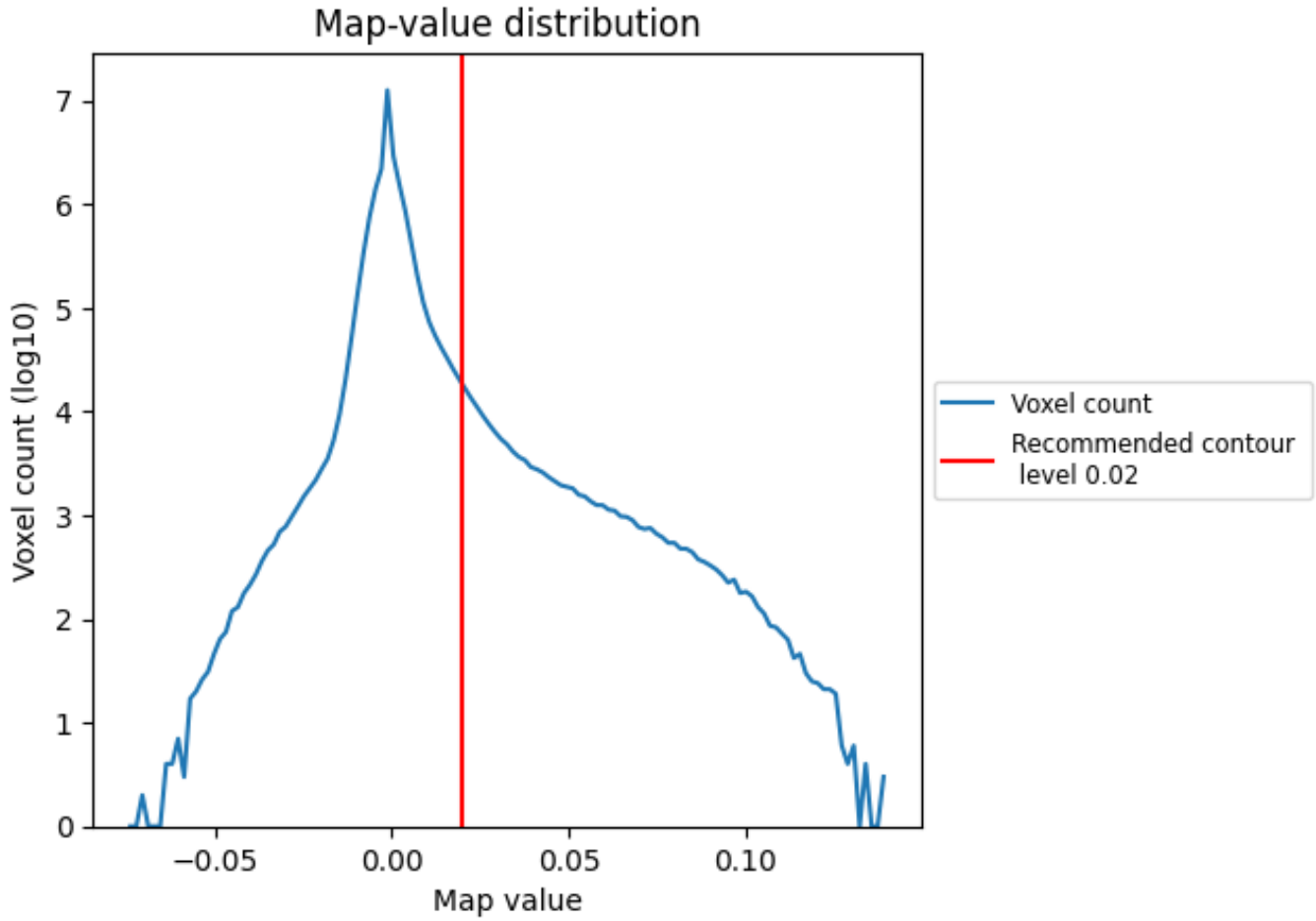
6.6 Mask visualisation (i)

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

7 Map analysis

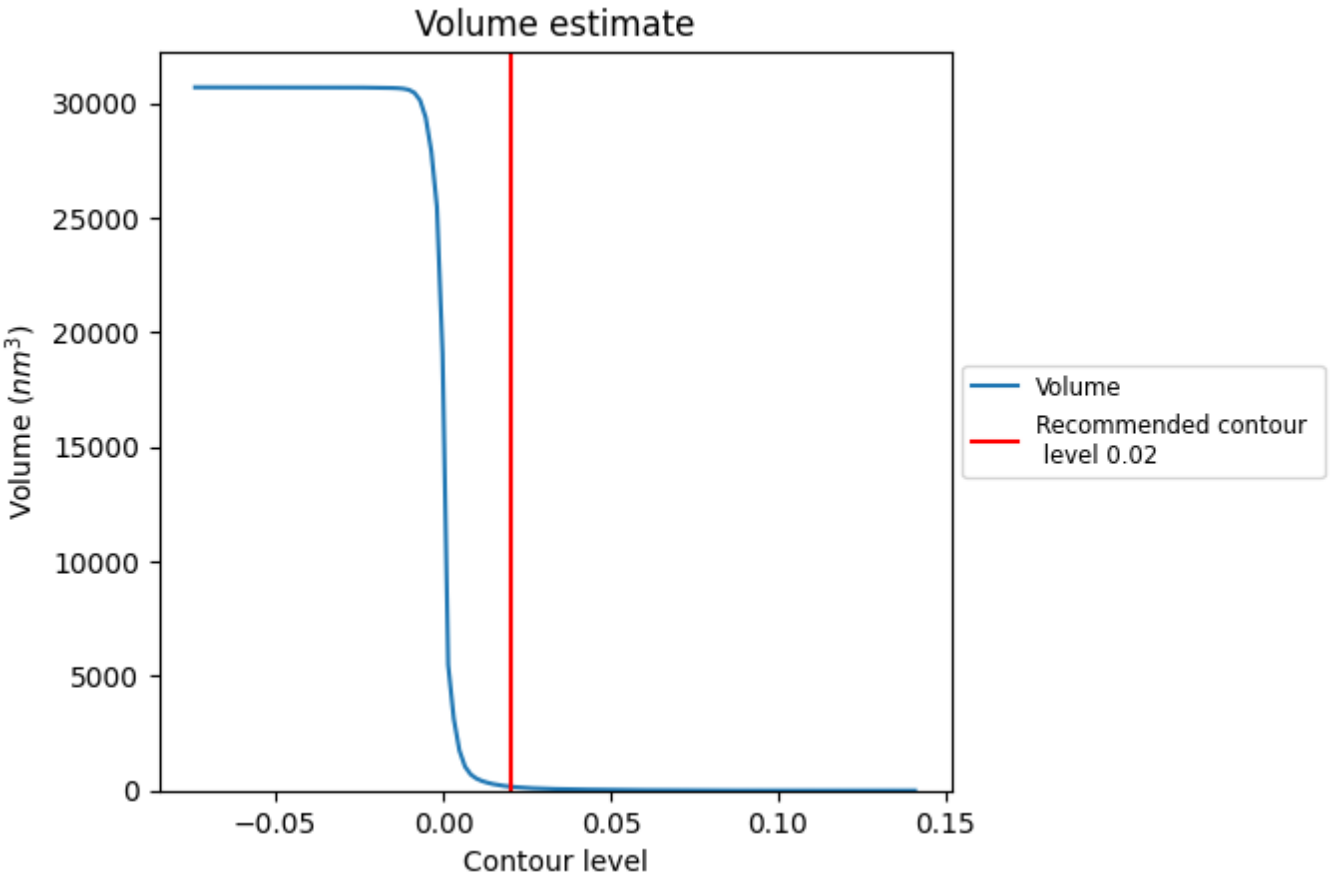
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

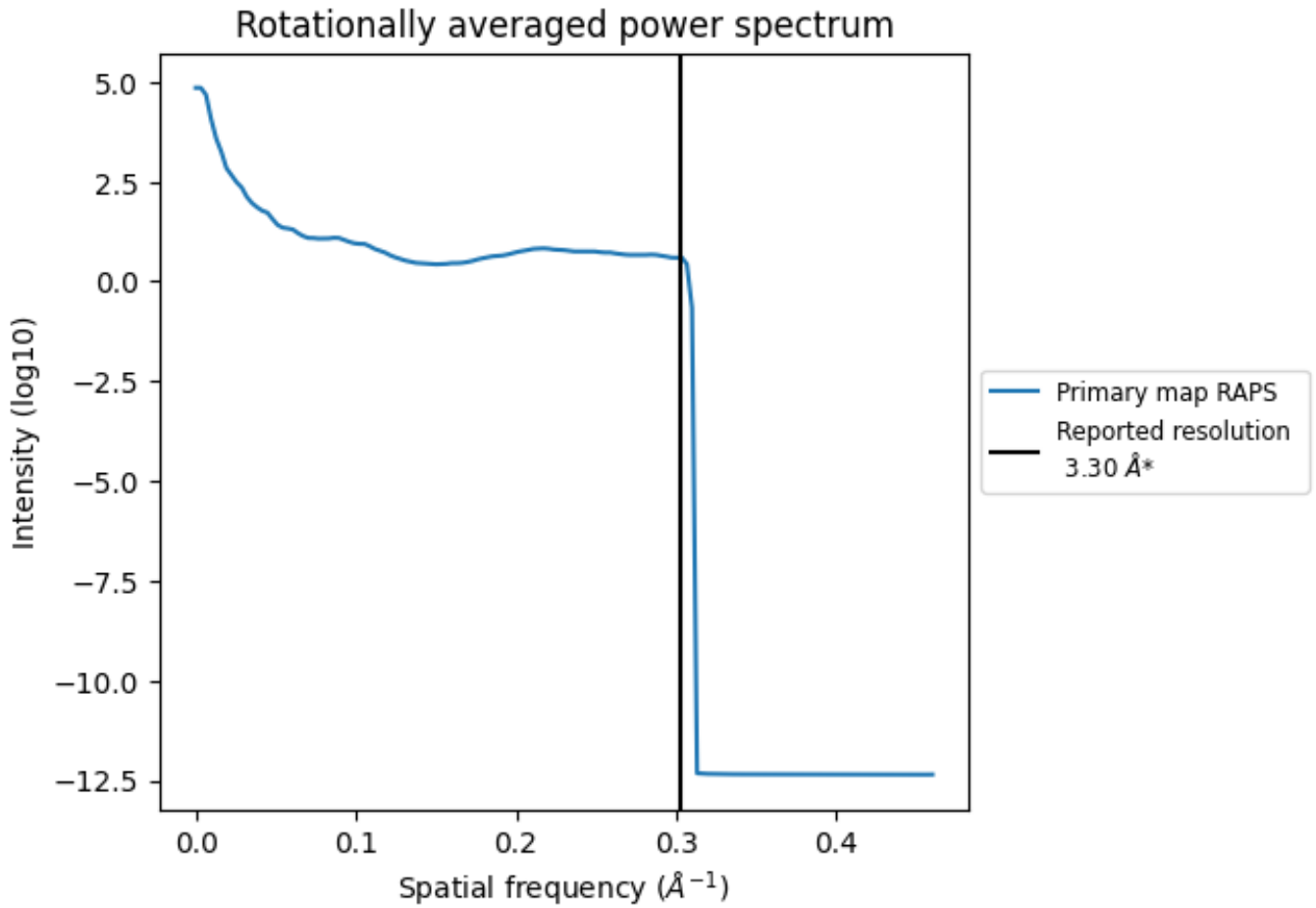
7.2 Volume estimate



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 156 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 0.303 $Å^{-1}$

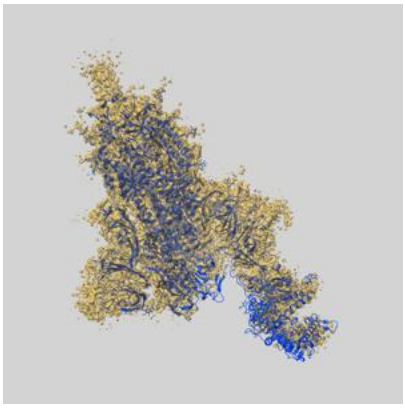
8 Fourier-Shell correlation

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

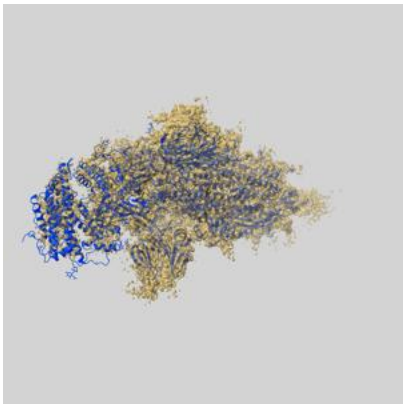
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30896 and PDB model 7DX5. Per-residue inclusion information can be found in section 3 on page 11.

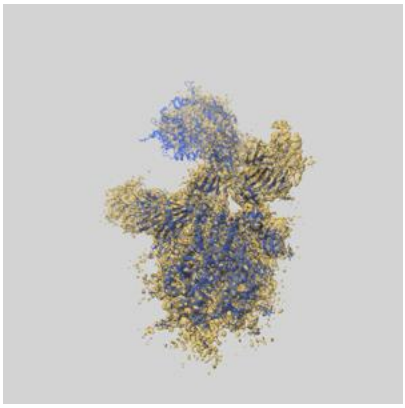
9.1 Map-model overlay



X



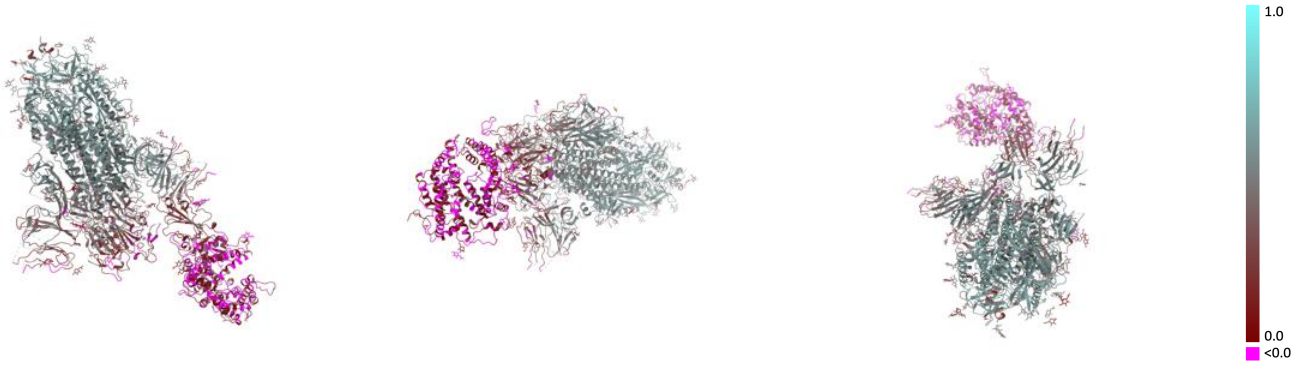
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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)



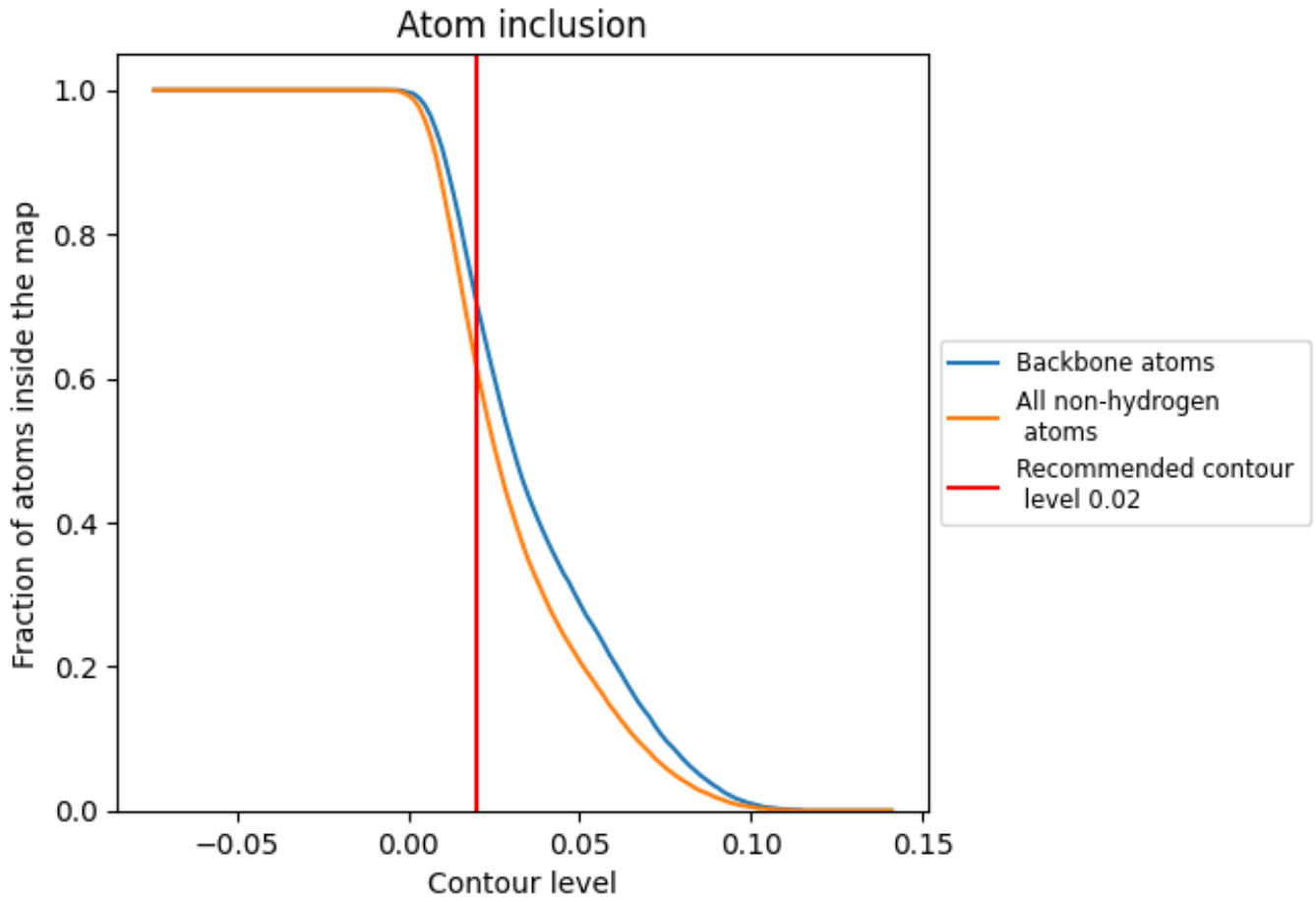
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.3670
A	0.7180	0.4250
B	0.7700	0.4660
C	0.7040	0.4240
D	0.0770	0.0380
E	0.5360	0.2990
F	0.2860	0.1300
G	0.7860	0.5090
H	0.5710	0.3660
I	0.5360	0.4610
J	0.8210	0.5450
K	0.7860	0.4110
L	0.0000	-0.0530
M	0.3930	0.2350
N	0.7500	0.4480
O	0.6070	0.4310
P	0.8210	0.4590
Q	0.6070	0.3440
R	0.0710	0.1400
S	0.1430	-0.0580
T	0.4290	0.2840
U	0.7500	0.4870
V	0.7500	0.3810
W	0.4640	0.2670
X	0.7500	0.4510
Y	0.6430	0.3290
Z	0.1430	0.0050
a	0.0000	0.1120
b	0.0000	0.0070
c	0.0000	-0.0970
d	0.0000	0.1070

