Full wwPDB EM Validation Report (i)

Mar 8, 2026 – 08:09 AM UTC

PDB ID	:	7CZW / pdb_00007czw
EMDB ID	:	EMD-30519
Title	:	S protein of SARS-CoV-2 in complex bound with P5A-2G7
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.
Deposited on	:	2020-09-09
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

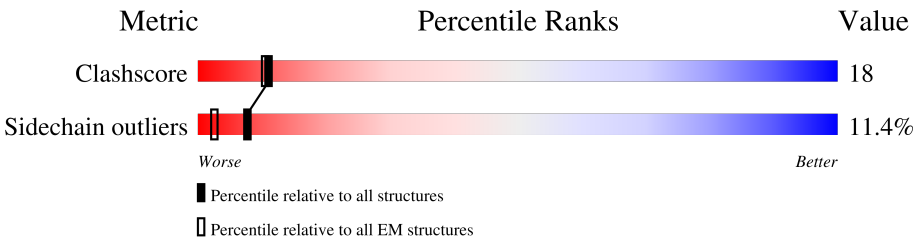
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

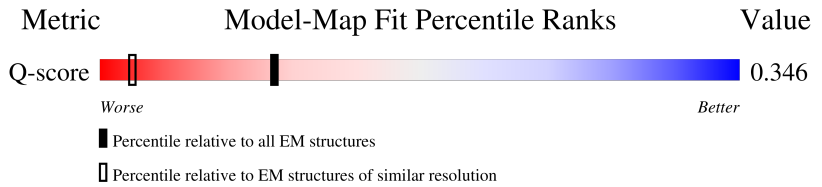
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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% 55% 21% • 22%
1	B	1283	7% 57% 18% • 23%
1	C	1283	18% 56% 19% • 22%
2	H	458	50% 30% 19% • 50%
2	J	458	50% 29% 19% • 50%

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Mol	Chain	Length	Quality of chain
3	L	217	98% 46% 48% 5%
3	N	217	99% 48% 47%
4	D	2	50% 100%
4	E	2	100% 100%
4	F	2	50% 50%
4	G	2	50% 50%
4	I	2	50% 50%
4	K	2	50% 50%
4	M	2	50% 50%
4	O	2	100% 50% 50%
4	P	2	50% 100%
4	Q	2	50% 50%
4	R	2	50% 50%
4	S	2	100%
4	T	2	100%
4	U	2	50% 50% 50%
4	V	2	100% 100%
4	W	2	50% 50% 50%
4	X	2	50% 50%
4	Y	2	100%
4	Z	2	50% 50% 50%
4	a	2	100%
4	b	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31004 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
			Total	C	N	O	S		
1	A	1006	7863	5019	1308	1500	36	0	0
1	B	982	7696	4920	1279	1462	35	0	0
1	C	1004	7853	5014	1307	1496	36	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	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	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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 Immunoglobulin heavy variable 4-61,chain H of P5A-2G7,Epididymis luminal protein 214.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	230	1727	1094	286	341	6	0	0
2	J	230	1727	1094	286	341	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	27	ASP	GLY	conflict	UNP A0A0C4DH41
J	27	ASP	GLY	conflict	UNP A0A0C4DH41

- Molecule 3 is a protein called IGL c2312_light_IGLV2-14_IGLJ2,IGL@ protein.

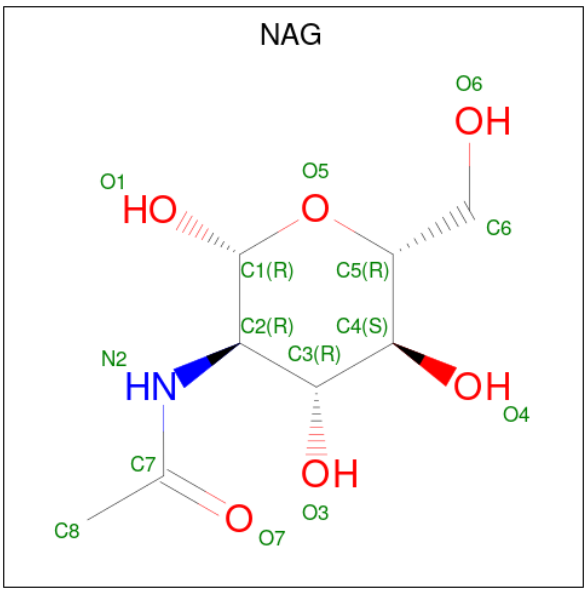
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	214	1579	983	262	329	5	0	0
3	N	214	1579	983	262	329	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0
4	G	2	28	16	2	10	0	0
4	I	2	28	16	2	10	0	0
4	K	2	28	16	2	10	0	0
4	M	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16	2	10	0	0
4	U	2	28	16	2	10	0	0
4	V	2	28	16	2	10	0	0
4	W	2	28	16	2	10	0	0
4	X	2	28	16	2	10	0	0
4	Y	2	28	16	2	10	0	0
4	Z	2	28	16	2	10	0	0
4	a	2	28	16	2	10	0	0
4	b	2	28	16	2	10	0	0

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

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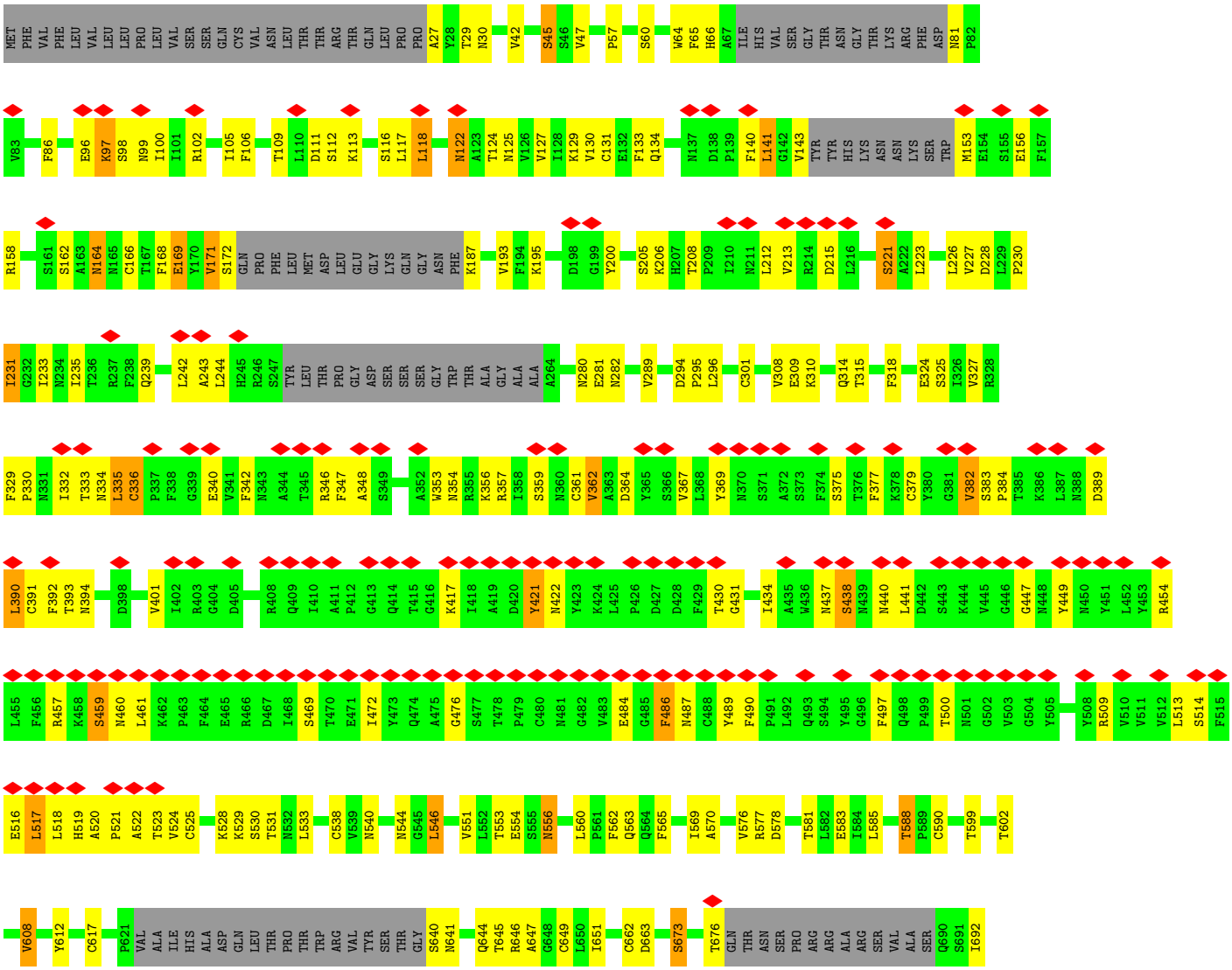
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8	1	5	0
5	C	1	14	8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

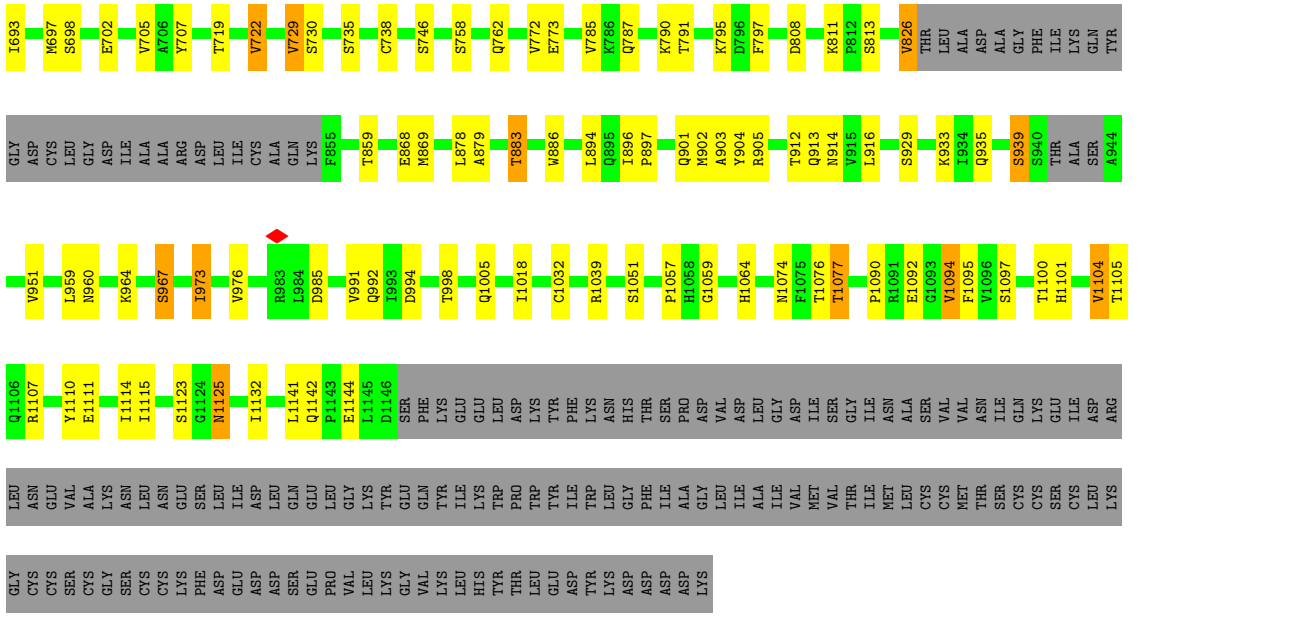
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

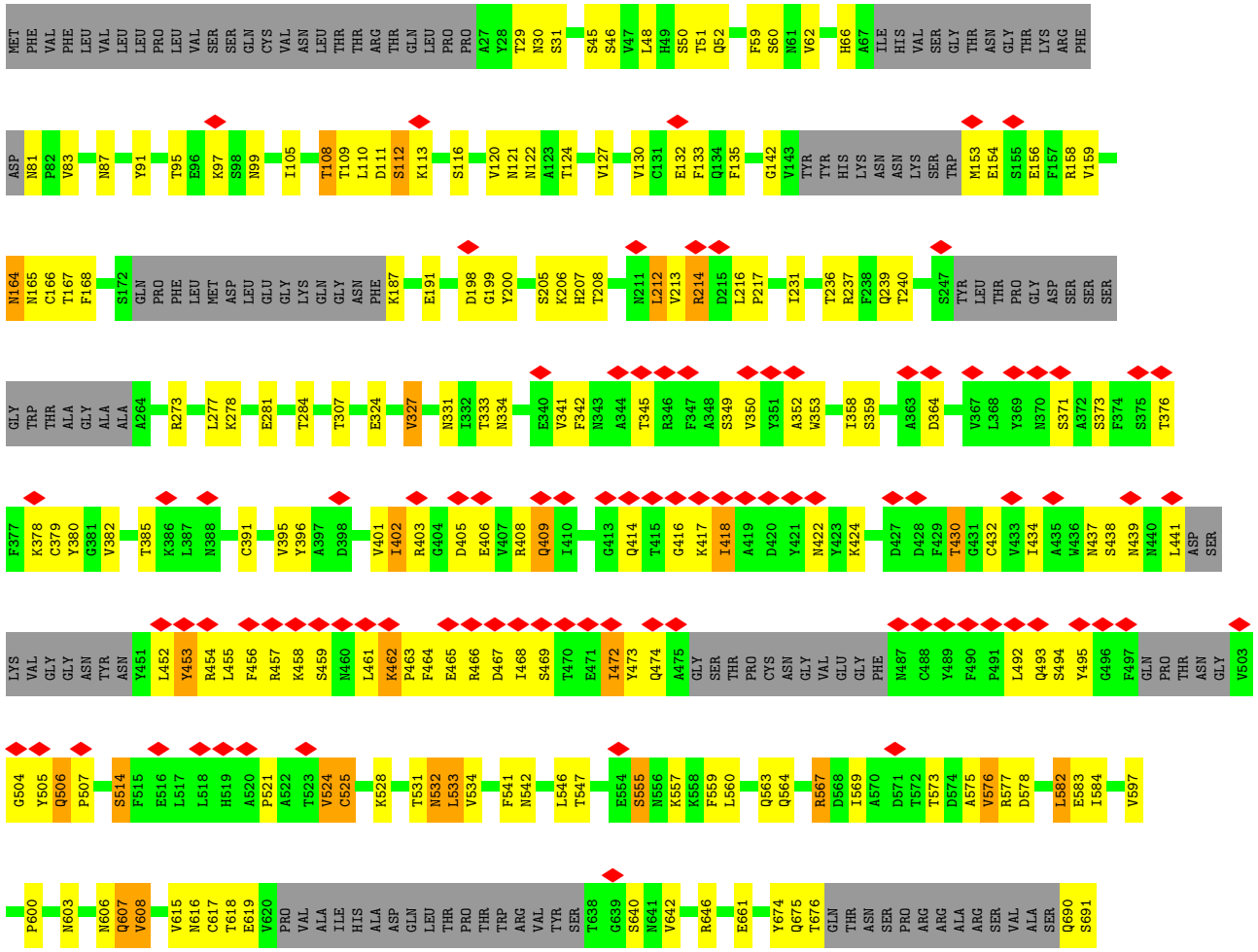
Chain A: 12% 55% 21% • 22%

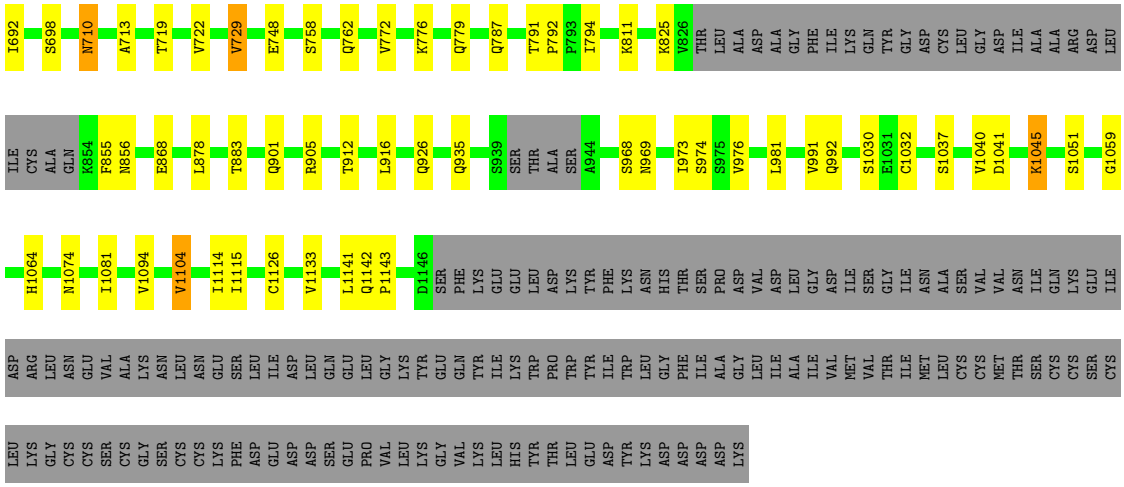




- Molecule 1: Spike glycoprotein

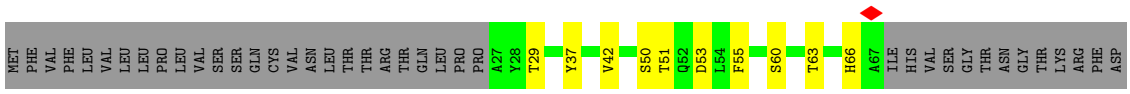
Chain B:

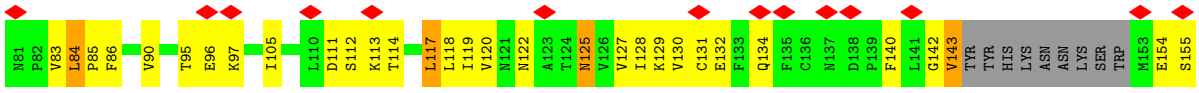


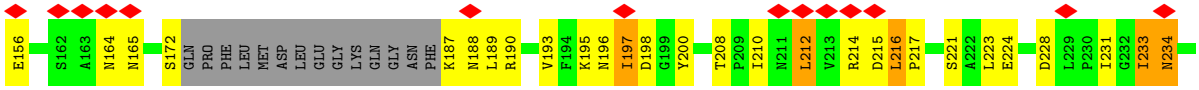


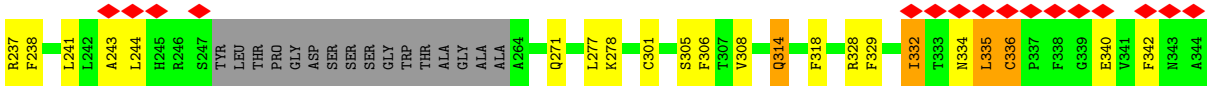
- Molecule 1: Spike glycoprotein

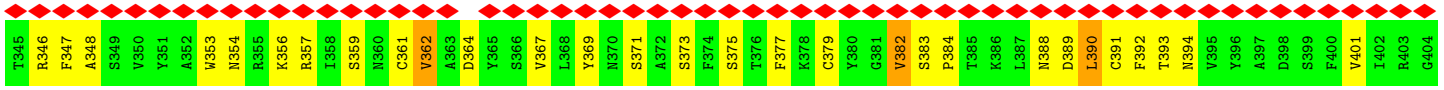
Chain C:

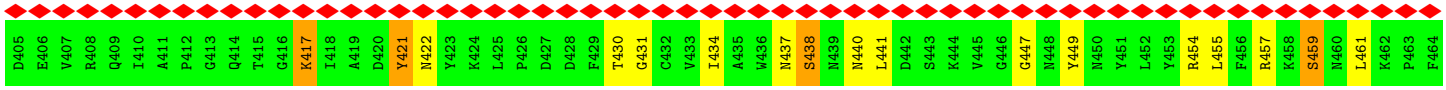


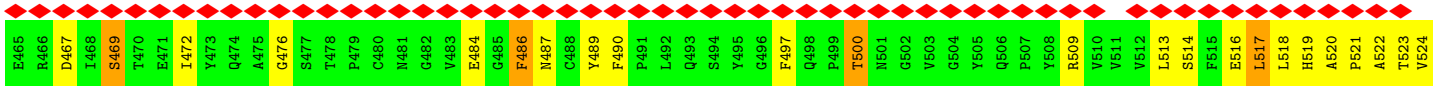


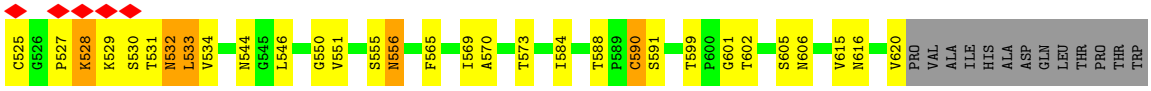


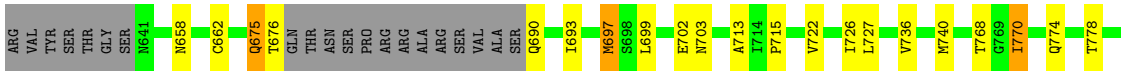


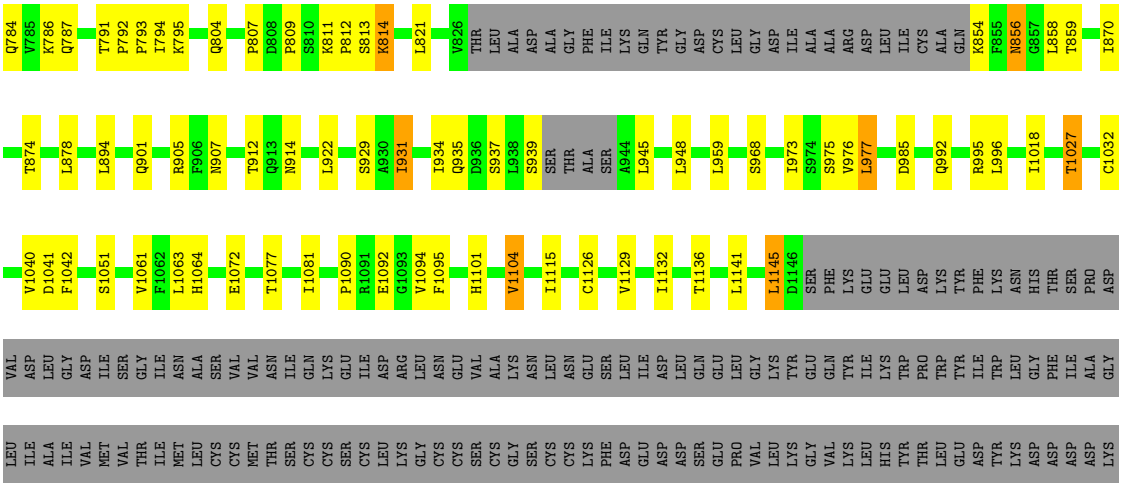






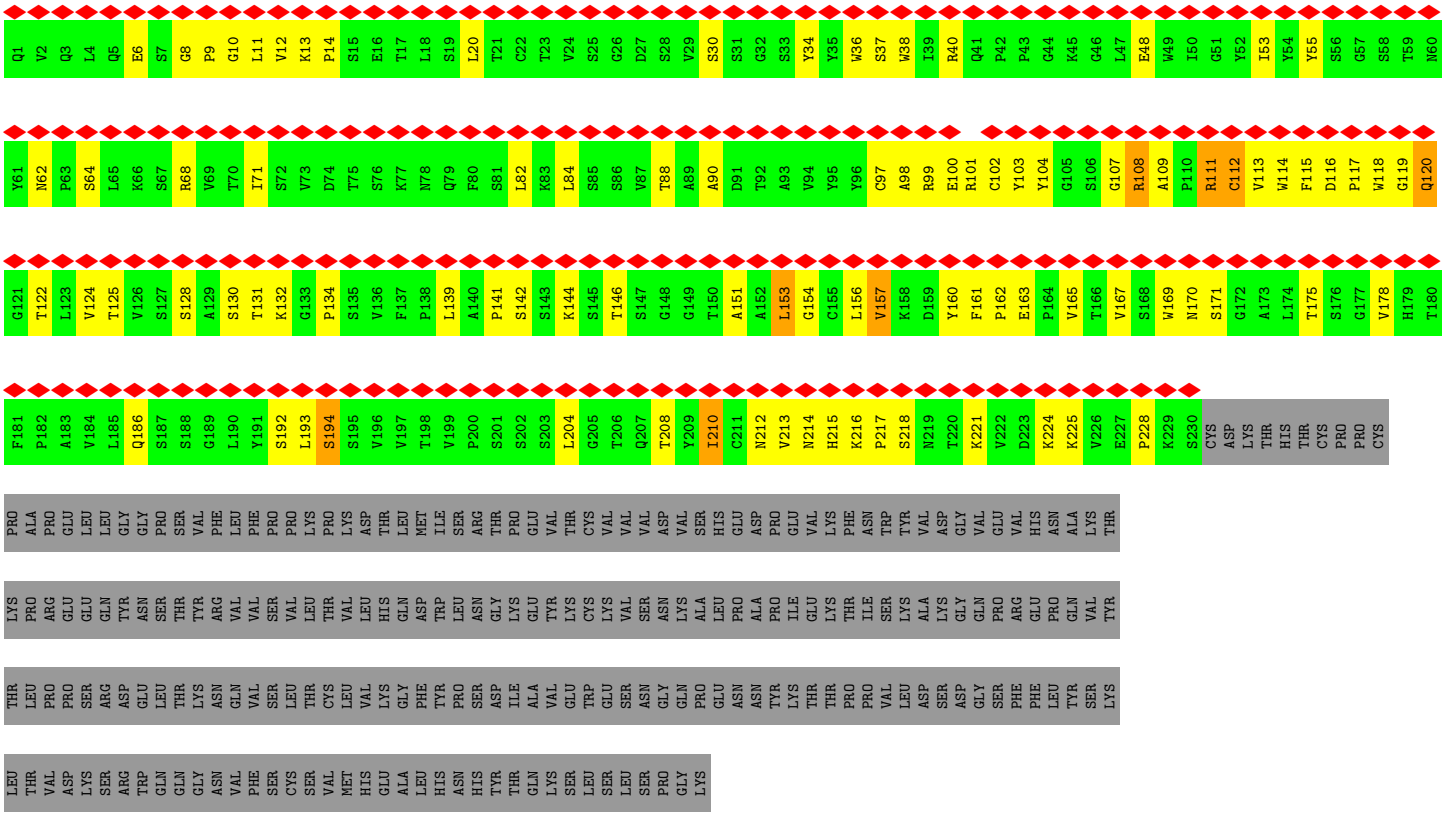






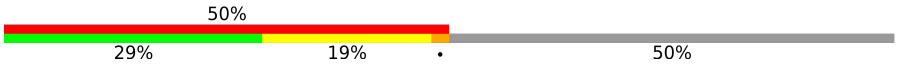
• Molecule 2: Immunoglobulin heavy variable 4-61,chain H of P5A-2G7,Epididymis luminal protein 214

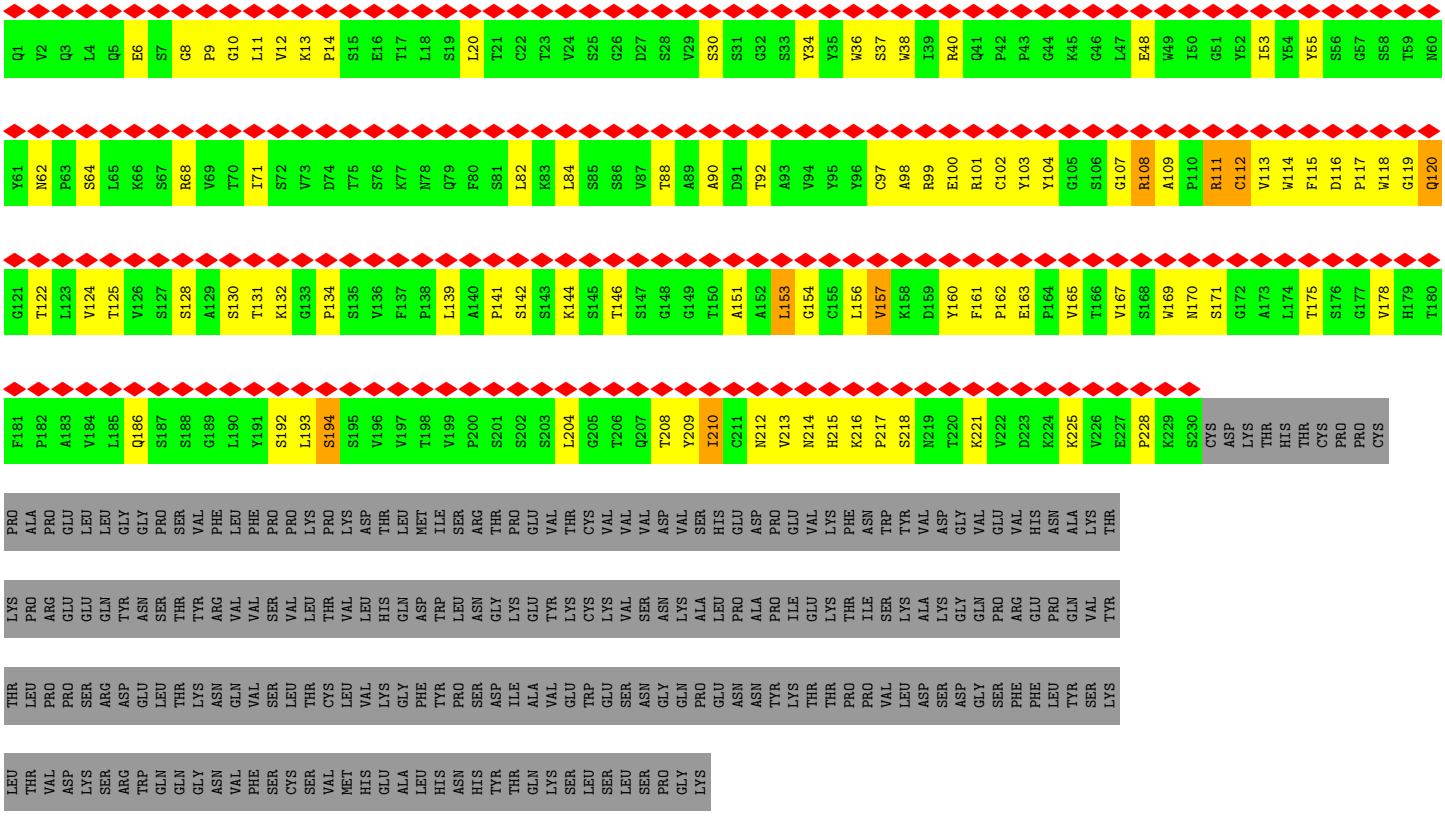
Chain H:



• Molecule 2: Immunoglobulin heavy variable 4-61,chain H of P5A-2G7,Epididymis luminal protein 214

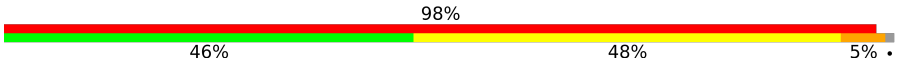
Chain J:

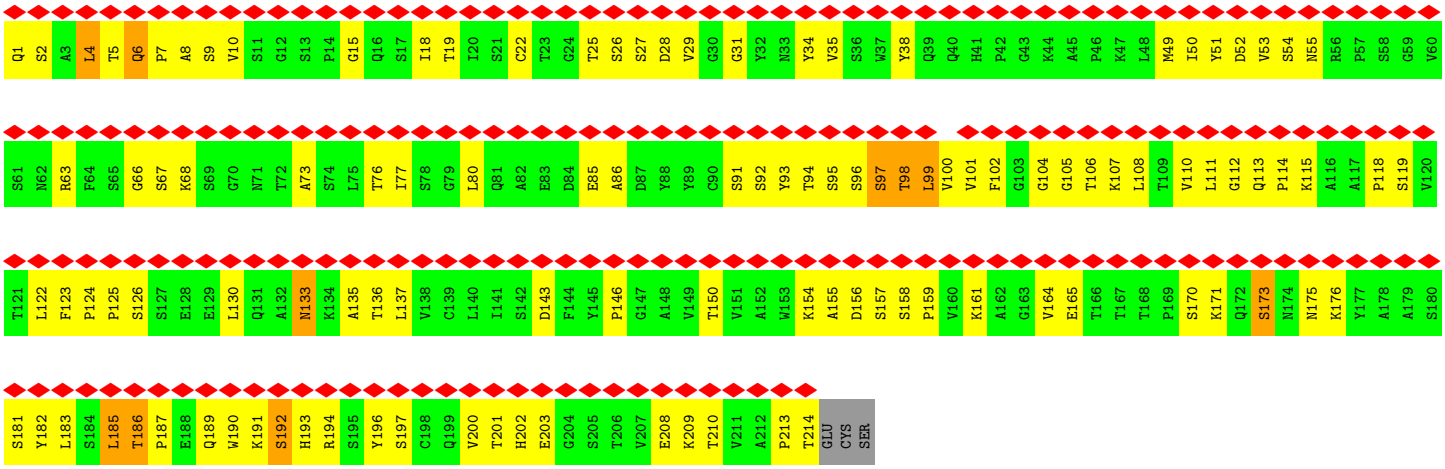




- Molecule 3: IGL c2312_light_IGLV2-14_IGLJ2,IGL@ protein

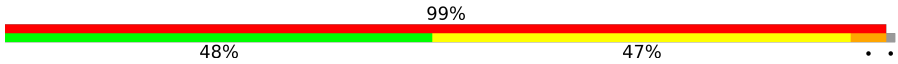
Chain L:

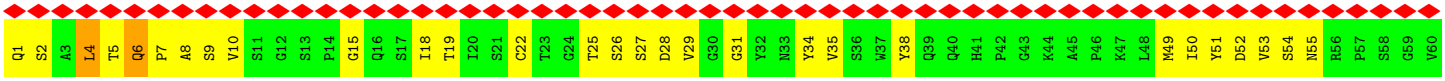




- Molecule 3: IGL c2312_light_IGLV2-14_IGLJ2,IGL@ protein

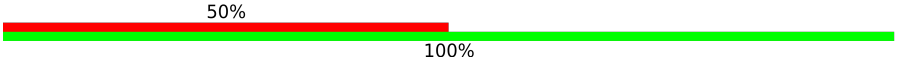
Chain N:





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

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

Chain I:

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

Chain K: 50% 50%

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

Chain M: 50% 50%

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

Chain O: 100% 50% 50%

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

Chain P: 50% 100%

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

Chain Q: 50% 50%

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

Chain R: 50% 50%

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

Chain S: 100%

NAG1 NAG2

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

Chain T: 100%

NAG1 NAG2

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

Chain U: 50% 50% 50%

NAG1 NAG2

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

Chain V: 100% 100%

NAG1 NAG2

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

Chain W: 50% 50% 50%

NAG1 NAG2

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

Chain X: 50% 50%

NAG1 NAG2

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

Chain Y: 100%

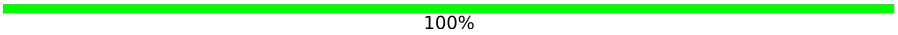
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

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

Chain a:

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

Chain b: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211771	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	0.267	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	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 (i)

5.1 Standard geometry (i)

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	0.52	0/8039	0.61	2/10936 (0.0%)
1	B	0.43	0/7864	0.59	2/10691 (0.0%)
1	C	0.52	0/8028	0.59	3/10919 (0.0%)
2	H	0.32	0/1774	0.58	0/2424
2	J	0.32	0/1774	0.58	0/2424
3	L	0.34	0/1616	0.58	0/2206
3	N	0.34	0/1616	0.58	0/2206
All	All	0.46	0/30711	0.59	7/41806 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	PHE	CA-C-N	5.89	132.80	121.54
1	A	86	PHE	C-N-CA	5.89	132.80	121.54
1	C	156	GLU	N-CA-C	5.87	115.85	108.45
1	C	588	THR	CA-C-N	-5.51	114.11	119.78
1	C	588	THR	C-N-CA	-5.51	114.11	119.78
1	B	212	LEU	CA-C-N	-5.39	117.63	123.08
1	B	212	LEU	C-N-CA	-5.39	117.63	123.08

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	7863	0	7659	241	0
1	B	7696	0	7514	151	0
1	C	7853	0	7653	242	0
2	H	1727	0	1691	171	0
2	J	1727	0	1691	172	0
3	L	1579	0	1527	123	0
3	N	1579	0	1527	124	0
4	D	28	0	25	0	0
4	E	28	0	25	3	0
4	F	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	3	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	2	0
4	b	28	0	25	0	0
5	A	126	0	117	4	0
5	B	154	0	142	10	0
5	C	112	0	104	2	0
All	All	31004	0	30150	1116	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 18.

All (1116) 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)
2:H:116:ASP:HB3	2:H:117:PRO:CD	1.44	1.47
5:B:1410:NAG:O4	5:B:1411:NAG:C1	1.63	1.46
2:J:116:ASP:HB3	2:J:117:PRO:CD	1.44	1.43
1:A:335:LEU:HA	1:A:362:VAL:CG1	1.54	1.33
2:H:111:ARG:HB3	3:L:93:TYR:CZ	1.64	1.33
2:J:111:ARG:HB3	3:N:93:TYR:CZ	1.64	1.33
1:C:490:PHE:CD2	2:J:104:TYR:CD2	2.20	1.29
1:C:417:LYS:NZ	1:C:455:LEU:HB2	1.42	1.29
2:H:111:ARG:HB3	3:L:93:TYR:CE2	1.69	1.28
1:A:490:PHE:CD2	2:H:104:TYR:CD2	2.20	1.28
1:A:490:PHE:CE2	2:H:104:TYR:CE2	2.23	1.27
2:J:111:ARG:HB3	3:N:93:TYR:CE2	1.69	1.27
1:C:490:PHE:CE2	2:J:104:TYR:CE2	2.23	1.27
1:C:490:PHE:HE2	2:J:104:TYR:CE2	1.53	1.26
1:A:490:PHE:HE2	2:H:104:TYR:CE2	1.53	1.26
1:C:335:LEU:HA	1:C:362:VAL:CG1	1.66	1.26
1:A:490:PHE:CE2	2:H:104:TYR:CD2	2.27	1.23
1:C:490:PHE:CE2	2:J:104:TYR:CD2	2.27	1.22
1:A:335:LEU:CA	1:A:362:VAL:HG13	1.68	1.20
2:H:101:ARG:HB2	2:H:114:TRP:CZ2	1.76	1.20
2:H:113:VAL:HG23	2:H:114:TRP:CD1	1.78	1.19
2:J:101:ARG:HB2	2:J:114:TRP:CZ2	1.76	1.19
2:H:113:VAL:HG23	2:H:114:TRP:HD1	1.00	1.17
2:J:113:VAL:HG23	2:J:114:TRP:CD1	1.78	1.16
2:J:113:VAL:HG23	2:J:114:TRP:HD1	1.00	1.15
2:J:116:ASP:CB	2:J:117:PRO:CD	2.24	1.15
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.14
1:C:523:THR:HG22	1:C:524:VAL:H	0.97	1.14
2:H:116:ASP:CB	2:H:117:PRO:CD	2.24	1.14
3:L:5:THR:HG23	3:L:104:GLY:H	1.09	1.14
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.12
2:H:100:GLU:CD	2:H:115:PHE:HE1	1.57	1.12
2:J:100:GLU:CD	2:J:115:PHE:HE1	1.57	1.12
3:N:5:THR:HG23	3:N:104:GLY:H	1.09	1.11
1:A:523:THR:HG22	1:A:524:VAL:H	0.97	1.10
1:A:334:ASN:O	1:A:362:VAL:HG12	1.51	1.10
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.07
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.06
1:C:335:LEU:CA	1:C:362:VAL:HG13	1.85	1.06
1:C:486:PHE:CD1	2:J:114:TRP:CH2	2.44	1.05
1:A:486:PHE:CD1	2:H:114:TRP:CH2	2.44	1.04
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:ARG:CB	2:H:114:TRP:CZ2	2.40	1.04
3:L:5:THR:CG2	3:L:104:GLY:H	1.71	1.04
2:J:102:CYS:HA	2:J:112:CYS:HA	1.38	1.03
1:A:486:PHE:CZ	3:L:51:TYR:CE2	2.46	1.03
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.03
3:N:5:THR:CG2	3:N:104:GLY:H	1.71	1.03
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.02
2:J:101:ARG:CB	2:J:114:TRP:CZ2	2.40	1.02
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.02
3:N:6:GLN:HB3	3:N:7:PRO:HD3	1.40	1.02
1:C:486:PHE:CZ	3:N:51:TYR:CE2	2.46	1.01
2:J:116:ASP:HB3	2:J:117:PRO:HD2	1.02	1.01
1:A:523:THR:HG22	1:A:524:VAL:N	1.72	1.01
1:B:422:ASN:HD21	1:B:455:LEU:H	1.09	1.01
5:B:1410:NAG:C4	5:B:1411:NAG:C1	2.38	1.01
2:H:13:LYS:HB3	2:H:14:PRO:HD2	1.42	1.01
2:H:102:CYS:HA	2:H:112:CYS:HA	1.38	1.01
1:C:523:THR:HG22	1:C:524:VAL:N	1.72	1.00
2:J:13:LYS:HB3	2:J:14:PRO:HD2	1.42	1.00
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.01	1.00
1:C:486:PHE:CE1	2:J:114:TRP:CZ3	2.50	1.00
2:J:111:ARG:CB	3:N:93:TYR:CE2	2.45	1.00
1:A:486:PHE:CE1	2:H:114:TRP:CZ3	2.50	0.99
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.92	0.99
2:J:101:ARG:CB	2:J:114:TRP:CE2	2.46	0.99
2:H:111:ARG:CB	3:L:93:TYR:CE2	2.45	0.99
1:A:521:PRO:CG	1:B:199:GLY:HA3	1.93	0.99
1:A:521:PRO:HG3	1:B:199:GLY:CA	1.92	0.99
2:H:116:ASP:HB3	2:H:117:PRO:HD2	1.02	0.99
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.92	0.98
3:L:6:GLN:HB3	3:L:7:PRO:HD3	1.40	0.98
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:C:676:THR:HA	1:C:690:GLN:HB3	1.46	0.98
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.98
2:H:101:ARG:CB	2:H:114:TRP:CE2	2.46	0.98
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.98
2:J:116:ASP:HB3	2:J:117:PRO:HD3	1.46	0.98
2:H:116:ASP:HB3	2:H:117:PRO:HD3	1.46	0.97
3:N:85:GLU:CD	3:N:110:VAL:HG23	1.89	0.97
2:H:101:ARG:CG	2:H:114:TRP:CZ2	2.48	0.97
3:L:85:GLU:CD	3:L:110:VAL:HG23	1.90	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:GLN:HE21	1:C:675:GLN:HA	1.27	0.96
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.96
2:J:101:ARG:CG	2:J:114:TRP:CZ2	2.48	0.95
2:H:100:GLU:CD	2:H:115:PHE:CE1	2.44	0.95
2:H:100:GLU:HG2	2:H:115:PHE:CD1	2.02	0.95
2:J:101:ARG:CG	2:J:114:TRP:HZ2	1.79	0.95
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.94
2:H:101:ARG:CG	2:H:114:TRP:HZ2	1.79	0.94
2:J:100:GLU:CD	2:J:115:PHE:CE1	2.44	0.94
1:C:335:LEU:HA	1:C:362:VAL:HG13	0.96	0.94
2:J:100:GLU:HG2	2:J:115:PHE:CD1	2.02	0.94
2:J:116:ASP:CB	2:J:117:PRO:HD3	1.96	0.94
1:A:521:PRO:HG3	1:B:199:GLY:HA3	1.50	0.94
2:H:116:ASP:CB	2:H:117:PRO:HD3	1.96	0.93
2:J:101:ARG:HB2	2:J:114:TRP:CE2	2.03	0.93
1:B:577:ARG:HH11	1:B:582:LEU:HD13	1.32	0.93
2:H:101:ARG:HB2	2:H:114:TRP:CE2	2.03	0.93
2:H:11:LEU:HG	2:H:161:PHE:CE2	2.04	0.92
3:N:85:GLU:CD	3:N:110:VAL:CG2	2.42	0.92
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.92
1:A:530:SER:O	1:A:531:THR:HG22	1.70	0.92
3:L:85:GLU:CD	3:L:110:VAL:CG2	2.43	0.92
1:C:334:ASN:O	1:C:362:VAL:HG12	1.69	0.91
2:J:11:LEU:HG	2:J:161:PHE:CE2	2.04	0.91
1:C:417:LYS:NZ	1:C:455:LEU:CB	2.32	0.91
2:H:101:ARG:HB3	2:H:114:TRP:NE1	1.86	0.90
2:J:101:ARG:HB3	2:J:114:TRP:NE1	1.86	0.90
1:A:490:PHE:CD2	2:H:104:TYR:HD2	1.89	0.90
2:H:113:VAL:HG11	3:L:34:TYR:HB3	1.53	0.90
3:L:5:THR:HG21	3:L:105:GLY:H	1.37	0.89
1:C:417:LYS:HE3	2:J:55:TYR:OH	1.72	0.89
1:C:417:LYS:HZ3	1:C:455:LEU:HB2	1.05	0.89
1:C:490:PHE:CD2	2:J:104:TYR:HD2	1.89	0.88
2:H:111:ARG:HD2	3:L:93:TYR:HE2	1.39	0.88
2:J:100:GLU:HG2	2:J:115:PHE:CE1	2.09	0.88
2:J:113:VAL:HG11	3:N:34:TYR:HB3	1.53	0.88
3:N:5:THR:HG21	3:N:105:GLY:H	1.37	0.88
1:C:417:LYS:HZ2	1:C:455:LEU:HB2	1.33	0.87
1:A:486:PHE:HD1	2:H:114:TRP:CH2	1.90	0.87
1:A:521:PRO:CB	1:B:199:GLY:HA3	2.03	0.87
2:H:100:GLU:HG2	2:H:115:PHE:CE1	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:CB	3:L:7:PRO:HD3	2.05	0.87
2:H:116:ASP:CG	2:H:117:PRO:HD3	2.00	0.87
1:A:521:PRO:HB3	1:B:199:GLY:HA3	1.55	0.87
3:N:6:GLN:CB	3:N:7:PRO:HD3	2.05	0.87
1:C:486:PHE:HD1	2:J:114:TRP:CH2	1.90	0.87
1:C:417:LYS:NZ	1:C:455:LEU:HD12	1.88	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.76	0.86
2:J:101:ARG:CD	2:J:114:TRP:HZ2	1.89	0.86
2:J:111:ARG:HD2	3:N:93:TYR:HE2	1.39	0.86
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.86
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.85
2:J:116:ASP:CG	2:J:117:PRO:HD3	2.00	0.85
1:B:577:ARG:HD3	1:B:582:LEU:CD1	2.07	0.85
1:C:490:PHE:HD2	2:J:104:TYR:CD2	1.93	0.84
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	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
2:H:101:ARG:CD	2:H:114:TRP:HZ2	1.89	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.83
2:J:101:ARG:HD3	2:J:114:TRP:HZ2	1.43	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:C:127:VAL:HG21	5:C:1402:NAG:H5	1.59	0.83
3:L:51:TYR:CE1	3:L:55:ASN:HB2	2.12	0.83
1:A:335:LEU:HA	1:A:362:VAL:HG13	0.85	0.83
1:C:676:THR:C	1:C:690:GLN:HE21	1.86	0.83
3:N:51:TYR:CE1	3:N:55:ASN:HB2	2.13	0.83
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:C:417:LYS:HZ3	1:C:455:LEU:CB	1.91	0.82
2:J:120:GLN:HA	2:J:120:GLN:NE2	1.94	0.82
3:N:6:GLN:HB3	3:N:7:PRO:CD	2.09	0.82
1:A:490:PHE:HD2	2:H:104:TYR:CD2	1.93	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:B:452:LEU:HG	1:B:492:LEU:HD22	1.63	0.81
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.61	0.81
1:A:486:PHE:CE1	2:H:114:TRP:CH2	2.69	0.81
2:H:101:ARG:HD3	2:H:114:TRP:HZ2	1.43	0.81
2:H:102:CYS:HA	2:H:112:CYS:CA	2.11	0.80
1:B:214:ARG:H	1:B:214:ARG:HH21	1.30	0.80
2:H:113:VAL:C	2:H:114:TRP:CD1	2.59	0.80
2:H:120:GLN:HA	2:H:120:GLN:NE2	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:SER:O	1:A:531:THR:CG2	2.28	0.80
2:J:13:LYS:HB3	2:J:14:PRO:CD	2.12	0.80
2:J:113:VAL:C	2:J:114:TRP:CD1	2.59	0.80
1:A:489:TYR:HD1	2:H:101:ARG:NH2	1.79	0.80
2:H:13:LYS:HB3	2:H:14:PRO:CD	2.12	0.80
3:L:6:GLN:HB3	3:L:7:PRO:CD	2.10	0.79
1:A:521:PRO:HG3	1:B:199:GLY:C	2.07	0.79
2:H:100:GLU:CG	2:H:115:PHE:CE1	2.66	0.79
2:H:101:ARG:CB	2:H:114:TRP:NE1	2.46	0.79
2:J:100:GLU:CG	2:J:115:PHE:CE1	2.66	0.79
1:A:390:LEU:HD23	1:A:391:CYS:H	1.48	0.79
1:A:417:LYS:HE3	2:H:55:TYR:CE2	2.18	0.78
1:C:489:TYR:HD1	2:J:101:ARG:NH2	1.80	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.48	0.78
1:C:486:PHE:CE1	2:J:114:TRP:CH2	2.69	0.78
1:A:335:LEU:CA	1:A:362:VAL:CG1	2.42	0.77
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.77
2:H:113:VAL:CG2	2:H:114:TRP:HD1	1.91	0.77
2:J:100:GLU:OE2	2:J:115:PHE:HE1	1.66	0.77
2:J:102:CYS:HA	2:J:112:CYS:CA	2.11	0.77
2:J:101:ARG:CB	2:J:114:TRP:NE1	2.46	0.77
1:C:329:PHE:CE1	1:C:544:ASN:HA	2.19	0.77
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.77
2:J:101:ARG:HG2	2:J:114:TRP:CZ2	2.18	0.77
2:H:100:GLU:OE2	2:H:115:PHE:HE1	1.66	0.77
2:H:101:ARG:HG2	2:H:114:TRP:CZ2	2.18	0.77
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.76
1:C:527:PRO:C	1:C:528:LYS:HG2	2.09	0.76
3:L:5:THR:HG23	3:L:104:GLY:N	1.95	0.76
2:J:113:VAL:CG2	2:J:114:TRP:HD1	1.91	0.76
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.76
1:A:486:PHE:CZ	3:L:51:TYR:CZ	2.74	0.76
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.76
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:C:486:PHE:CZ	3:N:51:TYR:CZ	2.74	0.75
1:C:675:GLN:HA	1:C:675:GLN:NE2	1.99	0.75
2:J:116:ASP:CB	2:J:117:PRO:HD2	1.99	0.75
2:H:111:ARG:CB	3:L:93:TYR:CZ	2.59	0.74
1:A:530:SER:C	1:A:531:THR:CG2	2.61	0.74
1:C:676:THR:C	1:C:690:GLN:NE2	2.45	0.74
2:J:100:GLU:CG	2:J:115:PHE:HE1	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HA	1:A:362:VAL:HG12	1.67	0.73
1:C:490:PHE:CE2	2:J:104:TYR:HE2	2.03	0.73
1:A:490:PHE:CE2	2:H:104:TYR:HE2	2.03	0.73
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.73
1:B:577:ARG:HH11	1:B:582:LEU:CD1	2.01	0.73
2:J:113:VAL:O	2:J:114:TRP:CD1	2.42	0.73
3:N:5:THR:HG23	3:N:104:GLY:N	1.95	0.73
2:H:100:GLU:CG	2:H:115:PHE:HE1	2.00	0.73
1:B:164:ASN:ND2	5:B:1403:NAG:O6	2.22	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
2:J:111:ARG:CB	3:N:93:TYR:CZ	2.59	0.72
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.72
2:H:113:VAL:O	2:H:114:TRP:CD1	2.42	0.72
3:L:85:GLU:OE1	3:L:110:VAL:CG2	2.38	0.72
3:N:85:GLU:OE1	3:N:110:VAL:CG2	2.38	0.72
1:C:335:LEU:CA	1:C:362:VAL:CG1	2.57	0.72
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.72
2:H:101:ARG:HD3	2:H:114:TRP:CZ2	2.24	0.72
3:N:5:THR:CG2	3:N:104:GLY:N	2.50	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.21	0.71
1:C:417:LYS:HZ2	1:C:455:LEU:HD12	1.54	0.71
1:B:124:THR:OG1	5:B:1402:NAG:N2	2.22	0.71
3:L:5:THR:CG2	3:L:104:GLY:N	2.50	0.71
2:J:111:ARG:HD2	3:N:93:TYR:CE2	2.24	0.71
1:C:359:SER:O	1:C:524:VAL:CG1	2.39	0.71
5:B:1410:NAG:H4	5:B:1411:NAG:C1	2.21	0.70
2:J:101:ARG:HD3	2:J:114:TRP:CZ2	2.24	0.70
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.70
1:A:336:CYS:SG	1:A:361:CYS:CB	2.79	0.70
1:A:359:SER:O	1:A:524:VAL:CG1	2.39	0.70
3:N:85:GLU:OE1	3:N:110:VAL:HG21	1.92	0.70
1:B:153:MET:HE3	1:B:154:GLU:HG3	1.72	0.70
1:C:417:LYS:HZ2	1:C:455:LEU:CD1	2.04	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.70
1:A:124:THR:HG21	5:A:1402:NAG:HN2	1.56	0.70
1:A:530:SER:C	1:A:531:THR:HG23	2.16	0.69
1:B:391:CYS:HA	1:B:525:CYS:HB2	1.73	0.69
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69
2:H:111:ARG:HD2	3:L:93:TYR:CE2	2.24	0.69
3:L:85:GLU:OE1	3:L:110:VAL:HG21	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:NH1	1:B:582:LEU:HD13	2.07	0.69
1:C:569:ILE:H	1:C:569:ILE:HD12	1.56	0.69
3:N:7:PRO:O	3:N:106:THR:HG22	1.92	0.69
2:H:100:GLU:HG2	2:H:115:PHE:HD1	1.56	0.69
3:L:7:PRO:O	3:L:106:THR:HG22	1.92	0.69
2:H:97:CYS:O	2:H:119:GLY:N	2.26	0.69
1:C:233:ILE:HG12	1:C:234:ASN:H	1.58	0.69
2:J:97:CYS:O	2:J:119:GLY:N	2.26	0.69
3:L:8:ALA:O	3:L:106:THR:HA	1.93	0.68
1:A:335:LEU:CB	1:A:362:VAL:HG13	2.23	0.68
1:A:486:PHE:CD1	2:H:114:TRP:CZ3	2.80	0.68
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.74	0.68
2:J:11:LEU:HD13	2:J:11:LEU:O	1.94	0.68
2:H:11:LEU:O	2:H:11:LEU:HD13	1.94	0.68
2:J:99:ARG:CG	2:J:117:PRO:HD2	2.24	0.68
2:H:11:LEU:HG	2:H:161:PHE:HE2	1.55	0.68
2:H:99:ARG:CG	2:H:117:PRO:HD2	2.23	0.68
1:B:403:ARG:NH2	1:B:405:ASP:OD2	2.27	0.68
3:L:27:SER:HA	3:L:31:GLY:H	1.59	0.68
1:B:406:GLU:HG3	1:B:418:ILE:HG13	1.75	0.67
3:N:8:ALA:O	3:N:106:THR:HA	1.93	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:C:486:PHE:CD1	2:J:114:TRP:CZ3	2.80	0.67
1:A:336:CYS:HG	1:A:361:CYS:CB	2.06	0.67
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.67
1:A:310:LYS:NZ	1:A:663:ASP:OD1	2.27	0.67
1:B:97:LYS:HD3	1:B:97:LYS:H	1.60	0.67
3:N:6:GLN:CB	3:N:7:PRO:CD	2.69	0.67
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.66
3:N:6:GLN:OE1	3:N:6:GLN:HA	1.96	0.66
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.66
1:C:85:PRO:HA	1:C:237:ARG:HA	1.78	0.66
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.66
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.59	0.66
1:B:577:ARG:NH1	1:B:582:LEU:CD1	2.58	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
2:J:100:GLU:HG2	2:J:115:PHE:HD1	1.56	0.66
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.78	0.66
1:C:489:TYR:CD1	2:J:101:ARG:NH2	2.64	0.65
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:C:486:PHE:CZ	3:N:51:TYR:CD2	2.84	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.65
3:N:27:SER:HA	3:N:31:GLY:H	1.59	0.65
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.76	0.65
1:A:486:PHE:CZ	3:L:51:TYR:CD2	2.84	0.65
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.78	0.65
2:J:11:LEU:HG	2:J:161:PHE:HE2	1.55	0.65
1:B:358:ILE:HB	1:B:395:VAL:HB	1.78	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:A:705:VAL:HB	1:B:883:THR:HG21	1.78	0.65
1:B:455:LEU:HD21	1:B:457:ARG:HG3	1.78	0.65
3:N:51:TYR:O	3:N:52:ASP:HB3	1.97	0.65
1:C:417:LYS:HZ2	1:C:455:LEU:CB	2.00	0.65
2:H:116:ASP:CB	2:H:117:PRO:HD2	1.99	0.65
3:L:6:GLN:OE1	3:L:6:GLN:HA	1.95	0.65
1:A:489:TYR:CD1	2:H:101:ARG:NH2	2.64	0.65
1:A:417:LYS:HE3	2:H:55:TYR:CZ	2.32	0.64
2:J:214:ASN:HB3	2:J:221:LYS:HE2	1.79	0.64
1:B:108:THR:HA	1:B:236:THR:HG22	1.79	0.64
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.64
3:L:6:GLN:CB	3:L:7:PRO:CD	2.69	0.64
1:A:521:PRO:CG	1:B:199:GLY:CA	2.61	0.64
3:L:112:GLY:O	3:L:113:GLN:HG2	1.97	0.64
1:B:350:VAL:HG22	1:B:453:TYR:HB2	1.78	0.64
1:C:676:THR:HA	1:C:690:GLN:CB	2.25	0.64
1:A:523:THR:HG22	1:A:524:VAL:HG22	1.79	0.64
1:B:472:ILE:HD13	1:B:474:GLN:HB3	1.79	0.64
1:C:391:CYS:SG	1:C:523:THR:O	2.56	0.64
2:J:116:ASP:OD1	2:J:117:PRO:HD3	1.98	0.64
1:A:391:CYS:SG	1:A:523:THR:O	2.56	0.64
1:B:607:GLN:O	1:B:608:VAL:HG23	1.98	0.64
1:C:523:THR:HG22	1:C:524:VAL:HG22	1.79	0.63
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.63
1:A:484:GLU:HB3	2:H:103:TYR:CE1	2.33	0.63
2:H:116:ASP:OD1	2:H:117:PRO:HD3	1.98	0.63
2:H:214:ASN:HB3	2:H:221:LYS:HE2	1.79	0.63
3:L:125:PRO:HD3	3:L:137:LEU:HD22	1.80	0.63
1:A:486:PHE:CE2	3:L:51:TYR:CZ	2.87	0.63
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.63
1:C:196:ASN:ND2	1:C:200:TYR:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:51:TYR:O	3:L:52:ASP:HB3	1.97	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:C:486:PHE:CE2	3:N:51:TYR:CZ	2.87	0.63
2:J:114:TRP:O	2:J:115:PHE:HB2	1.98	0.63
1:C:417:LYS:NZ	1:C:455:LEU:CD1	2.58	0.62
2:H:139:LEU:HD11	2:H:156:LEU:HB2	1.81	0.62
3:N:125:PRO:HD3	3:N:137:LEU:HD22	1.80	0.62
1:B:111:ASP:OD1	1:B:112:SER:N	2.31	0.62
1:C:484:GLU:HB3	2:J:103:TYR:CE1	2.33	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
2:H:114:TRP:O	2:H:115:PHE:HB2	1.98	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	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
2:H:167:VAL:HG22	2:H:213:VAL:HG22	1.81	0.62
2:J:10:GLY:O	2:J:12:VAL:N	2.33	0.62
3:N:146:PRO:HG2	3:N:202:HIS:CE1	2.34	0.62
1:B:454:ARG:HH21	1:B:493:GLN:HG3	1.63	0.62
3:N:137:LEU:HB2	3:N:183:LEU:HB3	1.82	0.62
2:J:139:LEU:HD11	2:J:156:LEU:HB2	1.81	0.62
3:N:85:GLU:CD	3:N:110:VAL:HG21	2.25	0.62
3:N:112:GLY:O	3:N:113:GLN:HG2	1.99	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:B:560:LEU:H	1:B:563:GLN:HE21	1.45	0.61
3:L:137:LEU:HB2	3:L:183:LEU:HB3	1.82	0.61
3:L:146:PRO:HG2	3:L:202:HIS:CE1	2.35	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
3:L:51:TYR:CD1	3:L:55:ASN:HB2	2.35	0.61
1:B:391:CYS:CA	1:B:525:CYS:HB2	2.30	0.61
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.61
2:H:118:TRP:O	2:H:119:GLY:O	2.19	0.61
3:N:51:TYR:CD1	3:N:55:ASN:HB2	2.35	0.61
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.61
2:J:167:VAL:HG22	2:J:213:VAL:HG22	1.81	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:C:457:ARG:NH1	1:C:459:SER:O	2.33	0.61
2:H:10:GLY:O	2:H:12:VAL:N	2.33	0.61
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.60
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.60
1:C:112:SER:HB2	1:C:113:LYS:HD3	1.83	0.60
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.60
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.84	0.60
3:L:85:GLU:CD	3:L:110:VAL:HG21	2.26	0.60
3:L:97:SER:C	3:L:99:LEU:H	2.08	0.60
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.17	0.60
3:N:97:SER:C	3:N:99:LEU:H	2.08	0.60
3:L:2:SER:O	3:L:4:LEU:CD1	2.50	0.60
2:J:118:TRP:O	2:J:119:GLY:O	2.19	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.50	0.60
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.84	0.59
3:N:2:SER:O	3:N:4:LEU:CD1	2.50	0.59
1:B:206:LYS:HD2	1:B:207:HIS:H	1.68	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:C:95:THR:HG22	1:C:96:GLU:H	1.66	0.59
3:L:18:ILE:H	3:L:77:ILE:HG22	1.67	0.59
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.59
2:J:53:ILE:HD11	2:J:71:ILE:HB	1.84	0.59
3:L:101:VAL:HG12	3:L:102:PHE:N	2.18	0.59
3:N:91:SER:O	3:N:92:SER:HB3	2.03	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:C:486:PHE:HE1	2:J:114:TRP:CZ3	2.17	0.59
2:J:8:GLY:N	2:J:9:PRO:CD	2.66	0.59
3:L:98:THR:O	3:L:100:VAL:N	2.36	0.59
3:N:154:LYS:HG2	3:N:155:ALA:O	2.03	0.59
1:C:361:CYS:N	1:C:524:VAL:HG12	2.18	0.58
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.58
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.58
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.58
1:A:486:PHE:HE1	2:H:114:TRP:CZ3	2.17	0.58
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.58
1:A:521:PRO:HB3	1:B:198:ASP:O	2.03	0.58
1:B:452:LEU:HD21	1:B:492:LEU:HD13	1.85	0.58
1:C:335:LEU:HA	1:C:362:VAL:HG12	1.78	0.58
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.86	0.58
1:C:599:THR:HG22	1:C:601:GLY:H	1.67	0.58
3:L:154:LYS:HG2	3:L:155:ALA:O	2.03	0.58
2:J:88:THR:HG23	2:J:90:ALA:H	1.68	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:C:486:PHE:CE1	2:J:114:TRP:CE3	2.92	0.58
3:L:91:SER:O	3:L:92:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.58
2:H:88:THR:HG23	2:H:90:ALA:H	1.68	0.58
2:J:11:LEU:CG	2:J:161:PHE:CE2	2.85	0.58
4:Z:2:NAG:H3	4:Z:2:NAG:H83	1.86	0.58
1:C:417:LYS:HE3	2:J:55:TYR:HH	1.68	0.58
2:H:53:ILE:HD11	2:H:71:ILE:HB	1.84	0.58
3:N:51:TYR:CE1	3:N:55:ASN:CB	2.86	0.58
3:N:18:ILE:H	3:N:77:ILE:HG22	1.67	0.58
2:H:8:GLY:N	2:H:9:PRO:CD	2.66	0.58
2:J:101:ARG:HG2	2:J:114:TRP:CE2	2.38	0.58
3:N:98:THR:O	3:N:100:VAL:N	2.36	0.58
1:A:334:ASN:C	1:A:362:VAL:HG12	2.29	0.58
1:B:214:ARG:HD3	1:B:214:ARG:N	2.18	0.58
2:H:101:ARG:HG2	2:H:114:TRP:CE2	2.38	0.58
3:L:15:GLY:H	3:L:80:LEU:HB2	1.69	0.58
3:L:118:PRO:HD3	3:L:202:HIS:HD2	1.69	0.57
3:N:118:PRO:HD3	3:N:202:HIS:HD2	1.69	0.57
1:A:361:CYS:N	1:A:524:VAL:HG12	2.18	0.57
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.57
1:A:486:PHE:CE1	2:H:114:TRP:CE3	2.92	0.57
5:A:1405:NAG:H3	5:A:1405:NAG:H83	1.86	0.57
1:C:490:PHE:HD2	2:J:104:TYR:CG	2.21	0.57
2:J:163:GLU:CD	2:J:163:GLU:H	2.12	0.57
3:N:15:GLY:H	3:N:80:LEU:HB2	1.69	0.57
1:A:490:PHE:HD2	2:H:104:TYR:CG	2.21	0.57
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.83	0.57
2:H:163:GLU:CD	2:H:163:GLU:H	2.12	0.57
3:N:101:VAL:HG12	3:N:102:PHE:N	2.18	0.57
1:A:486:PHE:CE1	3:L:51:TYR:CE2	2.92	0.57
2:H:107:GLY:O	2:H:108:ARG:HB3	2.05	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
2:J:107:GLY:O	2:J:108:ARG:HB3	2.05	0.57
2:H:34:TYR:CD2	2:H:99:ARG:NH1	2.73	0.57
3:L:51:TYR:CE1	3:L:55:ASN:CB	2.86	0.57
3:L:110:VAL:HG12	3:L:110:VAL:O	2.05	0.57
2:J:34:TYR:CD2	2:J:99:ARG:NH1	2.72	0.57
2:H:11:LEU:CG	2:H:161:PHE:HE2	2.18	0.57
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.57
5:B:1405:NAG:H83	5:B:1405:NAG:H3	1.87	0.57
1:B:408:ARG:O	1:B:414:GLN:NE2	2.32	0.56
1:C:417:LYS:CE	2:J:55:TYR:OH	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.56
2:J:111:ARG:CD	3:N:93:TYR:CE2	2.88	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:490:PHE:CE2	2:H:104:TYR:HD2	2.10	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:B:213:VAL:HB	1:B:214:ARG:HD3	1.87	0.56
1:C:336:CYS:SG	1:C:361:CYS:CB	2.93	0.56
1:C:486:PHE:CE1	3:N:51:TYR:CE2	2.92	0.56
4:a:2:NAG:H3	4:a:2:NAG:H83	1.87	0.56
1:C:519:HIS:O	1:C:519:HIS:ND1	2.38	0.56
3:L:4:LEU:CD1	3:L:4:LEU:H	2.19	0.56
2:J:11:LEU:CG	2:J:161:PHE:HE2	2.18	0.56
2:H:134:PRO:HB2	2:H:157:VAL:HG23	1.88	0.56
3:L:208:GLU:OE1	3:L:210:THR:OG1	2.24	0.56
2:J:134:PRO:HB2	2:J:157:VAL:HG23	1.88	0.56
3:N:49:MET:SD	3:N:49:MET:N	2.79	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:B:105:ILE:HG13	1:B:110:LEU:HD11	1.87	0.56
2:H:102:CYS:HA	2:H:112:CYS:CB	2.36	0.56
1:A:391:CYS:SG	1:A:524:VAL:O	2.64	0.56
1:B:187:LYS:NZ	1:B:213:VAL:HG13	2.21	0.56
2:H:101:ARG:CG	2:H:114:TRP:CE2	2.85	0.56
3:N:208:GLU:OE1	3:N:210:THR:OG1	2.24	0.56
5:C:1405:NAG:H3	5:C:1405:NAG:H83	1.88	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:C:359:SER:O	1:C:524:VAL:HG11	2.06	0.56
2:H:111:ARG:CD	3:L:93:TYR:CE2	2.88	0.56
2:J:214:ASN:HD22	2:J:216:LYS:HE3	1.71	0.56
3:N:4:LEU:CD1	3:N:4:LEU:H	2.18	0.56
4:I:2:NAG:H3	4:I:2:NAG:H83	1.87	0.56
4:V:1:NAG:H61	4:V:2:NAG:HN2	1.71	0.56
2:J:102:CYS:HA	2:J:112:CYS:CB	2.36	0.55
1:A:342:PHE:HB3	4:E:1:NAG:H82	1.87	0.55
2:H:11:LEU:CG	2:H:161:PHE:CE2	2.85	0.55
2:J:101:ARG:HG2	2:J:114:TRP:NE1	2.21	0.55
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.55
2:H:8:GLY:N	2:H:9:PRO:HD3	2.21	0.55
3:L:49:MET:SD	3:L:49:MET:N	2.79	0.55
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.55
1:B:577:ARG:CD	1:B:582:LEU:HD13	2.35	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:C:113:LYS:HD2	1:C:164:ASN:HD21	1.71	0.55
1:C:391:CYS:SG	1:C:524:VAL:O	2.64	0.55
1:C:490:PHE:CD2	2:J:104:TYR:CG	2.91	0.55
2:H:214:ASN:HD22	2:H:216:LYS:HE3	1.71	0.55
2:J:37:SER:OG	2:J:38:TRP:N	2.37	0.55
2:J:100:GLU:CG	2:J:115:PHE:CD1	2.84	0.55
3:N:164:VAL:HA	3:N:182:TYR:O	2.07	0.55
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
3:N:110:VAL:HG12	3:N:110:VAL:O	2.05	0.55
1:B:661:GLU:OE2	1:B:698:SER:OG	2.25	0.55
2:H:101:ARG:HG2	2:H:114:TRP:NE1	2.21	0.55
1:A:486:PHE:HE1	2:H:114:TRP:CE3	2.25	0.55
1:C:342:PHE:HB3	4:V:1:NAG:H82	1.88	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
2:H:99:ARG:HG2	2:H:117:PRO:HD2	1.89	0.55
2:J:8:GLY:N	2:J:9:PRO:HD3	2.21	0.55
1:B:352:ALA:HB2	1:B:468:ILE:HD12	1.88	0.55
1:C:129:LYS:HD3	1:C:131:CYS:SG	2.46	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.54
3:L:25:THR:OG1	3:L:26:SER:N	2.40	0.54
3:L:164:VAL:HA	3:L:182:TYR:O	2.07	0.54
1:A:551:VAL:HB	1:A:588:THR:HG23	1.88	0.54
2:H:100:GLU:OE2	2:H:115:PHE:CE1	2.53	0.54
2:J:10:GLY:O	2:J:12:VAL:HG23	2.07	0.54
1:A:521:PRO:HB2	1:B:200:TYR:CE1	2.43	0.54
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.90	0.54
2:H:10:GLY:O	2:H:12:VAL:HG23	2.07	0.54
3:L:53:VAL:O	3:L:53:VAL:HG22	2.08	0.54
1:A:417:LYS:CD	2:H:55:TYR:OH	2.55	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
2:H:154:GLY:HA2	2:H:169:TRP:HZ2	1.73	0.54
1:B:166:CYS:SG	1:B:167:THR:N	2.81	0.54
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.54
2:H:37:SER:OG	2:H:38:TRP:N	2.37	0.54
2:J:154:GLY:HA2	2:J:169:TRP:HZ2	1.73	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:C:417:LYS:HZ1	1:C:455:LEU:HD12	1.68	0.54
1:C:486:PHE:HE1	2:J:114:TRP:CE3	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.54
2:J:99:ARG:HG2	2:J:117:PRO:HD2	1.89	0.54
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.72	0.54
1:A:359:SER:O	1:A:524:VAL:HG11	2.06	0.53
1:B:165:ASN:OD1	5:B:1403:NAG:N2	2.40	0.53
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.53
1:C:421:TYR:HA	1:C:461:LEU:HG	1.90	0.53
2:H:194:SER:HB2	3:L:182:TYR:OH	2.08	0.53
3:N:53:VAL:O	3:N:53:VAL:HG22	2.07	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.53
1:B:333:THR:OG1	1:B:334:ASN:N	2.42	0.53
2:H:131:THR:OG1	2:H:162:PRO:CG	2.56	0.53
2:H:141:PRO:HG3	2:H:153:LEU:HD23	1.90	0.53
2:J:101:ARG:HG2	2:J:114:TRP:HE1	1.73	0.53
2:J:194:SER:HB2	3:N:182:TYR:OH	2.08	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:C:97:LYS:HB3	1:C:187:LYS:HA	1.89	0.53
2:J:34:TYR:CG	2:J:99:ARG:NH1	2.77	0.53
2:J:101:ARG:CG	2:J:114:TRP:CE2	2.85	0.53
3:N:1:GLN:HE22	3:N:96:SER:HB3	1.73	0.53
4:G:2:NAG:H83	4:G:2:NAG:H3	1.90	0.53
1:C:476:GLY:H	1:C:487:ASN:HB3	1.74	0.53
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.53
1:C:449:TYR:HB3	2:J:107:GLY:HA2	1.91	0.53
2:H:101:ARG:HG2	2:H:114:TRP:HE1	1.73	0.53
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.53
2:H:144:LYS:O	3:L:209:LYS:NZ	2.41	0.53
3:N:113:GLN:CD	3:N:114:PRO:HD2	2.34	0.53
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.53
2:J:144:LYS:O	3:N:209:LYS:NZ	2.41	0.53
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.91	0.53
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.53
1:B:402:ILE:O	1:B:507:PRO:HA	2.09	0.53
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.53
1:C:417:LYS:CE	1:C:455:LEU:HB2	2.35	0.53
1:C:417:LYS:HD3	1:C:455:LEU:HA	1.91	0.53
2:J:141:PRO:HG3	2:J:153:LEU:HD23	1.89	0.52
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.72	0.52
2:H:62:ASN:ND2	2:H:64:SER:OG	2.43	0.52
1:A:57:PRO:O	1:A:60:SER:OG	2.25	0.52
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:ASN:ND2	2:J:64:SER:OG	2.43	0.52
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.52
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.52
3:L:67:SER:OG	3:L:68:LYS:N	2.43	0.52
1:B:112:SER:O	1:B:113:LYS:HB2	2.10	0.52
1:B:424:LYS:HB3	1:B:463:PRO:HA	1.92	0.52
2:H:34:TYR:CG	2:H:99:ARG:NH1	2.77	0.52
2:J:131:THR:OG1	2:J:162:PRO:CG	2.57	0.52
1:B:403:ARG:HA	1:B:495:TYR:OH	2.10	0.52
1:B:457:ARG:NH2	1:B:469:SER:O	2.43	0.52
1:C:113:LYS:HD3	1:C:113:LYS:N	2.25	0.52
1:C:193:VAL:HG23	1:C:223:LEU:HD23	1.91	0.52
2:H:11:LEU:HD23	2:H:125:THR:HG23	1.92	0.52
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.52
3:L:1:GLN:HE22	3:L:96:SER:HB3	1.74	0.52
3:N:136:THR:HA	3:N:183:LEU:O	2.09	0.52
1:B:555:SER:OG	1:B:584:ILE:O	2.28	0.52
1:A:449:TYR:HB3	2:H:107:GLY:HA2	1.91	0.52
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.45	0.52
1:C:1101:HIS:CD2	4:a:1:NAG:H5	2.45	0.52
3:L:189:GLN:HA	3:L:192:SER:HB3	1.91	0.52
2:J:100:GLU:OE2	2:J:115:PHE:CE1	2.52	0.52
1:B:380:TYR:O	1:B:430:THR:HA	2.11	0.51
1:C:83:VAL:HG22	1:C:237:ARG:HD2	1.92	0.51
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.07	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
2:H:100:GLU:HA	2:H:115:PHE:HA	1.92	0.51
3:L:136:THR:HA	3:L:183:LEU:O	2.09	0.51
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.51
1:B:560:LEU:H	1:B:563:GLN:NE2	2.08	0.51
1:C:449:TYR:CE2	2:J:109:ALA:HA	2.46	0.51
3:L:113:GLN:CD	3:L:114:PRO:HD2	2.35	0.51
1:A:521:PRO:HD3	1:B:199:GLY:HA2	1.92	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51
2:J:101:ARG:CG	2:J:114:TRP:NE1	2.74	0.51
3:N:189:GLN:HA	3:N:192:SER:HB3	1.91	0.51
2:J:101:ARG:HB3	2:J:114:TRP:HE1	1.74	0.51
2:J:101:ARG:HB3	2:J:114:TRP:CE2	2.28	0.51
3:N:67:SER:OG	3:N:68:LYS:N	2.43	0.51
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.45	0.51
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4:LEU:CD1	3:N:4:LEU:N	2.73	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
2:H:99:ARG:HE	2:H:117:PRO:CD	2.24	0.51
1:C:113:LYS:H	1:C:132:GLU:HB3	1.76	0.51
1:C:523:THR:CG2	1:C:524:VAL:N	2.45	0.51
2:J:99:ARG:HE	2:J:117:PRO:CD	2.24	0.51
1:C:97:LYS:HD3	1:C:187:LYS:HA	1.93	0.51
2:H:101:ARG:CG	2:H:114:TRP:NE1	2.74	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.92	0.50
1:A:490:PHE:HE2	2:H:104:TYR:HE2	1.38	0.50
3:L:4:LEU:CD1	3:L:4:LEU:N	2.73	0.50
2:J:170:ASN:ND2	2:J:208:THR:O	2.45	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.77	0.50
1:A:449:TYR:CE2	2:H:109:ALA:HA	2.46	0.50
2:H:101:ARG:CG	2:H:114:TRP:HE1	2.24	0.50
3:N:91:SER:O	3:N:92:SER:CB	2.60	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
2:H:170:ASN:ND2	2:H:208:THR:O	2.45	0.50
2:J:114:TRP:O	3:N:38:TYR:OH	2.23	0.50
2:H:113:VAL:C	2:H:114:TRP:HD1	2.16	0.50
3:N:25:THR:OG1	3:N:26:SER:N	2.40	0.50
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.50
1:A:964:LYS:HE3	1:C:570:ALA:HA	1.93	0.50
1:B:675:GLN:HA	1:B:690:GLN:HG3	1.93	0.50
2:J:11:LEU:HD23	2:J:125:THR:HG23	1.92	0.50
1:A:200:TYR:CZ	1:C:521:PRO:HB2	2.47	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
1:B:616:ASN:HB3	1:B:618:THR:HG22	1.94	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
3:L:29:VAL:HG12	3:L:94:THR:HG22	1.94	0.50
2:J:100:GLU:HA	2:J:115:PHE:HA	1.92	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.50
1:B:350:VAL:HG23	1:B:422:ASN:HD22	1.76	0.50
2:H:40:ARG:NE	2:H:48:GLU:OE2	2.45	0.50
3:N:63:ARG:HB3	3:N:77:ILE:HG13	1.94	0.50
1:B:112:SER:N	1:B:133:PHE:O	2.45	0.49
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.49
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.12	0.49
2:H:114:TRP:C	3:L:38:TYR:HH	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:THR:OG1	2:H:162:PRO:HG2	2.12	0.49
3:L:63:ARG:HB3	3:L:77:ILE:HG13	1.94	0.49
4:S:1:NAG:H62	4:S:2:NAG:H2	1.93	0.49
1:B:31:SER:O	1:B:59:PHE:HA	2.10	0.49
2:H:130:SER:O	2:H:161:PHE:CD2	2.65	0.49
2:J:130:SER:O	2:J:161:PHE:CD2	2.65	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
2:J:40:ARG:NE	2:J:48:GLU:OE2	2.45	0.49
2:H:134:PRO:HD3	2:H:215:HIS:HD1	1.78	0.49
3:L:91:SER:O	3:L:92:SER:CB	2.60	0.49
3:N:52:ASP:O	3:N:53:VAL:HB	2.13	0.49
3:N:122:LEU:HD21	3:N:137:LEU:HD12	1.94	0.49
3:N:155:ALA:HB1	3:N:193:HIS:CD2	2.48	0.49
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.49
1:C:332:ILE:HD12	1:C:332:ILE:O	2.13	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.13	0.49
3:L:122:LEU:HD21	3:L:137:LEU:HD12	1.94	0.49
2:J:101:ARG:CG	2:J:114:TRP:HE1	2.24	0.49
1:B:331:ASN:HD22	4:O:1:NAG:H83	1.78	0.49
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.13	0.49
3:L:202:HIS:CE1	3:L:203:GLU:HG2	2.48	0.49
1:C:117:LEU:HB2	1:C:130:VAL:HG22	1.94	0.49
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.49
2:J:108:ARG:HD2	2:J:108:ARG:O	2.12	0.49
2:J:120:GLN:HA	2:J:120:GLN:HE21	1.74	0.49
2:J:131:THR:OG1	2:J:162:PRO:HG2	2.12	0.49
3:N:85:GLU:OE1	3:N:110:VAL:HG23	2.05	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.49
1:C:329:PHE:HE1	1:C:544:ASN:HA	1.75	0.49
3:L:52:ASP:O	3:L:53:VAL:HB	2.13	0.49
3:N:101:VAL:CG1	3:N:102:PHE:N	2.76	0.49
3:N:29:VAL:HG12	3:N:94:THR:HG22	1.94	0.49
3:N:85:GLU:OE2	3:N:110:VAL:HB	2.13	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.48
2:J:134:PRO:HD3	2:J:215:HIS:HD1	1.78	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.96	0.48
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.48
2:H:34:TYR:CD1	2:H:99:ARG:NH1	2.82	0.48
3:L:101:VAL:CG1	3:L:102:PHE:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:TYR:CD1	2:J:99:ARG:NH1	2.82	0.48
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.95	0.48
1:B:457:ARG:NH1	1:B:467:ASP:HB3	2.28	0.48
3:L:85:GLU:OE2	3:L:110:VAL:HB	2.13	0.48
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.94	0.48
1:C:550:GLY:CA	1:C:590:CYS:SG	2.90	0.48
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.48
1:B:281:GLU:OE2	5:B:1405:NAG:H81	2.14	0.48
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.96	0.48
3:L:191:LYS:NZ	3:L:214:THR:OG1	2.47	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
3:L:155:ALA:HB1	3:L:193:HIS:CD2	2.48	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:C:675:GLN:NE2	1:C:675:GLN:CA	2.73	0.48
2:H:108:ARG:HD2	2:H:108:ARG:O	2.13	0.48
3:L:22:CYS:N	3:L:73:ALA:O	2.47	0.48
2:J:34:TYR:CZ	2:J:99:ARG:NH1	2.82	0.48
3:N:35:VAL:HG23	3:N:53:VAL:HA	1.95	0.48
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.48
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.94	0.48
2:H:34:TYR:CZ	2:H:99:ARG:NH1	2.82	0.48
2:H:101:ARG:HG2	2:H:114:TRP:HZ2	1.60	0.48
3:N:194:ARG:O	3:N:213:PRO:HD2	2.13	0.48
3:N:202:HIS:CE1	3:N:203:GLU:HG2	2.48	0.48
1:C:118:LEU:O	1:C:128:ILE:HA	2.14	0.48
1:C:197:ILE:HG22	1:C:198:ASP:H	1.78	0.48
2:H:162:PRO:HB2	2:H:215:HIS:NE2	2.29	0.48
3:N:191:LYS:NZ	3:N:214:THR:OG1	2.47	0.48
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.77	0.48
2:H:165:VAL:HG22	2:H:215:HIS:CD2	2.49	0.48
3:L:194:ARG:O	3:L:213:PRO:HD2	2.13	0.48
2:J:162:PRO:HB2	2:J:215:HIS:NE2	2.29	0.48
1:B:576:VAL:O	1:B:584:ILE:HA	2.13	0.47
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.47
1:B:557:LYS:NZ	1:B:575:ALA:HB2	2.29	0.47
1:C:140:PHE:CE2	1:C:244:LEU:HB2	2.49	0.47
3:L:4:LEU:O	3:L:6:GLN:N	2.43	0.47
1:B:459:SER:C	1:B:461:LEU:H	2.22	0.47
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.47
2:H:146:THR:HG23	2:H:151:ALA:HB2	1.96	0.47
2:J:165:VAL:HG22	2:J:215:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:113:GLN:NE2	3:N:114:PRO:HD2	2.29	0.47
1:A:45:SER:O	1:A:47:VAL:HG22	2.14	0.47
3:L:85:GLU:OE1	3:L:110:VAL:HG23	2.05	0.47
1:A:230:PRO:HB2	1:C:521:PRO:HG2	1.95	0.47
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:C:605:SER:OG	1:C:606:ASN:N	2.47	0.47
3:L:4:LEU:N	3:L:4:LEU:HD12	2.30	0.47
2:J:146:THR:HG23	2:J:151:ALA:HB2	1.96	0.47
3:N:107:LYS:NZ	3:N:108:LEU:O	2.46	0.47
1:B:748:GLU:CD	1:B:981:LEU:HD21	2.39	0.47
1:C:66:HIS:CE1	1:C:214:ARG:HH22	2.32	0.47
1:C:143:VAL:C	1:C:154:GLU:HA	2.39	0.47
1:C:278:LYS:HB2	1:C:306:PHE:CZ	2.50	0.47
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.47
2:H:120:GLN:HA	2:H:120:GLN:HE21	1.74	0.47
3:L:35:VAL:HG23	3:L:53:VAL:HA	1.95	0.47
3:L:191:LYS:HD2	3:L:191:LYS:HA	1.75	0.47
2:J:139:LEU:HB3	3:N:123:PHE:CD2	2.49	0.47
1:B:577:ARG:HD3	1:B:582:LEU:HD11	1.92	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
2:H:114:TRP:O	3:L:38:TYR:OH	2.23	0.47
3:L:173:SER:O	3:L:175:ASN:ND2	2.47	0.47
3:N:22:CYS:N	3:N:73:ALA:O	2.47	0.47
3:N:97:SER:C	3:N:99:LEU:N	2.73	0.47
3:N:124:PRO:HA	3:N:137:LEU:HD13	1.97	0.47
1:A:361:CYS:H	1:A:524:VAL:HG12	1.79	0.47
1:B:403:ARG:NH2	1:B:504:GLY:O	2.47	0.47
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.97	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.47
2:J:99:ARG:HG3	2:J:117:PRO:HD2	1.97	0.47
2:J:101:ARG:HG2	2:J:114:TRP:HZ2	1.60	0.47
3:N:4:LEU:N	3:N:4:LEU:HD12	2.30	0.47
3:N:173:SER:O	3:N:175:ASN:ND2	2.47	0.47
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.47
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.47
3:L:97:SER:C	3:L:99:LEU:N	2.73	0.47
3:L:155:ALA:O	3:L:157:SER:N	2.48	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.46
1:A:490:PHE:CD2	2:H:104:TYR:CG	2.91	0.46
1:C:66:HIS:HE1	1:C:214:ARG:HH22	1.62	0.46
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:GLU:CG	2:H:115:PHE:CD1	2.84	0.46
2:H:120:GLN:NE2	2:H:120:GLN:CA	2.73	0.46
2:H:139:LEU:HB3	3:L:123:PHE:CD2	2.49	0.46
2:J:101:ARG:CD	2:J:114:TRP:CZ2	2.78	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
3:L:49:MET:HG2	3:L:50:ILE:HG12	1.97	0.46
3:N:165:GLU:O	3:N:181:SER:HA	2.15	0.46
1:A:985:ASP:OD1	1:A:985:ASP:N	2.46	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
2:J:34:TYR:CE2	2:J:99:ARG:NH1	2.76	0.46
3:N:49:MET:HG2	3:N:50:ILE:HG12	1.97	0.46
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:B:603:ASN:OD1	5:B:1407:NAG:N2	2.49	0.46
3:L:124:PRO:HA	3:L:137:LEU:HD13	1.97	0.46
3:L:146:PRO:HG2	3:L:202:HIS:HE1	1.80	0.46
2:J:142:SER:HB3	2:J:144:LYS:HG2	1.98	0.46
3:N:155:ALA:O	3:N:157:SER:N	2.48	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
2:J:215:HIS:CD2	2:J:217:PRO:HD2	2.51	0.46
1:A:127:VAL:HG11	5:A:1402:NAG:H61	1.98	0.46
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.46
1:B:532:ASN:ND2	1:B:533:LEU:H	2.14	0.46
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.51	0.46
3:L:86:ALA:O	3:L:107:LYS:NZ	2.43	0.46
3:L:165:GLU:O	3:L:181:SER:HA	2.15	0.46
2:J:20:LEU:HD21	2:J:124:VAL:HG21	1.98	0.46
2:J:111:ARG:H	2:J:111:ARG:HG2	1.52	0.46
3:N:2:SER:O	3:N:4:LEU:HD12	2.16	0.46
1:A:327:VAL:HG12	1:A:530:SER:HA	1.97	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.46
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	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
2:H:142:SER:HB3	2:H:144:LYS:HG2	1.98	0.46
1:B:424:LYS:HG3	1:B:461:LEU:O	2.16	0.46
1:B:567:ARG:HE	1:B:567:ARG:HB3	1.48	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.46
1:C:361:CYS:H	1:C:524:VAL:HG12	1.79	0.46
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.46
2:J:114:TRP:C	3:N:38:TYR:HH	2.20	0.46
1:B:437:ASN:HD21	1:B:506:GLN:HE21	1.64	0.45
1:C:486:PHE:HZ	3:N:51:TYR:CD2	2.34	0.45
3:L:2:SER:O	3:L:4:LEU:HD12	2.16	0.45
3:N:85:GLU:CG	3:N:110:VAL:HG23	2.46	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
3:L:107:LYS:NZ	3:L:108:LEU:O	2.46	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:A:335:LEU:O	1:A:362:VAL:O	2.33	0.45
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.99	0.45
2:H:38:TRP:CD2	2:H:82:LEU:HD23	2.52	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
3:L:4:LEU:H	3:L:4:LEU:HD13	1.81	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:393:THR:HA	1:A:523:THR:HB	1.97	0.45
1:A:417:LYS:CE	2:H:55:TYR:OH	2.65	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:C:37:TYR:HA	1:C:223:LEU:H	1.81	0.45
2:H:34:TYR:CE1	2:H:99:ARG:NH1	2.85	0.45
2:J:34:TYR:CE1	2:J:99:ARG:NH1	2.85	0.45
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.45
1:C:314:GLN:HE21	1:C:314:GLN:HB2	1.56	0.45
3:L:171:LYS:HB3	3:L:171:LYS:HE2	1.79	0.45
2:J:186:GLN:OE1	2:J:192:SER:OG	2.31	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:353:TRP:CD1	1:B:353:TRP:H	2.34	0.45
3:N:4:LEU:H	3:N:4:LEU:HD13	1.81	0.45
1:A:417:LYS:HE3	2:H:55:TYR:OH	2.16	0.45
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.45
1:C:676:THR:CA	1:C:690:GLN:HE21	2.29	0.45
2:H:215:HIS:CD2	2:H:217:PRO:HD2	2.51	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
3:L:54:SER:OG	3:L:66:GLY:O	2.35	0.45
2:J:38:TRP:CD2	2:J:82:LEU:HD23	2.52	0.45
3:N:4:LEU:O	3:N:6:GLN:N	2.43	0.45
1:B:437:ASN:OD1	1:B:438:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:PRO:HG3	1:B:564:GLN:NE2	2.32	0.45
1:B:521:PRO:HG3	1:B:564:GLN:HE21	1.81	0.45
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.45
2:H:20:LEU:HD21	2:H:124:VAL:HG21	1.98	0.45
3:L:19:THR:HA	3:L:76:THR:HA	1.99	0.45
3:L:154:LYS:HE2	3:L:155:ALA:C	2.42	0.45
2:J:114:TRP:CE3	2:J:115:PHE:O	2.71	0.45
2:J:160:TYR:OH	2:J:193:LEU:HD23	2.17	0.45
1:A:449:TYR:O	2:H:107:GLY:HA2	2.17	0.44
1:A:676:THR:HB	1:A:693:ILE:HG21	1.98	0.44
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.44
1:C:484:GLU:HB3	2:J:103:TYR:HE1	1.81	0.44
3:L:197:SER:HB2	3:L:209:LYS:O	2.17	0.44
2:J:102:CYS:CA	2:J:112:CYS:HB3	2.47	0.44
3:N:54:SER:OG	3:N:66:GLY:O	2.35	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:A:523:THR:CG2	1:A:524:VAL:N	2.45	0.44
1:C:449:TYR:O	2:J:107:GLY:HA2	2.17	0.44
3:L:113:GLN:NE2	3:L:114:PRO:HD2	2.33	0.44
3:N:146:PRO:HG2	3:N:202:HIS:HE1	1.81	0.44
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:B:350:VAL:HG11	1:B:402:ILE:HG23	2.00	0.44
1:B:472:ILE:H	1:B:472:ILE:HG13	1.56	0.44
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.44
3:L:51:TYR:C	3:L:53:VAL:H	2.25	0.44
3:N:85:GLU:OE2	3:N:110:VAL:CG2	2.65	0.44
3:N:154:LYS:HE2	3:N:155:ALA:C	2.42	0.44
3:N:197:SER:HB2	3:N:209:LYS:O	2.17	0.44
1:C:521:PRO:O	1:C:522:ALA:CB	2.66	0.44
2:H:8:GLY:H	2:H:9:PRO:CD	2.31	0.44
2:H:34:TYR:CE2	2:H:99:ARG:NH1	2.76	0.44
1:A:521:PRO:HG3	1:B:199:GLY:O	2.14	0.44
1:B:376:THR:CG2	1:B:378:LYS:HG3	2.48	0.44
1:B:454:ARG:NH2	1:B:456:PHE:HZ	2.16	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:C:142:GLY:H	1:C:243:ALA:HA	1.83	0.44
2:H:186:GLN:OE1	2:H:192:SER:OG	2.31	0.44
2:H:99:ARG:HG3	2:H:117:PRO:HD2	1.97	0.44
2:J:120:GLN:NE2	2:J:120:GLN:CA	2.73	0.44
2:J:210:ILE:HG23	2:J:225:LYS:HD2	2.00	0.44
1:B:453:TYR:HD1	1:B:453:TYR:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.85	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.44
2:H:102:CYS:CA	2:H:112:CYS:HB3	2.47	0.44
2:H:114:TRP:CE3	2:H:115:PHE:O	2.71	0.44
2:J:92:THR:O	2:J:92:THR:OG1	2.34	0.44
2:J:113:VAL:O	2:J:115:PHE:N	2.44	0.44
3:N:19:THR:HA	3:N:76:THR:HA	1.99	0.44
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.44
2:H:160:TYR:OH	2:H:193:LEU:HD23	2.17	0.44
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.44
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.44
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.77	0.44
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.44
2:H:169:TRP:HD1	2:H:178:VAL:HG13	1.83	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.43
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.84	0.43
1:C:533:LEU:O	1:C:533:LEU:HG	2.17	0.43
2:J:169:TRP:HD1	2:J:178:VAL:HG13	1.83	0.43
3:N:51:TYR:C	3:N:53:VAL:H	2.25	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.00	0.43
1:B:167:THR:HG22	1:B:168:PHE:H	1.82	0.43
1:C:84:LEU:HD13	1:C:238:PHE:CE1	2.52	0.43
3:L:9:SER:C	3:L:10:VAL:HG23	2.43	0.43
1:B:439:ASN:HB3	1:B:506:GLN:HB2	1.99	0.43
2:H:68:ARG:HD2	2:H:84:LEU:HD11	2.00	0.43
3:L:85:GLU:OE2	3:L:110:VAL:CG2	2.66	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:C:132:GLU:CD	1:C:165:ASN:HB2	2.43	0.43
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:B:559:PHE:O	1:B:560:LEU:HD13	2.18	0.43
1:C:119:ILE:HG13	1:C:128:ILE:HG23	2.01	0.43
3:N:9:SER:C	3:N:10:VAL:HG23	2.43	0.43
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
1:B:364:ASP:OD1	1:B:364:ASP:N	2.50	0.43
3:L:28:ASP:OD1	3:L:28:ASP:N	2.51	0.43
3:L:111:LEU:HD23	3:L:111:LEU:HA	1.87	0.43
2:J:36:TRP:CE3	2:J:99:ARG:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:VAL:C	2:J:114:TRP:HD1	2.16	0.43
3:N:186:THR:HG23	3:N:189:GLN:HB2	2.01	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:B:121:ASN:O	1:B:121:ASN:ND2	2.49	0.43
3:L:4:LEU:C	3:L:6:GLN:H	2.27	0.43
2:J:68:ARG:HD2	2:J:84:LEU:HD11	2.00	0.43
1:A:230:PRO:CB	1:C:521:PRO:HG2	2.49	0.43
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.43
2:H:162:PRO:HD2	2:H:215:HIS:CE1	2.54	0.43
2:J:102:CYS:HA	2:J:112:CYS:HB3	2.00	0.43
3:N:28:ASP:OD1	3:N:28:ASP:N	2.51	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:B:91:TYR:OH	1:B:191:GLU:HG2	2.19	0.43
2:J:157:VAL:HG13	2:J:193:LEU:HG	2.01	0.43
1:A:484:GLU:HB3	2:H:103:TYR:HE1	1.81	0.43
1:B:462:LYS:H	1:B:462:LYS:HD3	1.84	0.43
2:H:214:ASN:HB3	2:H:221:LYS:CE	2.49	0.43
4:E:1:NAG:H61	4:E:2:NAG:N2	2.33	0.43
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
5:B:1410:NAG:O4	5:B:1411:NAG:O5	2.28	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.42
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.42
3:L:85:GLU:CG	3:L:110:VAL:HG23	2.47	0.42
3:N:125:PRO:HG2	3:N:135:ALA:HB1	2.01	0.42
3:N:191:LYS:HA	3:N:191:LYS:HD2	1.75	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:A:127:VAL:HG21	5:A:1402:NAG:H5	2.01	0.42
1:A:869:MET:HE1	1:C:697:MET:HG3	2.00	0.42
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.00	0.42
2:H:102:CYS:HA	2:H:112:CYS:HB3	2.00	0.42
2:H:170:ASN:OD1	2:H:210:ILE:HG13	2.19	0.42
3:L:122:LEU:HD23	3:L:123:PHE:N	2.34	0.42
3:L:143:ASP:HA	3:L:176:LYS:HG3	2.01	0.42
2:J:8:GLY:H	2:J:9:PRO:CD	2.31	0.42
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.42
2:J:193:LEU:HD12	2:J:194:SER:N	2.34	0.42
1:B:29:THR:OG1	1:B:30:ASN:N	2.50	0.42
2:H:36:TRP:CE3	2:H:99:ARG:HB3	2.54	0.42
3:L:2:SER:O	3:L:4:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:125:PRO:HG2	3:L:135:ALA:HB1	2.01	0.42
2:J:214:ASN:HB3	2:J:221:LYS:CE	2.49	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:C:417:LYS:NZ	1:C:455:LEU:CG	2.82	0.42
1:C:740:MET:HE2	1:C:740:MET:HB2	1.91	0.42
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.42
3:L:186:THR:HG23	3:L:189:GLN:HB2	2.01	0.42
1:B:472:ILE:CD1	1:B:474:GLN:HB3	2.47	0.42
1:C:233:ILE:HG12	1:C:234:ASN:N	2.28	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
2:H:204:LEU:HB3	2:H:228:PRO:HG3	2.02	0.42
3:L:156:ASP:OD1	3:L:194:ARG:N	2.52	0.42
3:N:194:ARG:HA	3:N:194:ARG:HD2	1.67	0.42
3:N:53:VAL:O	3:N:54:SER:OG	2.26	0.42
3:N:156:ASP:OD1	3:N:194:ARG:N	2.52	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:567:ARG:HG2	1:C:42:VAL:HG11	2.02	0.42
2:J:162:PRO:HD2	2:J:215:HIS:CE1	2.54	0.42
2:J:204:LEU:HB3	2:J:228:PRO:HG3	2.02	0.42
3:N:122:LEU:HD23	3:N:123:PHE:N	2.34	0.42
3:N:143:ASP:HA	3:N:176:LYS:HG3	2.01	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.42
1:B:341:VAL:HG23	1:B:342:PHE:HD1	1.84	0.42
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.42
2:J:170:ASN:OD1	2:J:210:ILE:HG13	2.19	0.42
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.55	0.42
1:A:460:ASN:OD1	1:A:460:ASN:N	2.53	0.42
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.42
1:B:187:LYS:HZ3	1:B:213:VAL:HG13	1.84	0.42
1:B:495:TYR:CZ	1:B:507:PRO:HG3	2.55	0.42
2:H:157:VAL:HG13	2:H:193:LEU:HG	2.01	0.42
2:H:210:ILE:HG23	2:H:225:LYS:HD2	2.00	0.42
3:L:137:LEU:HD23	3:L:185:LEU:HD11	2.02	0.42
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.41
1:C:556:ASN:HD22	1:C:556:ASN:HA	1.53	0.41
2:H:193:LEU:HD12	2:H:194:SER:N	2.34	0.41
3:L:155:ALA:HA	3:L:196:TYR:CD1	2.55	0.41
3:N:187:PRO:HA	3:N:190:TRP:HB3	2.02	0.41
1:B:376:THR:O	1:B:434:ILE:HA	2.20	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.41
2:H:215:HIS:HD2	2:H:217:PRO:HD2	1.86	0.41
3:L:194:ARG:HA	3:L:194:ARG:HD2	1.67	0.41
3:N:4:LEU:C	3:N:6:GLN:H	2.27	0.41
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.71	0.41
1:C:122:ASN:ND2	1:C:125:ASN:HB2	2.35	0.41
2:H:98:ALA:HB2	2:H:118:TRP:HA	2.03	0.41
2:H:111:ARG:H	2:H:111:ARG:HG2	1.52	0.41
3:L:5:THR:O	3:L:7:PRO:HD2	2.21	0.41
3:L:126:SER:O	3:L:130:LEU:HG	2.19	0.41
3:L:191:LYS:NZ	3:L:213:PRO:HB2	2.36	0.41
3:N:189:GLN:O	3:N:196:TYR:OH	2.39	0.41
4:W:1:NAG:H83	4:W:1:NAG:H3	2.02	0.41
1:B:81:ASN:O	1:B:239:GLN:NE2	2.54	0.41
1:B:142:GLY:O	1:B:156:GLU:HG3	2.20	0.41
1:C:117:LEU:HD22	1:C:231:ILE:HD12	2.03	0.41
1:C:530:SER:C	1:C:531:THR:HG23	2.45	0.41
1:C:532:ASN:HB2	1:C:533:LEU:H	1.68	0.41
2:J:6:GLU:HB2	2:J:122:THR:HG23	2.02	0.41
2:J:98:ALA:HB2	2:J:118:TRP:HA	2.03	0.41
3:N:126:SER:O	3:N:130:LEU:HG	2.19	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.50	0.41
1:A:295:PRO:HB2	1:A:608:VAL:HG11	2.01	0.41
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.41
1:B:506:GLN:HA	1:B:507:PRO:HD3	1.94	0.41
2:H:112:CYS:C	2:H:113:VAL:HG13	2.46	0.41
2:H:118:TRP:C	2:H:119:GLY:O	2.64	0.41
2:J:30:SER:HA	2:J:55:TYR:HB2	2.03	0.41
2:J:118:TRP:C	2:J:119:GLY:O	2.64	0.41
1:B:187:LYS:HG2	1:B:212:LEU:O	2.21	0.41
1:C:111:ASP:CG	1:C:112:SER:H	2.28	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
2:H:6:GLU:HB2	2:H:122:THR:HG23	2.02	0.41
2:H:30:SER:HA	2:H:55:TYR:HB2	2.02	0.41
3:N:5:THR:O	3:N:7:PRO:HD2	2.21	0.41
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
2:H:101:ARG:CD	2:H:114:TRP:CZ2	2.78	0.41
3:L:133:ASN:OD1	3:L:133:ASN:N	2.54	0.41
1:A:226:LEU:HB3	1:A:227:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:PHE:O	1:B:547:THR:HA	2.20	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41
2:H:224:LYS:HD2	2:H:224:LYS:HA	1.92	0.41
2:J:111:ARG:HB3	3:N:93:TYR:OH	2.12	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.21	0.41
1:C:188:ASN:HB2	1:C:190:ARG:HH11	1.86	0.41
1:C:388:ASN:OD1	1:C:527:PRO:HD2	2.21	0.41
1:C:532:ASN:OD1	1:C:532:ASN:N	2.46	0.41
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.41
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.41
3:L:155:ALA:O	3:L:156:ASP:C	2.64	0.41
3:L:159:PRO:HB2	3:L:161:LYS:NZ	2.36	0.41
2:J:112:CYS:C	2:J:113:VAL:HG13	2.46	0.41
3:N:191:LYS:NZ	3:N:213:PRO:HB2	2.36	0.41
1:B:132:GLU:HG3	1:B:165:ASN:HB2	2.02	0.41
1:B:403:ARG:NE	1:B:505:TYR:HD1	2.19	0.41
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.41
3:N:137:LEU:HD23	3:N:185:LEU:HD11	2.02	0.41
4:V:1:NAG:H61	4:V:2:NAG:N2	2.33	0.41
1:B:794:ILE:H	1:B:794:ILE:HG13	1.69	0.40
1:C:467:ASP:OD1	1:C:469:SER:OG	2.39	0.40
2:J:215:HIS:HD2	2:J:217:PRO:HD2	1.86	0.40
3:N:159:PRO:HB2	3:N:161:LYS:NZ	2.36	0.40
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.40
1:A:332:ILE:O	1:A:333:THR:HG23	2.21	0.40
1:B:273:ARG:HA	1:B:273:ARG:HD3	1.70	0.40
1:B:458:LYS:HE2	1:B:458:LYS:HB2	1.79	0.40
1:B:646:ARG:O	1:B:646:ARG:HG3	2.22	0.40
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.40
3:L:187:PRO:HA	3:L:190:TRP:HB3	2.02	0.40
3:N:2:SER:O	3:N:4:LEU:HD13	2.19	0.40
3:N:155:ALA:HA	3:N:196:TYR:CD1	2.55	0.40
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.56	0.40
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.78	0.40
1:B:578:ASP:N	1:B:583:GLU:O	2.37	0.40
1:C:371:SER:C	1:C:373:SER:H	2.30	0.40
2:J:209:TYR:H	2:J:225:LYS:HE3	1.87	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:135:PHE:HE1	1:B:159:VAL:HG12	1.86	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.40
3:N:9:SER:O	3:N:10:VAL:HG23	2.21	0.40
3:N:96:SER:OG	3:N:97:SER:N	2.53	0.40
1:A:879:ALA:O	1:A:883:THR:HB	2.22	0.40
1:C:335:LEU:CB	1:C:362:VAL:HG13	2.46	0.40
1:C:369:TYR:CZ	1:C:384:PRO:HB2	2.57	0.40
1:C:615:VAL:HG12	1:C:616:ASN:O	2.20	0.40
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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	881/1122 (78%)	770 (87%)	111 (13%)	4 15
1	B	862/1122 (77%)	756 (88%)	106 (12%)	4 16
1	C	879/1122 (78%)	773 (88%)	106 (12%)	5 16
2	H	199/410 (48%)	185 (93%)	14 (7%)	14 40
2	J	199/410 (48%)	185 (93%)	14 (7%)	14 40
3	L	180/183 (98%)	162 (90%)	18 (10%)	7 24
3	N	180/183 (98%)	163 (91%)	17 (9%)	8 27
All	All	3380/4552 (74%)	2994 (89%)	386 (11%)	8 19

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
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
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	318	PHE
1	A	324	GLU
1	A	325	SER
1	A	335	LEU
1	A	336	CYS
1	A	362	VAL
1	A	375	SER
1	A	382	VAL
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	459	SER
1	A	469	SER
1	A	472	ILE

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Mol	Chain	Res	Type
1	A	486	PHE
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
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	599	THR
1	A	602	THR
1	A	608	VAL
1	A	673	SER
1	A	692	ILE
1	A	698	SER
1	A	702	GLU
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	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU

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Mol	Chain	Res	Type
1	A	929	SER
1	A	939	SER
1	A	951	VAL
1	A	960	ASN
1	A	967	SER
1	A	973	ILE
1	A	976	VAL
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	45	SER
1	B	46	SER
1	B	48	LEU
1	B	50	SER
1	B	51	THR
1	B	52	GLN
1	B	60	SER
1	B	62	VAL
1	B	66	HIS
1	B	87	ASN
1	B	95	THR
1	B	99	ASN
1	B	108	THR
1	B	109	THR
1	B	112	SER
1	B	116	SER

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Mol	Chain	Res	Type
1	B	120	VAL
1	B	122	ASN
1	B	127	VAL
1	B	158	ARG
1	B	164	ASN
1	B	205	SER
1	B	208	THR
1	B	214	ARG
1	B	240	THR
1	B	277	LEU
1	B	278	LYS
1	B	284	THR
1	B	307	THR
1	B	324	GLU
1	B	327	VAL
1	B	345	THR
1	B	349	SER
1	B	359	SER
1	B	371	SER
1	B	373	SER
1	B	382	VAL
1	B	385	THR
1	B	401	VAL
1	B	402	ILE
1	B	409	GLN
1	B	417	LYS
1	B	418	ILE
1	B	430	THR
1	B	441	LEU
1	B	453	TYR
1	B	462	LYS
1	B	464	PHE
1	B	465	GLU
1	B	472	ILE
1	B	473	TYR
1	B	494	SER
1	B	506	GLN
1	B	514	SER
1	B	524	VAL
1	B	525	CYS
1	B	528	LYS
1	B	531	THR

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Mol	Chain	Res	Type
1	B	532	ASN
1	B	533	LEU
1	B	534	VAL
1	B	555	SER
1	B	567	ARG
1	B	569	ILE
1	B	576	VAL
1	B	582	LEU
1	B	597	VAL
1	B	606	ASN
1	B	607	GLN
1	B	608	VAL
1	B	615	VAL
1	B	617	CYS
1	B	619	GLU
1	B	640	SER
1	B	642	VAL
1	B	676	THR
1	B	710	ASN
1	B	729	VAL
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

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Mol	Chain	Res	Type
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1133	VAL
1	B	1141	LEU
1	C	29	THR
1	C	50	SER
1	C	51	THR
1	C	60	SER
1	C	63	THR
1	C	84	LEU
1	C	86	PHE
1	C	90	VAL
1	C	114	THR
1	C	117	LEU
1	C	120	VAL
1	C	125	ASN
1	C	143	VAL
1	C	155	SER
1	C	172	SER
1	C	195	LYS
1	C	197	ILE
1	C	208	THR
1	C	212	LEU
1	C	215	ASP
1	C	216	LEU
1	C	221	SER
1	C	224	GLU
1	C	233	ILE
1	C	234	ASN
1	C	271	GLN
1	C	277	LEU
1	C	301	CYS
1	C	305	SER
1	C	308	VAL
1	C	314	GLN
1	C	318	PHE
1	C	332	ILE
1	C	335	LEU
1	C	336	CYS
1	C	362	VAL

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Mol	Chain	Res	Type
1	C	375	SER
1	C	382	VAL
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	417	LYS
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	459	SER
1	C	469	SER
1	C	472	ILE
1	C	486	PHE
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	532	ASN
1	C	533	LEU
1	C	534	VAL
1	C	546	LEU
1	C	551	VAL
1	C	555	SER
1	C	556	ASN
1	C	573	THR
1	C	584	ILE
1	C	590	CYS
1	C	591	SER
1	C	602	THR
1	C	620	VAL
1	C	658	ASN
1	C	675	GLN
1	C	693	ILE
1	C	697	MET
1	C	699	LEU
1	C	727	LEU
1	C	768	THR
1	C	770	ILE
1	C	778	THR

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Mol	Chain	Res	Type
1	C	787	GLN
1	C	791	THR
1	C	814	LYS
1	C	856	ASN
1	C	859	THR
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	H	108	ARG
2	H	111	ARG
2	H	112	CYS
2	H	120	GLN
2	H	128	SER
2	H	132	LYS
2	H	153	LEU
2	H	157	VAL
2	H	171	SER
2	H	175	THR
2	H	194	SER
2	H	210	ILE
2	H	212	ASN
2	H	218	SER

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Mol	Chain	Res	Type
3	L	4	LEU
3	L	6	GLN
3	L	95	SER
3	L	97	SER
3	L	98	THR
3	L	99	LEU
3	L	115	LYS
3	L	119	SER
3	L	133	ASN
3	L	150	THR
3	L	158	SER
3	L	170	SER
3	L	173	SER
3	L	185	LEU
3	L	186	THR
3	L	192	SER
3	L	200	VAL
3	L	201	THR
2	J	108	ARG
2	J	111	ARG
2	J	112	CYS
2	J	120	GLN
2	J	128	SER
2	J	132	LYS
2	J	153	LEU
2	J	157	VAL
2	J	171	SER
2	J	175	THR
2	J	194	SER
2	J	210	ILE
2	J	212	ASN
2	J	218	SER
3	N	4	LEU
3	N	6	GLN
3	N	95	SER
3	N	97	SER
3	N	98	THR
3	N	99	LEU
3	N	119	SER
3	N	133	ASN
3	N	150	THR
3	N	158	SER

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Mol	Chain	Res	Type
3	N	170	SER
3	N	173	SER
3	N	185	LEU
3	N	186	THR
3	N	192	SER
3	N	200	VAL
3	N	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	334	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	450	ASN
1	A	498	GLN
1	A	556	ASN
1	A	644	GLN
1	A	658	ASN
1	A	675	GLN
1	A	690	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	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1010	GLN
1	A	1054	GLN
1	A	1113	GLN
1	A	1125	ASN
1	B	52	GLN
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	188	ASN
1	B	245	HIS
1	B	334	ASN
1	B	422	ASN
1	B	460	ASN
1	B	487	ASN
1	B	506	GLN
1	B	532	ASN
1	B	540	ASN
1	B	563	GLN
1	B	607	GLN
1	B	613	GLN
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	30	ASN
1	C	188	ASN
1	C	207	HIS
1	C	271	GLN
1	C	314	GLN
1	C	321	GLN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	450	ASN
1	C	498	GLN
1	C	542	ASN
1	C	556	ASN
1	C	606	ASN

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Mol	Chain	Res	Type
1	C	641	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
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	1106	GLN
1	C	1125	ASN
2	H	60	ASN
2	H	78	ASN
2	H	120	GLN
2	H	219	ASN
3	L	39	GLN
3	L	40	GLN
3	L	113	GLN
3	L	175	ASN
3	L	199	GLN
2	J	60	ASN
2	J	78	ASN
2	J	120	GLN
2	J	219	ASN
3	N	39	GLN
3	N	40	GLN
3	N	113	GLN
3	N	175	ASN
3	N	199	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4	14,14,15	0.49	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.61	0
4	NAG	E	1	1,4	14,14,15	0.53	0	17,19,21	0.58	0
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	F	1	1,4	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	0.48	0
4	NAG	G	1	1,4	14,14,15	0.36	0	17,19,21	0.74	0
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
4	NAG	I	1	1,4	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
4	NAG	I	2	4	14,14,15	0.44	0	17,19,21	1.48	3 (17%)
4	NAG	K	1	1,4	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.67	0
4	NAG	M	1	1,4	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
4	NAG	M	2	4	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	O	1	1,4	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	O	2	4	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	P	1	1,4	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	P	2	4	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	Q	1	1,4	14,14,15	0.36	0	17,19,21	1.15	1 (5%)
4	NAG	Q	2	4	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	R	1	1,4	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
4	NAG	R	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	S	1	1,4	14,14,15	0.71	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	S	2	4	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
4	NAG	T	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	T	2	4	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	U	1	1,4	14,14,15	0.40	0	17,19,21	0.59	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	0.58	0
4	NAG	V	2	4	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	W	1	1,4	14,14,15	0.23	0	17,19,21	1.43	2 (11%)
4	NAG	W	2	4	14,14,15	0.19	0	17,19,21	0.52	0
4	NAG	X	1	1,4	14,14,15	0.50	0	17,19,21	0.72	1 (5%)
4	NAG	X	2	4	14,14,15	0.40	0	17,19,21	0.48	0
4	NAG	Y	1	1,4	14,14,15	0.37	0	17,19,21	0.42	0
4	NAG	Y	2	4	14,14,15	0.20	0	17,19,21	0.76	0
4	NAG	Z	1	1,4	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	Z	2	4	14,14,15	0.60	1 (7%)	17,19,21	1.39	2 (11%)
4	NAG	a	1	1,4	14,14,15	0.62	1 (7%)	17,19,21	0.45	0
4	NAG	a	2	4	14,14,15	0.32	0	17,19,21	1.44	2 (11%)
4	NAG	b	1	1,4	14,14,15	0.41	0	17,19,21	0.44	0
4	NAG	b	2	4	14,14,15	0.25	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	6/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	3/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	6/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	5/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	O5-C1	-2.56	1.39	1.43
4	K	1	NAG	O5-C1	-2.46	1.39	1.43
4	I	1	NAG	O5-C1	-2.24	1.39	1.43
4	a	1	NAG	O5-C1	-2.06	1.40	1.43
4	Z	2	NAG	C1-C2	2.00	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	1	NAG	C2-N2-C7	4.93	129.50	122.90
4	a	2	NAG	C2-N2-C7	4.65	129.14	122.90
4	I	2	NAG	C2-N2-C7	4.64	129.11	122.90
4	G	2	NAG	C2-N2-C7	4.60	129.07	122.90
4	Z	2	NAG	C2-N2-C7	4.60	129.07	122.90
4	Q	1	NAG	C1-O5-C5	3.27	116.57	112.19
4	I	2	NAG	C1-C2-N2	2.59	114.52	110.43
4	a	2	NAG	C1-C2-N2	2.50	114.37	110.43
4	G	2	NAG	C1-C2-N2	2.46	114.31	110.43
4	S	1	NAG	O4-C4-C3	-2.36	104.81	110.38
4	X	1	NAG	C1-O5-C5	2.29	115.25	112.19
4	R	1	NAG	C1-O5-C5	2.23	115.18	112.19
4	M	1	NAG	C1-O5-C5	2.20	115.14	112.19
4	I	2	NAG	C1-O5-C5	2.15	115.07	112.19
4	W	1	NAG	C1-C2-N2	2.14	113.80	110.43
4	U	2	NAG	C1-O5-C5	2.08	114.98	112.19
4	F	1	NAG	C1-O5-C5	2.08	114.97	112.19
4	Z	2	NAG	C1-C2-N2	2.02	113.62	110.43
4	S	2	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	W	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	W	1	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C4-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
4	K	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
4	Z	2	NAG	C1-C2-N2-C7
4	a	2	NAG	C1-C2-N2-C7
4	V	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	R	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
4	V	1	NAG	3	0
4	a	2	NAG	1	0
4	S	1	NAG	1	0
4	Z	2	NAG	1	0
4	W	1	NAG	1	0
4	a	1	NAG	1	0
4	S	2	NAG	1	0

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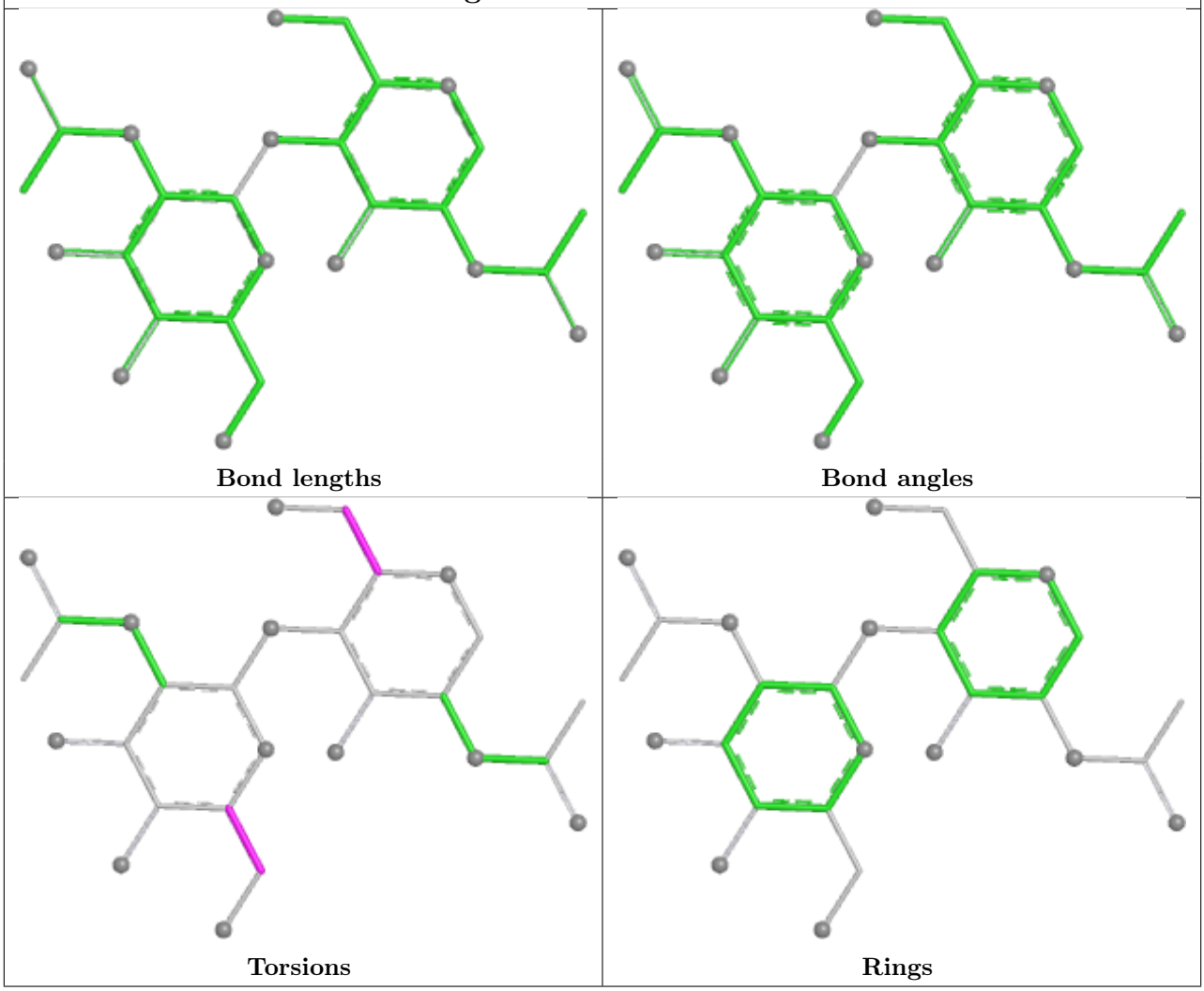
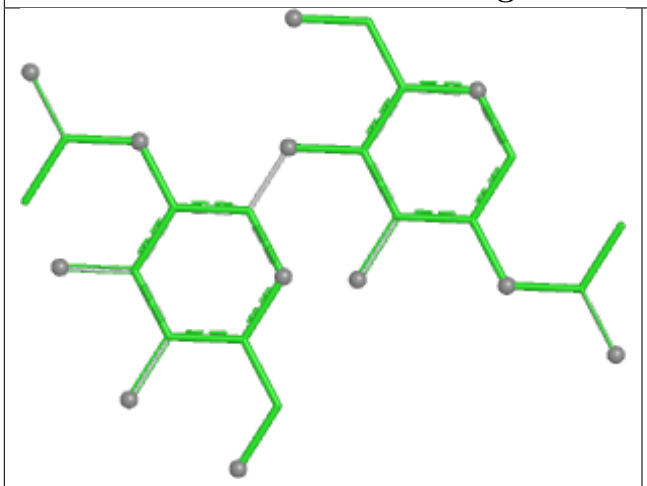
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
4	V	2	NAG	2	0
4	G	2	NAG	1	0
4	O	1	NAG	1	0
4	E	1	NAG	3	0

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

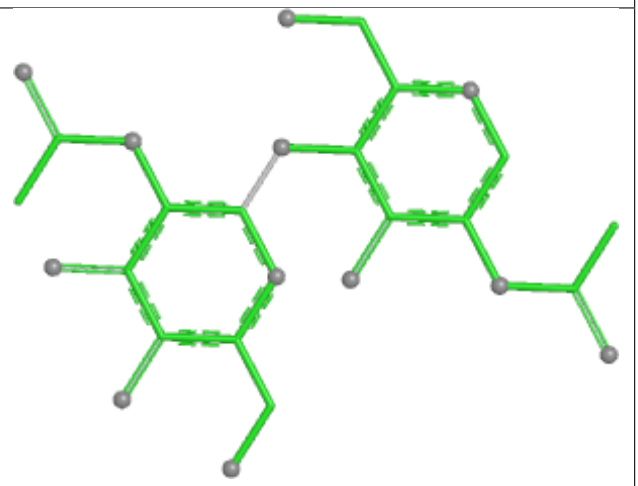
Oligosaccharide Chain D



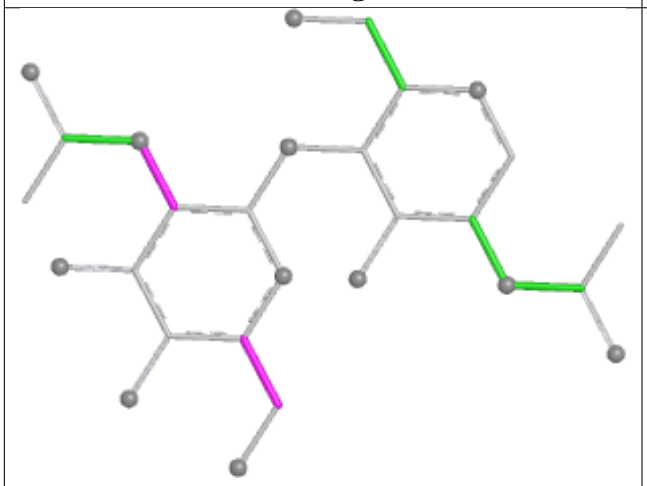
Oligosaccharide Chain E



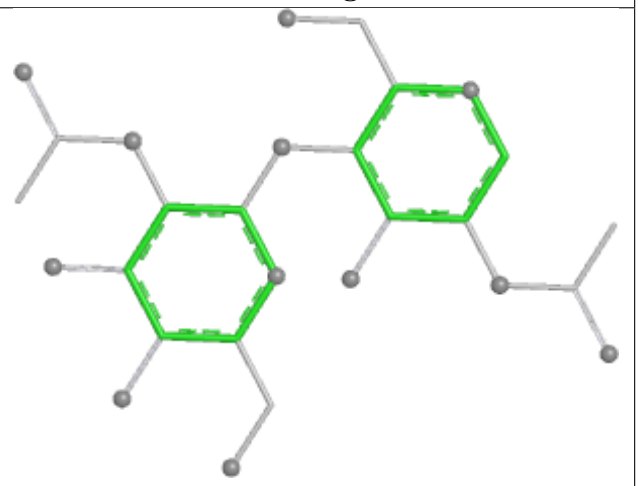
Bond lengths



Bond angles

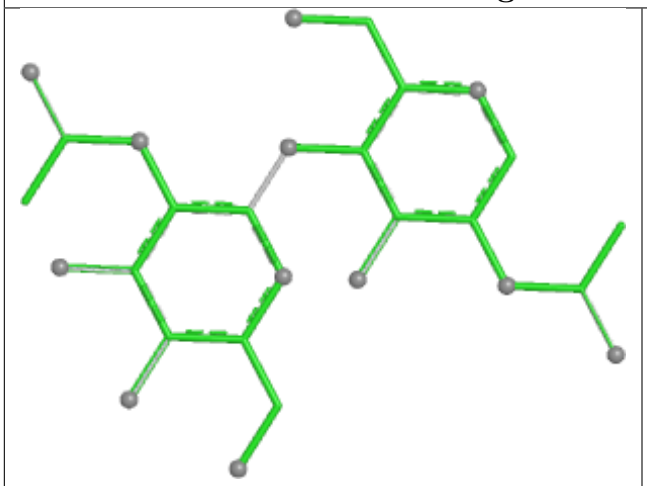


Torsions

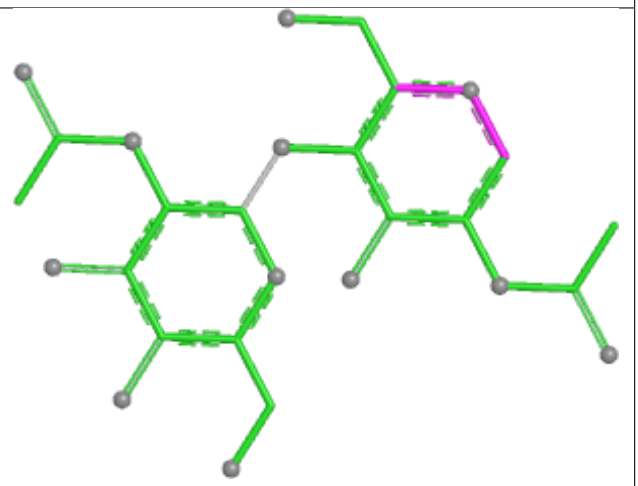


Rings

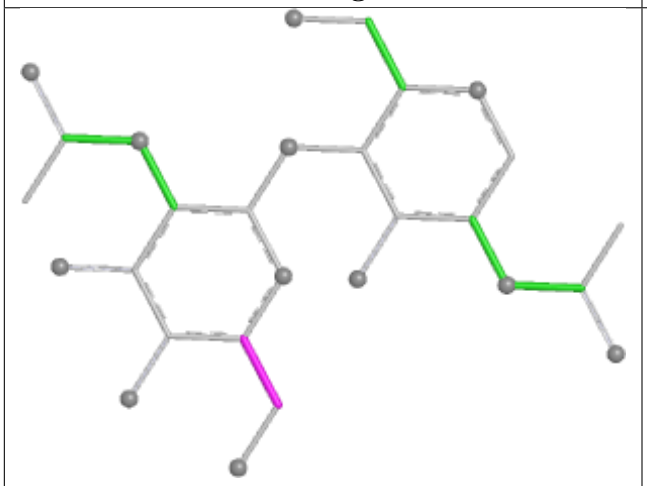
Oligosaccharide Chain F



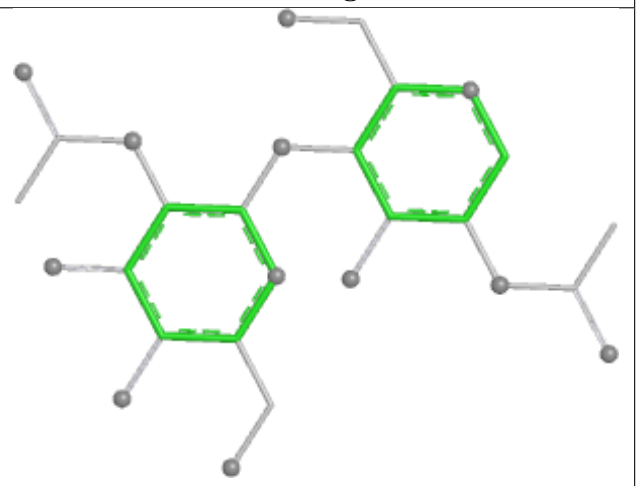
Bond lengths



Bond angles

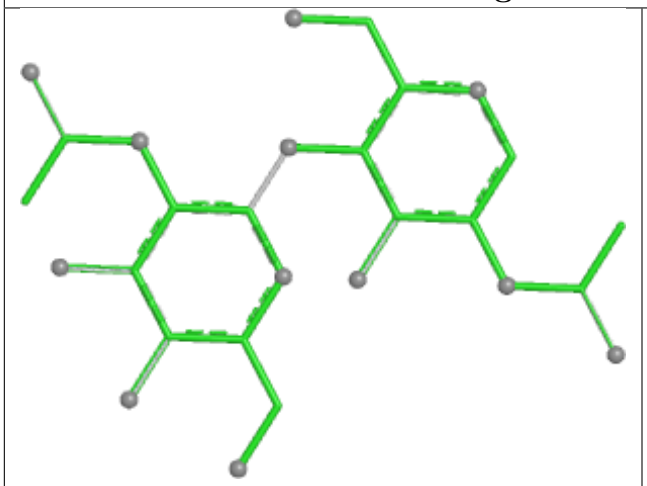


Torsions

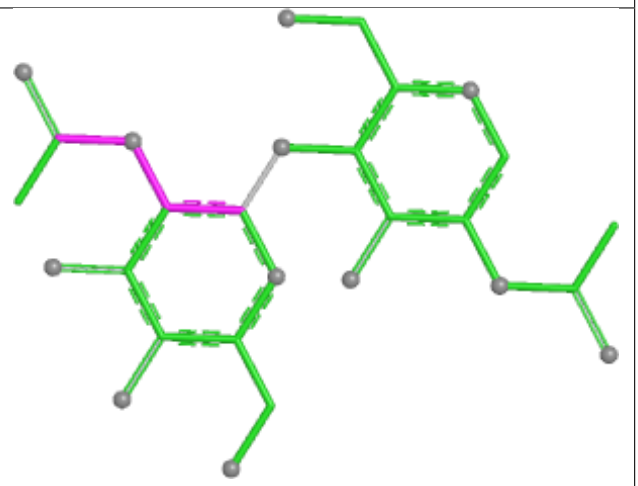


Rings

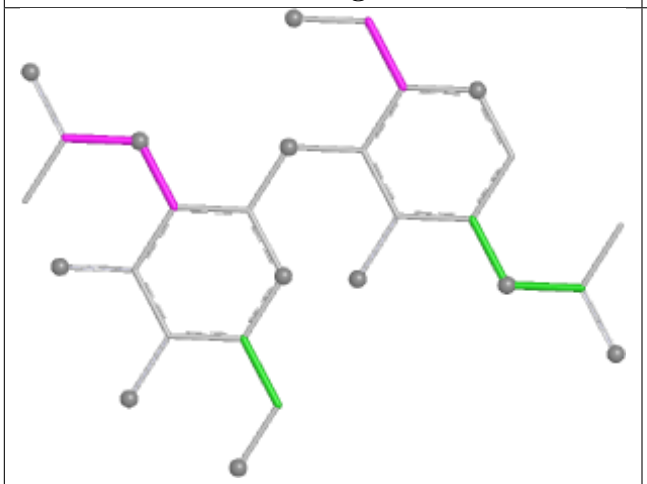
Oligosaccharide Chain G



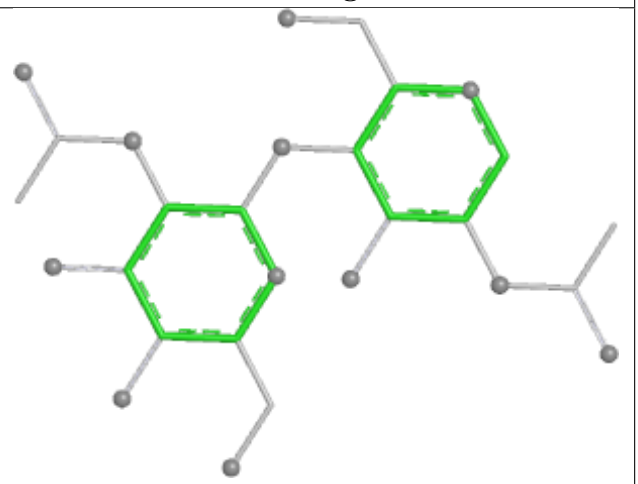
Bond lengths



Bond angles

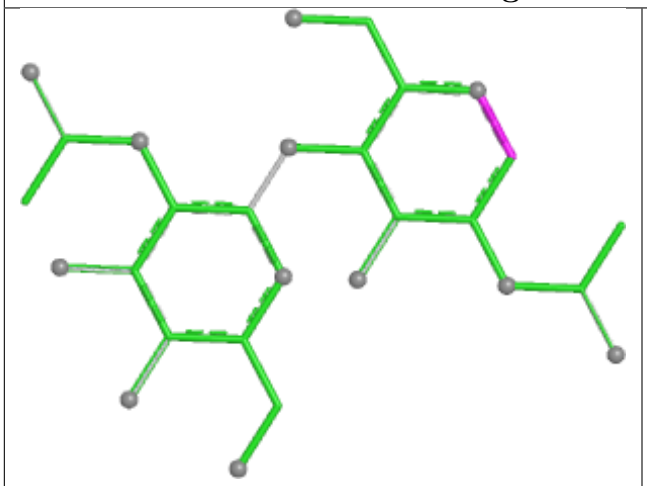


Torsions

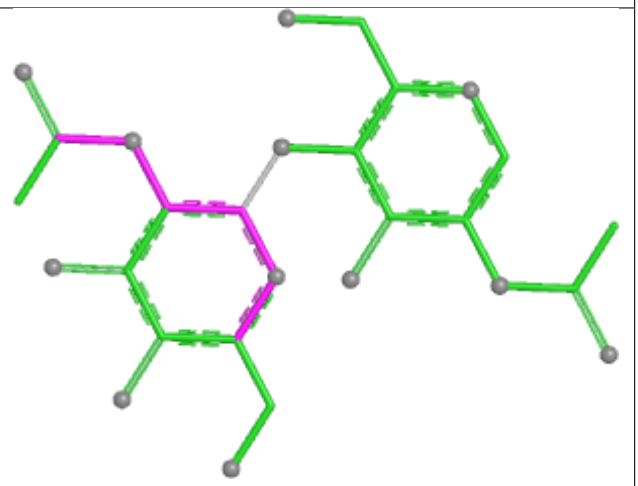


Rings

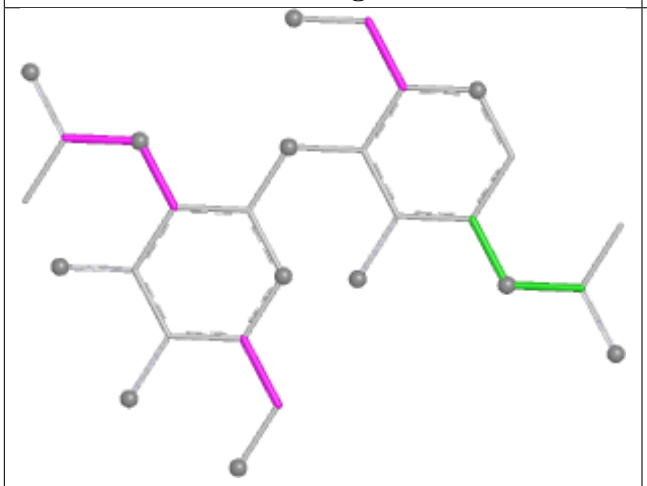
Oligosaccharide Chain I



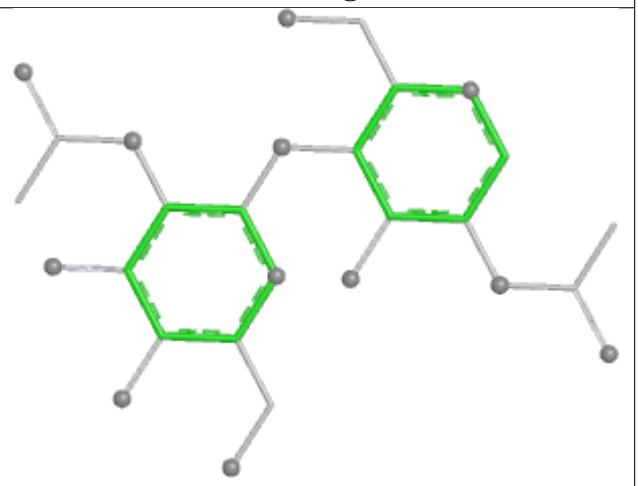
Bond lengths



Bond angles

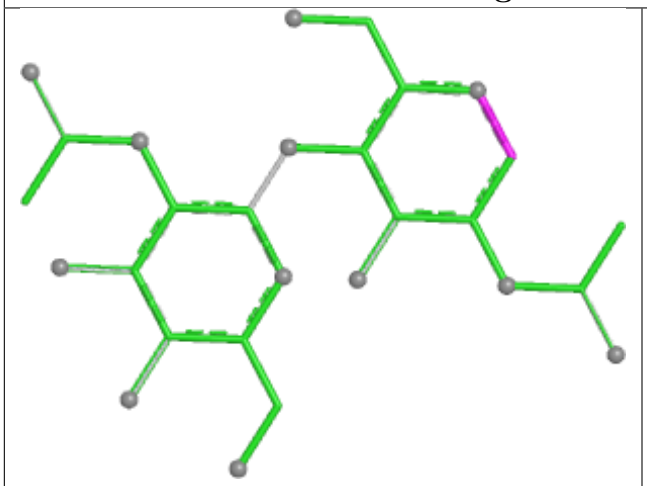


Torsions

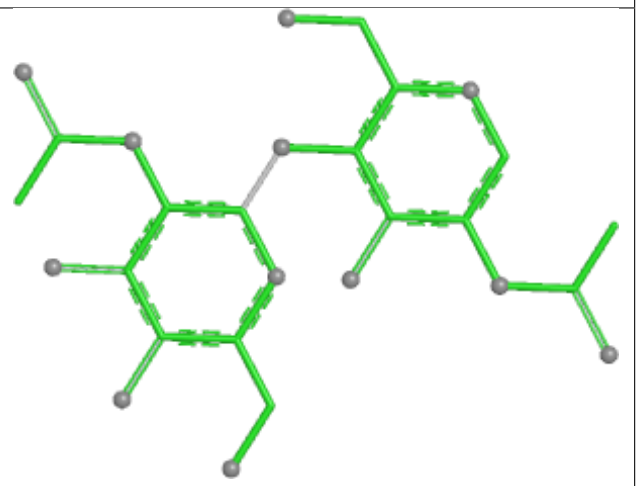


Rings

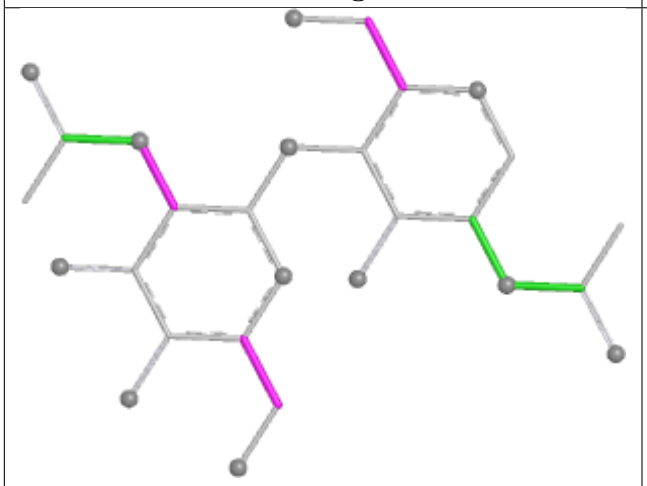
Oligosaccharide Chain K



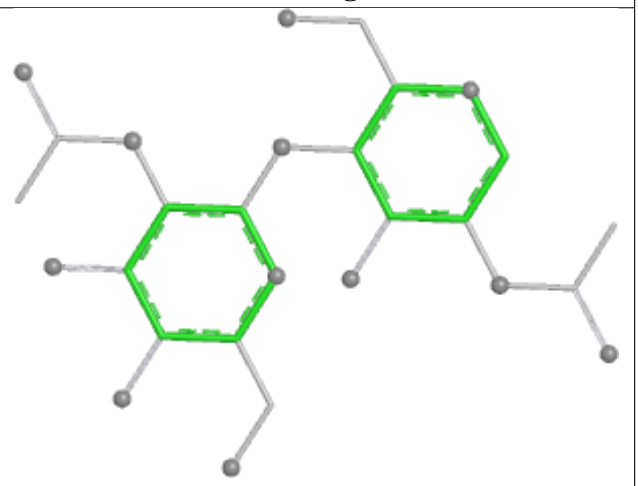
Bond lengths



Bond angles

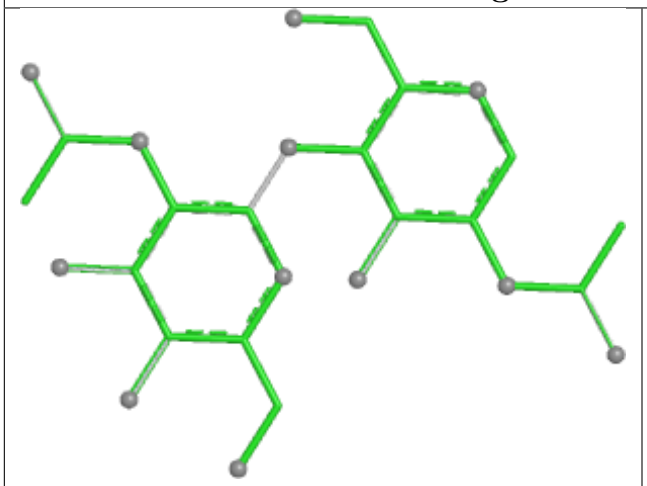


Torsions

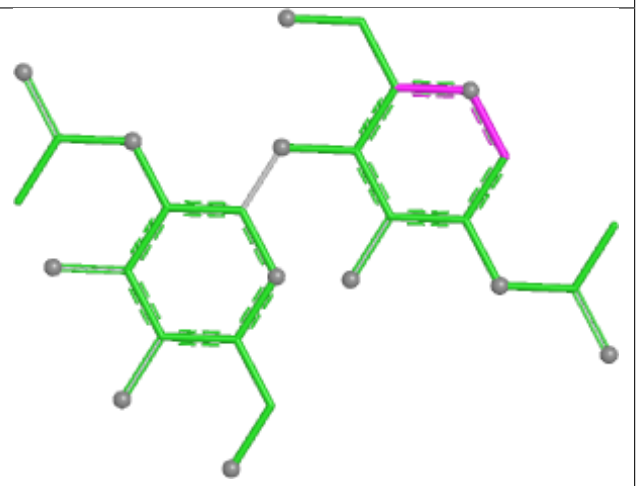


Rings

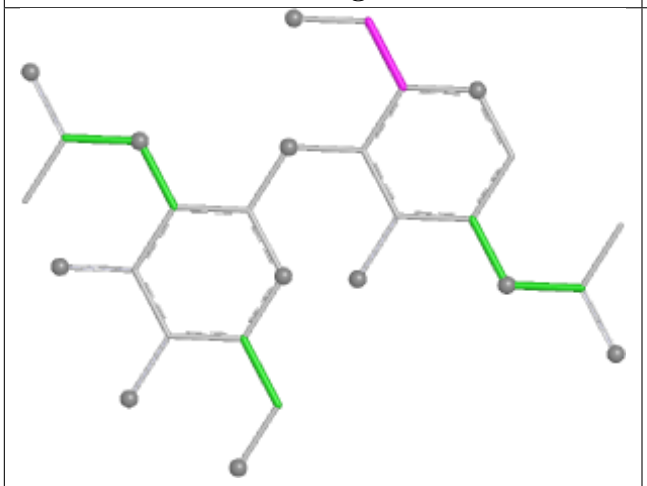
Oligosaccharide Chain M



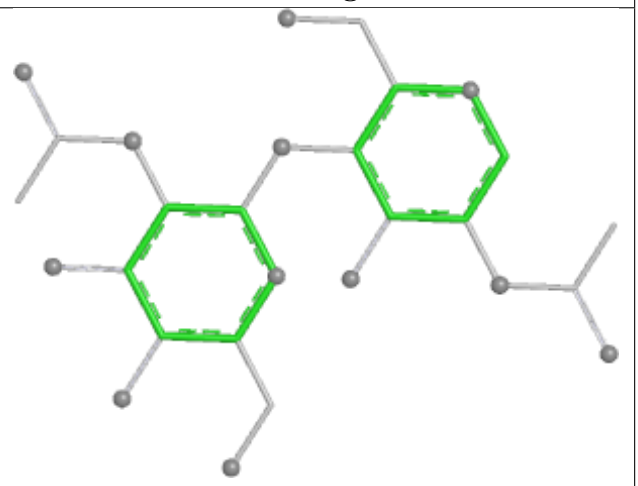
Bond lengths



Bond angles

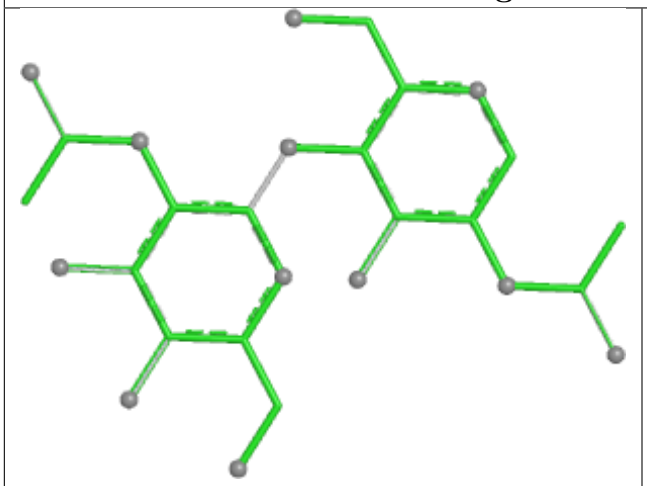


Torsions

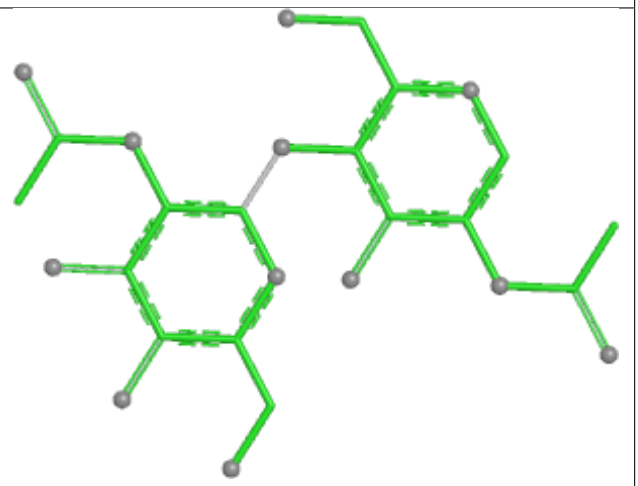


Rings

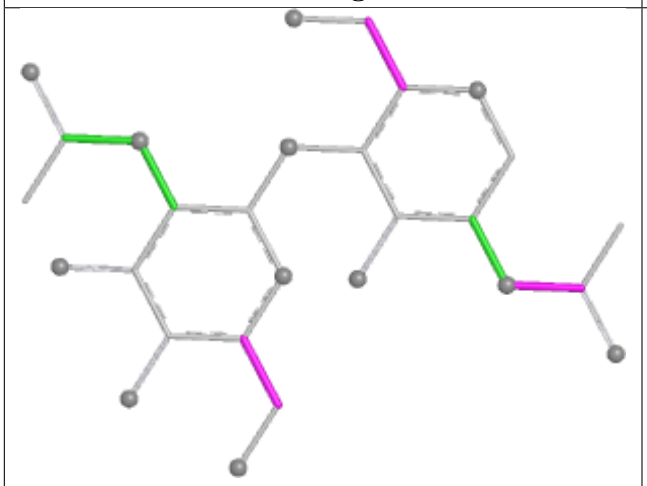
Oligosaccharide Chain O



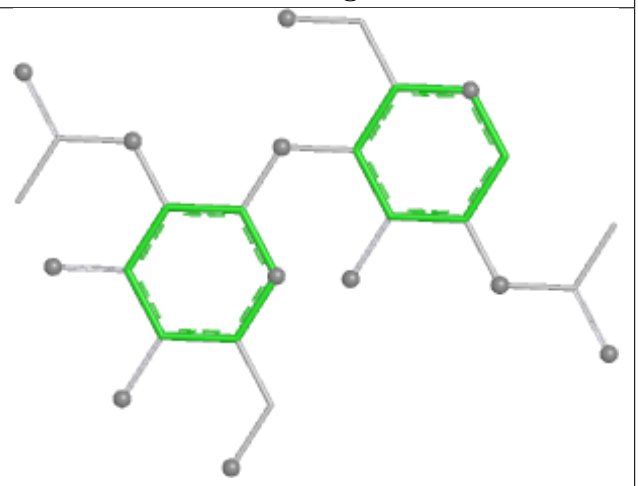
Bond lengths



Bond angles

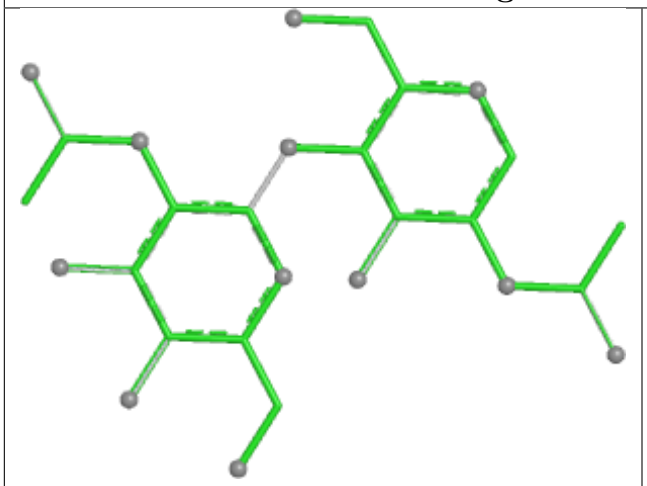


Torsions

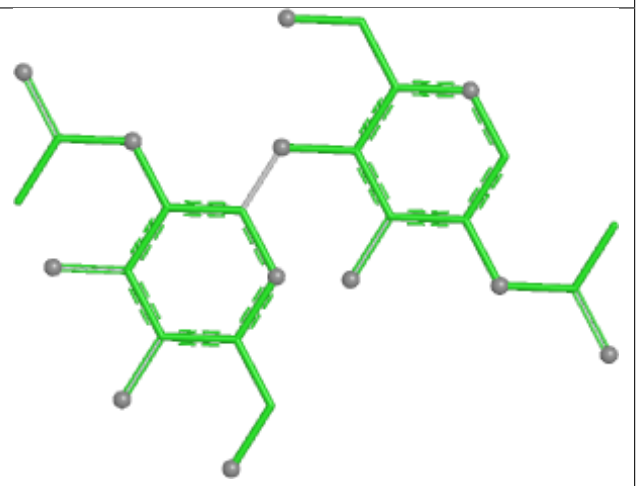


Rings

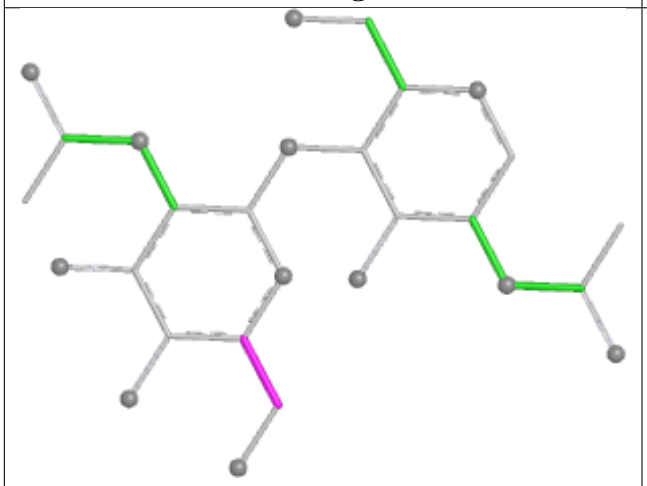
Oligosaccharide Chain P



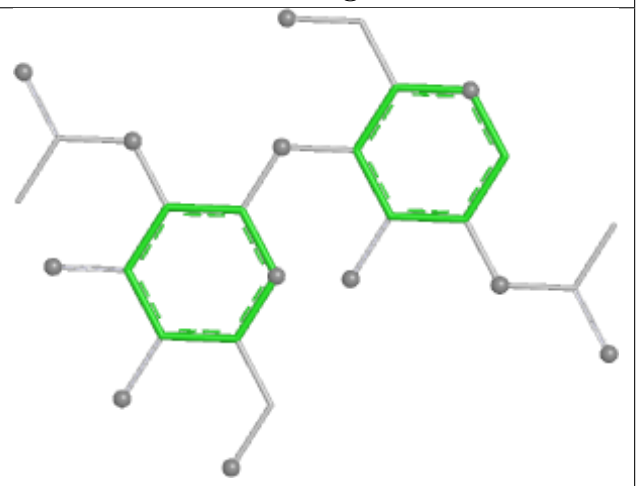
Bond lengths



Bond angles

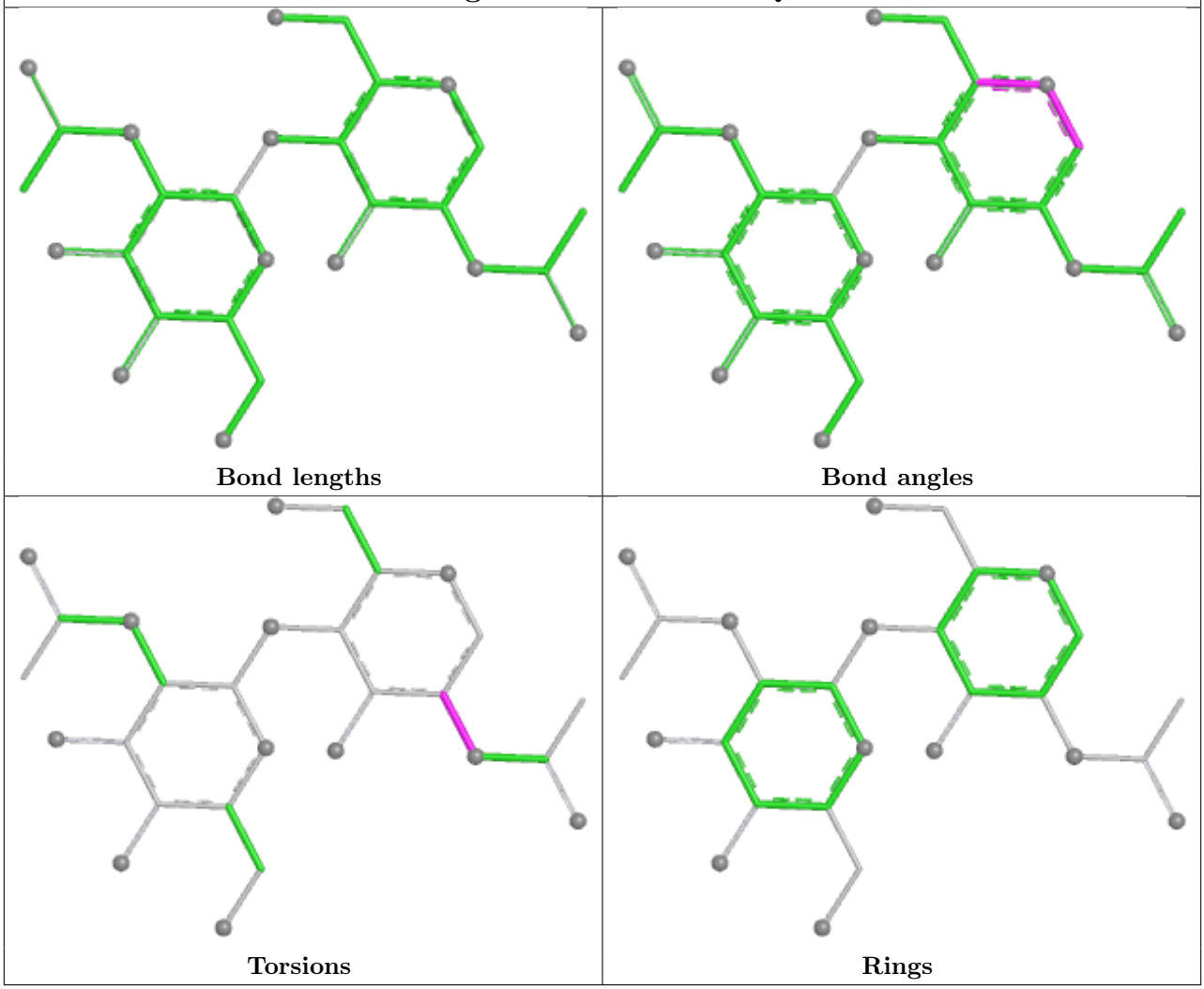


Torsions

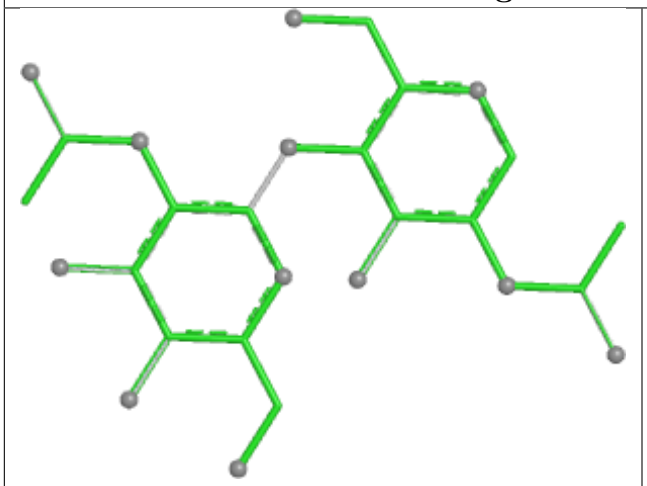


Rings

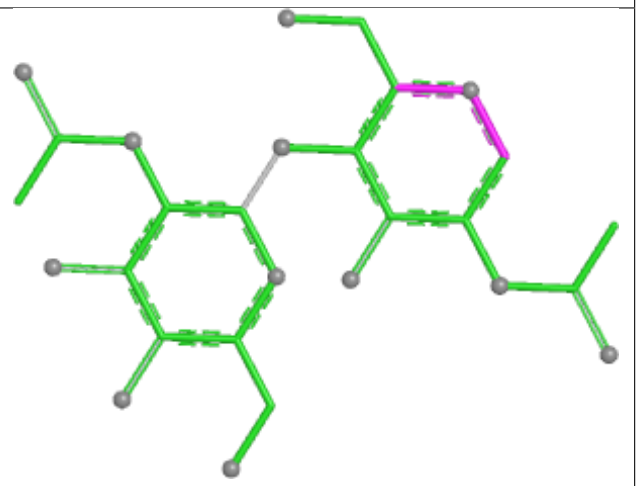
Oligosaccharide Chain Q



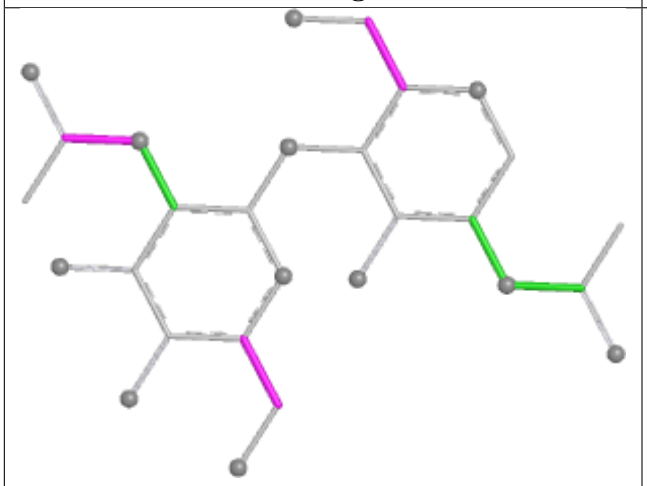
Oligosaccharide Chain R



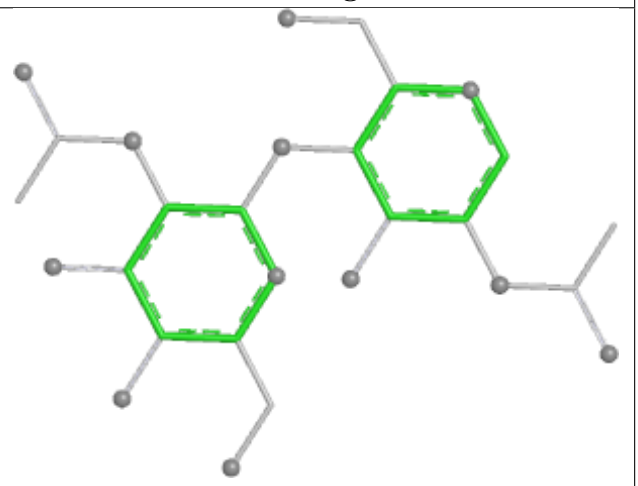
Bond lengths



Bond angles

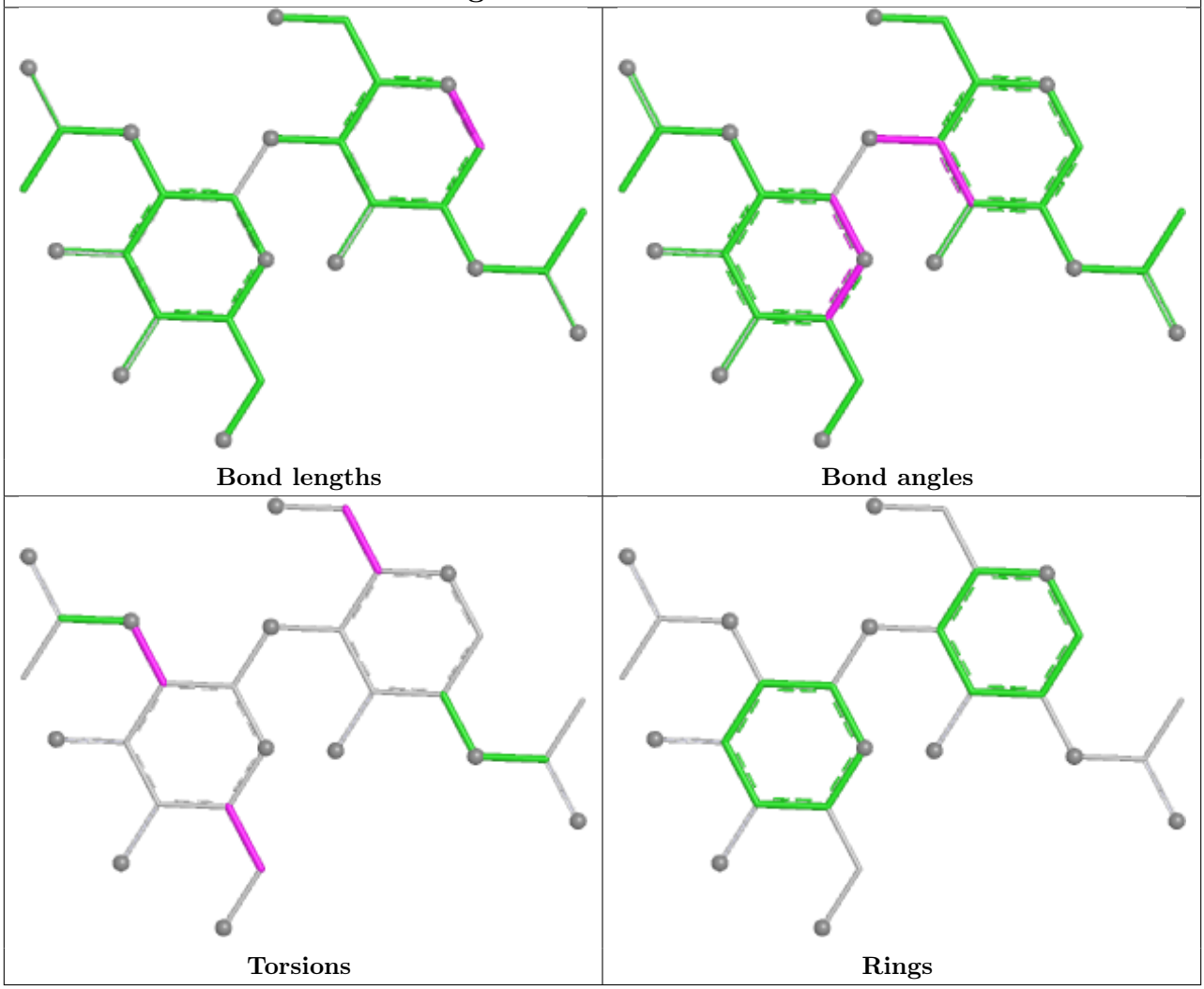


Torsions

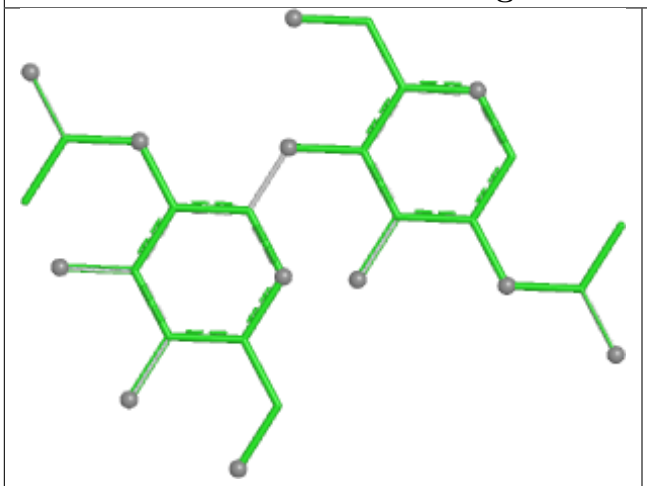


Rings

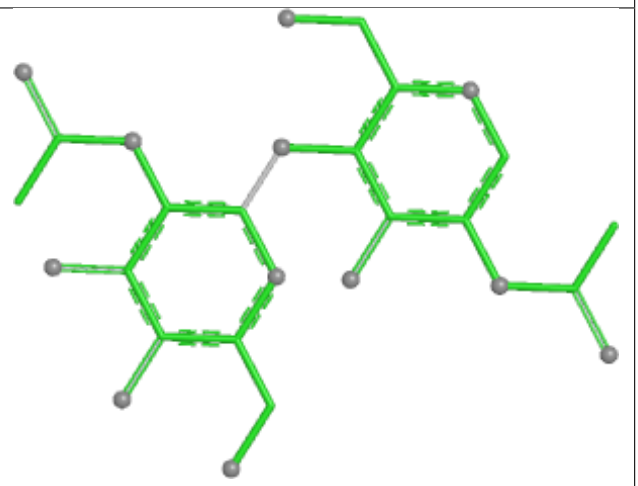
Oligosaccharide Chain S



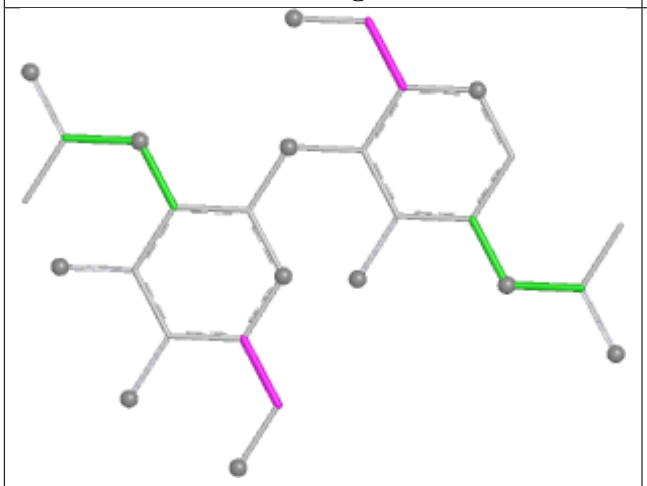
Oligosaccharide Chain T



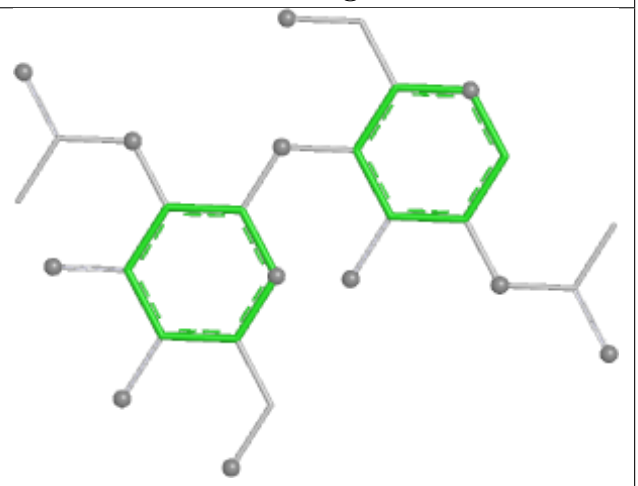
Bond lengths



Bond angles

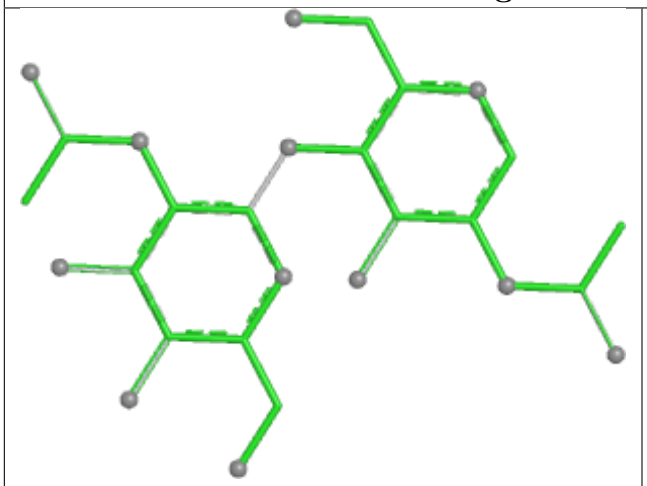


Torsions

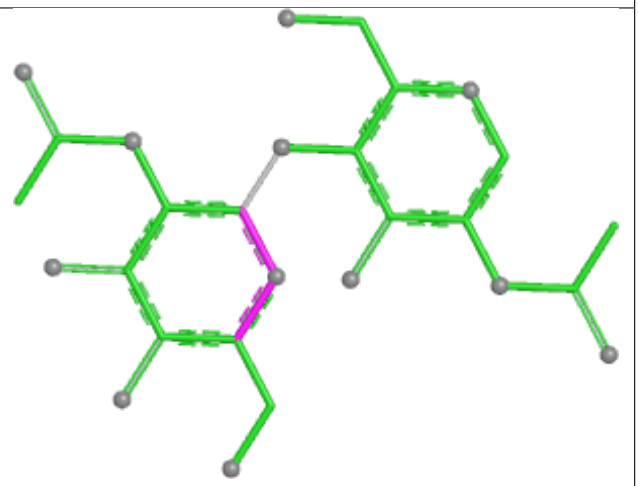


Rings

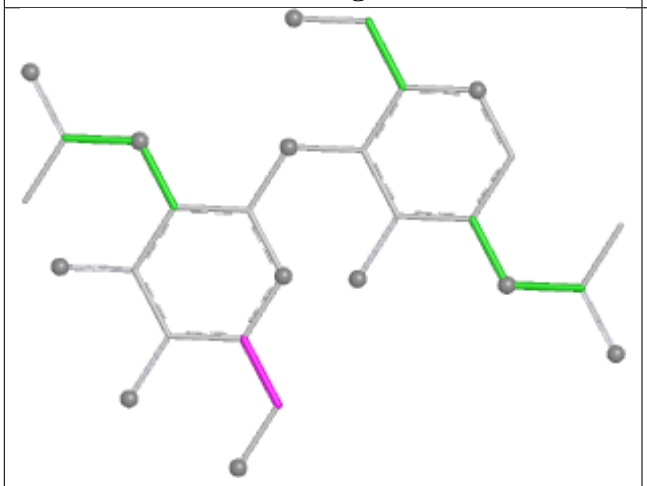
Oligosaccharide Chain U



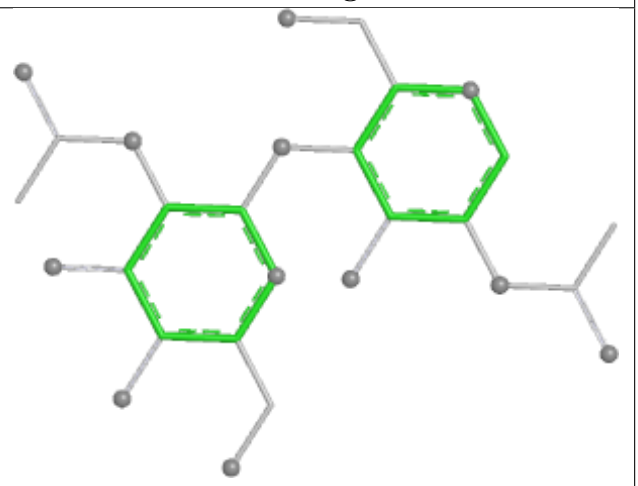
Bond lengths



Bond angles

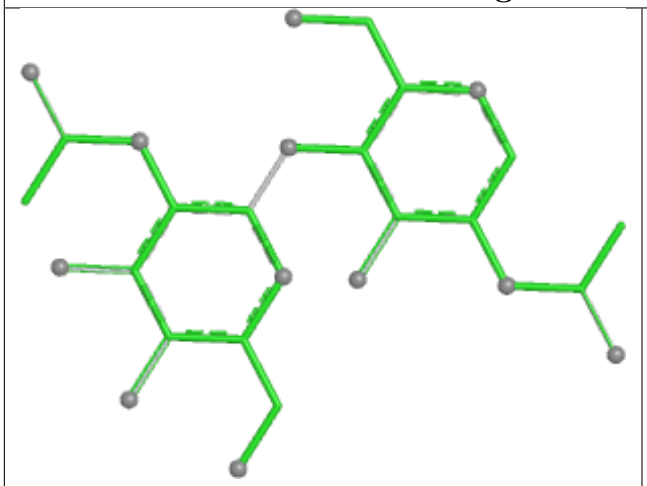


Torsions

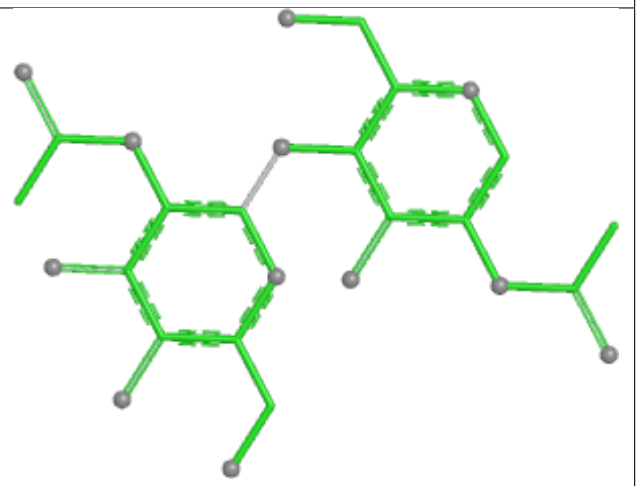


Rings

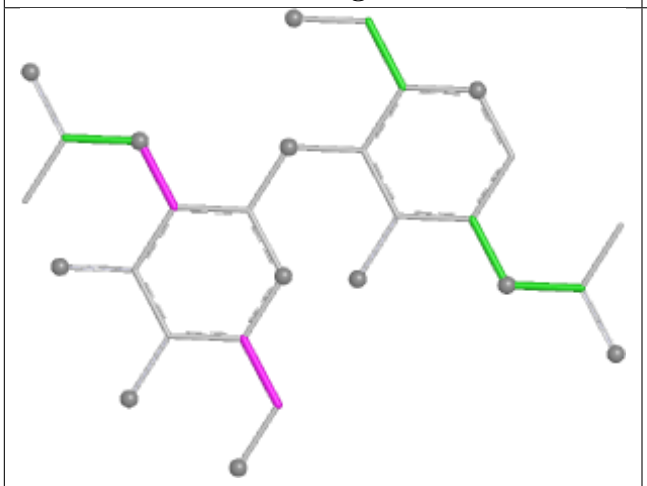
Oligosaccharide Chain V



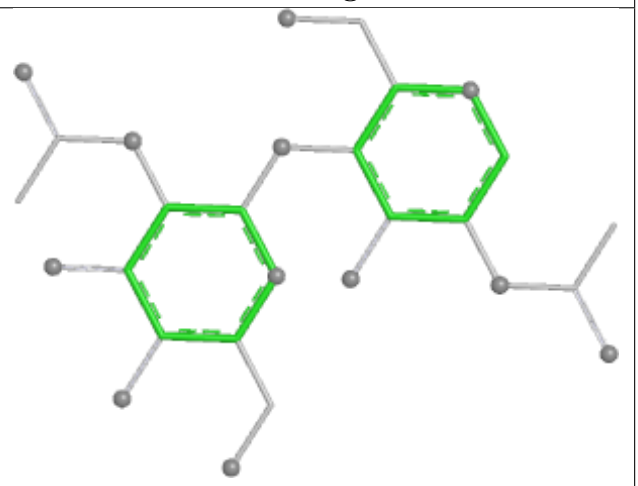
Bond lengths



Bond angles

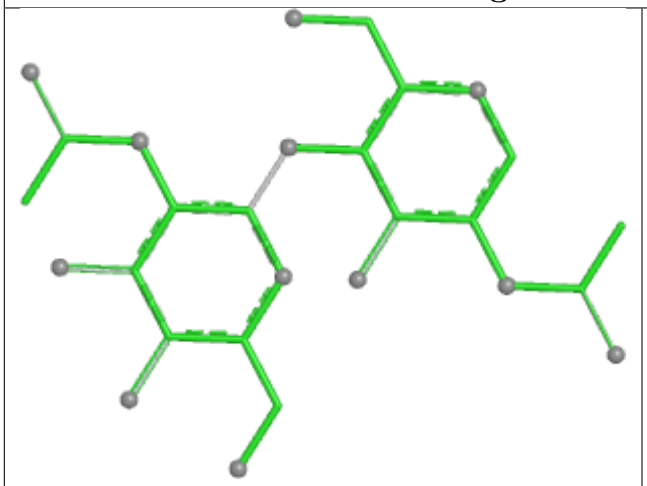


Torsions

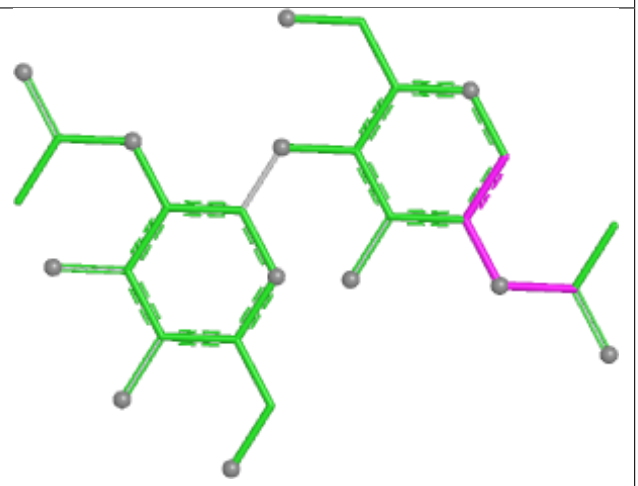


Rings

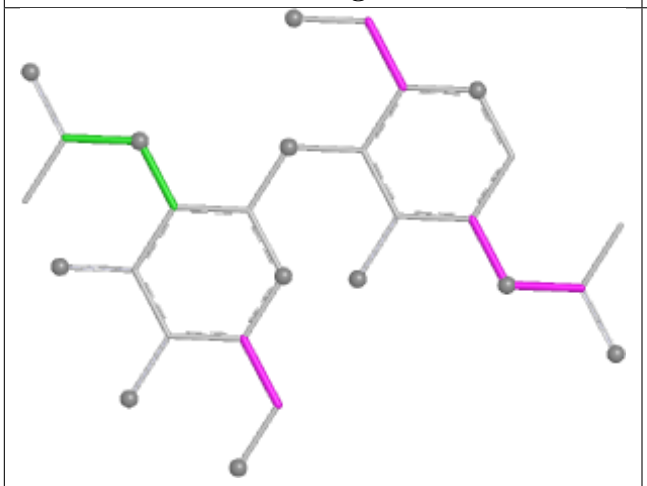
Oligosaccharide Chain W



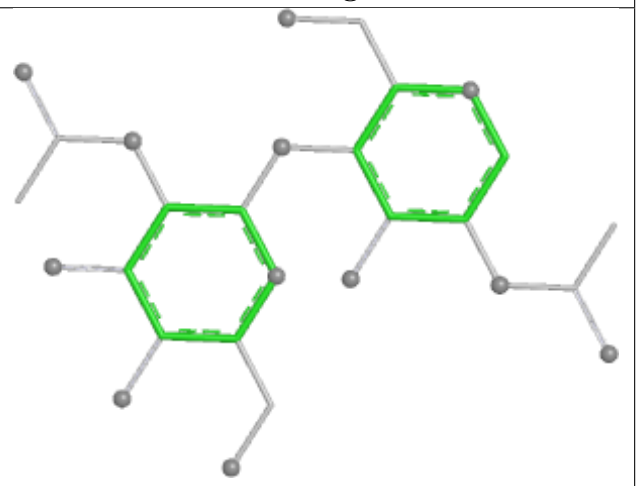
Bond lengths



Bond angles

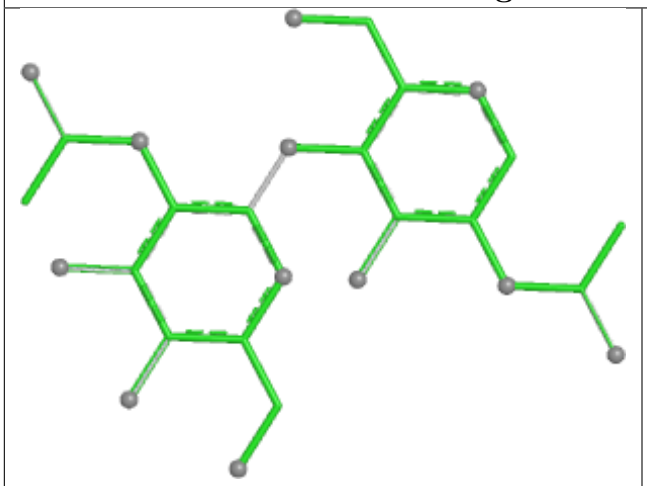


Torsions

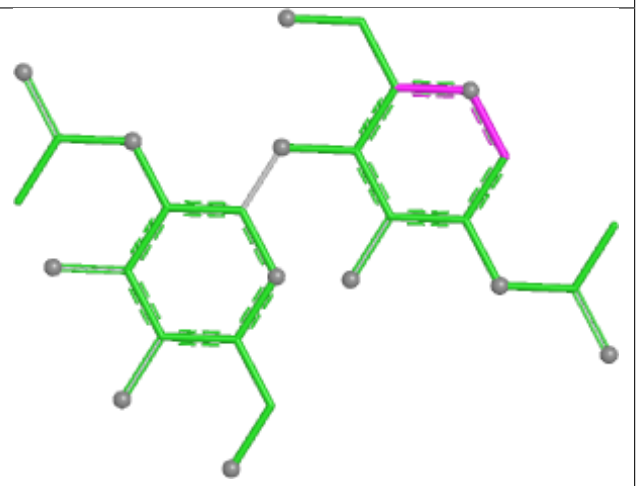


Rings

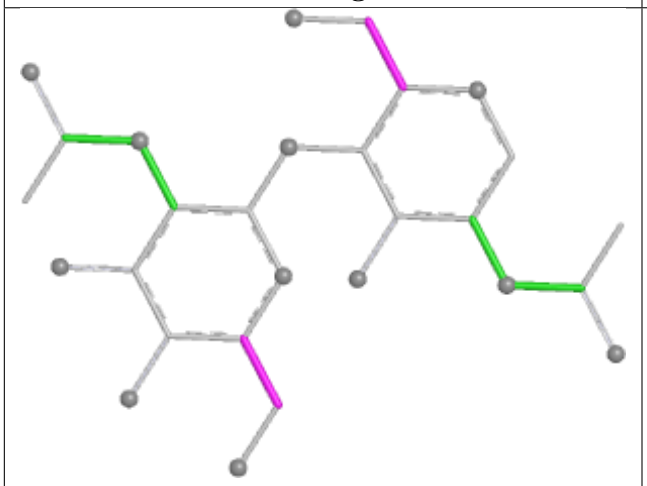
Oligosaccharide Chain X



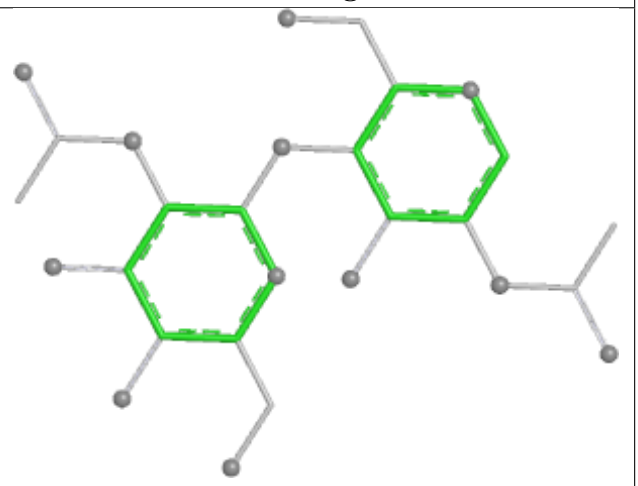
Bond lengths



Bond angles

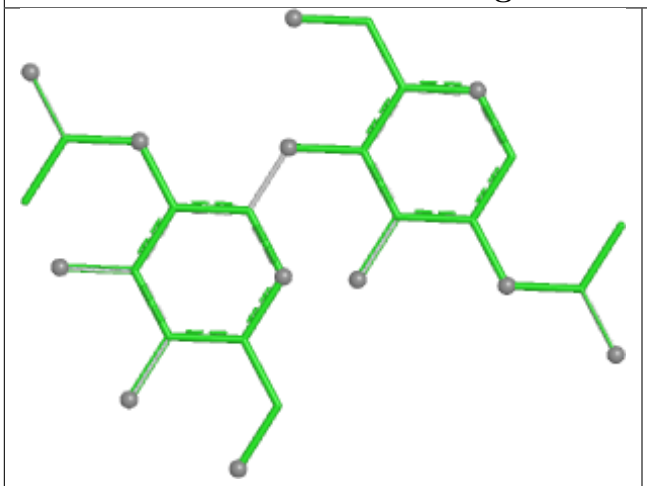


Torsions

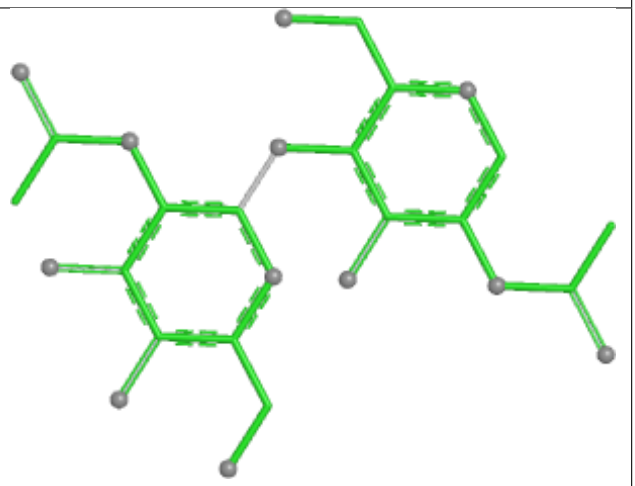


Rings

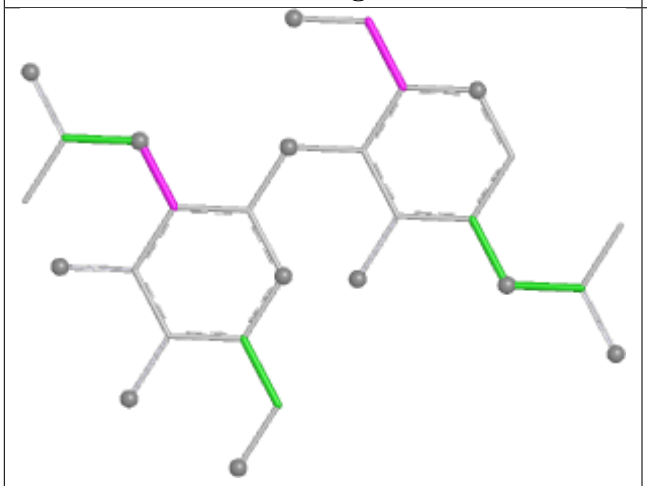
Oligosaccharide Chain Y



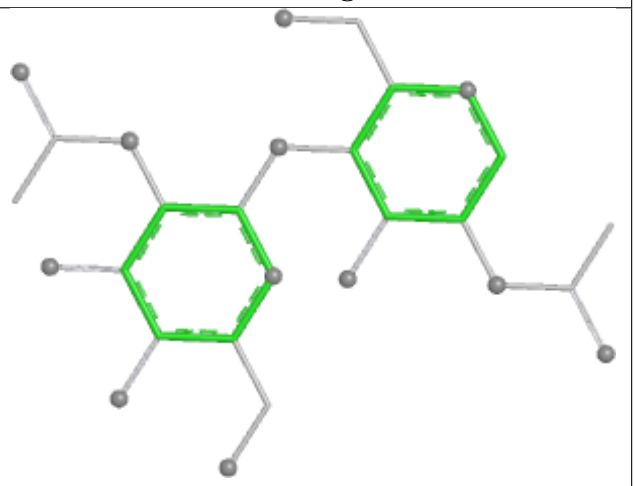
Bond lengths



Bond angles

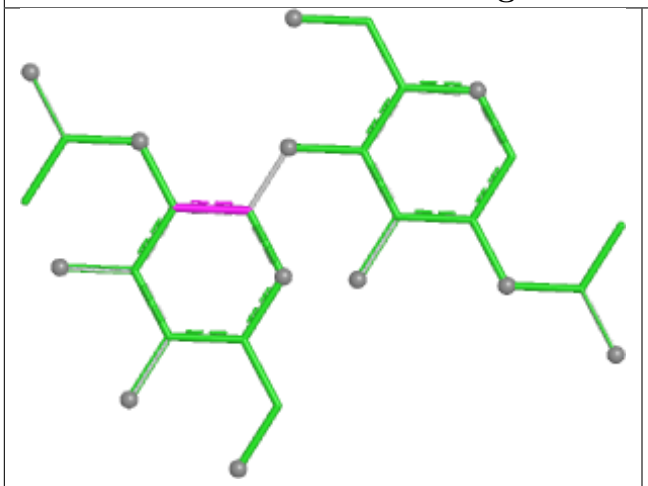


Torsions

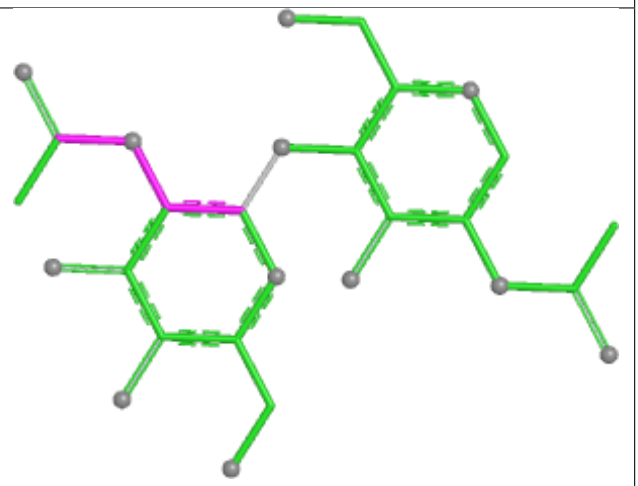


Rings

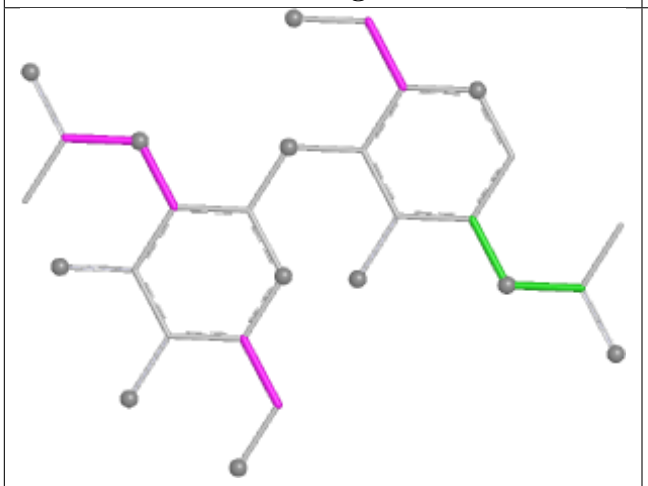
Oligosaccharide Chain Z



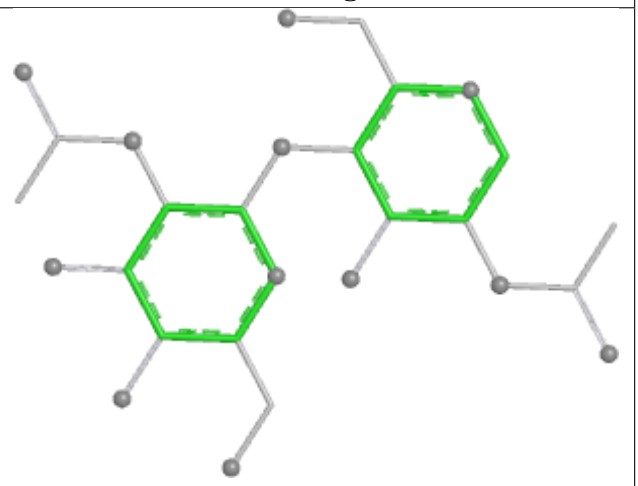
Bond lengths



Bond angles

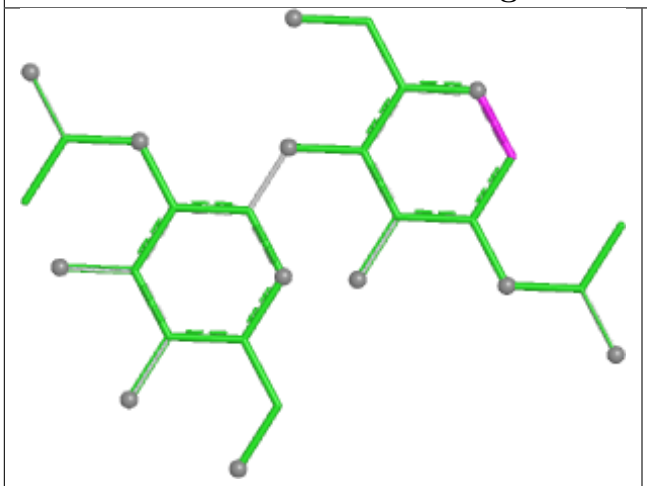


Torsions

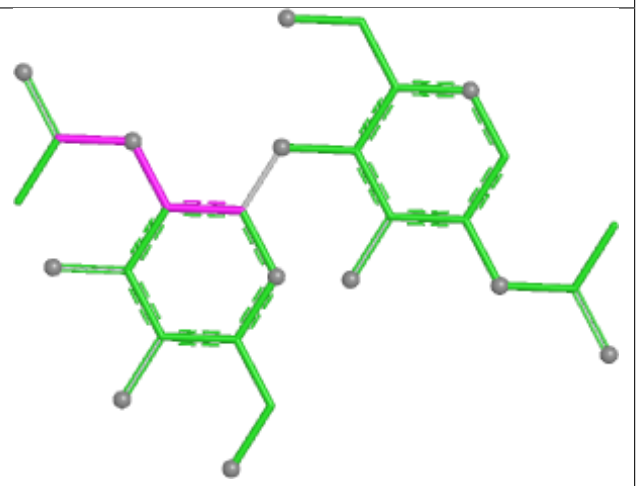


Rings

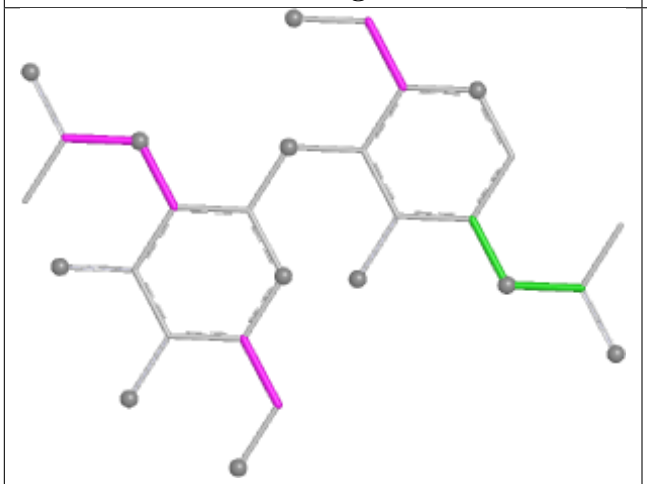
Oligosaccharide Chain a



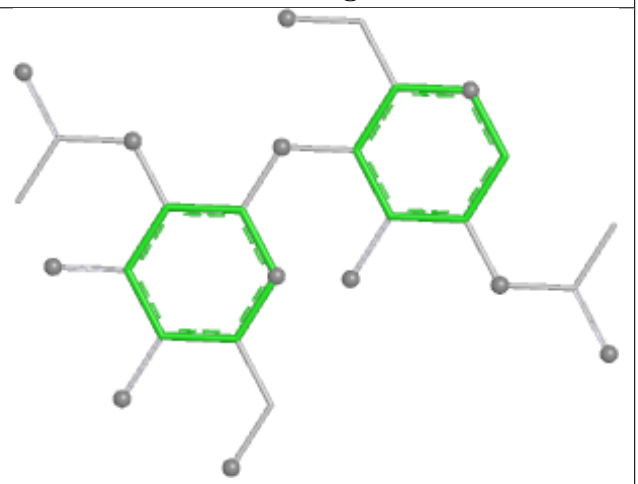
Bond lengths



Bond angles

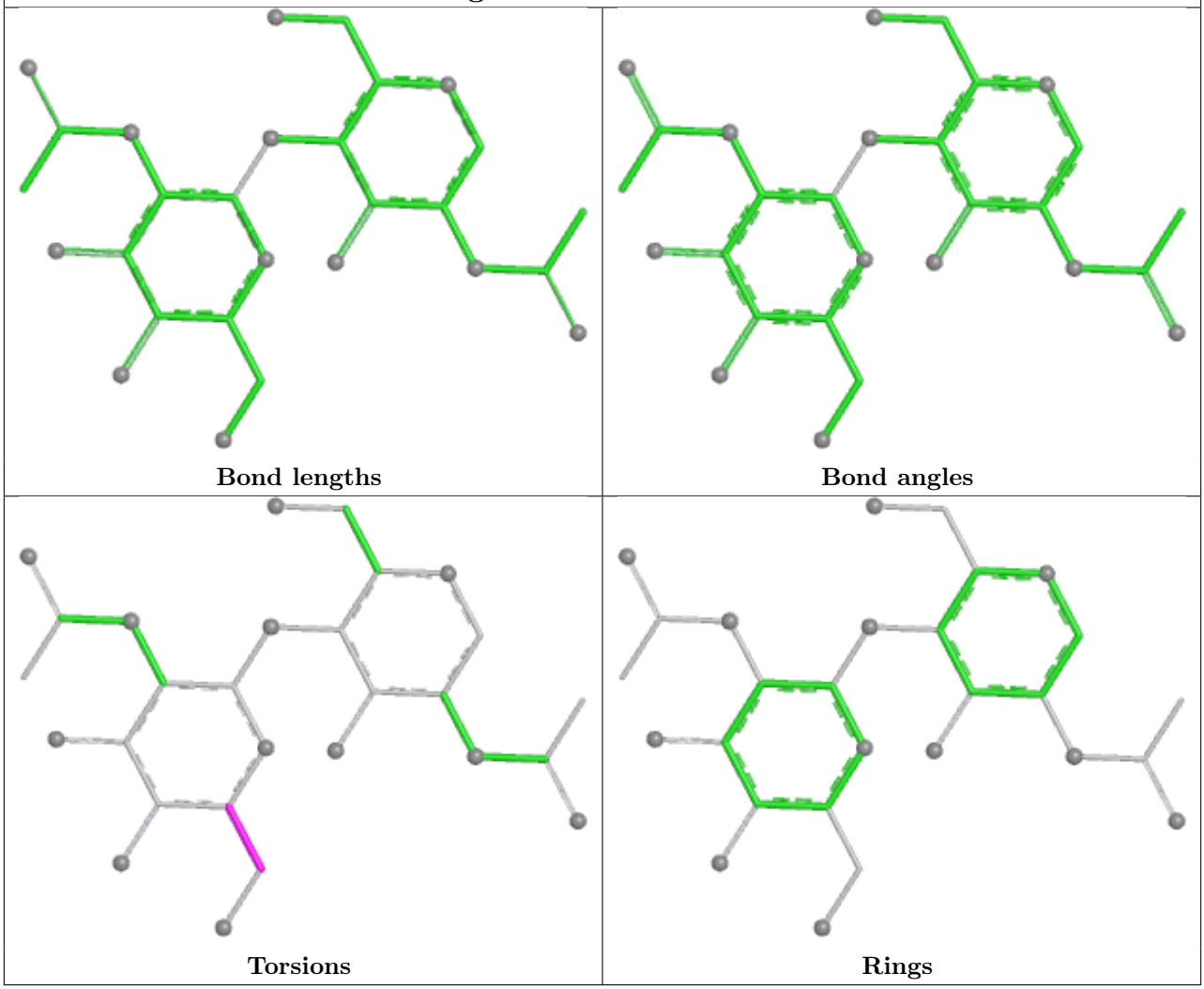


Torsions



Rings

Oligosaccharide Chain b



5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1405	1	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
5	NAG	C	1408	1	14,14,15	0.15	0	17,19,21	0.59	0
5	NAG	B	1405	1	14,14,15	0.39	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1403	1	14,14,15	0.19	0	17,19,21	0.43	0
5	NAG	B	1410	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
5	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.56	0
5	NAG	B	1402	1	14,14,15	0.34	0	17,19,21	0.66	0
5	NAG	B	1406	1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
5	NAG	C	1401	1	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
5	NAG	B	1404	1	14,14,15	0.35	0	17,19,21	0.60	0
5	NAG	A	1408	1	14,14,15	0.33	0	17,19,21	0.40	0
5	NAG	C	1403	1	14,14,15	0.51	0	17,19,21	0.48	0
5	NAG	A	1409	1	14,14,15	0.48	0	17,19,21	0.36	0
5	NAG	B	1409	1	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	C	1407	1	14,14,15	0.39	0	17,19,21	0.66	0
5	NAG	B	1407	1	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
5	NAG	C	1406	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	C	1402	1	14,14,15	0.44	0	17,19,21	0.59	0
5	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	C	1404	1	14,14,15	0.30	0	17,19,21	0.38	0
5	NAG	B	1403	1	14,14,15	0.30	0	17,19,21	0.42	0
5	NAG	C	1405	1	14,14,15	0.39	0	17,19,21	1.37	2 (11%)
5	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.44	0
5	NAG	B	1411	-	14,14,15	0.35	0	17,19,21	0.43	0
5	NAG	A	1404	1	14,14,15	0.48	0	17,19,21	0.54	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	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})
5	A	1405	NAG	C2-N2-C7	4.60	129.07	122.90
5	C	1405	NAG	C2-N2-C7	4.55	128.99	122.90
5	B	1405	NAG	C2-N2-C7	4.39	128.78	122.90
5	C	1401	NAG	C1-O5-C5	2.90	116.08	112.19
5	B	1406	NAG	C1-O5-C5	2.58	115.64	112.19
5	C	1405	NAG	C1-C2-N2	2.46	114.30	110.43
5	B	1407	NAG	C1-O5-C5	2.43	115.44	112.19
5	B	1410	NAG	C8-C7-N2	2.33	119.99	116.12
5	B	1405	NAG	C1-C2-N2	2.33	114.10	110.43
5	B	1410	NAG	C2-N2-C7	-2.17	119.99	122.90
5	A	1405	NAG	C1-C2-N2	2.07	113.70	110.43

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1408	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	A	1406	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	A	1409	NAG	C4-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	1409	NAG	O5-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6
5	A	1405	NAG	C8-C7-N2-C2
5	A	1405	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	C	1406	NAG	C8-C7-N2-C2
5	C	1406	NAG	O7-C7-N2-C2
5	B	1407	NAG	C4-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	C	1407	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	B	1406	NAG	C3-C2-N2-C7
5	B	1407	NAG	C3-C2-N2-C7
5	C	1407	NAG	C3-C2-N2-C7
5	A	1405	NAG	C1-C2-N2-C7
5	B	1405	NAG	C1-C2-N2-C7
5	B	1406	NAG	C1-C2-N2-C7
5	B	1407	NAG	C1-C2-N2-C7
5	C	1405	NAG	C1-C2-N2-C7
5	C	1407	NAG	C1-C2-N2-C7
5	A	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7
5	C	1403	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

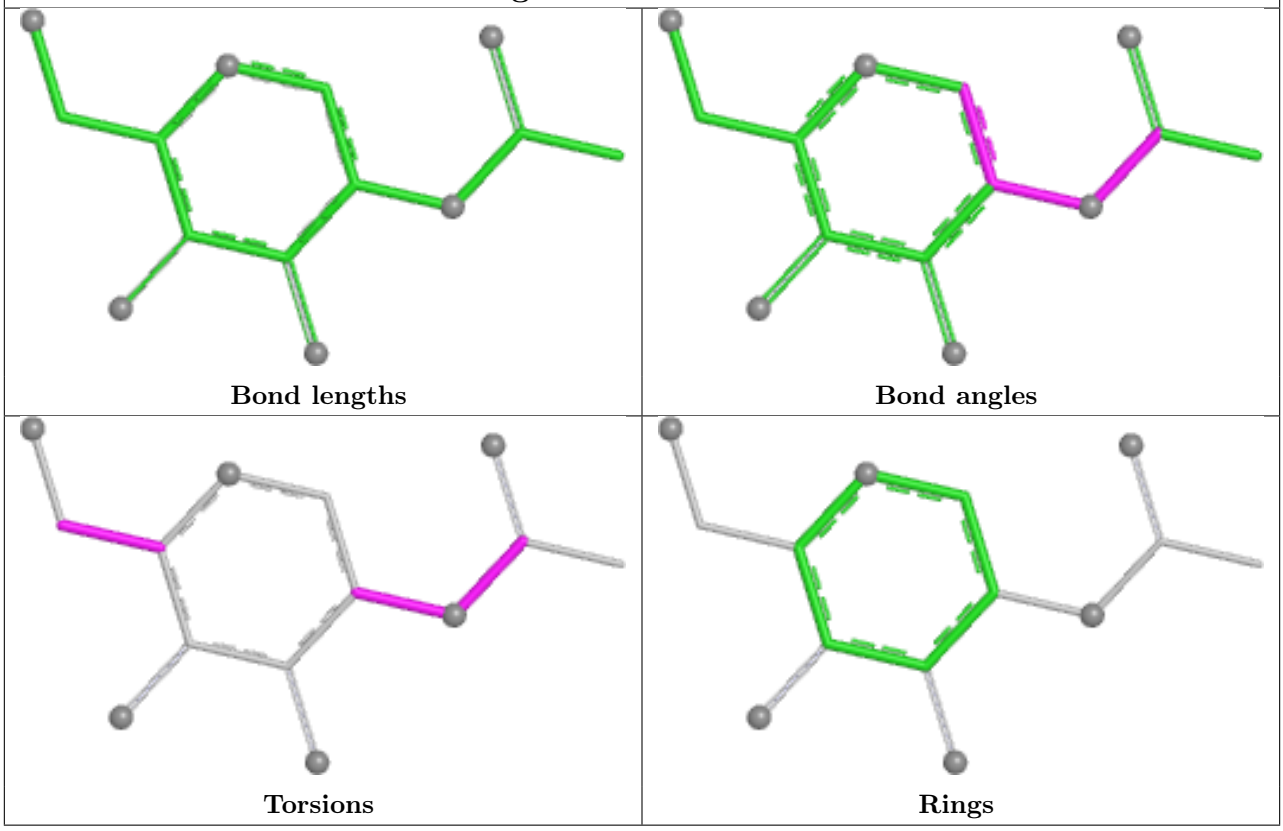
10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1405	NAG	1	0
5	B	1405	NAG	2	0
5	B	1410	NAG	4	0
5	B	1402	NAG	1	0
5	B	1407	NAG	1	0
5	C	1402	NAG	1	0
5	A	1402	NAG	3	0
5	B	1403	NAG	2	0
5	C	1405	NAG	1	0
5	B	1411	NAG	4	0

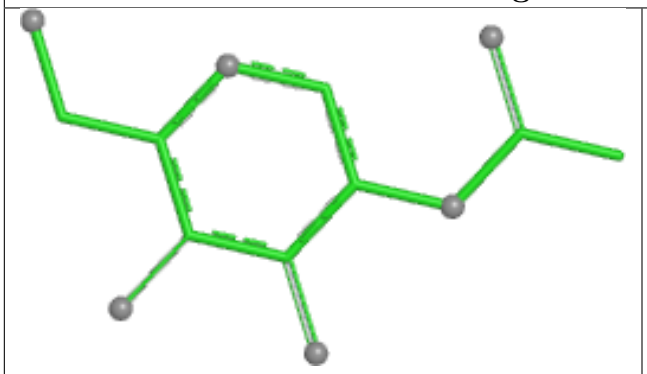
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

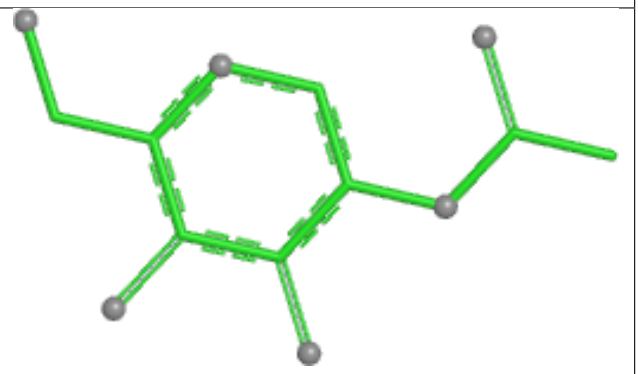
Ligand NAG A 1405



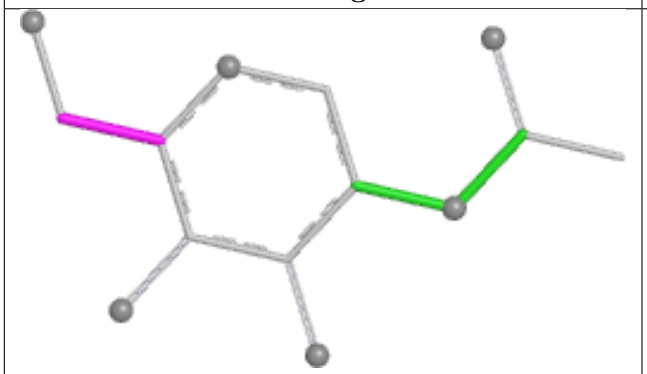
Ligand NAG C 1408



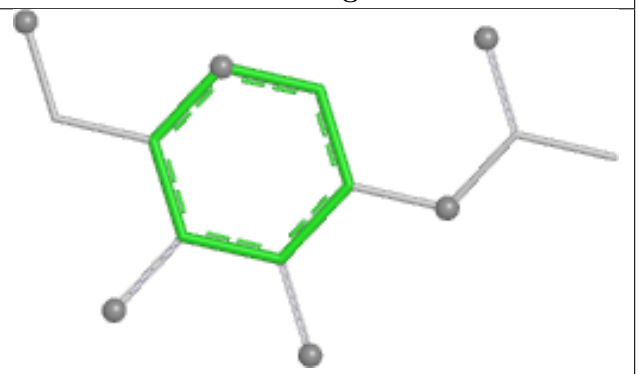
Bond lengths



Bond angles

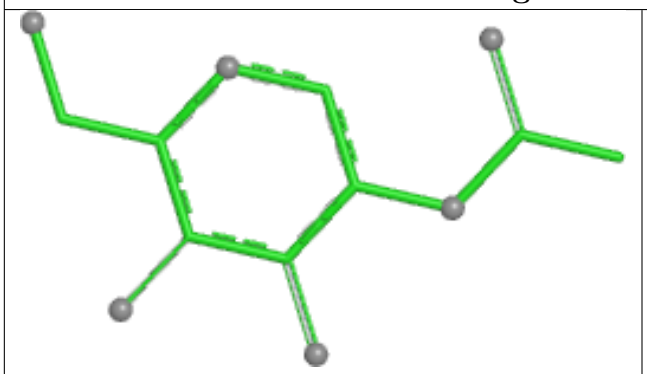


Torsions



Rings

Ligand NAG B 1405



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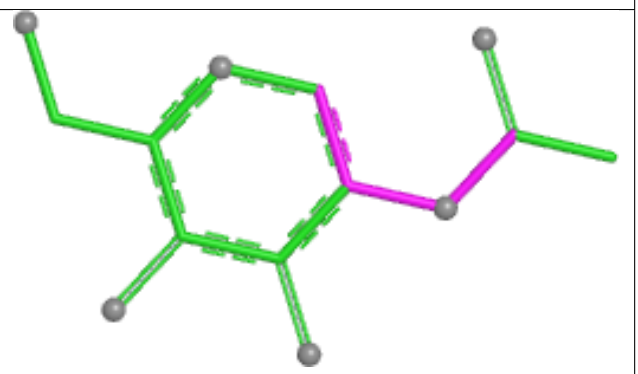
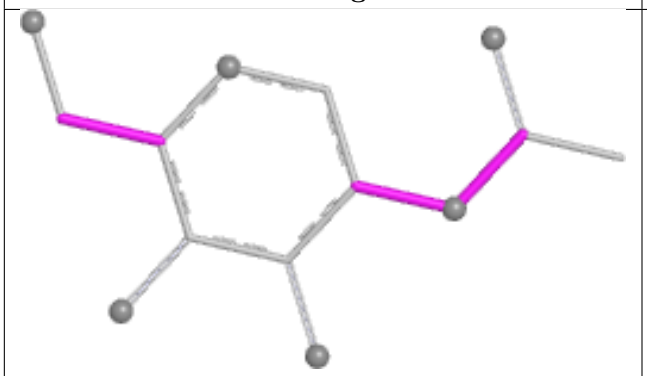


Bond angles



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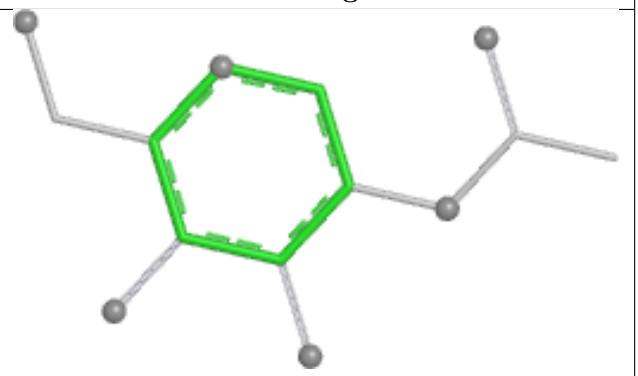
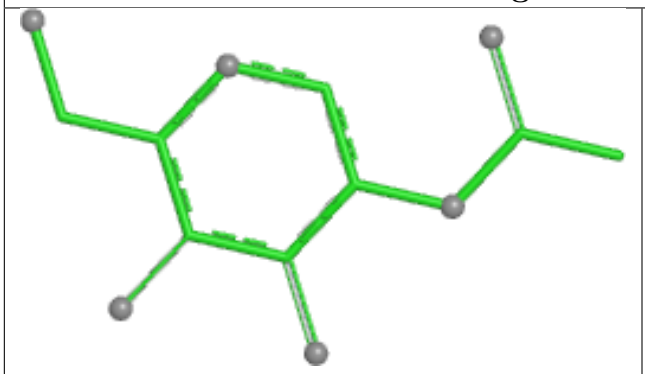
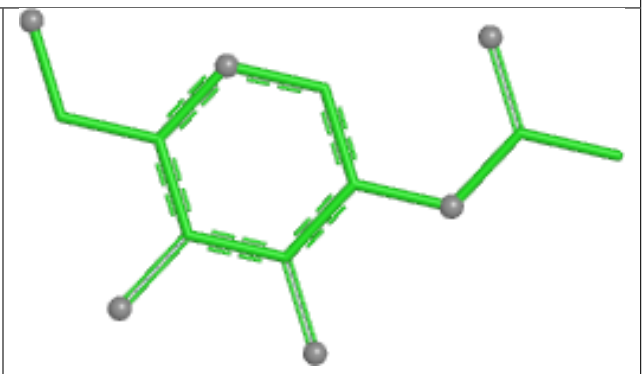


Rings

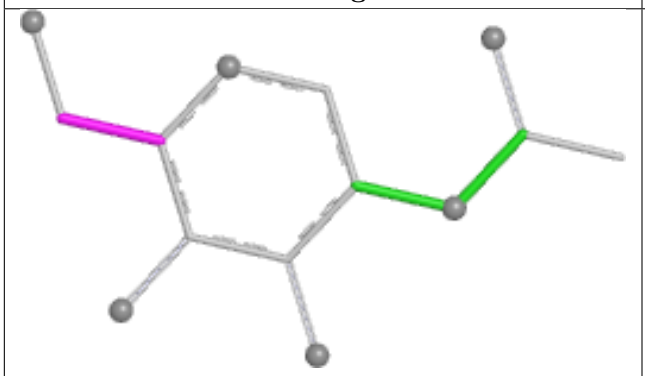
Ligand NAG A 1403



Bond lengths



Bond angles



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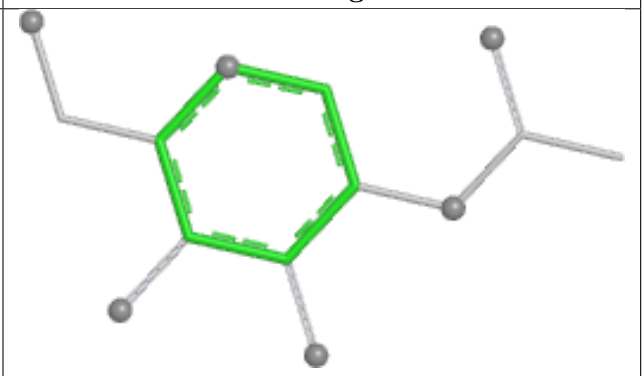

Rings

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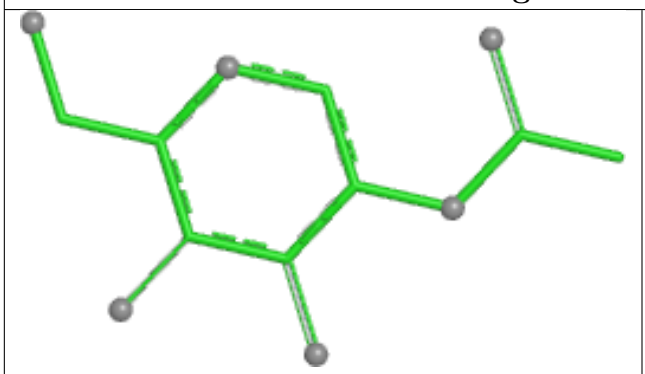

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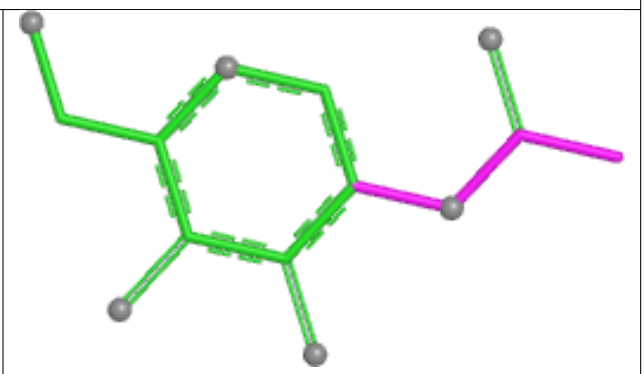
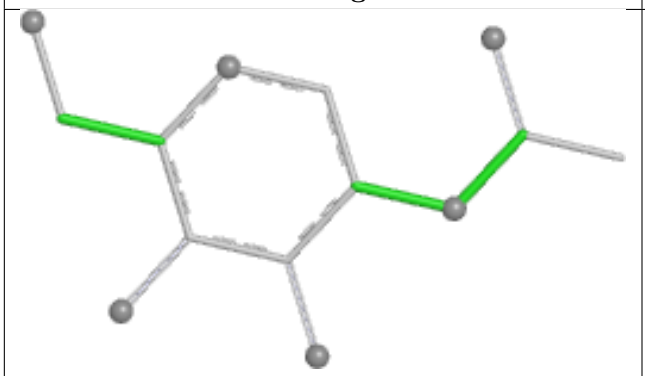


Bond angles



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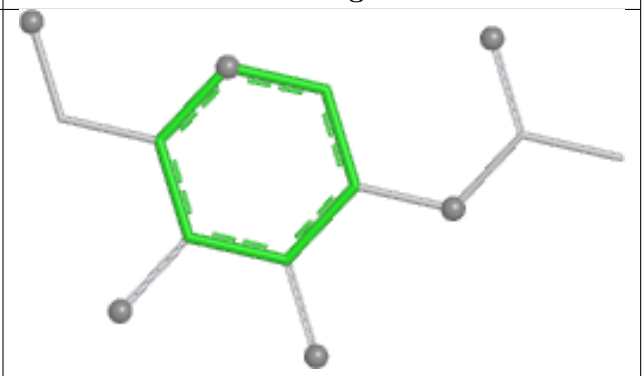

Rings

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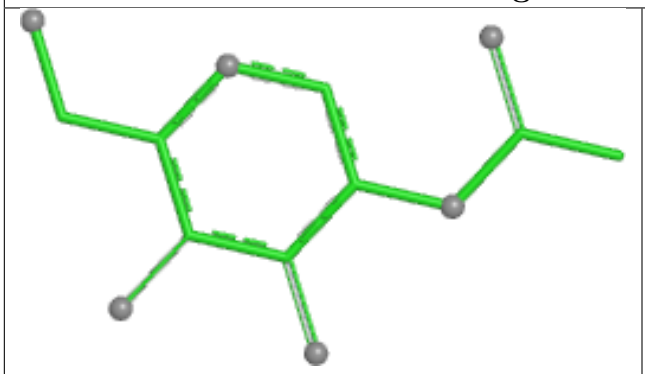

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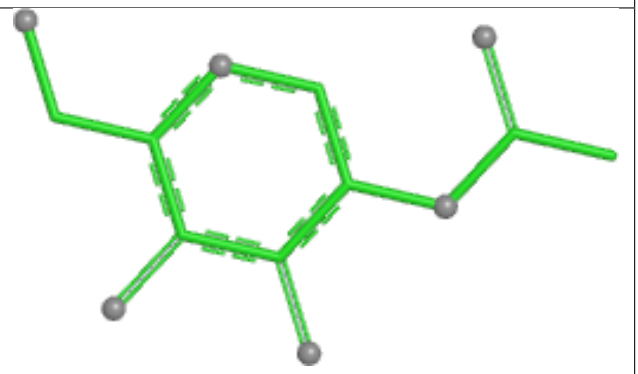

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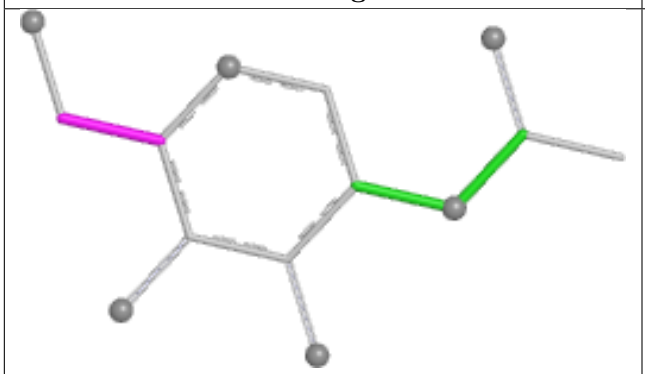
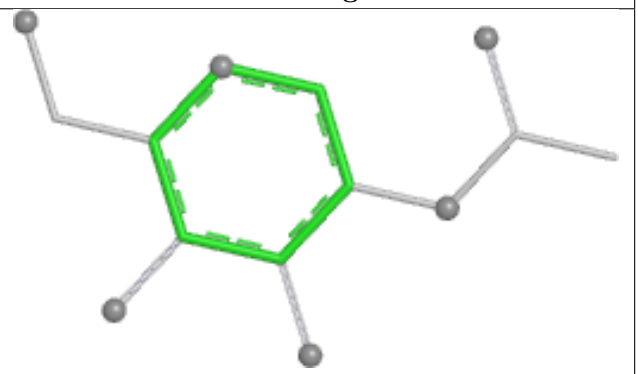
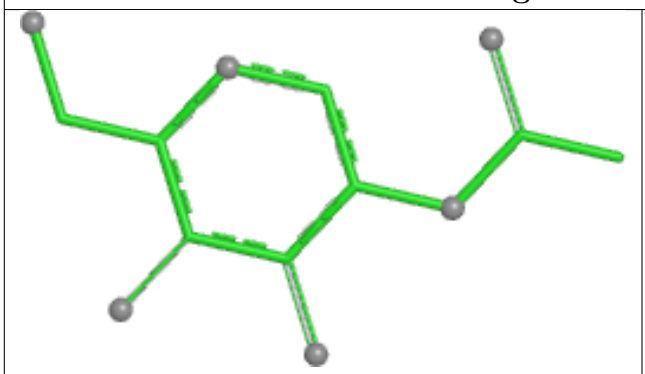


Torsions



Rings

Ligand NAG B 1402



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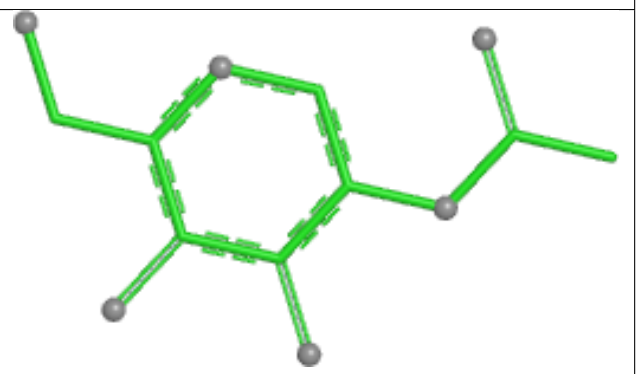
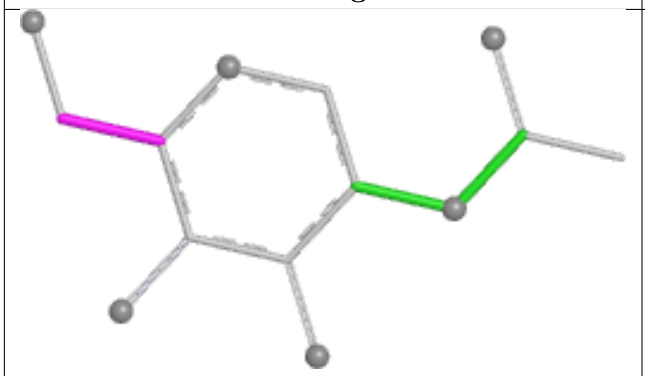


Bond angles



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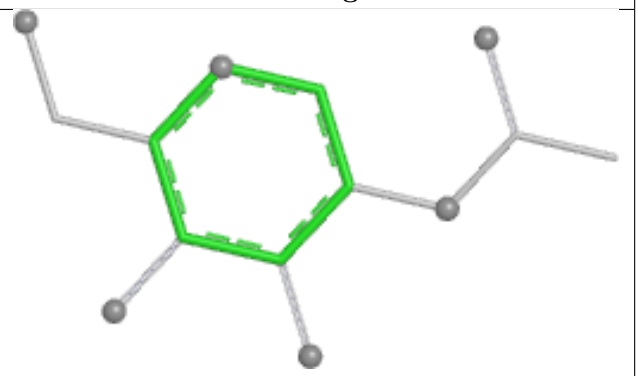
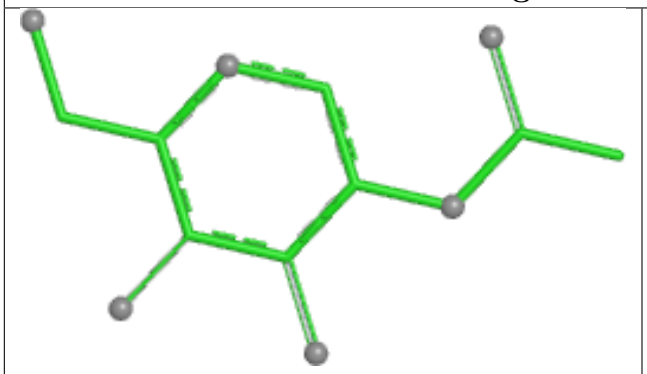


Rings

Ligand NAG B 1406



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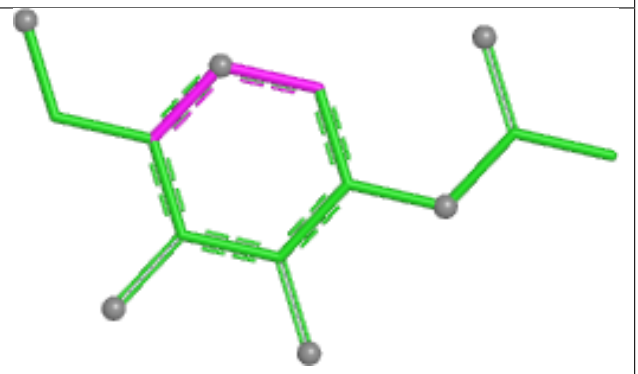
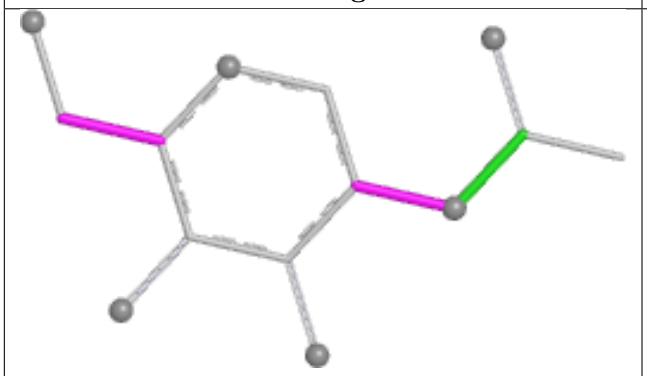
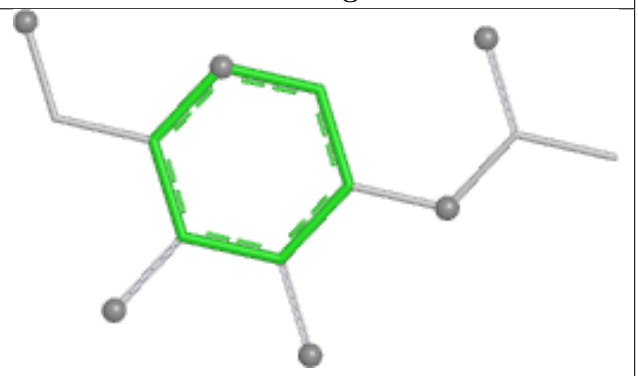


Bond angles

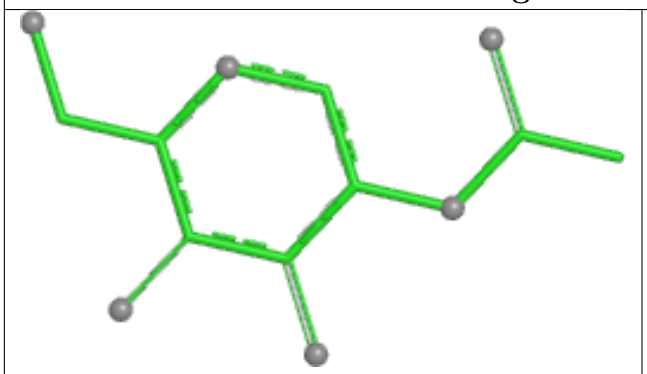


Torsions



Rings

Ligand NAG C 1401



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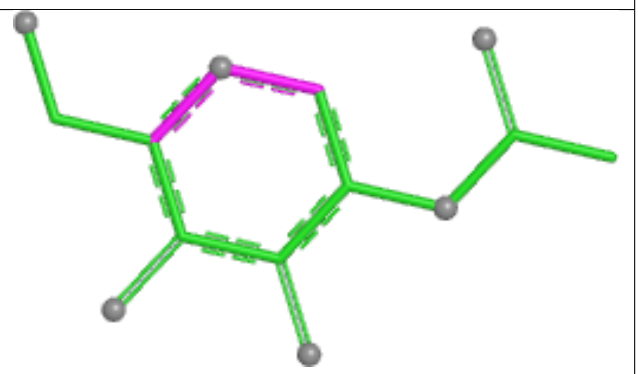
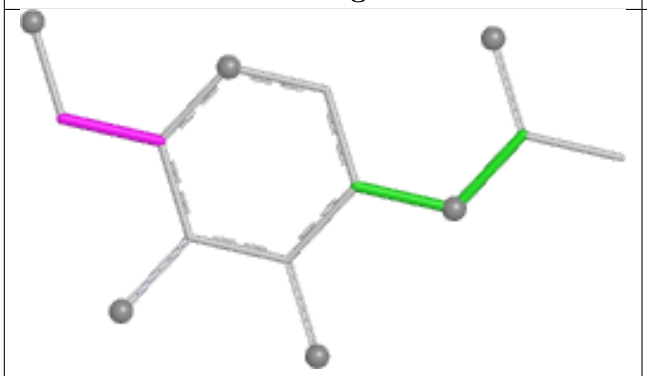
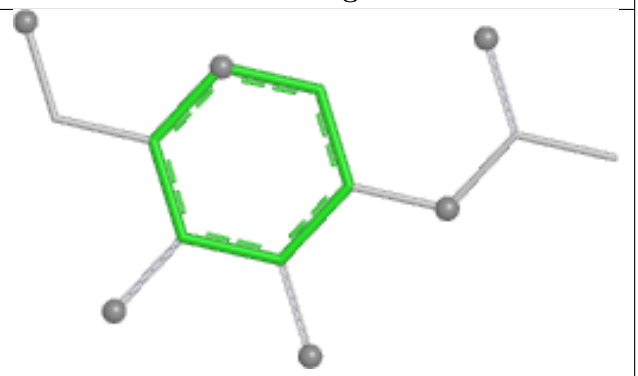


Bond angles

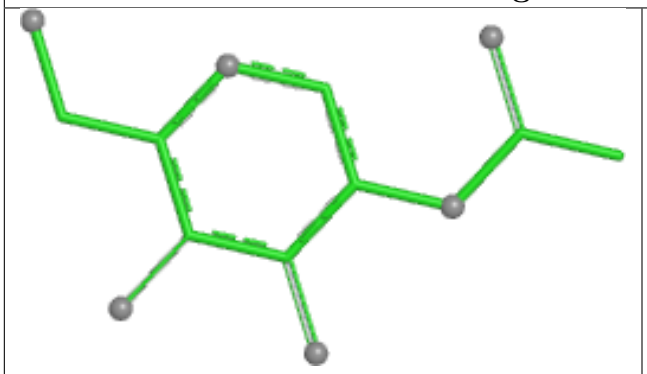


Torsions



Rings

Ligand NAG B 1404



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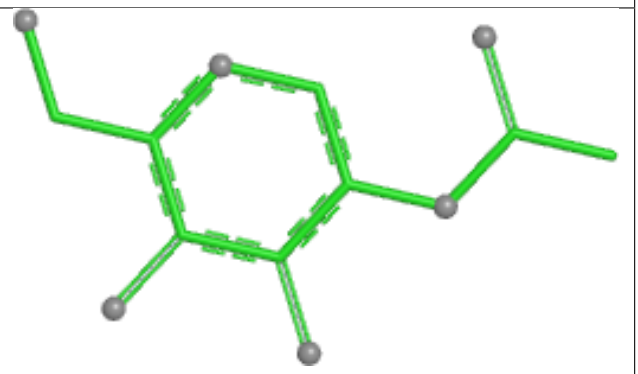

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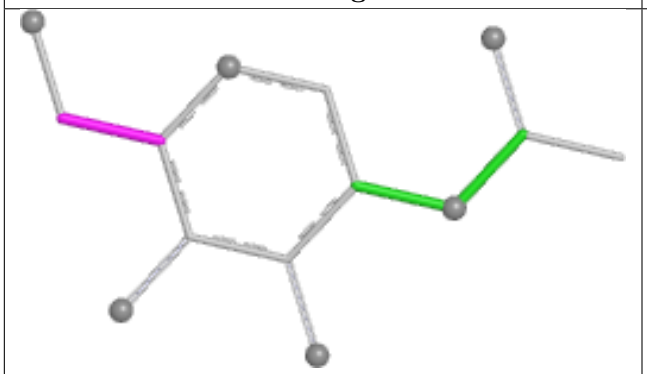
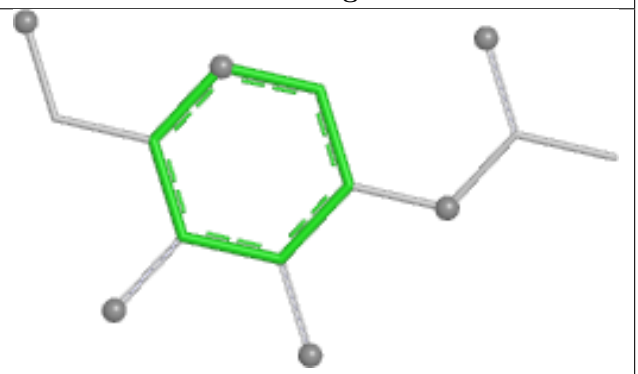
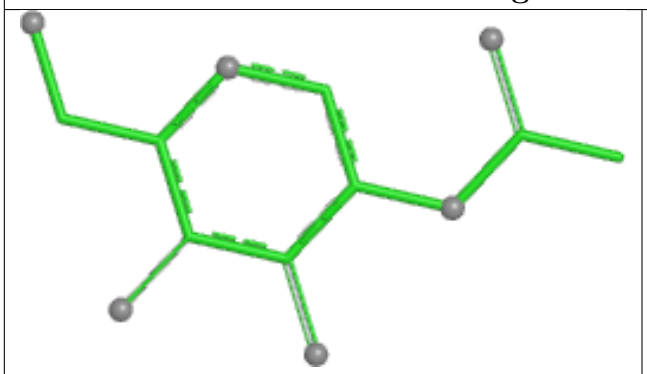


Torsions



Rings

Ligand NAG A 1408



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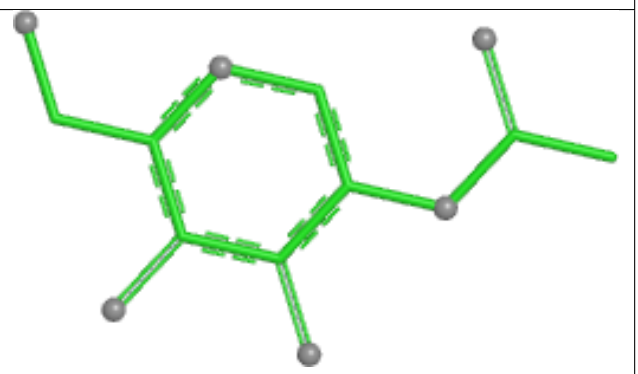
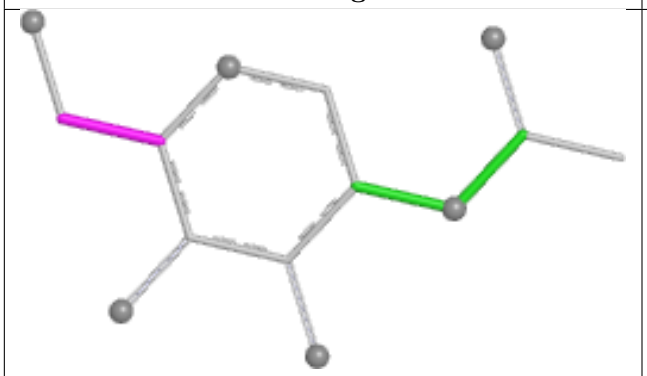


Bond angles



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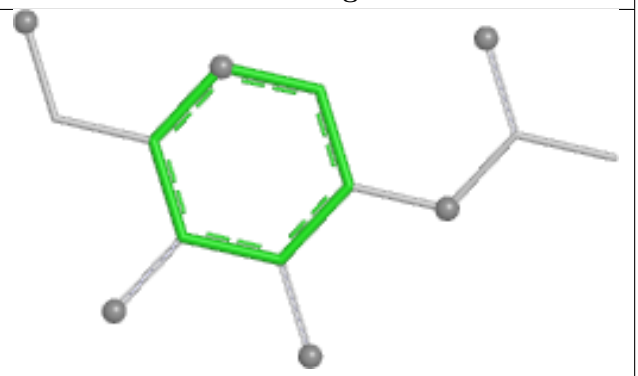
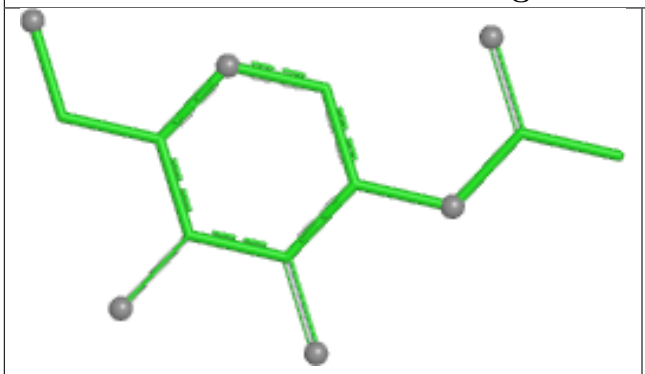
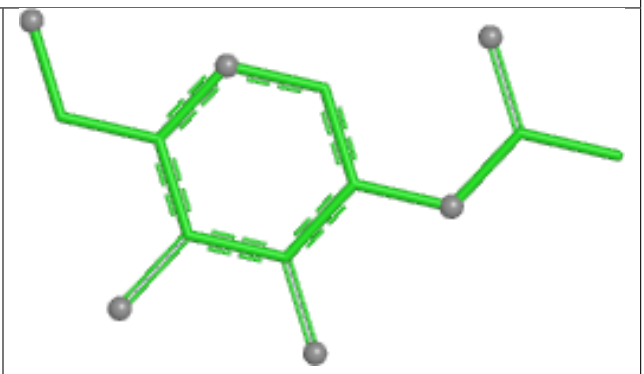


Rings

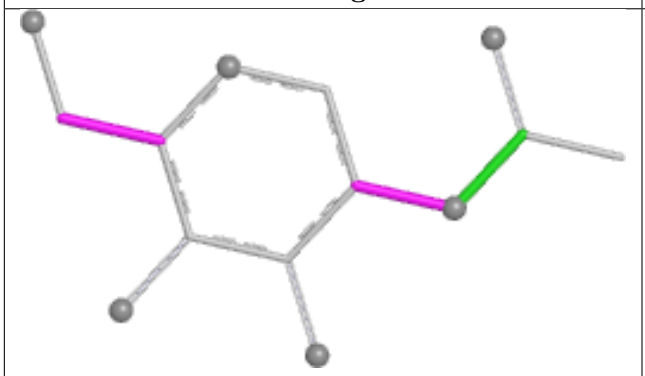
Ligand NAG C 1403



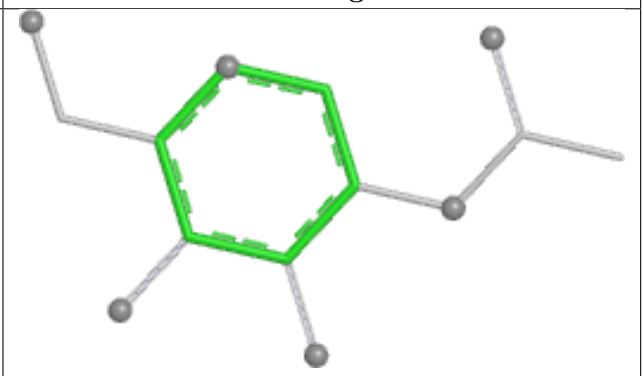
Bond lengths



Bond angles

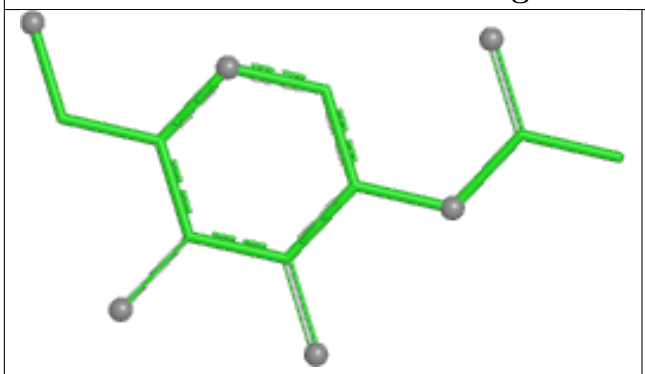


Torsions



Rings

Ligand NAG A 1409



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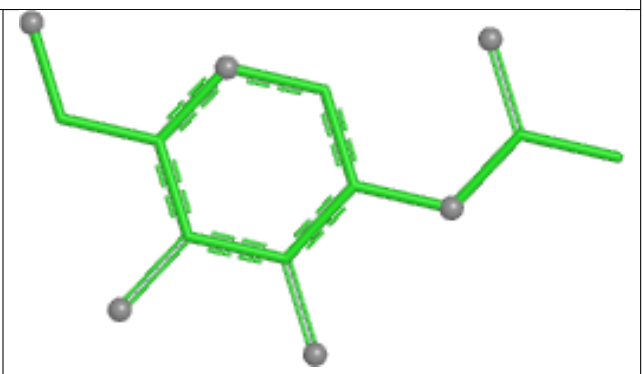
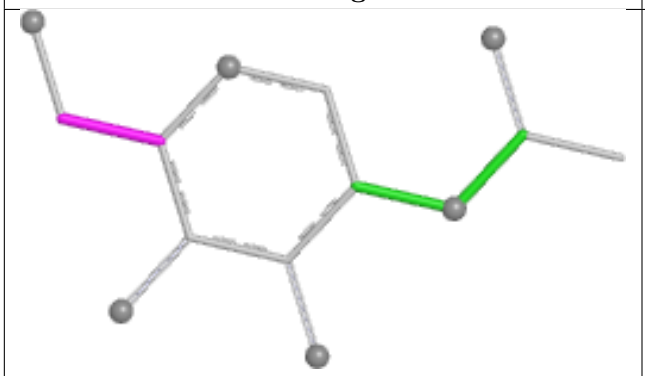


Bond angles



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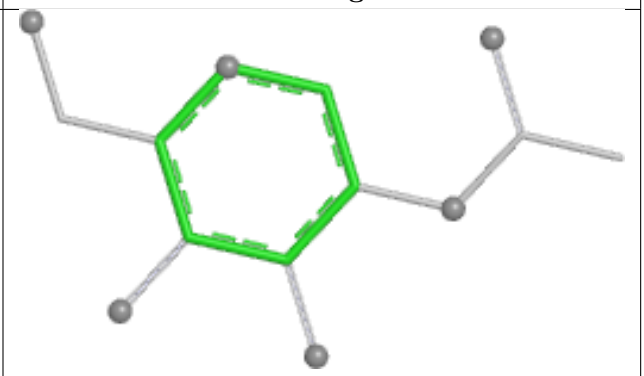
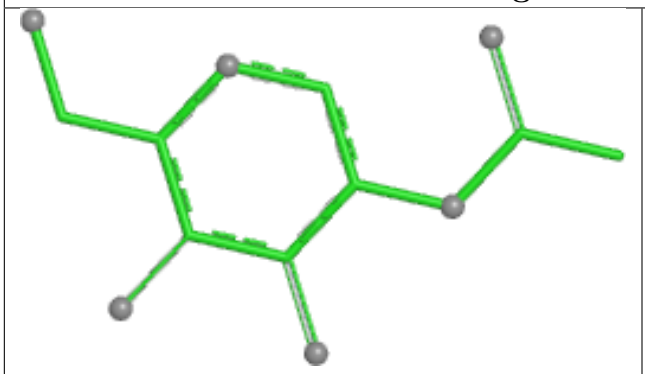


Rings

Ligand NAG B 1409



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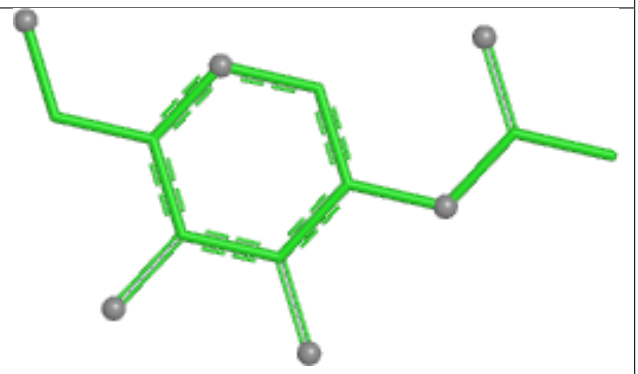
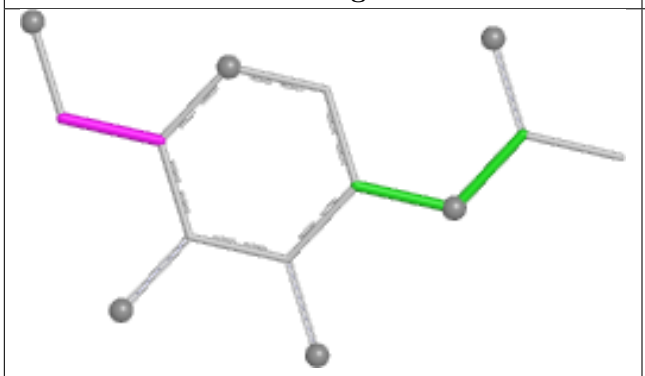


Bond angles



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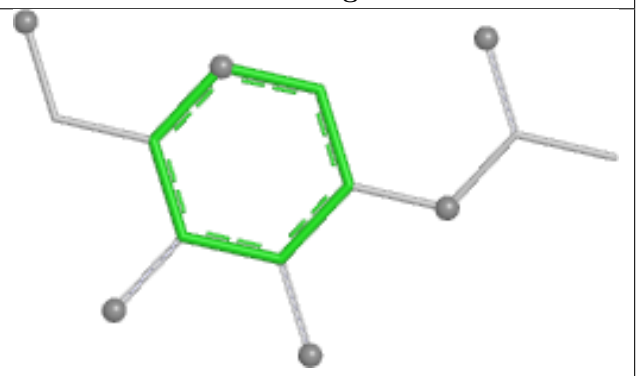
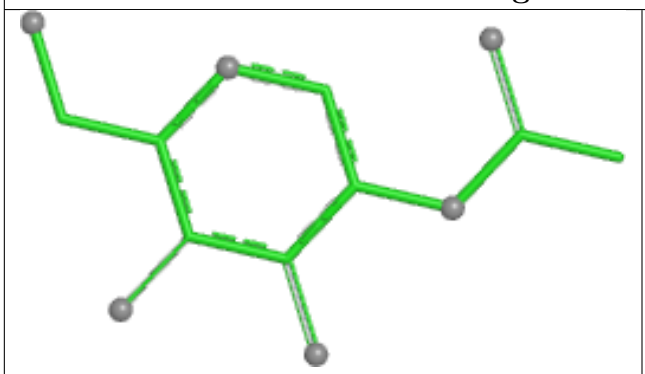


Rings

Ligand NAG C 1407



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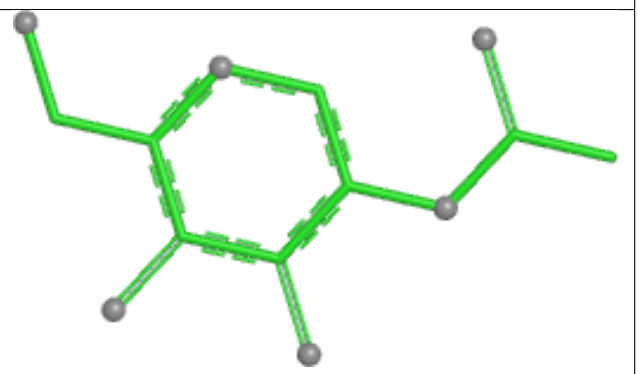
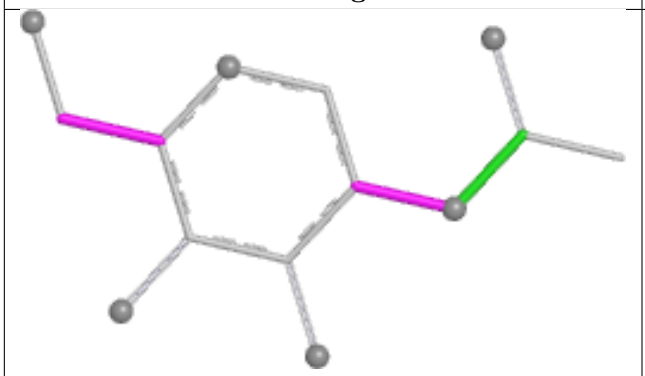


Bond angles



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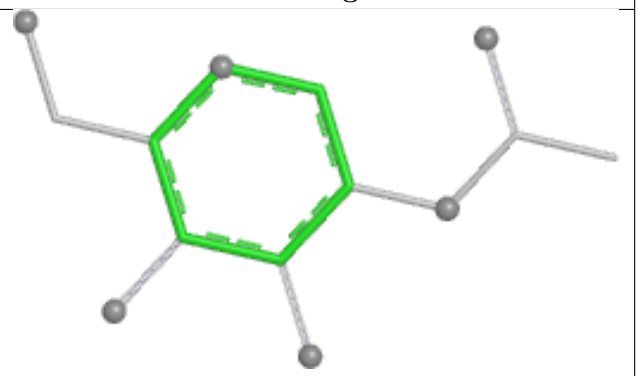

Rings

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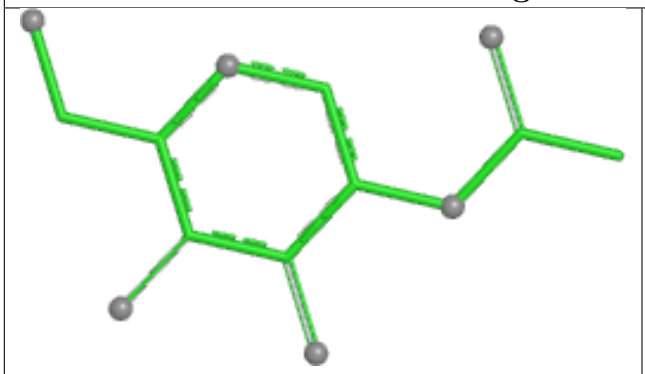

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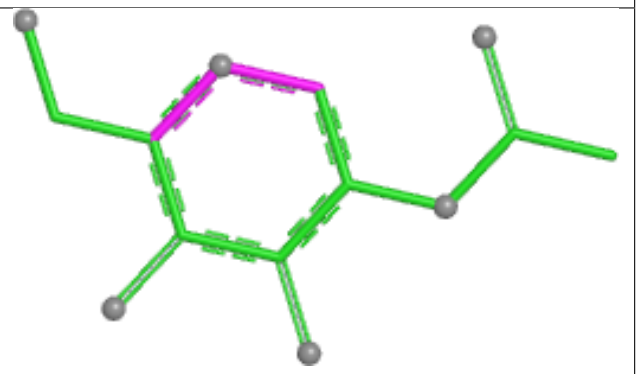
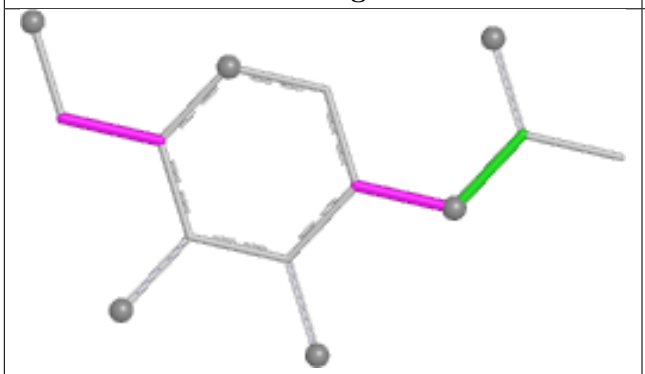


Bond angles



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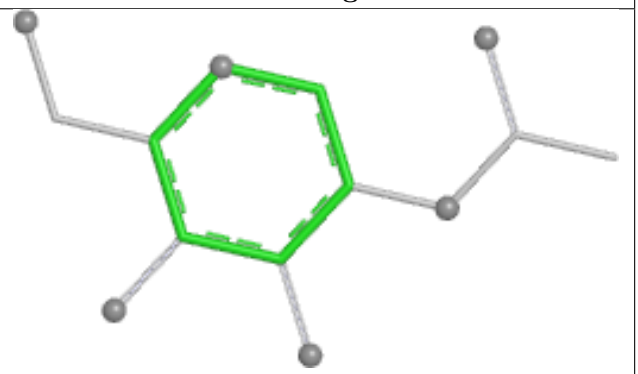
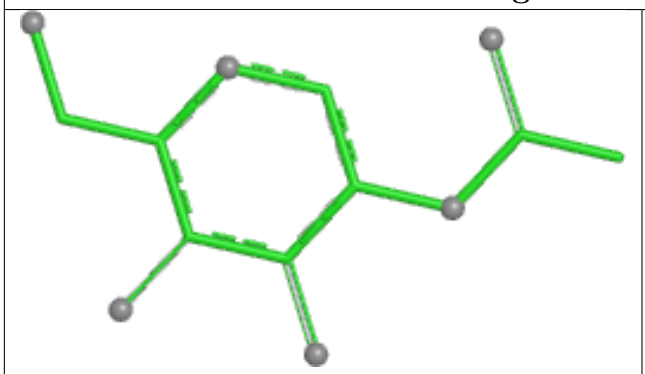


Rings

Ligand NAG C 1406



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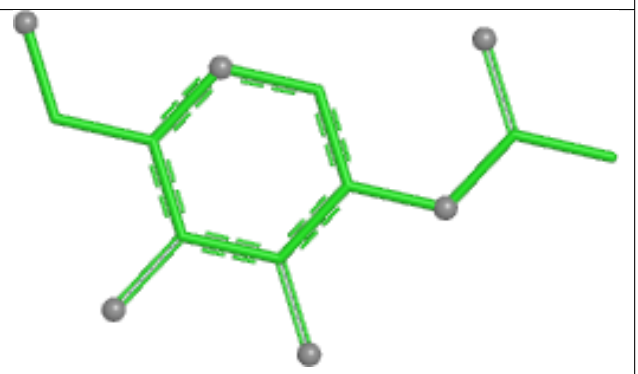
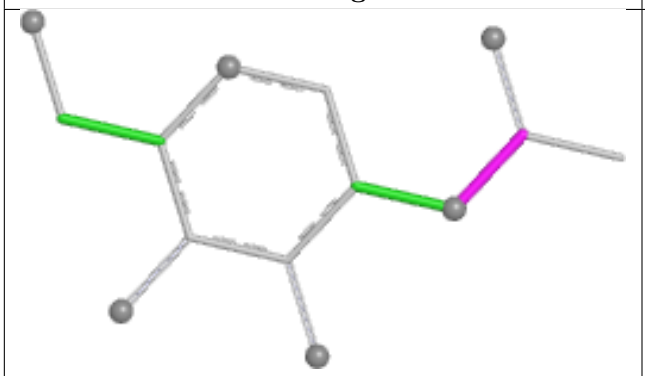


Bond angles



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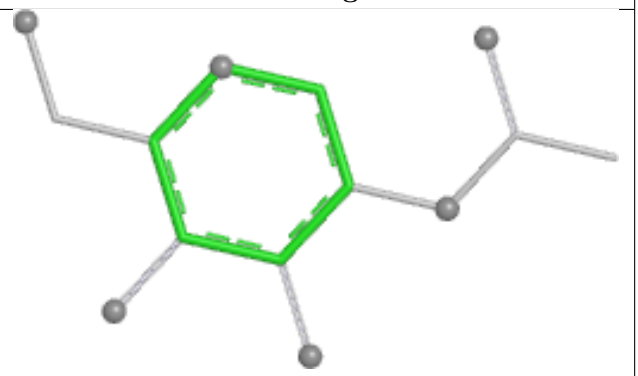
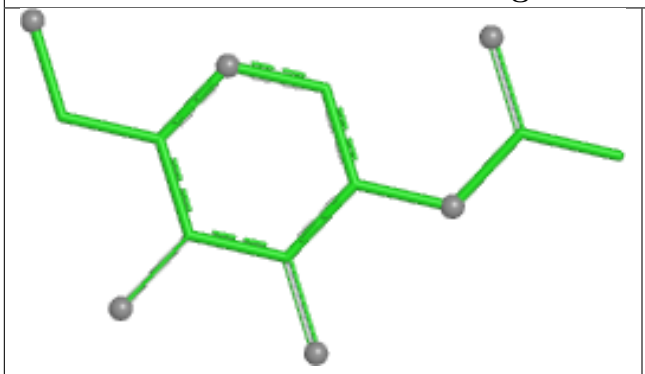


Rings

Ligand NAG A 1407



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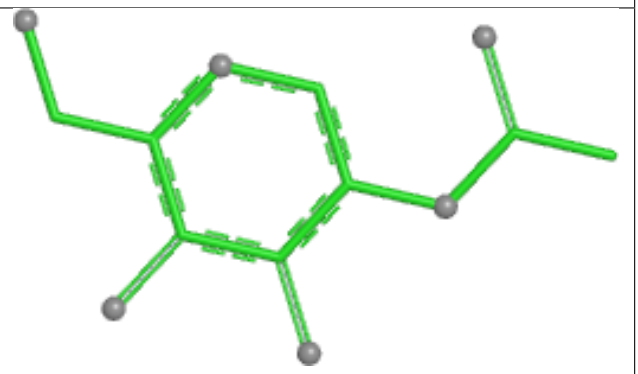
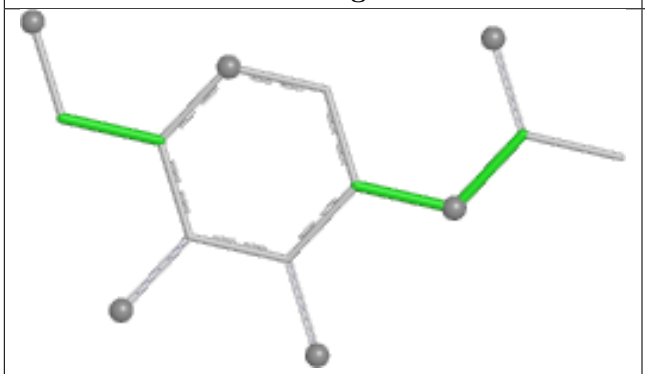


Bond angles



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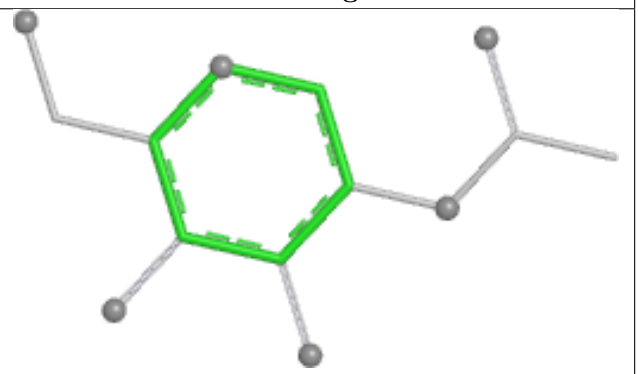
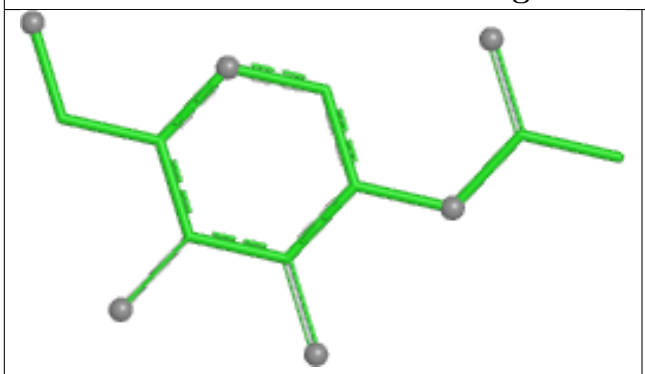


Rings

Ligand NAG C 1402



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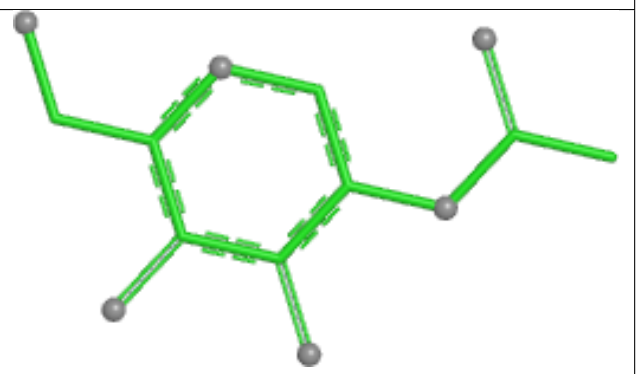
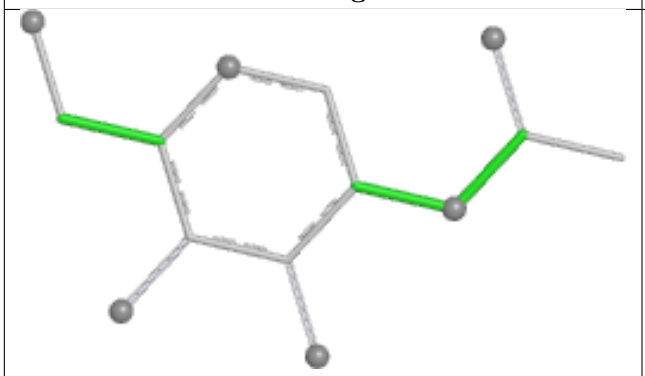


Bond angles



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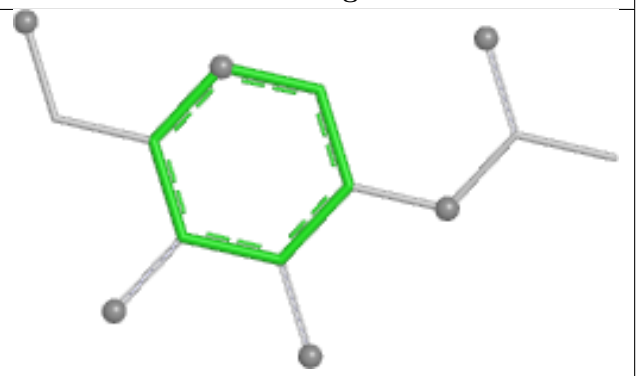
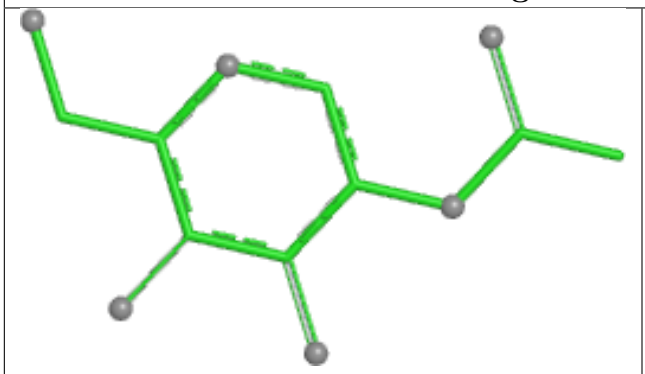


Rings

Ligand NAG A 1402



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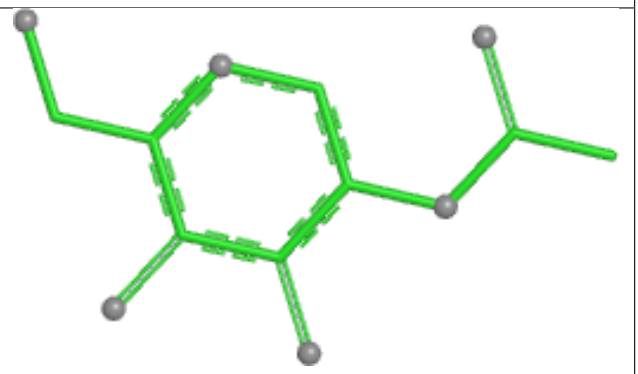
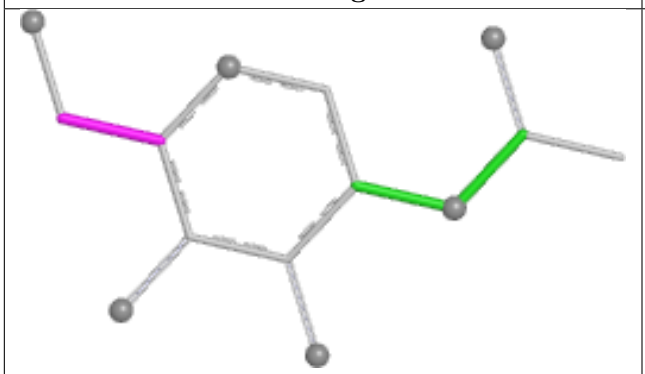


Bond angles



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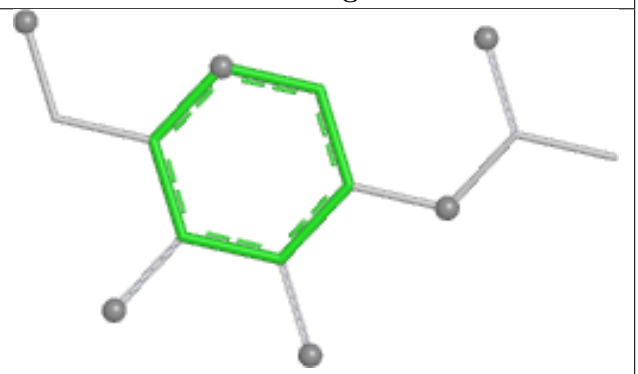
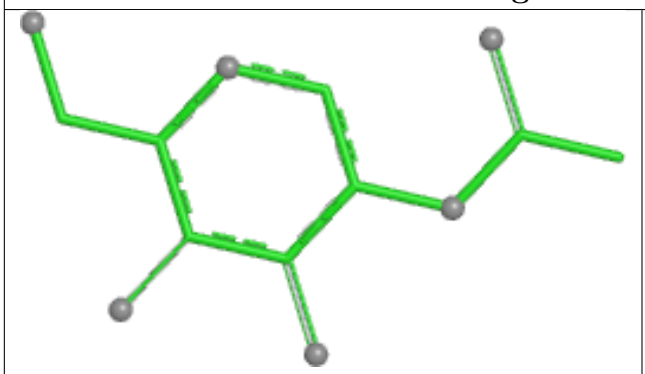


Rings

Ligand NAG A 1401



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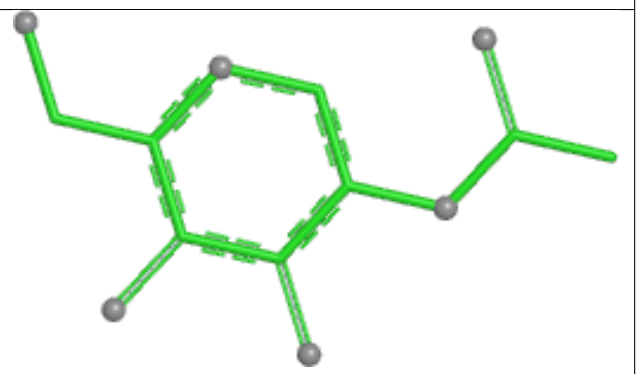

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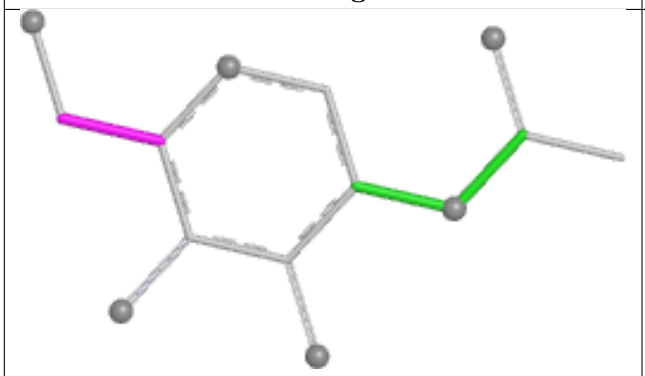

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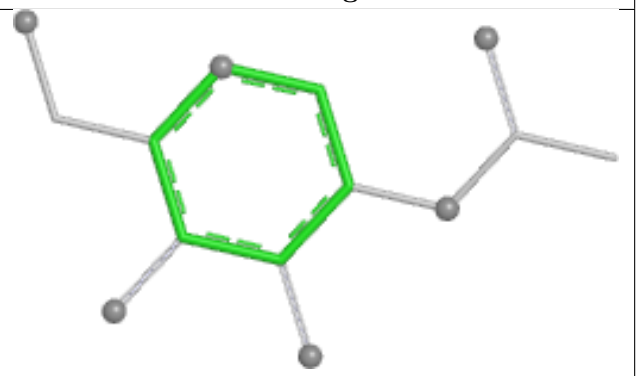
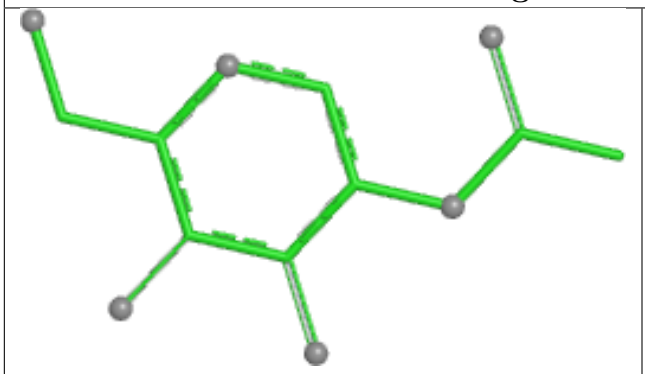


Rings

Ligand NAG A 1406



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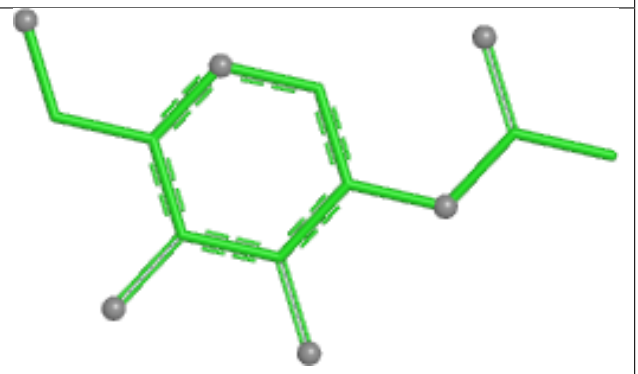
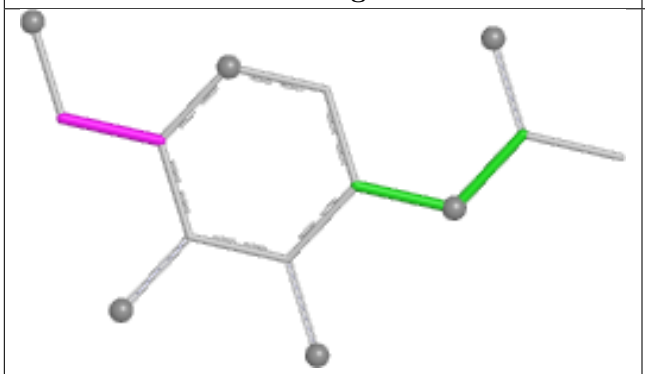


Bond angles



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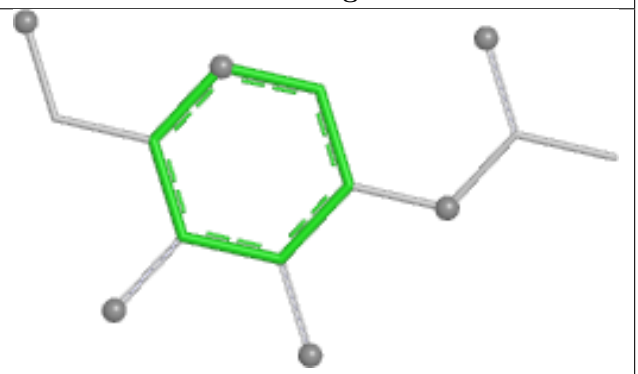
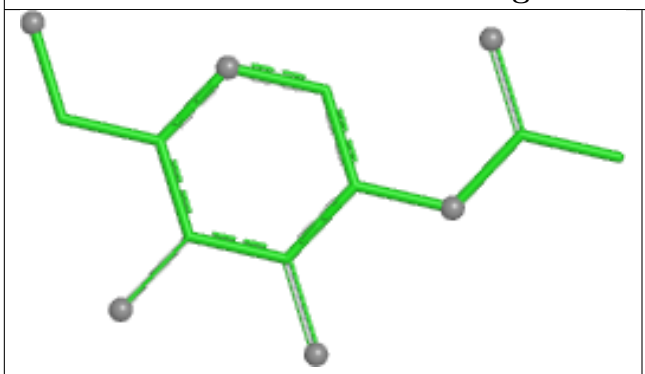


Rings

Ligand NAG C 1404



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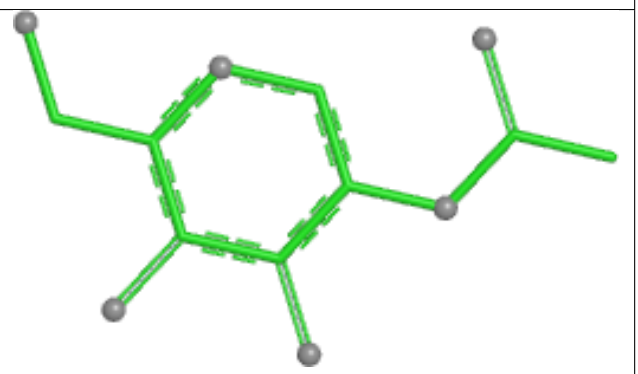
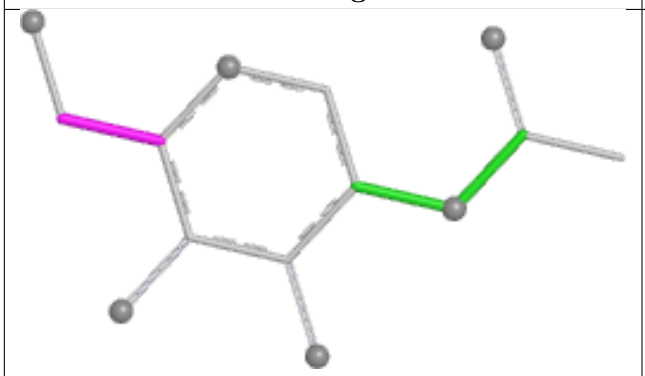


Bond angles



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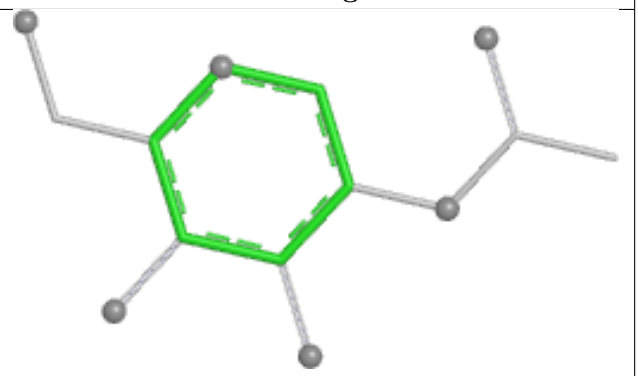
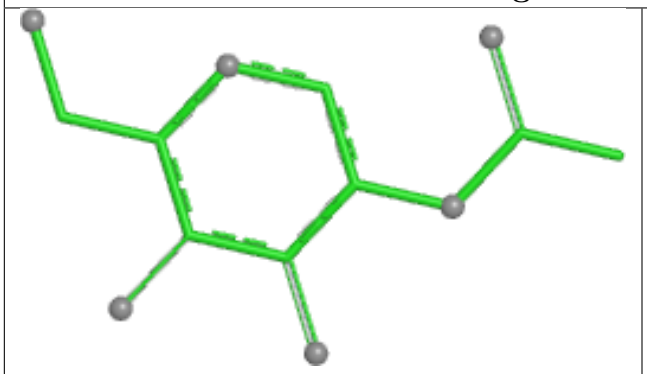


Rings

Ligand NAG B 1403



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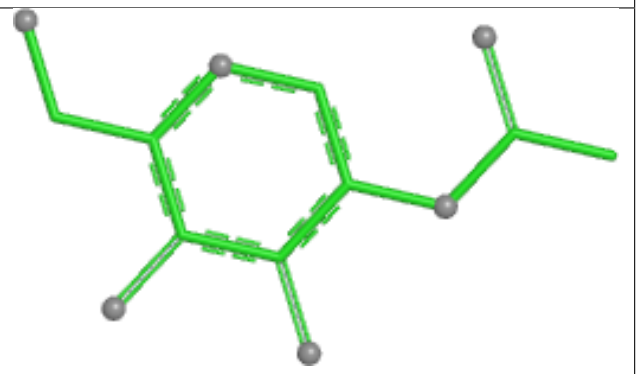
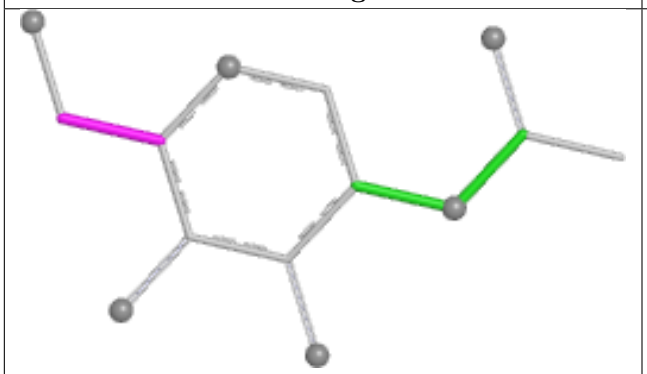


Bond angles



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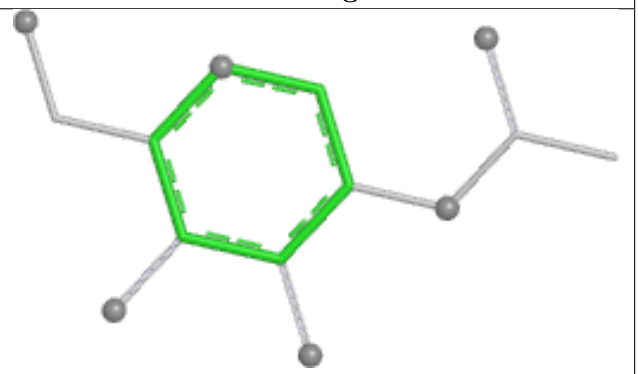
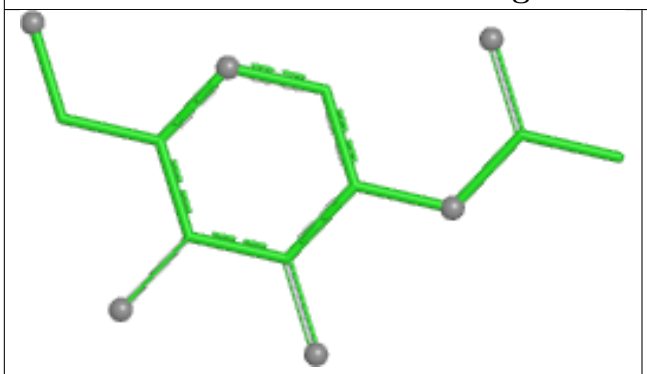
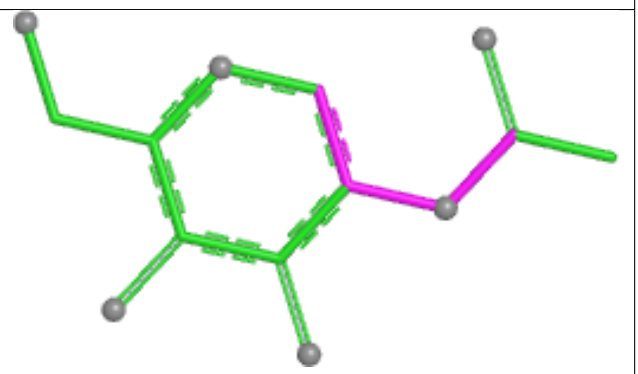


Rings

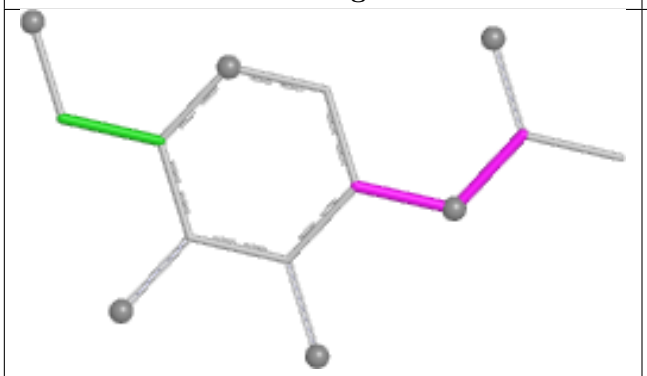
Ligand NAG C 1405



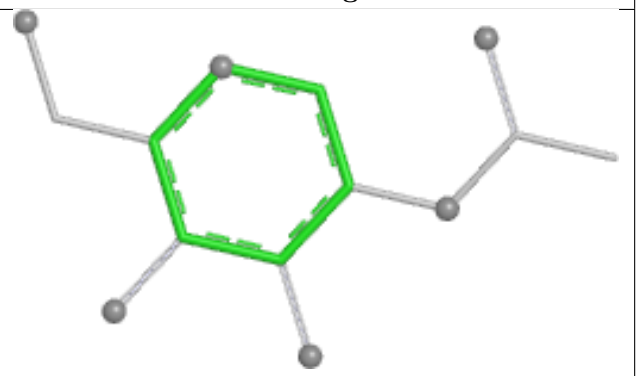
Bond lengths



Bond angles

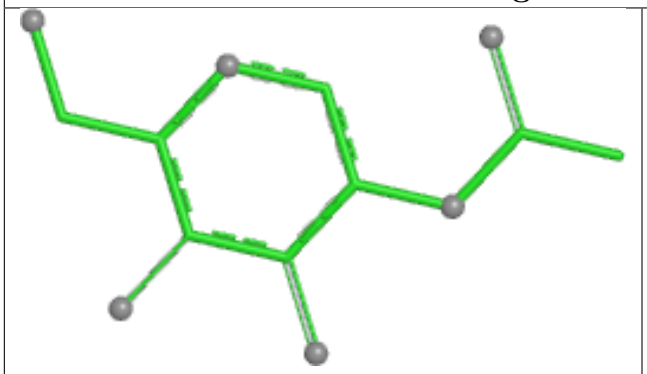


Torsions

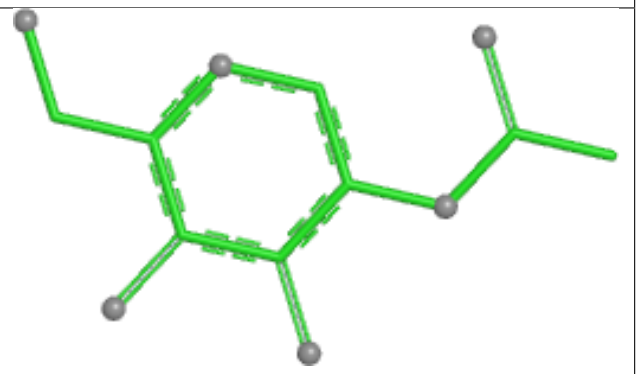


Rings

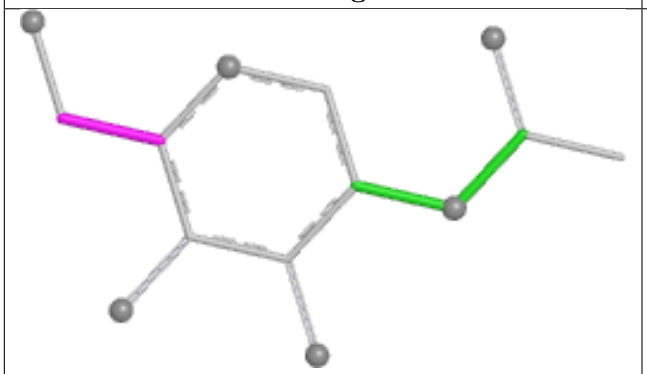
Ligand NAG B 1408



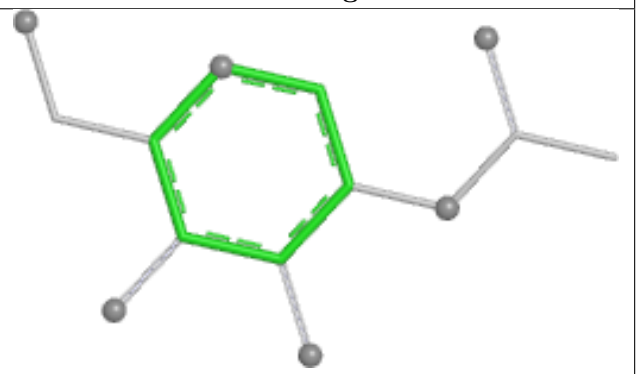
Bond lengths



Bond angles

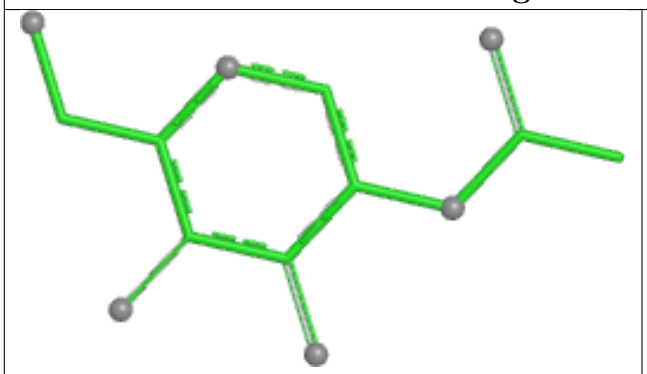


Torsions

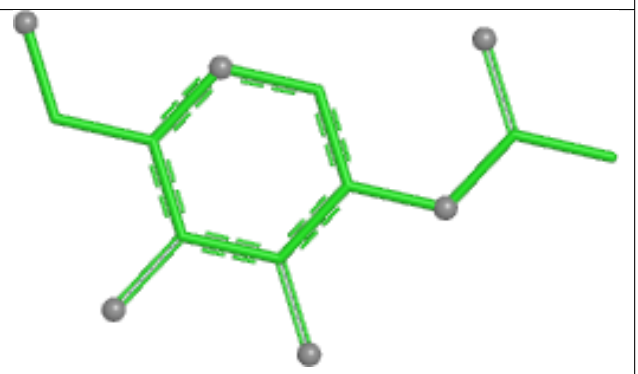


Rings

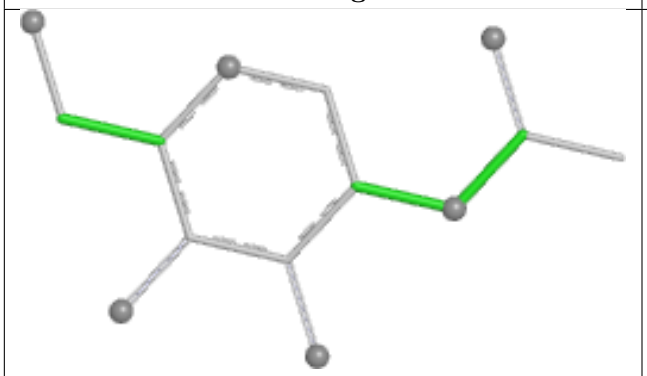
Ligand NAG B 1411



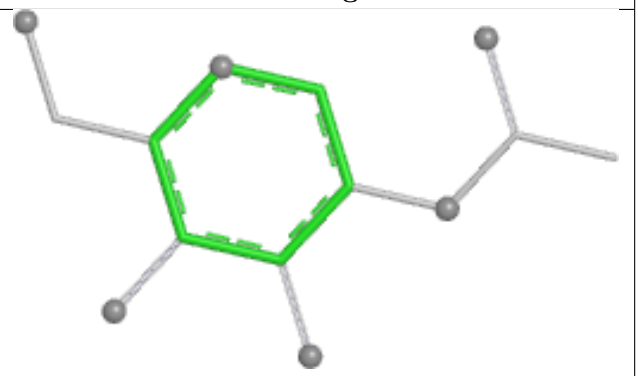
Bond lengths



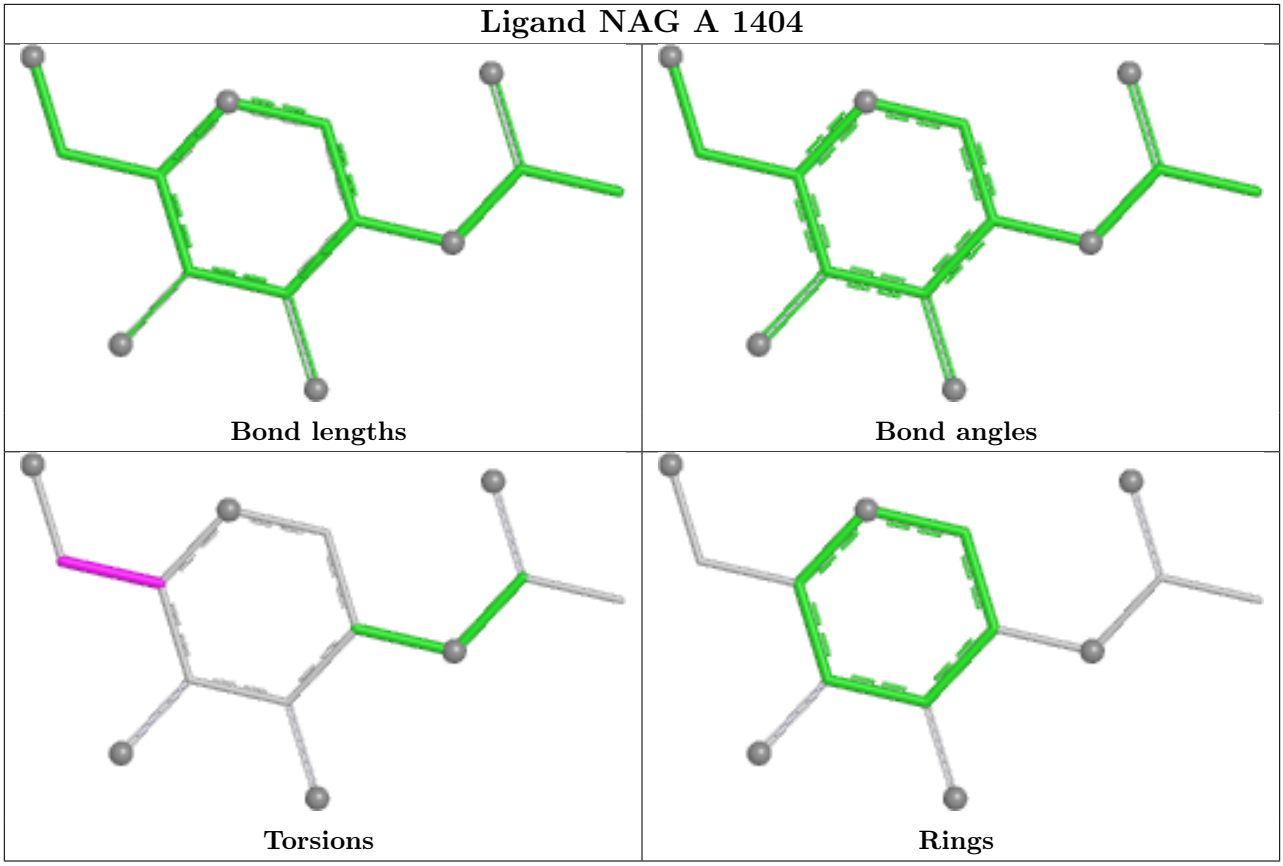
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

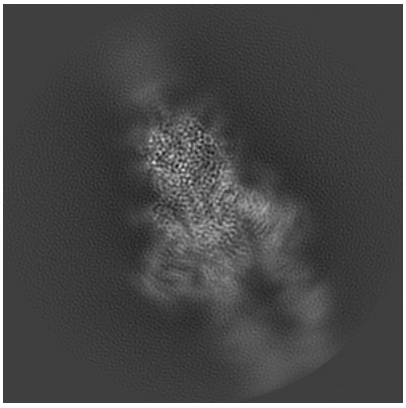
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30519. These allow visual inspection of the internal detail of the map and identification of artifacts.

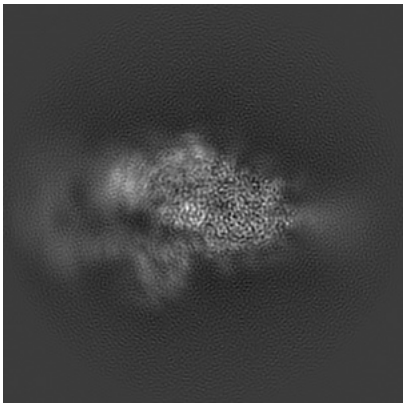
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

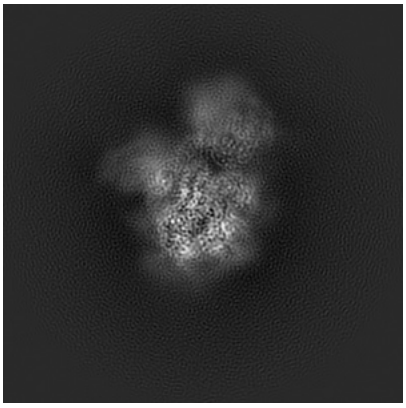
6.1.1 Primary map



X



Y

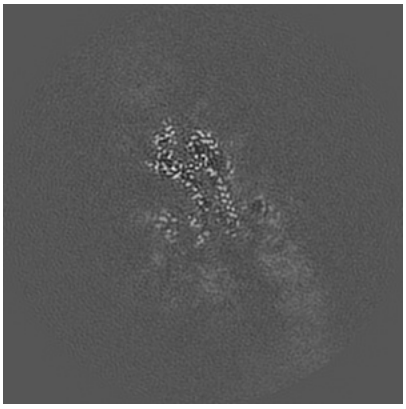


Z

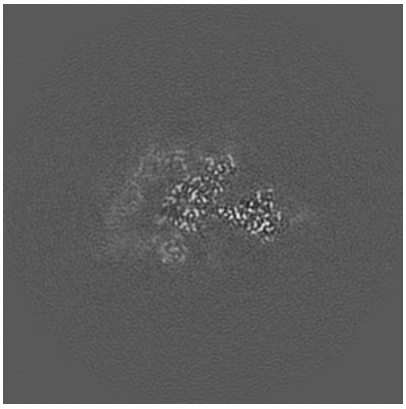
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

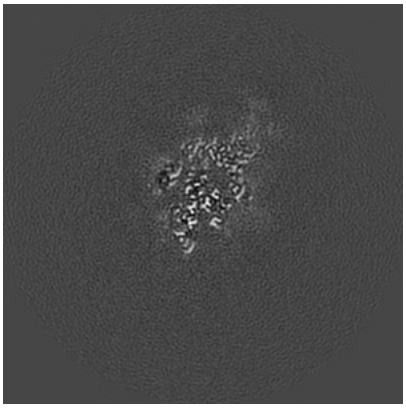
6.2.1 Primary map



X Index: 144



Y Index: 144

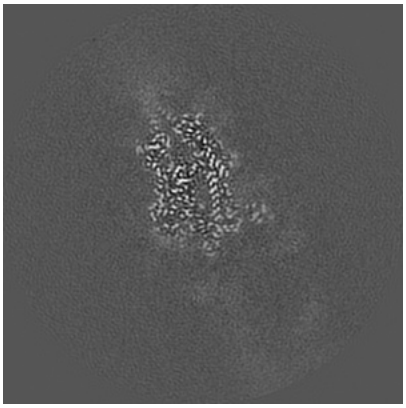


Z Index: 144

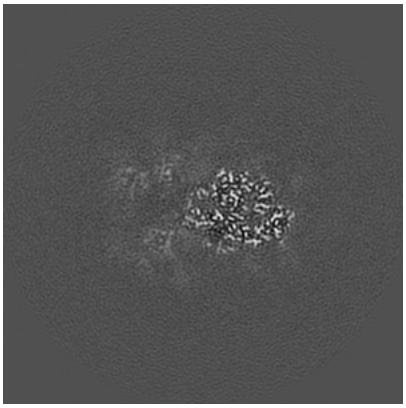
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

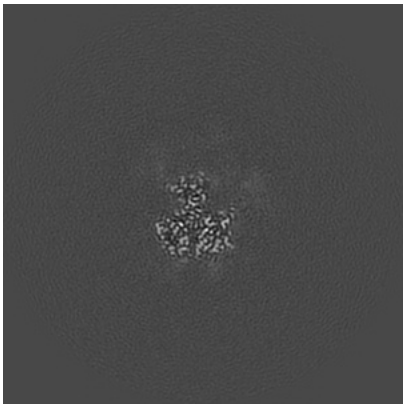
6.3.1 Primary map



X Index: 131



Y Index: 133

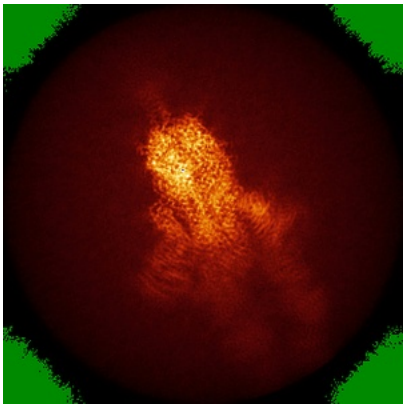


Z Index: 168

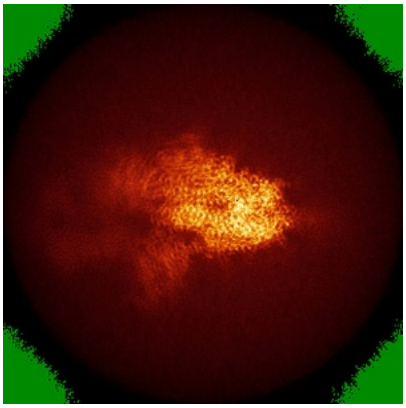
The images above show the largest variance slices of the map in three orthogonal directions.

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

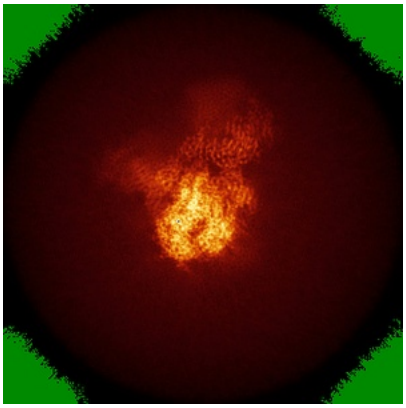
6.4.1 Primary map



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.

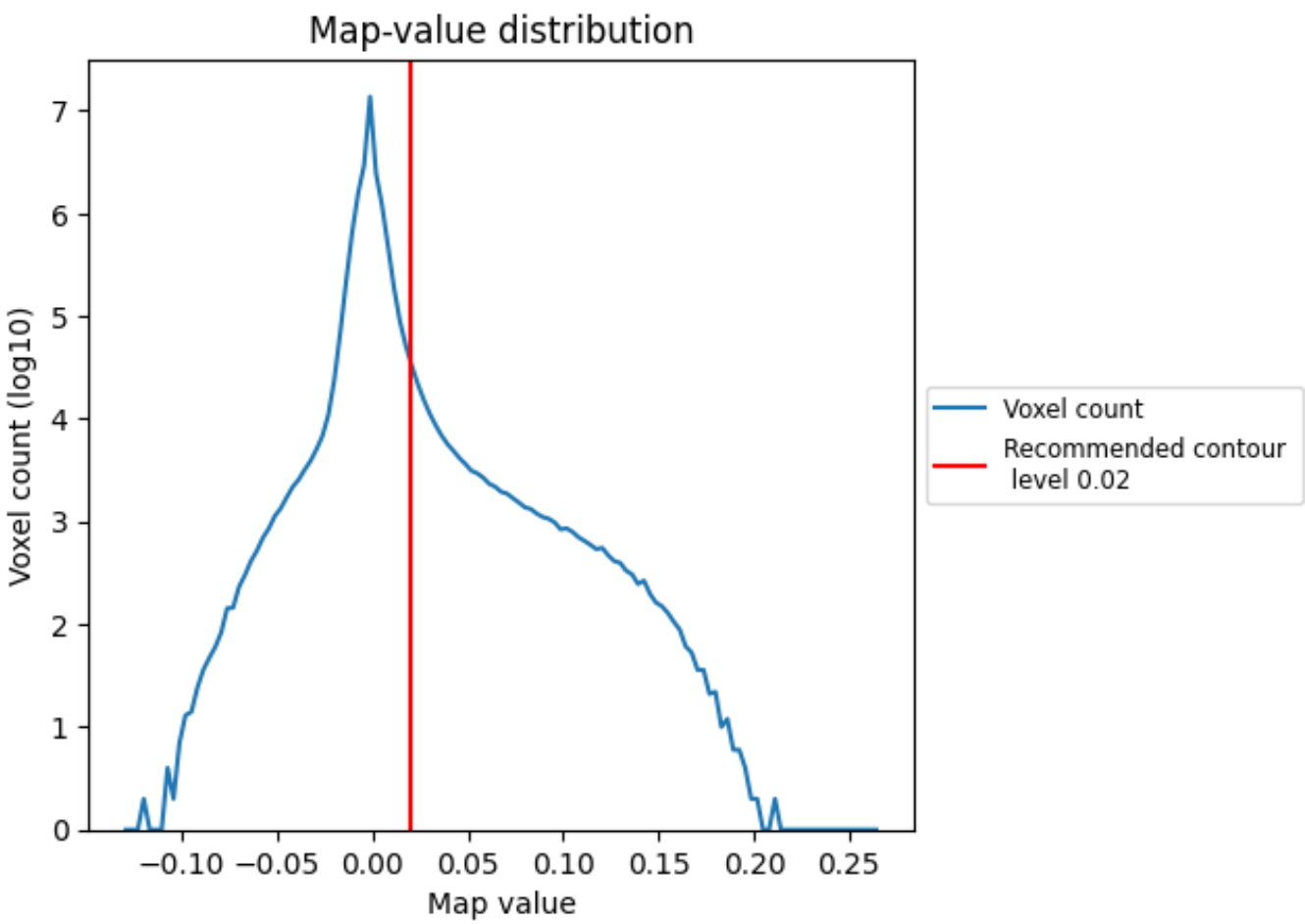
6.6 Mask visualisation (i)

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

7 Map analysis (i)

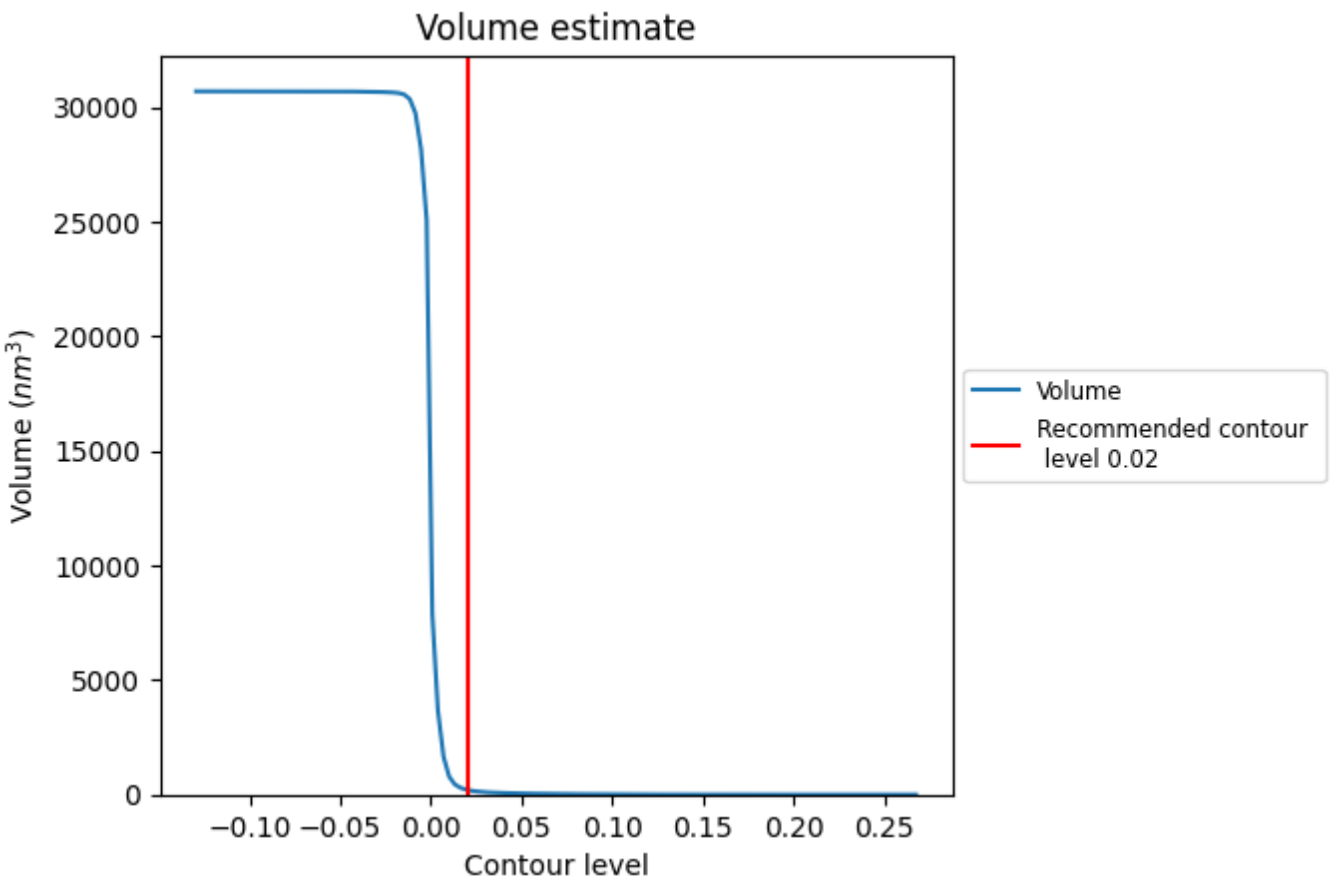
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

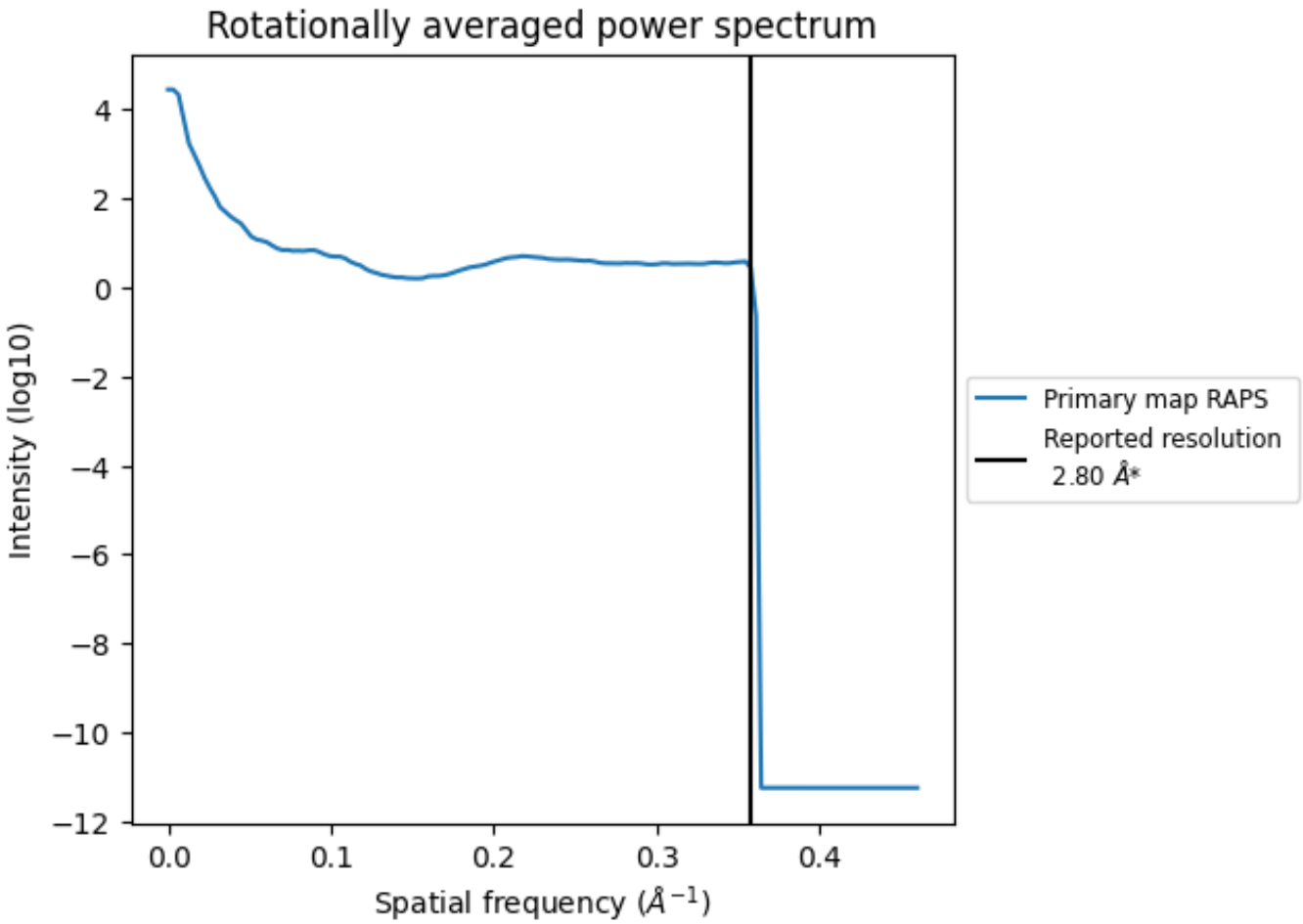
7.2 Volume estimate (i)



The volume at the recommended contour level is 207 nm^3; this corresponds to an approximate mass of 187 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 0.357 Å^{-1}

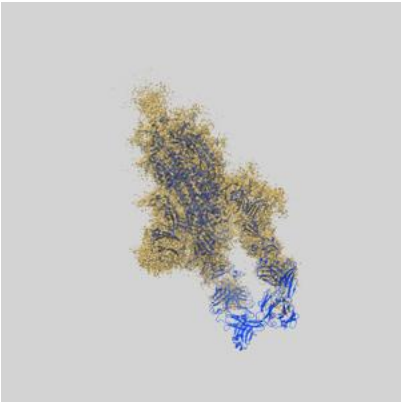
8 Fourier-Shell correlation (i)

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

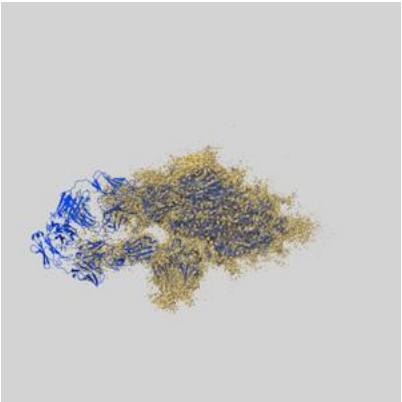
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30519 and PDB model 7CZW. Per-residue inclusion information can be found in section 3 on page 9.

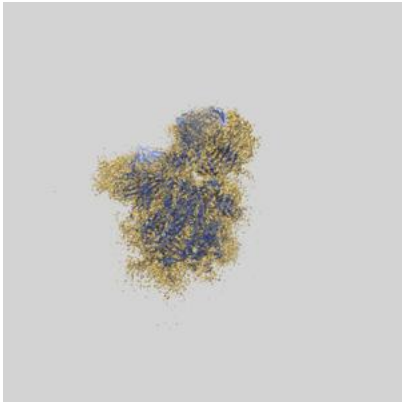
9.1 Map-model overlay (i)



X



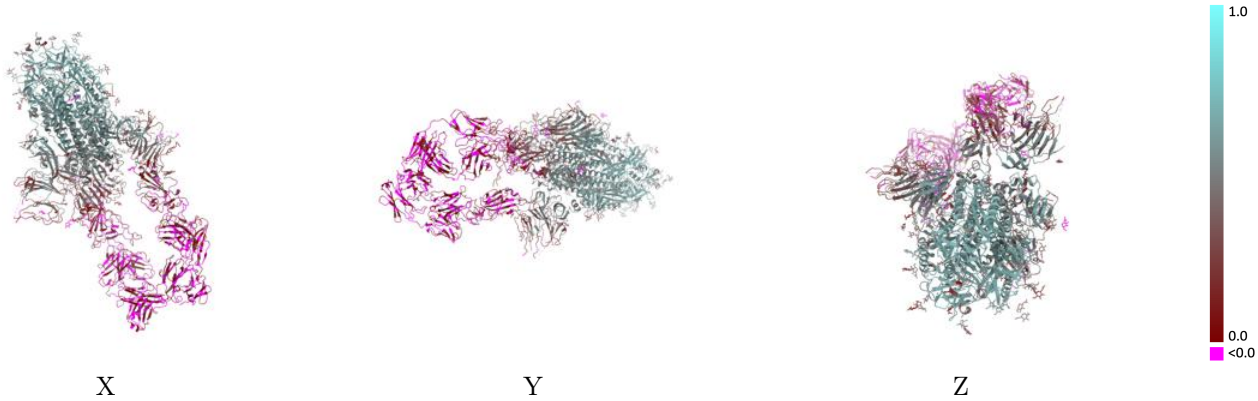
Y



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)

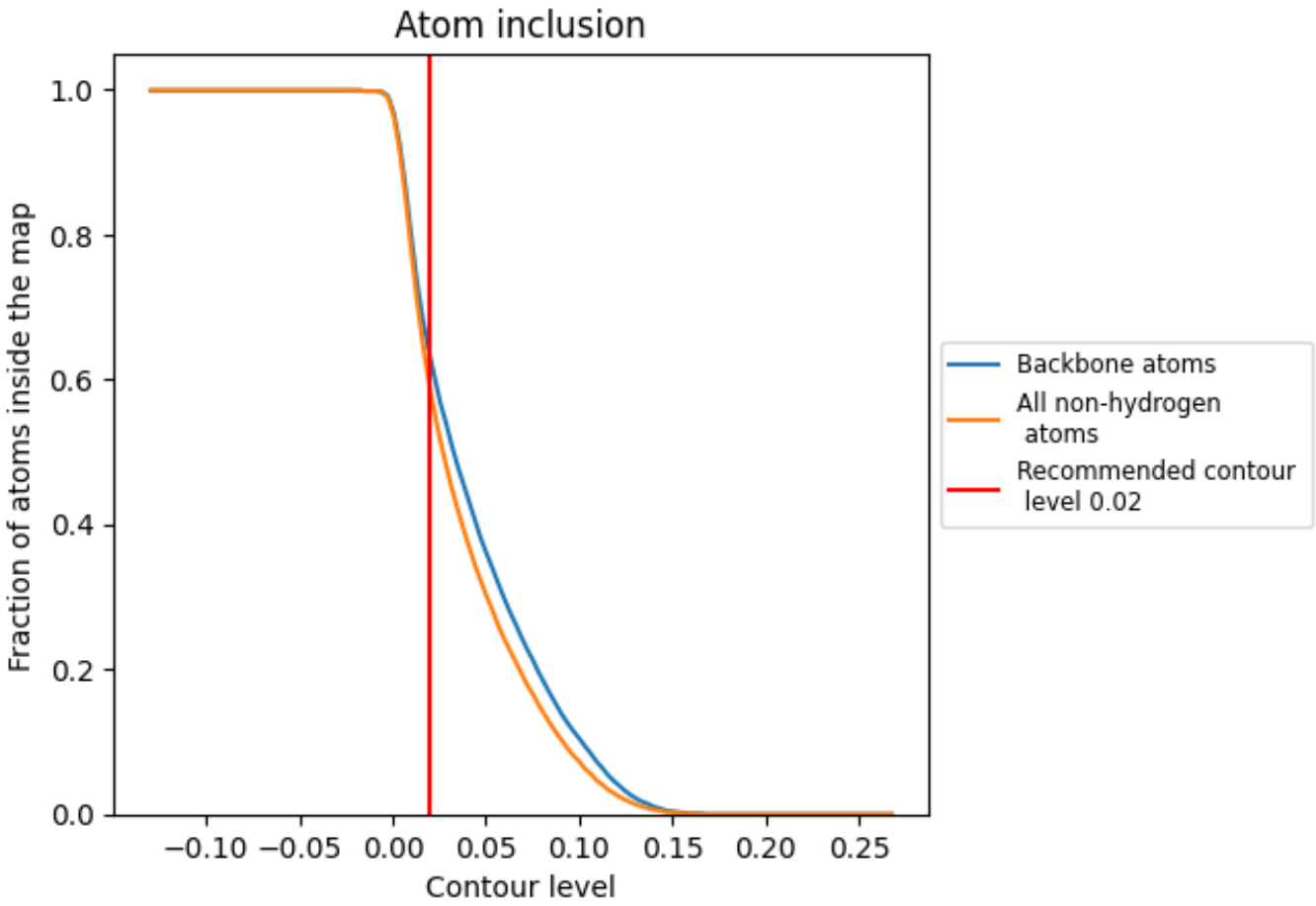


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 63% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.5890	0.3460
A	0.7470	0.4310
B	0.7930	0.4710
C	0.6970	0.4150
D	0.6430	0.2330
E	0.2860	0.1720
F	0.8930	0.5550
G	0.7140	0.3450
H	0.0420	0.0280
I	0.7140	0.4950
J	0.0140	0.0160
K	0.8210	0.5040
L	0.0210	0.0060
M	0.7500	0.4340
N	0.0090	-0.0050
O	0.2500	0.1880
P	0.6070	0.2710
Q	0.8930	0.5210
R	0.7500	0.3920
S	0.8210	0.4200
T	0.6790	0.4010
U	0.3930	0.2570
V	0.0000	0.0490
W	0.4640	0.3500
X	0.8210	0.4970
Y	0.6790	0.3910
Z	0.5360	0.2870
a	0.7500	0.4190
b	0.6070	0.3280