Full wwPDB EM Validation Report ⓘ

Nov 18, 2024 – 01:07 PM JST

PDB ID	:	8XZ8
EMDB ID	:	EMD-38789
Title	:	BA.2.86 Spike in complex with bovine ACE2 (bound 1 ACE2)
Authors	:	Yue, C.; Liu, P.
Deposited on	:	2024-01-21
Resolution	:	3.65 Å(reported)

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

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

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

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

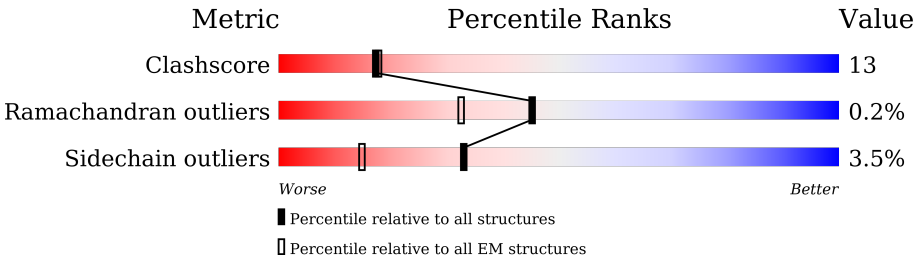
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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%

Mol	Chain	Length	Quality of chain
1	A	804	48% 25% • 26%
2	B	1206	58% 29% • 12%
2	C	1206	59% 28% • 12%
2	D	1206	59% 28% • 12%
3	E	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	100%
3	I	2	100%

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Mol	Chain	Length	Quality of chain
3	J	2	100%
3	K	2	100%
3	L	2	100%
3	M	2	100%
3	N	2	100%
3	O	2	100%
3	P	2	100%
3	Q	2	100%
3	R	2	100%
3	S	2	100%
3	T	2	100%
3	U	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 30785 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	596	Total	C	N	O	S	0	0
			4906	3136	815	925	30		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
2	C	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
2	D	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		

There are 219 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	-	insertion	UNP P0DTC2
B	18	LEU	-	insertion	UNP P0DTC2
B	19	PHE	-	insertion	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2
C	18	LEU	-	insertion	UNP P0DTC2
C	19	PHE	-	insertion	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
D	-2	ALA	-	expression tag	UNP P0DTC2
D	-1	THR	-	expression tag	UNP P0DTC2
D	16	MET	-	insertion	UNP P0DTC2
D	17	PRO	-	insertion	UNP P0DTC2
D	18	LEU	-	insertion	UNP P0DTC2
D	19	PHE	-	insertion	UNP P0DTC2
D	22	ILE	THR	conflict	UNP P0DTC2
D	24	THR	ARG	conflict	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2
D	50	LEU	SER	conflict	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	127	PHE	VAL	conflict	UNP P0DTC2
D	143	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	157	SER	PHE	conflict	UNP P0DTC2
D	158	GLY	ARG	conflict	UNP P0DTC2
D	?	-	ASN	deletion	UNP P0DTC2
D	212	ILE	LEU	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	216	PHE	LEU	variant	UNP P0DTC2
D	245	ASN	HIS	conflict	UNP P0DTC2
D	264	ASP	ALA	conflict	UNP P0DTC2
D	332	VAL	ILE	conflict	UNP P0DTC2
D	339	HIS	GLY	conflict	UNP P0DTC2
D	356	THR	LYS	conflict	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	403	LYS	ARG	conflict	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	HIS	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	446	SER	GLY	variant	UNP P0DTC2
D	450	ASP	ASN	conflict	UNP P0DTC2
D	452	TRP	LEU	conflict	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	481	LYS	ASN	conflict	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	484	LYS	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	554	LYS	GLU	conflict	UNP P0DTC2
D	570	VAL	ALA	conflict	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	621	SER	PRO	conflict	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	ARG	PRO	variant	UNP P0DTC2
D	683	ALA	ARG	conflict	UNP P0DTC2
D	685	ALA	ARG	conflict	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	939	PHE	SER	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			25	14	1	10		
3	F	2	Total	C	N	O	0	0
			25	14	1	10		
3	G	2	Total	C	N	O	0	0
			25	14	1	10		
3	H	2	Total	C	N	O	0	0
			25	14	1	10		
3	I	2	Total	C	N	O	0	0
			25	14	1	10		
3	J	2	Total	C	N	O	0	0
			25	14	1	10		
3	K	2	Total	C	N	O	0	0
			25	14	1	10		
3	L	2	Total	C	N	O	0	0
			25	14	1	10		
3	M	2	Total	C	N	O	0	0
			25	14	1	10		
3	N	2	Total	C	N	O	0	0
			25	14	1	10		
3	O	2	Total	C	N	O	0	0
			25	14	1	10		
3	P	2	Total	C	N	O	0	0
			25	14	1	10		
3	Q	2	Total	C	N	O	0	0
			25	14	1	10		
3	R	2	Total	C	N	O	0	0
			25	14	1	10		
3	S	2	Total	C	N	O	0	0
			25	14	1	10		
3	T	2	Total	C	N	O	0	0
			25	14	1	10		
3	U	2	Total	C	N	O	0	0
			25	14	1	10		

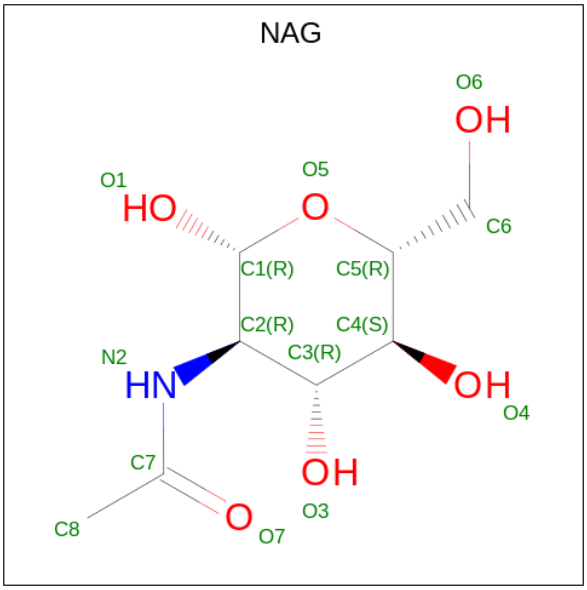
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Cl 1 1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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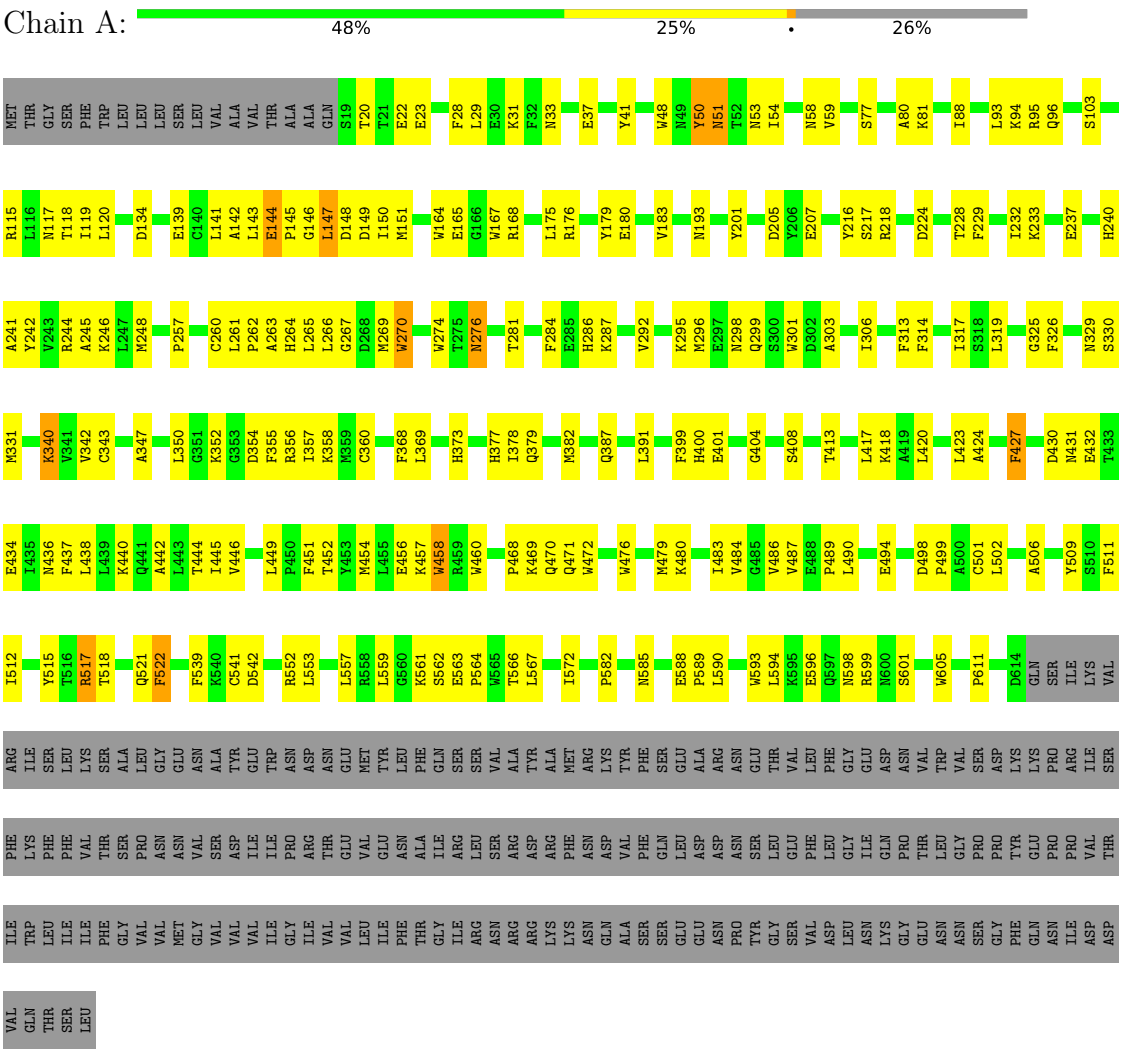
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

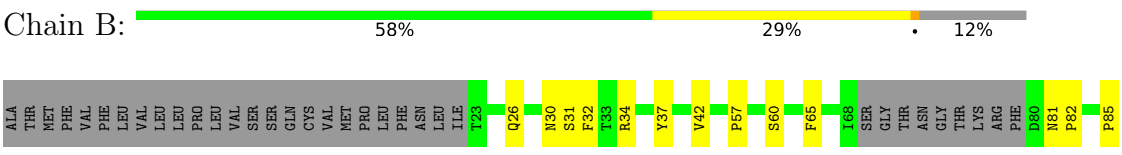
- Molecule 1: Angiotensin-converting enzyme

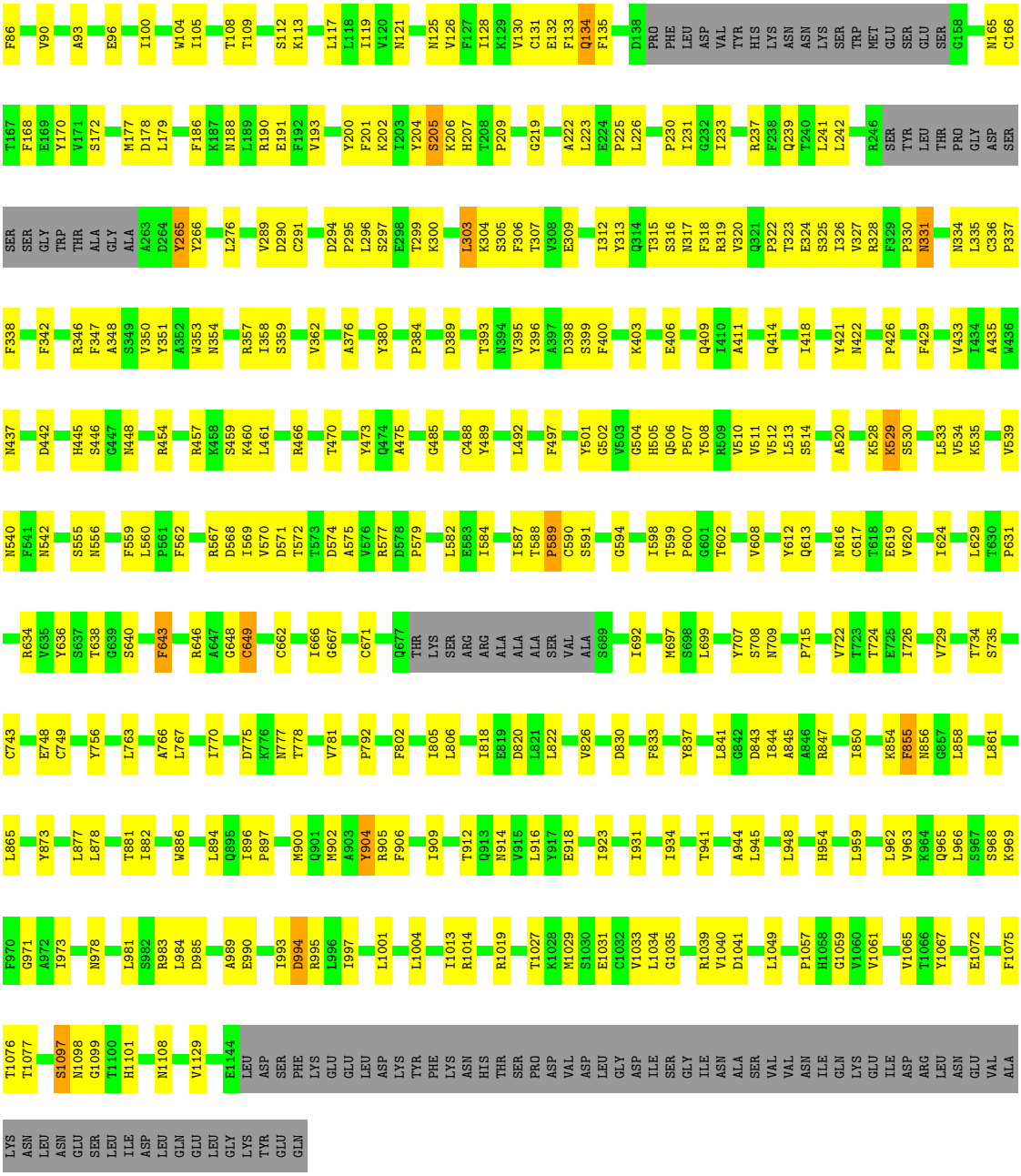
Chain A:



- Molecule 2: Spike glycoprotein

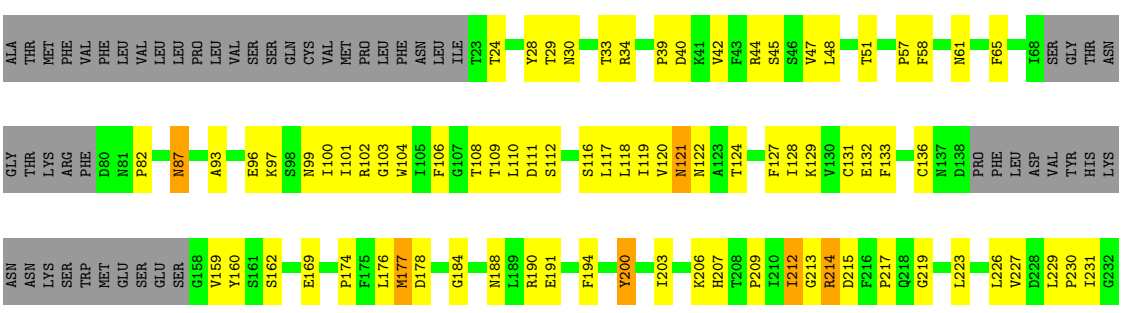
Chain B:

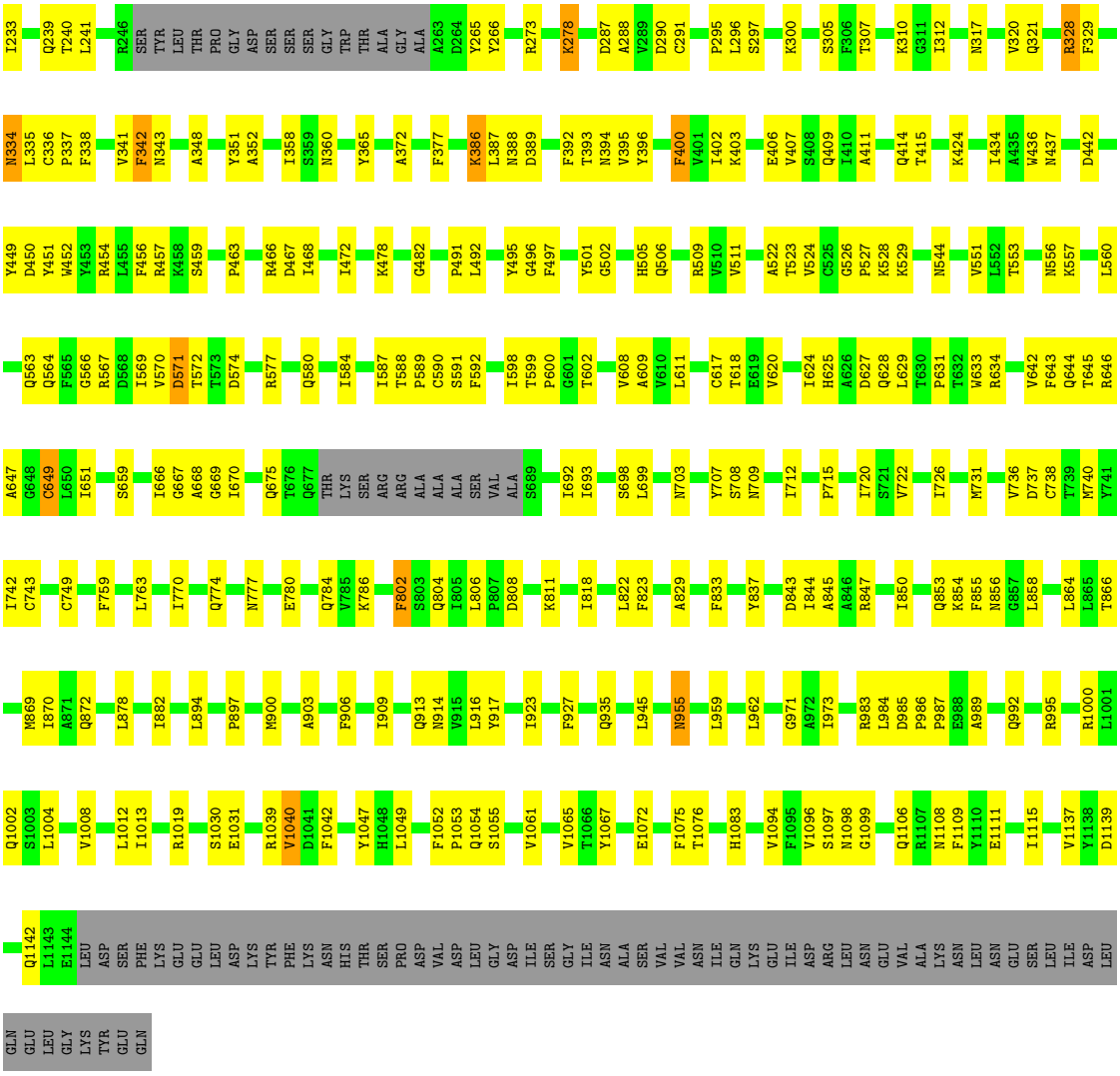




• Molecule 2: Spike glycoprotein

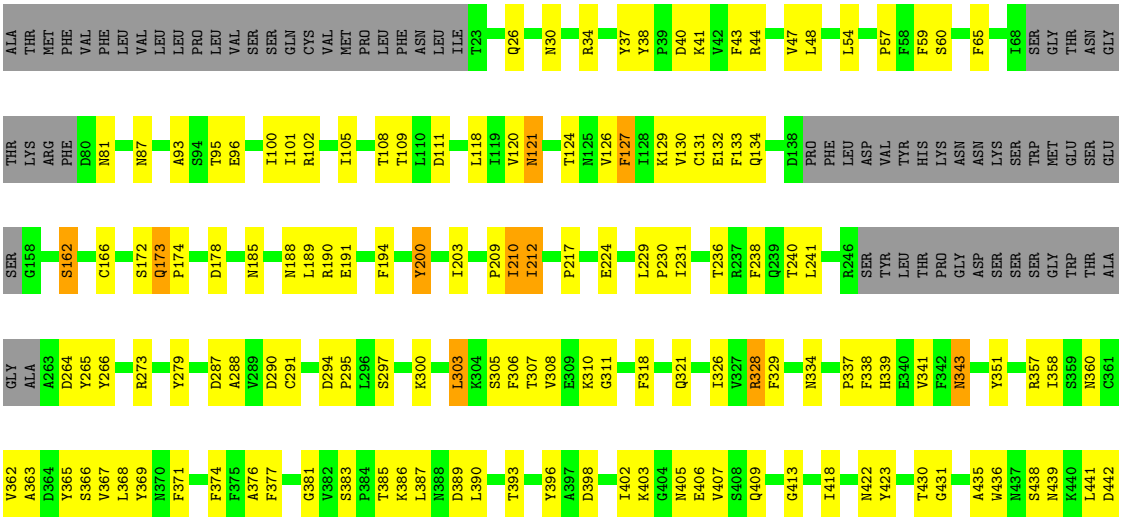
Chain C:

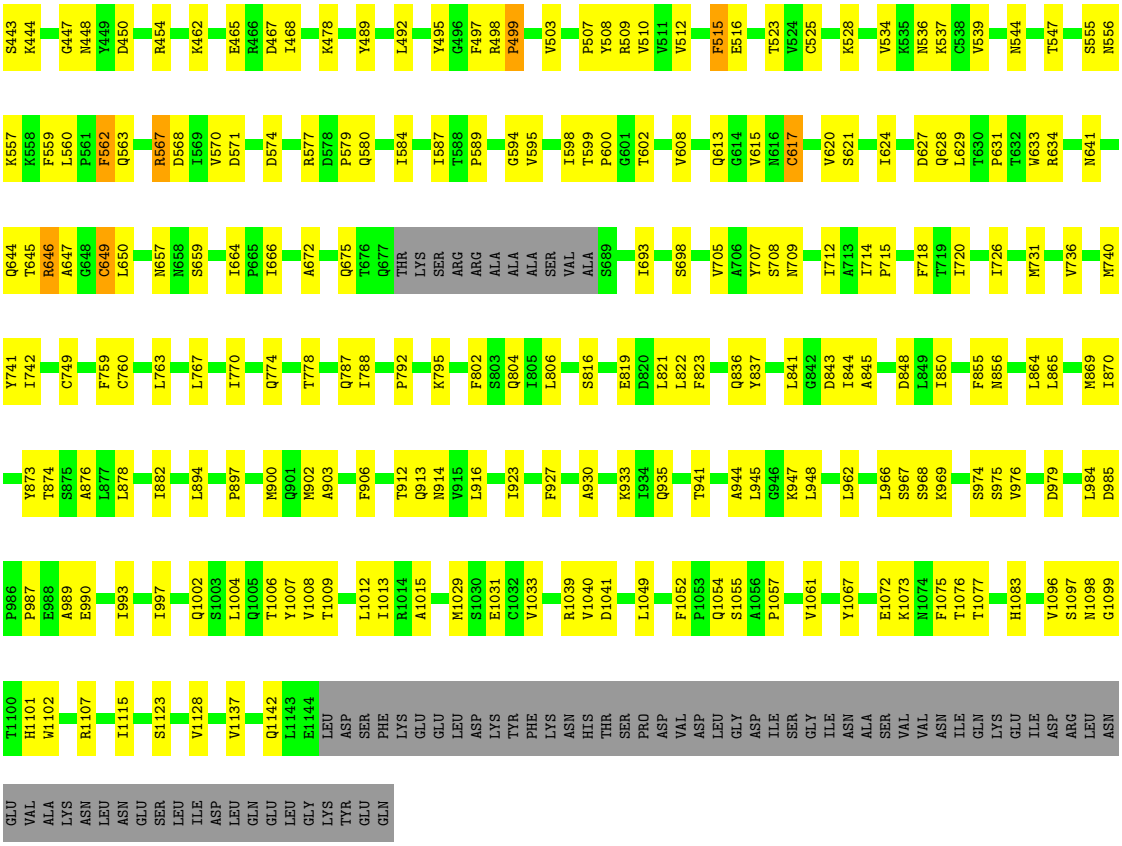




• Molecule 2: Spike glycoprotein

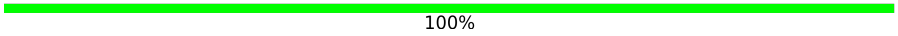
Chain D:





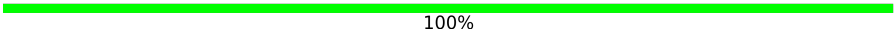
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



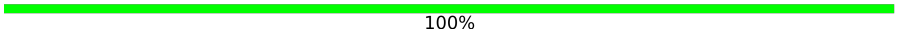
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



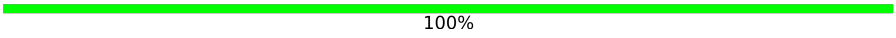
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

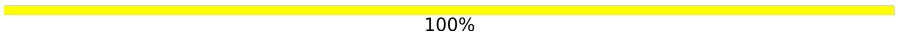


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

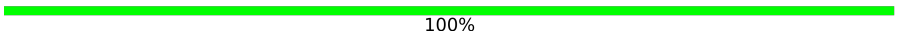
Chain H:



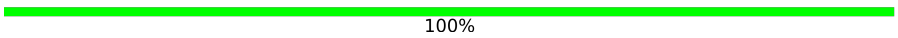
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

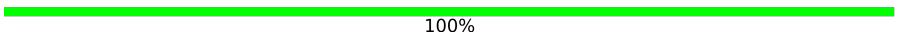
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

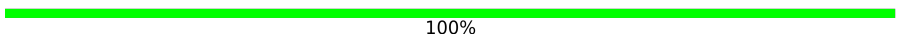
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

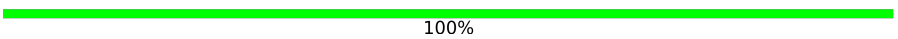
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

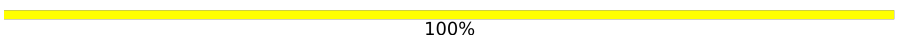
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

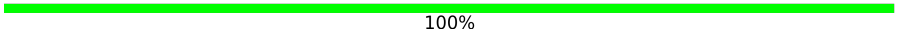
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

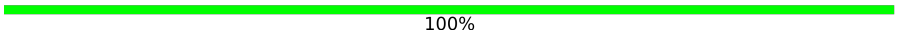
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 

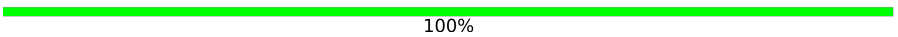
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

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

Chain Q: 

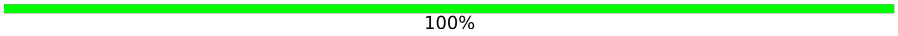
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 

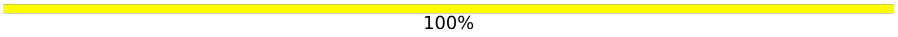
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

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

Chain T: 

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

Chain U: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, BMA, CL

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	0.27	0/5043	0.52	0/6838
2	B	0.27	0/8516	0.50	0/11591
2	C	0.26	0/8516	0.50	0/11591
2	D	0.26	0/8516	0.50	0/11591
All	All	0.26	0/30591	0.50	0/41611

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4906	0	4691	134	0
2	B	8316	0	8103	240	0
2	C	8316	0	8104	246	0
2	D	8316	0	8104	261	0
3	E	25	0	22	0	0
3	F	25	0	22	0	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	25	0	22	0	0
3	K	25	0	22	0	0
3	L	25	0	22	0	0
3	M	25	0	22	0	0
3	N	25	0	22	0	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
3	R	25	0	22	0	0
3	S	25	0	22	0	0
3	T	25	0	22	0	0
3	U	25	0	22	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	70	0	65	0	0
6	B	154	0	140	1	0
6	C	140	0	130	1	0
6	D	140	0	130	3	0
All	All	30785	0	29841	812	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 13.

All (812) 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:B:334:ASN:OD1	2:B:362:VAL:HG13	1.58	1.00
2:D:617:CYS:HA	2:D:620:VAL:HG12	1.56	0.88
2:C:212:ILE:HG22	2:C:213:GLY:H	1.39	0.87
2:C:777:ASN:HD21	2:C:1019:ARG:HA	1.45	0.82
2:C:352:ALA:HA	2:C:466:ARG:HD2	1.59	0.82
2:D:188:ASN:HA	2:D:209:PRO:HA	1.63	0.80
1:A:483:ILE:HG23	1:A:484:VAL:HG23	1.64	0.80
2:C:644:GLN:HA	2:C:649:CYS:HB2	1.64	0.79
2:C:131:CYS:SG	2:C:132:GLU:N	2.57	0.78
2:B:426:PRO:HG2	2:B:429:PHE:HB2	1.66	0.77
2:C:351:TYR:CE2	2:C:452:TRP:HB2	2.19	0.77
2:B:984:LEU:HB3	2:B:989:ALA:HB2	1.66	0.76
2:D:310:LYS:HG2	2:D:664:ILE:HD11	1.68	0.76
2:B:276:LEU:HD11	2:B:304:LYS:HA	1.68	0.75
2:D:555:SER:HB3	2:D:584:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:ASP:HB2	2:B:850:ILE:HD12	1.68	0.74
2:D:559:PHE:HB2	2:D:584:ILE:HD11	1.71	0.73
1:A:457:LYS:HD2	1:A:460:TRP:HD1	1.53	0.73
2:D:329:PHE:HB2	2:D:528:LYS:HG3	1.70	0.73
1:A:54:ILE:HG21	1:A:340:LYS:HE3	1.69	0.73
2:B:735:SER:HB3	2:B:861:LEU:HD11	1.70	0.73
2:B:726:ILE:HG12	2:B:1061:VAL:HG22	1.70	0.72
2:D:65:PHE:HB2	2:D:265:TYR:HB2	1.71	0.72
2:C:617:CYS:HA	2:C:620:VAL:HG12	1.71	0.72
2:B:646:ARG:HG3	2:C:833:PHE:HB2	1.72	0.72
2:B:1013:ILE:HG21	2:C:1012:LEU:HD12	1.70	0.71
2:D:311:GLY:HA2	2:D:664:ILE:HD12	1.73	0.70
1:A:53:ASN:O	1:A:58:ASN:ND2	2.23	0.70
2:D:339:HIS:O	2:D:343:ASN:HB2	1.90	0.70
2:D:131:CYS:SG	2:D:132:GLU:N	2.63	0.70
2:D:200:TYR:HA	2:D:230:PRO:HA	1.74	0.70
2:B:108:THR:HG22	2:B:109:THR:HG23	1.74	0.70
2:B:575:ALA:HB1	2:B:584:ILE:HD11	1.74	0.70
2:D:454:ARG:NH1	2:D:467:ASP:O	2.23	0.70
2:C:903:ALA:HB1	2:C:913:GLN:HB3	1.72	0.69
2:C:858:LEU:HD11	2:C:962:LEU:HD13	1.74	0.69
2:C:65:PHE:HB2	2:C:265:TYR:HB3	1.75	0.69
2:B:569:ILE:HD12	2:B:569:ILE:H	1.57	0.69
2:D:557:LYS:HB2	2:D:584:ILE:HG21	1.74	0.69
2:B:777:ASN:HD21	2:B:1019:ARG:HA	1.58	0.68
2:C:556:ASN:HB2	2:D:844:ILE:HG23	1.75	0.68
2:B:617:CYS:HA	2:B:620:VAL:HG12	1.76	0.68
2:B:501:TYR:O	2:B:506:GLN:NE2	2.26	0.68
2:D:659:SER:HB3	2:D:698:SER:HB3	1.75	0.68
2:B:65:PHE:HB2	2:B:265:TYR:HB3	1.74	0.68
2:C:659:SER:HB3	2:C:698:SER:HB2	1.76	0.68
2:D:503:VAL:O	2:D:508:TYR:OH	2.11	0.67
2:B:560:LEU:O	2:B:577:ARG:NH2	2.27	0.67
2:C:627:ASP:HA	2:C:634:ARG:HH22	1.58	0.67
2:D:802:PHE:HB3	2:D:806:LEU:HD13	1.77	0.67
2:D:742:ILE:HG22	2:D:997:ILE:HD12	1.75	0.66
2:B:724:THR:HB	2:B:934:ILE:HD11	1.78	0.66
2:B:900:MET:SD	2:D:1077:THR:OG1	2.52	0.66
2:C:34:ARG:NH1	2:C:191:GLU:OE2	2.27	0.66
2:C:522:ALA:H	2:C:544:ASN:HD21	1.42	0.66
2:C:360:ASN:H	2:C:523:THR:HB	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:VAL:HG12	2:B:512:VAL:HG13	1.76	0.65
2:B:844:ILE:HG23	2:D:556:ASN:HB3	1.78	0.65
2:B:1041:ASP:HB3	2:C:1030:SER:HB3	1.78	0.65
2:C:624:ILE:HA	2:C:634:ARG:HH21	1.61	0.65
2:C:351:TYR:HE2	2:C:452:TRP:HB2	1.62	0.65
2:D:560:LEU:HD22	2:D:562:PHE:HD1	1.59	0.65
2:B:485:GLY:H	2:B:488:CYS:HB2	1.60	0.65
2:C:296:LEU:O	2:C:300:LYS:HG3	1.97	0.65
2:C:34:ARG:NH2	2:C:219:GLY:O	2.30	0.65
2:D:310:LYS:HG3	2:D:600:PRO:HA	1.79	0.64
1:A:325:GLY:O	1:A:329:ASN:ND2	2.30	0.64
2:B:912:THR:OG1	2:B:914:ASN:OD1	2.15	0.64
2:D:365:TYR:HA	2:D:368:LEU:HD23	1.79	0.64
2:B:131:CYS:SG	2:B:132:GLU:N	2.71	0.64
1:A:424:ALA:HB3	1:A:427:PHE:HE1	1.62	0.64
2:D:105:ILE:HG23	2:D:241:LEU:HD11	1.79	0.64
2:D:804:GLN:NE2	2:D:935:GLN:OE1	2.31	0.64
2:B:802:PHE:HB3	2:B:806:LEU:HD23	1.79	0.64
2:D:644:GLN:HA	2:D:649:CYS:HB2	1.79	0.64
2:D:720:ILE:HD12	2:D:923:ILE:HD11	1.79	0.64
1:A:479:MET:O	1:A:483:ILE:HG22	1.98	0.63
2:B:1077:THR:OG1	2:C:900:MET:SD	2.57	0.63
2:C:328:ARG:NE	2:C:580:GLN:OE1	2.30	0.63
2:B:354:ASN:HA	6:B:1310:NAG:H83	1.81	0.63
2:C:985:ASP:OD1	2:C:986:PRO:HD2	1.99	0.63
2:D:442:ASP:OD1	2:D:509:ARG:NH2	2.31	0.63
2:B:778:THR:HG22	2:B:865:LEU:HD12	1.81	0.63
2:C:646:ARG:HB2	2:C:668:ALA:HB1	1.80	0.63
2:B:290:ASP:OD1	2:B:291:CYS:N	2.32	0.63
2:C:411:ALA:HB3	2:C:414:GLN:HG3	1.81	0.63
2:C:1076:THR:HB	2:C:1097:SER:HB3	1.80	0.63
2:C:667:GLY:HA2	2:D:864:LEU:HA	1.80	0.62
2:D:447:GLY:HA2	2:D:499:PRO:HD2	1.81	0.62
1:A:331:MET:H	1:A:358:LYS:HE3	1.64	0.62
2:B:353:TRP:HE1	2:B:466:ARG:HB2	1.65	0.62
1:A:489:PRO:HA	1:A:611:PRO:HG2	1.82	0.62
2:B:1075:PHE:O	2:B:1076:THR:OG1	2.18	0.62
2:C:454:ARG:HG2	2:C:492:LEU:HB3	1.82	0.62
2:D:443:SER:HB2	2:D:499:PRO:HA	1.82	0.62
2:C:34:ARG:NH2	2:C:217:PRO:O	2.33	0.62
2:C:802:PHE:HB3	2:C:806:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:858:LEU:HD11	2:B:962:LEU:HD23	1.83	0.61
2:D:927:PHE:HZ	2:D:1052:PHE:HE2	1.48	0.61
2:D:290:ASP:OD1	2:D:291:CYS:N	2.33	0.61
2:C:176:LEU:HD22	2:C:190:ARG:HD2	1.83	0.61
2:C:454:ARG:NH1	2:C:467:ASP:O	2.28	0.61
2:D:736:VAL:HG11	2:D:1004:LEU:HD11	1.81	0.61
1:A:95:ARG:HH22	1:A:564:PRO:HG3	1.65	0.61
2:B:833:PHE:HB2	2:D:646:ARG:HG2	1.82	0.61
2:D:462:LYS:HB2	2:D:465:GLU:HG3	1.81	0.61
2:D:627:ASP:HA	2:D:634:ARG:HH22	1.65	0.61
2:D:1075:PHE:O	2:D:1076:THR:OG1	2.19	0.61
2:B:85:PRO:HA	2:B:237:ARG:HE	1.66	0.61
1:A:451:PHE:HE2	1:A:502:LEU:HD21	1.66	0.61
2:D:129:LYS:HG3	2:D:133:PHE:HZ	1.66	0.61
2:C:48:LEU:HD13	2:C:305:SER:HA	1.83	0.61
2:D:624:ILE:HA	2:D:634:ARG:HH21	1.66	0.60
2:C:229:LEU:HD12	2:C:230:PRO:HD2	1.82	0.60
2:C:731:MET:SD	2:C:955:ASN:ND2	2.73	0.60
2:C:742:ILE:O	2:C:1000:ARG:NH1	2.33	0.60
2:B:330:PRO:O	2:B:331:ASN:C	2.40	0.60
1:A:287:LYS:HG3	1:A:432:GLU:HB2	1.84	0.60
2:D:439:ASN:O	2:D:443:SER:OG	2.19	0.60
2:B:312:ILE:HB	2:B:598:ILE:HG22	1.84	0.60
1:A:240:HIS:HB3	1:A:244:ARG:HH21	1.67	0.60
1:A:287:LYS:HZ3	1:A:430:ASP:HB3	1.67	0.60
2:B:400:PHE:HB2	2:B:510:VAL:HG13	1.83	0.60
2:C:450:ASP:OD1	2:C:450:ASP:N	2.35	0.60
2:C:804:GLN:NE2	2:C:935:GLN:OE1	2.31	0.60
2:D:599:THR:HB	2:D:608:VAL:HG12	1.83	0.60
2:D:763:LEU:HD11	2:D:1004:LEU:HG	1.82	0.60
2:C:1075:PHE:O	2:C:1076:THR:OG1	2.16	0.60
2:C:116:SER:N	2:C:131:CYS:O	2.24	0.59
2:C:780:GLU:O	2:C:784:GLN:NE2	2.35	0.59
2:B:325:SER:HB2	2:B:540:ASN:HD22	1.67	0.59
2:D:763:LEU:HG	2:D:1008:VAL:HG21	1.82	0.59
1:A:262:PRO:HD2	1:A:265:LEU:HD12	1.82	0.59
2:B:327:VAL:HG12	2:B:542:ASN:HB3	1.84	0.59
2:D:369:TYR:HA	2:D:374:PHE:HE2	1.67	0.59
1:A:242:TYR:OH	1:A:594:LEU:O	2.15	0.59
1:A:88:ILE:HD11	1:A:93:LEU:HB3	1.84	0.59
2:B:96:GLU:OE1	2:B:100:ILE:N	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ASN:ND2	2:D:240:THR:O	2.29	0.59
2:D:406:GLU:HA	2:D:409:GLN:HB3	1.85	0.59
2:D:560:LEU:HD22	2:D:562:PHE:CD1	2.37	0.59
2:B:577:ARG:HD3	2:B:582:LEU:HD13	1.84	0.59
2:B:699:LEU:HD13	2:C:872:GLN:HG2	1.84	0.59
2:C:643:PHE:HE2	2:C:670:ILE:HG13	1.68	0.59
2:C:290:ASP:OD1	2:C:291:CYS:N	2.36	0.59
2:C:590:CYS:O	2:D:837:TYR:OH	2.15	0.59
1:A:142:ALA:O	1:A:144:GLU:N	2.35	0.59
1:A:480:LYS:HB3	1:A:486:VAL:HB	1.84	0.59
2:D:984:LEU:HB3	2:D:989:ALA:HB2	1.85	0.58
2:C:987:PRO:HG2	2:D:413:GLY:HA3	1.84	0.58
2:D:96:GLU:OE1	2:D:100:ILE:N	2.34	0.58
1:A:522:PHE:HB3	1:A:582:PRO:HB2	1.85	0.58
2:B:589:PRO:HB3	2:C:855:PHE:HA	1.85	0.58
2:B:1076:THR:HB	2:B:1097:SER:HB3	1.85	0.58
2:C:39:PRO:HG2	2:C:51:THR:HG21	1.85	0.58
1:A:436:ASN:O	1:A:440:LYS:HG2	2.04	0.58
2:C:627:ASP:OD1	2:C:634:ARG:NH1	2.35	0.58
2:D:124:THR:OG1	6:D:1301:NAG:O7	2.21	0.58
2:B:117:LEU:HD13	2:B:130:VAL:HG22	1.85	0.58
2:C:321:GLN:N	2:C:628:GLN:O	2.36	0.58
2:C:296:LEU:HB3	2:C:608:VAL:HG11	1.84	0.58
1:A:552:ARG:NH2	1:A:572:ILE:O	2.37	0.58
2:C:442:ASP:OD1	2:C:509:ARG:NH2	2.34	0.57
2:D:1009:THR:O	2:D:1013:ILE:HG12	2.03	0.57
2:C:178:ASP:OD1	2:C:178:ASP:N	2.37	0.57
2:C:212:ILE:HG22	2:C:213:GLY:N	2.17	0.57
2:C:609:ALA:HB2	2:C:692:ILE:HD12	1.86	0.57
2:D:595:VAL:HG21	2:D:633:TRP:HH2	1.69	0.57
2:C:703:ASN:ND2	2:D:787:GLN:OE1	2.38	0.57
2:C:456:PHE:HB2	2:C:491:PRO:HA	1.86	0.57
1:A:141:LEU:HD22	1:A:146:GLY:HA3	1.86	0.57
2:D:381:GLY:HA3	2:D:430:THR:HG23	1.86	0.57
2:D:1002:GLN:O	2:D:1006:THR:HG23	2.05	0.57
2:B:112:SER:HB2	2:B:134:GLN:HA	1.86	0.57
2:B:502:GLY:O	2:B:504:GLY:N	2.35	0.57
2:D:454:ARG:HG2	2:D:492:LEU:HB3	1.86	0.57
2:D:856:ASN:HD22	2:D:966:LEU:HD12	1.68	0.57
1:A:242:TYR:CE2	1:A:594:LEU:HB3	2.40	0.56
1:A:598:ASN:OD1	1:A:601:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:MET:SD	2:C:177:MET:N	2.78	0.56
1:A:387:GLN:NE2	1:A:559:LEU:O	2.34	0.56
2:B:205:SER:HB3	2:B:226:LEU:HG	1.86	0.56
2:B:230:PRO:HG2	2:D:357:ARG:HD2	1.87	0.56
2:C:566:GLY:HA2	2:D:43:PHE:H	1.70	0.56
2:B:393:THR:HG21	2:B:520:ALA:HB3	1.88	0.56
2:D:363:ALA:N	2:D:525:CYS:O	2.37	0.56
2:D:450:ASP:OD1	2:D:450:ASP:N	2.36	0.56
2:D:930:ALA:HA	2:D:933:LYS:HG2	1.88	0.56
1:A:292:VAL:HA	1:A:295:LYS:HD2	1.88	0.56
2:D:185:ASN:OD1	2:D:212:ILE:HG22	2.06	0.56
2:B:320:VAL:N	2:B:591:SER:OG	2.39	0.56
2:C:406:GLU:HA	2:C:409:GLN:HB3	1.88	0.56
2:C:731:MET:HG3	2:C:774:GLN:HE22	1.70	0.56
2:C:971:GLY:O	2:C:995:ARG:NH1	2.38	0.56
1:A:246:LYS:HD3	1:A:281:THR:HA	1.87	0.56
1:A:267:GLY:O	1:A:276:ASN:ND2	2.37	0.56
2:B:856:ASN:OD1	2:B:966:LEU:HD12	2.05	0.56
2:D:126:VAL:HG22	2:D:172:SER:H	1.69	0.56
2:C:312:ILE:HG13	2:C:598:ILE:HG12	1.88	0.56
2:C:389:ASP:OD1	2:C:389:ASP:N	2.38	0.56
1:A:350:LEU:HB2	1:A:354:ASP:O	2.06	0.55
2:C:337:PRO:HD2	2:C:358:ILE:HG23	1.87	0.55
2:C:599:THR:HB	2:C:608:VAL:HG12	1.87	0.55
1:A:301:TRP:HE1	1:A:306:ILE:HG13	1.71	0.55
1:A:149:ASP:OD1	1:A:150:ILE:N	2.39	0.55
2:B:307:THR:HA	2:B:602:THR:HG21	1.87	0.55
2:D:120:VAL:HG13	2:D:127:PHE:HB3	1.88	0.55
2:D:945:LEU:HD12	2:D:948:LEU:HD12	1.88	0.55
2:B:826:VAL:HB	2:B:1057:PRO:HG2	1.88	0.55
2:D:912:THR:OG1	2:D:914:ASN:OD1	2.17	0.55
2:D:976:VAL:HG12	2:D:979:ASP:H	1.72	0.55
1:A:438:LEU:HD21	1:A:590:LEU:HB2	1.88	0.55
2:B:1098:ASN:OD1	2:B:1101:HIS:N	2.39	0.55
2:D:326:ILE:HG13	2:D:539:VAL:HG11	1.89	0.55
2:B:334:ASN:OD1	2:B:334:ASN:C	2.45	0.55
2:B:599:THR:HB	2:B:608:VAL:HG12	1.87	0.55
2:D:580:GLN:OE1	6:D:1310:NAG:O3	2.25	0.55
2:D:598:ILE:HD12	2:D:650:LEU:HD21	1.89	0.55
2:D:328:ARG:NH1	2:D:544:ASN:OD1	2.39	0.55
1:A:217:SER:OG	1:A:218:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:718:PHE:HE2	2:D:923:ILE:HD13	1.71	0.55
2:C:386:LYS:NZ	2:D:985:ASP:OD1	2.40	0.55
2:C:403:LYS:HE2	2:C:495:TYR:HE1	1.72	0.55
2:C:454:ARG:HH22	2:C:467:ASP:HB3	1.71	0.55
2:B:855:PHE:HB2	2:D:589:PRO:HG3	1.89	0.54
2:B:909:ILE:HD13	2:B:1049:LEU:HD21	1.89	0.54
2:C:589:PRO:HG3	2:D:855:PHE:HA	1.89	0.54
2:B:348:ALA:HB3	2:B:354:ASN:HB2	1.88	0.54
2:C:133:PHE:HA	2:C:162:SER:HB2	1.89	0.54
2:C:577:ARG:HA	2:C:584:ILE:HA	1.87	0.54
1:A:470:GLN:HA	1:A:494:GLU:HG2	1.90	0.54
2:B:1075:PHE:HB3	2:B:1097:SER:O	2.07	0.54
2:B:421:TYR:HA	2:B:457:ARG:HH21	1.73	0.54
2:B:667:GLY:HA2	2:C:864:LEU:HA	1.89	0.54
2:C:278:LYS:HG2	2:C:287:ASP:H	1.72	0.54
1:A:387:GLN:NE2	1:A:562:SER:OG	2.41	0.54
2:B:132:GLU:N	2:B:166:CYS:SG	2.67	0.54
2:D:645:THR:HG23	2:D:647:ALA:H	1.71	0.54
1:A:175:LEU:O	1:A:175:LEU:HD23	2.07	0.54
2:C:927:PHE:HZ	2:C:1052:PHE:HE2	1.54	0.54
2:C:93:ALA:HB3	2:C:266:TYR:HB2	1.90	0.54
2:D:48:LEU:HD13	2:D:305:SER:HA	1.90	0.54
2:D:816:SER:H	2:D:819:GLU:HG3	1.72	0.54
1:A:472:TRP:N	1:A:494:GLU:OE1	2.41	0.54
1:A:476:TRP:CE3	1:A:499:PRO:HG2	2.43	0.54
2:C:40:ASP:N	2:C:40:ASP:OD1	2.40	0.54
2:C:707:TYR:HD2	2:D:792:PRO:HG3	1.72	0.54
2:D:307:THR:HA	2:D:602:THR:HG21	1.89	0.54
2:D:406:GLU:N	2:D:406:GLU:OE1	2.41	0.54
1:A:452:THR:HG23	1:A:511:PHE:HB3	1.90	0.53
1:A:117:ASN:HA	1:A:120:LEU:HD23	1.89	0.53
1:A:413:THR:OG1	1:A:542:ASP:OD1	2.21	0.53
2:B:941:THR:HG21	2:B:944:ALA:HB2	1.90	0.53
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.91	0.53
2:B:93:ALA:HB3	2:B:266:TYR:HB2	1.91	0.53
2:B:241:LEU:HD12	2:B:242:LEU:H	1.72	0.53
2:B:590:CYS:O	2:C:837:TYR:OH	2.20	0.53
2:C:342:PHE:HZ	2:C:434:ILE:HG21	1.72	0.53
2:C:388:ASN:HB3	2:C:527:PRO:HD2	1.90	0.53
1:A:326:PHE:CE1	1:A:355:PHE:HB2	2.44	0.53
2:B:454:ARG:HG2	2:B:492:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:843:ASP:O	2:C:845:ALA:N	2.41	0.53
1:A:207:GLU:OE2	1:A:218:ARG:NE	2.38	0.53
1:A:245:ALA:HA	1:A:248:MET:HG3	1.90	0.53
2:B:126:VAL:HG22	2:B:172:SER:H	1.74	0.53
2:C:551:VAL:HB	2:C:588:THR:HB	1.91	0.53
2:D:334:ASN:ND2	2:D:360:ASN:O	2.40	0.53
2:B:411:ALA:HB3	2:B:414:GLN:HG3	1.91	0.53
2:C:320:VAL:N	2:C:591:SER:OG	2.41	0.53
1:A:326:PHE:HE1	1:A:355:PHE:HB2	1.74	0.53
2:D:906:PHE:CD2	2:D:916:LEU:HB2	2.43	0.53
1:A:48:TRP:HD1	1:A:350:LEU:HD21	1.72	0.52
1:A:356:ARG:HB2	1:A:358:LYS:HZ1	1.74	0.52
1:A:469:LYS:HD3	1:A:472:TRP:CD1	2.44	0.52
2:B:357:ARG:NH2	2:B:359:SER:OG	2.40	0.52
1:A:262:PRO:HG3	1:A:611:PRO:HG3	1.91	0.52
1:A:296:MET:HB2	1:A:301:TRP:HB2	1.91	0.52
2:B:729:VAL:HG11	2:B:781:VAL:HG11	1.91	0.52
2:D:93:ALA:HB3	2:D:266:TYR:HB2	1.91	0.52
1:A:20:THR:OG1	1:A:23:GLU:OE1	2.26	0.52
1:A:51:ASN:ND2	1:A:342:VAL:O	2.37	0.52
2:B:105:ILE:HG12	2:B:239:GLN:HB2	1.90	0.52
2:C:715:PRO:HD3	2:D:894:LEU:HD13	1.92	0.52
2:D:34:ARG:NH2	2:D:217:PRO:O	2.42	0.52
2:B:715:PRO:HD3	2:C:894:LEU:HD13	1.90	0.52
2:D:326:ILE:HD11	2:D:534:VAL:HG12	1.92	0.52
2:D:560:LEU:H	2:D:563:GLN:HG3	1.74	0.52
1:A:29:LEU:HD11	1:A:96:GLN:HB3	1.90	0.52
1:A:264:HIS:ND1	1:A:489:PRO:HG2	2.24	0.52
2:B:230:PRO:O	2:D:396:TYR:OH	2.27	0.52
2:B:971:GLY:O	2:B:995:ARG:NH1	2.42	0.52
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.45	0.52
1:A:146:GLY:O	1:A:148:ASP:N	2.43	0.52
2:B:200:TYR:HA	2:B:230:PRO:HA	1.92	0.52
2:D:557:LYS:HB2	2:D:584:ILE:HD13	1.92	0.52
1:A:117:ASN:OD1	1:A:118:THR:N	2.42	0.52
2:B:31:SER:OG	2:B:60:SER:N	2.42	0.52
2:B:574:ASP:O	2:B:587:ILE:N	2.43	0.52
2:B:1027:THR:O	2:B:1031:GLU:HG3	2.10	0.52
2:B:841:LEU:HD23	2:B:841:LEU:H	1.75	0.52
2:B:897:PRO:HG2	2:B:900:MET:HG3	1.92	0.52
2:B:350:VAL:HG11	2:B:422:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:PRO:HG2	2:D:489:TYR:CZ	2.45	0.51
2:C:117:LEU:HD22	2:C:119:ILE:HD11	1.91	0.51
2:C:118:LEU:C	2:C:119:ILE:HD13	2.30	0.51
2:D:130:VAL:HG21	2:D:231:ILE:HD12	1.92	0.51
2:D:351:TYR:HE2	2:D:468:ILE:HG13	1.75	0.51
2:D:367:VAL:O	2:D:371:PHE:HB2	2.10	0.51
1:A:77:SER:O	1:A:81:LYS:HG2	2.09	0.51
2:B:334:ASN:OD1	2:B:362:VAL:CG1	2.46	0.51
2:B:886:TRP:HB3	2:B:1035:GLY:HA2	1.93	0.51
2:D:714:ILE:HD12	2:D:1096:VAL:HG21	1.91	0.51
2:B:358:ILE:HB	2:B:395:VAL:HB	1.91	0.51
2:B:1029:MET:O	2:B:1033:VAL:HB	2.10	0.51
2:D:559:PHE:H	2:D:584:ILE:HD11	1.75	0.51
2:D:897:PRO:HG2	2:D:900:MET:SD	2.51	0.51
1:A:165:GLU:HG3	1:A:490:LEU:HD12	1.91	0.51
2:C:712:ILE:HD13	2:C:1094:VAL:HG11	1.92	0.51
2:B:112:SER:HA	2:B:132:GLU:HG2	1.91	0.51
2:C:1075:PHE:HB3	2:C:1097:SER:O	2.11	0.51
2:B:894:LEU:HD13	2:D:715:PRO:HD3	1.91	0.51
2:C:589:PRO:O	2:D:837:TYR:OH	2.29	0.51
2:D:34:ARG:NH1	2:D:191:GLU:OE2	2.41	0.51
2:D:749:CYS:SG	2:D:997:ILE:HD11	2.50	0.51
1:A:431:ASN:O	1:A:434:GLU:HG3	2.10	0.51
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.25	0.51
2:C:973:ILE:HG12	2:C:992:GLN:HE21	1.76	0.51
2:D:133:PHE:HA	2:D:162:SER:HB2	1.93	0.51
2:C:352:ALA:HB2	2:C:468:ILE:HD12	1.93	0.51
2:B:330:PRO:HA	2:B:579:PRO:HB2	1.92	0.51
2:B:629:LEU:HG	2:B:631:PRO:HD2	1.93	0.50
2:C:903:ALA:HB2	2:C:916:LEU:HD22	1.93	0.50
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	1.94	0.50
2:B:403:LYS:HD2	2:B:505:HIS:HB3	1.92	0.50
2:C:214:ARG:HG3	2:C:215:ASP:H	1.76	0.50
2:C:853:GLN:HB2	2:C:858:LEU:HB2	1.94	0.50
2:D:360:ASN:H	2:D:523:THR:HB	1.75	0.50
2:D:1076:THR:HB	2:D:1097:SER:HB3	1.93	0.50
2:B:699:LEU:HD21	2:C:869:MET:HB2	1.93	0.50
2:C:472:ILE:HA	2:C:491:PRO:HD3	1.93	0.50
1:A:585:ASN:HA	1:A:588:GLU:HG2	1.94	0.50
2:B:406:GLU:HA	2:B:409:GLN:HB3	1.93	0.50
2:C:592:PHE:CZ	2:D:740:MET:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:986:PRO:HA	2:C:989:ALA:HB3	1.94	0.50
2:B:204:TYR:HA	2:B:225:PRO:HA	1.92	0.50
2:B:600:PRO:HD3	2:B:692:ILE:HD11	1.94	0.50
2:D:118:LEU:HG	2:D:120:VAL:HG12	1.94	0.50
1:A:22:GLU:N	1:A:22:GLU:OE1	2.43	0.49
1:A:418:LYS:HG2	1:A:423:LEU:HD22	1.94	0.49
2:C:206:LYS:HB3	2:C:223:LEU:HD13	1.94	0.49
2:C:336:CYS:HB2	2:C:338:PHE:CE2	2.47	0.49
2:C:1013:ILE:HD13	2:D:1012:LEU:HB3	1.93	0.49
2:D:287:ASP:OD1	2:D:288:ALA:N	2.45	0.49
2:D:376:ALA:HB3	2:D:435:ALA:HB3	1.94	0.49
1:A:357:ILE:C	1:A:358:LYS:HZ2	2.16	0.49
2:B:459:SER:OG	2:B:460:LYS:N	2.45	0.49
2:B:916:LEU:HD12	2:B:923:ILE:HG21	1.93	0.49
2:B:985:ASP:OD2	2:D:383:SER:OG	2.20	0.49
1:A:48:TRP:CD1	1:A:350:LEU:HD21	2.47	0.49
2:C:737:ASP:OD1	2:C:738:CYS:N	2.45	0.49
2:C:188:ASN:HA	2:C:209:PRO:HA	1.94	0.49
2:C:563:GLN:HA	2:D:41:LYS:HB3	1.94	0.49
2:C:618:THR:OG1	6:C:1305:NAG:O6	2.30	0.49
2:C:909:ILE:HG12	2:C:1047:TYR:HB3	1.93	0.49
2:D:295:PRO:HG3	2:D:633:TRP:CE3	2.48	0.49
2:D:843:ASP:O	2:D:845:ALA:N	2.45	0.49
2:B:81:ASN:HD21	2:B:239:GLN:HB3	1.77	0.49
2:B:886:TRP:HZ3	2:B:905:ARG:HD3	1.78	0.49
2:B:965:GLN:O	2:B:968:SER:OG	2.30	0.49
2:C:878:LEU:O	2:C:882:ILE:HG23	2.12	0.49
2:C:457:ARG:NE	2:C:459:SER:O	2.45	0.49
2:C:736:VAL:HG11	2:C:1004:LEU:HD11	1.94	0.49
2:D:617:CYS:O	2:D:621:SER:CB	2.61	0.49
2:D:874:THR:HG21	2:D:1054:GLN:HA	1.94	0.49
1:A:444:THR:HG23	1:A:445:ILE:HG12	1.95	0.49
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.95	0.49
2:D:305:SER:OG	2:D:306:PHE:N	2.46	0.49
2:D:337:PRO:HD2	2:D:358:ILE:HG23	1.95	0.49
1:A:563:GLU:HG3	1:A:567:LEU:HD23	1.94	0.49
2:B:193:VAL:HG13	2:B:204:TYR:HD1	1.78	0.49
2:B:612:TYR:O	2:B:648:GLY:HA3	2.13	0.49
2:D:617:CYS:O	2:D:621:SER:N	2.42	0.49
2:B:299:THR:O	2:B:303:LEU:HG	2.12	0.49
2:C:44:ARG:HD3	2:C:47:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:858:LEU:HD21	2:C:962:LEU:HD22	1.95	0.49
2:C:104:TRP:CD1	2:C:240:THR:HG23	2.48	0.48
2:C:763:LEU:HD22	2:C:1008:VAL:HG21	1.94	0.48
2:D:37:TYR:OH	2:D:54:LEU:O	2.24	0.48
2:D:57:PRO:HG3	2:D:273:ARG:HD2	1.95	0.48
1:A:391:LEU:HA	1:A:561:LYS:HB2	1.95	0.48
2:B:42:VAL:CG1	2:D:567:ARG:HB2	2.44	0.48
2:B:983:ARG:HA	2:D:390:LEU:HD21	1.95	0.48
2:D:30:ASN:HD21	2:D:59:PHE:HD1	1.62	0.48
2:D:87:ASN:OD1	2:D:87:ASN:N	2.45	0.48
2:D:303:LEU:HD12	2:D:308:VAL:HG12	1.96	0.48
2:D:1029:MET:O	2:D:1033:VAL:HB	2.13	0.48
2:C:449:TYR:HA	2:C:496:GLY:HA2	1.96	0.48
2:D:795:LYS:HE3	2:D:806:LEU:HD23	1.94	0.48
1:A:168:ARG:HB3	1:A:498:ASP:OD1	2.13	0.48
1:A:229:PHE:O	1:A:233:LYS:HG2	2.13	0.48
2:C:983:ARG:HG2	2:C:984:LEU:HD12	1.95	0.48
2:B:969:LYS:NZ	2:B:973:ILE:O	2.46	0.48
2:C:102:ARG:HH21	2:C:122:ASN:HA	1.78	0.48
1:A:541:CYS:SG	1:A:542:ASP:N	2.86	0.48
2:C:457:ARG:NH1	2:C:467:ASP:OD2	2.46	0.48
1:A:458:TRP:HB3	1:A:476:TRP:CE2	2.49	0.48
2:B:326:ILE:HG23	2:B:539:VAL:HG21	1.95	0.48
2:C:200:TYR:HA	2:C:230:PRO:HA	1.96	0.48
2:C:822:LEU:HD22	2:C:945:LEU:HD11	1.95	0.48
1:A:134:ASP:N	1:A:139:GLU:OE2	2.41	0.48
2:B:376:ALA:HB3	2:B:435:ALA:HB3	1.96	0.48
2:B:574:ASP:OD2	2:C:847:ARG:N	2.35	0.48
2:B:707:TYR:HE1	2:C:897:PRO:HA	1.79	0.48
2:D:403:LYS:O	2:D:407:VAL:HG23	2.14	0.48
2:B:624:ILE:HD11	2:B:629:LEU:HD22	1.95	0.48
1:A:216:TYR:CE1	1:A:566:THR:HG21	2.49	0.48
1:A:458:TRP:HB3	1:A:476:TRP:CZ2	2.49	0.48
1:A:539:PHE:HE2	1:A:589:PRO:HG2	1.79	0.48
2:B:666:ILE:HG12	2:B:671:CYS:HA	1.94	0.48
2:B:896:ILE:HG12	2:D:712:ILE:HG13	1.95	0.48
2:D:385:THR:OG1	2:D:386:LYS:N	2.47	0.48
2:D:770:ILE:HD11	2:D:1012:LEU:HD23	1.96	0.48
2:B:822:LEU:HD22	2:B:945:LEU:HD21	1.95	0.47
2:D:194:PHE:HD1	2:D:203:ILE:HG13	1.79	0.47
2:C:858:LEU:HD12	2:C:959:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:878:LEU:O	2:D:882:ILE:HG23	2.14	0.47
1:A:144:GLU:H	1:A:145:PRO:HD2	1.78	0.47
1:A:476:TRP:HE3	1:A:499:PRO:HG2	1.79	0.47
2:B:978:ASN:HB3	2:D:547:THR:HG23	1.96	0.47
1:A:468:PRO:HD2	1:A:471:GLN:NE2	2.29	0.47
2:B:990:GLU:OE2	2:B:990:GLU:N	2.46	0.47
2:C:1040:VAL:C	2:C:1042:PHE:H	2.18	0.47
1:A:553:LEU:O	1:A:557:LEU:HG	2.14	0.47
2:C:564:GLN:OE1	2:C:577:ARG:NH1	2.47	0.47
2:D:741:TYR:HD2	2:D:1004:LEU:HD22	1.80	0.47
1:A:241:ALA:O	1:A:244:ARG:HG2	2.15	0.47
2:B:305:SER:OG	2:B:306:PHE:N	2.47	0.47
2:B:350:VAL:HG11	2:B:418:ILE:HD11	1.97	0.47
2:C:29:THR:OG1	2:C:30:ASN:N	2.48	0.47
2:B:191:GLU:O	2:B:205:SER:HA	2.14	0.47
2:B:843:ASP:O	2:B:845:ALA:N	2.46	0.47
2:D:594:GLY:O	2:D:613:GLN:N	2.38	0.47
2:D:666:ILE:HD11	2:D:672:ALA:HB2	1.97	0.47
2:D:1073:LYS:HB2	2:D:1075:PHE:CZ	2.50	0.47
2:D:1075:PHE:HB3	2:D:1097:SER:O	2.15	0.47
2:D:1098:ASN:OD1	2:D:1099:GLY:N	2.48	0.47
1:A:50:TYR:CE1	1:A:59:VAL:HA	2.50	0.47
2:B:396:TYR:HB2	2:B:514:SER:HB3	1.95	0.47
2:B:473:TYR:HD2	2:B:489:TYR:HB2	1.80	0.47
2:B:125:ASN:ND2	2:B:172:SER:O	2.46	0.47
2:B:906:PHE:CD2	2:B:916:LEU:HB2	2.50	0.47
2:C:112:SER:HA	2:C:132:GLU:HG2	1.96	0.47
2:C:295:PRO:HG3	2:C:633:TRP:CD1	2.50	0.47
2:C:472:ILE:HD13	2:C:482:GLY:O	2.14	0.47
2:C:866:THR:OG1	2:C:869:MET:HG2	2.15	0.47
1:A:303:ALA:O	1:A:306:ILE:HG22	2.15	0.46
2:B:113:LYS:HB3	2:B:113:LYS:HE2	1.71	0.46
2:D:568:ASP:OD1	2:D:568:ASP:N	2.48	0.46
2:C:231:ILE:HG22	2:C:233:ILE:HG23	1.98	0.46
2:C:906:PHE:HA	2:C:909:ILE:HG22	1.97	0.46
2:D:229:LEU:HD23	2:D:229:LEU:H	1.81	0.46
2:D:969:LYS:HE3	2:D:974:SER:HA	1.97	0.46
1:A:417:LEU:HB3	1:A:423:LEU:HB2	1.98	0.46
2:B:1039:ARG:NE	2:C:1031:GLU:OE2	2.46	0.46
2:C:290:ASP:O	2:C:297:SER:HB3	2.15	0.46
2:C:526:GLY:O	2:C:528:LYS:NZ	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1039:ARG:NE	2:D:1031:GLU:OE2	2.48	0.46
2:C:1083:HIS:HB2	2:C:1137:VAL:HG12	1.97	0.46
2:D:131:CYS:HB2	2:D:166:CYS:HB3	1.76	0.46
2:B:26:GLN:HE22	2:B:82:PRO:HG3	1.80	0.46
2:B:328:ARG:HG3	2:B:579:PRO:HG2	1.98	0.46
2:B:570:VAL:HG23	2:B:572:THR:HG23	1.97	0.46
2:B:931:ILE:O	2:B:934:ILE:HG22	2.15	0.46
2:D:441:LEU:HD22	2:D:509:ARG:HH12	1.80	0.46
1:A:263:ALA:N	1:A:487:VAL:O	2.45	0.46
2:B:294:ASP:OD2	2:B:296:LEU:HB3	2.16	0.46
2:C:829:ALA:O	2:C:850:ILE:HD11	2.15	0.46
2:C:1002:GLN:HG3	2:D:759:PHE:HZ	1.80	0.46
2:B:317:ASN:HA	2:B:594:GLY:HA2	1.98	0.46
2:B:914:ASN:ND2	2:D:1123:SER:OG	2.48	0.46
2:C:553:THR:HG21	2:D:841:LEU:HB2	1.97	0.46
2:C:878:LEU:HD11	2:C:1052:PHE:HB3	1.96	0.46
2:C:906:PHE:CD2	2:C:916:LEU:HB2	2.50	0.46
1:A:442:ALA:O	1:A:446:VAL:HG22	2.15	0.46
1:A:451:PHE:HA	1:A:454:MET:HE3	1.97	0.46
1:A:456:GLU:HG3	1:A:460:TRP:NE1	2.30	0.46
2:B:1098:ASN:OD1	2:B:1099:GLY:N	2.49	0.46
2:C:502:GLY:O	2:C:506:GLN:HG2	2.15	0.46
2:D:389:ASP:OD1	2:D:389:ASP:N	2.45	0.46
2:D:650:LEU:HD23	2:D:650:LEU:HA	1.83	0.46
1:A:33:ASN:O	1:A:37:GLU:HG2	2.16	0.46
2:B:178:ASP:OD1	2:B:178:ASP:N	2.49	0.46
2:B:225:PRO:HG2	2:D:562:PHE:CE2	2.51	0.46
2:D:303:LEU:H	2:D:303:LEU:HG	1.54	0.46
2:B:322:PRO:HB3	2:B:539:VAL:HA	1.97	0.46
2:B:847:ARG:NH2	2:D:587:ILE:O	2.47	0.46
2:C:119:ILE:HD12	2:C:128:ILE:HG23	1.98	0.46
2:B:556:ASN:H	2:C:844:ILE:HG23	1.81	0.46
2:C:743:CYS:HB3	2:C:749:CYS:HB3	1.82	0.46
2:D:444:LYS:HG2	2:D:448:ASN:HB2	1.97	0.46
2:D:848:ASP:OD1	2:D:848:ASP:N	2.48	0.46
2:B:328:ARG:HD3	2:B:530:SER:HB3	1.97	0.45
2:D:328:ARG:NH1	2:D:579:PRO:HG2	2.31	0.45
1:A:193:ASN:HB3	1:A:201:TYR:HE2	1.81	0.45
2:B:457:ARG:CZ	2:B:461:LEU:HG	2.47	0.45
2:B:1129:VAL:HG13	2:C:917:TYR:HB3	1.97	0.45
2:C:334:ASN:OD1	2:C:334:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:PRO:O	2:D:341:VAL:HG23	2.16	0.45
2:D:448:ASN:H	2:D:498:ARG:HG2	1.80	0.45
2:B:132:GLU:OE1	2:B:165:ASN:ND2	2.43	0.45
2:B:792:PRO:HG3	2:D:707:TYR:HD2	1.82	0.45
2:B:878:LEU:O	2:B:882:ILE:HG23	2.16	0.45
2:B:1098:ASN:CG	2:B:1101:HIS:H	2.18	0.45
2:D:1083:HIS:HB2	2:D:1137:VAL:HG12	1.98	0.45
1:A:456:GLU:HG2	1:A:512:ILE:HG13	1.98	0.45
2:B:384:PRO:HG2	2:D:489:TYR:CE2	2.51	0.45
2:B:568:ASP:OD1	2:B:572:THR:OG1	2.24	0.45
2:B:878:LEU:HA	2:B:881:THR:HG22	1.99	0.45
2:C:96:GLU:OE1	2:C:100:ILE:N	2.40	0.45
2:C:307:THR:HA	2:C:602:THR:HG21	1.99	0.45
2:D:57:PRO:HB2	2:D:60:SER:HB3	1.98	0.45
1:A:314:PHE:HD1	1:A:319:LEU:HD12	1.82	0.45
2:C:850:ILE:O	2:C:853:GLN:HG2	2.17	0.45
2:D:778:THR:HG22	2:D:865:LEU:HD12	1.98	0.45
1:A:343:CYS:HB2	1:A:360:CYS:N	2.32	0.45
2:C:87:ASN:O	2:C:87:ASN:ND2	2.48	0.45
2:C:358:ILE:HB	2:C:395:VAL:HB	1.99	0.45
2:C:853:GLN:HB2	2:C:858:LEU:CB	2.46	0.45
2:D:178:ASP:OD1	2:D:178:ASP:N	2.50	0.45
2:D:617:CYS:O	2:D:621:SER:HB2	2.17	0.45
2:B:560:LEU:HD12	2:B:562:PHE:HE1	1.81	0.45
2:C:770:ILE:HD11	2:C:1012:LEU:HD13	1.98	0.45
2:B:206:LYS:HD2	2:B:222:ALA:O	2.17	0.45
2:C:310:LYS:HG3	2:C:600:PRO:HA	1.99	0.45
2:C:402:ILE:HB	2:C:406:GLU:HB3	1.99	0.45
1:A:518:THR:O	1:A:521:GLN:HG3	2.16	0.45
2:C:436:TRP:HZ3	2:C:511:VAL:HG22	1.81	0.45
2:C:570:VAL:O	2:C:572:THR:HG23	2.17	0.45
2:C:629:LEU:HD23	2:C:631:PRO:HG2	1.98	0.45
2:C:699:LEU:HB3	2:D:873:TYR:CZ	2.52	0.45
2:D:105:ILE:HG22	2:D:118:LEU:HD13	1.99	0.45
2:D:294:ASP:OD1	2:D:295:PRO:HD2	2.16	0.45
2:D:398:ASP:OD2	2:D:423:TYR:OH	2.32	0.45
2:B:1072:GLU:N	2:B:1072:GLU:OE1	2.50	0.45
2:C:101:ILE:HG23	2:C:241:LEU:O	2.17	0.45
2:D:173:GLN:HG2	2:D:174:PRO:HD2	1.99	0.45
2:D:577:ARG:HA	2:D:584:ILE:HA	1.99	0.45
2:D:941:THR:HG21	2:D:944:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:TYR:O	1:A:183:VAL:HG23	2.18	0.44
1:A:502:LEU:O	1:A:506:ALA:HB2	2.17	0.44
2:B:42:VAL:HG11	2:D:567:ARG:HE	1.82	0.44
2:D:318:PHE:HD2	2:D:629:LEU:HD11	1.82	0.44
1:A:292:VAL:HG12	1:A:295:LYS:HD2	2.00	0.44
2:B:37:TYR:HA	2:B:223:LEU:HB3	2.00	0.44
2:C:365:TYR:CZ	2:C:387:LEU:HG	2.53	0.44
2:C:770:ILE:O	2:C:774:GLN:HG3	2.17	0.44
2:D:109:THR:OG1	2:D:111:ASP:OD1	2.36	0.44
1:A:244:ARG:HH12	1:A:260:CYS:HA	1.82	0.44
1:A:270:TRP:CD2	1:A:502:LEU:HG	2.52	0.44
1:A:326:PHE:O	1:A:330:SER:OG	2.18	0.44
2:B:336:CYS:SG	2:B:337:PRO:HD2	2.57	0.44
2:B:954:HIS:HB3	2:B:1014:ARG:NH1	2.32	0.44
2:D:321:GLN:N	2:D:628:GLN:O	2.35	0.44
2:D:534:VAL:HG13	2:D:539:VAL:HG21	1.99	0.44
2:D:788:ILE:HG23	2:D:876:ALA:HB2	2.00	0.44
2:D:903:ALA:HB1	2:D:913:GLN:HB3	1.97	0.44
2:B:567:ARG:HD2	2:C:42:VAL:HG11	2.00	0.44
2:B:802:PHE:CD1	2:B:805:ILE:HD11	2.53	0.44
2:D:731:MET:HE1	2:D:1015:ALA:HA	2.00	0.44
1:A:81:LYS:NZ	1:A:103:SER:HB3	2.32	0.44
2:B:342:PHE:CE1	2:B:511:VAL:HG11	2.52	0.44
2:B:445:HIS:O	2:B:446:SER:OG	2.30	0.44
2:C:190:ARG:HD3	2:C:207:HIS:CE1	2.52	0.44
2:C:403:LYS:O	2:C:407:VAL:HG23	2.17	0.44
2:D:497:PHE:CE1	2:D:507:PRO:HA	2.52	0.44
2:C:108:THR:O	2:C:109:THR:OG1	2.36	0.44
2:C:437:ASN:HD21	2:C:506:GLN:HB3	1.82	0.44
2:C:1075:PHE:HB2	2:C:1096:VAL:HG22	2.00	0.44
2:C:1106:GLN:HB2	2:C:1109:PHE:O	2.17	0.44
2:D:209:PRO:C	2:D:210:ILE:HG13	2.38	0.44
2:D:229:LEU:HD12	2:D:231:ILE:HD11	2.00	0.44
2:D:962:LEU:HD12	2:D:1007:TYR:CG	2.52	0.44
1:A:295:LYS:O	1:A:298:ASN:HB2	2.18	0.44
2:B:555:SER:HB3	2:B:584:ILE:HG23	1.99	0.44
2:D:131:CYS:HB3	2:D:133:PHE:CE1	2.52	0.44
2:D:328:ARG:HH21	2:D:580:GLN:CD	2.21	0.44
2:D:365:TYR:CE2	2:D:387:LEU:HG	2.53	0.44
1:A:164:TRP:NE1	1:A:269:MET:O	2.50	0.44
2:B:319:ARG:HE	2:C:740:MET:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:850:ILE:O	2:C:854:LYS:HG2	2.18	0.44
2:C:854:LYS:HA	2:C:854:LYS:HD2	1.83	0.44
2:D:44:ARG:HB3	2:D:47:VAL:HG11	1.99	0.44
2:D:821:LEU:HD11	2:D:935:GLN:HG3	2.00	0.44
2:D:822:LEU:HD22	2:D:945:LEU:HD11	1.99	0.44
2:C:365:TYR:CE1	2:C:387:LEU:HG	2.52	0.44
2:D:567:ARG:HD3	2:D:571:ASP:HA	2.00	0.44
2:D:985:ASP:HB3	2:D:987:PRO:HD2	1.99	0.44
2:D:1049:LEU:HD11	2:D:1067:TYR:HB2	2.00	0.44
2:C:342:PHE:HE2	2:C:372:ALA:HB2	1.83	0.43
2:D:969:LYS:HE2	2:D:969:LYS:HB3	1.74	0.43
2:B:30:ASN:HB3	2:B:32:PHE:CE1	2.52	0.43
2:B:296:LEU:HB2	2:B:608:VAL:HG11	2.00	0.43
2:B:533:LEU:HD23	2:B:535:LYS:HE3	1.99	0.43
2:B:902:MET:HE1	2:B:1049:LEU:HD13	1.99	0.43
2:D:402:ILE:HD11	2:D:510:VAL:HG21	2.00	0.43
2:B:643:PHE:O	2:B:649:CYS:HA	2.18	0.43
2:B:763:LEU:HD11	2:B:1004:LEU:HG	2.00	0.43
2:C:574:ASP:O	2:C:587:ILE:N	2.48	0.43
2:C:642:VAL:HG22	2:C:651:ILE:HD13	2.00	0.43
2:D:537:LYS:HE2	2:D:537:LYS:HB2	1.75	0.43
2:B:190:ARG:HD3	2:B:207:HIS:CE1	2.52	0.43
2:B:290:ASP:O	2:B:297:SER:HB3	2.18	0.43
2:B:631:PRO:O	2:B:634:ARG:NH2	2.51	0.43
2:C:24:THR:HG21	2:C:82:PRO:HG3	2.00	0.43
2:C:870:ILE:HG22	2:C:1055:SER:HB2	1.99	0.43
2:B:300:LYS:HG2	2:B:305:SER:O	2.19	0.43
2:C:611:LEU:HD22	2:C:666:ILE:HG23	2.01	0.43
2:D:95:THR:HB	2:D:189:LEU:HG	2.00	0.43
2:D:975:SER:O	2:D:975:SER:OG	2.30	0.43
1:A:446:VAL:HA	1:A:449:LEU:HD23	1.99	0.43
2:B:276:LEU:HB3	2:B:289:VAL:HG23	2.00	0.43
2:B:318:PHE:HD2	2:B:629:LEU:HD11	1.84	0.43
2:C:33:THR:HG23	2:C:58:PHE:CZ	2.53	0.43
2:C:393:THR:OG1	2:C:394:ASN:N	2.51	0.43
2:C:1031:GLU:OE1	2:C:1039:ARG:HD3	2.19	0.43
1:A:31:LYS:HG3	2:B:489:TYR:HD2	1.83	0.43
1:A:41:TYR:HE2	1:A:352:LYS:HB2	1.84	0.43
2:C:720:ILE:HD12	2:C:923:ILE:HG23	2.01	0.43
2:D:822:LEU:HD11	2:D:1061:VAL:HG11	2.01	0.43
2:D:990:GLU:HA	2:D:993:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:CYS:HB2	1:A:487:VAL:HG23	2.01	0.43
2:C:569:ILE:HG23	2:D:47:VAL:HG23	2.00	0.43
2:B:347:PHE:HD2	2:B:399:SER:HB2	1.84	0.43
2:C:124:THR:O	2:C:174:PRO:HD3	2.19	0.43
2:D:111:ASP:HA	2:D:134:GLN:O	2.19	0.43
2:D:418:ILE:HG23	2:D:422:ASN:HB2	2.00	0.43
2:D:870:ILE:HG22	2:D:1055:SER:HB2	2.00	0.43
1:A:237:GLU:HG2	1:A:605:TRP:CH2	2.54	0.43
2:B:437:ASN:HA	2:B:508:TYR:HD1	1.84	0.43
2:C:119:ILE:HG22	2:C:119:ILE:O	2.19	0.43
2:C:348:ALA:O	2:C:400:PHE:HA	2.19	0.43
2:C:666:ILE:HB	2:C:670:ILE:O	2.19	0.43
2:C:708:SER:OG	2:C:709:ASN:N	2.52	0.43
1:A:266:LEU:HD12	1:A:274:TRP:NE1	2.34	0.42
2:B:748:GLU:HG3	2:B:981:LEU:HD11	2.01	0.42
2:C:392:PHE:HD1	2:C:524:VAL:HG13	1.84	0.42
2:C:403:LYS:HG2	2:C:505:HIS:HA	2.01	0.42
2:C:645:THR:HG23	2:C:647:ALA:H	1.84	0.42
2:C:818:ILE:HB	2:C:1054:GLN:OE1	2.20	0.42
2:D:188:ASN:N	2:D:188:ASN:OD1	2.51	0.42
2:D:767:LEU:HD23	2:D:767:LEU:HA	1.86	0.42
2:B:334:ASN:O	2:B:335:LEU:HD22	2.18	0.42
2:B:403:LYS:HB3	2:B:505:HIS:HA	2.01	0.42
2:B:616:ASN:O	2:B:619:GLU:HB2	2.19	0.42
2:C:627:ASP:HA	2:C:634:ARG:NH2	2.29	0.42
2:D:290:ASP:O	2:D:297:SER:HB3	2.19	0.42
2:D:770:ILE:O	2:D:774:GLN:HG2	2.18	0.42
2:B:529:LYS:HD2	2:B:529:LYS:HA	1.45	0.42
2:B:918:GLU:HG2	2:D:1128:VAL:HG21	2.01	0.42
2:B:1031:GLU:OE2	2:D:1039:ARG:NE	2.32	0.42
2:C:906:PHE:HE1	2:C:1049:LEU:HD11	1.84	0.42
2:B:389:ASP:OD1	2:B:389:ASP:N	2.46	0.42
2:B:497:PHE:CE2	2:B:507:PRO:HB3	2.54	0.42
2:C:317:ASN:OD1	2:C:317:ASN:N	2.52	0.42
2:C:1098:ASN:OD1	2:C:1099:GLY:N	2.52	0.42
2:D:338:PHE:HB3	2:D:368:LEU:HD11	2.01	0.42
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.87	0.42
2:B:559:PHE:HB3	2:B:577:ARG:NH2	2.34	0.42
2:C:97:LYS:HE2	2:C:184:GLY:HA3	2.02	0.42
2:C:424:LYS:HG3	2:C:463:PRO:HA	2.01	0.42
2:C:571:ASP:HB2	2:D:967:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:GLU:HG2	2:D:418:ILE:HD12	2.02	0.42
2:D:708:SER:OG	2:D:709:ASN:N	2.52	0.42
2:B:948:LEU:HD22	2:B:1059:GLY:HA3	2.01	0.42
2:C:478:LYS:HE3	2:C:478:LYS:HB2	1.93	0.42
2:C:497:PHE:HA	2:C:501:TYR:HE2	1.85	0.42
2:D:393:THR:OG1	2:D:516:GLU:OE1	2.37	0.42
2:B:276:LEU:CD1	2:B:304:LYS:HA	2.45	0.42
2:B:295:PRO:O	2:B:299:THR:HG22	2.20	0.42
2:B:818:ILE:O	2:B:822:LEU:HG	2.20	0.42
2:B:886:TRP:CZ3	2:B:905:ARG:HD3	2.55	0.42
2:D:422:ASN:ND2	2:D:454:ARG:O	2.30	0.42
2:D:902:MET:HB3	2:D:916:LEU:HD11	2.02	0.42
1:A:205:ASP:N	1:A:205:ASP:OD1	2.52	0.42
2:B:34:ARG:NH2	2:B:219:GLY:O	2.53	0.42
2:B:315:THR:OG1	2:B:316:SER:N	2.53	0.42
2:C:102:ARG:HH12	2:C:176:LEU:HD12	1.85	0.42
2:C:110:LEU:HD11	2:C:239:GLN:HG3	2.00	0.42
2:D:726:ILE:HD13	2:D:1061:VAL:HG23	2.02	0.42
2:B:877:LEU:HA	2:B:877:LEU:HD23	1.85	0.42
2:B:905:ARG:O	2:B:909:ILE:HG23	2.20	0.42
2:C:669:GLY:HA2	2:D:869:MET:CE	2.49	0.42
2:D:188:ASN:HD21	2:D:190:ARG:HH21	1.66	0.42
1:A:373:HIS:HA	1:A:404:GLY:O	2.20	0.42
2:B:662:CYS:HB2	2:B:697:MET:SD	2.60	0.42
2:B:638:THR:HG23	2:B:640:SER:H	1.85	0.41
2:D:124:THR:O	2:D:174:PRO:HD3	2.20	0.41
2:D:300:LYS:HG2	2:D:305:SER:O	2.19	0.41
2:D:574:ASP:O	2:D:587:ILE:N	2.49	0.41
1:A:28:PHE:CE2	1:A:80:ALA:HB2	2.55	0.41
1:A:167:TRP:CH2	1:A:501:CYS:HB3	2.55	0.41
1:A:352:LYS:HG2	2:B:505:HIS:CG	2.55	0.41
1:A:502:LEU:O	1:A:506:ALA:CB	2.68	0.41
2:B:398:ASP:HB3	2:B:400:PHE:HE1	1.85	0.41
2:B:837:TYR:OH	2:D:589:PRO:O	2.33	0.41
2:B:854:LYS:HA	2:B:854:LYS:HD2	1.88	0.41
2:C:109:THR:OG1	2:C:111:ASP:OD1	2.27	0.41
2:C:442:ASP:HB3	2:C:451:TYR:HE2	1.85	0.41
2:D:641:ASN:OD1	2:D:641:ASN:N	2.53	0.41
2:D:823:PHE:CD1	2:D:1057:PRO:HG3	2.56	0.41
1:A:401:GLU:HB3	1:A:517:ARG:HD2	2.03	0.41
2:B:104:TRP:HB2	2:B:119:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:ASN:HA	2:B:209:PRO:HA	2.02	0.41
2:B:350:VAL:HG23	2:B:400:PHE:CE2	2.55	0.41
2:B:708:SER:OG	2:B:709:ASN:N	2.52	0.41
2:C:396:TYR:OH	2:D:230:PRO:HB2	2.20	0.41
2:D:947:LYS:HE2	2:D:947:LYS:HB3	1.79	0.41
1:A:151:MET:HB2	1:A:164:TRP:CH2	2.55	0.41
1:A:228:THR:O	1:A:232:ILE:HB	2.20	0.41
2:B:57:PRO:HB2	2:B:60:SER:HB3	2.03	0.41
2:C:129:LYS:HE3	2:C:169:GLU:OE2	2.20	0.41
2:C:403:LYS:HE2	2:C:495:TYR:CE1	2.55	0.41
2:D:570:VAL:HG23	2:D:570:VAL:O	2.19	0.41
2:D:1097:SER:HB2	2:D:1102:TRP:CE3	2.55	0.41
2:D:1097:SER:HB2	2:D:1102:TRP:CD2	2.55	0.41
2:D:1115:ILE:HG22	2:D:1137:VAL:HG23	2.02	0.41
1:A:317:ILE:HD12	1:A:317:ILE:HA	1.81	0.41
2:B:231:ILE:HG22	2:B:233:ILE:HG23	2.02	0.41
2:B:470:THR:O	2:B:470:THR:OG1	2.37	0.41
2:B:475:ALA:HB3	2:B:489:TYR:HE1	1.85	0.41
2:C:106:PHE:HB2	2:C:117:LEU:HB2	2.01	0.41
2:C:203:ILE:HG22	2:C:227:VAL:O	2.20	0.41
2:D:108:THR:HG22	2:D:236:THR:HB	2.02	0.41
2:D:856:ASN:OD1	2:D:856:ASN:N	2.51	0.41
1:A:41:TYR:HD2	2:B:501:TYR:HH	1.67	0.41
1:A:260:CYS:HB2	1:A:487:VAL:CG2	2.50	0.41
2:B:119:ILE:HG23	2:B:128:ILE:HD12	2.02	0.41
2:B:398:ASP:O	2:B:511:VAL:HA	2.20	0.41
2:B:588:THR:HG22	2:B:589:PRO:HD2	2.02	0.41
2:C:136:CYS:HB2	2:C:159:VAL:O	2.20	0.41
2:C:1040:VAL:O	2:C:1042:PHE:N	2.52	0.41
2:C:1115:ILE:HG22	2:C:1137:VAL:HG23	2.03	0.41
2:D:836:GLN:NE2	2:D:850:ILE:HB	2.35	0.41
1:A:233:LYS:O	1:A:237:GLU:HG3	2.20	0.41
1:A:593:TRP:O	1:A:596:GLU:HG3	2.20	0.41
2:C:337:PRO:O	2:C:341:VAL:HG23	2.20	0.41
2:C:529:LYS:HD2	2:C:529:LYS:HA	1.80	0.41
2:C:914:ASN:HD21	2:C:1111:GLU:CD	2.24	0.41
2:C:1047:TYR:O	2:C:1067:TYR:N	2.47	0.41
2:D:101:ILE:O	2:D:102:ARG:NH1	2.49	0.41
2:D:131:CYS:HB3	2:D:133:PHE:CZ	2.56	0.41
2:D:386:LYS:O	2:D:390:LEU:HD11	2.21	0.41
2:D:436:TRP:NE1	2:D:438:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:O	1:A:119:ILE:HG13	2.21	0.41
2:B:202:LYS:HA	2:B:202:LYS:HD2	1.68	0.41
2:B:323:THR:OG1	2:B:324:GLU:N	2.54	0.41
2:C:57:PRO:HG3	2:C:273:ARG:HD2	2.03	0.41
2:C:853:GLN:HA	2:C:856:ASN:OD1	2.20	0.41
2:D:121:ASN:N	2:D:121:ASN:ND2	2.68	0.41
1:A:224:ASP:O	1:A:228:THR:HG23	2.21	0.41
1:A:377:HIS:O	1:A:400:HIS:NE2	2.41	0.41
2:B:193:VAL:HG13	2:B:204:TYR:CD1	2.54	0.41
2:B:309:GLU:O	2:B:313:TYR:OH	2.25	0.41
2:B:906:PHE:HE1	2:B:1067:TYR:CD2	2.39	0.41
2:C:99:ASN:ND2	2:C:101:ILE:O	2.48	0.41
2:C:121:ASN:OD1	2:C:121:ASN:N	2.53	0.41
2:C:415:THR:HG23	2:D:385:THR:HA	2.03	0.41
2:C:560:LEU:H	2:C:563:GLN:HG3	1.86	0.41
2:C:669:GLY:O	2:C:670:ILE:HD13	2.20	0.41
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.41	0.41
2:D:38:TYR:CE2	2:D:224:GLU:HG3	2.56	0.41
2:D:47:VAL:HG12	2:D:279:TYR:HB2	2.02	0.41
2:D:675:GLN:HG3	2:D:693:ILE:HD11	2.02	0.41
2:D:741:TYR:CD2	2:D:1004:LEU:HD22	2.56	0.41
2:B:734:THR:O	2:B:767:LEU:HD12	2.21	0.41
2:C:28:TYR:HD2	2:C:61:ASN:HB2	1.86	0.41
2:C:557:LYS:HD3	2:D:43:PHE:CD2	2.56	0.41
2:D:318:PHE:HZ	2:D:615:VAL:HG21	1.86	0.41
2:D:334:ASN:O	2:D:362:VAL:N	2.52	0.41
2:B:338:PHE:HD1	2:B:338:PHE:HA	1.78	0.40
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.95	0.40
2:B:904:TYR:CE2	2:D:1107:ARG:HG2	2.56	0.40
2:C:103:GLY:HA3	2:C:120:VAL:HA	2.02	0.40
2:C:133:PHE:HB3	2:C:160:TYR:HB2	2.02	0.40
2:B:959:LEU:O	2:B:963:VAL:HG23	2.22	0.40
2:B:997:ILE:O	2:B:1001:LEU:HB2	2.21	0.40
2:B:1040:VAL:HG13	2:C:1030:SER:O	2.22	0.40
2:C:631:PRO:HB3	2:C:633:TRP:CH2	2.55	0.40
2:C:726:ILE:HD12	2:C:1061:VAL:HG22	2.03	0.40
2:C:808:ASP:HB3	2:C:811:LYS:HD2	2.03	0.40
2:D:657:ASN:HB3	6:D:1306:NAG:O5	2.21	0.40
1:A:379:GLN:HA	1:A:382:MET:HG3	2.02	0.40
2:B:409:GLN:HE21	2:B:409:GLN:HB2	1.71	0.40
2:C:675:GLN:HB2	2:C:693:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:ASP:HB2	2:D:512:VAL:HG12	2.03	0.40
2:D:705:VAL:HG12	2:D:707:TYR:H	1.87	0.40
1:A:248:MET:CE	1:A:257:PRO:HA	2.51	0.40
1:A:369:LEU:HD13	1:A:408:SER:HB2	2.03	0.40
2:B:86:PHE:CD2	2:B:90:VAL:HG23	2.57	0.40
2:B:177:MET:H	2:B:207:HIS:CE1	2.40	0.40
2:B:766:ALA:O	2:B:770:ILE:HG12	2.21	0.40
2:B:1034:LEU:O	2:D:1040:VAL:HG21	2.22	0.40
2:C:287:ASP:OD1	2:C:288:ALA:N	2.53	0.40
2:C:1072:GLU:OE1	2:C:1072:GLU:N	2.55	0.40
2:D:209:PRO:O	2:D:210:ILE:HG13	2.21	0.40
2:D:1072:GLU:N	2:D:1072:GLU:OE1	2.55	0.40
1:A:176:ARG:O	1:A:180:GLU:HG3	2.22	0.40
1:A:284:PHE:CE1	1:A:286:HIS:HB2	2.56	0.40
1:A:347:ALA:HB1	1:A:378:ILE:HD11	2.04	0.40
1:A:522:PHE:HD1	1:A:522:PHE:HA	1.73	0.40
2:B:990:GLU:HA	2:B:993:ILE:HB	2.04	0.40
2:C:131:CYS:HB3	2:C:133:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/804 (74%)	570 (96%)	21 (4%)	3 (0%)	25	57
2	B	1053/1206 (87%)	969 (92%)	82 (8%)	2 (0%)	44	72
2	C	1053/1206 (87%)	965 (92%)	87 (8%)	1 (0%)	48	78
2	D	1053/1206 (87%)	978 (93%)	73 (7%)	2 (0%)	44	72
All	All	3753/4422 (85%)	3482 (93%)	263 (7%)	8 (0%)	45	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	ILE
2	D	210	ILE
2	D	499	PRO
1	A	147	LEU
2	B	331	ASN
1	A	143	LEU
1	A	144	GLU
2	B	534	VAL

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	525/711 (74%)	505 (96%)	20 (4%)	28	53
2	B	925/1054 (88%)	892 (96%)	33 (4%)	30	54
2	C	925/1054 (88%)	893 (96%)	32 (4%)	31	55
2	D	925/1054 (88%)	894 (97%)	31 (3%)	32	55
All	All	3300/3873 (85%)	3184 (96%)	116 (4%)	33	55

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
1	A	51	ASN
1	A	94	LYS
1	A	147	LEU
1	A	261	LEU
1	A	270	TRP
1	A	276	ASN
1	A	299	GLN
1	A	313	PHE
1	A	340	LYS
1	A	368	PHE
1	A	399	PHE
1	A	427	PHE
1	A	437	PHE

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Mol	Chain	Res	Type
1	A	458	TRP
1	A	509	TYR
1	A	515	TYR
1	A	517	ARG
1	A	522	PHE
1	A	599	ARG
2	B	121	ASN
2	B	133	PHE
2	B	134	GLN
2	B	135	PHE
2	B	168	PHE
2	B	170	TYR
2	B	179	LEU
2	B	186	PHE
2	B	201	PHE
2	B	205	SER
2	B	265	TYR
2	B	303	LEU
2	B	346	ARG
2	B	351	TYR
2	B	380	TYR
2	B	442	ASP
2	B	513	LEU
2	B	528	LYS
2	B	529	LYS
2	B	571	ASP
2	B	589	PRO
2	B	613	GLN
2	B	636	TYR
2	B	643	PHE
2	B	649	CYS
2	B	775	ASP
2	B	820	ASP
2	B	855	PHE
2	B	873	TYR
2	B	904	TYR
2	B	994	ASP
2	B	1097	SER
2	B	1108	ASN
2	C	45	SER
2	C	87	ASN
2	C	121	ASN

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Mol	Chain	Res	Type
2	C	127	PHE
2	C	177	MET
2	C	194	PHE
2	C	200	TYR
2	C	214	ARG
2	C	226	LEU
2	C	278	LYS
2	C	328	ARG
2	C	329	PHE
2	C	334	ASN
2	C	335	LEU
2	C	342	PHE
2	C	343	ASN
2	C	377	PHE
2	C	386	LYS
2	C	400	PHE
2	C	567	ARG
2	C	571	ASP
2	C	625	HIS
2	C	649	CYS
2	C	759	PHE
2	C	786	LYS
2	C	802	PHE
2	C	823	PHE
2	C	955	ASN
2	C	1040	VAL
2	C	1108	ASN
2	C	1139	ASP
2	C	1142	GLN
2	D	26	GLN
2	D	40	ASP
2	D	121	ASN
2	D	127	PHE
2	D	162	SER
2	D	173	GLN
2	D	200	TYR
2	D	212	ILE
2	D	238	PHE
2	D	264	ASP
2	D	303	LEU
2	D	328	ARG
2	D	343	ASN

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Mol	Chain	Res	Type
2	D	366	SER
2	D	377	PHE
2	D	405	ASN
2	D	478	LYS
2	D	495	TYR
2	D	515	PHE
2	D	536	ASN
2	D	562	PHE
2	D	567	ARG
2	D	617	CYS
2	D	631	PRO
2	D	646	ARG
2	D	649	CYS
2	D	760	CYS
2	D	968	SER
2	D	1041	ASP
2	D	1101	HIS
2	D	1142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
2	B	207	HIS
2	B	777	ASN
2	C	321	GLN
2	C	437	ASN
2	D	173	GLN
2	D	207	HIS

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)

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.21	0	17,19,21	0.41	0
3	BMA	E	2	3	11,11,12	0.60	0	15,15,17	0.77	0
3	NAG	F	1	3,2	14,14,15	0.21	0	17,19,21	0.41	0
3	BMA	F	2	3	11,11,12	0.60	0	15,15,17	0.77	0
3	NAG	G	1	3,2	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	G	2	3	11,11,12	0.60	0	15,15,17	0.70	0
3	NAG	H	1	3,2	14,14,15	0.22	0	17,19,21	0.42	0
3	BMA	H	2	3	11,11,12	0.61	0	15,15,17	0.75	0
3	NAG	I	1	3,2	14,14,15	0.90	1 (7%)	17,19,21	0.90	1 (5%)
3	BMA	I	2	3	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
3	NAG	J	1	3,2	14,14,15	0.25	0	17,19,21	0.39	0
3	BMA	J	2	3	11,11,12	0.62	0	15,15,17	0.82	0
3	NAG	K	1	3,2	14,14,15	0.21	0	17,19,21	0.41	0
3	BMA	K	2	3	11,11,12	0.62	0	15,15,17	0.69	0
3	NAG	L	1	3,2	14,14,15	0.22	0	17,19,21	0.43	0
3	BMA	L	2	3	11,11,12	0.62	0	15,15,17	0.74	0
3	NAG	M	1	3,2	14,14,15	0.26	0	17,19,21	0.47	0
3	BMA	M	2	3	11,11,12	0.61	0	15,15,17	0.68	0
3	NAG	N	1	3,2	14,14,15	0.22	0	17,19,21	0.46	0
3	BMA	N	2	3	11,11,12	0.59	0	15,15,17	0.71	0
3	NAG	O	1	3,2	14,14,15	0.94	1 (7%)	17,19,21	0.94	1 (5%)
3	BMA	O	2	3	11,11,12	0.55	0	15,15,17	1.10	1 (6%)
3	NAG	P	1	3,2	14,14,15	0.27	0	17,19,21	0.39	0
3	BMA	P	2	3	11,11,12	0.58	0	15,15,17	0.76	0
3	NAG	Q	1	3,2	14,14,15	0.22	0	17,19,21	0.39	0
3	BMA	Q	2	3	11,11,12	0.57	0	15,15,17	0.72	0
3	NAG	R	1	3,2	14,14,15	0.19	0	17,19,21	0.41	0
3	BMA	R	2	3	11,11,12	0.59	0	15,15,17	0.79	0
3	NAG	S	1	3,2	14,14,15	0.26	0	17,19,21	0.47	0
3	BMA	S	2	3	11,11,12	0.59	0	15,15,17	0.73	0
3	NAG	T	1	3,2	14,14,15	0.24	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	T	2	3	11,11,12	0.62	0	15,15,17	0.74	0
3	NAG	U	1	3,2	14,14,15	1.25	1 (7%)	17,19,21	1.23	1 (5%)
3	BMA	U	2	3	11,11,12	0.61	0	15,15,17	1.26	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,2	-	1/6/23/26	0/1/1/1
3	BMA	H	2	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,2	-	1/6/23/26	0/1/1/1
3	BMA	J	2	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	K	2	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	L	2	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	M	2	3	-	1/2/19/22	0/1/1/1
3	NAG	N	1	3,2	-	0/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	0/2/19/22	0/1/1/1
3	NAG	P	1	3,2	-	1/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	Q	2	3	-	0/2/19/22	0/1/1/1
3	NAG	R	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	R	2	3	-	1/2/19/22	0/1/1/1
3	NAG	S	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	S	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	1	3,2	-	0/6/23/26	0/1/1/1
3	BMA	T	2	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,2	-	2/6/23/26	0/1/1/1
3	BMA	U	2	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	-4.32	1.36	1.43
3	O	1	NAG	O5-C1	-3.29	1.38	1.43
3	I	1	NAG	O5-C1	-3.13	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C3-C4-C5	3.52	116.52	110.24
3	U	2	BMA	C1-O5-C5	2.75	115.91	112.19
3	I	2	BMA	C1-O5-C5	2.73	115.89	112.19
3	O	2	BMA	C1-O5-C5	2.52	115.61	112.19
3	O	1	NAG	C3-C4-C5	2.47	114.64	110.24
3	I	1	NAG	C3-C4-C5	2.30	114.33	110.24
3	U	2	BMA	C1-C2-C3	2.07	112.21	109.67
3	U	2	BMA	O5-C1-C2	2.03	113.91	110.77
3	I	2	BMA	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

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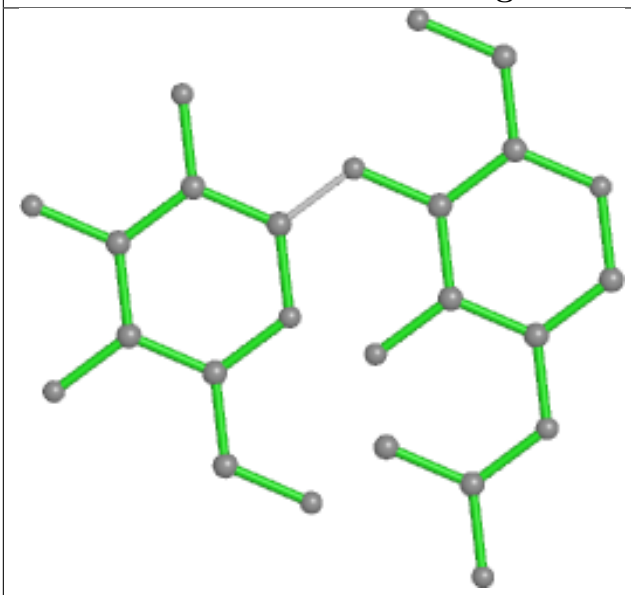
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	R	2	BMA	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	M	2	BMA	O5-C5-C6-O6

There are no ring outliers.

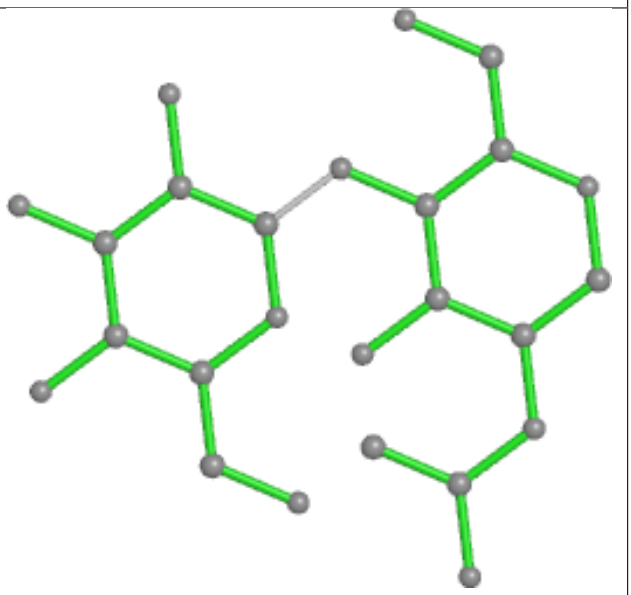
No monomer is involved in short contacts.

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

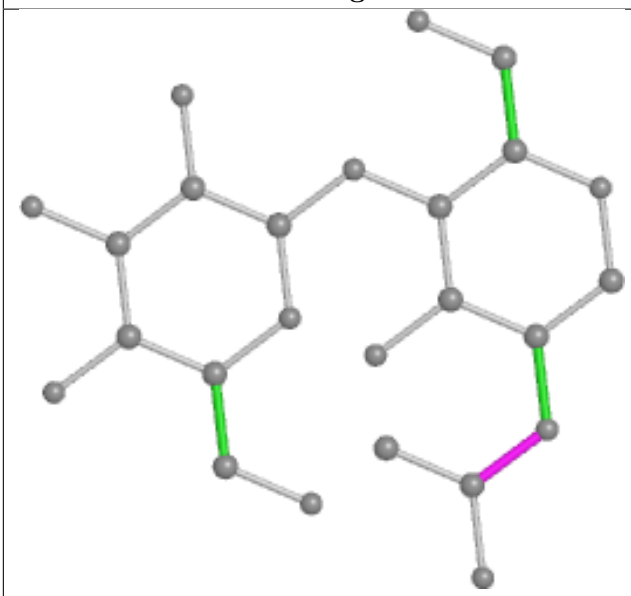
Oligosaccharide Chain E



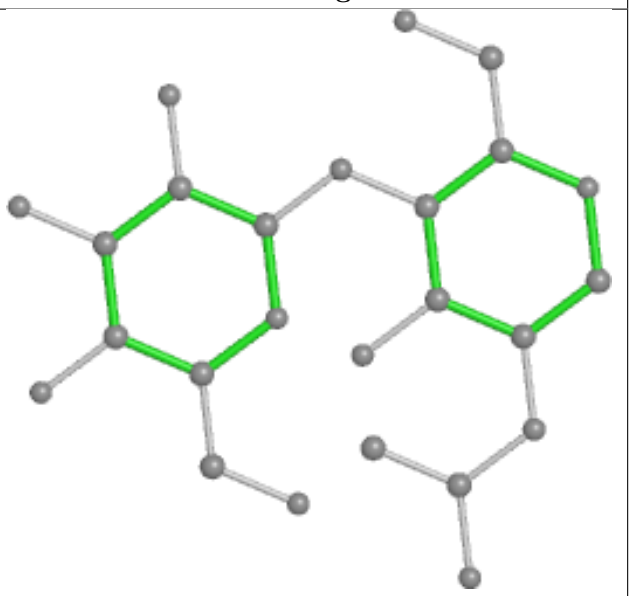
Bond lengths



Bond angles

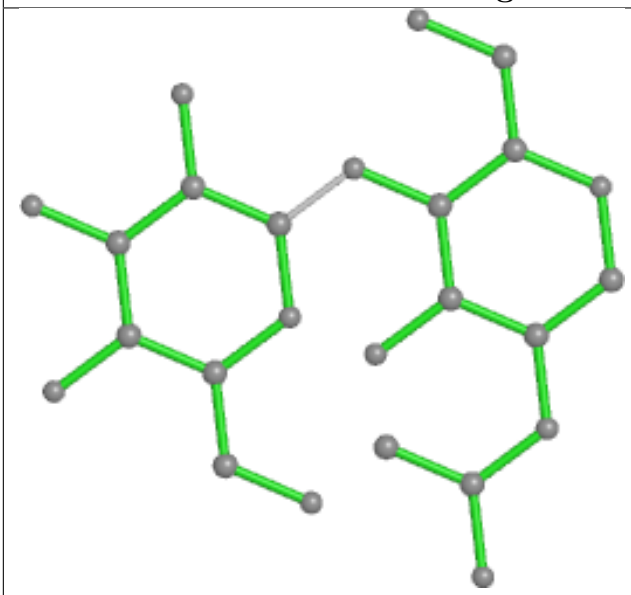


Torsions

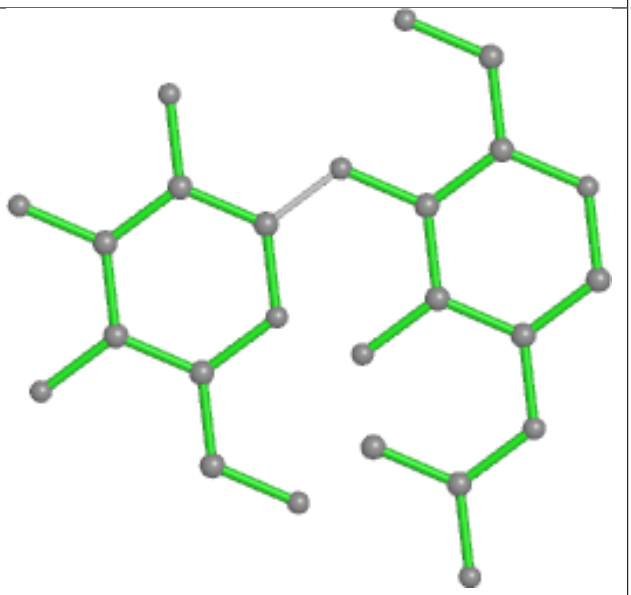


Rings

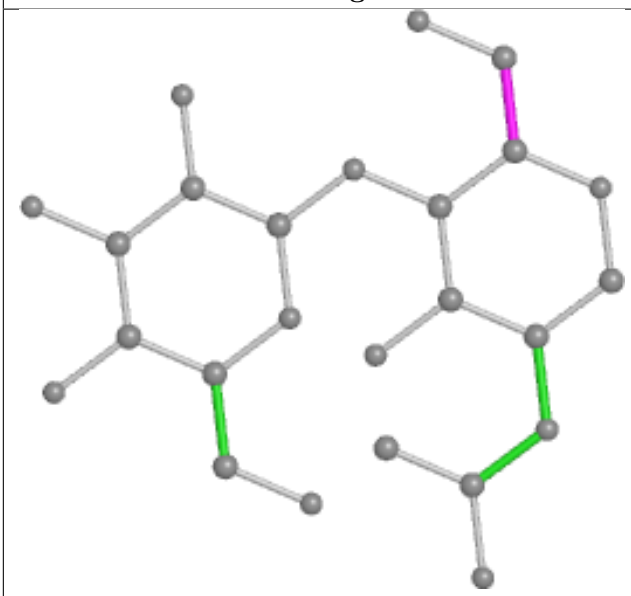
Oligosaccharide Chain F



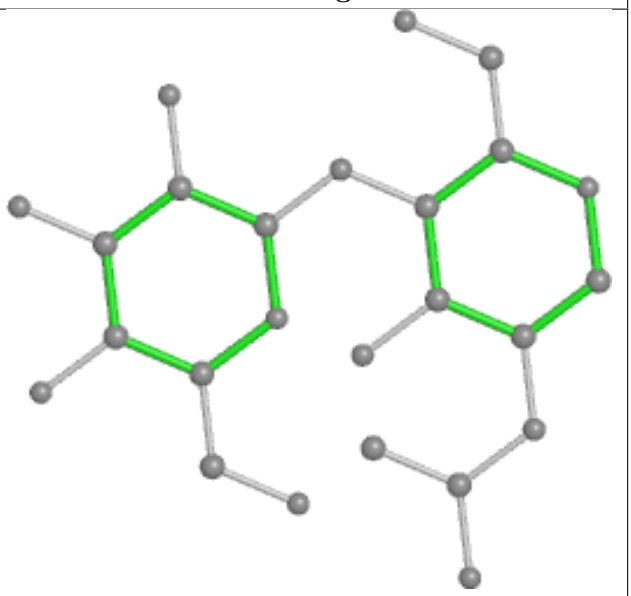
Bond lengths



Bond angles

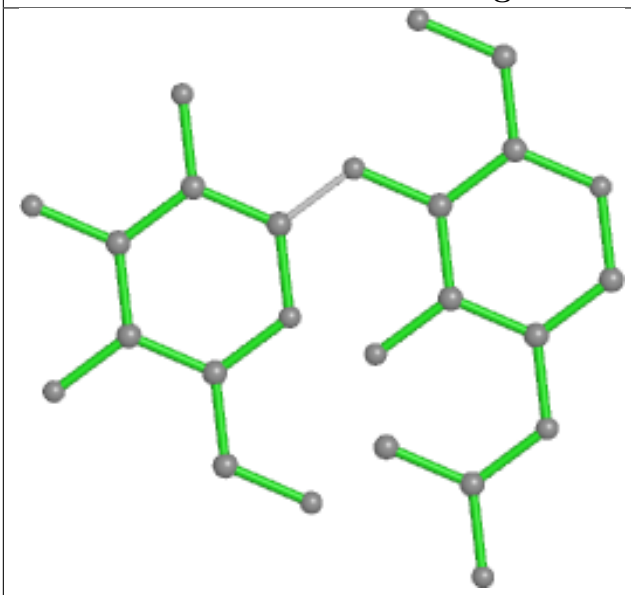


Torsions

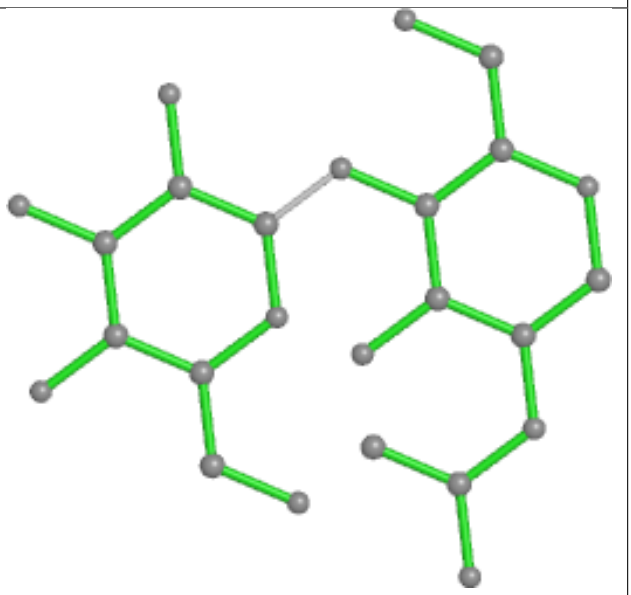


Rings

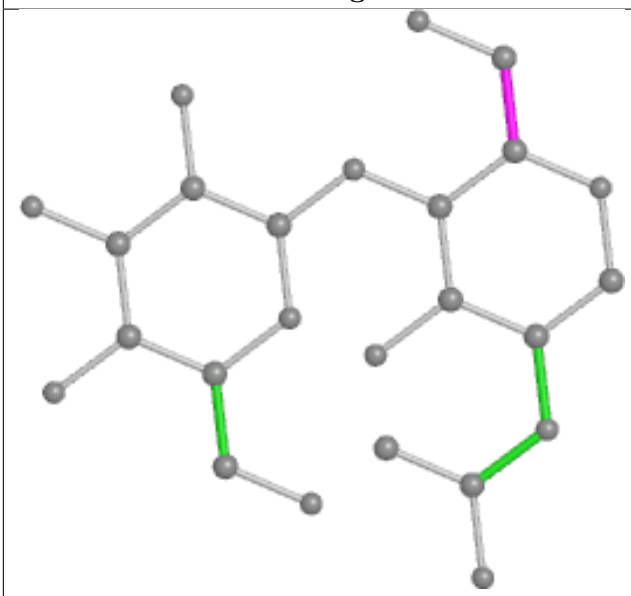
Oligosaccharide Chain G



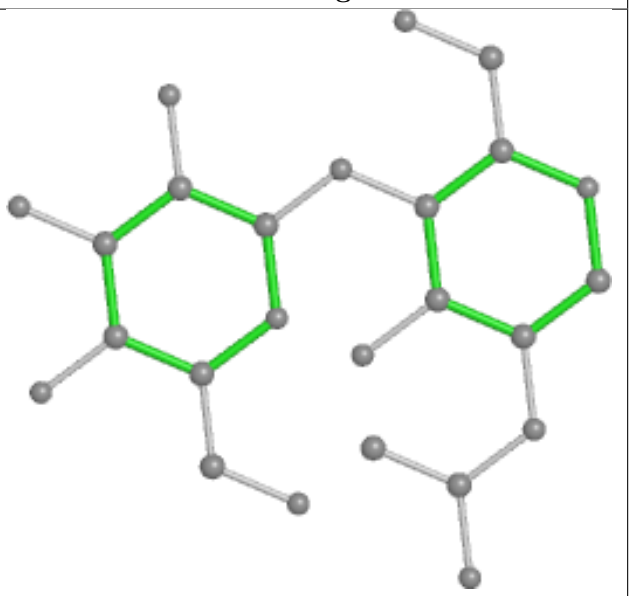
Bond lengths



Bond angles

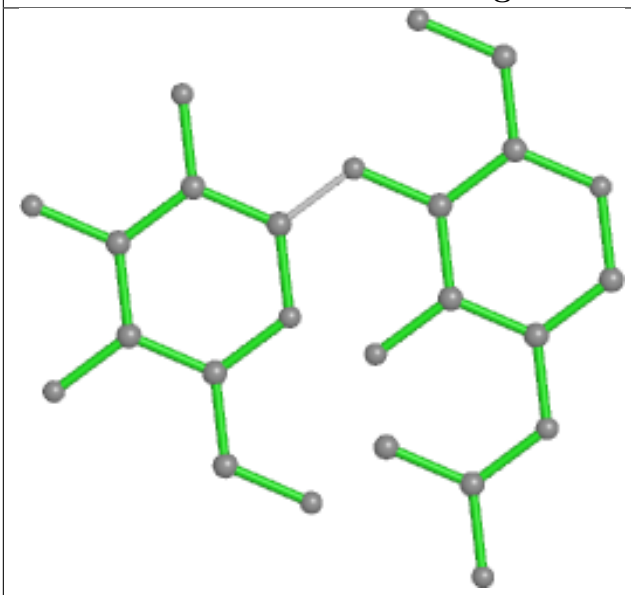


Torsions

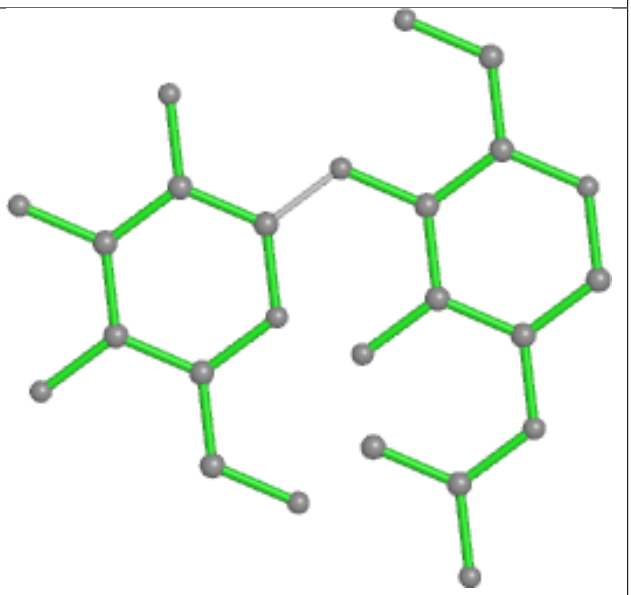


Rings

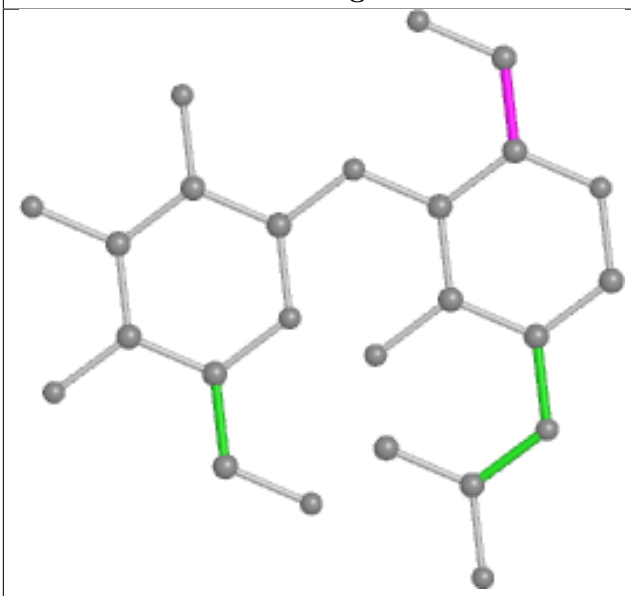
Oligosaccharide Chain H



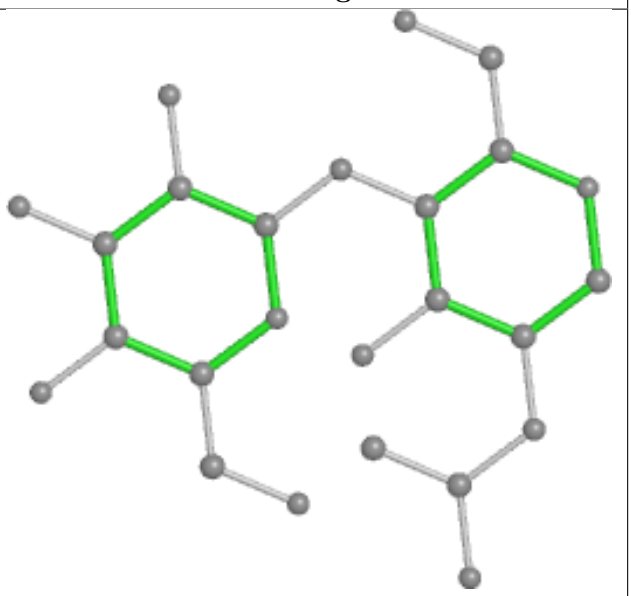
Bond lengths



Bond angles

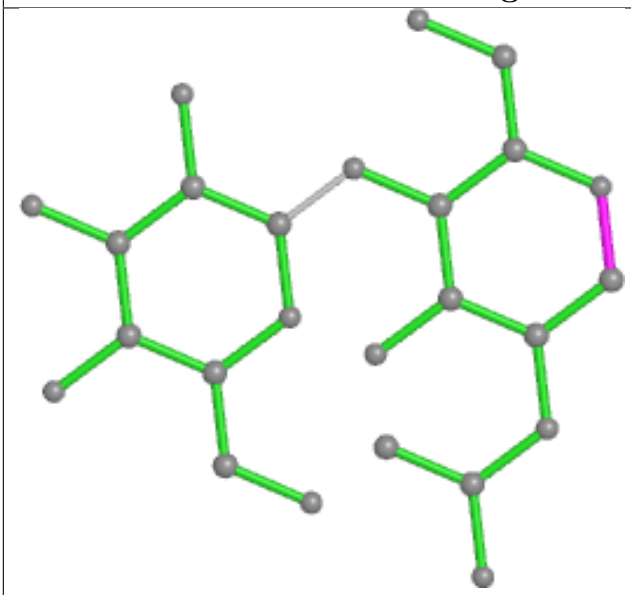


Torsions

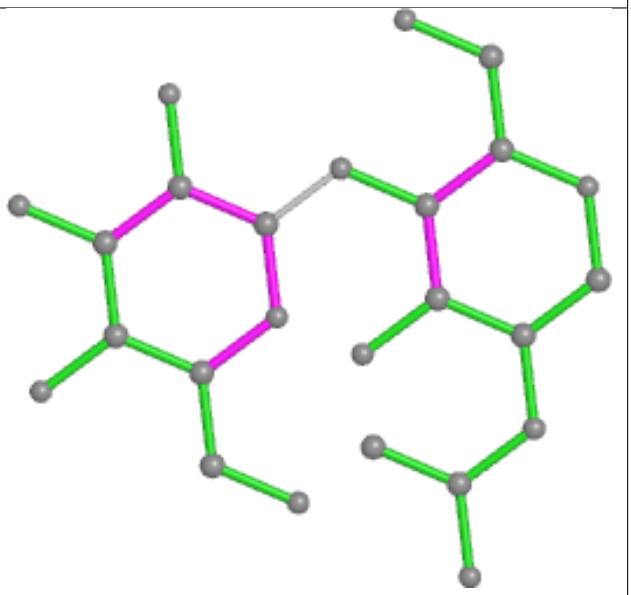


Rings

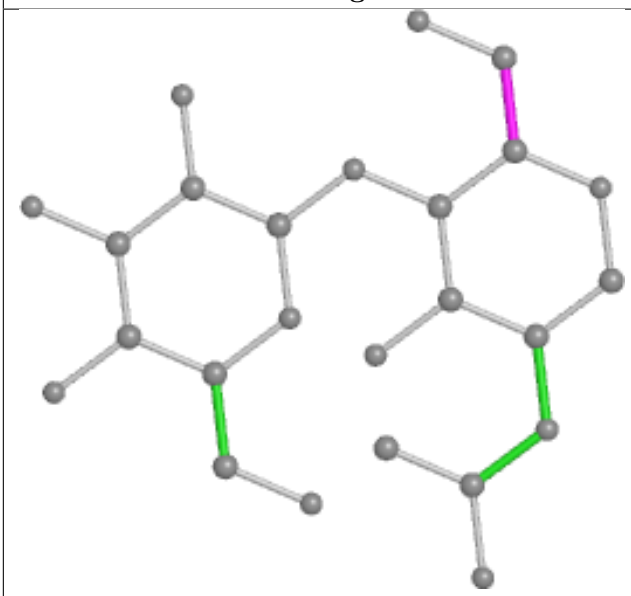
Oligosaccharide Chain I



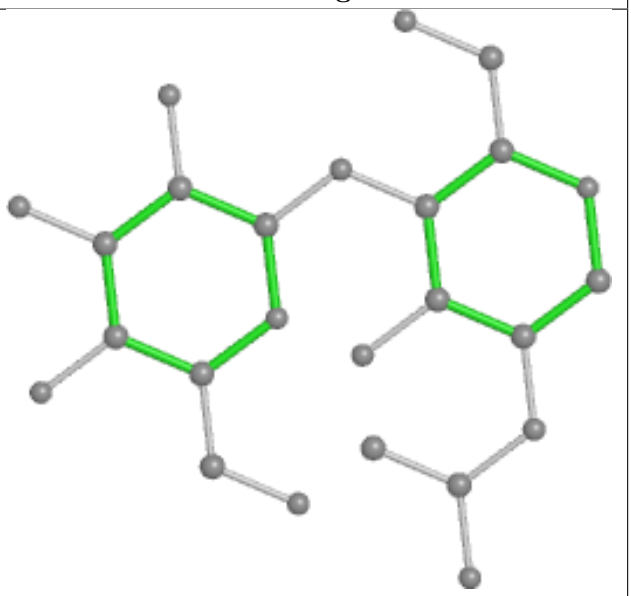
Bond lengths



Bond angles

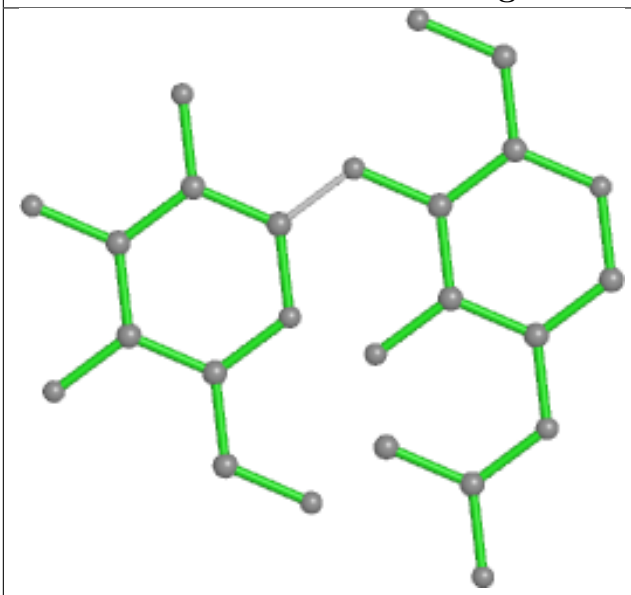


Torsions

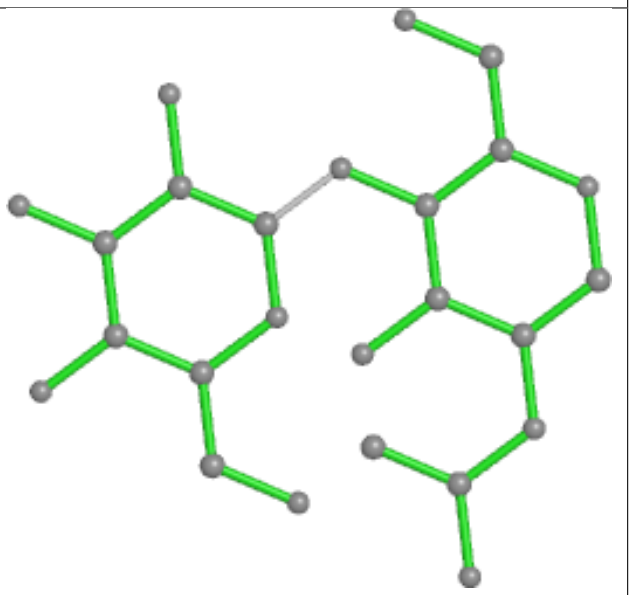


Rings

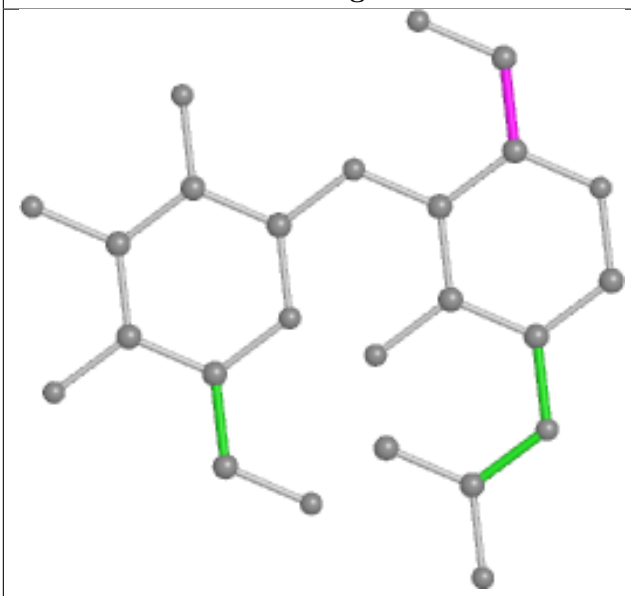
Oligosaccharide Chain J



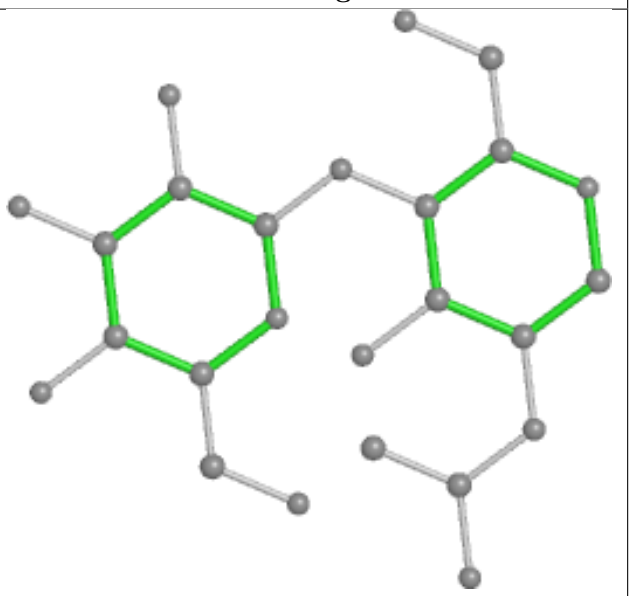
Bond lengths



Bond angles

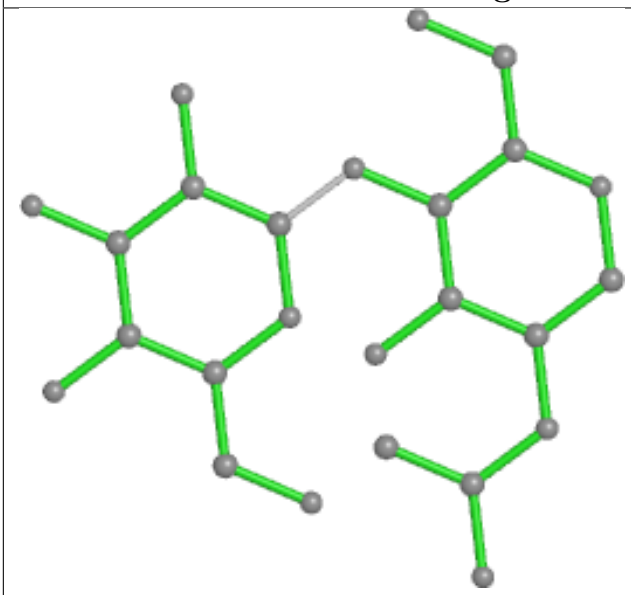


Torsions

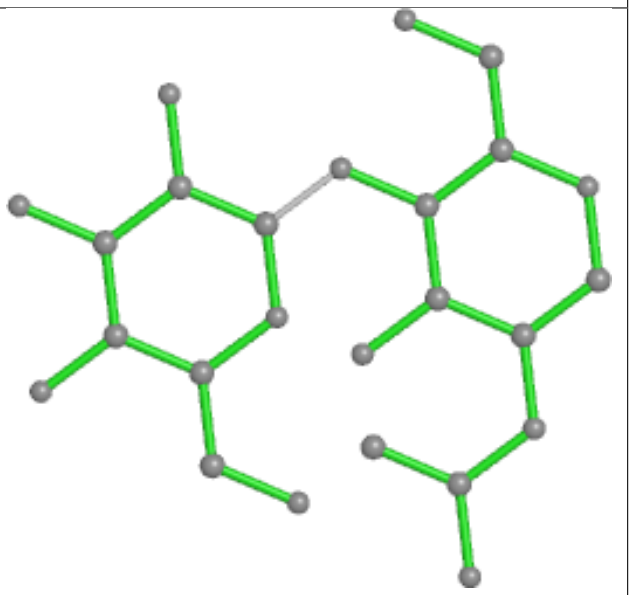


Rings

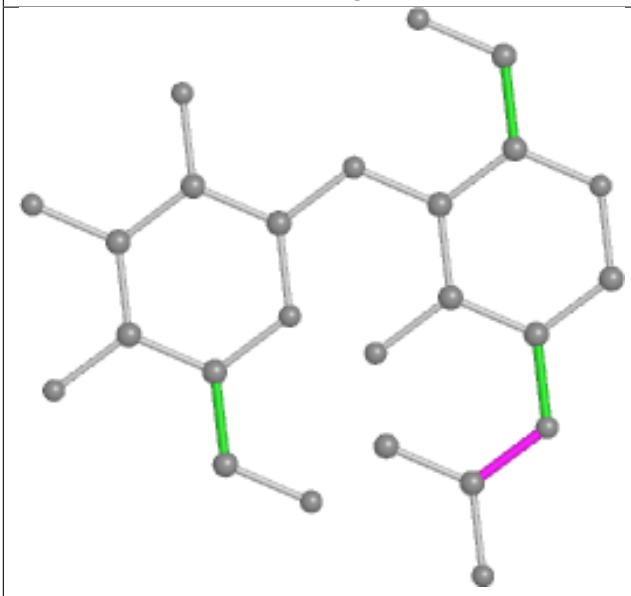
Oligosaccharide Chain K



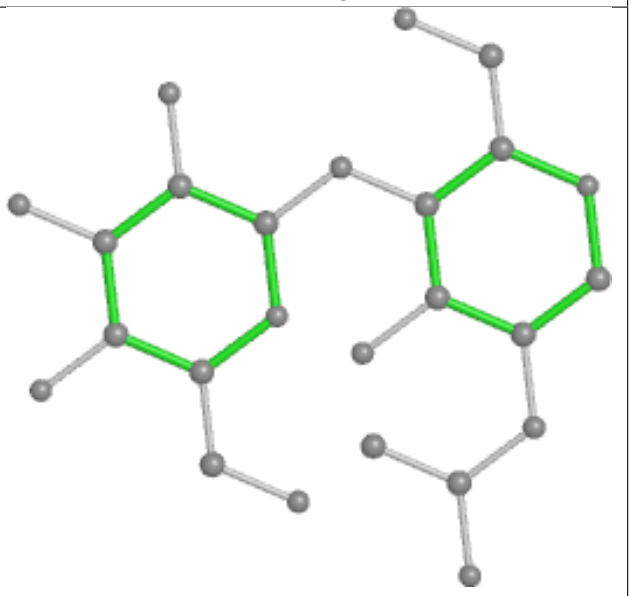
Bond lengths



Bond angles

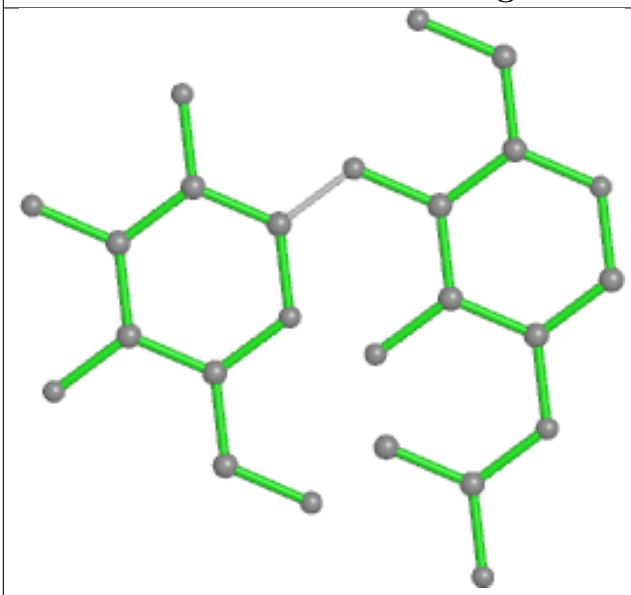


Torsions

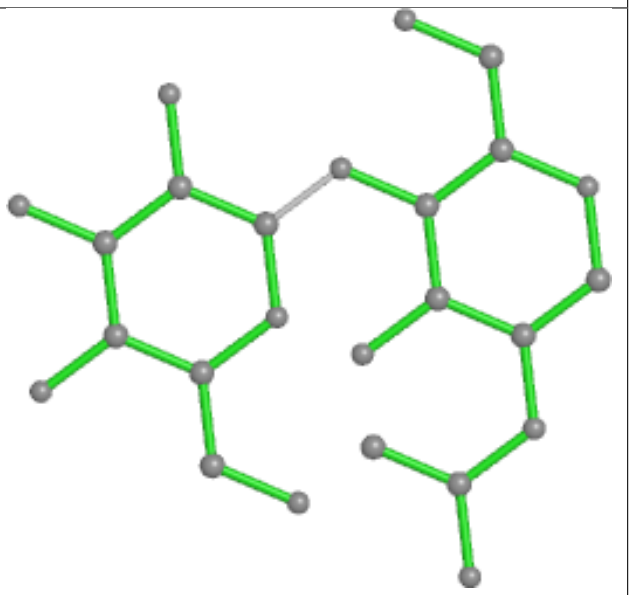


Rings

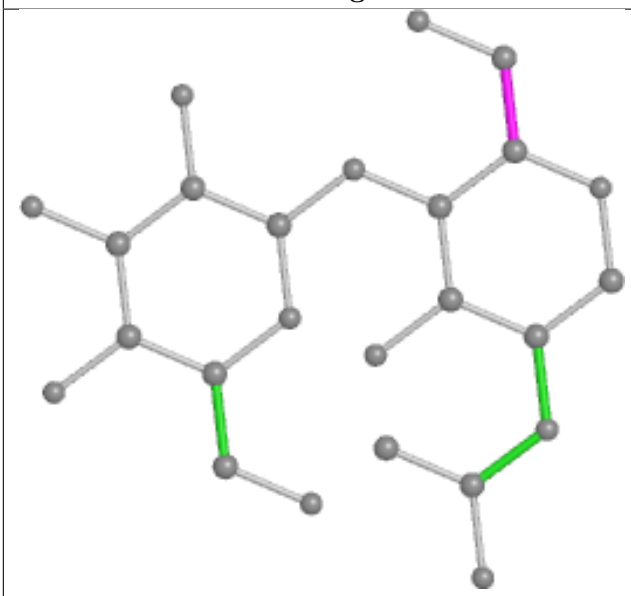
Oligosaccharide Chain L



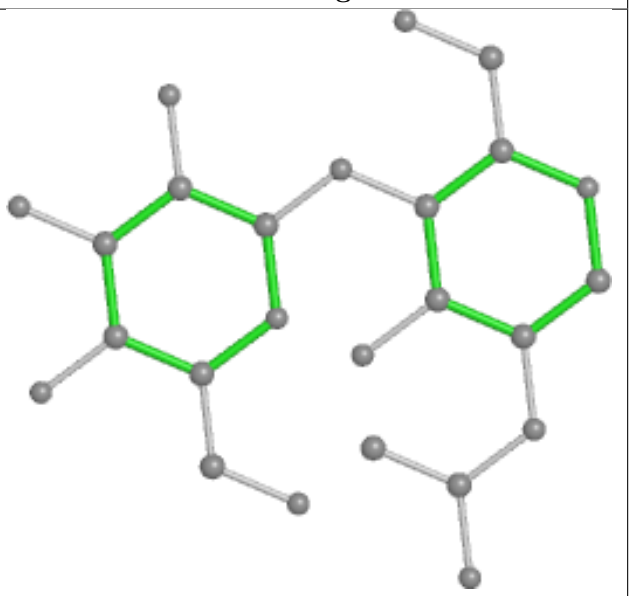
Bond lengths



Bond angles

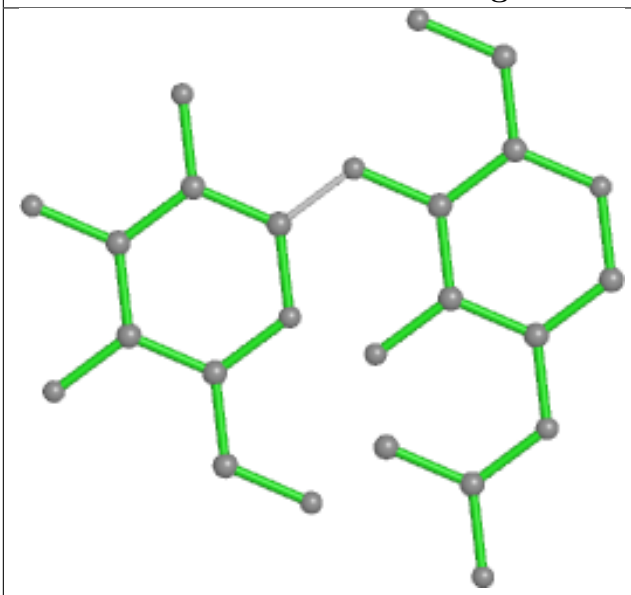


Torsions

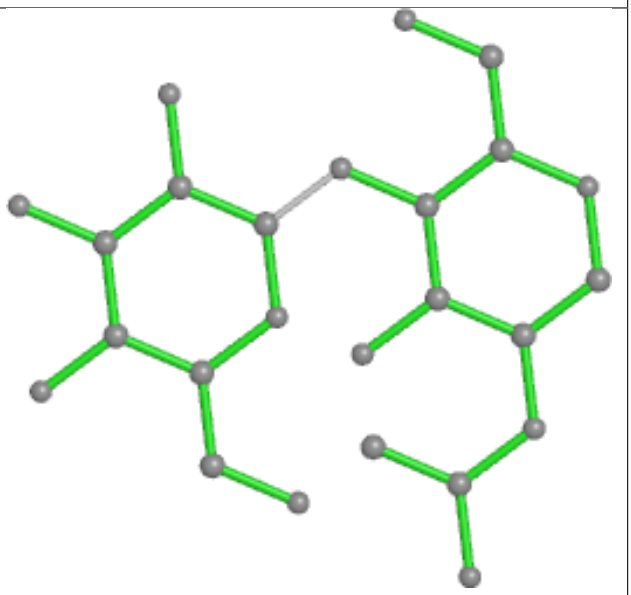


Rings

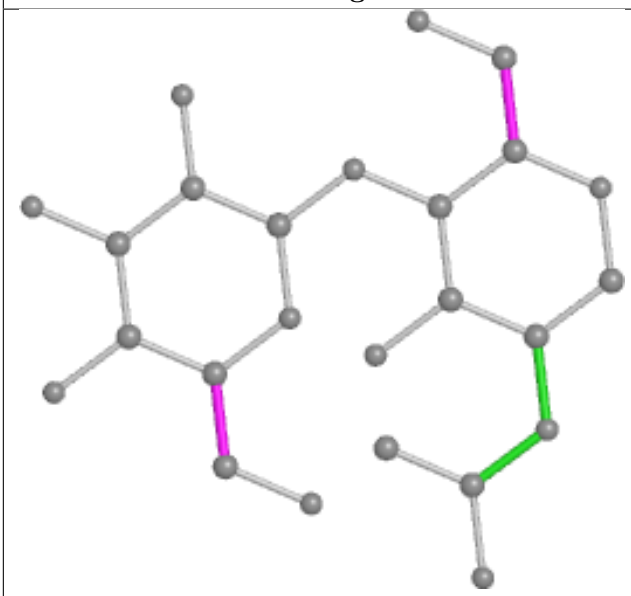
Oligosaccharide Chain M



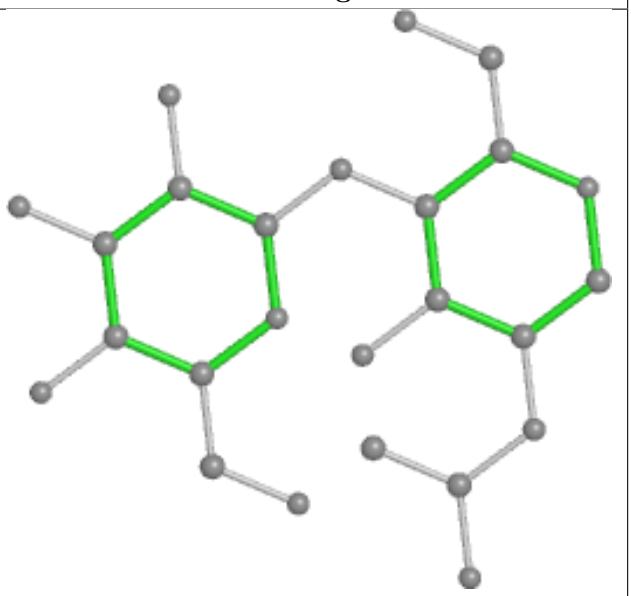
Bond lengths



Bond angles

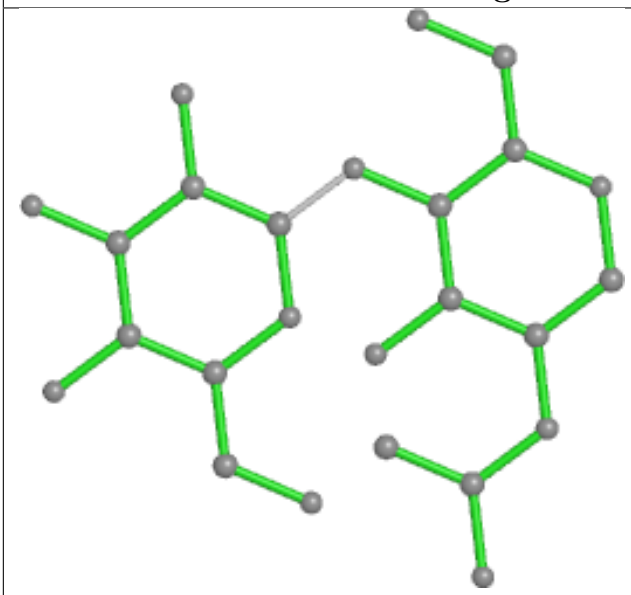


Torsions

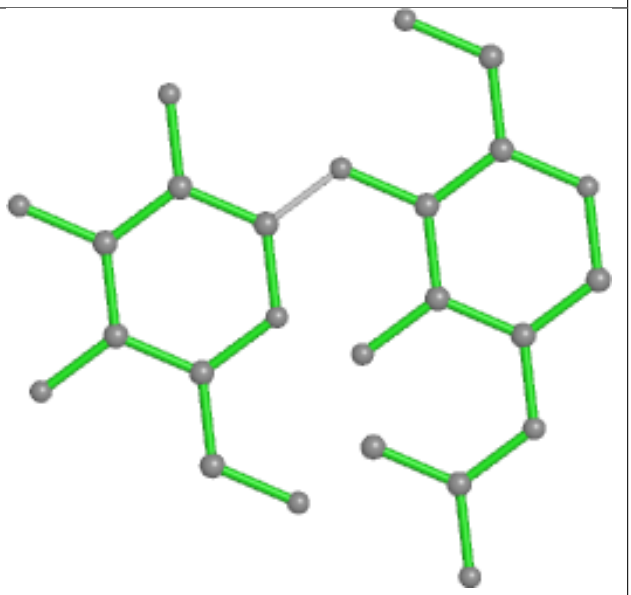


Rings

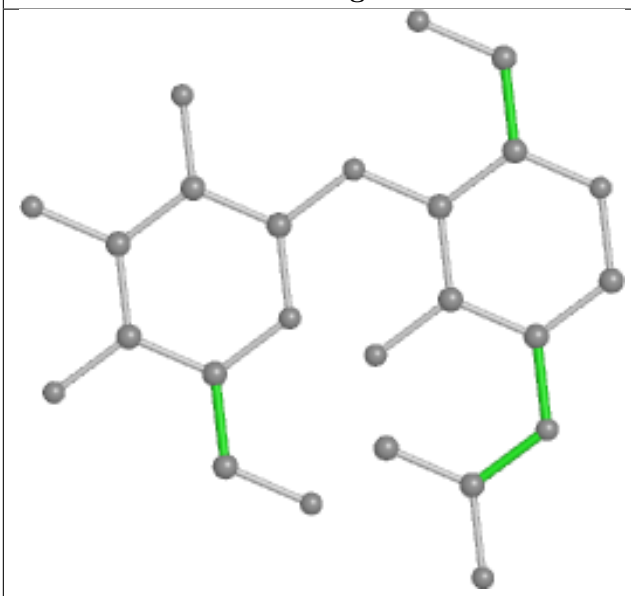
Oligosaccharide Chain N



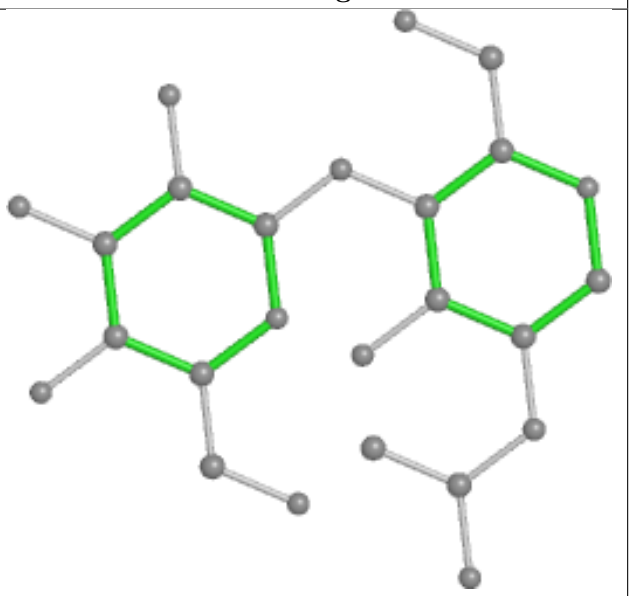
Bond lengths



Bond angles

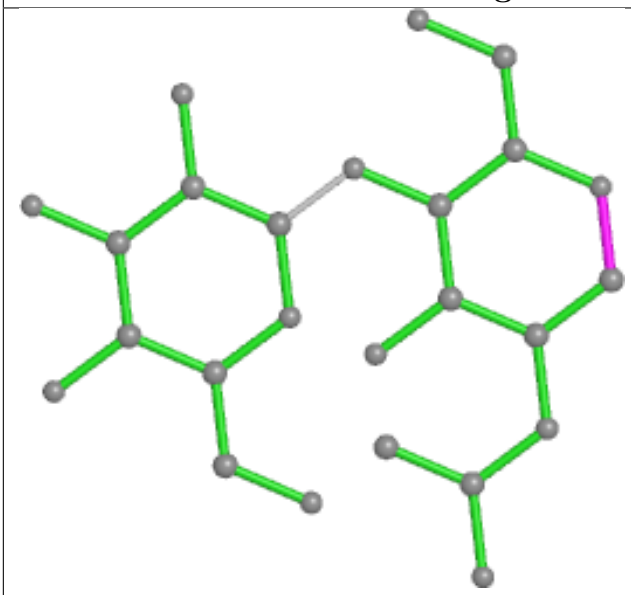


Torsions

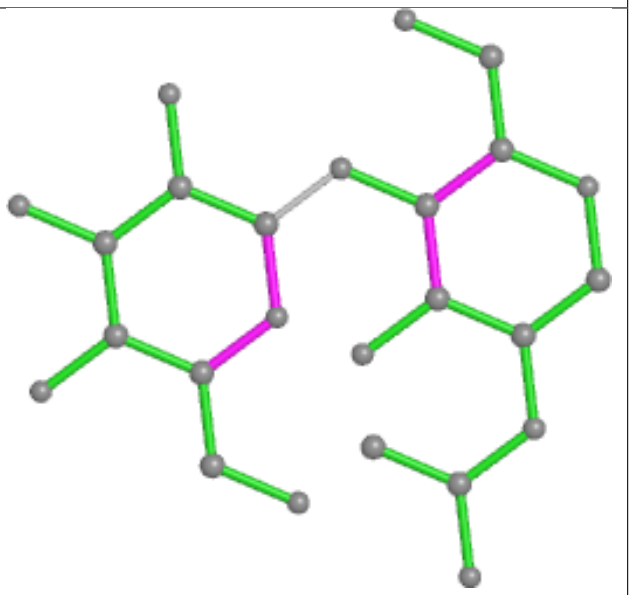


Rings

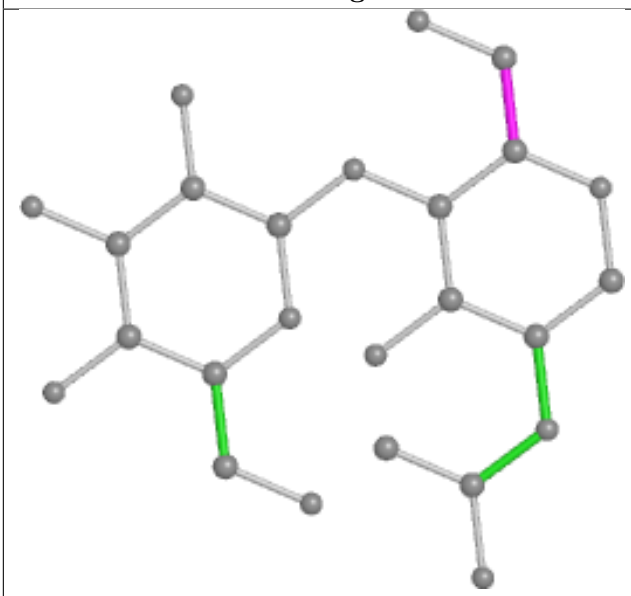
Oligosaccharide Chain O



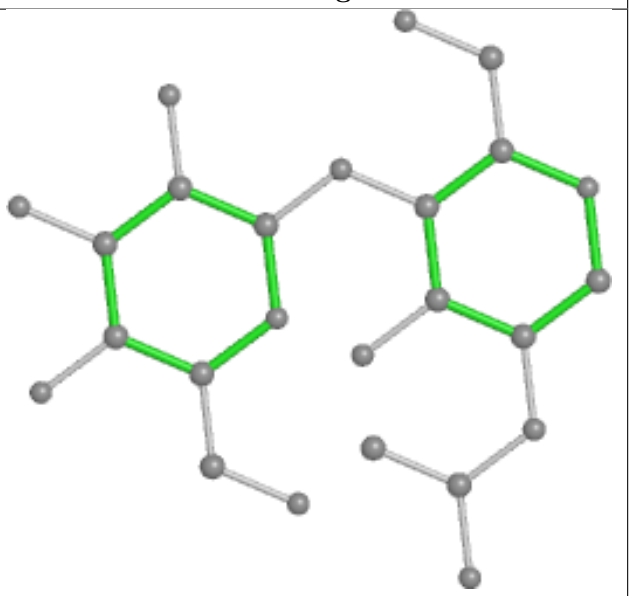
Bond lengths



Bond angles

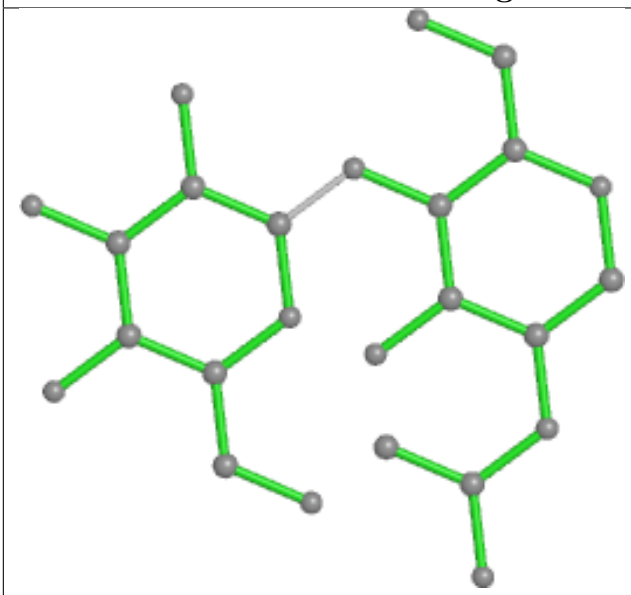


Torsions

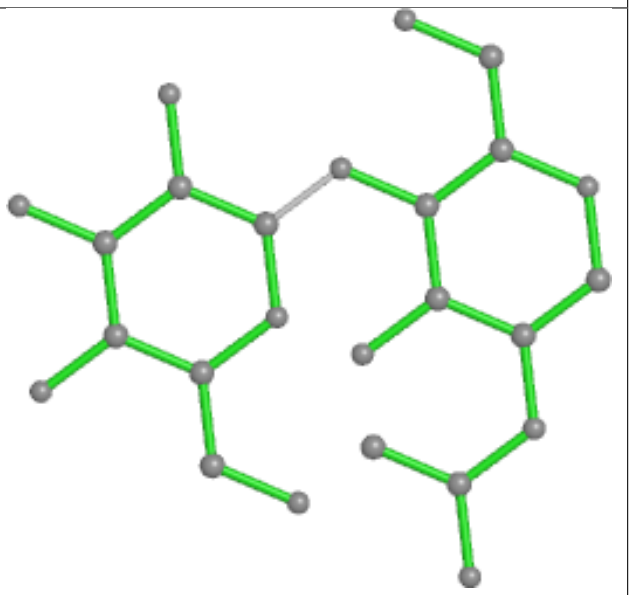


Rings

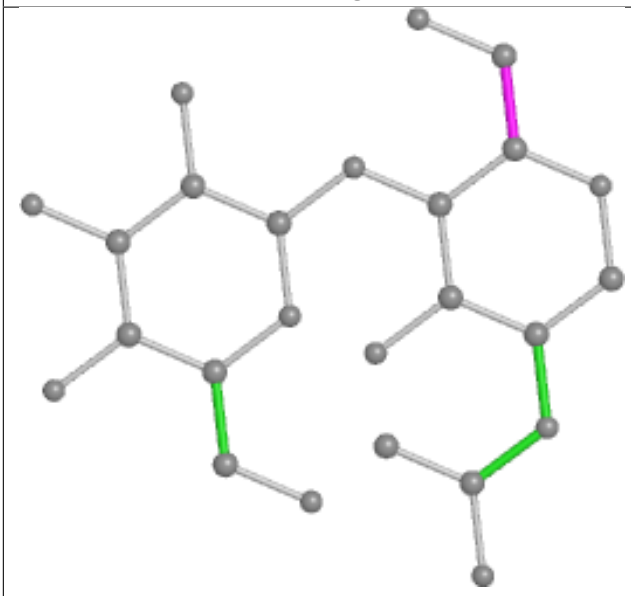
Oligosaccharide Chain P



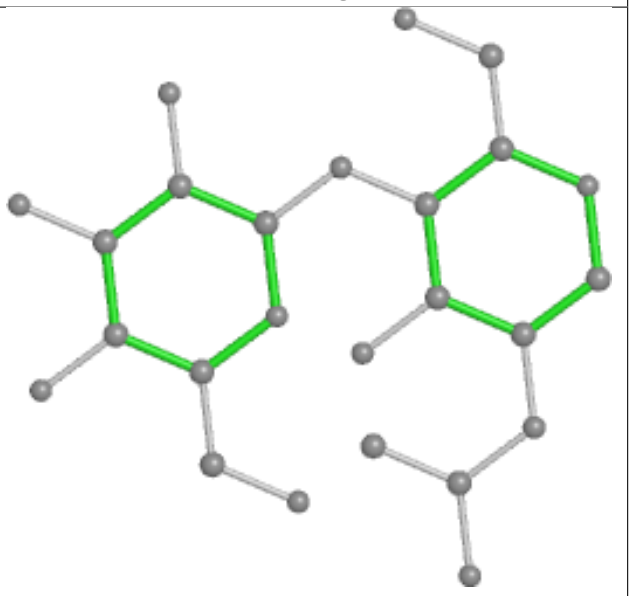
Bond lengths



Bond angles

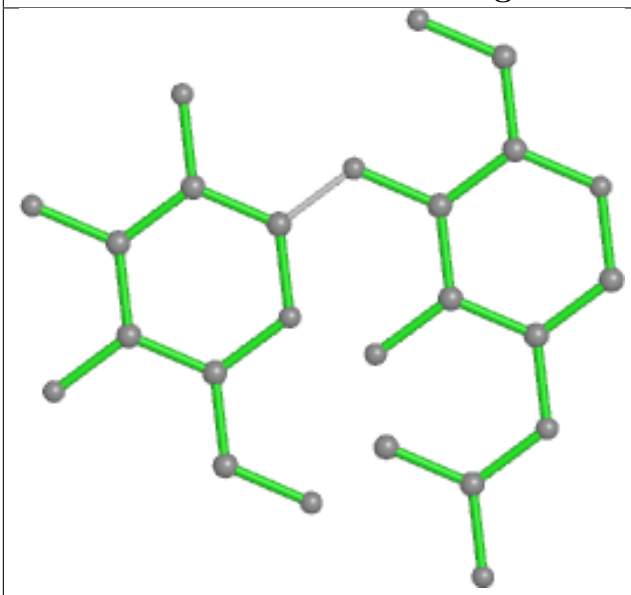


Torsions

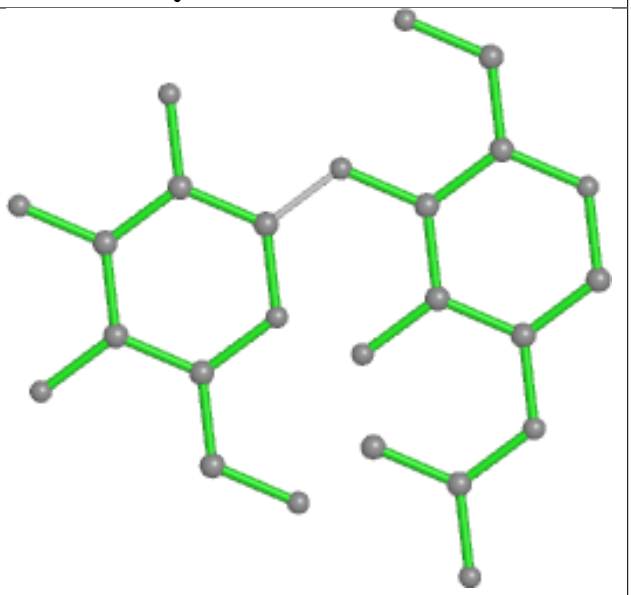


Rings

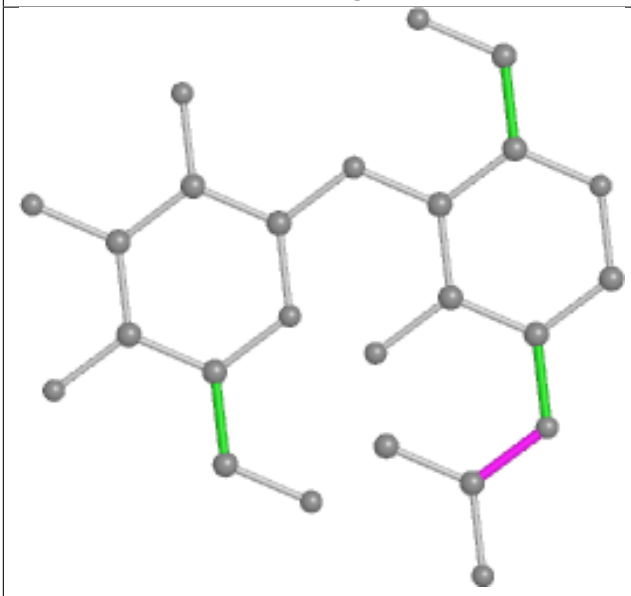
Oligosaccharide Chain Q



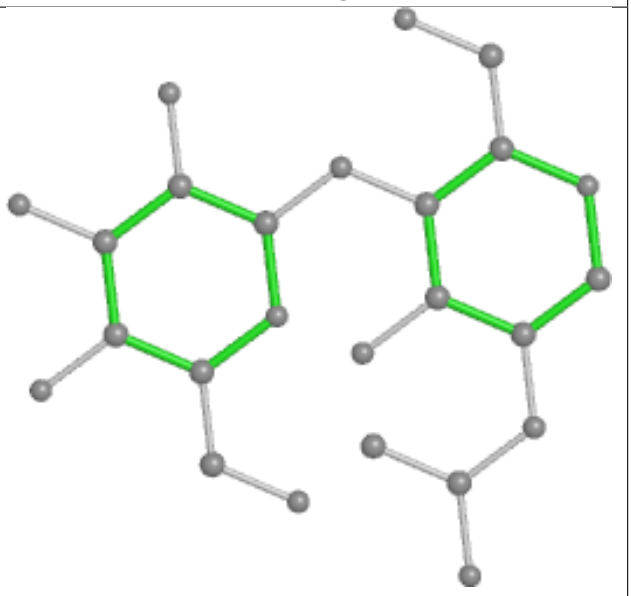
Bond lengths



Bond angles

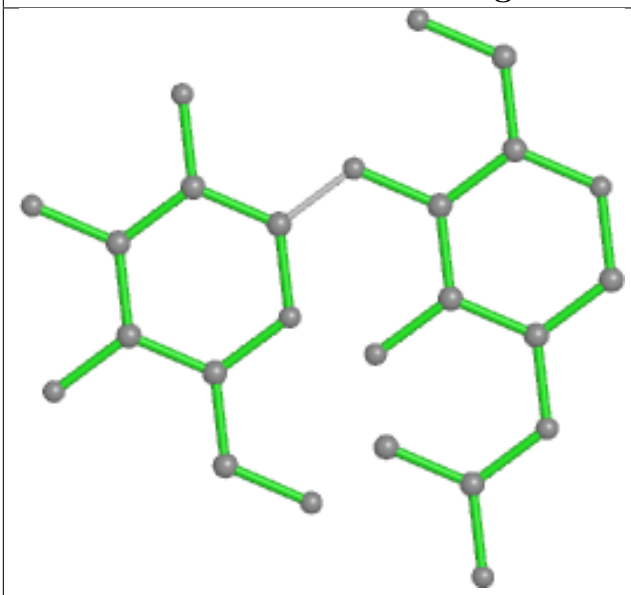


Torsions

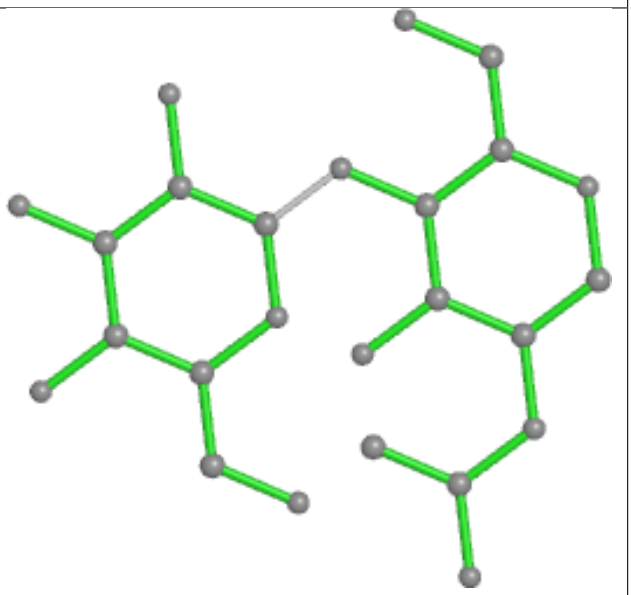


Rings

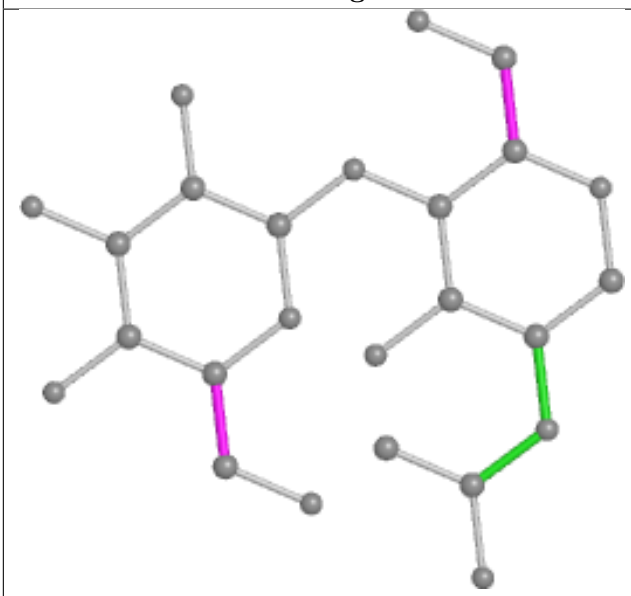
Oligosaccharide Chain R



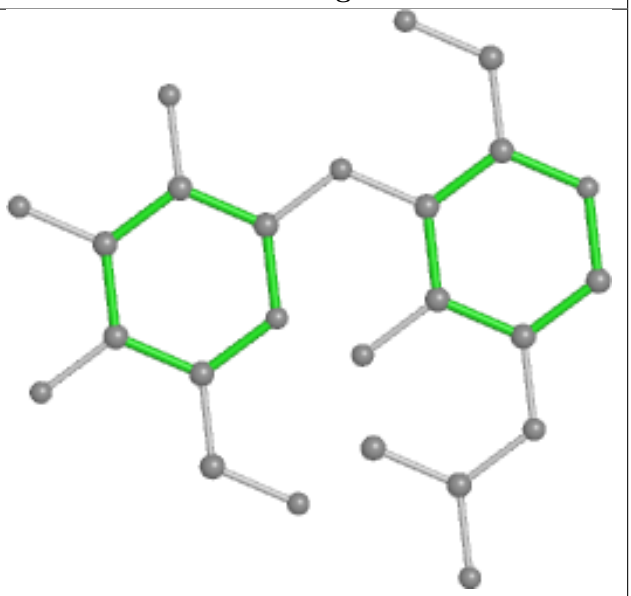
Bond lengths



Bond angles

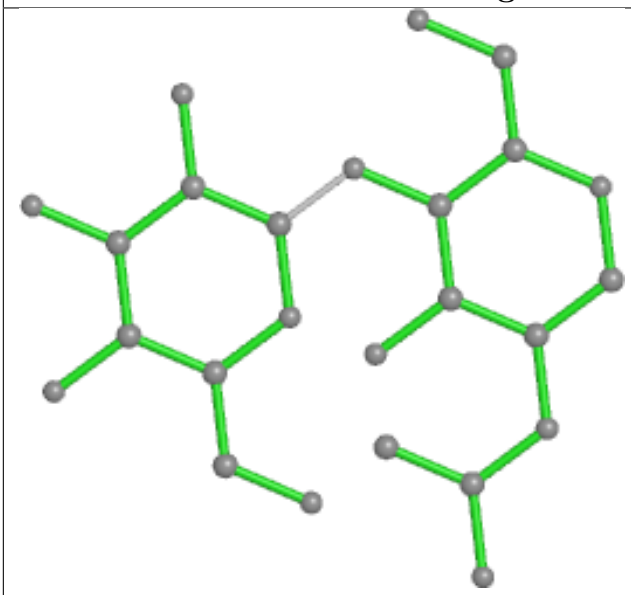


Torsions

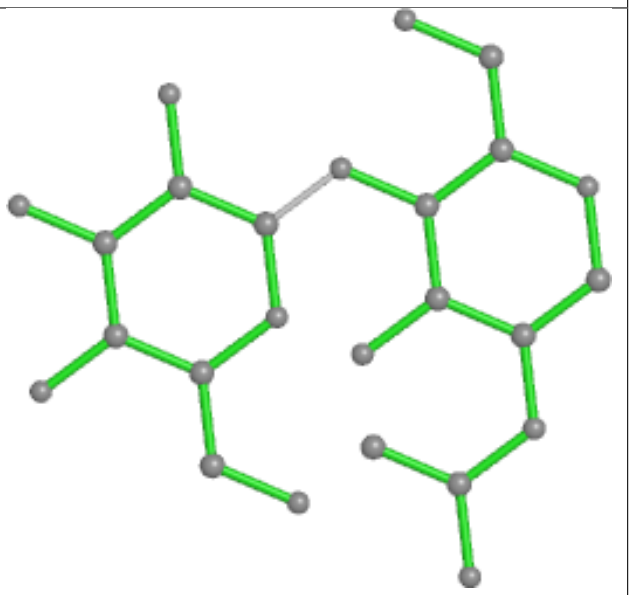


Rings

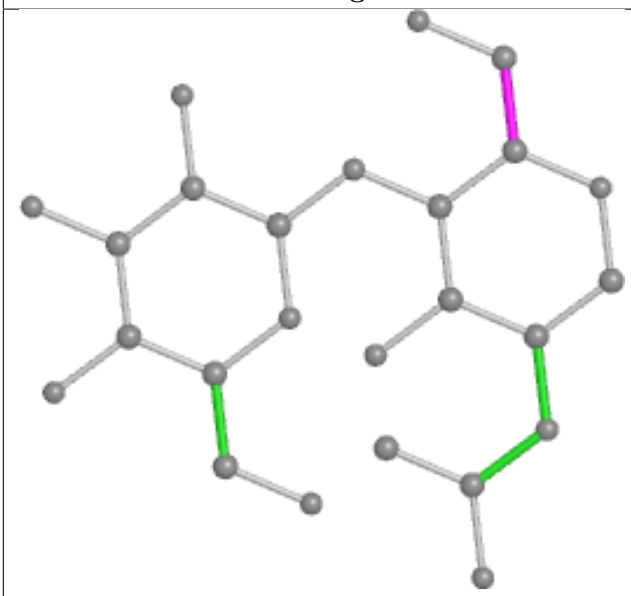
Oligosaccharide Chain S



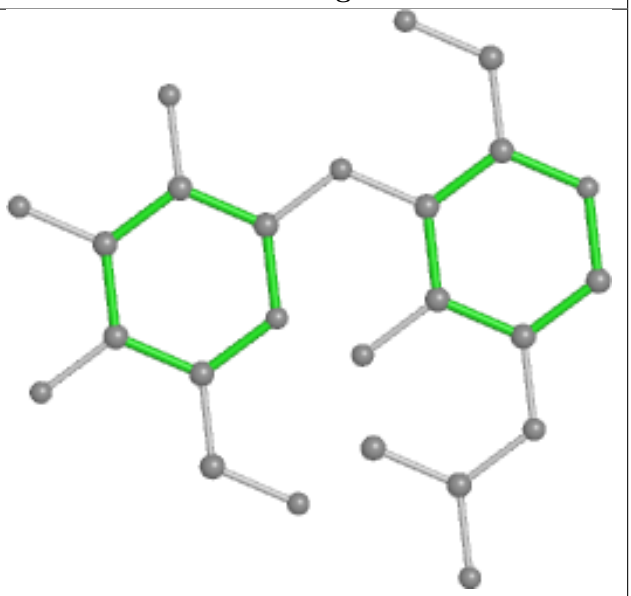
Bond lengths



Bond angles

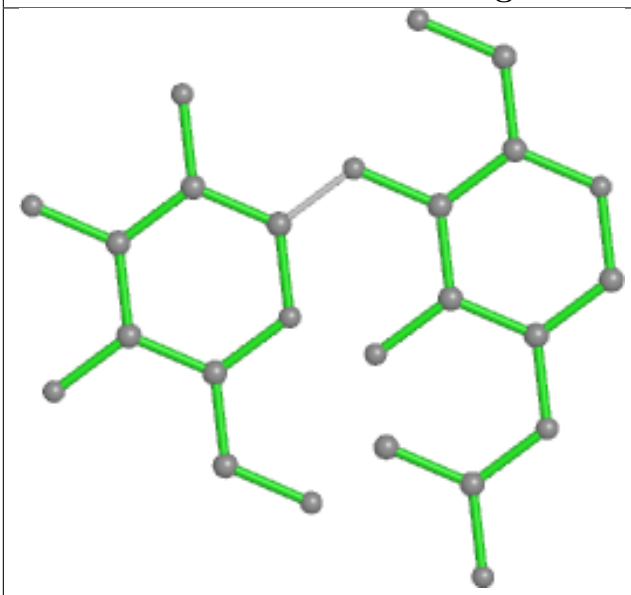


Torsions

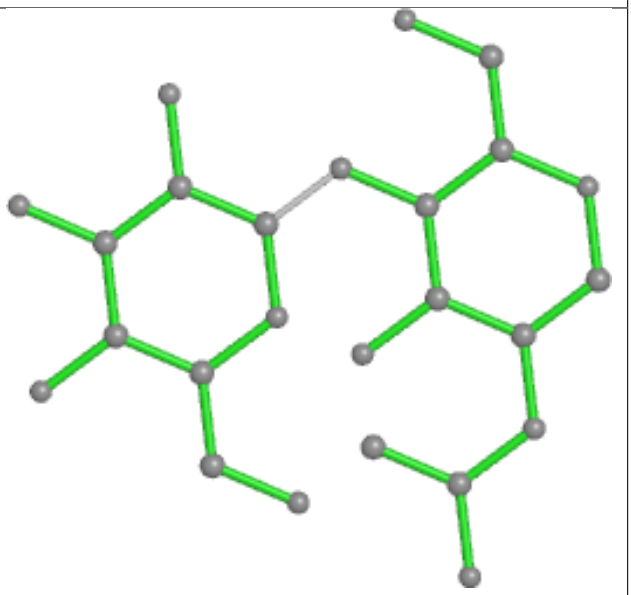


Rings

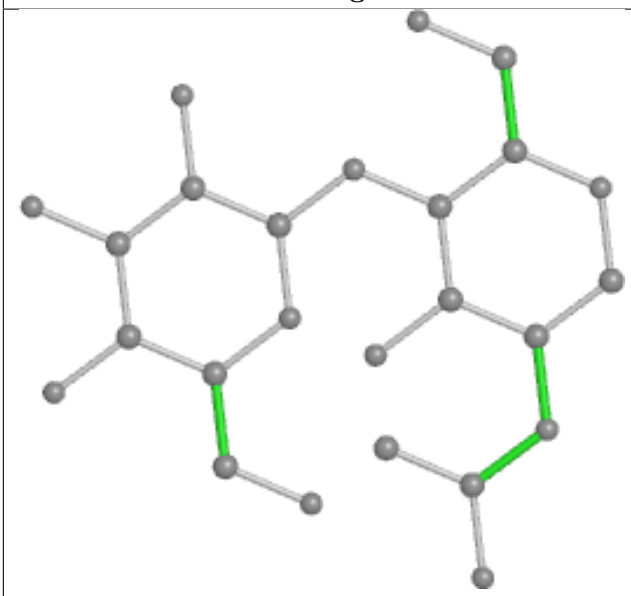
Oligosaccharide Chain T



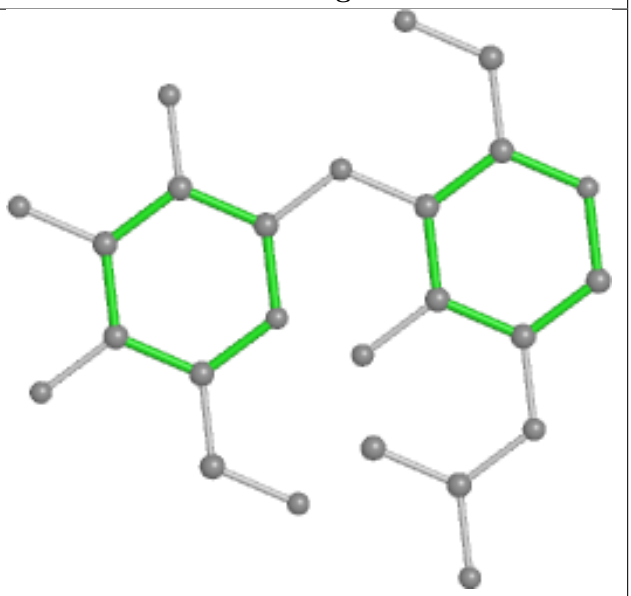
Bond lengths



Bond angles

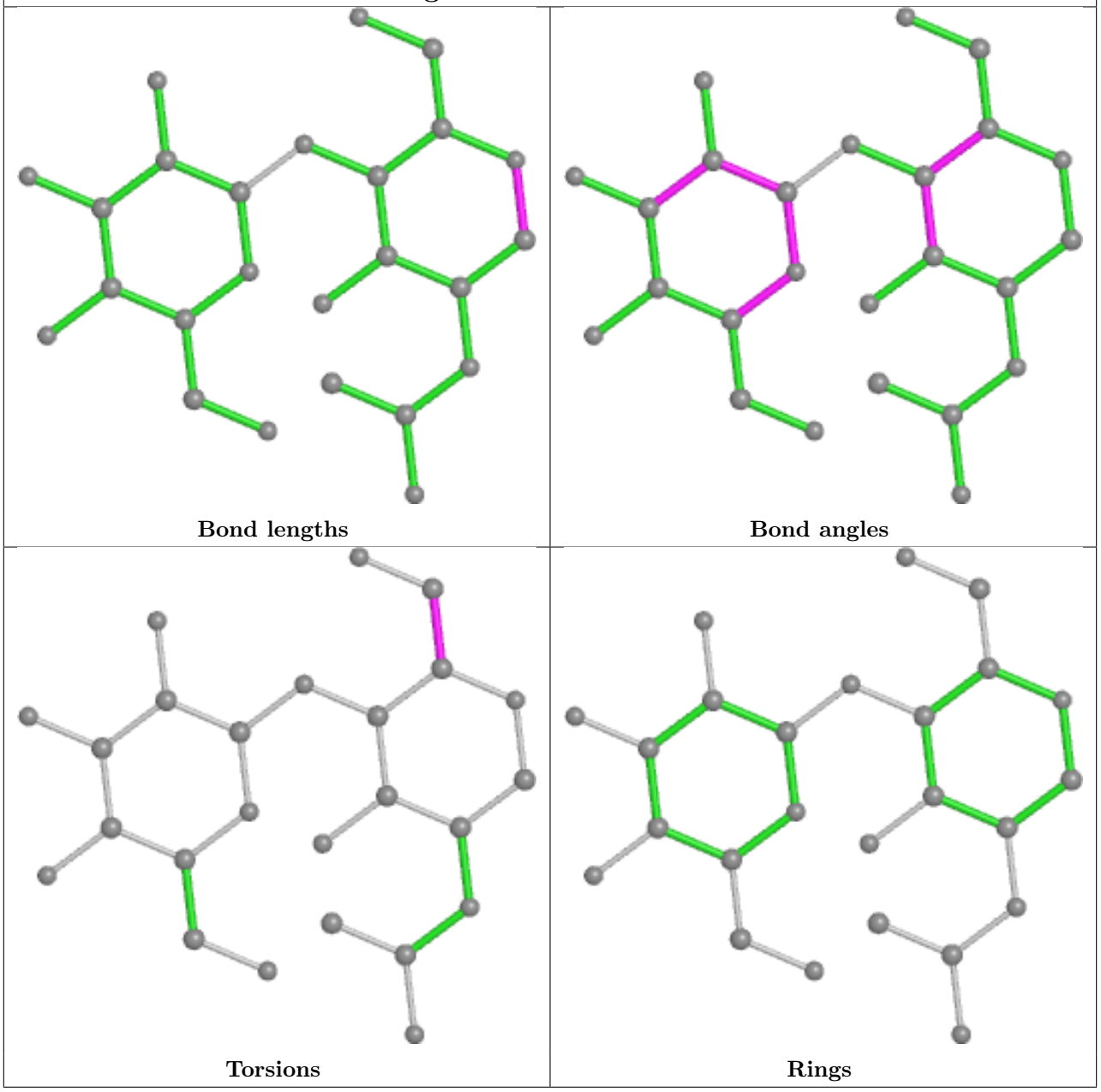


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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	$\#\|Z\|>2$
6	NAG	C	1303	2	14,14,15	1.05	2 (14%)	17,19,21	0.87	1 (5%)
6	NAG	B	1311	2	14,14,15	0.29	0	17,19,21	0.48	0
6	NAG	C	1310	2	14,14,15	0.42	0	17,19,21	0.40	0
6	NAG	D	1301	2	14,14,15	0.25	0	17,19,21	0.56	0
6	NAG	C	1309	2	14,14,15	0.19	0	17,19,21	0.42	0
6	NAG	B	1301	2	14,14,15	0.28	0	17,19,21	0.53	0
6	NAG	D	1303	2	14,14,15	0.40	0	17,19,21	0.49	0
6	NAG	D	1302	2	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	B	1304	2	14,14,15	0.23	0	17,19,21	0.38	0
6	NAG	C	1307	2	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	D	1306	2	14,14,15	0.36	0	17,19,21	0.40	0
6	NAG	D	1310	2	14,14,15	0.28	0	17,19,21	0.38	0
6	NAG	B	1308	2	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	B	1303	2	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	C	1302	2	14,14,15	0.21	0	17,19,21	0.37	0
6	NAG	A	905	1	14,14,15	0.25	0	17,19,21	0.49	0
6	NAG	C	1304	2	14,14,15	0.24	0	17,19,21	0.37	0
6	NAG	C	1306	2	14,14,15	0.34	0	17,19,21	0.40	0
6	NAG	D	1305	2	14,14,15	0.30	0	17,19,21	1.39	2 (11%)
6	NAG	A	904	1	14,14,15	0.81	1 (7%)	17,19,21	1.48	3 (17%)
6	NAG	D	1307	2	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	A	902	1	14,14,15	0.34	0	17,19,21	0.36	0
6	NAG	B	1306	2	14,14,15	0.35	0	17,19,21	1.35	1 (5%)
6	NAG	B	1305	2	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	D	1309	2	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	B	1309	2	14,14,15	0.34	0	17,19,21	0.60	1 (5%)
6	NAG	B	1302	2	14,14,15	0.23	0	17,19,21	0.38	0
6	NAG	B	1307	2	14,14,15	0.39	0	17,19,21	0.40	0
6	NAG	D	1304	2	14,14,15	0.24	0	17,19,21	0.34	0
6	NAG	B	1310	-	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1301	2	14,14,15	0.25	0	17,19,21	0.54	0
6	NAG	A	906	1	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	A	903	1	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	C	1305	2	14,14,15	0.29	0	17,19,21	1.36	2 (11%)
6	NAG	C	1308	2	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
6	NAG	D	1308	2	14,14,15	0.32	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1303	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1310	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1301	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1303	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1302	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1310	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	2	-	4/6/23/26	0/1/1/1
6	NAG	C	1302	2	-	0/6/23/26	0/1/1/1
6	NAG	A	905	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1304	2	-	1/6/23/26	0/1/1/1
6	NAG	C	1306	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1305	2	-	0/6/23/26	0/1/1/1
6	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1306	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1309	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1309	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1302	2	-	1/6/23/26	0/1/1/1
6	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1304	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1301	2	-	2/6/23/26	0/1/1/1
6	NAG	A	906	1	-	4/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1305	2	-	0/6/23/26	0/1/1/1
6	NAG	C	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1308	2	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	C1-C2	2.93	1.56	1.52
6	C	1303	NAG	O5-C1	2.52	1.47	1.43
6	A	904	NAG	C1-C2	2.38	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1305	NAG	C1-O5-C5	4.98	118.94	112.19
6	B	1306	NAG	C1-O5-C5	4.92	118.86	112.19
6	C	1305	NAG	C1-O5-C5	4.90	118.83	112.19
6	A	904	NAG	C1-O5-C5	4.62	118.45	112.19
6	C	1303	NAG	C1-O5-C5	3.06	116.33	112.19
6	A	904	NAG	C2-N2-C7	2.31	126.20	122.90
6	D	1305	NAG	C3-C4-C5	2.12	114.02	110.24
6	B	1309	NAG	C1-O5-C5	2.08	115.01	112.19
6	D	1308	NAG	C1-O5-C5	2.07	115.00	112.19
6	C	1308	NAG	C1-O5-C5	2.05	114.97	112.19
6	A	904	NAG	C1-C2-N2	2.04	113.97	110.49
6	C	1305	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	906	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	D	1310	NAG	C4-C5-C6-O6
6	D	1307	NAG	O5-C5-C6-O6
6	D	1308	NAG	C4-C5-C6-O6
6	B	1311	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	D	1308	NAG	O5-C5-C6-O6
6	A	906	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	D	1310	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	B	1309	NAG	C4-C5-C6-O6
6	C	1310	NAG	C4-C5-C6-O6
6	D	1303	NAG	C4-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	D	1309	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1307	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	B	1311	NAG	C4-C5-C6-O6
6	D	1307	NAG	C4-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	C	1310	NAG	O5-C5-C6-O6
6	D	1302	NAG	O5-C5-C6-O6
6	A	905	NAG	C4-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6
6	B	1308	NAG	C4-C5-C6-O6
6	D	1306	NAG	O5-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	A	906	NAG	C8-C7-N2-C2
6	A	906	NAG	O7-C7-N2-C2
6	B	1303	NAG	C8-C7-N2-C2
6	B	1303	NAG	O7-C7-N2-C2
6	B	1309	NAG	C8-C7-N2-C2
6	B	1309	NAG	O7-C7-N2-C2
6	B	1310	NAG	C8-C7-N2-C2
6	B	1310	NAG	O7-C7-N2-C2
6	C	1308	NAG	C8-C7-N2-C2
6	C	1308	NAG	O7-C7-N2-C2
6	C	1310	NAG	C8-C7-N2-C2
6	C	1310	NAG	O7-C7-N2-C2
6	D	1308	NAG	C8-C7-N2-C2
6	D	1308	NAG	O7-C7-N2-C2
6	D	1310	NAG	C8-C7-N2-C2
6	D	1310	NAG	O7-C7-N2-C2
6	D	1303	NAG	O5-C5-C6-O6
6	D	1302	NAG	C4-C5-C6-O6
6	A	905	NAG	O5-C5-C6-O6
6	D	1309	NAG	C4-C5-C6-O6
6	D	1304	NAG	O5-C5-C6-O6
6	D	1306	NAG	C4-C5-C6-O6
6	D	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	A	904	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	B	1302	NAG	O5-C5-C6-O6
6	C	1307	NAG	C4-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	A	905	NAG	C3-C2-N2-C7
6	C	1301	NAG	C3-C2-N2-C7
6	D	1301	NAG	C3-C2-N2-C7
6	D	1304	NAG	C4-C5-C6-O6
6	B	1310	NAG	C4-C5-C6-O6
6	B	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1301	NAG	1	0
6	D	1306	NAG	1	0
6	D	1310	NAG	1	0
6	B	1310	NAG	1	0
6	C	1305	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.