Full wwPDB EM Validation Report ⓘ

Aug 8, 2024 – 10:15 PM JST

PDB ID	:	8X5Q
EMDB ID	:	EMD-38072
Title	:	SARS-CoV-2 BA.2.75 Spike with K356T mutation (3 RBD down)
Authors	:	Yue, C.; Liu, P.
Deposited on	:	2023-11-17
Resolution	:	3.47 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:

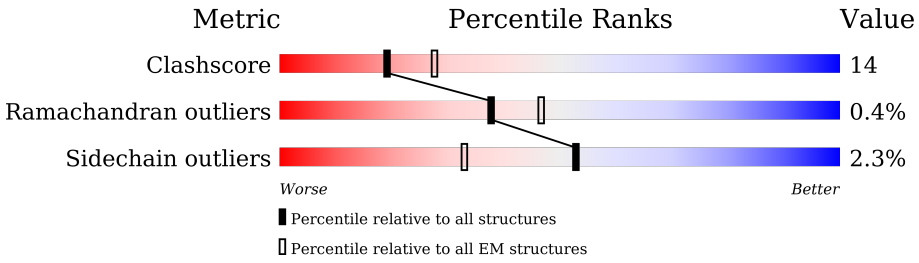
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.47 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1270	59% 26% • 14%
1	B	1270	58% 27% • 14%
1	C	1270	58% 26% • 14%
2	D	2	100%
2	E	2	100%
2	F	2	100%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	2	50% 50%
2	K	2	100%
2	L	2	100%
2	M	2	100%
2	N	2	100%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	50% 50%
2	R	2	100%
2	S	2	100%
2	T	2	100%
2	U	2	100%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26208 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1086	Total	C	N	O	S	0	0
			8442	5395	1405	1605	37		
1	A	1086	Total	C	N	O	S	0	0
			8442	5395	1405	1605	37		
1	B	1086	Total	C	N	O	S	0	0
			8442	5395	1405	1605	37		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	22	ILE	THR	variant	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	142	ASP	GLY	variant	UNP P0DTC2
C	147	GLU	LYS	variant	UNP P0DTC2
C	152	ARG	TRP	variant	UNP P0DTC2
C	157	LEU	PHE	variant	UNP P0DTC2
C	210	VAL	ILE	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	257	SER	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	engineered mutation	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	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	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	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	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	147	GLU	LYS	variant	UNP P0DTC2
A	152	ARG	TRP	variant	UNP P0DTC2
A	157	LEU	PHE	variant	UNP P0DTC2
A	210	VAL	ILE	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	257	SER	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	engineered mutation	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	22	ILE	THR	variant	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	142	ASP	GLY	variant	UNP P0DTC2
B	147	GLU	LYS	variant	UNP P0DTC2
B	152	ARG	TRP	variant	UNP P0DTC2
B	157	LEU	PHE	variant	UNP P0DTC2
B	210	VAL	ILE	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	257	SER	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	engineered mutation	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	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	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2

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

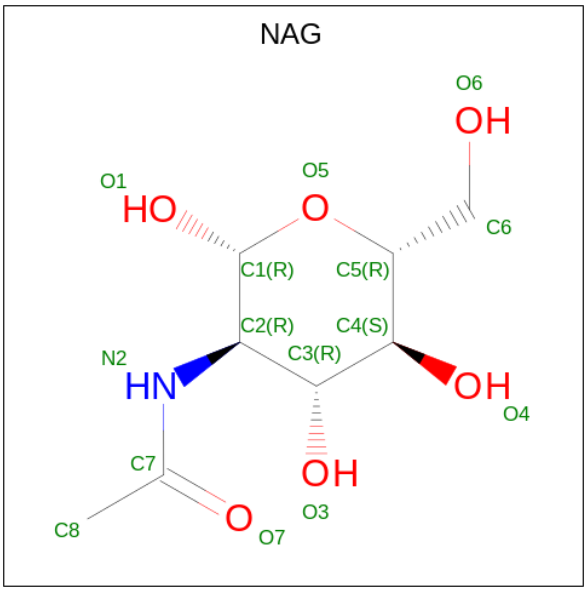
Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	2	Total C N O 28 16 2 10	0	0
2	E	2	Total C N O 28 16 2 10	0	0
2	F	2	Total C N O 28 16 2 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

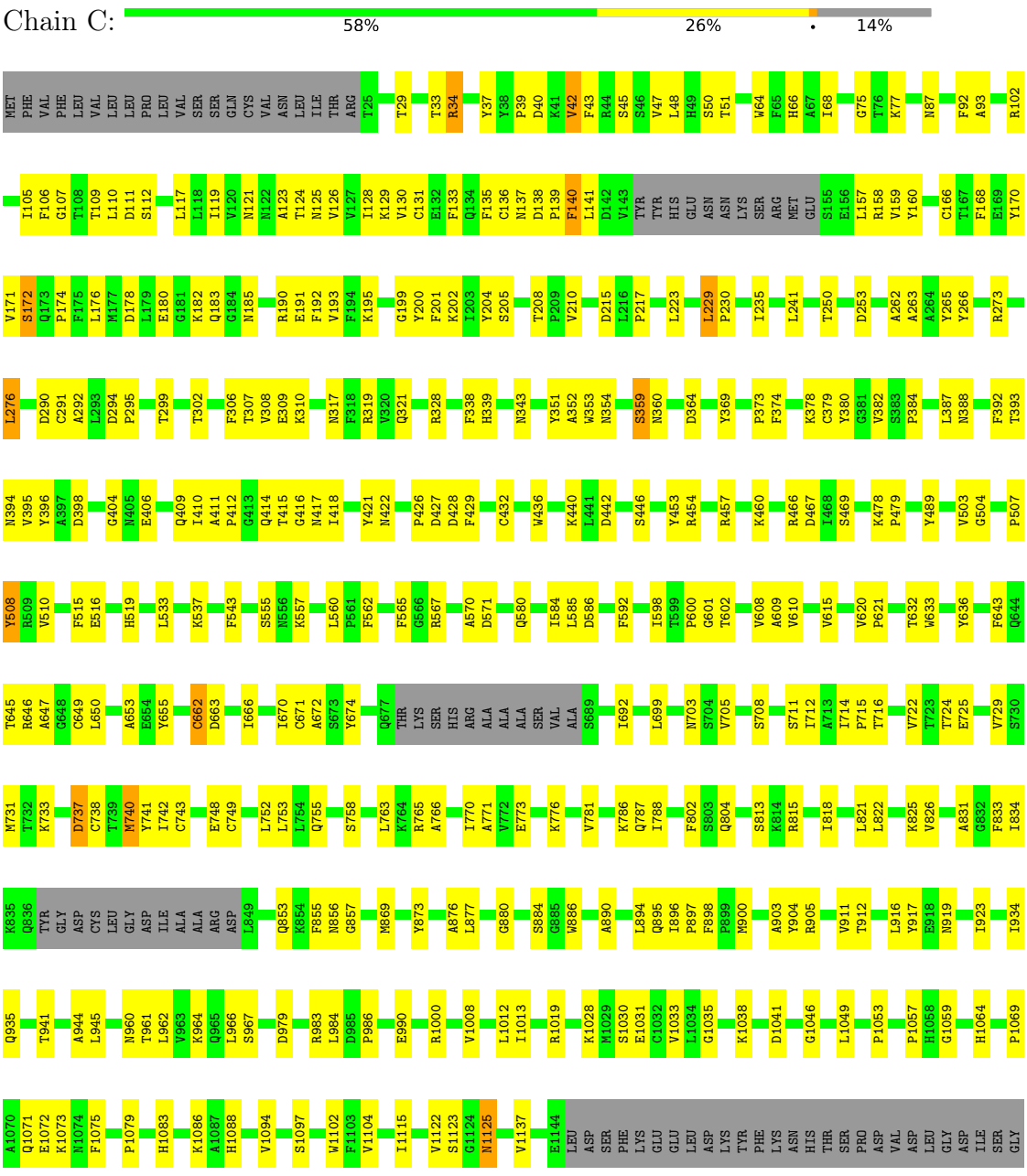
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0

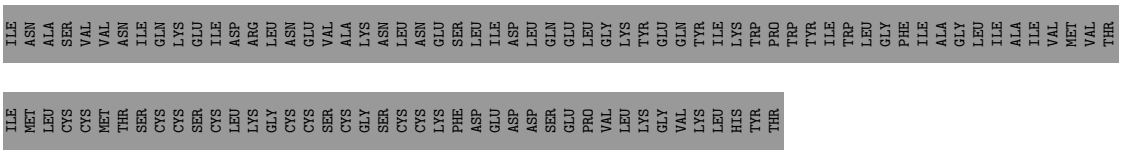
3 Residue-property plots (i)

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

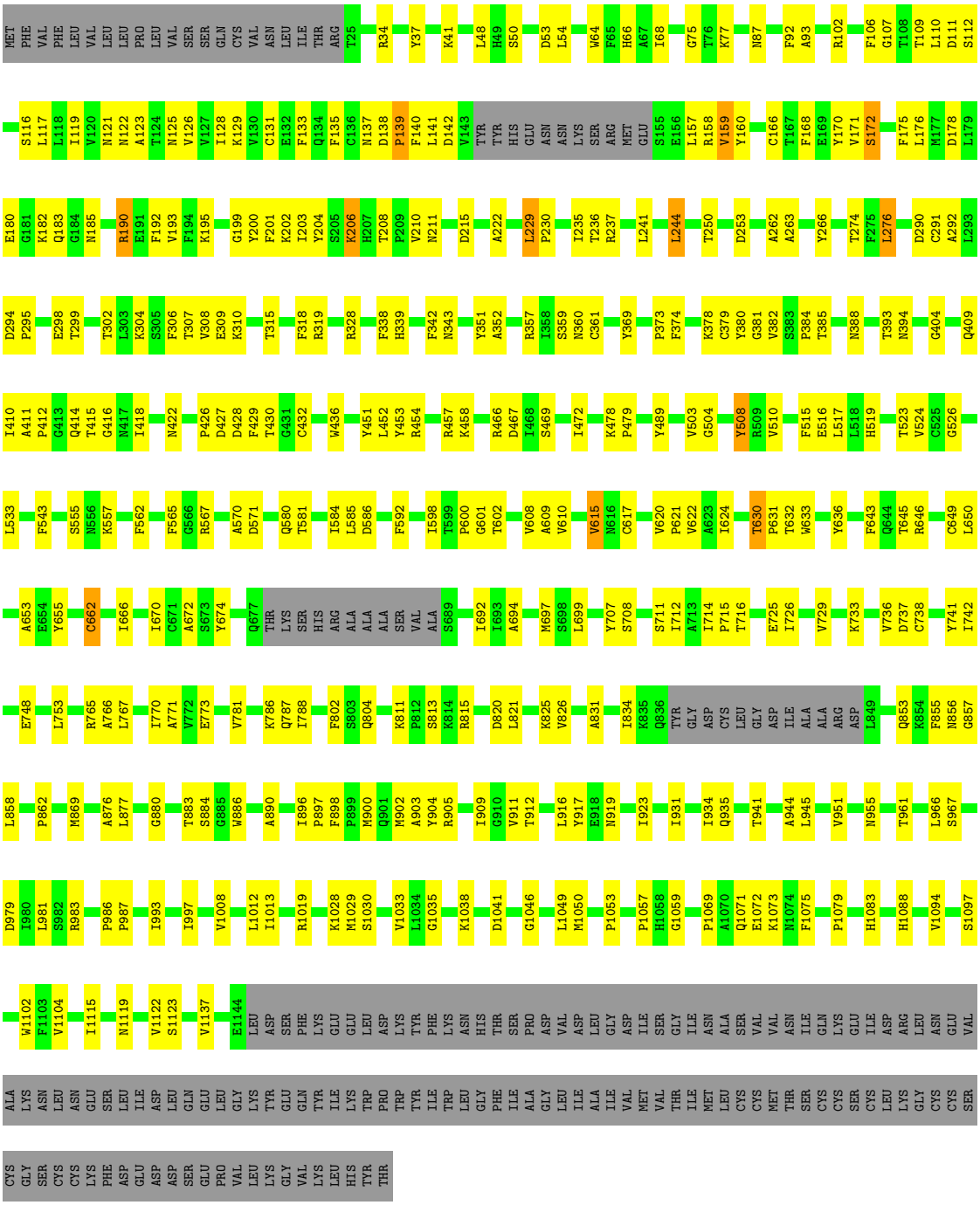
Chain C:





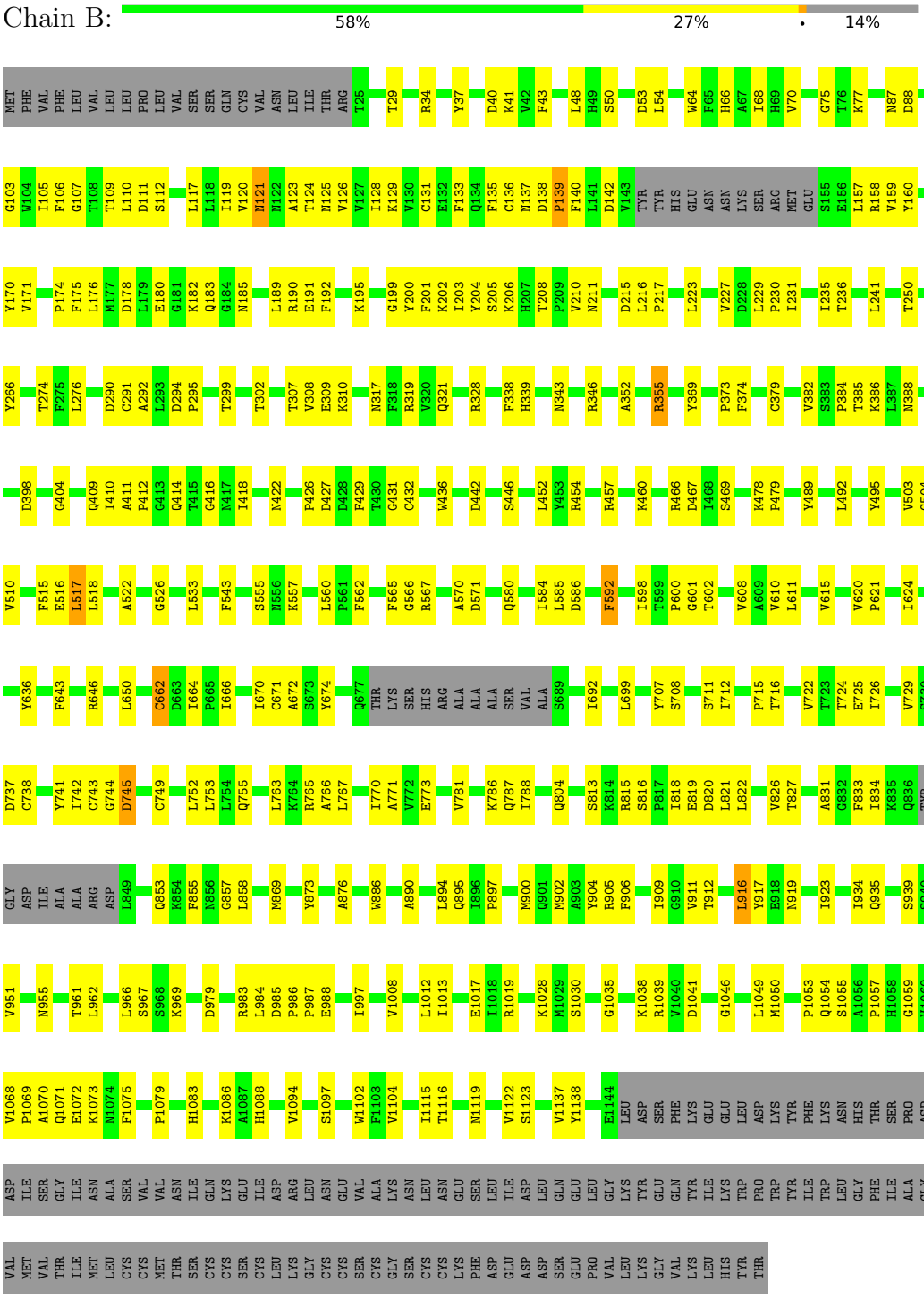
• Molecule 1: Spike glycoprotein

Chain A:



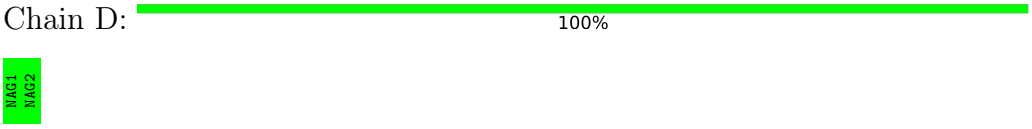
• Molecule 1: Spike glycoprotein

Chain B:



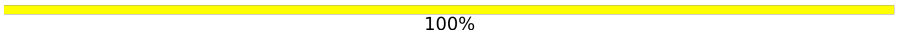
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



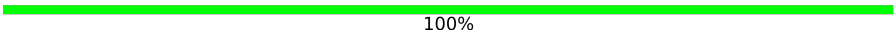
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



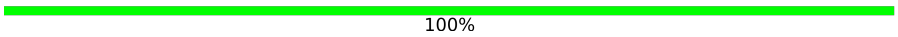
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:



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

Chain H:

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

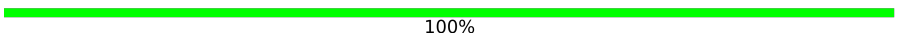
Chain I:

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

Chain J:

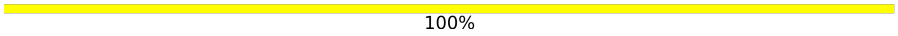
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



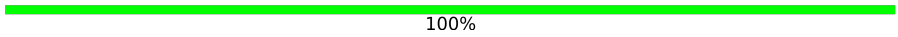
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



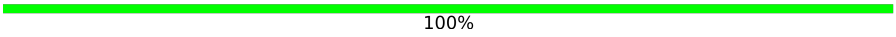
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:



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

Chain O:

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

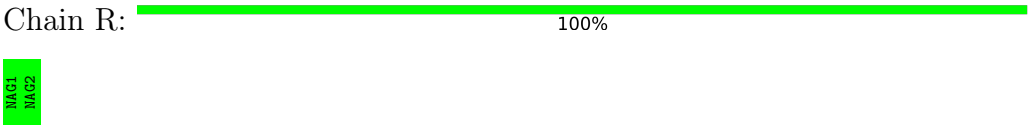
Chain P:

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

Chain Q:

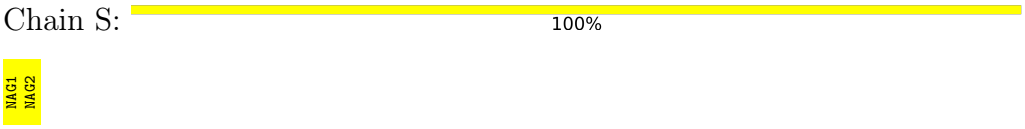
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



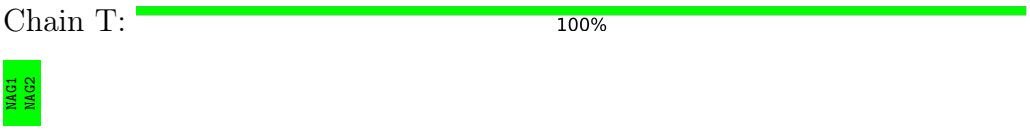
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



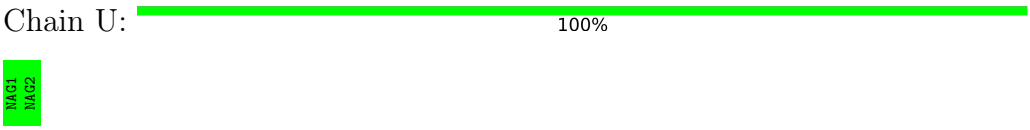
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:



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

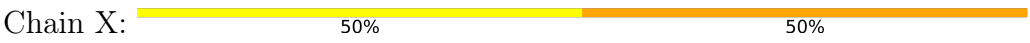
Chain V:

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

Chain W:

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

Chain X:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163826	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 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

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	0.33	0/8644	0.51	0/11776
1	B	0.32	0/8644	0.51	0/11776
1	C	0.34	0/8644	0.51	0/11776
All	All	0.33	0/25932	0.51	0/35328

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain
1	B	355	ARG	Sidechain
1	B	567	ARG	Sidechain
1	C	273	ARG	Sidechain
1	C	34	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8442	0	8221	260	0
1	B	8442	0	8221	270	0
1	C	8442	0	8221	282	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	2	0
2	K	28	0	25	0	0
2	L	28	0	25	1	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
2	P	28	0	25	1	0
2	Q	28	0	25	2	0
2	R	28	0	25	0	0
2	S	28	0	25	1	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	1	0
2	W	28	0	25	0	0
2	X	28	0	25	1	0
3	A	98	0	91	2	0
3	B	98	0	91	1	0
3	C	98	0	91	2	0
All	All	26208	0	25461	736	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 14.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HD3	1:C:121:ASN:O	1.47	1.13
1:A:102:ARG:HD2	1:A:140:PHE:CZ	1.89	1.06
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.56	0.88
1:A:102:ARG:HD2	1:A:140:PHE:HZ	1.37	0.87
1:C:102:ARG:CD	1:C:121:ASN:O	2.23	0.87
1:A:916:LEU:HD12	1:A:923:ILE:HD13	1.60	0.83
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.61	0.83
1:C:916:LEU:HD12	1:C:923:ILE:HD13	1.61	0.83
1:B:557:LYS:HB2	1:B:584:ILE:HG21	1.62	0.81
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.61	0.80
1:B:176:LEU:HB2	1:B:190:ARG:HE	1.49	0.77
1:A:393:THR:HB	1:A:516:GLU:HG3	1.66	0.76
1:B:742:ILE:HG23	1:B:997:ILE:HD12	1.66	0.76
1:B:821:LEU:HD22	1:B:935:GLN:HG3	1.66	0.76
1:C:708:SER:HB3	1:C:711:SER:HB3	1.67	0.76
1:B:708:SER:HB3	1:B:711:SER:HB3	1.67	0.75
1:A:738:CYS:O	1:A:742:ILE:HB	1.87	0.74
1:C:204:TYR:HB3	1:C:223:LEU:HG	1.69	0.74
1:B:34:ARG:NH2	1:B:217:PRO:O	2.20	0.74
1:C:1030:SER:HB3	1:B:1041:ASP:HB3	1.69	0.73
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.21	0.73
1:C:1125:ASN:ND2	1:C:1125:ASN:O	2.21	0.73
1:C:141:LEU:HD23	1:C:158:ARG:HG3	1.70	0.73
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.71	0.73
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.72	0.72
1:B:984:LEU:HD13	1:B:988:GLU:HG3	1.72	0.72
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.71	0.71
1:C:199:GLY:HA3	1:C:230:PRO:HA	1.73	0.70
1:A:141:LEU:HD23	1:A:158:ARG:HG3	1.71	0.70
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.24	0.70
1:C:139:PRO:HG2	1:C:158:ARG:HB3	1.71	0.70
1:C:178:ASP:OD1	1:C:190:ARG:NH2	2.25	0.70
1:B:738:CYS:O	1:B:742:ILE:HB	1.91	0.70
1:A:961:THR:HG21	1:B:765:ARG:HH22	1.57	0.69
1:C:384:PRO:HA	1:C:387:LEU:HB2	1.75	0.69
1:C:1041:ASP:HB3	1:A:1030:SER:HB3	1.74	0.68
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.24	0.68
1:C:68:ILE:HA	1:C:250:THR:HB	1.74	0.68
1:A:68:ILE:HA	1:A:250:THR:HB	1.74	0.68
1:B:369:TYR:HA	1:B:374:PHE:HE1	1.58	0.68
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	1.75	0.68
1:C:716:THR:OG1	1:C:1071:GLN:NE2	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:THR:OG1	1:B:1071:GLN:NE2	2.28	0.67
1:A:716:THR:OG1	1:A:1071:GLN:NE2	2.28	0.67
1:C:765:ARG:HH22	1:B:961:THR:HG21	1.60	0.67
1:A:519:HIS:HB3	1:A:565:PHE:HB2	1.77	0.66
1:A:50:SER:HB3	1:A:276:LEU:HD12	1.77	0.66
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.25	0.66
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.77	0.66
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.77	0.66
1:B:64:TRP:HB3	1:B:263:ALA:HB3	1.76	0.66
1:A:64:TRP:HB3	1:A:263:ALA:HB3	1.78	0.65
1:A:195:LYS:HE3	1:A:202:LYS:HG2	1.79	0.65
1:A:116:SER:HB2	1:A:237:ARG:HH22	1.62	0.65
1:C:64:TRP:HB3	1:C:263:ALA:HB3	1.77	0.65
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.78	0.65
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.80	0.64
1:C:50:SER:HB3	1:C:276:LEU:HD12	1.78	0.64
1:B:128:ILE:HG12	1:B:170:TYR:HB3	1.80	0.63
1:C:317:ASN:ND2	1:A:737:ASP:OD2	2.32	0.63
1:B:666:ILE:HB	1:B:670:ILE:O	1.99	0.62
1:A:199:GLY:HA3	1:A:230:PRO:HA	1.81	0.62
1:B:102:ARG:O	1:B:121:ASN:ND2	2.32	0.62
1:C:393:THR:HB	1:C:516:GLU:HG3	1.80	0.62
1:A:821:LEU:HD22	1:A:935:GLN:HG3	1.80	0.62
1:B:379:CYS:HA	1:B:432:CYS:HB2	1.81	0.62
1:C:984:LEU:O	1:B:386:LYS:NZ	2.21	0.62
1:C:387:LEU:HD11	1:C:392:PHE:HZ	1.64	0.62
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.82	0.62
1:B:516:GLU:O	1:B:518:LEU:N	2.33	0.62
1:B:886:TRP:HH2	1:B:904:TYR:HB3	1.64	0.62
1:C:555:SER:HB2	1:C:586:ASP:HB2	1.81	0.62
1:B:418:ILE:HG12	1:B:422:ASN:HD22	1.63	0.61
1:B:37:TYR:HB3	1:B:223:LEU:HB3	1.83	0.61
1:C:961:THR:HG21	1:A:765:ARG:HH22	1.65	0.61
1:C:712:ILE:O	1:C:1075:PHE:N	2.31	0.61
1:B:897:PRO:HG2	1:B:900:MET:HB2	1.83	0.61
1:C:195:LYS:HE3	1:C:202:LYS:HG2	1.82	0.61
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.82	0.61
1:B:199:GLY:HA3	1:B:230:PRO:HA	1.83	0.61
1:C:897:PRO:HG2	1:C:900:MET:HB2	1.83	0.60
1:C:92:PHE:CE2	1:C:265:TYR:HE1	2.18	0.60
1:C:570:ALA:HB2	1:A:853:GLN:NE2	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HD21	1:B:869:MET:HB2	1.83	0.60
1:C:129:LYS:HE2	1:C:133:PHE:HZ	1.66	0.60
1:A:129:LYS:HE2	1:A:133:PHE:HZ	1.67	0.60
1:A:711:SER:O	1:B:895:GLN:NE2	2.34	0.60
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.83	0.60
1:B:138:ASP:H	1:B:139:PRO:HD2	1.66	0.60
1:A:359:SER:OG	1:A:360:ASN:N	2.35	0.60
1:A:570:ALA:HB2	1:B:853:GLN:NE2	2.15	0.60
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.84	0.60
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.83	0.60
1:B:107:GLY:H	1:B:235:ILE:HG23	1.66	0.60
1:B:393:THR:HB	1:B:516:GLU:HG3	1.82	0.60
1:B:555:SER:HB2	1:B:586:ASP:HB2	1.82	0.60
1:A:571:ASP:HB3	1:B:967:SER:HB3	1.83	0.60
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.83	0.60
1:C:102:ARG:NH1	1:C:140:PHE:CZ	2.70	0.60
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.84	0.60
1:C:379:CYS:HA	1:C:432:CYS:HB2	1.85	0.59
1:A:712:ILE:O	1:A:1075:PHE:N	2.32	0.59
1:C:199:GLY:CA	1:C:230:PRO:HA	2.33	0.59
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.84	0.59
1:C:609:ALA:HB1	1:C:650:LEU:HD21	1.85	0.59
1:A:369:TYR:HA	1:A:374:PHE:HE1	1.66	0.59
1:B:129:LYS:HE2	1:B:133:PHE:HZ	1.67	0.59
1:B:138:ASP:N	1:B:139:PRO:HD2	2.17	0.59
1:B:712:ILE:O	1:B:1075:PHE:N	2.33	0.59
1:A:415:THR:HB	1:B:385:THR:HB	1.84	0.59
1:B:369:TYR:HA	1:B:374:PHE:CE1	2.37	0.59
1:C:107:GLY:H	1:C:235:ILE:HG23	1.69	0.58
1:C:478:LYS:HD2	1:C:479:PRO:HD2	1.85	0.58
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.85	0.58
1:B:48:LEU:HD12	1:B:276:LEU:HD21	1.84	0.58
1:C:580:GLN:O	3:C:1304:NAG:O3	2.22	0.58
1:A:379:CYS:HA	1:A:432:CYS:HB2	1.83	0.58
1:C:369:TYR:HA	1:C:374:PHE:HE1	1.68	0.58
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.84	0.58
1:A:192:PHE:HA	1:A:204:TYR:O	2.04	0.58
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.83	0.58
1:B:941:THR:HG21	1:B:944:ALA:HB2	1.85	0.58
1:C:307:THR:HA	1:C:602:THR:HG21	1.86	0.58
1:C:738:CYS:O	1:C:742:ILE:HB	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:THR:HG21	1:A:944:ALA:HB2	1.86	0.57
1:C:941:THR:HG21	1:C:944:ALA:HB2	1.85	0.57
1:B:580:GLN:O	3:B:1305:NAG:O3	2.22	0.57
1:C:853:GLN:NE2	1:B:570:ALA:HB2	2.18	0.57
1:A:107:GLY:H	1:A:235:ILE:HG23	1.69	0.57
1:C:763:LEU:HD11	1:C:1008:VAL:HG21	1.86	0.57
1:C:359:SER:OG	1:C:360:ASN:N	2.37	0.57
1:C:894:LEU:HD21	1:B:715:PRO:HD3	1.86	0.57
1:C:967:SER:HB3	1:B:571:ASP:HB2	1.86	0.57
1:B:204:TYR:HB3	1:B:223:LEU:HG	1.86	0.57
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.86	0.57
1:C:415:THR:HB	1:A:385:THR:HB	1.86	0.57
1:A:102:ARG:CD	1:A:140:PHE:HZ	2.14	0.57
1:C:571:ASP:HB2	1:A:967:SER:HB3	1.86	0.57
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.87	0.57
1:A:580:GLN:O	3:A:1304:NAG:O3	2.22	0.57
1:B:979:ASP:OD1	1:B:983:ARG:NH2	2.36	0.57
1:C:1125:ASN:HD22	1:C:1125:ASN:C	2.03	0.57
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.87	0.57
1:C:138:ASP:HA	1:C:159:VAL:HG23	1.87	0.56
1:A:135:PHE:HB3	1:A:160:TYR:HA	1.87	0.56
1:C:359:SER:OG	1:C:360:ASN:OD1	2.23	0.56
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.87	0.56
1:C:896:ILE:HG22	1:B:712:ILE:HG13	1.87	0.56
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.87	0.56
1:C:138:ASP:HB2	1:C:241:LEU:HD23	1.85	0.56
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.86	0.56
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.86	0.56
1:C:699:LEU:HD21	1:A:869:MET:HB2	1.87	0.56
1:A:307:THR:HA	1:A:602:THR:HG21	1.88	0.56
1:B:608:VAL:O	1:B:636:TYR:OH	2.21	0.56
1:C:457:ARG:NE	1:C:467:ASP:OD2	2.30	0.56
1:B:643:PHE:HB3	1:B:650:LEU:HB3	1.87	0.56
1:A:357:ARG:HB3	1:A:357:ARG:NH1	2.21	0.56
1:C:643:PHE:CD2	1:C:655:TYR:HB2	2.41	0.56
1:C:714:ILE:HD11	1:C:1094:VAL:HG11	1.88	0.56
1:B:902:MET:SD	1:B:1050:MET:HE3	2.45	0.56
1:C:409:GLN:NE2	1:C:416:GLY:HA3	2.22	0.55
1:C:712:ILE:HG13	1:A:896:ILE:HG22	1.87	0.55
1:B:135:PHE:HB3	1:B:160:TYR:HA	1.87	0.55
1:B:307:THR:HA	1:B:602:THR:HG21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:VAL:O	1:C:636:TYR:OH	2.20	0.55
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.29	0.55
1:B:516:GLU:C	1:B:518:LEU:H	2.10	0.55
1:B:902:MET:SD	1:B:1050:MET:CE	2.95	0.55
1:A:570:ALA:HB2	1:B:853:GLN:HE21	1.72	0.55
1:A:979:ASP:OD1	1:A:983:ARG:NH2	2.40	0.55
1:C:176:LEU:HB2	1:C:190:ARG:NE	2.22	0.55
1:C:560:LEU:HD12	1:C:562:PHE:HE1	1.70	0.55
1:C:869:MET:HB2	1:B:699:LEU:HD21	1.89	0.55
1:B:92:PHE:CE2	1:B:265:TYR:HE1	2.25	0.55
1:C:138:ASP:N	1:C:139:PRO:HD3	2.22	0.55
1:C:886:TRP:HH2	1:C:904:TYR:HB3	1.71	0.55
1:C:135:PHE:HB3	1:C:160:TYR:HA	1.88	0.54
1:A:102:ARG:HD2	1:A:140:PHE:CE2	2.38	0.54
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.87	0.54
1:C:737:ASP:OD1	1:C:857:GLY:HA3	2.08	0.54
1:B:37:TYR:OH	1:B:54:LEU:O	2.26	0.54
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.90	0.54
1:C:190:ARG:HB3	1:C:192:PHE:HE2	1.73	0.54
1:C:215:ASP:OD1	1:C:215:ASP:N	2.41	0.54
1:B:119:ILE:HA	1:B:128:ILE:HG22	1.90	0.54
1:B:178:ASP:OD1	1:B:190:ARG:NH2	2.41	0.54
1:B:199:GLY:CA	1:B:230:PRO:HA	2.38	0.54
1:A:178:ASP:HA	1:A:190:ARG:HH22	1.73	0.54
1:B:29:THR:HB	1:B:64:TRP:HE1	1.72	0.54
1:C:102:ARG:CG	1:C:121:ASN:O	2.55	0.54
1:C:394:ASN:OD1	1:C:395:VAL:N	2.41	0.54
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.90	0.54
1:C:592:PHE:HE1	1:A:855:PHE:HD1	1.56	0.53
1:C:1038:LYS:NZ	1:A:1038:LYS:HZ2	2.06	0.53
1:A:409:GLN:NE2	1:A:416:GLY:HA3	2.22	0.53
1:A:138:ASP:N	1:A:139:PRO:HD2	2.23	0.53
1:A:428:ASP:OD1	1:A:428:ASP:N	2.40	0.53
1:A:902:MET:SD	1:A:1050:MET:CE	2.97	0.53
1:C:1125:ASN:ND2	1:C:1125:ASN:C	2.62	0.53
1:B:215:ASP:OD1	1:B:215:ASP:N	2.41	0.53
1:B:478:LYS:NZ	1:B:479:PRO:O	2.41	0.53
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.35	0.53
1:C:369:TYR:HA	1:C:374:PHE:CE1	2.44	0.53
1:A:418:ILE:HG12	1:A:422:ASN:HD22	1.73	0.53
1:B:788:ILE:HG23	1:B:876:ALA:HB2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:LEU:HD21	1:B:939:SER:HB2	1.89	0.53
1:B:109:THR:O	1:B:111:ASP:N	2.42	0.53
1:A:608:VAL:O	1:A:636:TYR:OH	2.22	0.53
1:A:643:PHE:O	1:A:649:CYS:SG	2.67	0.53
1:C:440:LYS:HE3	1:C:440:LYS:HA	1.91	0.53
1:A:138:ASP:HA	1:A:159:VAL:HG23	1.89	0.53
1:C:128:ILE:HG12	1:C:170:TYR:HB3	1.90	0.53
1:C:171:VAL:HG12	1:C:172:SER:N	2.24	0.53
1:C:40:ASP:HB3	1:C:42:VAL:HG22	1.91	0.53
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.44	0.53
1:A:359:SER:OG	1:A:360:ASN:OD1	2.25	0.53
1:A:369:TYR:HA	1:A:374:PHE:CE1	2.42	0.53
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.24	0.53
1:A:37:TYR:OH	1:A:53:ASP:OD1	2.27	0.52
1:A:620:VAL:HG13	1:A:621:PRO:HD3	1.91	0.52
1:B:111:ASP:OD1	1:B:112:SER:N	2.42	0.52
1:B:410:ILE:HD11	1:B:510:VAL:HG11	1.91	0.52
1:C:412:PRO:HB3	1:C:427:ASP:HA	1.91	0.52
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	1.92	0.52
1:C:570:ALA:HB2	1:A:853:GLN:HE21	1.74	0.52
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.74	0.52
1:A:478:LYS:NZ	1:A:479:PRO:O	2.42	0.52
1:C:853:GLN:O	1:C:855:PHE:N	2.40	0.52
1:C:1019:ARG:NH2	1:B:1017:GLU:HG2	2.24	0.52
1:A:388:ASN:O	1:A:526:GLY:HA3	2.10	0.52
1:B:816:SER:HB2	1:B:819:GLU:HG3	1.91	0.52
1:A:48:LEU:HD12	1:A:276:LEU:HD21	1.92	0.52
1:B:611:LEU:HB2	1:B:650:LEU:HG	1.90	0.52
1:C:168:PHE:HE2	1:C:229:LEU:HD13	1.73	0.52
1:A:853:GLN:O	1:A:855:PHE:N	2.39	0.52
1:A:215:ASP:N	1:A:215:ASP:OD1	2.42	0.52
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.90	0.52
1:C:180:GLU:HG3	1:C:182:LYS:H	1.75	0.52
1:C:200:TYR:O	1:C:202:LYS:HD2	2.09	0.52
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.45	0.52
1:A:708:SER:HA	3:A:1306:NAG:H82	1.92	0.51
1:B:180:GLU:HG3	1:B:182:LYS:H	1.74	0.51
1:B:620:VAL:HG13	1:B:621:PRO:HD3	1.93	0.51
1:C:87:ASN:OD1	1:C:87:ASN:N	2.44	0.51
1:C:708:SER:HA	3:C:1306:NAG:H82	1.92	0.51
2:V:1:NAG:H3	2:V:2:NAG:O5	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD23	1:A:306:PHE:HE1	1.76	0.51
1:A:609:ALA:HB1	1:A:650:LEU:HD21	1.90	0.51
1:A:630:THR:HG23	1:A:631:PRO:HD3	1.93	0.51
1:B:457:ARG:NE	1:B:467:ASP:OD2	2.31	0.51
1:A:180:GLU:HG3	1:A:182:LYS:H	1.75	0.51
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.45	0.51
1:C:64:TRP:CE2	1:C:266:TYR:HE2	2.28	0.51
1:C:290:ASP:OD1	1:C:291:CYS:N	2.43	0.51
1:C:724:THR:HG23	1:C:934:ILE:HD11	1.92	0.51
1:A:206:LYS:HG3	1:A:222:ALA:O	2.10	0.51
1:A:1038:LYS:NZ	1:B:1038:LYS:HZ2	2.09	0.51
1:A:128:ILE:HG12	1:A:170:TYR:HB3	1.92	0.51
1:B:388:ASN:O	1:B:526:GLY:HA3	2.11	0.51
1:B:737:ASP:OD1	1:B:857:GLY:HA3	2.10	0.51
1:C:886:TRP:HB3	1:C:1035:GLY:HA2	1.91	0.51
1:B:308:VAL:O	1:B:602:THR:N	2.43	0.51
1:A:352:ALA:HA	1:A:466:ARG:HD3	1.93	0.51
1:C:111:ASP:OD1	1:C:112:SER:N	2.41	0.50
1:C:195:LYS:HE2	1:C:204:TYR:HE2	1.76	0.50
1:A:373:PRO:HD2	1:A:436:TRP:CD1	2.46	0.50
1:C:418:ILE:HG12	1:C:422:ASN:HD22	1.76	0.50
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.92	0.50
1:A:382:VAL:HG23	1:B:983:ARG:HG3	1.92	0.50
1:C:716:THR:HG21	1:C:1073:LYS:HD3	1.94	0.50
1:A:87:ASN:OD1	1:A:87:ASN:N	2.43	0.50
1:A:290:ASP:OD1	1:A:291:CYS:N	2.44	0.50
1:B:1068:VAL:HG12	1:B:1070:ALA:H	1.77	0.50
1:C:620:VAL:HG13	1:C:621:PRO:HD3	1.93	0.50
1:C:853:GLN:HE21	1:B:570:ALA:HB2	1.77	0.50
1:A:208:THR:HG22	1:A:210:VAL:HG22	1.93	0.50
1:B:355:ARG:HG3	1:B:398:ASP:OD1	2.10	0.50
1:C:666:ILE:HB	1:C:670:ILE:O	2.12	0.50
1:A:909:ILE:HG13	1:A:911:VAL:HG23	1.94	0.50
1:B:716:THR:HG21	1:B:1073:LYS:HD3	1.92	0.50
1:A:902:MET:SD	1:A:1050:MET:HE3	2.51	0.50
1:B:68:ILE:HA	1:B:250:THR:HB	1.94	0.50
1:C:48:LEU:HD12	1:C:276:LEU:HD21	1.93	0.50
1:A:309:GLU:HA	1:A:601:GLY:HA2	1.94	0.50
1:C:208:THR:HG22	1:C:210:VAL:HG22	1.94	0.50
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.52	0.50
1:B:208:THR:HG22	1:B:210:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:VAL:HG11	1:B:633:TRP:CH2	2.47	0.50
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.75	0.49
1:A:742:ILE:HG23	1:A:997:ILE:HD12	1.94	0.49
1:A:825:LYS:HG2	1:A:945:LEU:HG	1.94	0.49
1:B:290:ASP:OD1	1:B:291:CYS:N	2.43	0.49
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.93	0.49
1:C:126:VAL:O	1:C:171:VAL:HA	2.12	0.49
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.12	0.49
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.12	0.49
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.13	0.49
1:B:555:SER:OG	1:B:557:LYS:HG2	2.12	0.49
1:C:373:PRO:HD2	1:C:436:TRP:CD1	2.48	0.49
1:C:382:VAL:HG23	1:A:983:ARG:HG3	1.93	0.49
1:A:109:THR:O	1:A:111:ASP:N	2.44	0.49
1:A:183:GLN:HG3	1:A:185:ASN:H	1.78	0.49
1:A:737:ASP:OD1	1:A:857:GLY:HA3	2.12	0.49
1:B:87:ASN:N	1:B:87:ASN:OD1	2.44	0.49
1:B:138:ASP:O	1:B:139:PRO:C	2.51	0.49
1:C:1038:LYS:HZ2	1:B:1038:LYS:HZ2	1.59	0.49
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.48	0.49
1:B:183:GLN:HG3	1:B:185:ASN:H	1.77	0.49
1:C:75:GLY:O	1:C:77:LYS:N	2.41	0.49
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.94	0.49
1:B:200:TYR:O	1:B:202:LYS:HD2	2.12	0.49
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.95	0.49
1:C:911:VAL:O	1:C:912:THR:OG1	2.30	0.49
1:C:1038:LYS:HZ2	1:B:1038:LYS:NZ	2.10	0.49
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.95	0.49
1:A:645:THR:HG23	1:A:670:ILE:HG13	1.93	0.49
1:A:742:ILE:HG21	1:A:753:LEU:HD22	1.93	0.49
1:B:176:LEU:HB2	1:B:190:ARG:HH21	1.76	0.49
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.95	0.49
1:A:199:GLY:CA	1:A:230:PRO:HA	2.43	0.49
1:A:766:ALA:O	1:A:770:ILE:HG12	2.13	0.49
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.35	0.49
1:C:43:PHE:H	1:B:566:GLY:HA2	1.77	0.49
1:A:121:ASN:OD1	1:A:122:ASN:N	2.45	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.49
1:B:742:ILE:HG21	1:B:753:LEU:HD22	1.95	0.49
1:C:309:GLU:HA	1:C:601:GLY:HA2	1.95	0.49
1:A:707:TYR:HE2	1:B:897:PRO:HA	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PRO:HD2	1:B:436:TRP:CD1	2.48	0.49
1:C:752:LEU:O	1:C:755:GLN:HG2	2.13	0.48
1:A:430:THR:HG21	1:A:517:LEU:HD21	1.95	0.48
1:C:183:GLN:HG3	1:C:185:ASN:H	1.78	0.48
1:C:352:ALA:HA	1:C:466:ARG:HD3	1.96	0.48
1:C:119:ILE:HA	1:C:128:ILE:HG22	1.95	0.48
1:C:821:LEU:HD22	1:C:935:GLN:HG3	1.94	0.48
1:A:119:ILE:HA	1:A:128:ILE:HG22	1.95	0.48
1:A:716:THR:HG21	1:A:1073:LYS:HD3	1.94	0.48
1:B:309:GLU:HA	1:B:601:GLY:HA2	1.95	0.48
1:B:766:ALA:O	1:B:770:ILE:HG12	2.14	0.48
1:B:853:GLN:O	1:B:855:PHE:N	2.39	0.48
1:C:105:ILE:HD11	1:C:241:LEU:HD21	1.96	0.48
1:C:109:THR:O	1:C:111:ASP:N	2.42	0.48
1:C:157:LEU:HG	1:C:158:ARG:H	1.77	0.48
1:C:897:PRO:HD3	1:B:711:SER:O	2.13	0.48
1:A:811:LYS:HD3	1:A:820:ASP:OD2	2.14	0.48
1:B:75:GLY:O	1:B:77:LYS:N	2.42	0.48
1:B:105:ILE:HD11	1:B:241:LEU:HD21	1.95	0.48
1:C:378:LYS:NZ	1:C:380:TYR:OH	2.47	0.48
1:C:643:PHE:O	1:C:650:LEU:N	2.33	0.48
1:C:646:ARG:HH22	1:A:831:ALA:HB3	1.78	0.48
1:A:646:ARG:HH22	1:B:831:ALA:HB3	1.78	0.48
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.96	0.48
1:B:64:TRP:CE2	1:B:266:TYR:HE1	2.31	0.48
1:B:560:LEU:HD12	1:B:562:PHE:HE1	1.79	0.48
1:B:729:VAL:HG11	1:B:781:VAL:HG11	1.96	0.48
1:C:1079:PRO:HB3	1:A:917:TYR:CZ	2.48	0.48
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	1.95	0.48
1:A:1088:HIS:CD2	1:A:1122:VAL:HB	2.49	0.48
1:B:40:ASP:OD1	1:B:40:ASP:N	2.47	0.48
1:C:1088:HIS:CD2	1:C:1122:VAL:HB	2.49	0.48
1:B:1088:HIS:CD2	1:B:1122:VAL:HB	2.49	0.48
1:A:378:LYS:NZ	1:A:380:TYR:OH	2.47	0.48
1:C:519:HIS:HD1	1:C:565:PHE:HD2	1.61	0.48
1:B:911:VAL:O	1:B:912:THR:OG1	2.31	0.48
1:C:715:PRO:HG3	1:C:1069:PRO:HB3	1.96	0.47
1:C:967:SER:OG	1:C:967:SER:O	2.32	0.47
1:C:766:ALA:O	1:C:770:ILE:HG12	2.14	0.47
1:A:190:ARG:HB3	1:A:192:PHE:HE2	1.78	0.47
1:A:308:VAL:O	1:A:602:THR:N	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HB	1:A:670:ILE:O	2.14	0.47
2:E:1:NAG:H3	2:E:2:NAG:H83	1.95	0.47
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.95	0.47
1:C:983:ARG:HG3	1:B:382:VAL:HG23	1.95	0.47
1:A:75:GLY:O	1:A:77:LYS:N	2.41	0.47
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.96	0.47
1:B:53:ASP:OD1	1:B:54:LEU:N	2.47	0.47
1:B:379:CYS:HB2	1:B:384:PRO:HD3	1.96	0.47
1:C:737:ASP:OD2	1:B:317:ASN:ND2	2.46	0.47
1:A:911:VAL:O	1:A:912:THR:OG1	2.31	0.47
1:B:157:LEU:HG	1:B:158:ARG:H	1.78	0.47
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.50	0.47
1:B:191:GLU:O	1:B:205:SER:HA	2.14	0.47
1:C:276:LEU:HD23	1:C:306:PHE:HE1	1.78	0.47
1:C:729:VAL:HG11	1:C:781:VAL:HG11	1.97	0.47
1:A:339:HIS:CD2	1:A:343:ASN:HB3	2.49	0.47
1:A:662:CYS:SG	1:A:697:MET:HG3	2.55	0.47
1:A:707:TYR:CE2	1:B:897:PRO:HA	2.50	0.47
1:B:176:LEU:HB2	1:B:190:ARG:NE	2.25	0.47
1:B:715:PRO:HG3	1:B:1069:PRO:HB3	1.97	0.47
1:A:598:ILE:HG21	1:A:672:ALA:HB3	1.97	0.47
1:B:299:THR:HA	1:B:302:THR:HG22	1.97	0.47
1:C:633:TRP:HE3	1:C:633:TRP:O	1.98	0.47
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.97	0.47
1:A:897:PRO:HG2	1:A:900:MET:HB2	1.97	0.47
1:B:126:VAL:O	1:B:171:VAL:HA	2.14	0.47
1:C:379:CYS:HA	1:C:432:CYS:CB	2.44	0.47
1:C:426:PRO:HG2	1:C:429:PHE:HB2	1.97	0.47
1:C:645:THR:HG23	1:C:670:ILE:HG13	1.98	0.46
1:C:1012:LEU:HB3	1:B:1013:ILE:HD13	1.97	0.46
1:C:1013:ILE:HD13	1:A:1012:LEU:HB3	1.96	0.46
1:C:1094:VAL:HB	1:A:904:TYR:OH	2.14	0.46
1:A:379:CYS:HA	1:A:432:CYS:CB	2.45	0.46
1:B:352:ALA:HA	1:B:466:ARG:HD3	1.96	0.46
1:C:339:HIS:CD2	1:C:343:ASN:HB3	2.50	0.46
1:C:740:MET:HE1	1:B:592:PHE:HD1	1.80	0.46
1:A:292:ALA:HB1	1:A:632:THR:OG1	2.15	0.46
1:A:517:LEU:HD23	1:A:517:LEU:H	1.80	0.46
1:A:733:LYS:HE2	1:A:771:ALA:HB1	1.98	0.46
1:B:339:HIS:CD2	1:B:343:ASN:HB3	2.50	0.46
1:C:131:CYS:HB3	1:C:133:PHE:CZ	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:O	1:C:602:THR:N	2.45	0.46
1:A:200:TYR:HA	1:A:229:LEU:N	2.31	0.46
1:A:138:ASP:O	1:A:139:PRO:C	2.53	0.46
1:A:139:PRO:HG3	1:A:244:LEU:HD12	1.98	0.46
1:C:960:ASN:OD1	1:C:964:LYS:NZ	2.46	0.46
1:A:357:ARG:HB3	1:A:357:ARG:CZ	2.46	0.46
1:C:979:ASP:OD1	1:C:983:ARG:NH2	2.40	0.46
1:A:562:PHE:CD2	1:B:41:LYS:HD2	2.50	0.46
1:A:813:SER:OG	1:A:815:ARG:NH1	2.49	0.46
1:A:951:VAL:O	1:A:955:ASN:ND2	2.48	0.46
1:B:208:THR:O	1:B:211:ASN:ND2	2.48	0.46
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.98	0.46
2:J:1:NAG:H4	2:J:2:NAG:C7	2.46	0.46
2:Q:1:NAG:H4	2:Q:2:NAG:C7	2.46	0.46
1:A:385:THR:OG1	1:B:985:ASP:HB3	2.16	0.46
1:B:292:ALA:HB1	1:B:632:THR:OG1	2.15	0.46
2:P:1:NAG:H4	2:P:2:NAG:H2	1.80	0.46
1:C:131:CYS:HB2	1:C:166:CYS:HB3	1.66	0.46
1:C:299:THR:HA	1:C:302:THR:HG22	1.97	0.46
1:C:917:TYR:CZ	1:B:1079:PRO:HB3	2.51	0.46
1:A:1046:GLY:HA2	1:B:890:ALA:HA	1.98	0.46
1:B:610:VAL:HG11	1:B:633:TRP:HH2	1.81	0.46
1:B:819:GLU:HG2	1:B:1054:GLN:HB3	1.97	0.46
1:C:292:ALA:HB1	1:C:632:THR:OG1	2.15	0.46
1:C:742:ILE:HG21	1:C:753:LEU:HD22	1.98	0.45
1:A:295:PRO:HG3	1:A:633:TRP:CE3	2.52	0.45
1:C:643:PHE:O	1:C:649:CYS:SG	2.74	0.45
1:A:454:ARG:NH2	1:A:469:SER:H	2.13	0.45
1:A:919:ASN:O	1:A:923:ILE:HD12	2.16	0.45
1:A:967:SER:OG	1:A:967:SER:O	2.32	0.45
1:C:168:PHE:CE2	1:C:229:LEU:HD13	2.51	0.45
1:A:319:ARG:HH11	1:A:630:THR:HG21	1.81	0.45
1:A:897:PRO:HG2	1:A:900:MET:HG3	1.97	0.45
2:X:1:NAG:H4	2:X:2:NAG:C7	2.47	0.45
1:A:111:ASP:OD1	1:A:112:SER:N	2.43	0.45
1:A:567:ARG:HA	1:A:567:ARG:HD3	1.80	0.45
1:B:598:ILE:HG21	1:B:672:ALA:HB3	1.98	0.45
1:C:422:ASN:ND2	1:C:453:TYR:HB2	2.32	0.45
1:A:610:VAL:HG11	1:A:633:TRP:HH2	1.80	0.45
1:B:858:LEU:HD21	1:B:962:LEU:HD23	1.98	0.45
1:C:102:ARG:HG2	1:C:121:ASN:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.51	0.45
1:A:66:HIS:ND1	1:A:262:ALA:O	2.45	0.45
1:A:382:VAL:HG11	1:A:515:PHE:CD2	2.51	0.45
1:B:66:HIS:ND1	1:B:262:ALA:O	2.47	0.45
1:B:77:LYS:HA	1:B:77:LYS:HD2	1.76	0.45
1:B:102:ARG:NH1	1:B:140:PHE:CD2	2.84	0.45
1:B:379:CYS:HA	1:B:432:CYS:CB	2.46	0.45
1:C:406:GLU:OE1	1:C:418:ILE:HD12	2.17	0.45
1:C:519:HIS:CE1	1:C:567:ARG:HH21	2.34	0.45
1:C:967:SER:HB3	1:B:571:ASP:CB	2.46	0.45
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.45
1:A:729:VAL:HG11	1:A:781:VAL:HG11	1.99	0.45
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.98	0.45
1:A:1013:ILE:HD13	1:B:1012:LEU:HB3	1.99	0.45
1:A:1079:PRO:HB3	1:B:917:TYR:CZ	2.52	0.45
1:B:168:PHE:CE1	1:B:229:LEU:HD13	2.52	0.45
1:B:733:LYS:HE2	1:B:771:ALA:HB1	1.98	0.45
1:C:919:ASN:O	1:C:923:ILE:HD12	2.16	0.45
1:C:66:HIS:ND1	1:C:262:ALA:O	2.48	0.45
1:C:699:LEU:HD11	1:A:869:MET:HB2	1.99	0.45
1:C:1123:SER:O	1:C:1123:SER:OG	2.35	0.45
1:A:236:THR:O	1:A:236:THR:OG1	2.33	0.45
1:B:741:TYR:CE1	1:B:966:LEU:HD21	2.52	0.45
1:B:1073:LYS:HB3	1:B:1073:LYS:HE2	1.74	0.45
1:C:966:LEU:HD22	1:C:1000:ARG:HH11	1.82	0.44
1:A:208:THR:O	1:A:211:ASN:ND2	2.49	0.44
1:A:310:LYS:HG2	1:A:600:PRO:HA	1.97	0.44
1:A:318:PHE:CZ	1:A:615:VAL:HG21	2.52	0.44
1:A:714:ILE:HD11	1:A:1094:VAL:HG11	1.99	0.44
1:B:827:THR:O	1:B:827:THR:OG1	2.33	0.44
1:C:1079:PRO:HB3	1:A:917:TYR:CE1	2.52	0.44
1:A:562:PHE:HD2	1:B:41:LYS:HD2	1.82	0.44
1:B:309:GLU:N	1:B:309:GLU:OE1	2.51	0.44
1:C:543:PHE:HE2	1:C:585:LEU:HD12	1.83	0.44
1:B:813:SER:OG	1:B:815:ARG:NH1	2.51	0.44
1:B:986:PRO:N	1:B:987:PRO:HD2	2.32	0.44
1:C:77:LYS:HD2	1:C:77:LYS:HA	1.76	0.44
1:C:309:GLU:N	1:C:309:GLU:OE1	2.50	0.44
1:C:877:LEU:HD13	1:C:1033:VAL:HG11	2.00	0.44
1:A:1079:PRO:HB3	1:B:917:TYR:CE1	2.53	0.44
1:C:137:ASN:HB3	1:C:139:PRO:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ASP:OD1	1:C:428:ASP:N	2.45	0.44
1:C:742:ILE:CD1	1:C:1000:ARG:HB3	2.47	0.44
1:C:786:LYS:HG3	1:C:787:GLN:HG3	2.00	0.44
1:A:54:LEU:HB2	1:A:195:LYS:HD3	1.99	0.44
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.99	0.44
1:B:138:ASP:N	1:B:139:PRO:CD	2.80	0.44
2:L:1:NAG:H3	2:L:2:NAG:H83	1.99	0.44
1:C:1086:LYS:HE3	1:C:1086:LYS:HB2	1.70	0.44
1:A:309:GLU:N	1:A:309:GLU:OE1	2.50	0.44
1:C:39:PRO:HG2	1:C:51:THR:HG21	1.99	0.44
1:C:962:LEU:HD23	1:C:962:LEU:HA	1.85	0.44
1:C:310:LYS:HG2	1:C:600:PRO:HA	1.99	0.44
1:C:733:LYS:HE2	1:C:771:ALA:HB1	2.00	0.44
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.75	0.44
1:A:299:THR:HA	1:A:302:THR:HG22	2.00	0.44
1:B:543:PHE:HE2	1:B:585:LEU:HD12	1.83	0.44
1:B:819:GLU:HA	1:B:822:LEU:HD12	2.00	0.44
1:B:967:SER:O	1:B:967:SER:OG	2.31	0.44
2:S:1:NAG:H3	2:S:2:NAG:H83	1.99	0.44
1:C:592:PHE:CZ	1:A:855:PHE:HA	2.53	0.44
1:A:557:LYS:HD2	1:B:43:PHE:CD2	2.53	0.44
1:B:295:PRO:HG3	1:B:633:TRP:CE3	2.53	0.44
1:B:752:LEU:O	1:B:755:GLN:HG2	2.17	0.44
1:C:29:THR:HB	1:C:64:TRP:HE1	1.83	0.43
1:C:394:ASN:HD21	1:C:396:TYR:HE2	1.64	0.43
1:C:395:VAL:HG22	1:C:515:PHE:CD1	2.52	0.43
1:C:454:ARG:NH2	1:C:469:SER:H	2.15	0.43
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.83	0.43
1:A:504:GLY:HA3	1:B:373:PRO:O	2.18	0.43
1:C:364:ASP:OD1	1:C:388:ASN:ND2	2.51	0.43
1:C:853:GLN:HE22	1:C:856:ASN:ND2	2.16	0.43
1:A:126:VAL:O	1:A:171:VAL:HA	2.18	0.43
1:C:129:LYS:HE2	1:C:133:PHE:CZ	2.51	0.43
1:A:110:LEU:HD11	1:A:135:PHE:O	2.19	0.43
1:C:45:SER:O	1:C:47:VAL:HG23	2.18	0.43
1:C:620:VAL:CG1	1:C:621:PRO:HD3	2.49	0.43
1:A:592:PHE:HE1	1:B:855:PHE:HD1	1.65	0.43
1:A:748:GLU:N	1:A:748:GLU:OE1	2.49	0.43
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.00	0.43
1:B:818:ILE:O	1:B:822:LEU:HG	2.18	0.43
1:C:543:PHE:CE2	1:C:585:LEU:HD12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:GLN:HB2	1:B:969:LYS:HE2	2.00	0.43
1:C:825:LYS:HG2	1:C:945:LEU:HG	2.00	0.43
1:A:592:PHE:CZ	1:B:855:PHE:HA	2.53	0.43
1:B:543:PHE:CE2	1:B:585:LEU:HD12	2.53	0.43
1:C:776:LYS:HB3	1:C:776:LYS:HE2	1.90	0.43
1:C:831:ALA:HB3	1:B:646:ARG:HH22	1.84	0.43
1:A:1119:ASN:OD1	1:A:1119:ASN:N	2.46	0.43
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.70	0.43
1:A:138:ASP:HB2	1:A:241:LEU:HD23	2.00	0.43
1:A:877:LEU:HD13	1:A:1033:VAL:HG11	2.00	0.43
1:A:1029:MET:SD	1:A:1053:PRO:HG3	2.59	0.43
1:B:410:ILE:CD1	1:B:510:VAL:HG11	2.49	0.43
1:B:454:ARG:NH2	1:B:469:SER:H	2.16	0.43
1:C:712:ILE:HD12	1:C:1094:VAL:HG21	2.00	0.43
1:C:758:SER:O	1:C:758:SER:OG	2.33	0.43
1:A:171:VAL:HG12	1:A:172:SER:H	1.83	0.43
1:A:610:VAL:HG11	1:A:633:TRP:CH2	2.54	0.43
1:A:620:VAL:CG1	1:A:621:PRO:HD3	2.48	0.43
1:B:137:ASN:HB3	1:B:139:PRO:HD2	2.01	0.43
1:B:138:ASP:H	1:B:139:PRO:CD	2.31	0.43
1:B:767:LEU:HD21	1:B:1008:VAL:HG22	2.01	0.43
1:C:37:TYR:HB3	1:C:223:LEU:HB3	2.01	0.43
1:C:42:VAL:HA	1:B:565:PHE:O	2.19	0.43
1:C:66:HIS:CE1	1:C:250:THR:HA	2.54	0.43
1:C:382:VAL:HG11	1:C:515:PHE:CD2	2.54	0.43
1:C:504:GLY:HA3	1:A:373:PRO:O	2.19	0.43
1:A:600:PRO:HD3	1:A:692:ILE:HD11	2.01	0.43
1:B:310:LYS:HG2	1:B:600:PRO:HA	1.99	0.43
1:C:711:SER:O	1:A:897:PRO:HD3	2.18	0.43
1:C:818:ILE:O	1:C:822:LEU:HG	2.19	0.43
1:B:722:VAL:HA	1:B:1064:HIS:O	2.19	0.43
1:B:1123:SER:O	1:B:1123:SER:OG	2.36	0.43
1:A:451:TYR:O	1:A:452:LEU:HD13	2.19	0.42
1:A:617:CYS:HA	1:A:621:PRO:HG2	2.01	0.42
1:A:622:VAL:O	1:A:624:ILE:HG22	2.19	0.42
1:A:767:LEU:HD21	1:A:1008:VAL:HG22	2.01	0.42
1:B:452:LEU:HB3	1:B:492:LEU:HD22	2.01	0.42
1:B:643:PHE:O	1:B:650:LEU:N	2.45	0.42
1:A:137:ASN:HB3	1:A:139:PRO:HD2	2.00	0.42
1:A:276:LEU:HD11	1:A:304:LYS:HG2	2.01	0.42
1:A:458:LYS:HA	1:A:458:LYS:HD2	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HG2	1:B:120:VAL:HG23	2.00	0.42
1:A:116:SER:HB2	1:A:237:ARG:NH2	2.33	0.42
1:A:454:ARG:HH22	1:A:469:SER:H	1.68	0.42
1:A:543:PHE:HE2	1:A:585:LEU:HD12	1.84	0.42
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.34	0.42
1:B:103:GLY:H	1:B:241:LEU:HB2	1.84	0.42
1:B:124:THR:C	1:B:174:PRO:HD3	2.39	0.42
1:B:516:GLU:C	1:B:518:LEU:N	2.70	0.42
1:B:763:LEU:HD12	1:B:763:LEU:HA	1.78	0.42
1:C:110:LEU:HD11	1:C:135:PHE:O	2.19	0.42
1:C:171:VAL:HG12	1:C:172:SER:H	1.84	0.42
1:C:410:ILE:CD1	1:C:510:VAL:HG11	2.49	0.42
1:A:543:PHE:CE2	1:A:585:LEU:HD12	2.54	0.42
1:B:131:CYS:SG	1:B:166:CYS:N	2.92	0.42
1:B:826:VAL:HG11	1:B:1057:PRO:HB2	2.01	0.42
1:B:833:PHE:C	1:B:834:ILE:HD12	2.40	0.42
1:C:600:PRO:HD3	1:C:692:ILE:HD11	2.01	0.42
1:C:662:CYS:HB2	1:C:671:CYS:HB2	1.28	0.42
1:B:110:LEU:HD11	1:B:135:PHE:O	2.19	0.42
1:C:93:ALA:HB3	1:C:266:TYR:HB2	2.01	0.42
1:C:128:ILE:HD11	1:C:229:LEU:HD11	2.02	0.42
1:C:897:PRO:HA	1:B:707:TYR:CE2	2.55	0.42
1:A:129:LYS:HE2	1:A:133:PHE:CZ	2.53	0.42
1:A:472:ILE:HD13	1:A:472:ILE:HA	1.89	0.42
1:A:712:ILE:HD13	1:A:1094:VAL:HG21	2.02	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.88	0.42
1:B:1083:HIS:CG	1:B:1137:VAL:HG22	2.55	0.42
1:C:139:PRO:HD2	1:C:158:ARG:O	2.19	0.42
1:C:503:VAL:O	1:A:373:PRO:HB3	2.19	0.42
1:C:813:SER:OG	1:C:815:ARG:NH1	2.53	0.42
1:C:917:TYR:CE1	1:B:1079:PRO:HB3	2.54	0.42
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.77	0.42
1:C:373:PRO:O	1:B:504:GLY:HA3	2.20	0.42
1:C:897:PRO:HG2	1:C:900:MET:CB	2.50	0.42
1:A:853:GLN:HE22	1:A:856:ASN:ND2	2.17	0.42
1:A:1083:HIS:CG	1:A:1137:VAL:HG22	2.55	0.42
1:C:904:TYR:OH	1:B:1094:VAL:HB	2.20	0.42
1:A:786:LYS:HG3	1:A:787:GLN:HG3	2.01	0.42
1:A:1038:LYS:HZ2	1:B:1038:LYS:HZ2	1.66	0.42
1:B:195:LYS:HE3	1:B:202:LYS:HG2	2.02	0.42
1:B:206:LYS:HD2	1:B:206:LYS:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.54	0.42
1:B:662:CYS:HB2	1:B:671:CYS:HB2	1.33	0.42
1:C:34:ARG:NH2	1:C:217:PRO:O	2.53	0.42
1:C:763:LEU:HA	1:C:763:LEU:HD12	1.74	0.42
1:C:773:GLU:OE1	1:C:1019:ARG:HD3	2.20	0.42
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.38	0.42
1:A:410:ILE:HD11	1:A:510:VAL:HG11	2.02	0.42
1:A:748:GLU:OE2	1:A:981:LEU:HD11	2.20	0.42
1:B:203:ILE:HG13	1:B:227:VAL:HG12	2.01	0.42
1:B:620:VAL:CG1	1:B:621:PRO:HD3	2.49	0.42
1:B:744:GLY:O	1:B:745:ASP:C	2.59	0.42
1:C:130:VAL:O	1:C:130:VAL:HG12	2.20	0.41
1:C:373:PRO:HB3	1:B:503:VAL:O	2.19	0.41
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.55	0.41
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.38	0.41
1:B:900:MET:HA	1:B:917:TYR:OH	2.19	0.41
1:C:457:ARG:NH1	1:C:460:LYS:O	2.46	0.41
1:C:519:HIS:ND1	1:C:565:PHE:HD2	2.18	0.41
1:C:877:LEU:HD11	1:C:1053:PRO:CG	2.50	0.41
1:A:298:GLU:HG3	1:A:315:THR:HB	2.01	0.41
1:B:66:HIS:CE1	1:B:250:THR:HA	2.55	0.41
1:B:200:TYR:HA	1:B:229:LEU:N	2.35	0.41
1:B:319:ARG:O	1:B:321:GLN:NE2	2.51	0.41
1:B:624:ILE:HD12	1:B:629:LEU:HD13	2.02	0.41
1:C:880:GLY:O	1:C:884:SER:OG	2.32	0.41
1:C:890:ALA:HA	1:B:1046:GLY:HA2	2.02	0.41
1:A:253:ASP:OD1	1:A:253:ASP:N	2.53	0.41
1:A:503:VAL:O	1:B:373:PRO:HB3	2.20	0.41
1:A:877:LEU:HD11	1:A:1053:PRO:CG	2.50	0.41
1:A:993:ILE:O	1:A:997:ILE:HG12	2.20	0.41
1:B:391:CYS:HB3	1:B:522:ALA:CB	2.50	0.41
1:B:826:VAL:HB	1:B:1057:PRO:HG2	2.02	0.41
1:C:748:GLU:OE1	1:C:748:GLU:N	2.52	0.41
1:B:919:ASN:O	1:B:923:ILE:HD12	2.19	0.41
1:B:1116:THR:HG22	1:B:1138:TYR:HD2	1.85	0.41
1:C:124:THR:HA	1:C:174:PRO:HG3	2.03	0.41
1:C:319:ARG:O	1:C:321:GLN:NE2	2.52	0.41
1:C:986:PRO:O	1:C:990:GLU:HG3	2.21	0.41
1:A:931:ILE:O	1:A:934:ILE:HG22	2.20	0.41
1:B:175:PHE:CD1	1:B:203:ILE:HG21	2.55	0.41
1:B:962:LEU:HD12	1:B:962:LEU:HA	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ARG:HD3	1:C:567:ARG:HA	1.84	0.41
1:C:610:VAL:HG11	1:C:633:TRP:CH2	2.55	0.41
1:C:722:VAL:HA	1:C:1064:HIS:O	2.21	0.41
1:A:66:HIS:CE1	1:A:250:THR:HA	2.55	0.41
1:A:274:THR:HB	1:A:291:CYS:HB2	2.02	0.41
1:A:328:ARG:NH2	1:A:581:THR:OG1	2.52	0.41
1:B:102:ARG:HG3	1:B:121:ASN:O	2.21	0.41
1:B:328:ARG:HA	1:B:328:ARG:HD2	1.89	0.41
2:O:1:NAG:H3	2:O:2:NAG:O5	2.17	0.41
1:C:37:TYR:CE1	1:C:193:VAL:HG11	2.56	0.41
1:C:191:GLU:O	1:C:205:SER:HA	2.21	0.41
1:C:200:TYR:HA	1:C:229:LEU:N	2.35	0.41
1:C:705:VAL:HG21	1:A:883:THR:OG1	2.20	0.41
1:A:157:LEU:HG	1:A:158:ARG:H	1.85	0.41
1:A:736:VAL:HG22	1:A:858:LEU:HD23	2.02	0.41
1:B:54:LEU:HB2	1:B:195:LYS:HD3	2.03	0.41
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.02	0.41
1:B:742:ILE:HG22	1:B:743:CYS:SG	2.61	0.41
1:C:571:ASP:CB	1:A:967:SER:HB3	2.49	0.41
1:C:895:GLN:HE21	1:B:708:SER:H	1.68	0.41
1:C:903:ALA:N	1:C:916:LEU:HD22	2.35	0.41
1:C:1038:LYS:HZ2	1:A:1038:LYS:HZ2	1.68	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.21	0.41
1:A:328:ARG:HA	1:A:328:ARG:HD2	1.88	0.41
1:A:903:ALA:N	1:A:916:LEU:HD22	2.35	0.41
1:B:92:PHE:CE2	1:B:265:TYR:CE1	3.08	0.41
1:B:382:VAL:HG11	1:B:515:PHE:CD2	2.56	0.41
2:Q:1:NAG:H62	2:Q:2:NAG:H83	2.01	0.41
1:C:253:ASP:N	1:C:253:ASP:OD1	2.54	0.41
1:C:442:ASP:O	1:C:507:PRO:HG3	2.21	0.41
1:C:663:ASP:N	1:C:663:ASP:OD1	2.54	0.41
1:C:703:ASN:ND2	1:A:787:GLN:OE1	2.53	0.41
1:C:1046:GLY:HA2	1:A:890:ALA:HA	2.01	0.41
1:C:1083:HIS:CG	1:C:1137:VAL:HG22	2.55	0.41
1:A:131:CYS:SG	1:A:166:CYS:N	2.94	0.41
1:A:726:ILE:HG12	1:A:945:LEU:HD22	2.02	0.41
1:B:199:GLY:HA3	1:B:230:PRO:CA	2.50	0.41
1:B:236:THR:O	1:B:236:THR:OG1	2.35	0.41
1:B:274:THR:HB	1:B:291:CYS:HB2	2.03	0.41
2:J:1:NAG:H62	2:J:2:NAG:H83	2.02	0.41
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ARG:HH22	1:C:469:SER:H	1.68	0.41
1:C:519:HIS:HB3	1:C:565:PHE:HB2	2.03	0.41
1:C:562:PHE:CD2	1:A:41:LYS:HD2	2.57	0.41
1:C:653:ALA:HB2	1:C:692:ILE:HG22	2.03	0.41
1:A:175:PHE:CD1	1:A:203:ILE:HG21	2.56	0.41
1:A:880:GLY:O	1:A:884:SER:OG	2.31	0.41
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.56	0.41
1:B:951:VAL:O	1:B:955:ASN:ND2	2.53	0.41
1:C:351:TYR:HB3	1:C:453:TYR:HA	2.01	0.40
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.56	0.40
1:C:598:ILE:HG21	1:C:672:ALA:HB3	2.02	0.40
1:C:647:ALA:HB2	1:A:862:PRO:HG2	2.03	0.40
1:A:725:GLU:OE1	1:A:1028:LYS:HD3	2.21	0.40
1:A:1123:SER:O	1:A:1123:SER:OG	2.34	0.40
1:B:129:LYS:HE2	1:B:133:PHE:CZ	2.52	0.40
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.57	0.40
1:A:653:ALA:HB2	1:A:692:ILE:HG22	2.04	0.40
1:B:457:ARG:NH1	1:B:460:LYS:O	2.47	0.40
1:B:1119:ASN:OD1	1:B:1119:ASN:N	2.47	0.40
2:I:1:NAG:H4	2:I:2:NAG:H2	1.80	0.40
1:A:655:TYR:HA	1:A:694:ALA:O	2.21	0.40
1:B:50:SER:HA	1:B:276:LEU:HA	2.03	0.40
1:C:37:TYR:HA	1:C:223:LEU:HB3	2.03	0.40
1:C:354:ASN:O	1:C:398:ASP:HA	2.22	0.40
1:C:417:ASN:O	1:C:421:TYR:HB2	2.20	0.40
1:A:171:VAL:HG12	1:A:172:SER:N	2.37	0.40
1:A:351:TYR:HB3	1:A:453:TYR:HA	2.04	0.40
1:A:410:ILE:CD1	1:A:510:VAL:HG11	2.51	0.40
1:A:557:LYS:HD2	1:B:43:PHE:CE2	2.57	0.40
1:B:442:ASP:O	1:B:507:PRO:HG3	2.20	0.40
1:B:724:THR:HG23	1:B:934:ILE:HD11	2.03	0.40
1:B:725:GLU:OE1	1:B:1028:LYS:HD3	2.21	0.40
1:C:537:LYS:HB3	1:C:537:LYS:HE3	1.84	0.40
1:C:725:GLU:OE1	1:C:1028:LYS:HD3	2.21	0.40
1:C:833:PHE:C	1:C:834:ILE:HD12	2.41	0.40
1:C:1031:GLU:OE1	1:B:1039:ARG:NH2	2.55	0.40
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.74	0.40
1:B:346:ARG:HD2	1:B:346:ARG:HA	1.85	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	1078/1270 (85%)	976 (90%)	95 (9%)	7 (1%)	25	63
1	B	1078/1270 (85%)	974 (90%)	99 (9%)	5 (0%)	29	66
1	C	1078/1270 (85%)	974 (90%)	102 (10%)	2 (0%)	47	80
All	All	3234/3810 (85%)	2924 (90%)	296 (9%)	14 (0%)	38	70

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	SER
1	A	172	SER
1	B	517	LEU
1	C	123	ALA
1	A	139	PRO
1	A	142	ASP
1	B	139	PRO
1	B	142	ASP
1	A	159	VAL
1	B	123	ALA
1	A	123	ALA
1	B	159	VAL
1	A	381	GLY
1	A	834	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	940/1112 (84%)	921 (98%)	19 (2%)	55 79
1	B	940/1112 (84%)	916 (97%)	24 (3%)	46 73
1	C	940/1112 (84%)	917 (98%)	23 (2%)	49 75
All	All	2820/3336 (84%)	2754 (98%)	66 (2%)	53 76

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	33	THR
1	C	42	VAL
1	C	125	ASN
1	C	136	CYS
1	C	140	PHE
1	C	201	PHE
1	C	229	LEU
1	C	276	LEU
1	C	294	ASP
1	C	338	PHE
1	C	353	TRP
1	C	359	SER
1	C	446	SER
1	C	489	TYR
1	C	508	TYR
1	C	615	VAL
1	C	662	CYS
1	C	674	TYR
1	C	731	MET
1	C	737	ASP
1	C	740	MET
1	C	873	TYR
1	C	1125	ASN
1	A	34	ARG
1	A	125	ASN
1	A	176	LEU
1	A	201	PHE
1	A	206	LYS
1	A	229	LEU
1	A	244	LEU
1	A	276	LEU
1	A	294	ASP
1	A	338	PHE
1	A	342	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	361	CYS
1	A	394	ASN
1	A	489	TYR
1	A	508	TYR
1	A	615	VAL
1	A	630	THR
1	A	662	CYS
1	A	674	TYR
1	B	70	VAL
1	B	88	ASP
1	B	121	ASN
1	B	125	ASN
1	B	136	CYS
1	B	201	PHE
1	B	231	ILE
1	B	294	ASP
1	B	338	PHE
1	B	394	ASN
1	B	446	SER
1	B	489	TYR
1	B	495	TYR
1	B	517	LEU
1	B	592	PHE
1	B	615	VAL
1	B	662	CYS
1	B	674	TYR
1	B	731	MET
1	B	745	ASP
1	B	820	ASP
1	B	873	TYR
1	B	916	LEU
1	B	1055	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	804	GLN
1	C	856	ASN
1	C	895	GLN
1	C	1071	GLN
1	A	317	ASN
1	A	394	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	804	GLN
1	A	856	ASN
1	A	895	GLN
1	A	1071	GLN
1	B	125	ASN
1	B	394	ASN
1	B	422	ASN
1	B	804	GLN
1	B	853	GLN
1	B	1071	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.37	0	17,19,21	0.50	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	E	1	2,1	14,14,15	0.38	0	17,19,21	0.51	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	F	1	2,1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.38	0	17,19,21	0.35	0
2	NAG	G	1	2,1	14,14,15	0.33	0	17,19,21	0.34	0
2	NAG	G	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	H	1	2,1	14,14,15	0.40	0	17,19,21	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	H	2	2	14,14,15	0.39	0	17,19,21	0.70	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	I	2	2	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
2	NAG	J	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	0.67	0
2	NAG	J	2	2	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	K	1	2,1	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	L	1	2,1	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.40	0
2	NAG	M	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	M	2	2	14,14,15	0.38	0	17,19,21	0.34	0
2	NAG	N	1	2,1	14,14,15	0.34	0	17,19,21	0.34	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	O	1	2,1	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
2	NAG	O	2	2	14,14,15	0.41	0	17,19,21	0.52	0
2	NAG	P	1	2,1	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	P	2	2	14,14,15	0.64	1 (7%)	17,19,21	0.47	0
2	NAG	Q	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	0.67	0
2	NAG	Q	2	2	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	R	1	2,1	14,14,15	0.37	0	17,19,21	0.50	0
2	NAG	R	2	2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	S	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	S	2	2	14,14,15	0.28	0	17,19,21	0.40	0
2	NAG	T	1	2,1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	T	2	2	14,14,15	0.37	0	17,19,21	0.34	0
2	NAG	U	1	2,1	14,14,15	0.36	0	17,19,21	0.35	0
2	NAG	U	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	V	1	2,1	14,14,15	0.42	0	17,19,21	0.90	1 (5%)
2	NAG	V	2	2	14,14,15	0.42	0	17,19,21	0.53	0
2	NAG	W	1	2,1	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	W	2	2	14,14,15	0.61	1 (7%)	17,19,21	0.47	0
2	NAG	X	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	0.68	0
2	NAG	X	2	2	14,14,15	0.38	0	17,19,21	0.60	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	X	2	2	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1	NAG	O5-C1	-2.66	1.39	1.43
2	J	1	NAG	O5-C1	-2.65	1.39	1.43
2	X	1	NAG	O5-C1	-2.65	1.39	1.43
2	P	2	NAG	C1-C2	2.11	1.55	1.52
2	I	2	NAG	C1-C2	2.02	1.55	1.52
2	W	2	NAG	C1-C2	2.02	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	NAG	O5-C1-C2	3.02	116.06	111.29
2	V	1	NAG	O5-C1-C2	2.87	115.83	111.29
2	H	2	NAG	C2-N2-C7	2.30	126.18	122.90

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	R	1	NAG	C8-C7-N2-C2
2	R	1	NAG	O7-C7-N2-C2
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	L	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7
2	V	2	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	K	1	NAG	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

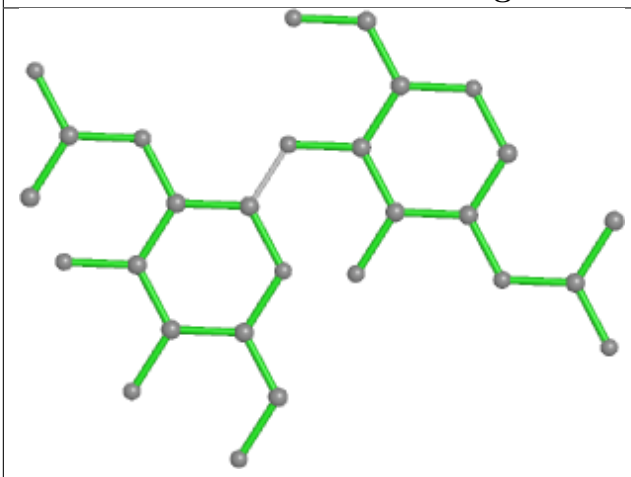
There are no ring outliers.

20 monomers are involved in 12 short contacts:

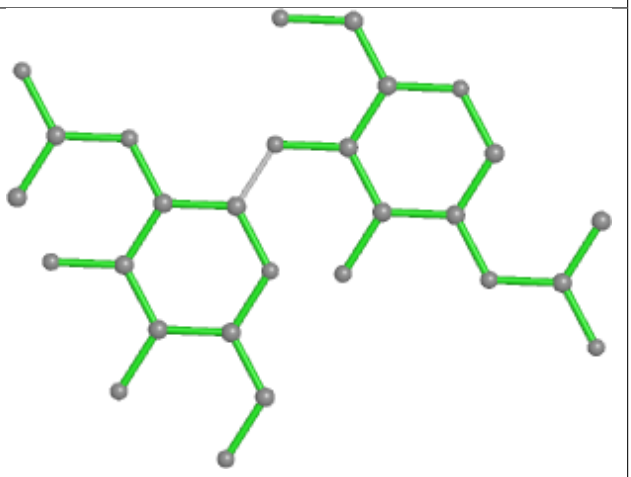
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	2	0
2	L	2	NAG	1	0
2	X	2	NAG	1	0
2	J	2	NAG	2	0
2	Q	2	NAG	2	0
2	P	2	NAG	1	0
2	L	1	NAG	1	0
2	X	1	NAG	1	0
2	J	1	NAG	2	0
2	O	1	NAG	1	0
2	S	2	NAG	1	0
2	E	2	NAG	1	0
2	P	1	NAG	1	0
2	V	2	NAG	1	0
2	S	1	NAG	1	0
2	I	2	NAG	1	0
2	V	1	NAG	1	0
2	E	1	NAG	1	0
2	O	2	NAG	1	0
2	I	1	NAG	1	0

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

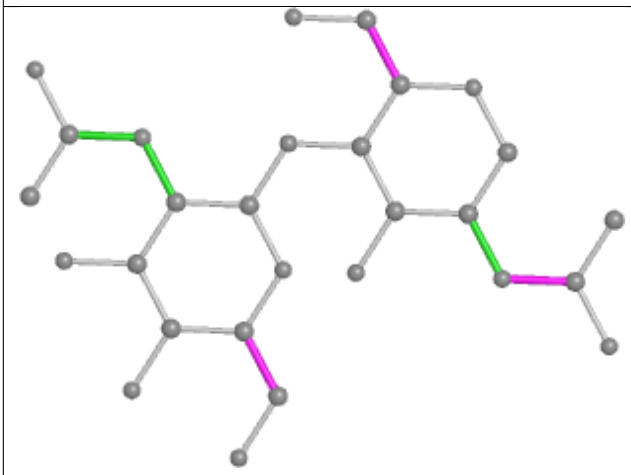
Oligosaccharide Chain D



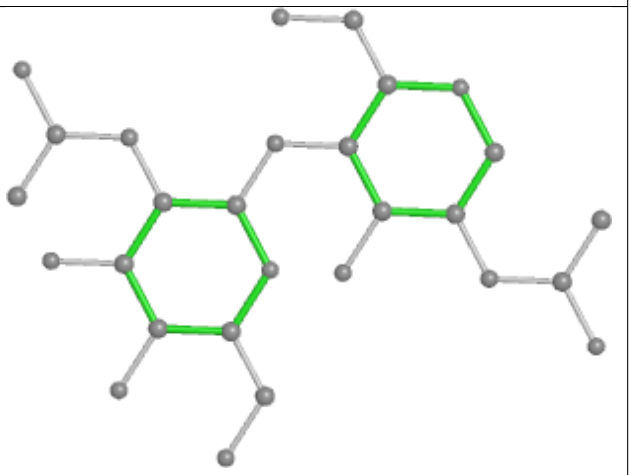
Bond lengths



Bond angles

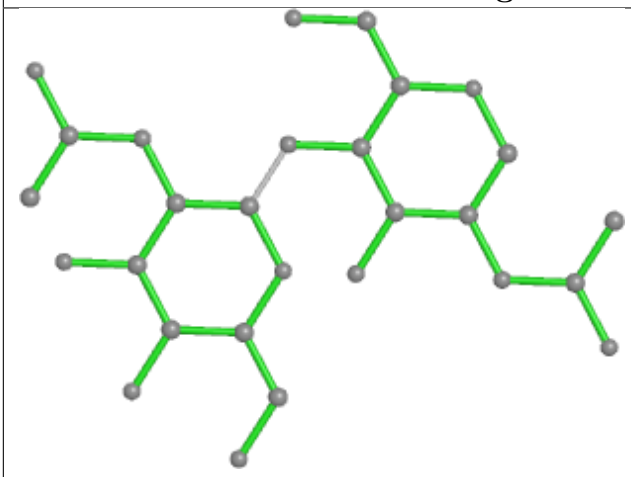


Torsions

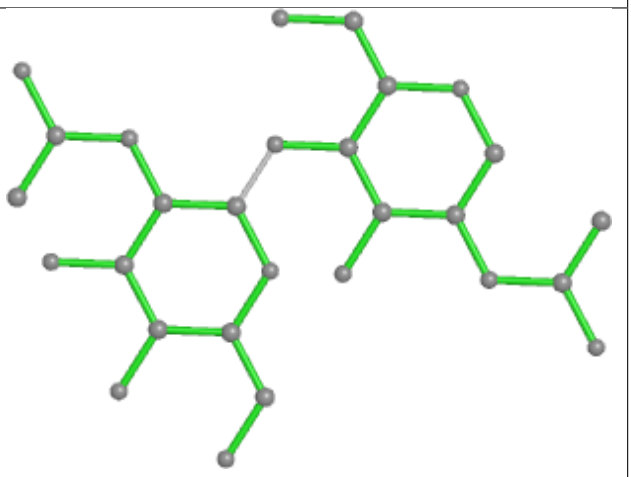


Rings

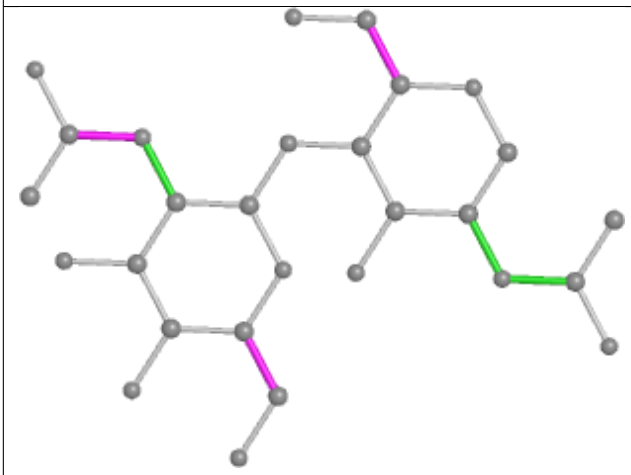
Oligosaccharide Chain E



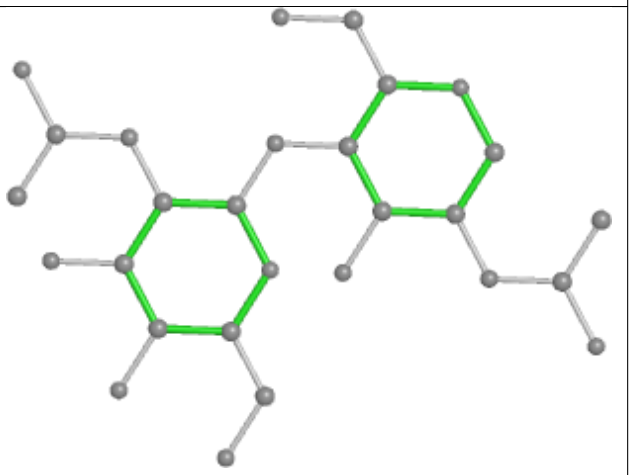
Bond lengths



Bond angles

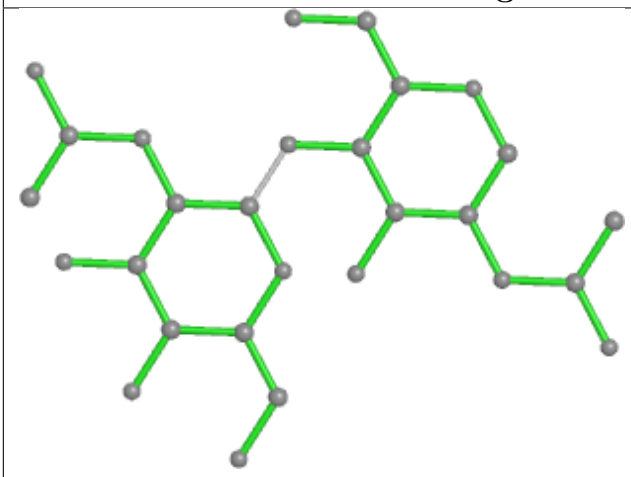


Torsions

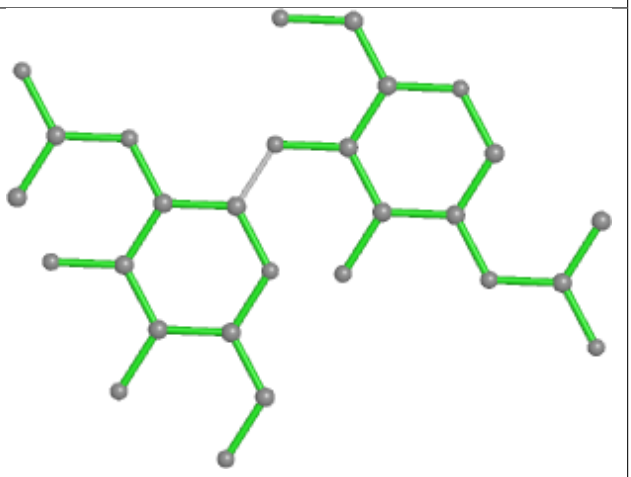


Rings

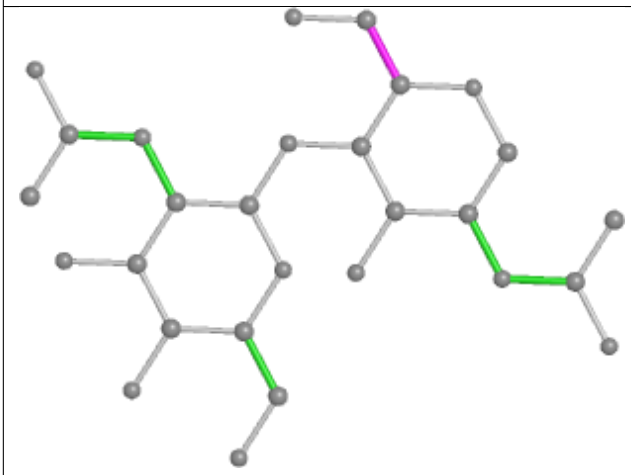
Oligosaccharide Chain F



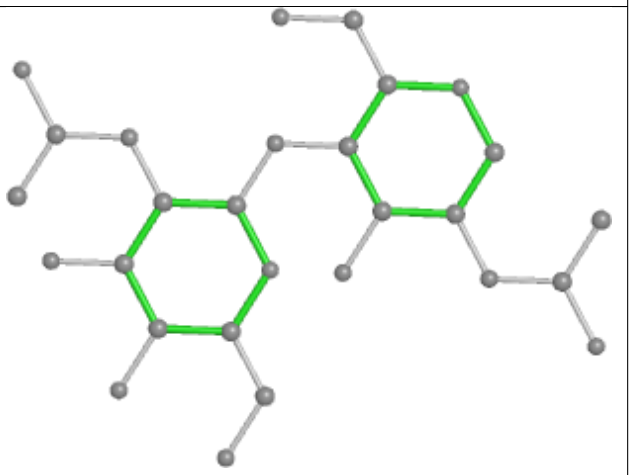
Bond lengths



Bond angles

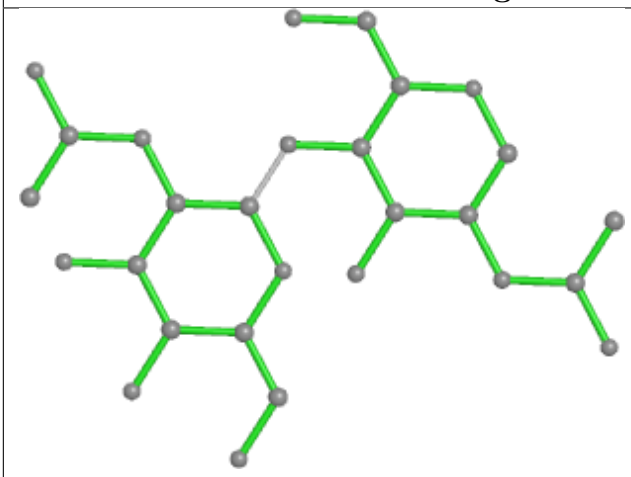


Torsions

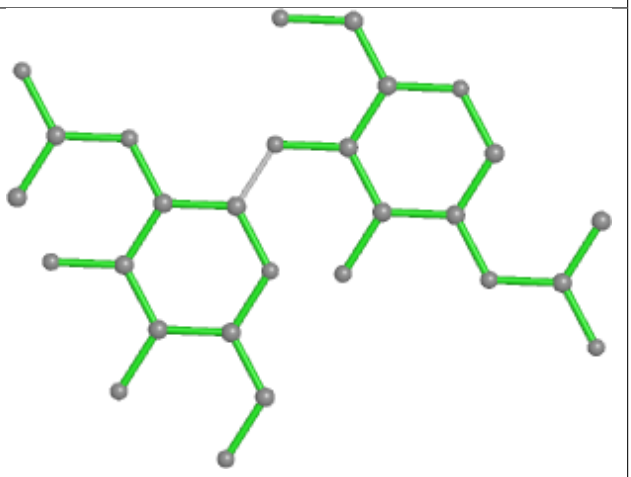


Rings

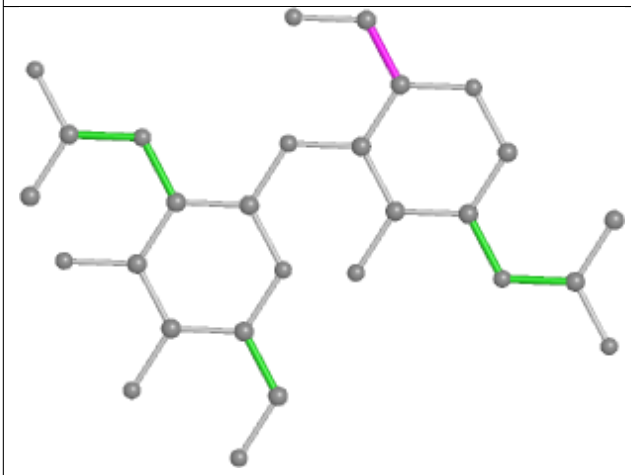
Oligosaccharide Chain G



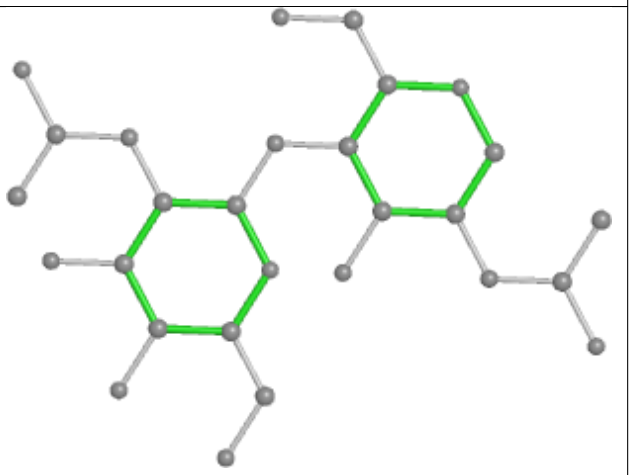
Bond lengths



Bond angles

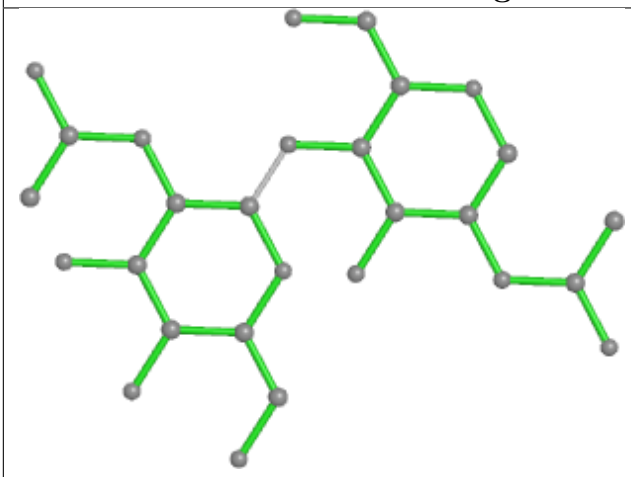


Torsions

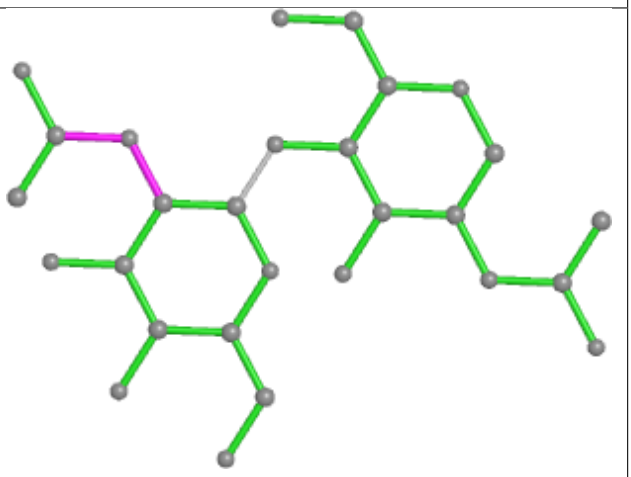


Rings

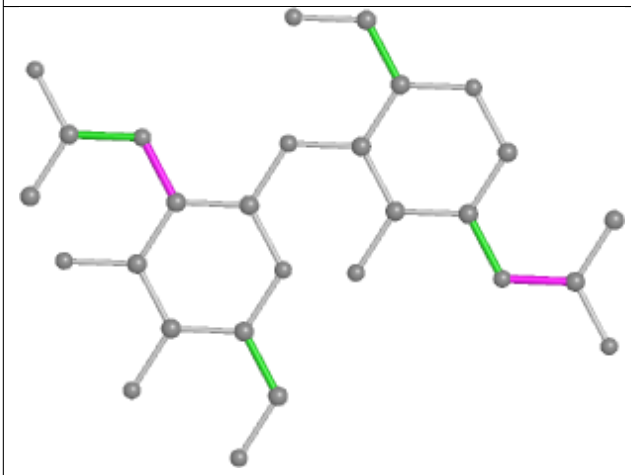
Oligosaccharide Chain H



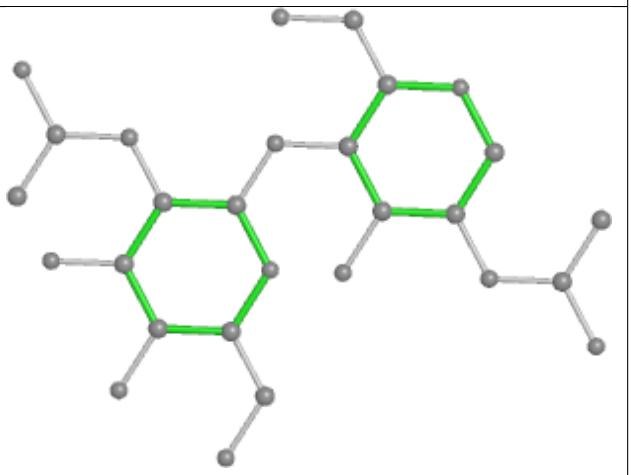
Bond lengths



Bond angles

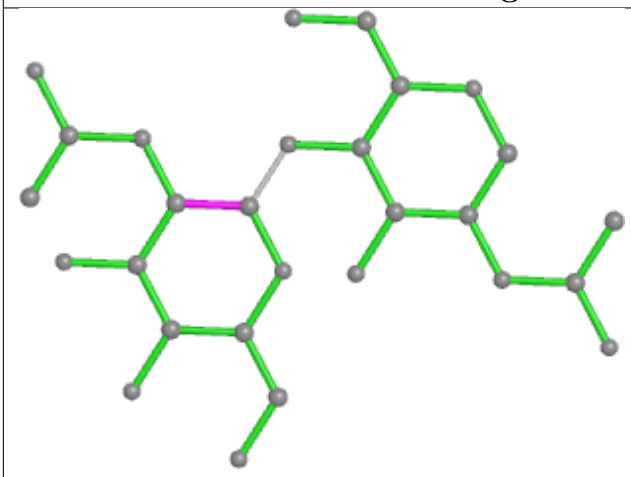


Torsions

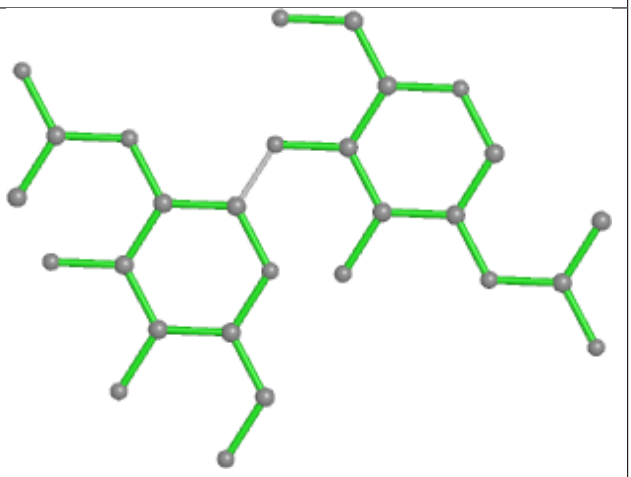


Rings

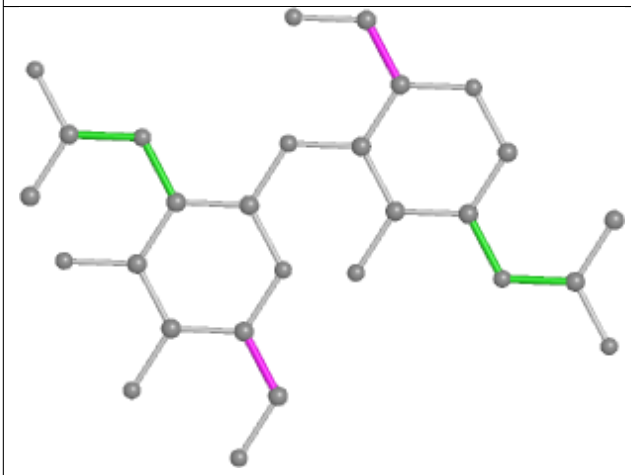
Oligosaccharide Chain I



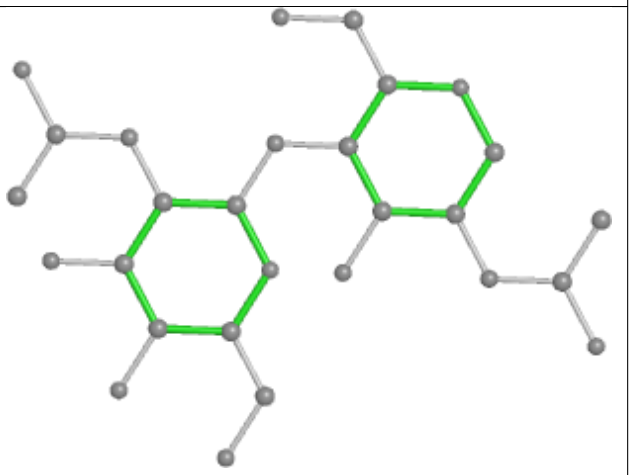
Bond lengths



Bond angles

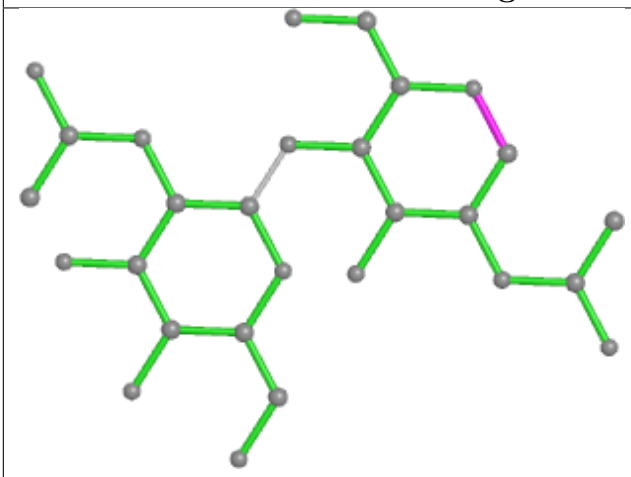


Torsions

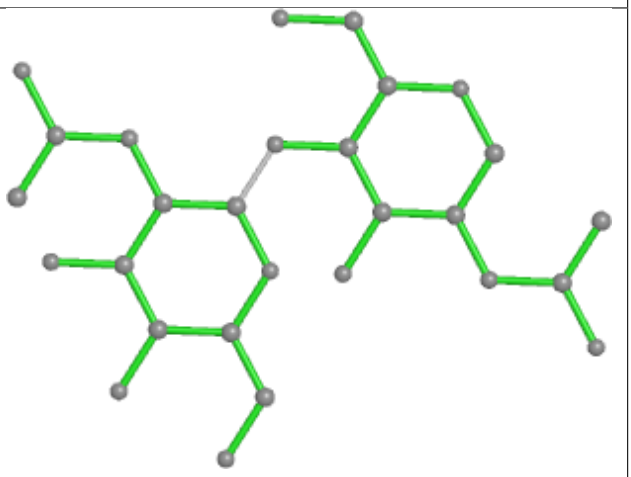


Rings

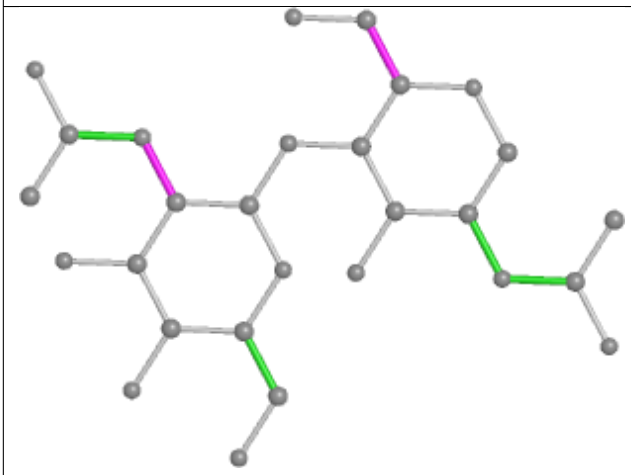
Oligosaccharide Chain J



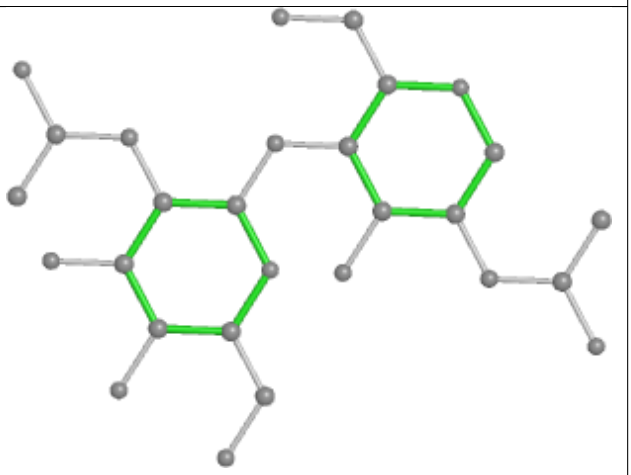
Bond lengths



Bond angles

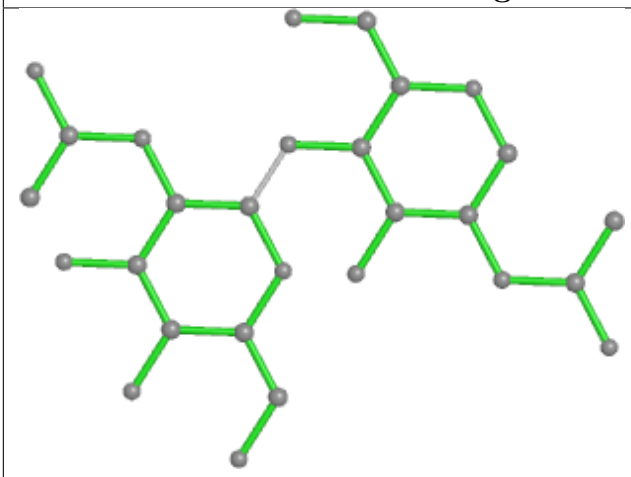


Torsions

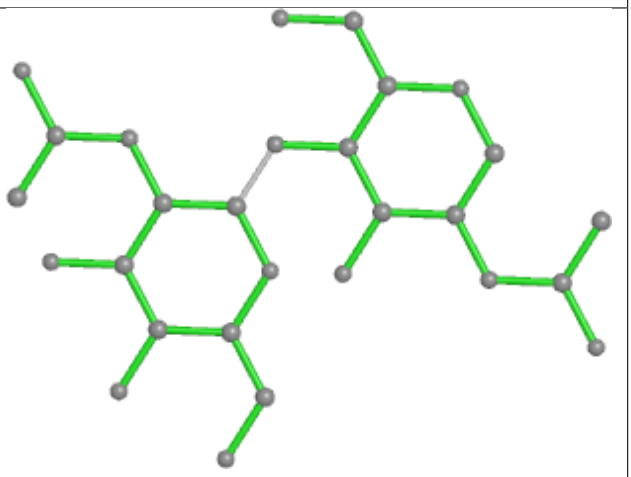


Rings

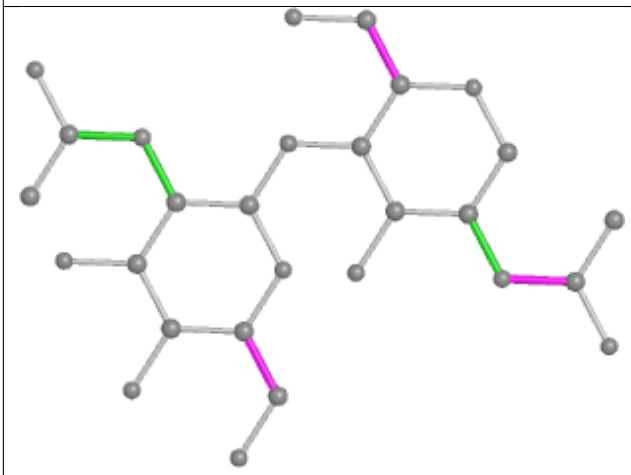
Oligosaccharide Chain K



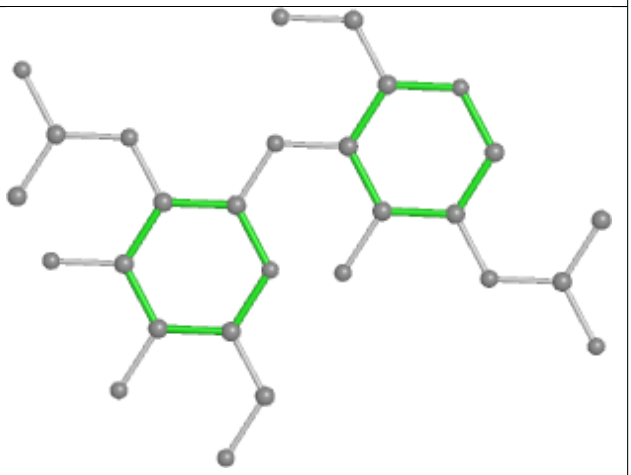
Bond lengths



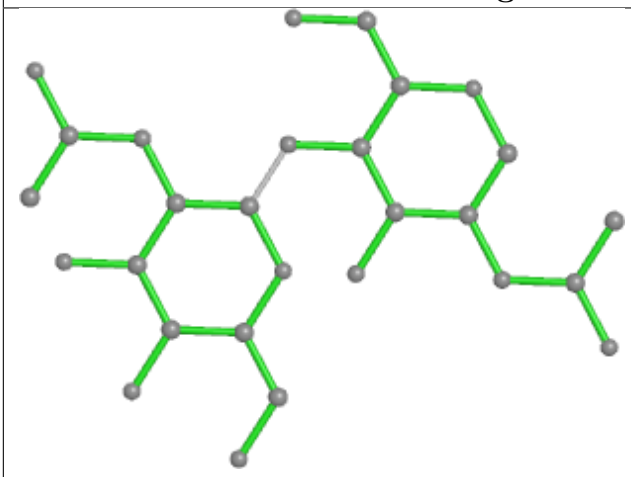
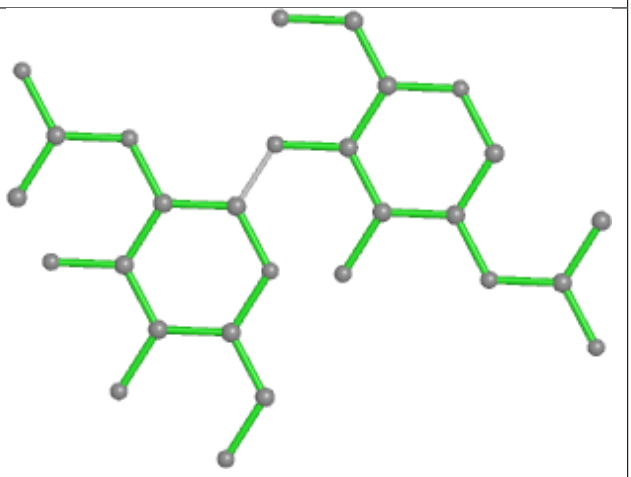
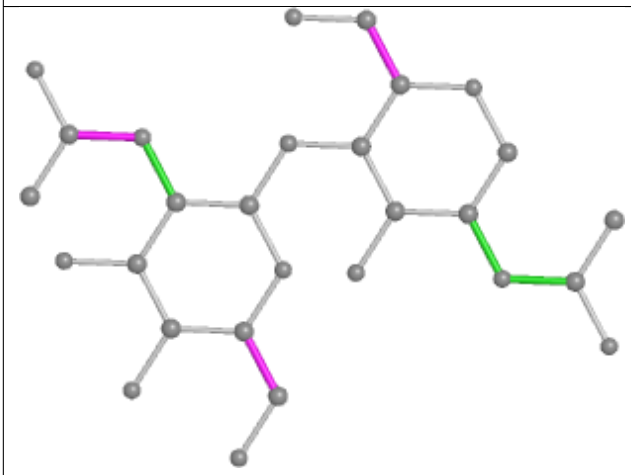
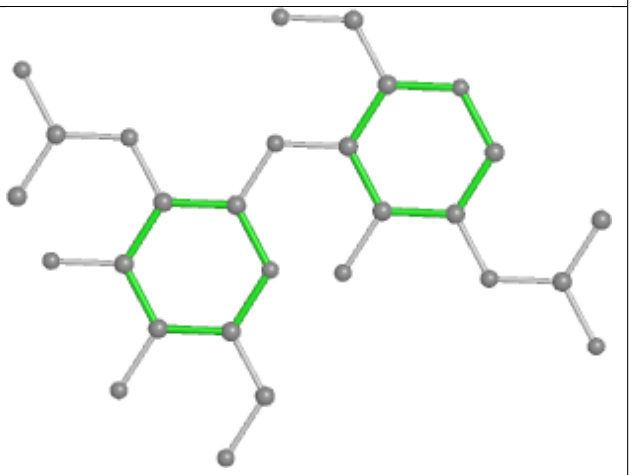
Bond angles

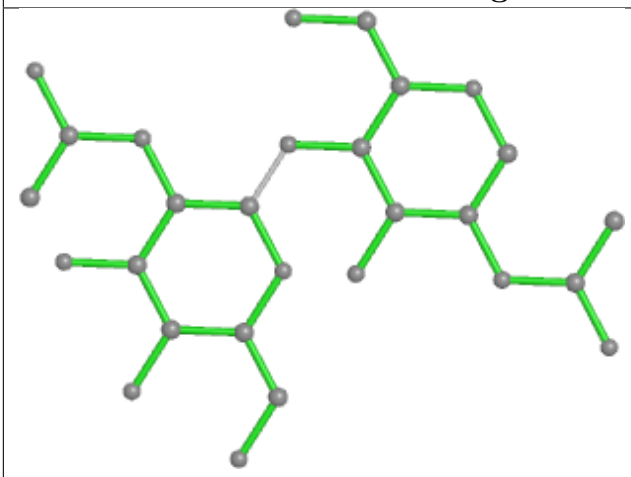
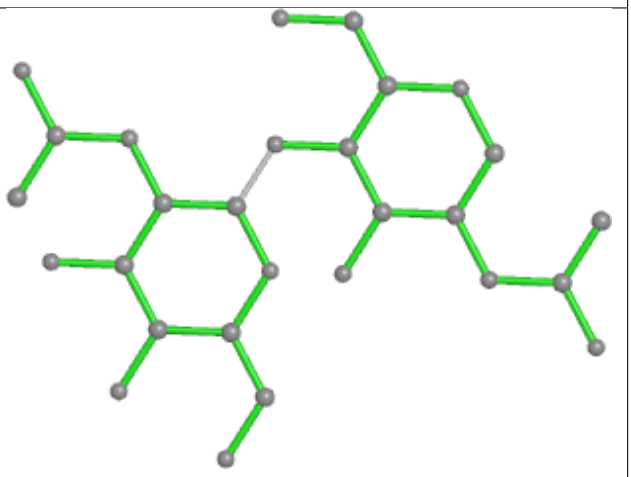
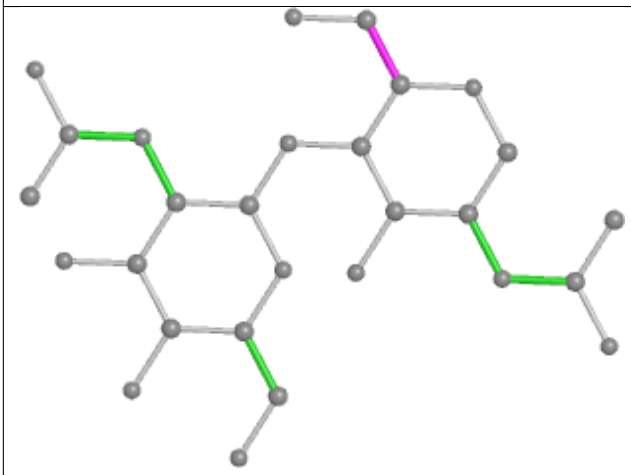
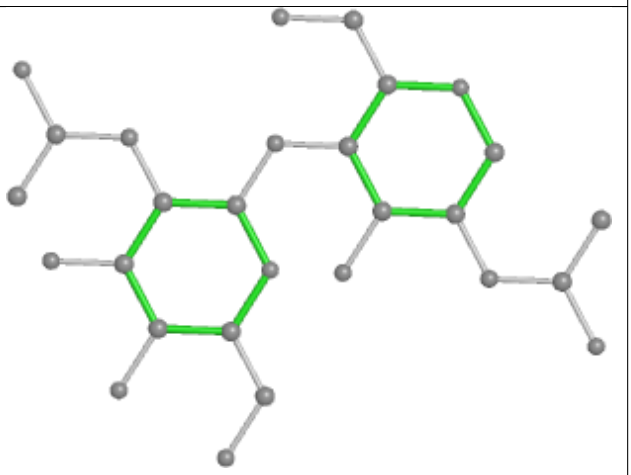


Torsions

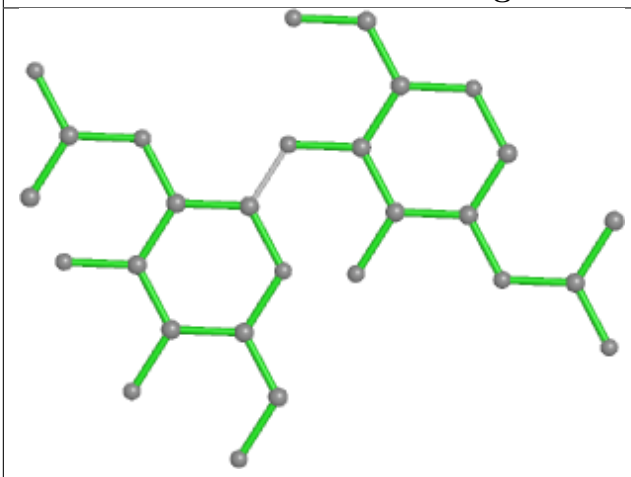


Rings

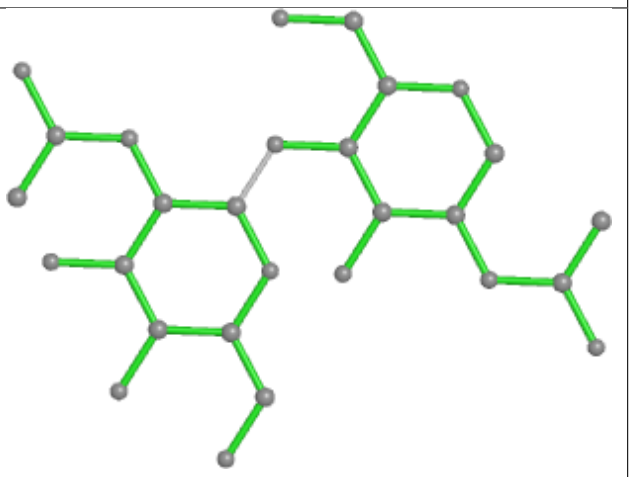
Oligosaccharide Chain L	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

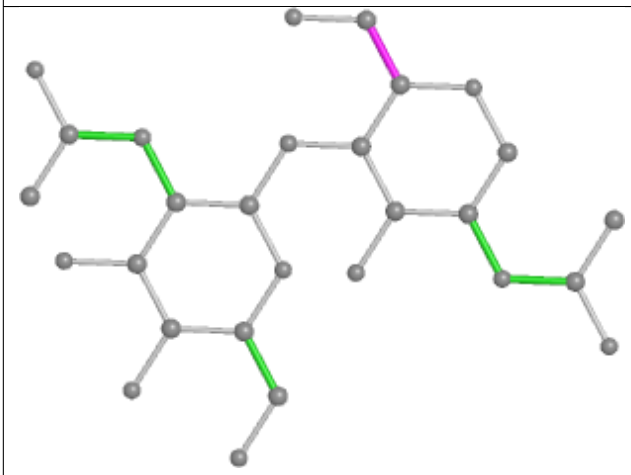
Oligosaccharide Chain N



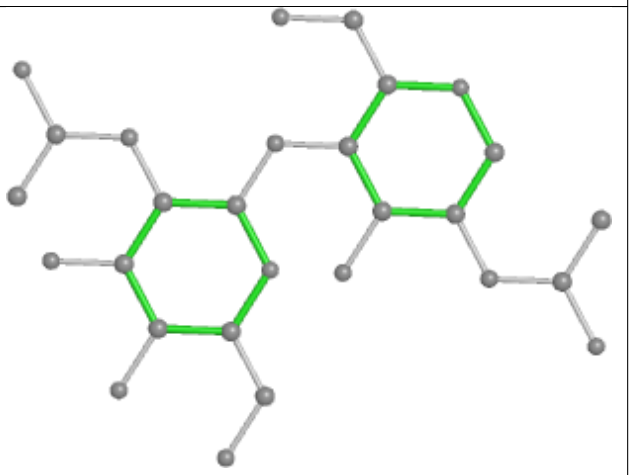
Bond lengths



Bond angles

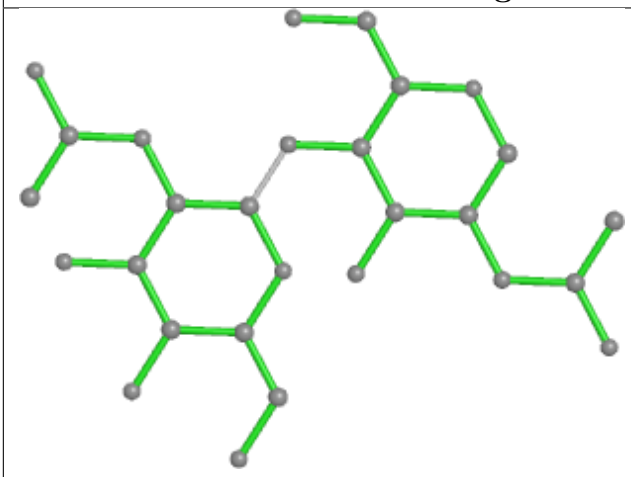


Torsions

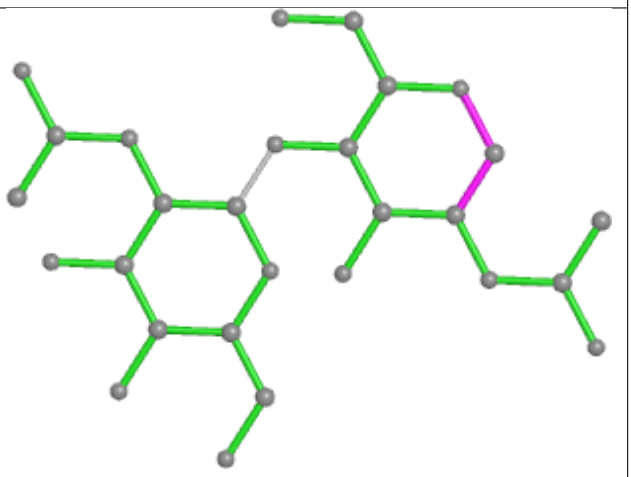


Rings

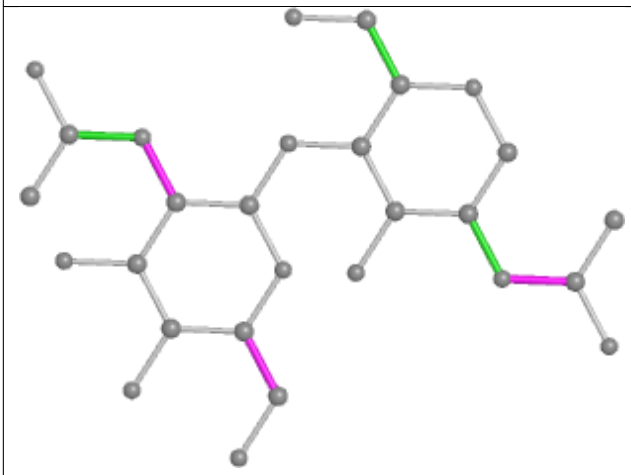
Oligosaccharide Chain O



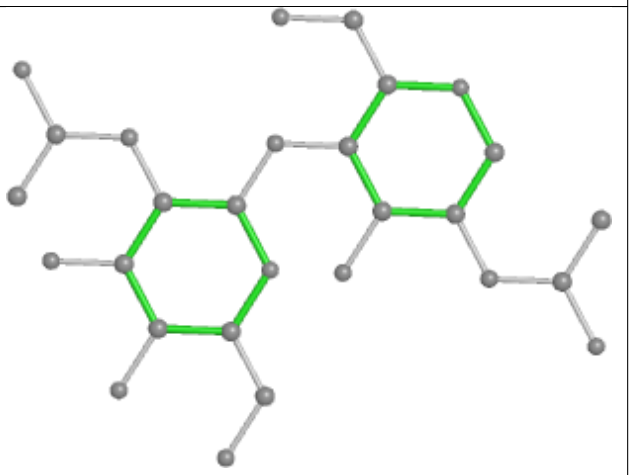
Bond lengths



Bond angles

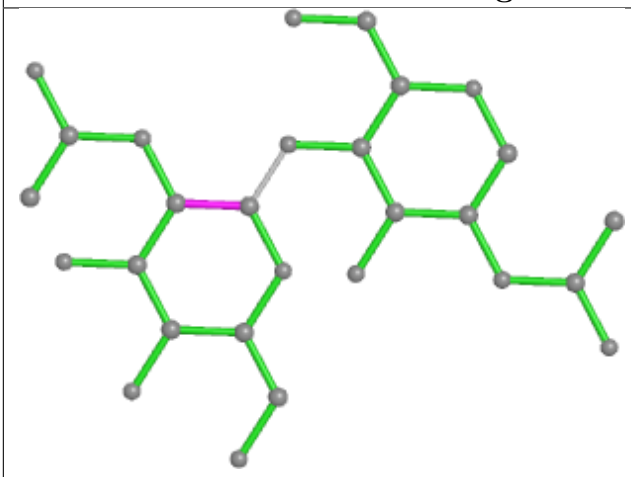


Torsions

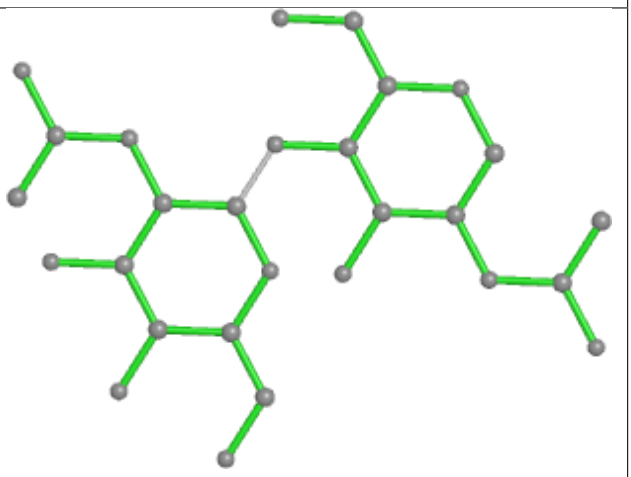


Rings

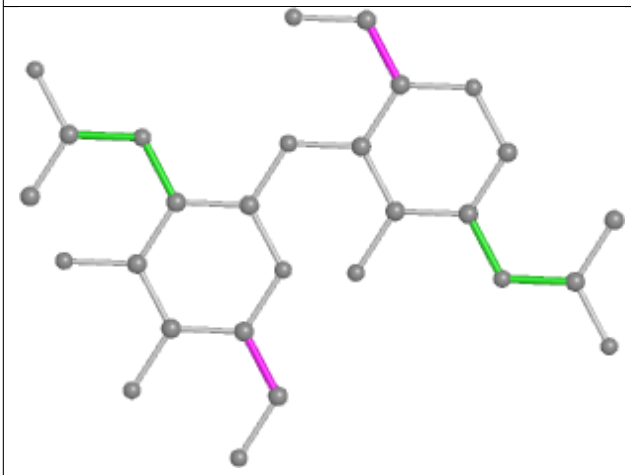
Oligosaccharide Chain P



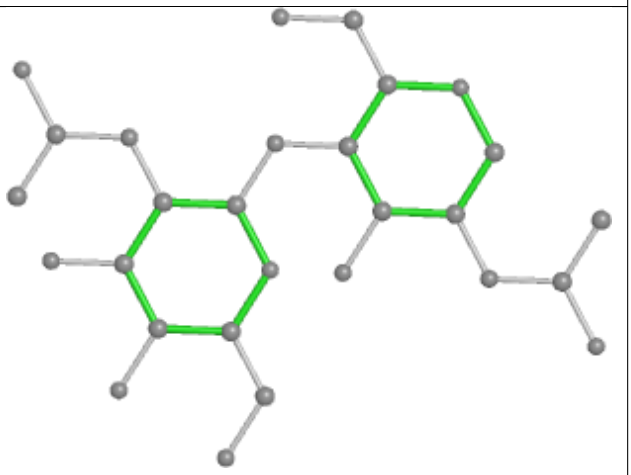
Bond lengths



Bond angles

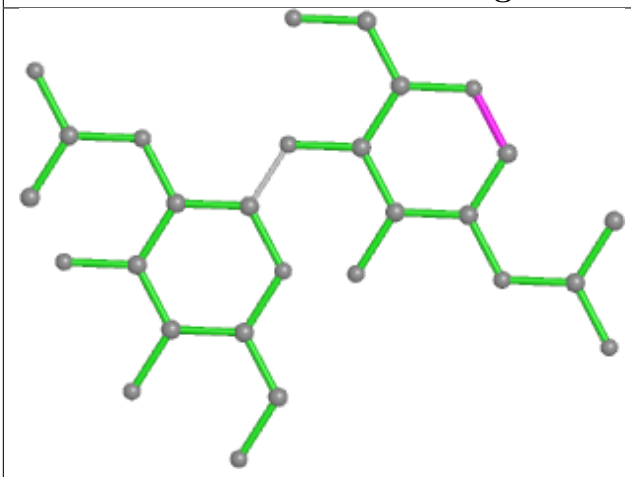


Torsions

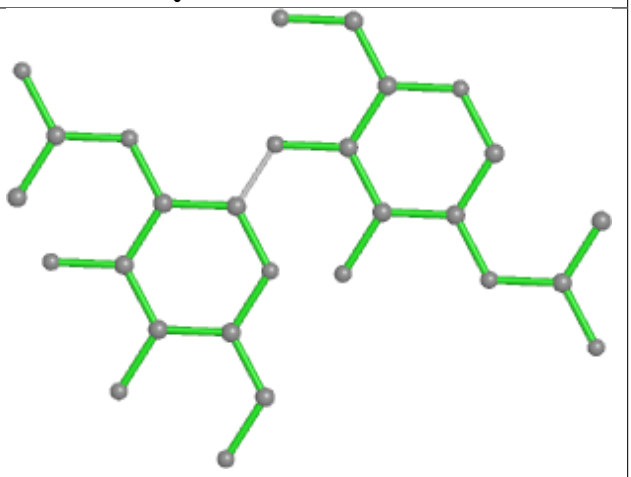


Rings

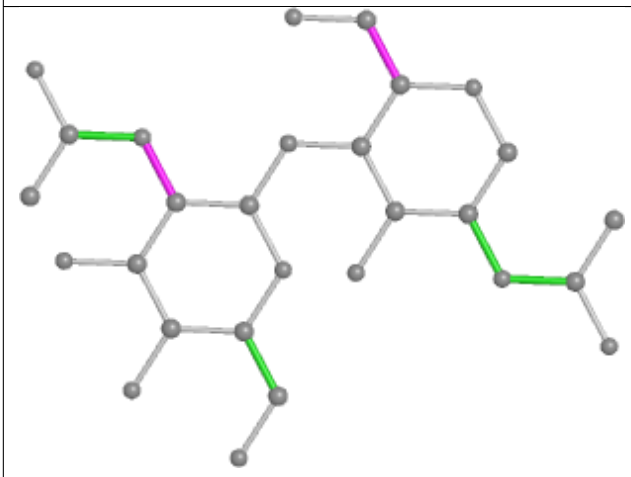
Oligosaccharide Chain Q



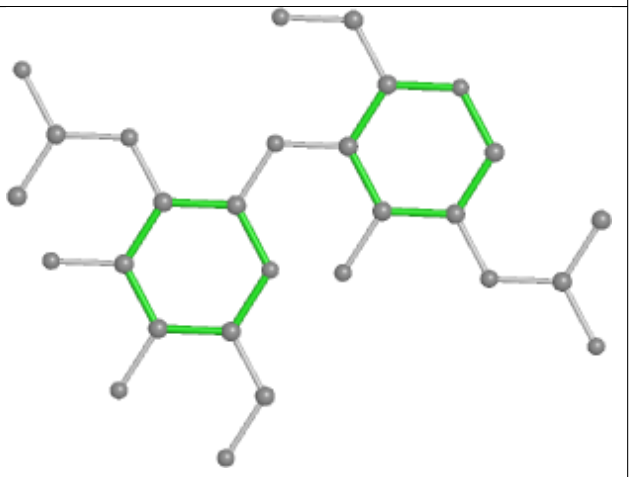
Bond lengths



Bond angles

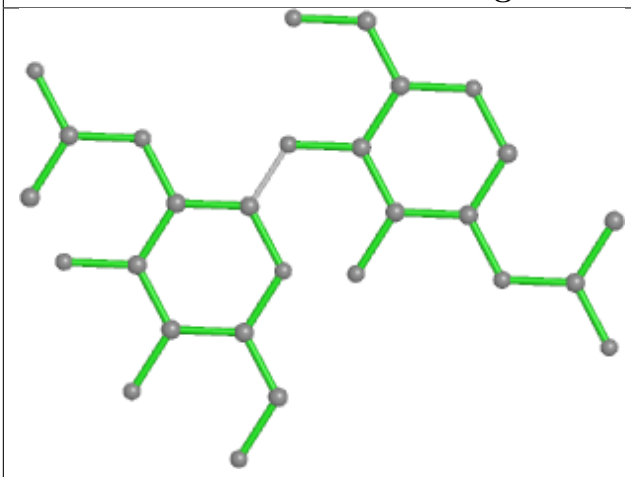


Torsions

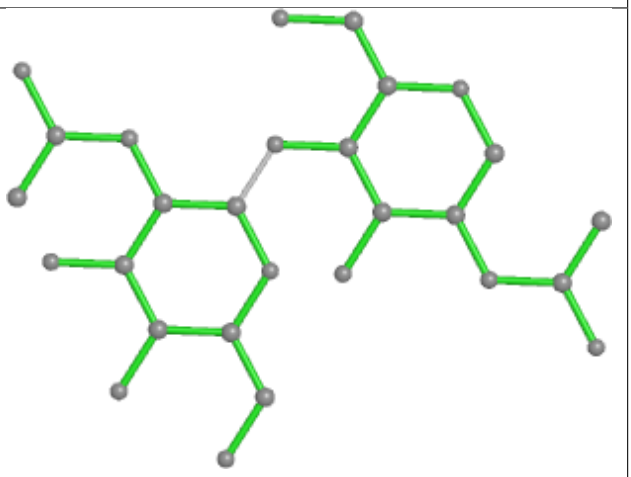


Rings

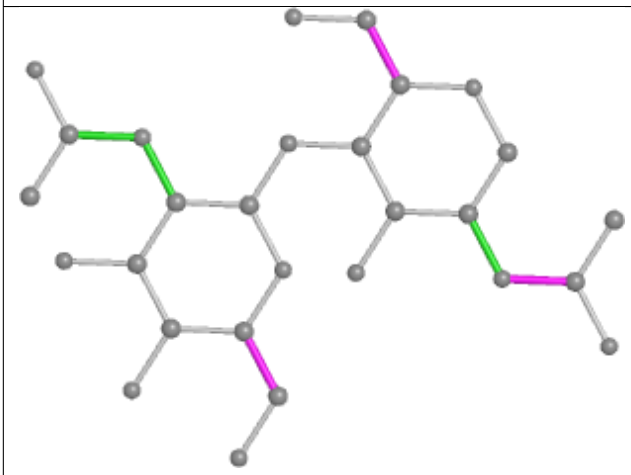
Oligosaccharide Chain R



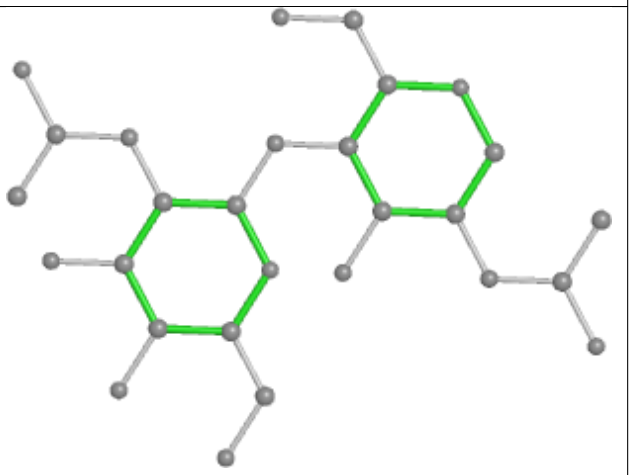
Bond lengths



Bond angles

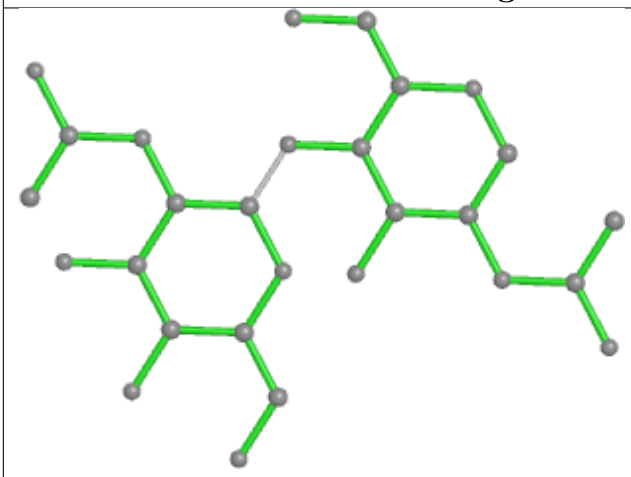


Torsions

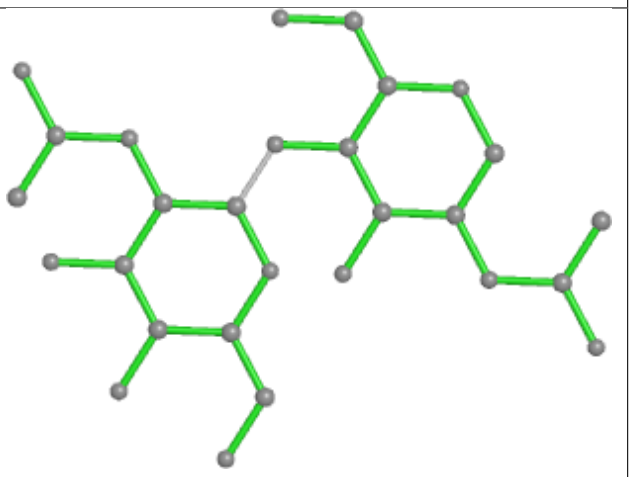


Rings

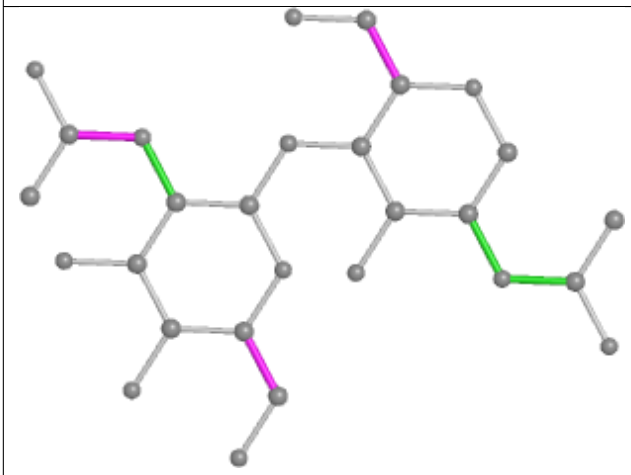
Oligosaccharide Chain S



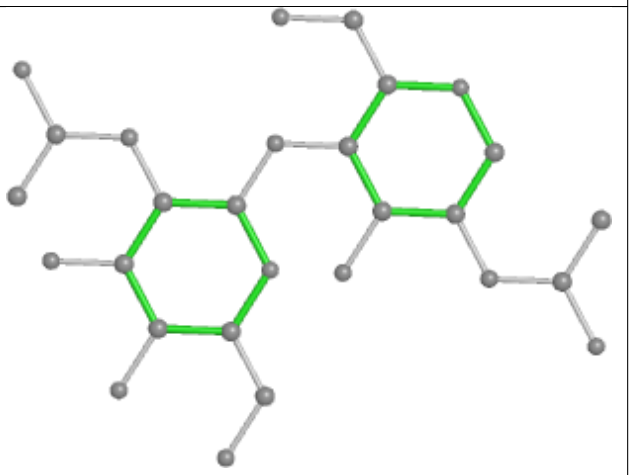
Bond lengths



Bond angles

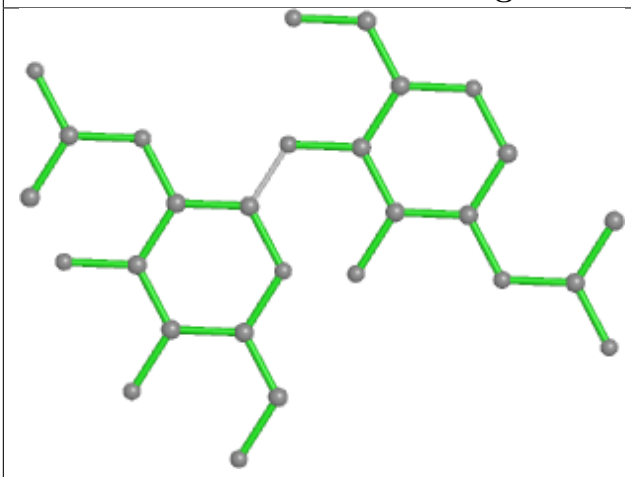


Torsions

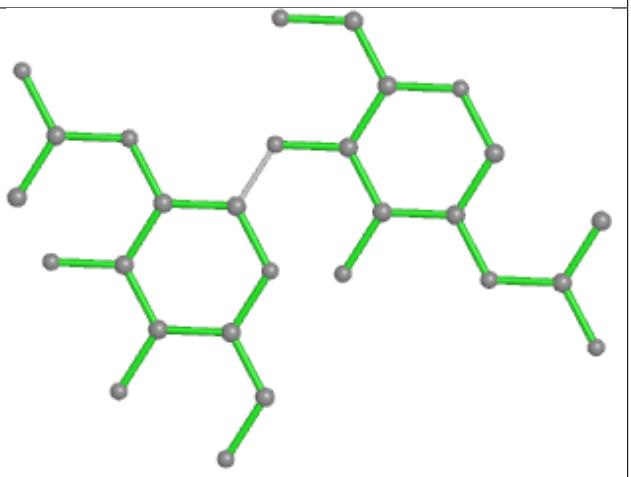


Rings

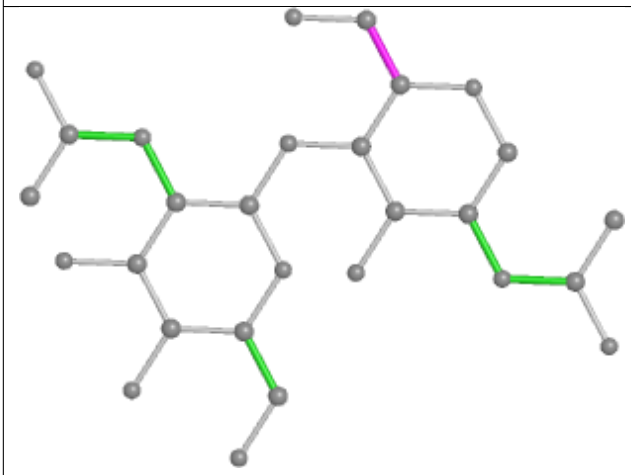
Oligosaccharide Chain T



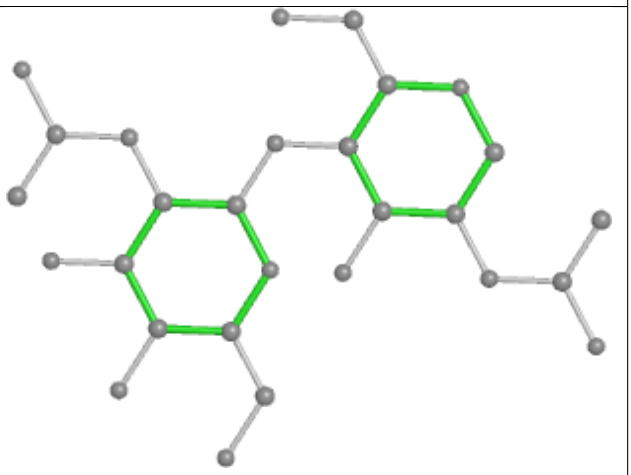
Bond lengths



Bond angles

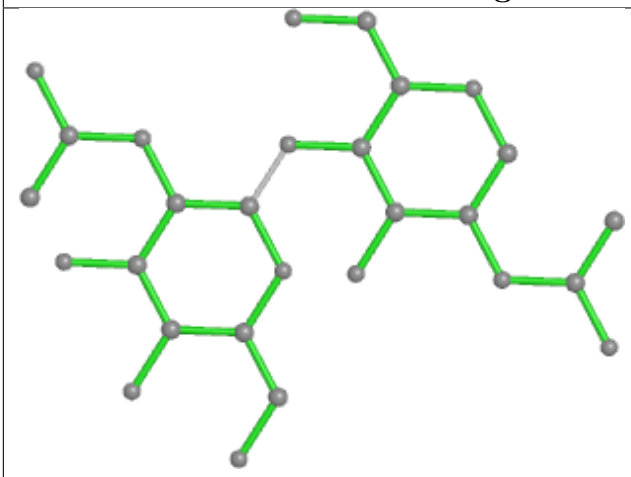


Torsions

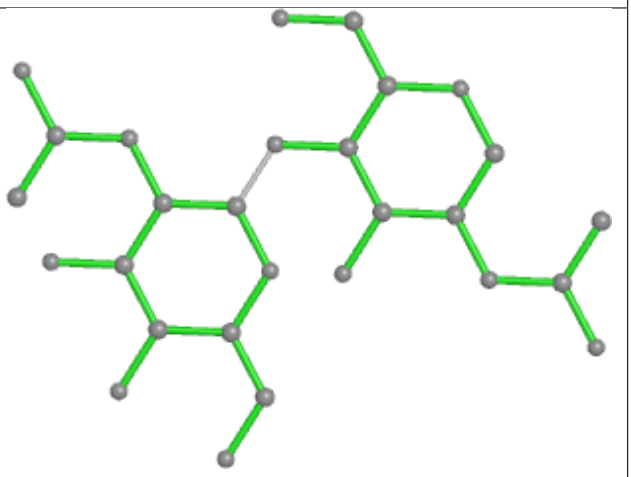


Rings

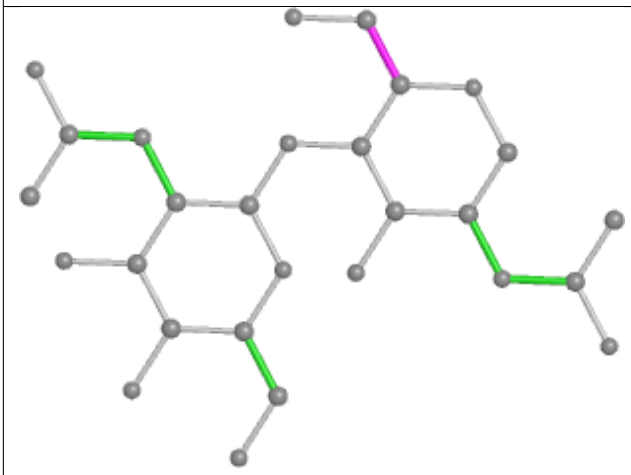
Oligosaccharide Chain U



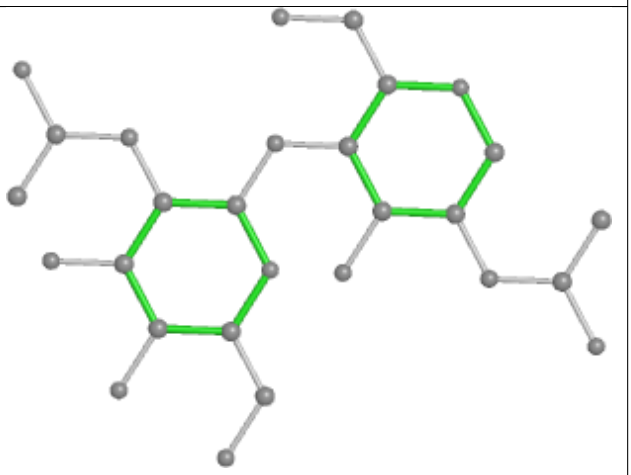
Bond lengths



Bond angles

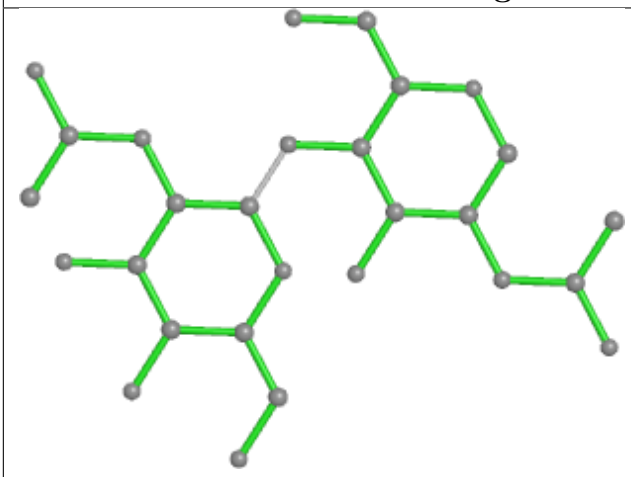


Torsions

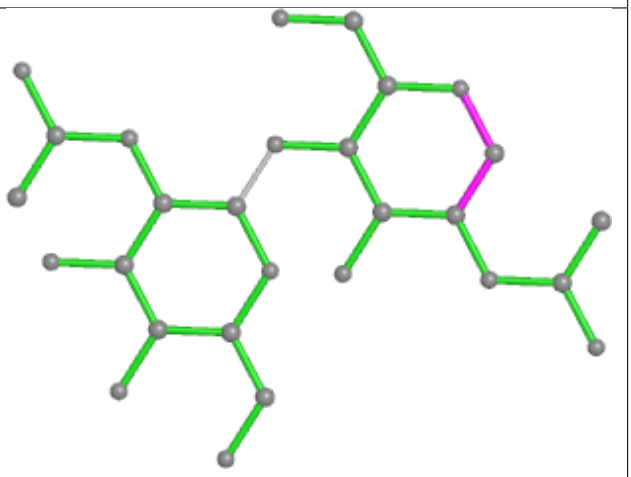


Rings

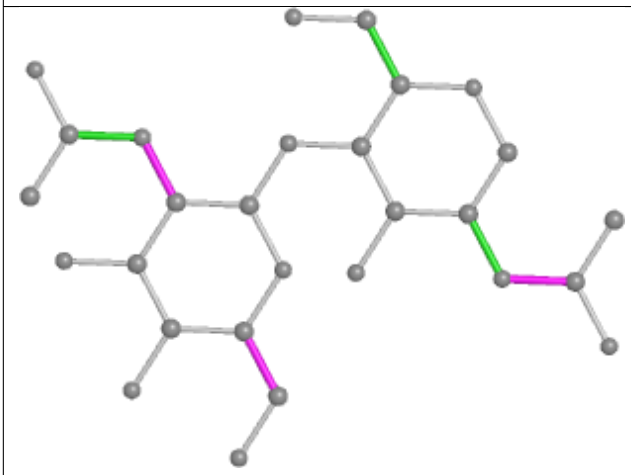
Oligosaccharide Chain V



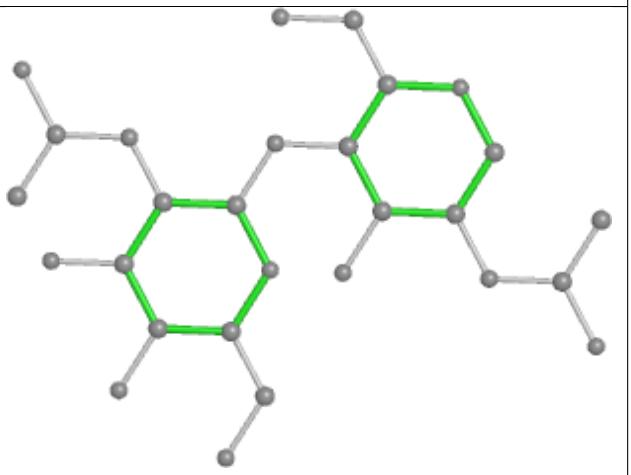
Bond lengths



Bond angles

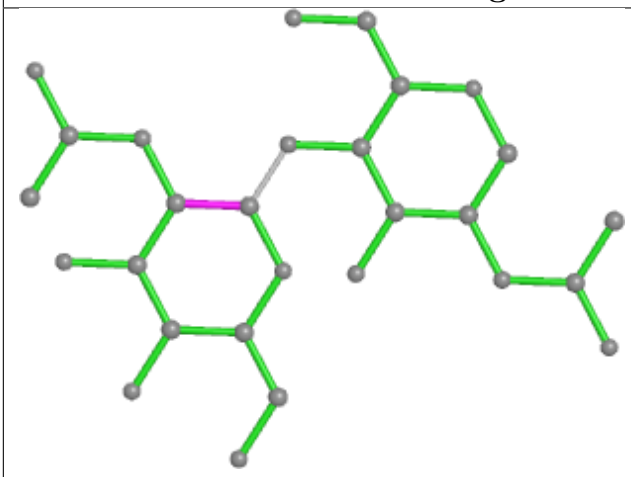


Torsions

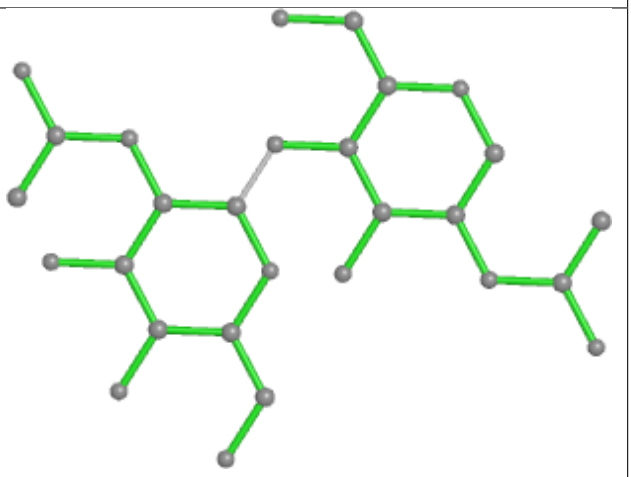


Rings

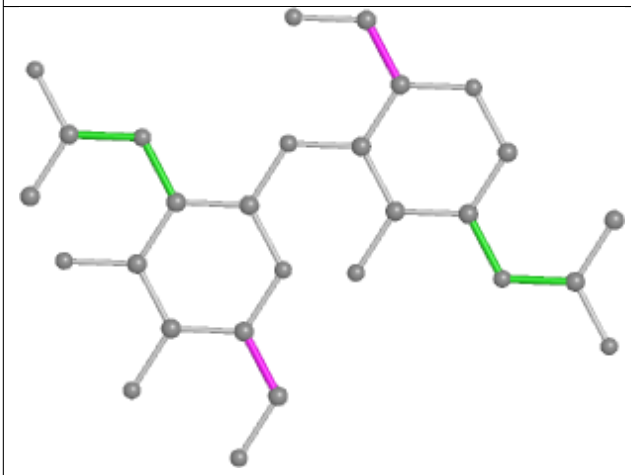
Oligosaccharide Chain W



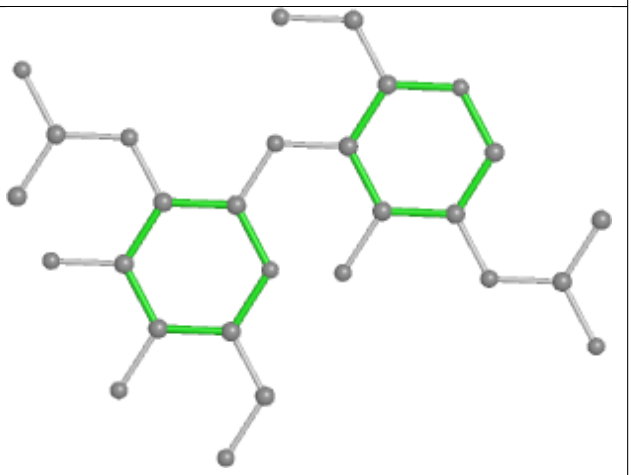
Bond lengths



Bond angles

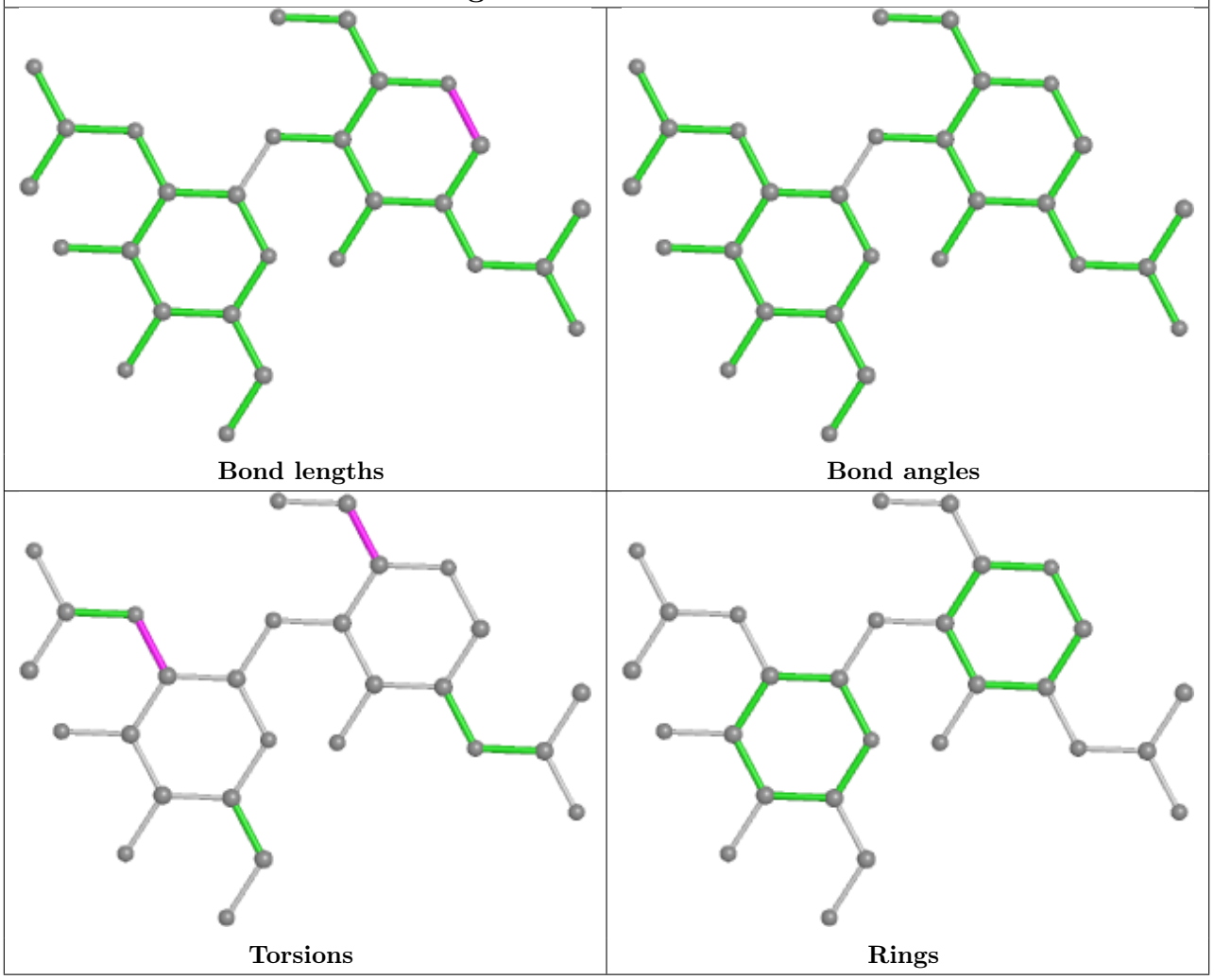


Torsions



Rings

Oligosaccharide Chain X



5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	0.41	0
3	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	B	1305	1	14,14,15	0.46	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1305	1	14,14,15	0.53	0	17,19,21	0.99	2 (11%)
3	NAG	A	1304	1	14,14,15	0.47	0	17,19,21	0.41	0
3	NAG	C	1307	1	14,14,15	0.18	0	17,19,21	0.53	0
3	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	B	1306	1	14,14,15	0.53	0	17,19,21	0.98	2 (11%)
3	NAG	C	1305	1	14,14,15	0.55	0	17,19,21	0.97	2 (11%)
3	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.55	0
3	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	B	1307	1	14,14,15	0.38	0	17,19,21	0.58	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	A	1306	1	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	C	1306	1	14,14,15	0.38	0	17,19,21	0.44	0
3	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1305	NAG	C1-O5-C5	2.86	116.07	112.19
3	B	1306	NAG	C1-O5-C5	2.78	115.96	112.19
3	C	1305	NAG	C1-O5-C5	2.77	115.94	112.19
3	A	1305	NAG	C3-C4-C5	2.25	114.26	110.24
3	C	1305	NAG	C3-C4-C5	2.25	114.25	110.24
3	B	1306	NAG	C3-C4-C5	2.25	114.25	110.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1307	NAG	C8-C7-N2-C2
3	B	1307	NAG	O7-C7-N2-C2
3	A	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1302	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1302	NAG	O7-C7-N2-C2
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	C	1305	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	1	0
3	B	1305	NAG	1	0
3	A	1304	NAG	1	0
3	A	1306	NAG	1	0
3	C	1306	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.