



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 01:10 PM UTC

PDB ID : 1GAC / pdb_00001gac
Title : NMR structure of asymmetric homodimer of a82846b, a glycopeptide antibiotic, complexed with its cell wall pentapeptide fragment
Authors : Kline, A.D.; Prowse, W.G.; Skelton, M.A.; Loncharich, R.J.
Deposited on : 1995-05-24

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 80 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (6) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 540 atoms, of which 252 are hydrogens and 0 are deuteriums.

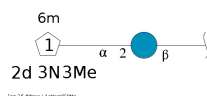
- Molecule 1 is a protein called CELL WALL PENTAPEPTIDE.

Mol	Chain	Residues	Atoms					Trace
1	A	5	Total	C	H	N	O	0
			69	20	36	6	7	
1	B	5	Total	C	H	N	O	0
			69	20	36	6	7	

- Molecule 2 is a protein called CHLOROORIENTICIN A.

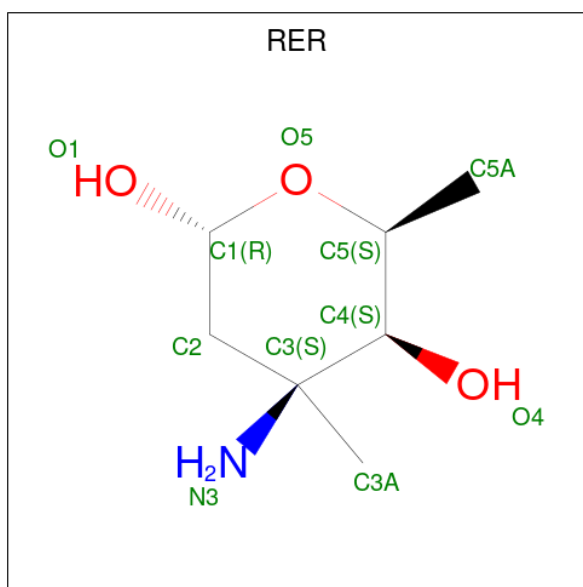
Mol	Chain	Residues	Atoms					Trace
2	C	7	Total	C	Cl	H	N	O
			130	53	2	50	8	17
2	D	7	Total	C	Cl	H	N	O
			130	53	2	50	8	17

- Molecule 3 is an oligosaccharide called vancosamine-(1-2)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					Trace
3	E	2	Total	C	H	N	O	0
			46	13	25	1	7	
3	F	2	Total	C	H	N	O	0
			46	13	25	1	7	

- Molecule 4 is vancosamine (CCD ID: RER) (formula: C₇H₁₅NO₃).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
4	C	1	25	7	15	1	2
4	D	1	25	7	15	1	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

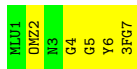
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

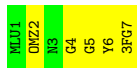
- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

B0C1
RER2

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

WUJ1	DKZ2	I13	G4	G5	Y6	3FG7
------	------	-----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

WUJ1	DKZ2	I13	G4	G5	Y6	3FG7
------	------	-----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

B0C1
RER2

4.2.2 Score per residue for model 2

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

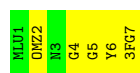
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.3 Score per residue for model 3

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.4 Score per residue for model 4

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

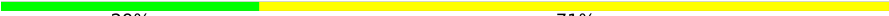
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.5 Score per residue for model 5

- Molecule 1: CELL WALL PENTAPEPTIDE



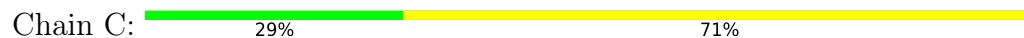
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.6 Score per residue for model 6

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

WU13
DW22
J3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

WU13
DW22
J3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  50% 50%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.7 Score per residue for model 7

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.8 Score per residue for model 8

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

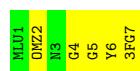
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.9 Score per residue for model 9

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.10 Score per residue for model 10

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

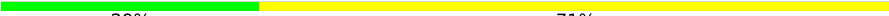
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.11 Score per residue for model 11

- Molecule 1: CELL WALL PENTAPEPTIDE



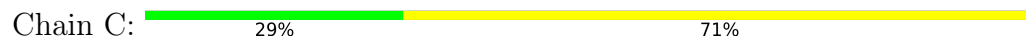
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

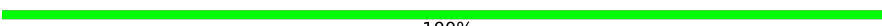
- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A

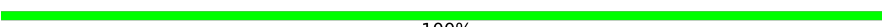


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

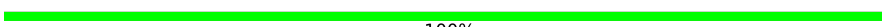
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

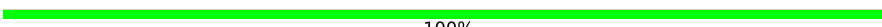
4.2.12 Score per residue for model 12

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

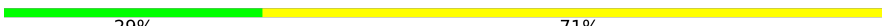
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

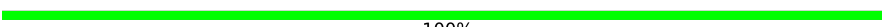
MLJ1
DNZ2
J3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLJ1
DNZ2
J3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.13 Score per residue for model 13

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.14 Score per residue for model 14

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

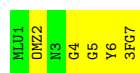
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.15 Score per residue for model 15

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.16 Score per residue for model 16

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

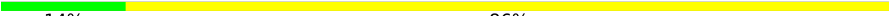
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.17 Score per residue for model 17

- Molecule 1: CELL WALL PENTAPEPTIDE



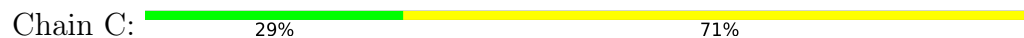
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

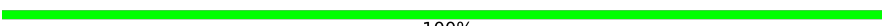
- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A

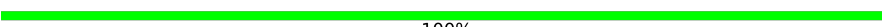


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

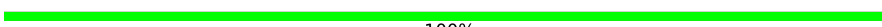
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.18 Score per residue for model 18

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

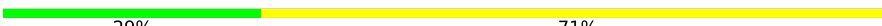
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  80% 20%

A1
E2
A5

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

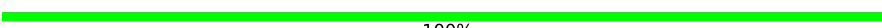
MLH3
ONW22
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLH3
ONW22
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.19 Score per residue for model 19

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

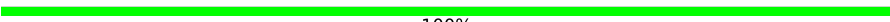
4.2.20 Score per residue for model 20

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

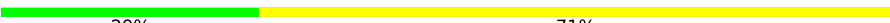
There are no outlier residues in this chain.

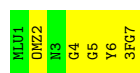
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

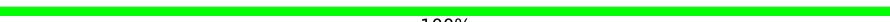


- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

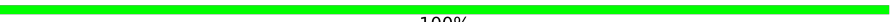


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.21 Score per residue for model 21

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.22 Score per residue for model 22

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.23 Score per residue for model 23

- Molecule 1: CELL WALL PENTAPEPTIDE



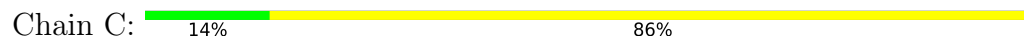
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

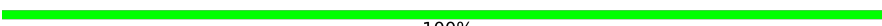
- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A

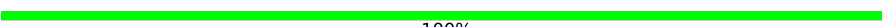


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

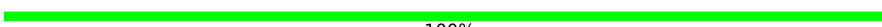
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

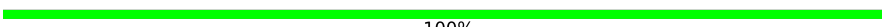
4.2.24 Score per residue for model 24

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

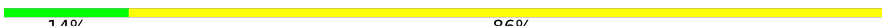
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

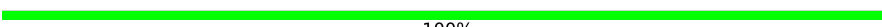
MLU1
DMZ2
J3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
DMZ2
J3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.25 Score per residue for model 25

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.26 Score per residue for model 26

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	REH2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	REH2
------	------

4.2.27 Score per residue for model 27

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	HER2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	HER2
------	------

4.2.28 Score per residue for model 28

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

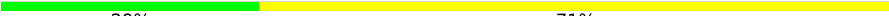
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:
29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:
100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:
100%



4.2.29 Score per residue for model 29

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:
100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:
100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:
14% 86%

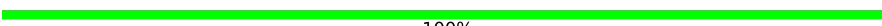


- Molecule 2: CHLOROORIENTICIN A

Chain D:
29% 71%

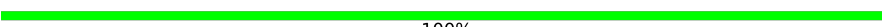


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

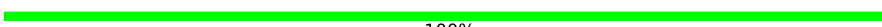
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

B0C1
RER2

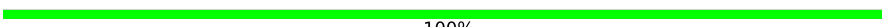
4.2.30 Score per residue for model 30

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

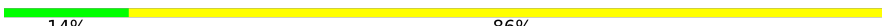
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

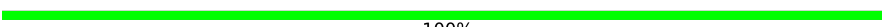
MLU1
DNZ2
I3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
DNZ2
I3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.31 Score per residue for model 31

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

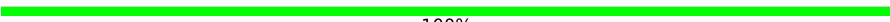
4.2.32 Score per residue for model 32

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

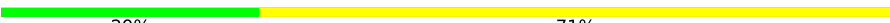
There are no outlier residues in this chain.

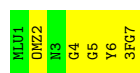
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

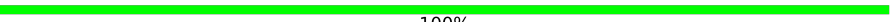


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.33 Score per residue for model 33

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.34 Score per residue for model 34

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

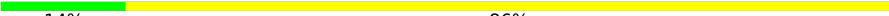
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%



- Molecule 2: CHLOROORIENTICIN A

Chain D:
29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:
100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:
100%



4.2.35 Score per residue for model 35

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:
100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:
100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:
29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:
29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.36 Score per residue for model 36

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1
DMZ2
R3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
DMZ2
R3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.37 Score per residue for model 37

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLH1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.38 Score per residue for model 38

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

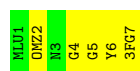
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.39 Score per residue for model 39

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.40 Score per residue for model 40

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

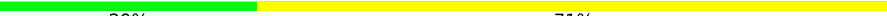
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.41 Score per residue for model 41

- Molecule 1: CELL WALL PENTAPEPTIDE



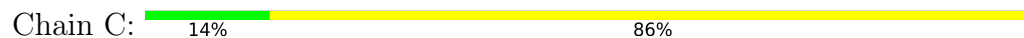
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

B0C1
RER2

4.2.42 Score per residue for model 42

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLU1
DNZ2
R3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
DNZ2
R3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.43 Score per residue for model 43

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
REF2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

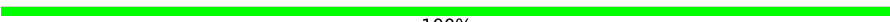
4.2.44 Score per residue for model 44

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

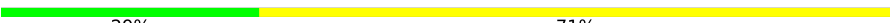
There are no outlier residues in this chain.

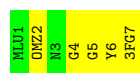
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

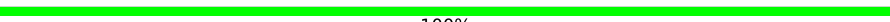


- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

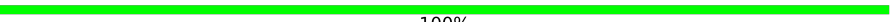


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.45 Score per residue for model 45

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	HER2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	HER2
------	------

4.2.46 Score per residue for model 46

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

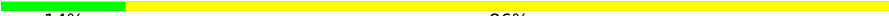
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F: 100%



4.2.47 Score per residue for model 47

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 100%

There are no outlier residues in this chain.

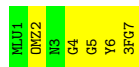
- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

B0C1
RER2

4.2.48 Score per residue for model 48

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

WU13
DW22
J3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

WU13
DW22
J3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

B0C1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.49 Score per residue for model 49

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
REF2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.50 Score per residue for model 50

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	REF2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	REF2
------	------

4.2.51 Score per residue for model 51

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.52 Score per residue for model 52

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

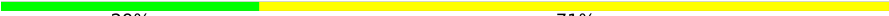
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F: 100%



4.2.53 Score per residue for model 53

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 80% 20%



- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4.2.54 Score per residue for model 54

- Molecule 1: CELL WALL PENTAPEPTIDE



There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

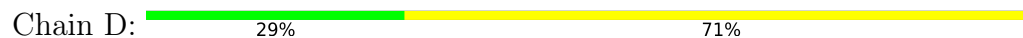


There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A



- Molecule 2: CHLOROORIENTICIN A



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.55 Score per residue for model 55

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLU13
OMZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
OMZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  50% 50%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.56 Score per residue for model 56

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

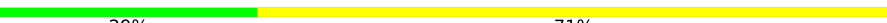
There are no outlier residues in this chain.

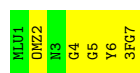
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

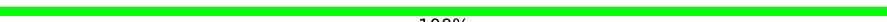


- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

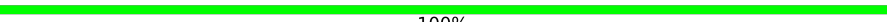


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.57 Score per residue for model 57

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	HER2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	HER2
------	------

4.2.58 Score per residue for model 58

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

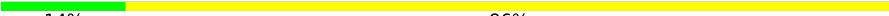
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F: 100%



4.2.59 Score per residue for model 59

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 71%

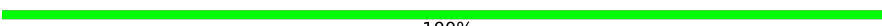


- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%

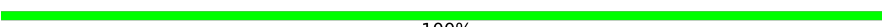


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

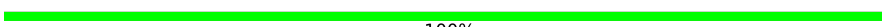
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

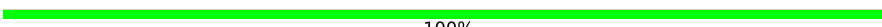
4.2.60 Score per residue for model 60

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

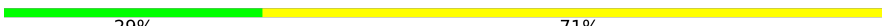
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

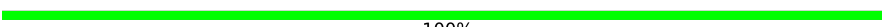
MLJ1
DNZ2
J3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLJ1
DNZ2
J3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.61 Score per residue for model 61

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLU1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
REF2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.62 Score per residue for model 62

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

MLJ1	ONZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	REK2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	REK2
------	------

4.2.63 Score per residue for model 63

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	HER2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	HER2
------	------

4.2.64 Score per residue for model 64

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

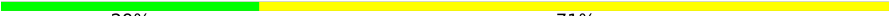
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

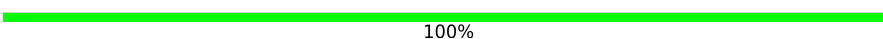


- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

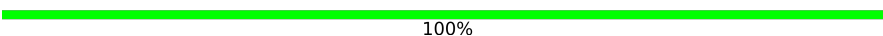


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



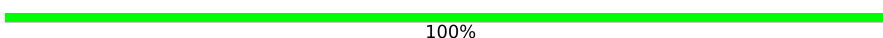
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.65 Score per residue for model 65

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

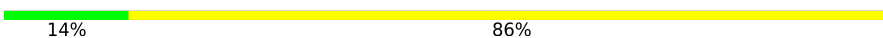
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

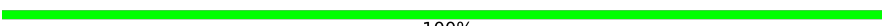


- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

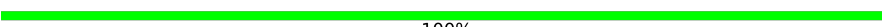


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

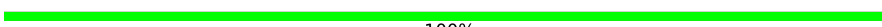
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

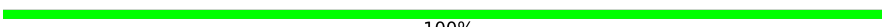
4.2.66 Score per residue for model 66

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

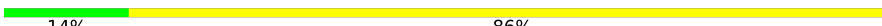
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

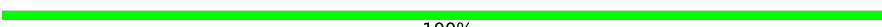
MLU1
DMZ2
I3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1
DMZ2
I3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.67 Score per residue for model 67

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.68 Score per residue for model 68

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

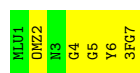
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.69 Score per residue for model 69

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

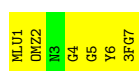
- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%



4.2.70 Score per residue for model 70

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

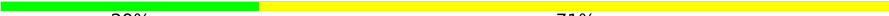
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 29% 71%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F: 100%



4.2.71 Score per residue for model 71

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 86%



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BC1
RER2

4.2.72 Score per residue for model 72

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

ML1
DN22
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

ML1
DN22
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.73 Score per residue for model 73

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1
DNZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
RER2

4.2.74 Score per residue for model 74

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	REK2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	REK2
------	------

4.2.75 Score per residue for model 75

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLU1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	HER2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	HER2
------	------

4.2.76 Score per residue for model 76

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

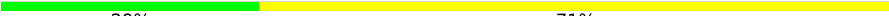
There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:
14% 86%

A horizontal bar representing the quality of Chain D. The bar is 100% long. The first 14% is green, and the remaining 86% is yellow.



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:
100%

A horizontal bar representing the quality of Chain E. The bar is 100% long and is entirely green.



- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:
100%

A horizontal bar representing the quality of Chain F. The bar is 100% long and is entirely green.



4.2.77 Score per residue for model 77

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:
100%

A horizontal bar representing the quality of Chain A. The bar is 100% long and is entirely green.

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:
100%

A horizontal bar representing the quality of Chain B. The bar is 100% long and is entirely green.

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:
14% 86%

A horizontal bar representing the quality of Chain C. The bar is 100% long. The first 14% is green, and the remaining 86% is yellow.



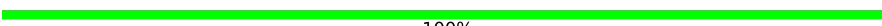
- Molecule 2: CHLOROORIENTICIN A

Chain D:
14% 86%

A horizontal bar representing the quality of Chain D. The bar is 100% long. The first 14% is green, and the remaining 86% is yellow.

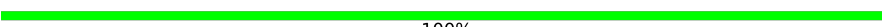


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BC1
RER2

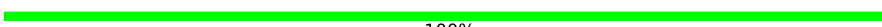
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BC1
RER2

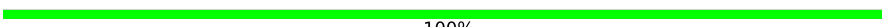
4.2.78 Score per residue for model 78

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

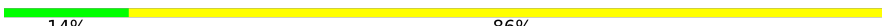
There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

ML1
DN22
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

ML1
DN22
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.79 Score per residue for model 79

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1
DMZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1
DMZ2
N3
G4
G5
Y6
3FG7

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1
REF2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1
REF2

4.2.80 Score per residue for model 80

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  14% 86%

MLJ1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 2: CHLOROORIENTICIN A

Chain D:  14% 86%

MLJ1	OMZ2	N3	G4	G5	Y6	3FG7
------	------	----	----	----	----	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:  100%

BGC1	REF2
------	------

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain F:  100%

BGC1	REF2
------	------

5 Refinement protocol and experimental data overview

Of the 80 calculated structures, 80 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CHARMM	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

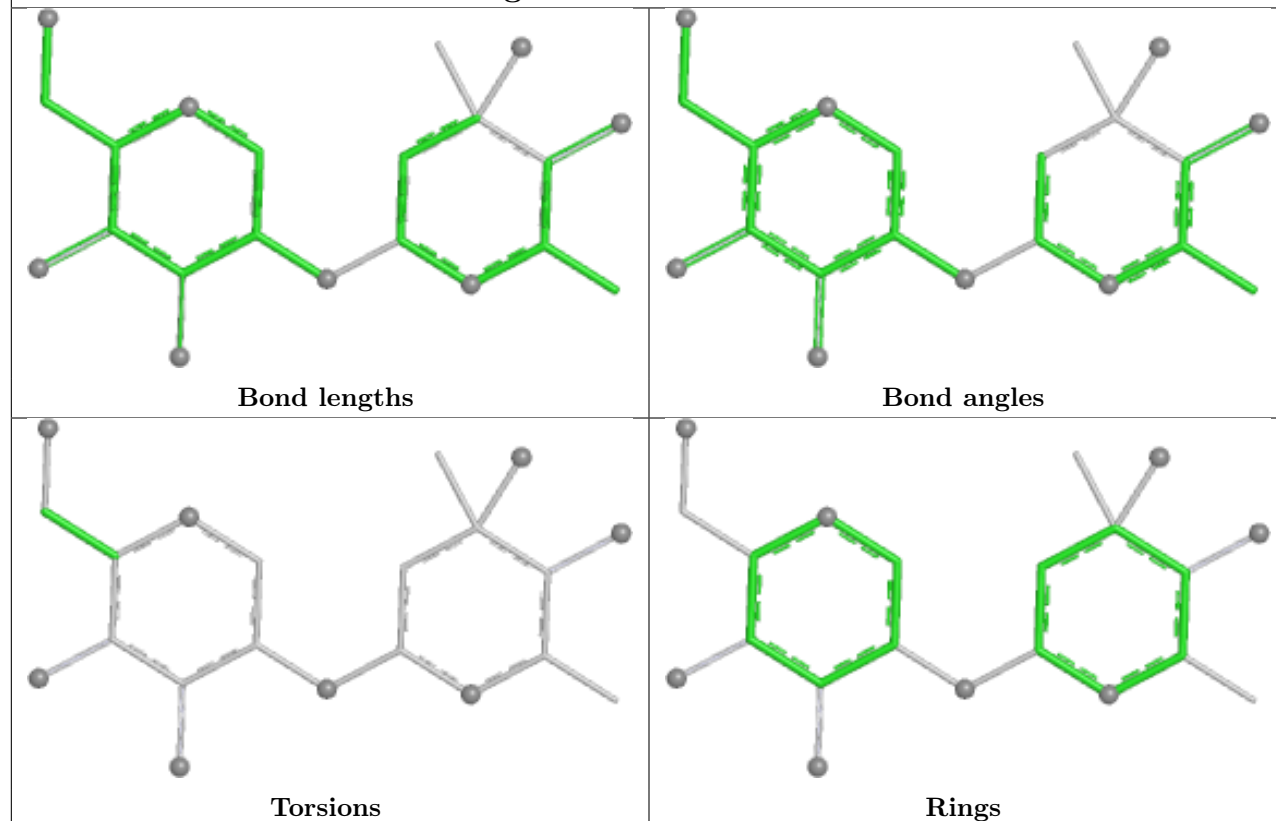
MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

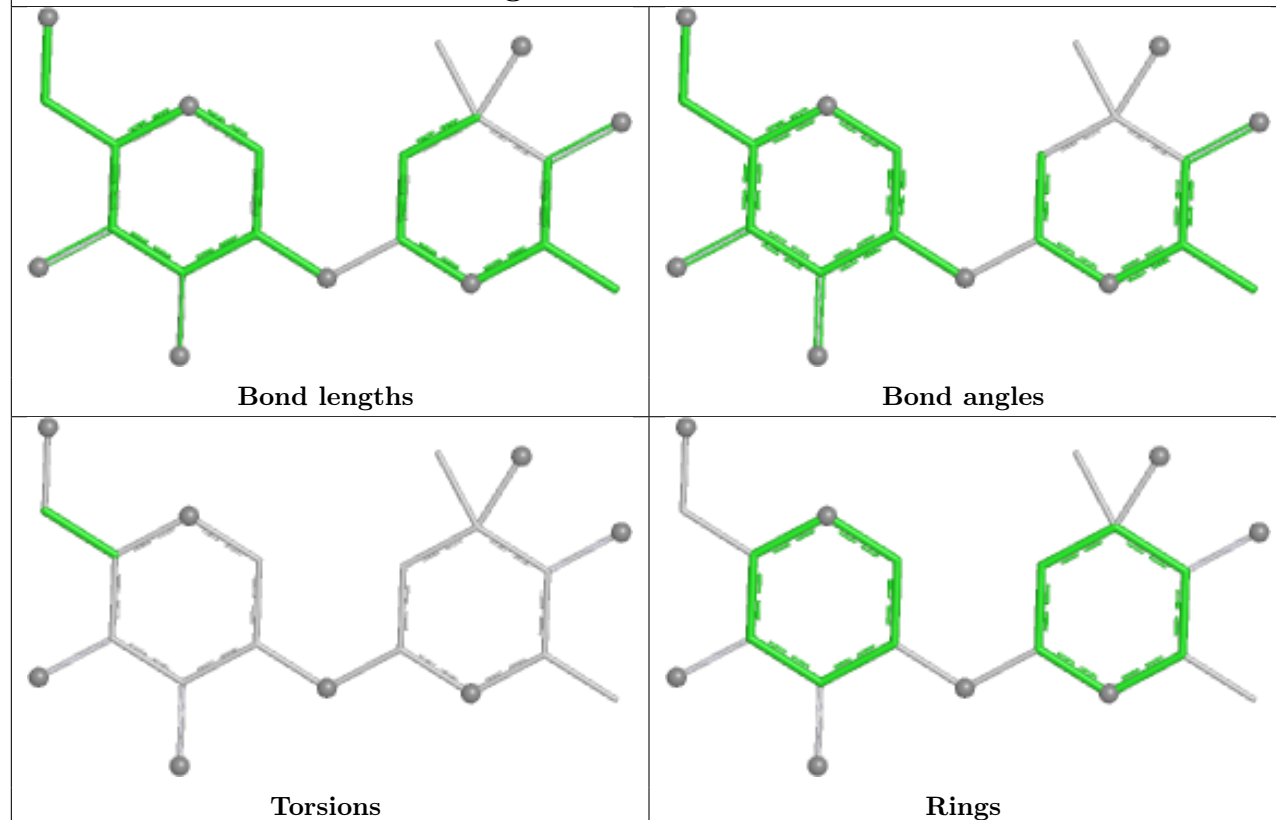
MolProbity failed to run properly - this section will have to be empty.

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



Oligosaccharide Chain F



6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided