Full wwPDB NMR Structure Validation Report (i)

Nov 6, 2023 – 06:35 AM EST

PDB ID	:	1GAC
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 (i) symbol.

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

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

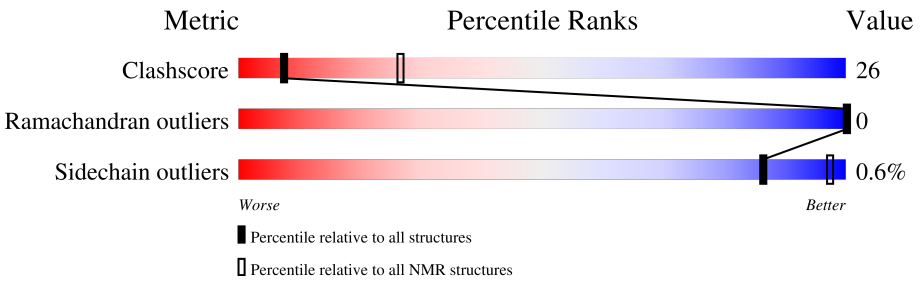
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	5	80% 20%
1	B	5	60% 40%
2	C	7	14% 29% 57%
2	D	7	14% 43% 43%
3	E	2	100%
3	F	2	100%

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

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
3	E	RER	2	80	-
3	F	RER	2	80	-
4	C	RER	10	80	-
4	D	RER	10	80	-

2 Ensemble composition and analysis (i)

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.

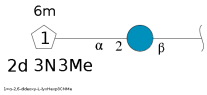
- Molecule 1 is a protein called CELL WALL PENTAPEPTIDE.

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

- Molecule 2 is a protein called CHLOROORIENTICIN A.

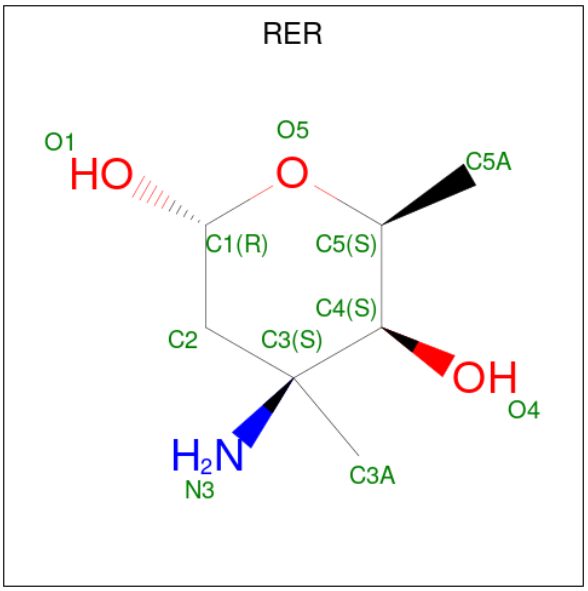
Mol	Chain	Residues	Atoms						Trace
			Total	C	Cl	H	N	O	
2	C	7	130	53	2	50	8	17	0
2	D	7	130	53	2	50	8	17	0

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



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

- Molecule 4 is vancosamine (three-letter code: RER) (formula: $C_7H_{15}NO_3$).



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

4 Residue-property plots (i)

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

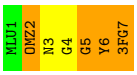
Chain A: 80% 20%

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

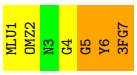
• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%



• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 100%

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

Chain F: 100%

BGC1 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: 80% 20%

A1 E2 A5

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1 E2 K3 A4 A5

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D: 29% 29% 43%

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%

4.2.2 Score per residue for model 2

- Molecule 1: CELL WALL PENTAPEPTIDE

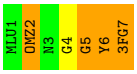
Chain A:

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

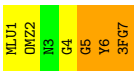
- Molecule 2: CHLOROORIENTICIN A

Chain C:



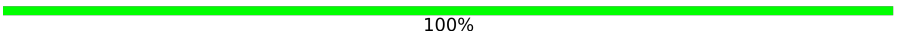
- Molecule 2: CHLOROORIENTICIN A

Chain D:



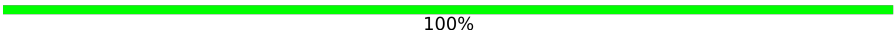
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.3 Score per residue for model 3

- Molecule 1: CELL WALL PENTAPEPTIDE

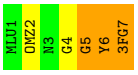
Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

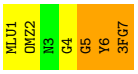
- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



- 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

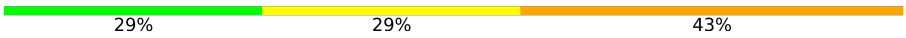
- Molecule 1: CELL WALL PENTAPEPTIDE

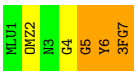
Chain A: 80% 20%

• Molecule 1: CELL WALL PENTAPEPTIDE

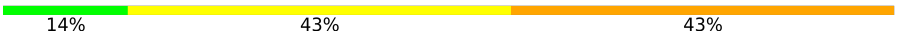
Chain B:

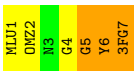
• Molecule 2: CHLOROORIENTICIN A

Chain C: 



• Molecule 2: CHLOROORIENTICIN A

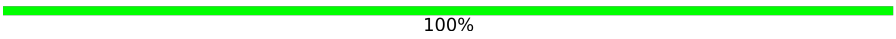
Chain D: 



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

Chain E:

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

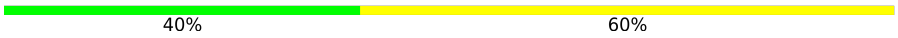
Chain F: 

4.2.5 Score per residue for model 5

• Molecule 1: CELL WALL PENTAPEPTIDE

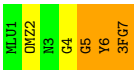
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

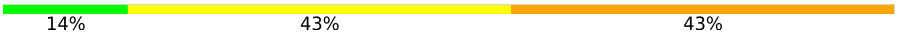
Chain B: 

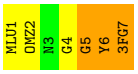
• Molecule 2: CHLOROORIENTICIN A

Chain C:

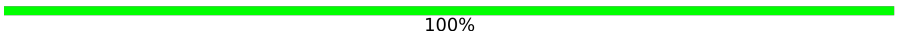


• Molecule 2: CHLOROORIENTICIN A

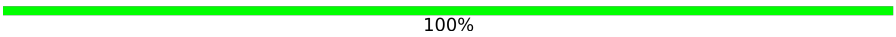
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.6 Score per residue for model 6

• Molecule 1: CELL WALL PENTAPEPTIDE

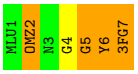
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

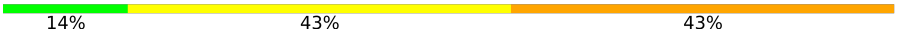
• Molecule 2: CHLOROORIENTICIN A

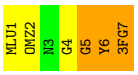
Chain C:



• Molecule 2: CHLOROORIENTICIN A

Chain D:



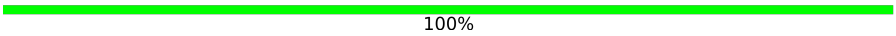


• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:

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

Chain F:



4.2.7 Score per residue for model 7

• Molecule 1: CELL WALL PENTAPEPTIDE

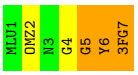
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

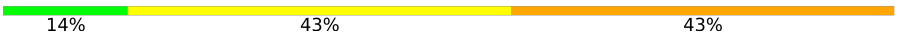
• Molecule 2: CHLOROORIENTICIN A

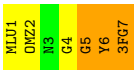
Chain C:



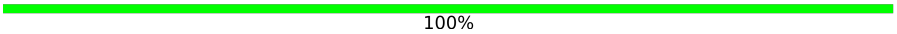
• Molecule 2: CHLOROORIENTICIN A

Chain D:

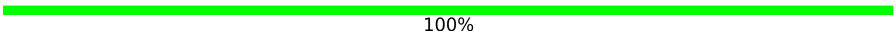




• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 

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

Chain F: 

4.2.8 Score per residue for model 8

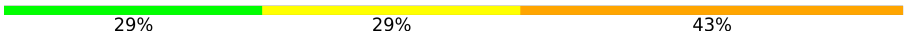
• Molecule 1: CELL WALL PENTAPEPTIDE

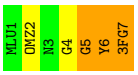
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

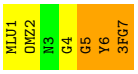
• Molecule 2: CHLOROORIENTICIN A

Chain C: 

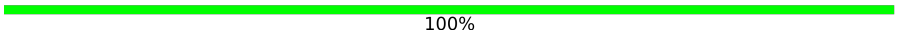


• Molecule 2: CHLOROORIENTICIN A

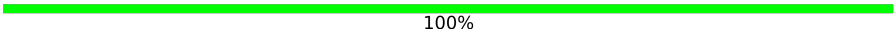
Chain D:



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

Chain E: 

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

Chain F: 

4.2.9 Score per residue for model 9

• Molecule 1: CELL WALL PENTAPEPTIDE

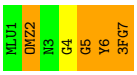
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

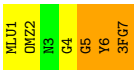
• Molecule 2: CHLOROORIENTICIN A

Chain C:



• Molecule 2: CHLOROORIENTICIN A

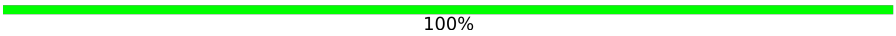
Chain D:



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

Chain E:

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

Chain F: 

4.2.10 Score per residue for model 10

- Molecule 1: CELL WALL PENTAPEPTIDE

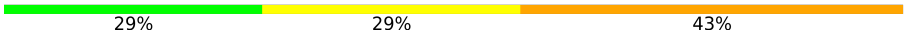
Chain A:

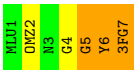
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

- Molecule 2: CHLOROORIENTICIN A

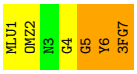
Chain C:





- Molecule 2: CHLOROORIENTICIN A

Chain D:

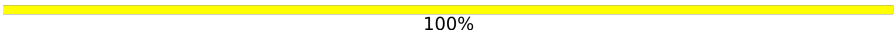


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:

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

Chain F:



4.2.11 Score per residue for model 11

- Molecule 1: CELL WALL PENTAPEPTIDE

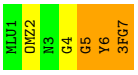
Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

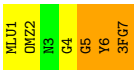
- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 50% 50%

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

Chain F: 100%

4.2.12 Score per residue for model 12

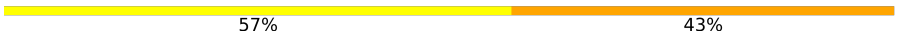
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 60% 40%

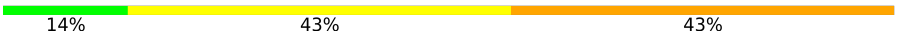
• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C: 

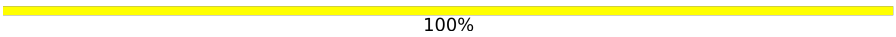
• Molecule 2: CHLOROORIENTICIN A

Chain D: 

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

Chain E:

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

Chain F: 

4.2.13 Score per residue for model 13

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

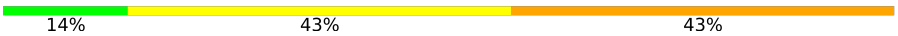
• Molecule 1: CELL WALL PENTAPEPTIDE

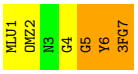
Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

• Molecule 2: CHLOROORIENTICIN A

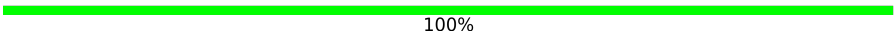
Chain D: 



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

Chain E:

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

Chain F: 

4.2.14 Score per residue for model 14

• Molecule 1: CELL WALL PENTAPEPTIDE

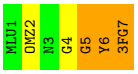
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

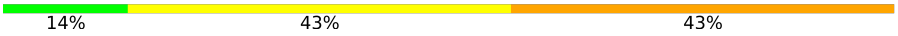
Chain B:

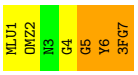
• Molecule 2: CHLOROORIENTICIN A

Chain C:



• Molecule 2: CHLOROORIENTICIN A

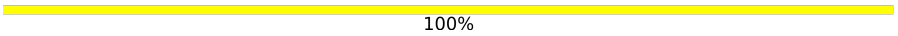
Chain D: 



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

Chain E:

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

Chain F: 

4.2.15 Score per residue for model 15

• Molecule 1: CELL WALL PENTAPEPTIDE

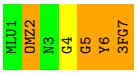
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

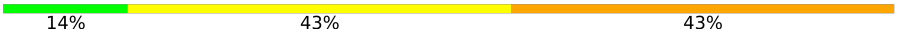
Chain B:

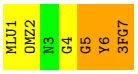
• Molecule 2: CHLOROORIENTICIN A

Chain C:



• Molecule 2: CHLOROORIENTICIN A

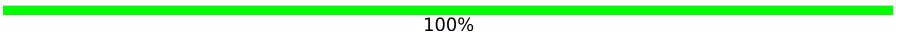
Chain D: 



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

Chain E:

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

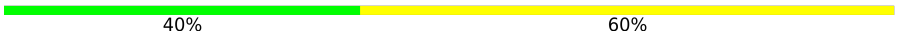
Chain F: 

4.2.16 Score per residue for model 16

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

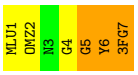
Chain B: 

• Molecule 2: CHLOROORIENTICIN A

Chain C:

• Molecule 2: CHLOROORIENTICIN A

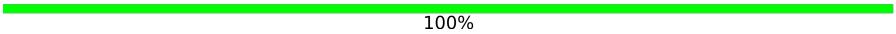
Chain D:



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

Chain E:

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

Chain F: 

4.2.17 Score per residue for model 17

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

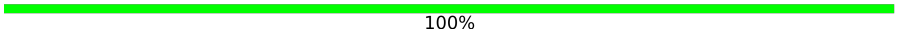
• Molecule 2: CHLOROORIENTICIN A

Chain C:

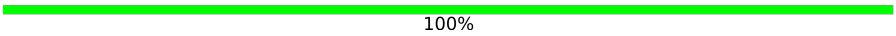
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.18 Score per residue for model 18

- Molecule 1: CELL WALL PENTAPEPTIDE

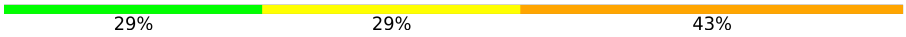
Chain A:

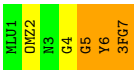
- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

- Molecule 2: CHLOROORIENTICIN A

Chain C:



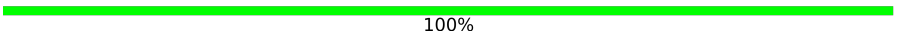


- Molecule 2: CHLOROORIENTICIN A

Chain D:

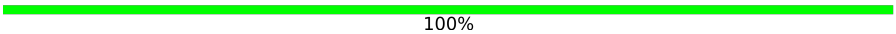
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.19 Score per residue for model 19

- Molecule 1: CELL WALL PENTAPEPTIDE

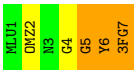
Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 40% 60%

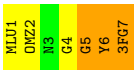
- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%



- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 50% 50%

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

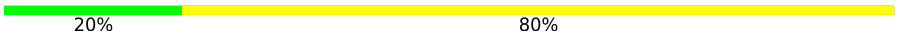
Chain F: 100%

4.2.20 Score per residue for model 20

- Molecule 1: CELL WALL PENTAPEPTIDE

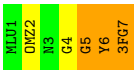
Chain A: 80% 20%

• Molecule 1: CELL WALL PENTAPEPTIDE

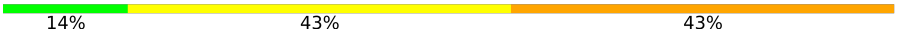
Chain B: 

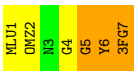
• Molecule 2: CHLOROORIENTICIN A

Chain C:

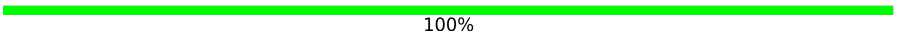


• Molecule 2: CHLOROORIENTICIN A

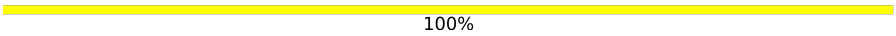
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.21 Score per residue for model 21

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

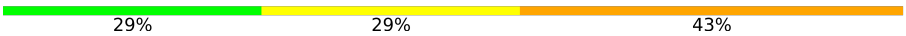
• Molecule 1: CELL WALL PENTAPEPTIDE

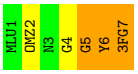
Chain B:

• Molecule 2: CHLOROORIENTICIN A

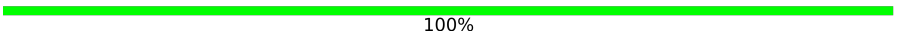
Chain C:

• Molecule 2: CHLOROORIENTICIN A

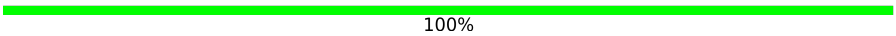
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.22 Score per residue for model 22

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

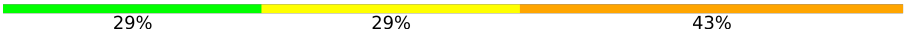
• Molecule 1: CELL WALL PENTAPEPTIDE

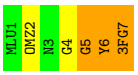
Chain B:

• Molecule 2: CHLOROORIENTICIN A

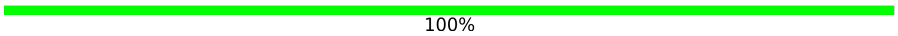
Chain C:

• Molecule 2: CHLOROORIENTICIN A

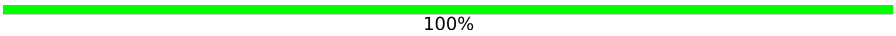
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.23 Score per residue for model 23

• Molecule 1: CELL WALL PENTAPEPTIDE

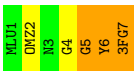
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

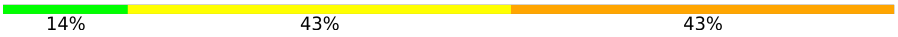
Chain B:

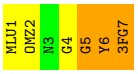
• Molecule 2: CHLOROORIENTICIN A

Chain C:



• Molecule 2: CHLOROORIENTICIN A

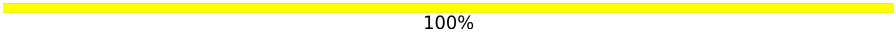
Chain D: 



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

Chain E:

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

Chain F: 

4.2.24 Score per residue for model 24

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

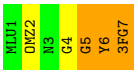
Chain B:

• Molecule 2: CHLOROORIENTICIN A

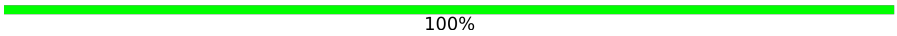
Chain C:

• Molecule 2: CHLOROORIENTICIN A

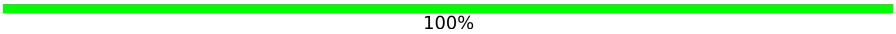
Chain D:



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

Chain E: 

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

Chain F: 

4.2.25 Score per residue for model 25

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

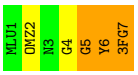
Chain B:

• Molecule 2: CHLOROORIENTICIN A

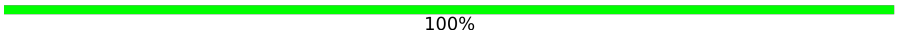
Chain C:

• Molecule 2: CHLOROORIENTICIN A

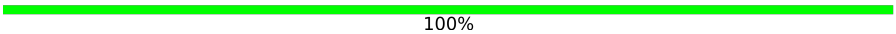
Chain D:



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

Chain E: 

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

Chain F: 

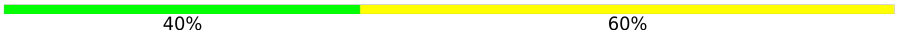
4.2.26 Score per residue for model 26

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

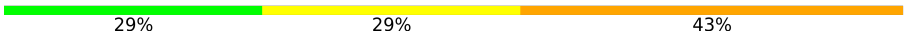
- Molecule 1: CELL WALL PENTAPEPTIDE

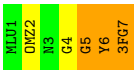
Chain B:



- Molecule 2: CHLOROORIENTICIN A

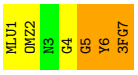
Chain C:





- Molecule 2: CHLOROORIENTICIN A

Chain D:

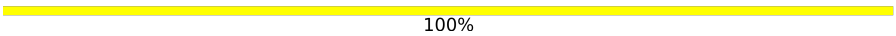


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:

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

Chain F:



4.2.27 Score per residue for model 27

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 80% 20%

A1 E2 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 29% 29% 43%

MLU1 OMZ2 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

4.2.28 Score per residue for model 28

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 80% 20%

A1 E2 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 29% 29% 43%

MLU1 OMZ2 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

4.2.29 Score per residue for model 29

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1 E2 K3 A4 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 29% 57%

MLU1 OMZ2 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

4.2.30 Score per residue for model 30

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 20% 80%

A1 E2 K3 A4 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

MLU1 OMZ2 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

4.2.31 Score per residue for model 31

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 20% 80%

A1 E2 K3 A4 A5

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

MLU1 OMZ2 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: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1 E2 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 43% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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

4.2.33 Score per residue for model 33

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1
E2
A5

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 20% 80%

A1
E2
K3
A4
A5

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1
OMZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

MLU1
OMZ2
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

4.2.34 Score per residue for model 34

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

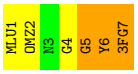
Chain B: 60% 40%

- Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 50% 50%

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

Chain F: 100%

4.2.35 Score per residue for model 35

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 60% 40%

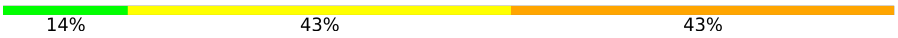
• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

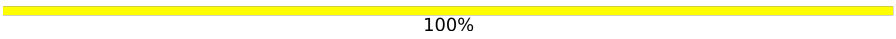
• Molecule 2: CHLOROORIENTICIN A

Chain D: 

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

Chain E:

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

Chain F: 

4.2.36 Score per residue for model 36

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

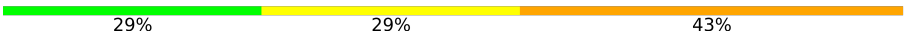
• Molecule 1: CELL WALL PENTAPEPTIDE

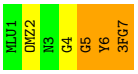
Chain B:

• Molecule 2: CHLOROORIENTICIN A

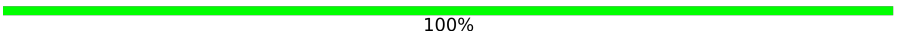
Chain C:

• Molecule 2: CHLOROORIENTICIN A

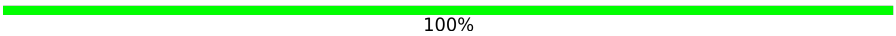
Chain D: 



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

Chain E: 

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

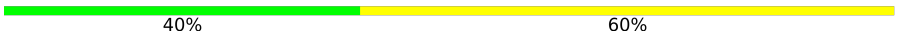
Chain F: 

4.2.37 Score per residue for model 37

• Molecule 1: CELL WALL PENTAPEPTIDE

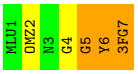
Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 

• Molecule 2: CHLOROORIENTICIN A

Chain C:



• Molecule 2: CHLOROORIENTICIN A

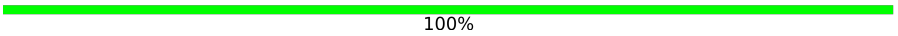
Chain D:

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

Chain E:

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

Chain F:



4.2.38 Score per residue for model 38

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

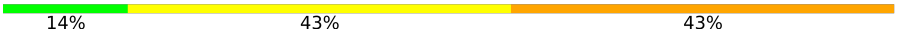
Chain B:

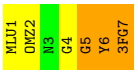
• Molecule 2: CHLOROORIENTICIN A

Chain C:

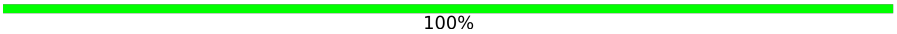
• Molecule 2: CHLOROORIENTICIN A

Chain D:

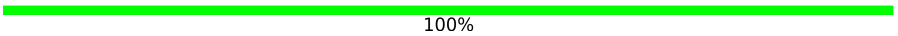




• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 

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

Chain F: 

4.2.39 Score per residue for model 39

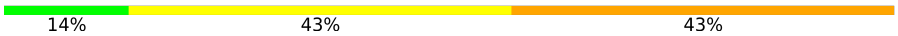
• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

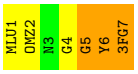
Chain B:

• Molecule 2: CHLOROORIENTICIN A

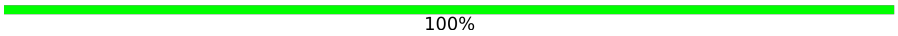
Chain C: 

• Molecule 2: CHLOROORIENTICIN A

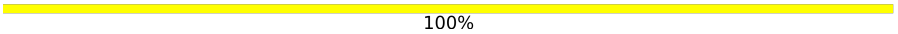
Chain D:



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

Chain E: 

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

Chain F: 

4.2.40 Score per residue for model 40

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

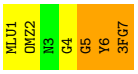
Chain B:

• Molecule 2: CHLOROORIENTICIN A

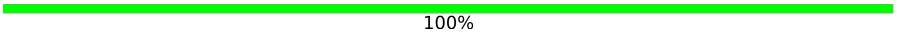
Chain C:

• Molecule 2: CHLOROORIENTICIN A

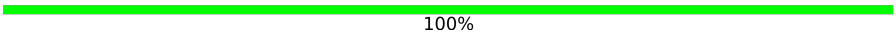
Chain D:



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

Chain E: 

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

Chain F: 

4.2.41 Score per residue for model 41

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

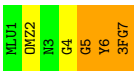
Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

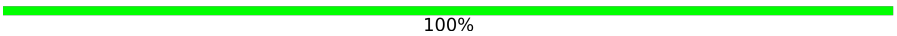
• Molecule 2: CHLOROORIENTICIN A

Chain D:



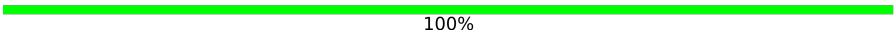
• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.42 Score per residue for model 42

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

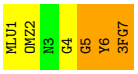
Chain B: 60% 40%

- Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 43% 43%

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 100%

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

Chain F: 100%

4.2.43 Score per residue for model 43

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 60% 40%

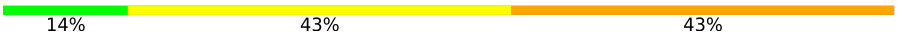
• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

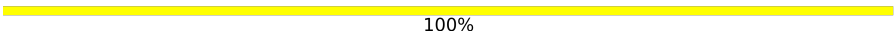
• Molecule 2: CHLOROORIENTICIN A

Chain D: 

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

Chain E:

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

Chain F: 

4.2.44 Score per residue for model 44

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

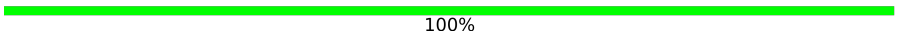
• Molecule 2: CHLOROORIENTICIN A

Chain C:

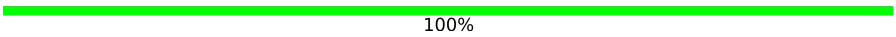
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.45 Score per residue for model 45

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

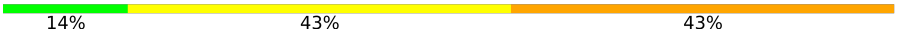
Chain B:

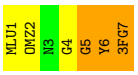
• Molecule 2: CHLOROORIENTICIN A

Chain C:

• Molecule 2: CHLOROORIENTICIN A

Chain D:



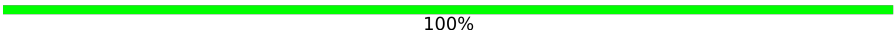


• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:

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

Chain F:



4.2.46 Score per residue for model 46

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

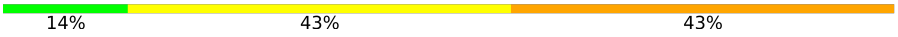
Chain B:

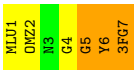
• Molecule 2: CHLOROORIENTICIN A

Chain C:

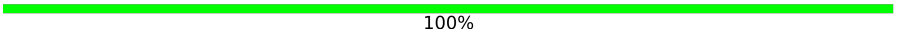
• Molecule 2: CHLOROORIENTICIN A

Chain D:

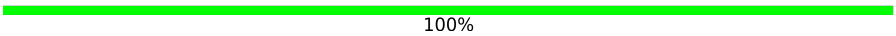




• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E: 

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

Chain F: 

4.2.47 Score per residue for model 47

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

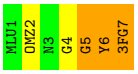
Chain B:

• Molecule 2: CHLOROORIENTICIN A

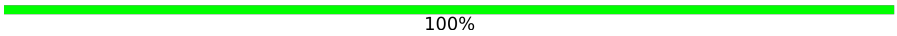
Chain C:

• Molecule 2: CHLOROORIENTICIN A

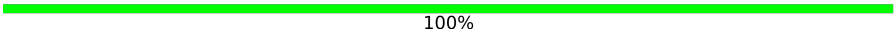
Chain D:



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

Chain E: 

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

Chain F: 

4.2.48 Score per residue for model 48

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

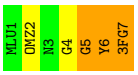
Chain B:

• Molecule 2: CHLOROORIENTICIN A

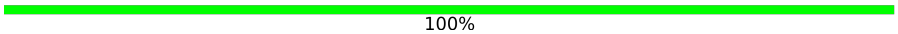
Chain C:

• Molecule 2: CHLOROORIENTICIN A

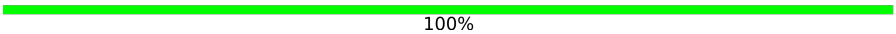
Chain D:



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

Chain E: 

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

Chain F: 

4.2.49 Score per residue for model 49

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

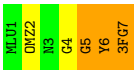
Chain B:

• Molecule 2: CHLOROORIENTICIN A

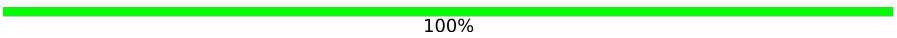
Chain C:

• Molecule 2: CHLOROORIENTICIN A

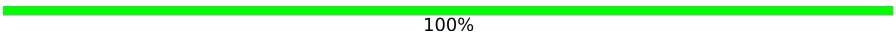
Chain D:



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

Chain E: 

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

Chain F: 

4.2.50 Score per residue for model 50

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1 E2 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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

4.2.51 Score per residue for model 51

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

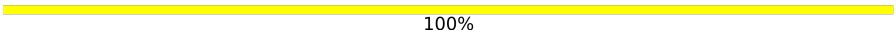
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E:

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

Chain F: 

4.2.52 Score per residue for model 52

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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: 50% 50%

BGC1 RER2

4.2.53 Score per residue for model 53

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 20% 60% 20%

A1 E2 K3 A4 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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

4.2.54 Score per residue for model 54

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1 E2 A5

- Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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

4.2.55 Score per residue for model 55

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

A1 E2 A5

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 40% 60%

A1 E2 K3 A4 A5

• Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%

MLU1 OMZ2 N3 G4 G5 Y6 3FG7

• Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%

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: 80% 20%

A1
E2
A5

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

A1
E2
A5

- Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

MLU1
OMZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D: 43% 57%

MLU1
OMZ2
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

4.2.57 Score per residue for model 57

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

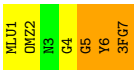
Chain B: 60% 40%

- Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 100%

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

Chain F: 100%

4.2.58 Score per residue for model 58

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

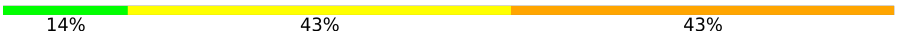
• Molecule 1: CELL WALL PENTAPEPTIDE

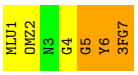
Chain B:

• Molecule 2: CHLOROORIENTICIN A

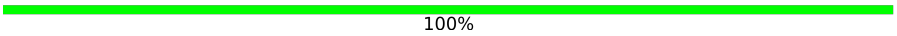
Chain C:

• Molecule 2: CHLOROORIENTICIN A

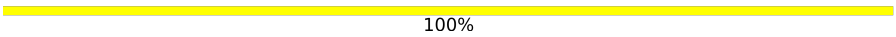
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.59 Score per residue for model 59

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

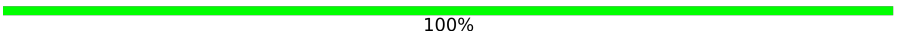
• Molecule 2: CHLOROORIENTICIN A

Chain C:

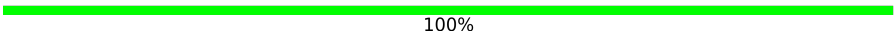
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.60 Score per residue for model 60

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

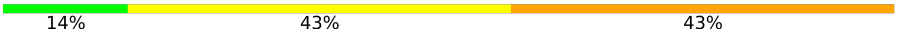
• Molecule 1: CELL WALL PENTAPEPTIDE

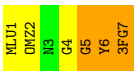
Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

• Molecule 2: CHLOROORIENTICIN A

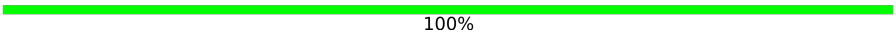
Chain D: 



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

Chain E:

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

Chain F: 

4.2.61 Score per residue for model 61

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

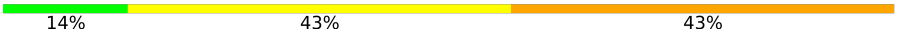
• Molecule 1: CELL WALL PENTAPEPTIDE

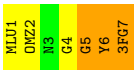
Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

• Molecule 2: CHLOROORIENTICIN A

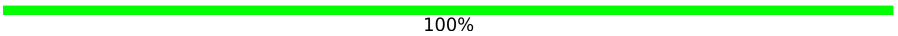
Chain D: 



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

Chain E:

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

Chain F: 

4.2.62 Score per residue for model 62

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

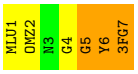
Chain B:

• Molecule 2: CHLOROORIENTICIN A

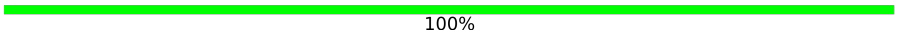
Chain C:

• Molecule 2: CHLOROORIENTICIN A

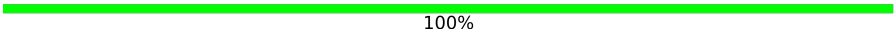
Chain D:



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

Chain E: 

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

Chain F: 

4.2.63 Score per residue for model 63

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

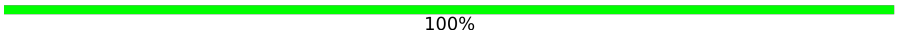
• Molecule 2: CHLOROORIENTICIN A

Chain C:

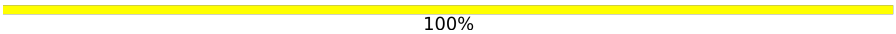
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.64 Score per residue for model 64

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

- Molecule 2: CHLOROORIENTICIN A

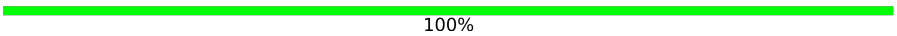
Chain C:

- Molecule 2: CHLOROORIENTICIN A

Chain D:

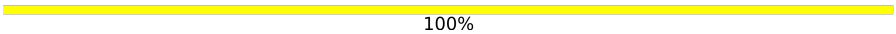
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.65 Score per residue for model 65

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

- Molecule 1: CELL WALL PENTAPEPTIDE

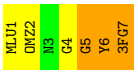
Chain B: 60% 40%

- Molecule 2: CHLOROORIENTICIN A

Chain C: 14% 29% 57%

- Molecule 2: CHLOROORIENTICIN A

Chain D: 14% 43% 43%



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

Chain E: 100%

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

Chain F: 100%

4.2.66 Score per residue for model 66

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A: 80% 20%

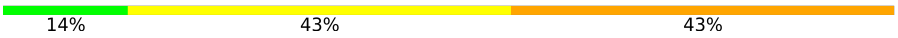
• Molecule 1: CELL WALL PENTAPEPTIDE

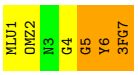
Chain B:

• Molecule 2: CHLOROORIENTICIN A

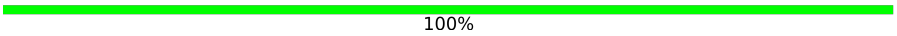
Chain C:

• Molecule 2: CHLOROORIENTICIN A

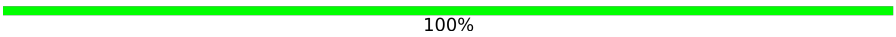
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.67 Score per residue for model 67

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

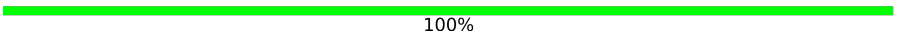
• Molecule 2: CHLOROORIENTICIN A

Chain C:

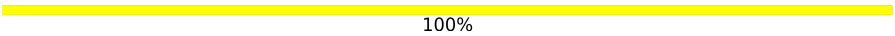
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.68 Score per residue for model 68

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

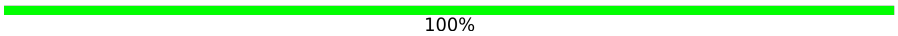
Chain C:

• Molecule 2: CHLOROORIENTICIN A

Chain D:

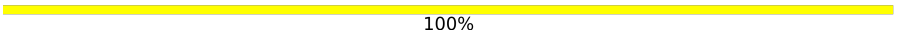
• Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.69 Score per residue for model 69

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

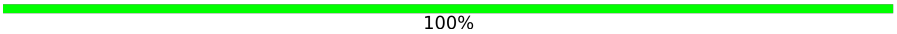
• Molecule 2: CHLOROORIENTICIN A

Chain C:

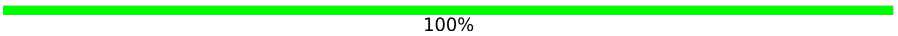
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

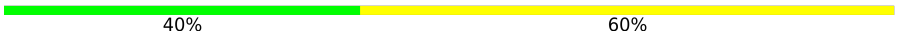
Chain F: 

4.2.70 Score per residue for model 70

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 

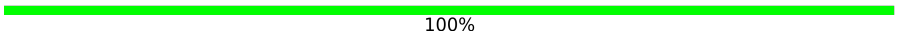
• Molecule 2: CHLOROORIENTICIN A

Chain C:

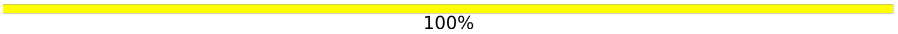
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.71 Score per residue for model 71

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

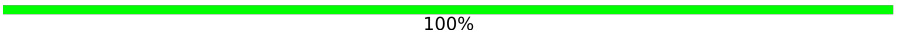
• Molecule 2: CHLOROORIENTICIN A

Chain C:

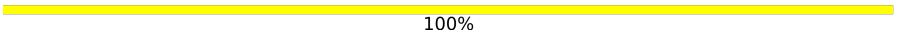
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.72 Score per residue for model 72

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

- Molecule 2: CHLOROORIENTICIN A

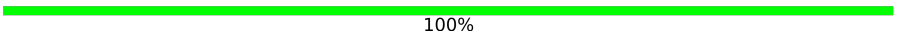
Chain C:

- Molecule 2: CHLOROORIENTICIN A

Chain D:

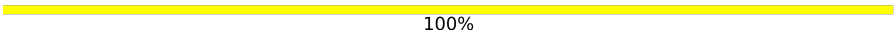
- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain E:



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

Chain F:



4.2.73 Score per residue for model 73

• Molecule 1: CELL WALL PENTAPEPTIDE

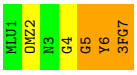
Chain A: 80% 20%

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B: 60% 40%

• Molecule 2: CHLOROORIENTICIN A

Chain C: 29% 29% 43%



• Molecule 2: CHLOROORIENTICIN A

Chain D: 43% 57%

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

Chain E: 50% 50%

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

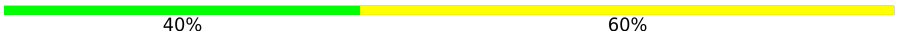
Chain F: 100%

4.2.74 Score per residue for model 74

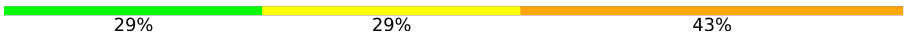
• Molecule 1: CELL WALL PENTAPEPTIDE

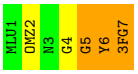
Chain A: 80% 20%

• Molecule 1: CELL WALL PENTAPEPTIDE

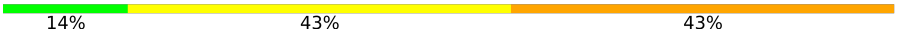
Chain B: 

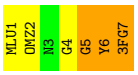
• Molecule 2: CHLOROORIENTICIN A

Chain C: 

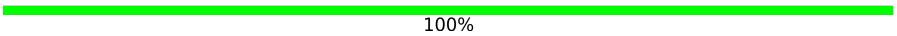


• Molecule 2: CHLOROORIENTICIN A

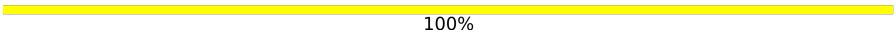
Chain D: 



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

Chain E: 

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

Chain F: 

4.2.75 Score per residue for model 75

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

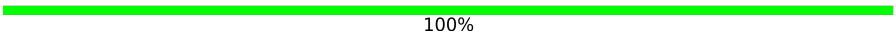
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E:

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

Chain F: 

4.2.76 Score per residue for model 76

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

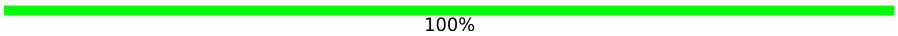
• Molecule 2: CHLOROORIENTICIN A

Chain C:

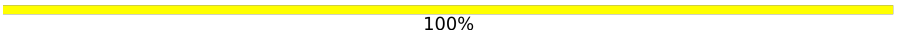
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.77 Score per residue for model 77

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

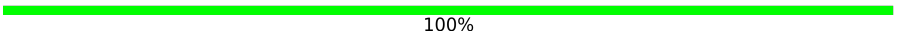
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E:

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

Chain F: 

4.2.78 Score per residue for model 78

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

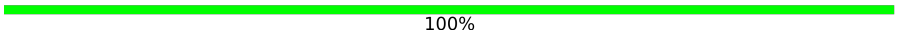
• Molecule 2: CHLOROORIENTICIN A

Chain C:

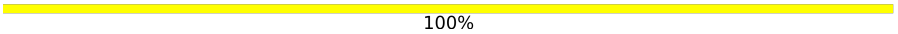
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E: 

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

Chain F: 

4.2.79 Score per residue for model 79

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

• Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

• Molecule 2: CHLOROORIENTICIN A

Chain C:

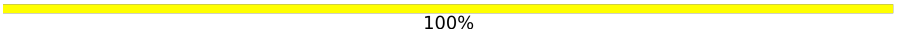
• Molecule 2: CHLOROORIENTICIN A

Chain D:

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

Chain E:

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

Chain F: 

4.2.80 Score per residue for model 80

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:

- Molecule 2: CHLOROORIENTICIN A

Chain C:

- Molecule 2: CHLOROORIENTICIN A

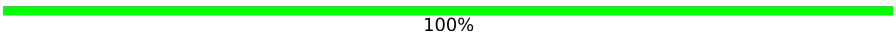
Chain D:

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

Chain E:

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

Chain F:



5 Refinement protocol and experimental data overview (i)

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)

Bond lengths and bond angles in the following residue types are not validated in this section: OMZ, RER, OMY, GHP, MLU, BGC, DAL, FGA, 3FG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	33	36	33	2±2
1	B	33	36	33	4±1
2	C	80	50	46	6±2
2	D	80	50	46	6±1
3	E	21	25	22	0±0
3	F	21	25	22	0±0
4	D	10	15	13	1±1
4	C	10	15	13	0±1
All	All	23040	20160	18220	1070

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 26.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:DAL:HB2	2:C:1:MLU:HD12	0.74	1.60	35	6
1:A:5:DAL:CB	2:C:1:MLU:HD12	0.70	2.15	35	6
1:A:5:DAL:CB	2:C:1:MLU:CD1	0.59	2.80	35	6
1:A:5:DAL:HB2	2:C:1:MLU:CD1	0.58	2.29	12	6
2:D:3:ASN:CG	2:D:4:GHP:H	0.58	2.02	29	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:3:ASN:HA	4:D:10:RER:H3A3	0.57	1.76	35	20
1:A:2:FGA:C	4:C:10:RER:C1	0.54	2.85	52	3
2:C:6:OMY:OCZ	3:F:2:RER:C5A	0.52	2.58	73	1
1:B:2:FGA:C	4:D:10:RER:O5	0.52	2.58	40	39
2:D:5:GHP:HC2	2:D:7:3FG:HN1	0.51	1.65	5	73
1:A:2:FGA:C	4:C:10:RER:O5	0.50	2.59	52	3
1:B:2:FGA:C	4:D:10:RER:C1	0.50	2.90	63	28
2:C:2:OMZ:C	2:C:3:ASN:CG	0.49	2.80	65	36
1:A:2:FGA:CA	4:C:10:RER:O5	0.49	2.61	80	3
1:B:2:FGA:CD	2:D:6:OMY:HD1	0.48	2.38	18	50
2:C:2:OMZ:O	2:C:3:ASN:OD1	0.48	2.32	43	39
1:A:5:DAL:C	2:C:4:GHP:C5	0.47	2.92	35	1
2:D:2:OMZ:C	2:D:3:ASN:CG	0.47	2.83	73	18
1:B:2:FGA:O	3:E:1:BGC:C6	0.47	2.63	1	2
1:B:1:ALA:O	2:C:2:OMZ:CL	0.46	2.71	46	2
1:A:2:FGA:CD	2:C:6:OMY:HD1	0.46	2.41	30	78
2:D:2:OMZ:O	2:D:3:ASN:OD1	0.46	2.32	73	1
2:C:2:OMZ:CL	3:E:1:BGC:O6	0.46	2.71	9	3
1:B:2:FGA:C	3:E:1:BGC:C6	0.46	2.94	1	1
1:B:5:DAL:HA	2:D:1:MLU:CD1	0.45	2.42	23	53
2:D:6:OMY:ODE	4:D:10:RER:H3A2	0.45	2.11	17	3
1:B:3:LYS:NZ	2:D:7:3FG:C	0.45	2.80	70	1
2:C:5:GHP:HC2	2:C:7:3FG:HN1	0.45	1.73	33	80
1:B:2:FGA:HB3	2:D:6:OMY:CB	0.44	2.42	29	39
2:D:5:GHP:C2	2:D:7:3FG:HN1	0.44	2.25	15	80
1:B:1:ALA:O	4:D:10:RER:O5	0.44	2.36	53	1
1:B:5:DAL:C	2:D:3:ASN:H	0.43	2.26	63	5
2:C:5:GHP:C2	2:C:7:3FG:N	0.43	2.82	38	80
1:A:2:FGA:OE1	2:C:6:OMY:HD1	0.43	2.13	52	3
2:D:5:GHP:C2	2:D:7:3FG:N	0.43	2.82	45	80
1:B:2:FGA:HB3	2:D:6:OMY:HB	0.43	1.88	44	23
2:C:5:GHP:C2	2:C:7:3FG:HN1	0.43	2.27	1	78
1:B:3:LYS:CE	2:D:7:3FG:OD2	0.42	2.67	60	1
1:B:3:LYS:CE	1:B:3:LYS:HA	0.42	2.43	14	1
2:C:3:ASN:OD1	2:C:4:GHP:N	0.42	2.53	13	4
1:B:4:DAL:O	2:D:1:MLU:CD1	0.42	2.67	80	1
2:C:5:GHP:O	2:D:5:GHP:N	0.42	2.53	54	1
1:B:2:FGA:OE1	2:D:6:OMY:HD1	0.42	2.15	44	38
2:D:3:ASN:OD1	2:D:4:GHP:N	0.42	2.53	70	1
1:A:2:FGA:HB3	4:C:10:RER:C1	0.42	2.45	73	2
2:C:1:MLU:O	2:C:3:ASN:ND2	0.41	2.53	43	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:5:GHP:N	2:D:5:GHP:O	0.41	2.53	73	3
1:A:5:DAL:CB	2:C:1:MLU:HD13	0.41	2.45	43	1
1:B:2:FGA:OE1	1:B:4:DAL:N	0.41	2.53	1	6
2:C:3:ASN:OD1	2:C:3:ASN:N	0.41	2.52	35	1
3:F:1:BGC:O2	3:F:2:RER:H3A2	0.41	2.15	43	28
1:B:3:LYS:O	2:D:7:3FG:CB	0.41	2.69	55	13
1:B:5:DAL:C	2:D:1:MLU:HD12	0.41	2.46	38	5
1:A:2:FGA:OE1	2:C:6:OMY:CD1	0.41	2.69	52	2
1:B:4:DAL:HA	2:D:4:GHP:O	0.40	2.16	29	2

6.3 Torsion angles (i)

6.3.1 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 NMR 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	0	-	-	-	-	
1	B	0	-	-	-	-	
2	C	1/7 (14%)	0±0 (0±0%)	1±0 (100±0%)	0±0 (0±0%)	100	100
2	D	1/7 (14%)	0±0 (0±0%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	160/1920 (8%)	0 (0%)	160 (100%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 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 NMR 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	1/1 (100%)	1±0 (98±16%)	0±0 (2±16%)	50	91
1	B	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
2	D	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	320/320 (100%)	318 (99%)	2 (1%)	86	97

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	3	LYS	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	FGA	A	2	1	6,7,9	0.71±0.03	0±0 (0±0%)
2	GHP	D	4	2,3	10,11,12	2.68±0.01	6±0 (60±2%)
2	MLU	D	1	2	7,8,9	0.45±0.01	0±0 (0±0%)
2	OMZ	D	2	2	12,14,15	2.56±0.01	6±0 (50±0%)
2	3FG	D	7	2	12,13,13	2.58±0.01	7±1 (55±4%)
2	OMY	D	6	2,4	12,14,15	2.51±0.02	6±0 (50±0%)
2	3FG	C	7	2	12,13,13	2.56±0.01	7±0 (54±4%)
2	GHP	C	4	2,3	10,11,12	2.69±0.01	6±0 (60±0%)
2	GHP	D	5	2	10,11,12	2.40±0.01	6±0 (59±1%)
1	FGA	B	2	1	6,7,9	0.82±0.08	0±0 (0±0%)
2	OMZ	C	2	2	12,14,15	2.60±0.01	6±0 (50±2%)
2	OMY	C	6	2,4	12,14,15	2.57±0.02	7±0 (56±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	GHP	C	5	2	10,11,12	2.41±0.01	6±0 (60±0%)
2	MLU	C	1	2	7,8,9	0.45±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	FGA	A	2	1	2,7,11	0.71±0.08	0±0 (0±0%)
2	GHP	D	4	2,3	11,14,16	1.14±0.08	0±0 (2±4%)
2	MLU	D	1	2	6,9,11	0.79±0.02	0±0 (0±0%)
2	OMZ	D	2	2	17,19,21	0.80±0.02	0±0 (0±0%)
2	3FG	D	7	2	14,18,18	0.83±0.04	0±0 (1±2%)
2	OMY	D	6	2,4	17,19,21	1.23±0.04	1±0 (5±0%)
2	3FG	C	7	2	14,18,18	0.79±0.01	0±0 (0±0%)
2	GHP	C	4	2,3	11,14,16	1.22±0.07	1±0 (11±3%)
2	GHP	D	5	2	11,14,16	1.38±0.05	3±0 (26±2%)
1	FGA	B	2	1	2,7,11	1.05±0.26	0±0 (1±7%)
2	OMZ	C	2	2	17,19,21	0.82±0.01	0±0 (0±0%)
2	OMY	C	6	2,4	17,19,21	1.25±0.08	1±0 (6±2%)
2	GHP	C	5	2	11,14,16	1.40±0.03	3±0 (27±0%)
2	MLU	C	1	2	6,9,11	0.81±0.02	0±0 (0±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	3FG	D	7	2	-	0±0,8,8,8	0±0,1,1,1
1	FGA	A	2	1	-	0±0,4,6,9	-
2	GHP	D	5	2	-	0±0,4,6,8	0±0,1,1,1
2	GHP	C	4	2,3	-	0±0,4,6,8	0±0,1,1,1
2	OMZ	C	2	2	-	0±0,9,10,12	0±0,1,1,1
2	MLU	D	1	2	-	0±0,5,8,10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GHP	C	5	2	-	0±0,4,6,8	0±0,1,1,1
2	MLU	C	1	2	-	0±0,5,8,10	-
2	3FG	C	7	2	-	0±0,8,8,8	0±0,1,1,1
2	OMY	D	6	2,4	-	0±0,9,10,12	0±0,1,1,1
2	OMZ	D	2	2	-	0±0,9,10,12	0±0,1,1,1
1	FGA	B	2	1	-	0±0,4,6,9	-
2	OMY	C	6	2,4	-	0±0,9,10,12	0±0,1,1,1
2	GHP	D	4	2,3	-	0±0,4,6,8	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	2	OMZ	CZ-CE1	4.99	1.44	1.39	55	80
2	D	2	OMZ	CZ-CE1	4.71	1.44	1.39	37	80
2	C	6	OMY	CZ-CE1	4.70	1.44	1.39	55	80
2	D	7	3FG	CG1-CB	4.56	1.46	1.39	53	80
2	D	6	OMY	CZ-CE1	4.45	1.43	1.39	60	80
2	C	7	3FG	CG1-CB	4.39	1.46	1.39	51	80
2	D	4	GHP	C3-C2	4.30	1.46	1.38	74	80
2	D	4	GHP	C6-C5	4.27	1.46	1.38	37	80
2	C	4	GHP	C3-C2	4.25	1.46	1.38	75	80
2	C	4	GHP	C6-C5	4.24	1.46	1.38	52	80
2	D	7	3FG	CG2-CB	4.14	1.45	1.39	26	80
2	C	7	3FG	CG2-CB	4.11	1.45	1.39	57	80
2	D	6	OMY	CD2-CG	3.85	1.45	1.39	55	80
2	C	6	OMY	CD2-CG	3.73	1.45	1.39	12	80
2	D	2	OMZ	CD1-CG	3.70	1.44	1.39	42	80
2	C	2	OMZ	CD2-CG	3.67	1.45	1.39	54	80
2	D	2	OMZ	CD2-CG	3.67	1.45	1.39	80	80
2	D	6	OMY	CD1-CG	3.65	1.44	1.39	19	80
2	D	6	OMY	CD2-CE2	3.61	1.45	1.38	63	80
2	C	6	OMY	CD2-CE2	3.57	1.45	1.38	35	80
2	C	5	GHP	C6-C1	3.53	1.44	1.39	4	80
2	D	5	GHP	C6-C1	3.53	1.44	1.39	60	80
2	C	2	OMZ	CD1-CG	3.47	1.44	1.39	16	80
2	C	5	GHP	C6-C5	3.46	1.45	1.38	76	80
2	D	5	GHP	C6-C5	3.45	1.45	1.38	49	80
2	D	4	GHP	C2-C1	3.44	1.44	1.39	72	80
2	C	4	GHP	C3-C4	3.42	1.45	1.38	77	80
2	C	6	OMY	CD1-CG	3.41	1.44	1.39	3	80
2	D	2	OMZ	CD1-CE1	3.39	1.44	1.38	66	80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	7	3FG	CG2-CD2	3.36	1.44	1.39	12	80
2	D	7	3FG	CG2-CD2	3.33	1.44	1.39	61	80
2	C	5	GHP	C5-C4	3.30	1.45	1.38	40	80
2	C	2	OMZ	CD1-CE1	3.29	1.43	1.38	6	80
2	C	2	OMZ	CE2-CD2	3.29	1.44	1.38	23	80
2	D	5	GHP	C5-C4	3.28	1.45	1.38	23	80
2	C	4	GHP	C2-C1	3.21	1.44	1.39	43	80
2	D	7	3FG	CZ-CD2	3.21	1.43	1.39	38	80
2	C	7	3FG	CZ-CD2	3.20	1.43	1.39	49	80
2	D	7	3FG	CZ-CD1	3.19	1.43	1.39	68	80
2	C	4	GHP	C5-C4	3.17	1.45	1.38	78	80
2	C	6	OMY	CD1-CE1	3.16	1.43	1.38	73	80
2	C	7	3FG	CZ-CD1	3.16	1.43	1.39	47	80
2	D	6	OMY	CD1-CE1	3.16	1.43	1.38	57	80
2	D	2	OMZ	CE2-CD2	3.13	1.44	1.38	73	80
2	D	4	GHP	C5-C4	3.07	1.44	1.38	29	80
2	C	6	OMY	CE2-CZ	3.03	1.44	1.39	35	80
2	D	4	GHP	C3-C4	3.00	1.44	1.38	29	80
2	D	6	OMY	CE2-CZ	2.92	1.44	1.39	17	80
2	D	2	OMZ	CE2-CZ	2.83	1.44	1.39	9	80
2	C	2	OMZ	CE2-CZ	2.76	1.44	1.39	62	80
2	D	7	3FG	CG1-CD1	2.75	1.43	1.39	77	80
2	D	5	GHP	C2-C1	2.74	1.43	1.39	73	80
2	C	5	GHP	C2-C1	2.73	1.43	1.39	66	80
2	C	7	3FG	CG1-CD1	2.70	1.43	1.39	21	80
2	C	4	GHP	C6-C1	2.67	1.43	1.39	18	80
2	D	4	GHP	C6-C1	2.63	1.43	1.39	52	80
2	D	5	GHP	C1-CA	2.52	1.49	1.52	29	79
2	D	5	GHP	C3-C4	2.49	1.43	1.38	16	80
2	C	5	GHP	C3-C4	2.49	1.43	1.38	77	80
2	C	5	GHP	C1-CA	2.38	1.50	1.52	38	80
2	C	6	OMY	OCZ-CZ	2.22	1.40	1.36	78	60
2	D	4	GHP	CA-C	2.21	1.55	1.51	53	6
2	D	7	3FG	OXT-C	2.10	1.23	1.30	29	53
2	C	7	3FG	OXT-C	2.04	1.23	1.30	78	43
2	C	2	OMZ	OH-CZ	2.03	1.40	1.36	43	5
2	D	7	3FG	CB-CA	2.02	1.54	1.52	44	4

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	6	OMY	CG-CB-CA	4.36	105.65	111.49	52	80
2	D	6	OMY	CG-CB-CA	4.36	105.65	111.49	42	80
2	D	5	GHP	C2-C1-CA	2.77	116.19	120.65	54	80
2	C	5	GHP	C2-C1-CA	2.72	116.27	120.65	78	80
2	C	5	GHP	C1-CA-N	2.58	118.58	112.40	76	80
2	D	5	GHP	C1-CA-N	2.51	118.40	112.40	11	74
2	C	4	GHP	C2-C3-C4	2.45	117.19	119.88	35	80
2	D	5	GHP	C6-C1-CA	2.41	124.54	120.65	7	80
2	C	5	GHP	C6-C1-CA	2.39	124.50	120.65	70	80
2	C	6	OMY	CD2-CG-CB	2.26	124.10	120.73	52	3
2	C	4	GHP	C6-C5-C4	2.23	117.43	119.88	43	20
1	B	2	FGA	CB-CG-CD	2.22	105.98	112.29	53	2
2	C	6	OMY	CD1-CG-CB	2.15	115.89	119.55	52	3
2	D	4	GHP	C2-C3-C4	2.14	117.53	119.88	29	19
2	D	7	3FG	CG1-CB-CA	2.12	123.07	119.71	19	14
2	D	4	GHP	C6-C5-C4	2.09	117.58	119.88	80	3
2	C	6	OMY	ODE-CB-CA	2.09	111.69	107.28	35	2
2	D	4	GHP	C2-C1-CA	2.04	123.93	120.65	42	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	BGC	E	1	2,3	11,11,12	0.82±0.03	0±0 (0±0%)
3	RER	E	2	3	6,10,11	0.87±0.01	0±0 (0±0%)
3	BGC	F	1	2,3	11,11,12	0.78±0.01	0±0 (0±0%)
3	RER	F	2	3	6,10,11	0.86±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	BGC	E	1	2,3	15,15,17	0.77±0.09	0±1 (3±3%)
3	RER	E	2	3	6,15,17	0.81±0.04	0±0 (0±0%)
3	BGC	F	1	2,3	15,15,17	0.77±0.06	0±0 (0±1%)
3	RER	F	2	3	6,15,17	0.80±0.06	0±0 (0±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	BGC	E	1	2,3	-	0±0,2,19,22	0±0,1,1,1
3	RER	E	2	3	1±0,1,4,4	-	0±0,1,1,1
3	BGC	F	1	2,3	-	0±0,2,19,22	0±0,1,1,1
3	RER	F	2	3	1±0,1,4,4	-	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	E	1	BGC	C1-C2-C3	2.64	112.91	109.67	55	6
3	E	1	BGC	O5-C1-C2	2.56	106.82	110.77	43	24
3	E	1	BGC	C1-O5-C5	2.56	115.66	112.19	32	6
3	F	1	BGC	C1-C2-C3	2.09	112.23	109.67	52	2

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

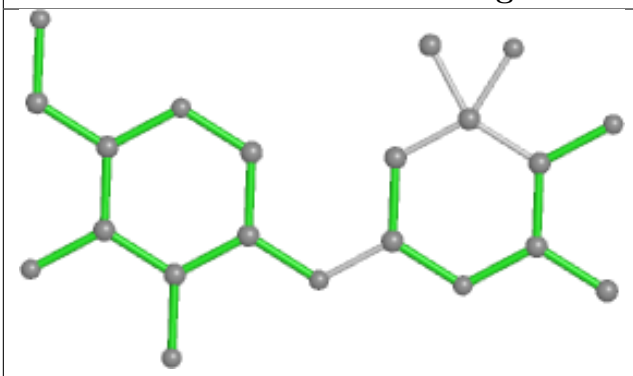
Mol	Chain	Res	Type	Atoms	Models (Total)
3	E	2	RER	C4	80
3	F	2	RER	C4	80

There are no torsion outliers.

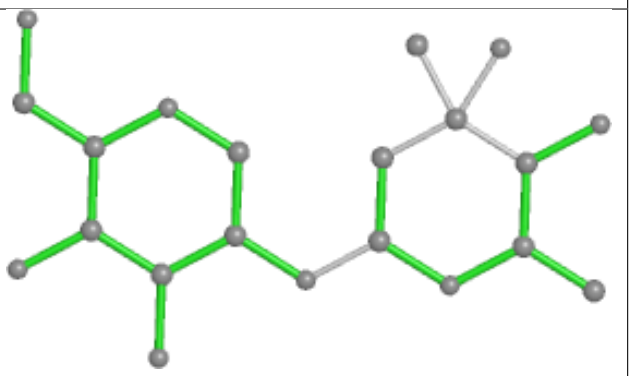
There are no ring outliers.

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

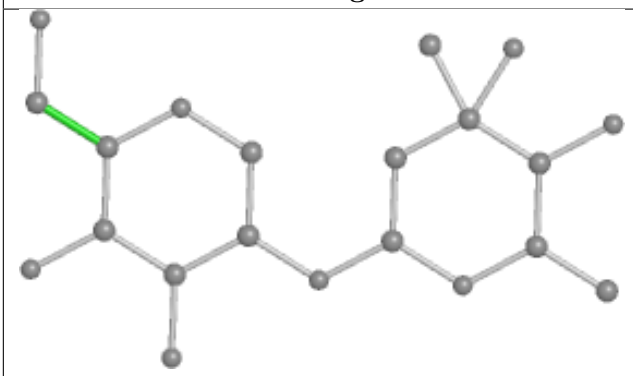
Oligosaccharide Chain E



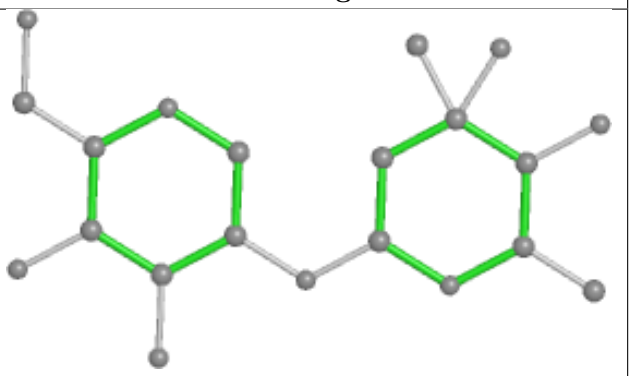
Bond lengths



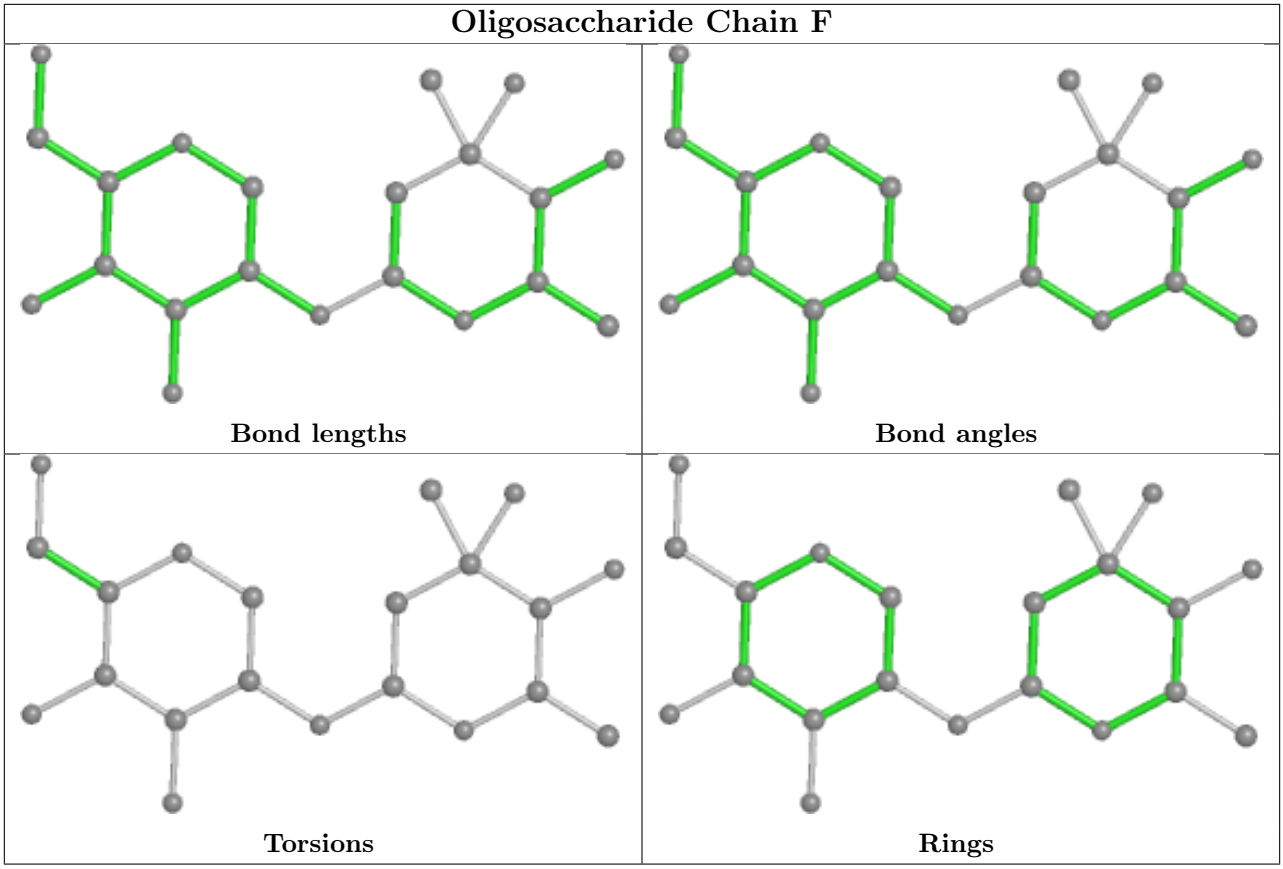
Bond angles



Torsions



Rings



6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	RER	D	10	2	6,10,11	0.92±0.04	0±0 (0±0%)
4	RER	C	10	2	6,10,11	0.94±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of

the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	RER	D	10	2	6,15,17	0.97±0.17	0±0 (3±7%)
4	RER	C	10	2	6,15,17	1.33±0.24	1±0 (20±7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RER	C	10	2	1±0,1,4,4	-	0±0,1,1,1
4	RER	D	10	2	1±0,1,4,4	-	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	C	10	RER	O5-C5-C4	3.21	104.29	110.03	31	79
4	D	10	RER	O5-C5-C4	2.45	105.64	110.03	54	18
4	C	10	RER	O5-C1-C2	2.21	114.49	111.38	78	18
4	D	10	RER	O5-C1-C2	2.08	108.45	111.38	29	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
4	C	10	RER	C4	80
4	D	10	RER	C4	80

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided