



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 01:00 PM UTC

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

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 80 models.

Cyrange was unable to find well-defined residues.

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

NmrClust was unable to cluster the ensemble.

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

3 Entry composition [i](#)

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

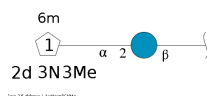
- Molecule 1 is a protein called CELL WALL PENTAPEPTIDE.

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

- Molecule 2 is a protein called CHLOROORIENTICIN A.

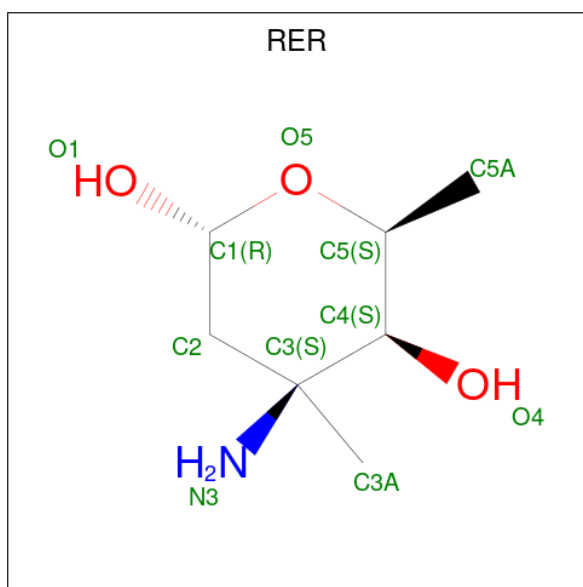
Mol	Chain	Residues	Atoms					Trace
2	C	7	Total	C	Cl	H	N	O
			130	53	2	50	8	17
2	D	7	Total	C	Cl	H	N	O
			130	53	2	50	8	17

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



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

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



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

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%



- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%



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

Chain E:  100%



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

Chain F:  100%

BC1
RER2

4.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 4.1 above.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CELL WALL PENTAPEPTIDE

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: CHLOROORIENTICIN A

Chain C:  29% 71%

HLH
OMZ2
N3
G4
G5
Y6
3FG7

- Molecule 2: CHLOROORIENTICIN A

Chain D:  29% 71%

HLH
OMZ2
N3
G4
G5
Y6
3FG7

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

Chain E:  100%

BC1
RER2

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

Chain F:  100%

BC1
RER2

5 Refinement protocol and experimental data overview

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

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

Software name	Classification	Version
CHARMM	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

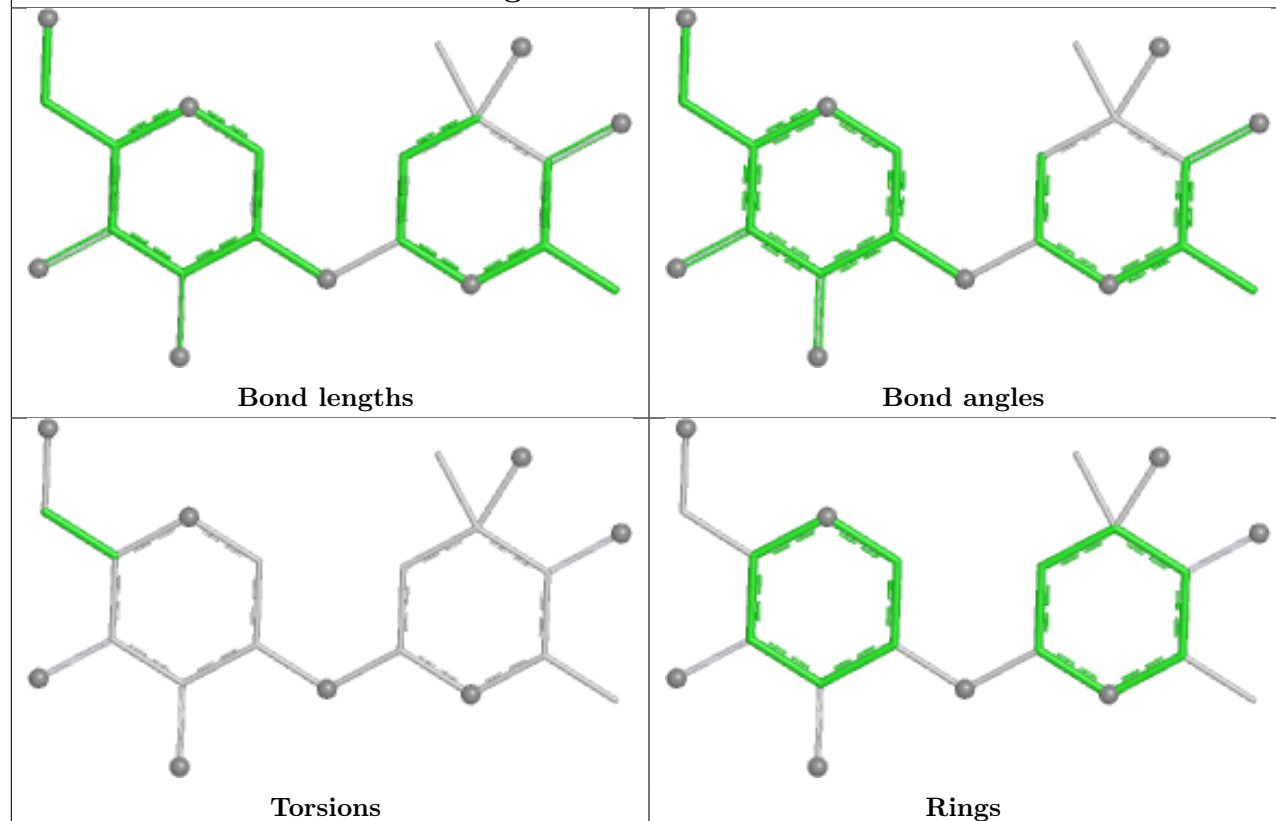
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6.5 Carbohydrates [i](#)

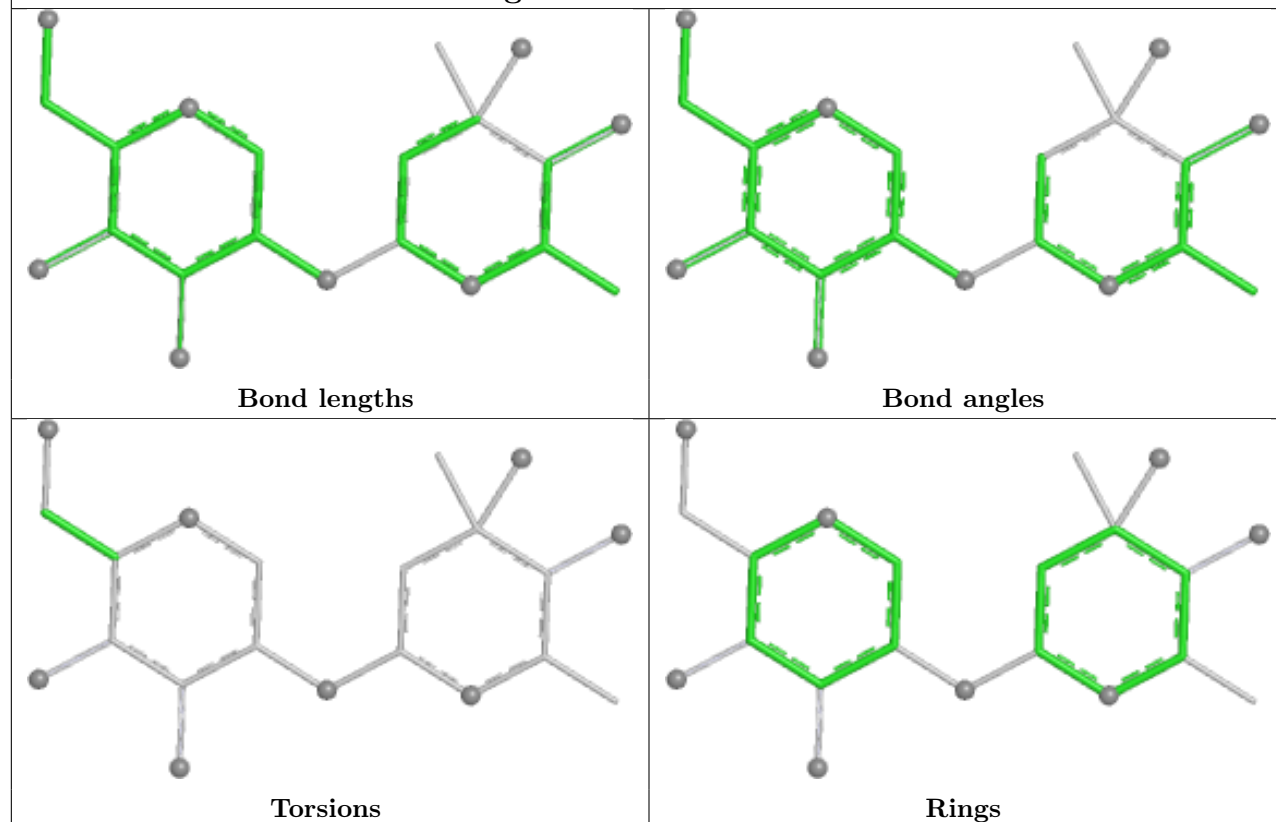
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The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F



6.6 Ligand geometry [i](#)

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6.7 Other polymers [i](#)

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6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided