Full wwPDB NMR Structure Validation Report (i)

Oct 17, 2021 – 09:38 AM EDT

PDB ID	:	1JAR
Title	:	Solution structure of lactam analogue (DDab)of HIV gp41 600-612 loop.
Authors	:	Phan Chan Du, A.; Limal, D.; Semetey, V.; Dali, H.; Jolivet, M.; Desgranges, C.; Cung, M.T.; Briand, J.P.; Petit, M.C.; Muller, S.
Deposited on	:	2001-05-31

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 following versions of software and data (see references (1)) were used in the production of this report:

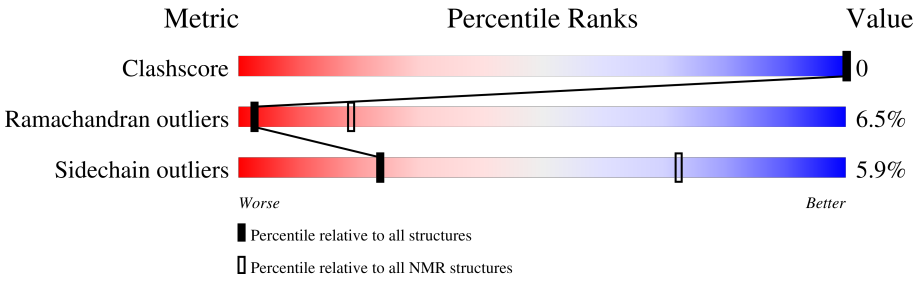
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	14	71% 29%

2 Ensemble composition and analysis (i)

This entry contains 49 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 199 atoms, of which 101 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	14	199	63	101	16	19	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P12488
A	5	ASP	CYS	engineered mutation	UNP P12488
A	11	DAB	CYS	engineered mutation	UNP P12488

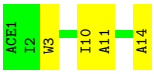
4 Residue-property plots (i)

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: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A:



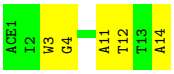
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A:

4.2.3 Score per residue for model 3

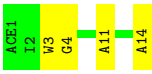
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

4.2.4 Score per residue for model 4

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

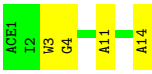
Chain A: 71% 29%



4.2.5 Score per residue for model 5

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

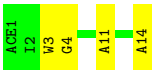
Chain A: 71% 29%



4.2.6 Score per residue for model 6

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

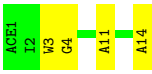
Chain A: 71% 29%



4.2.7 Score per residue for model 7

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

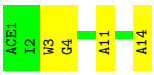
Chain A: 71% 29%



4.2.8 Score per residue for model 8

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

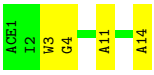
Chain A: 71% 29%



4.2.9 Score per residue for model 9

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

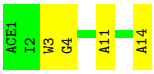
Chain A: 71% 29%



4.2.10 Score per residue for model 10

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 29%



4.2.11 Score per residue for model 11

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

4.2.12 Score per residue for model 12

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 14% 7%

4.2.13 Score per residue for model 13

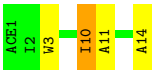
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

4.2.14 Score per residue for model 14

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

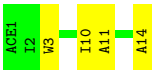
Chain A: 71% 21% 7%



4.2.15 Score per residue for model 15

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

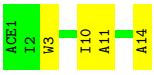
Chain A: 71% 29%



4.2.16 Score per residue for model 16

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

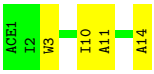
Chain A: 71% 29%



4.2.17 Score per residue for model 17

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

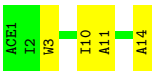
Chain A: 71% 29%



4.2.18 Score per residue for model 18

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

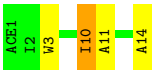
Chain A: 71% 29%



4.2.19 Score per residue for model 19

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

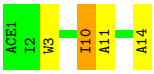
Chain A: 71% 21% 7%



4.2.20 Score per residue for model 20

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 21% 7%



4.2.21 Score per residue for model 21

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

4.2.22 Score per residue for model 22

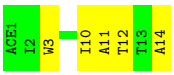
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 14% 7%

4.2.23 Score per residue for model 23

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 64% 36%



4.2.24 Score per residue for model 24

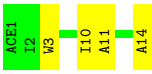
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

4.2.25 Score per residue for model 25

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

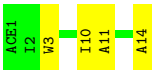
Chain A: 71% 29%



4.2.26 Score per residue for model 26

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

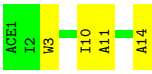
Chain A: 71% 29%



4.2.27 Score per residue for model 27

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

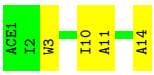
Chain A: 71% 29%



4.2.28 Score per residue for model 28

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

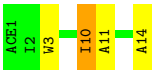
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

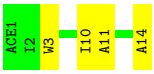
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

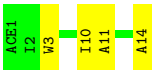
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

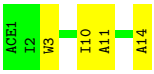
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

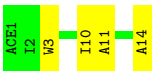
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

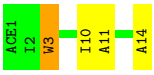
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

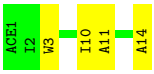
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

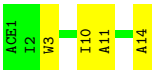
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

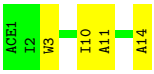
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

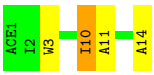
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 21% 7%



4.2.39 Score per residue for model 39

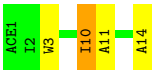
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 64% 29% 7%

4.2.40 Score per residue for model 40

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 21% 7%



4.2.41 Score per residue for model 41

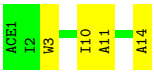
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 21% 7%

4.2.42 Score per residue for model 42

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

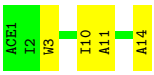
Chain A: 71% 29%



4.2.43 Score per residue for model 43

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

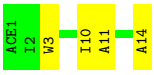
Chain A: 71% 29%



4.2.44 Score per residue for model 44

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 29%



4.2.45 Score per residue for model 45

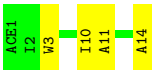
• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 86% 7% 7%

4.2.46 Score per residue for model 46

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

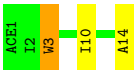
Chain A: 71% 29%



4.2.47 Score per residue for model 47

• Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

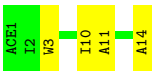
Chain A: 79% 14% 7%



4.2.48 Score per residue for model 48

- Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 71% 29%



4.2.49 Score per residue for model 49

- Molecule 1: DDab: (ACE)IWGDSGKLI(DAB)TTA ANALOGUE OF HIV GP41

Chain A: 79% 21%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynalmics, molecular dynamics, energy minimization.*

Of the 50 calculated structures, 49 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
DYANA	refinement	1.5
Discover	refinement	3

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: ACE, DAB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.40±0.02	1±0/89 (1.1± 0.0%)	1.28±0.06	1±0/117 (0.9± 0.1%)
All	All	1.40	49/4361 (1.1%)	1.28	50/5733 (0.9%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	14	ALA	C-OXT	7.75	1.38	1.23	47	49

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
1	A	3	TRP	CD1-NE1-CE2	-5.82	103.77	109.00	15	49
1	A	12	THR	CA-CB-CG2	5.12	119.56	112.40	23	1

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
All	All	4802	4949	4838	-

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 -.

There are no clashes.

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	11/14 (79%)	8±1 (70±5%)	3±1 (23±6%)	1±1 (6±5%)	2 18
All	All	539/686 (79%)	379 (70%)	125 (23%)	35 (6%)	2 18

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	10	ILE	25
1	A	4	GLY	8
1	A	12	THR	1
1	A	7	GLY	1

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	9/9 (100%)	8±0 (94±6%)	1±0 (6±6%)	23 72
All	All	441/441 (100%)	415 (94%)	26 (6%)	23 72

All 2 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	10	ILE	23

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Mol	Chain	Res	Type	Models (Total)
1	A	3	TRP	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	DAB	A	11	1	5,6,7	1.15±0.07	1±0 (16±7%)

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	DAB	A	11	1	1,6,8	0.14±0.11	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
1	DAB	A	11	1	-	0±0,4,5,7	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	DAB	CB-CA	2.60	1.57	1.53	41	40

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

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