

Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 08:41 PM EDT

PDB ID	:	1BAH
Title	:	A TWO DISULFIDE DERIVATIVE OF CHARYBDOTOXIN WITH DISUL-
		FIDE 13-33 REPLACED BY TWO ALPHA-AMINOBUTYRIC ACIDS,
		NMR, 30 STRUCTURES
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		Menez, A.
Deposited on	:	1996-06-06

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 (1)) were used in the production of this report:

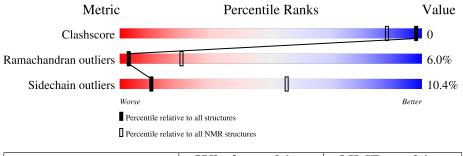
MolProbity		
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \ {f archive} \ (\#{f Entries})$
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	А	37	78%	11%	11%



2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 4 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model						
1	A:3-A:12, A:14-A:32, A:34-	0.41	4				
	A:37 (33)						

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 9, 11, 12, 14, 17, 21, 24, 25, 26, 29, 30
2	2, 3, 8, 18
3	13, 20, 28
4	6, 22, 27
Single-model clusters	7; 10; 15; 16; 19; 23



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 583 atoms, of which 288 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called CHARYBDOTOXIN.

Mol	Chain	Residues	Atoms					Trace	
1	٨	27	Total	С	Н	Ν	0	S	0
	A	37	583	178	288	57	55	5	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	13	ABA	CYS	modified residue	UNP P13487
А	33	ABA	CYS	modified residue	UNP P13487

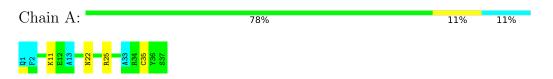


4 Residue-property plots (i)

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: CHARYBDOTOXIN

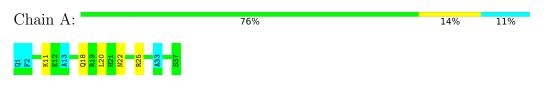


4.2 Scores per residue for each member of the ensemble

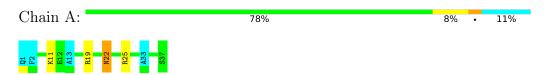
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CHARYBDOTOXIN



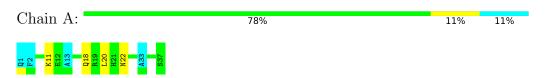
4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: CHARYBDOTOXIN



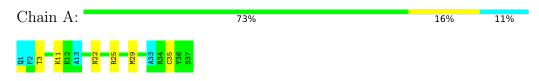
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: CHARYBDOTOXIN



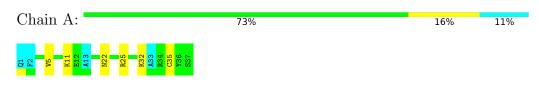
4.2.5 Score per residue for model 5

• Molecule 1: CHARYBDOTOXIN



4.2.6 Score per residue for model 6

• Molecule 1: CHARYBDOTOXIN



4.2.7 Score per residue for model 7





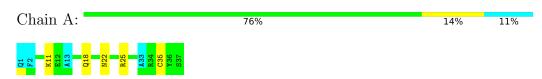
4.2.8 Score per residue for model 8

• Molecule 1: CHARYBDOTOXIN



4.2.9 Score per residue for model 9

• Molecule 1: CHARYBDOTOXIN



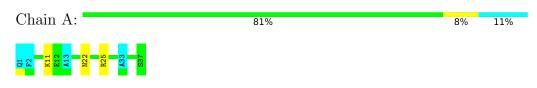
4.2.10 Score per residue for model 10

• Molecule 1: CHARYBDOTOXIN

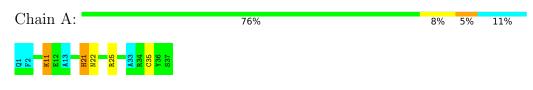
Chain A:	81%	5%	•	11%
91 11 11 11 11 11 11 11 11 11 11 11 11 1				

4.2.11 Score per residue for model 11

• Molecule 1: CHARYBDOTOXIN



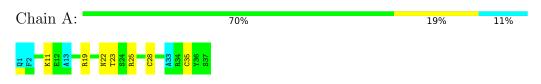
4.2.12 Score per residue for model 12





4.2.13 Score per residue for model 13

• Molecule 1: CHARYBDOTOXIN



4.2.14 Score per residue for model 14

• Molecule 1: CHARYBDOTOXIN

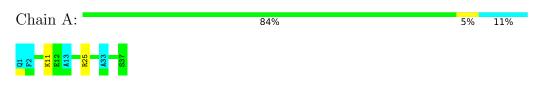


4.2.15 Score per residue for model 15

• Molecule 1: CHARYBDOTOXIN

Chain A:	73%	16%	11%
41 13 14 14 14 13 13 13 13 13 13 13 13 13 13 13 13 13	A33 R35 Y36 S37		

- 4.2.16 Score per residue for model 16
- Molecule 1: CHARYBDOTOXIN



4.2.17 Score per residue for model 17





4.2.18 Score per residue for model 18

• Molecule 1: CHARYBDOTOXIN



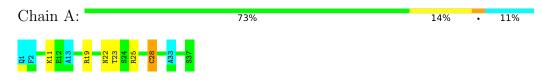
4.2.19 Score per residue for model 19

• Molecule 1: CHARYBDOTOXIN



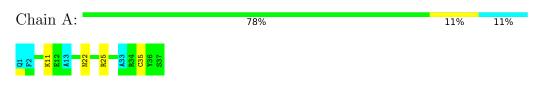
4.2.20 Score per residue for model 20

• Molecule 1: CHARYBDOTOXIN



4.2.21 Score per residue for model 21

• Molecule 1: CHARYBDOTOXIN



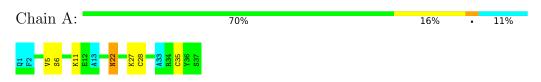
4.2.22 Score per residue for model 22





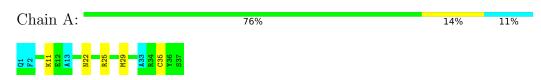
4.2.23 Score per residue for model 23

• Molecule 1: CHARYBDOTOXIN



4.2.24 Score per residue for model 24

• Molecule 1: CHARYBDOTOXIN

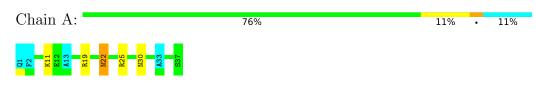


4.2.25 Score per residue for model 25

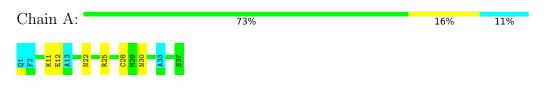
• Molecule 1: CHARYBDOTOXIN

Chain A:	78%	11%	11%
01 12 12 12 13 14 13 14 13 13 13 13 13 13 13 13 13 13 13 13 13			

4.2.26 Score per residue for model 26



- 4.2.27 Score per residue for model 27
- Molecule 1: CHARYBDOTOXIN



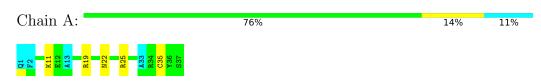


4.2.28 Score per residue for model 28

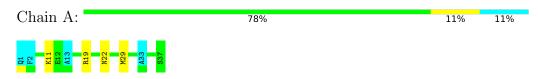
• Molecule 1: CHARYBDOTOXIN



4.2.29 Score per residue for model 29



- 4.2.30 Score per residue for model 30
- Molecule 1: CHARYBDOTOXIN





5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	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: PCA, ABA

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	E	Sond lengths	1	Bond angles		
	Chain	RMSZ	$\#Z{>}5$	RMSZ	#Z>5		
1	А	$1.06 {\pm} 0.01$	$0{\pm}0/265~(~0.0{\pm}~0.0\%)$	1.15 ± 0.03	$0\pm 0/348~(~0.0\pm~0.1\%)$		
All	All	1.06	0/7950~(~0.0%)	1.15	2/10440~(~0.0%)		

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

Mol	Chain	Chirality	Planarity
1	А	$0.0{\pm}0.0$	0.1 ± 0.2
All	All	0	2

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$	Moo Worst	dels Total
1	А	28	CYS	CA-CB-SG	5.21	123.39	114.00	28	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	А	21	HIS	Sidechain	1
1	А	36	TYR	Sidechain	1



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	А	264	259	259	0 ± 0
All	All	7920	7770	7770	5

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:21:HIS:HE1	1:A:35:CYS:SG	0.45	2.34	12	1
1:A:5:VAL:HG12	1:A:6:SER:H	0.42	1.75	23	3
1:A:21:HIS:CE1	1:A:35:CYS:SG	0.41	3.14	17	1

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		Allowed	Outliers	Percentiles	
1	А	32/37~(86%)	$21 \pm 1 (66 \pm 3\%)$	$9{\pm}1~(28{\pm}3\%)$	$2\pm0~(6\pm1\%)$	3	20
All	All	960/1110 (86%)	634 (66%)	268 (28%)	58~(6%)	3	20

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	11	LYS	29
1	А	22	ASN	29



6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
1	А	32/33~(97%)	$29 \pm 1 (90 \pm 4\%)$	3 ± 1 (10 $\pm4\%$)	10 55	
All	All	960/990~(97%)	860 (90%)	100 (10%)	10 55	

All 17 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	А	25	ARG	27
1	А	35	CYS	14
1	А	19	ARG	11
1	А	3	THR	7
1	А	28	CYS	6
1	А	29	MET	5
1	А	23	THR	5
1	А	18	GLN	4
1	А	22	ASN	3
1	А	11	LYS	3
1	А	21	HIS	3
1	А	20	LEU	2
1	А	5	VAL	2
1	А	32	LYS	2
1	А	27	LYS	2
1	А	12	GLU	2
1	А	30	ASN	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)

3 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	Turne	Chain	Dec	Tink		Bond ler	ngths
10101	туре	Unam	nes	LIIIK	Counts	RMSZ	#Z>2
1	PCA	А	1	1	7,8,9	$0.96{\pm}0.06$	$1\pm0 (11\pm5\%)$
1	ABA	А	13	1	4,5,6	$0.73 {\pm} 0.04$	0±0 (0±0%)
1	ABA	А	33	1	4,5,6	$0.80 {\pm} 0.03$	$0\pm0~(0\pm0\%)$

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	Dog	Link		Bond an	gles
MOI	rybe	Ullalli	nes		Counts	RMSZ	#Z>2
1	PCA	А	1	1	9,10,12	$1.19{\pm}0.05$	1±1 (7±7%)
1	ABA	А	13	1	1,5,7	$0.73 {\pm} 0.30$	0±0 (0±0%)
1	ABA	А	33	1	$1,\!5,\!7$	$0.69 {\pm} 0.36$	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	PCA	А	1	1	-	$0\pm 0,0,11,13$	$0\pm 0,1,1,1$
1	ABA	А	33	1	-	$0\pm 0,3,4,6$	-
1	ABA	А	13	1	-	$0\pm 0,3,4,6$	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$	Models	
								Worst	Total
1	А	1	PCA	CA-N	2.41	1.43	1.46	17	24

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



Mal	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathrm{Ideal}(^{o})$	Models	
10101								Worst	Total
1	А	1	PCA	CB-CG-CD	2.49	100.40	104.40	17	11
1	А	1	PCA	OE-CD-CG	2.15	123.01	126.76	27	8

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

