wwPDB NMR Structure Validation Summary Report (i)

Mar 5, 2022 – 01:36 PM EST

PDB ID	:	2JZJ
Title	:	Structure of CrCVNH (C. richardii CVNH)
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Deposited on	:	2008-01-09

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 (i) symbol.

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

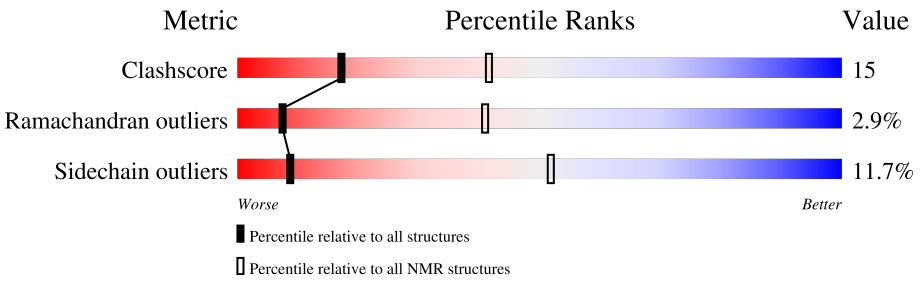
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	124	

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:102 (100)	0.20	12

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1550 atoms, of which 674 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cyanovirin-N homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1550	532	674	151	184	9	0

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: Cyanovirin-N homolog

Chain A: 56% 22% • • 13% 6%

M1 Q2 C3 N4 F5 C9 L14 Y17 I18 L19 D22 P30 N36 L37 G42 N45 G46 R47 Y50 P51 G52 L64 N65 D66 G67 H68 T71 A77 D78 S85 M86 D87 L88 V91 V92 G93 N94 S95 E100 P101 C102 R103 A104 S105 N106

A107 D108 H109 V110 L111 K112 S113 S114 S115 E116 LEU GLU HIS HIS HIS HIS HIS HIS

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 12. Colouring as in section 4.1 above.

- Molecule 1: Cyanovirin-N homolog

Chain A: 60% 18% • • 13% 6%

M1 Q2 F5 L14 Y17 I18 L19 D22 H29 P30 L37 G42 R47 L48 E49 Y50 P51 G52 L64 H68 T69 L70 T71 C74 D78 S85 L88 V91 V92 E100 P101 C102 R103 A104 S105 N106 A107 D108 H109 V110 L111 K112 S113 S114

S115 E116 LEU GLU HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 800 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CNS	structure solution	
ARIA	structure solution	
CNS	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.48±0.01	1±0/773 (0.1± 0.0%)	0.45±0.02	0±0/1050 (0.0± 0.0%)
All	All	0.48	26/23190 (0.1%)	0.45	3/31500 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	51	PRO	N-CA	-7.52	1.34	1.47	28	26

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	51	PRO	N-CA-CB	-5.47	96.59	102.60	10	3

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	755	576	669	22±3
All	All	22650	17280	20070	655

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 15.

5 of 99 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:VAL:HA	1:A:101:PRO:HA	0.90	1.43	14	25
1:A:50:TYR:HB2	1:A:91:VAL:HG11	0.77	1.54	21	1
1:A:19:LEU:HB2	1:A:37:LEU:HD21	0.77	1.57	23	30
1:A:50:TYR:CD2	1:A:51:PRO:HD3	0.76	2.15	19	25
1:A:14:LEU:HD22	1:A:64:LEU:HD23	0.75	1.58	27	27

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	100/124 (81%)	89±2 (89±2%)	8±2 (8±2%)	3±1 (3±1%)	7	41
All	All	3000/3720 (81%)	2682 (89%)	232 (8%)	86 (3%)	7	41

5 of 9 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	51	PRO	30
1	A	78	ASP	30
1	A	17	TYR	13
1	A	50	TYR	7
1	A	4	ASN	2

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	82/104 (79%)	72±2 (88±3%)	10±2 (12±3%)	9	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2460/3120 (79%)	2172 (88%)	288 (12%)	9 52

5 of 37 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	47	ARG	30
1	A	64	LEU	30
1	A	71	THR	30
1	A	85	SER	30
1	A	50	TYR	26

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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