wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2L0Z
Title	:	Solution structure of a zinc-binding domain from the Junin virus envelope glycoprotein
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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
http://wwpdb.org/validation/2016/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:

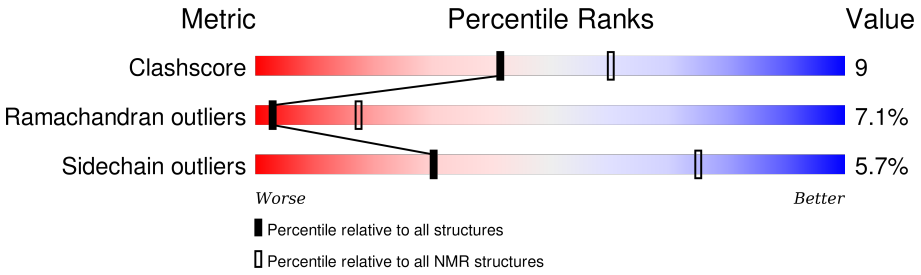
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	42	69% 26% 5%

2 Ensemble composition and analysis

This entry contains 21 models. Model 21 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:446-A:485 (40)	0.58	21

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 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 10, 12, 13, 14, 15, 18, 19, 20, 21
2	8, 16, 17
Single-model clusters	5; 9; 11

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 670 atoms, of which 335 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called glycoprotein G2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	42	668	206	335	73	51	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ACE	-	ACETYLATION	UNP P26313

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: glycoprotein G2

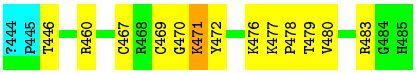
Chain A:

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

The representative model is number 21. Colouring as in section 4.1 above.

- Molecule 1: glycoprotein G2

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 56 calculated structures, 21 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
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACE

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	0.51±0.08	1±1/333 (0.2±0.2%)	0.54±0.07	0±1/446 (0.1±0.1%)
All	All	0.52	13/6993 (0.2%)	0.55	6/9366 (0.1%)

5 of 13 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
1	A	451	ARG	CD-NE	6.49	1.57	1.46	14	1
1	A	485	HIS	CB-CG	-6.08	1.39	1.50	20	1
1	A	472	TYR	CD2-CE2	6.04	1.48	1.39	21	1
1	A	481	TRP	CZ3-CH2	5.82	1.49	1.40	7	1
1	A	465	GLY	C-O	-5.60	1.14	1.23	4	1

5 of 6 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	468	ARG	NE-CZ-NH2	8.43	124.52	120.30	11	1
1	A	472	TYR	CG-CD2-CE2	-7.88	115.00	121.30	21	1
1	A	472	TYR	CB-CG-CD2	-6.94	116.84	121.00	21	1
1	A	468	ARG	NE-CZ-NH1	-5.57	117.52	120.30	11	1
1	A	481	TRP	CZ3-CH2-CZ2	-5.28	115.27	121.60	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	323	325	325	6±2
All	All	6825	6825	6824	121

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 9.

5 of 66 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:446:THR:HG22	1:A:483:ARG:HB2	0.75	1.57	5	4
1:A:448:ARG:HB3	1:A:479:THR:HB	0.73	1.60	15	3
1:A:467:CYS:SG	1:A:471:LYS:HB3	0.73	2.23	11	9
1:A:449:HIS:HB2	1:A:480:VAL:HB	0.71	1.59	16	6
1:A:446:THR:HG22	1:A:483:ARG:HG2	0.67	1.65	15	1

6.3 Torsion angles

6.3.1 Protein backbone

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	39/42 (93%)	30±3 (77±8%)	6±2 (16±5%)	3±1 (7±4%)	3	17
All	All	819/882 (93%)	634 (77%)	127 (16%)	58 (7%)	3	17

5 of 19 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	471	LYS	13
1	A	470	GLY	5
1	A	478	PRO	5

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Mol	Chain	Res	Type	Models (Total)
1	A	455	CYS	4
1	A	446	THR	4

6.3.2 Protein sidechains

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	34/35 (97%)	32±1 (94±4%)	2±1 (6±4%)	30	75
All	All	714/735 (97%)	673 (94%)	41 (6%)	30	75

5 of 13 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	479	THR	11
1	A	469	CYS	8
1	A	453	GLU	4
1	A	462	ASN	3
1	A	483	ARG	3

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

No chemical shift data were provided