wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2KGF
Title	:	N-terminal domain of capsid protein from the Mason-Pfizer monkey virus
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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:

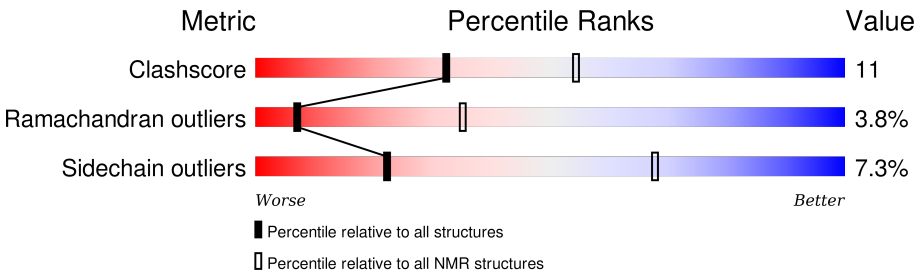
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	140	68% 11% • 17%

2 Ensemble composition and analysis (i)

This entry contains 50 models. Model 16 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:1-A:3, A:16-A:102, A:111-A:136 (116)	0.49	16

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 8 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 5, 11, 12, 15, 16, 17, 19, 20, 22, 26, 27, 28, 29, 30, 31, 33, 34, 40, 48
2	2, 8, 9, 10, 39, 41, 43, 45
3	3, 32, 42, 49, 50
4	6, 7, 13, 23, 38
5	21, 35, 37, 47
6	36, 44
7	4, 18
8	24, 46
Single-model clusters	14; 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1033 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p27.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2126	688	1033	190	212	3	0

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: Capsid protein p27

Chain A: 68% 11% • 17%

P1 V2 T3 E4 T5 V6 D7 G8 Q9 G10 Q11 A12 W13 R14 H15 A36 T37 L42 E46 V62 L66 D70 W74 R83 R88 D97 L101 T102 G103 S104 G105 N106 Y107 S108 S109 T110 Q113 Y116 A131 W132 R133 K134 L135 P136 V137 K138

G139 D140

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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: Capsid protein p27

Chain A: 61% 17% • • 17%

P1 V2 T3 E4 T5 V6 D7 G8 Q9 G10 Q11 A12 W13 R14 H15 K28 G35 A36 T37 T41 L42 A49 W52 N59 V62 R63 A64 V65 D70 W74 C82 R83 D84 T85 A86 K87 R88 W96 D97 M100 L101 T102 G103 S104 G105 N106 Y107 S108

S109 T110 Q123 I124 Q125 A131 W132 R133 K134 L135 P136 V137 K138 G139 D140

5 Refinement protocol and experimental data overview (i)

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

Of the 150 calculated structures, 50 were deposited, based on the following criterion: *10 structures for lowest energy*.

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

Software name	Classification	Version
CNS	refinement	

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 (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	0.88±0.03	0±0/940 (0.0±0.0%)	0.85±0.03	0±0/1283 (0.0±0.0%)
All	All	0.88	6/47000 (0.0%)	0.85	17/64150 (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	A	0.1±0.2	0.8±0.8
All	All	3	39

All 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	134	LYS	N-CA	6.66	1.59	1.46	50	3
1	A	132	TRP	CD1-NE1	-5.50	1.28	1.38	36	2
1	A	128	ALA	C-O	-5.20	1.13	1.23	27	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	134	LYS	N-CA-C	6.61	128.83	111.00	27	10
1	A	134	LYS	N-CA-CB	-5.89	99.99	110.60	35	2
1	A	1	PRO	N-CA-CB	5.63	110.06	103.30	47	2
1	A	16	HIS	N-CA-C	-5.20	96.95	111.00	39	1
1	A	116	TYR	CB-CA-C	-5.02	100.37	110.40	2	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	134	LYS	CA	3

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	A	133	ARG	Sidechain	22
1	A	88	ARG	Sidechain	9
1	A	83	ARG	Sidechain	8

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	914	877	875	20±3
All	All	45700	43850	43750	999

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 11.

5 of 214 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TRP:CG	1:A:132:TRP:HA	0.78	2.13	41	50
1:A:116:TYR:O	1:A:120:LEU:HB3	0.75	1.82	8	5
1:A:74:TRP:HA	1:A:131:ALA:O	0.70	1.85	24	50
1:A:134:LYS:N	1:A:134:LYS:HE2	0.70	2.01	30	2
1:A:69:GLY:C	1:A:135:LEU:HG	0.67	2.10	46	3

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	115/140 (82%)	103±2 (90±2%)	7±2 (6±2%)	4±1 (4±1%)	7 35
All	All	5750/7000 (82%)	5174 (90%)	358 (6%)	218 (4%)	7 35

5 of 17 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	132	TRP	44
1	A	102	THR	36
1	A	134	LYS	34
1	A	37	THR	33
1	A	136	PRO	21

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	93/111 (84%)	86±2 (93±2%)	7±2 (7±2%)	22 68
All	All	4650/5550 (84%)	4310 (93%)	340 (7%)	22 68

5 of 44 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	133	ARG	49
1	A	42	LEU	49
1	A	113	GLN	41
1	A	134	LYS	36
1	A	135	LEU	21

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 carbohydrates 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