wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1XU6
Title	:	Structure of the C-terminal domain from Trypanosoma brucei Variant Surface Glycoprotein MITat1.2
Authors	:	Chattopadhyay, A.; Jones, N.G.; Nietlispach, D.; Nielsen, P.R.; Voorheis, H.P.; Mott, H.R.; Carrington, M.
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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
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:

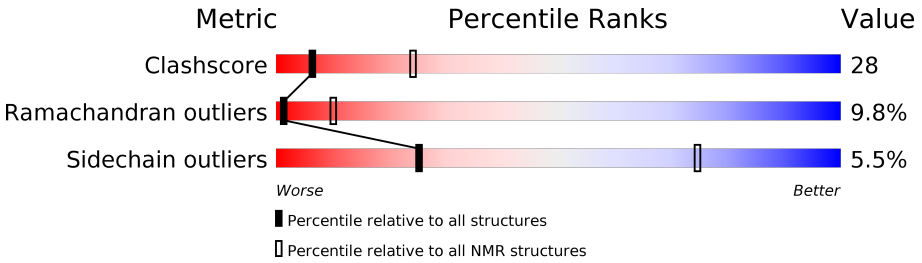
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	80	20% 24% • 54%

2 Ensemble composition and analysis (i)

This entry contains 60 models. Model 35 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:376-A:412 (37)	0.33	35

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 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 10, 11, 14, 16, 25, 26, 29, 30, 31, 33, 34, 35, 36, 37, 44, 49, 59, 60
2	2, 3, 7, 8, 12, 13, 17, 18, 19, 24, 32, 42, 45, 48, 51, 53, 56, 57
3	9, 20, 23, 27, 28, 38, 40, 41, 50, 52, 54, 55
4	22, 39, 43, 46
5	5, 15
Single-model clusters	21; 47; 58

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1188 atoms, of which 581 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Variant surface glycoprotein MITAT 1.2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	80	1188	357	581	111	134	5	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	GLY	-	CLONING ARTIFACT	UNP P26332
A	355	SER	-	CLONING ARTIFACT	UNP P26332
A	356	HIS	-	CLONING ARTIFACT	UNP P26332
A	357	MET	-	CLONING ARTIFACT	UNP P26332
A	358	LEU	-	CLONING ARTIFACT	UNP P26332

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: Variant surface glycoprotein MITAT 1.2

Chain A: 20% 24% • 54%

G354 S355 H356 M357 L358 E359 V360 L361 T362 Q363 K364 H365 K366 P367 A368 E369 S370 Q371 Q372 Q373 A374 A375 E376 S380 C381 N382 K383 K384 D385 E388 C389 K390 S391 P392 C393 H396 A399 E400 N401 K402 K403 C404 T405 L406 D407 E410 A411 K412 K413 V414 A415 D416 E417 T418 A419

K420 D421 G422 K423 T424 G425 N426 T427 N428 T429 T430 G431 S432 S433

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

The representative model is number 35. Colouring as in section 4.1 above.

- Molecule 1: Variant surface glycoprotein MITAT 1.2

Chain A: 23% 20% • • 54%

G354 S355 H356 M357 L358 E359 V360 L361 T362 Q363 K364 H365 K366 P367 A368 E369 S370 Q371 Q372 Q373 A374 A375 E376 C381 N382 K383 K384 D385 E388 C389 K390 S391 P392 C393 A399 E400 N401 K402 K403 L406 D407 K408 E409 E410 A411 K412 K413 V414 A415 D416 E417 T418 A419 K420 D421 G422

K423 T424 G425 N426 T427 N428 T429 T430 G431 S432 S433

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS, SIMULATED ANNEALING.*

Of the 100 calculated structures, 60 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	refinement	1.1
AZARA	structure solution	2.7
ANSIG	structure solution	3.3
CNS	structure solution	1.1
ARIA	structure solution	1.1

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)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	294	273	272	16±3
All	All	17640	16380	16320	964

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 28.

5 of 188 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:396:HIS:HB2	1:A:403:LYS:HB2	0.78	1.56	26	19
1:A:406:LEU:HD13	1:A:407:ASP:N	0.72	2.00	42	55
1:A:381:CYS:SG	1:A:404:CYS:HB3	0.72	2.24	5	1
1:A:385:ASP:H	1:A:388:GLU:HB2	0.70	1.46	50	32
1:A:399:ALA:HB1	1:A:403:LYS:HE2	0.67	1.66	45	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	37/80 (46%)	30±2 (80±4%)	4±2 (10±4%)	4±1 (10±3%)	1 10
All	All	2220/4800 (46%)	1774 (80%)	229 (10%)	217 (10%)	1 10

5 of 8 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	402	LYS	58
1	A	376	GLU	42
1	A	401	ASN	31
1	A	393	CYS	31
1	A	389	CYS	25

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	34/68 (50%)	32±1 (95±3%)	2±1 (5±3%)	25 74
All	All	2040/4080 (50%)	1928 (95%)	112 (5%)	25 74

5 of 18 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	384	LYS	30
1	A	401	ASN	22
1	A	412	LYS	11
1	A	397	ASN	7
1	A	402	LYS	7

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