Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 08:17 pm BST

PDB ID	:	1PJF
Title	:	Solid State NMR structure of the Pf1 Major Coat Protein in Magnetically Aligned Bacteriophage
Authors	:	Thiriot, D.S.; Nevzorov, A.A.; Zagyanskiy, L.; Wu, C.H.; Opella, S.J.
Deposited on	:	2003-06-02

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 following versions of software and data (see references (1)) were used in the production of this report:

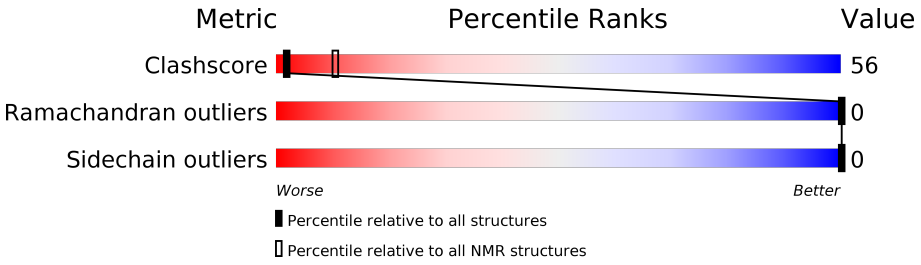
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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:
SOLID-STATE 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	46	48% 52%

2 Ensemble composition and analysis

This entry contains 27 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. The authors have identified model ? as representative, based on the following criterion: *nearest structure to the average of the 60 best ramachandran structures (based on a statistical ramachandran potential) out of 1000 total structures.*. No medoid model was calculated.

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:46 (46)	Not calculated	Not calculated

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 136 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COAT PROTEIN B.

Mol	Chain	Residues	Atoms			Trace
			Total	C	N	
1	A	46	136	91	45	2

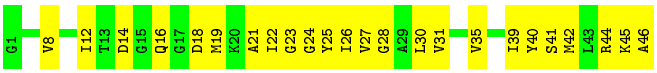
4 Residue-property plots (i)

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: COAT PROTEIN B

Chain A:



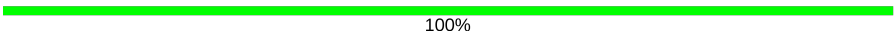
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: COAT PROTEIN B

Chain A:

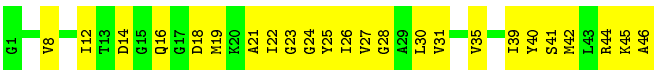


There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

- Molecule 1: COAT PROTEIN B

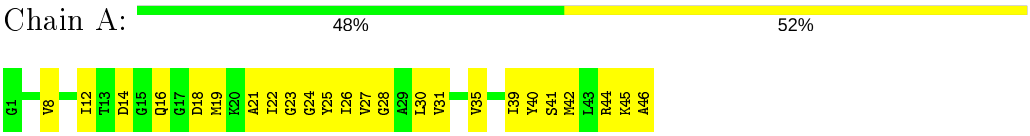
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: COAT PROTEIN B

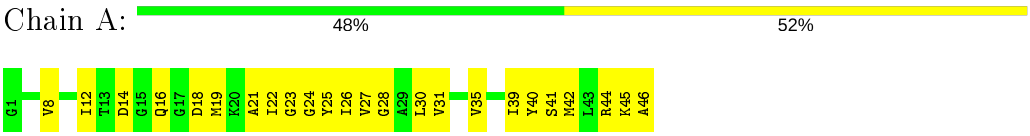
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: COAT PROTEIN B

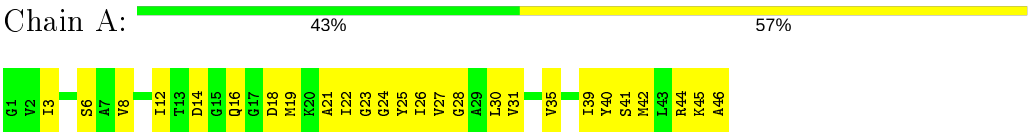
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: COAT PROTEIN B

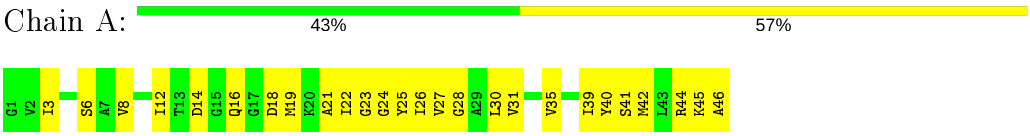
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: COAT PROTEIN B

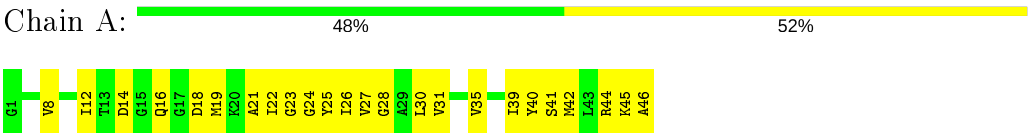
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: COAT PROTEIN B

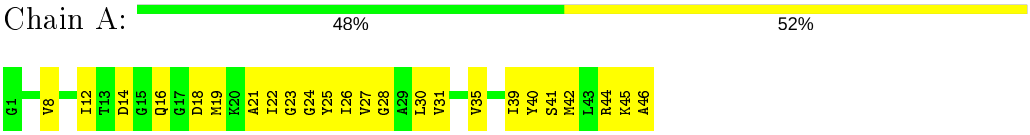
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: COAT PROTEIN B

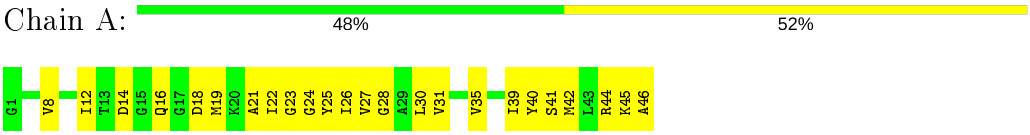
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: COAT PROTEIN B

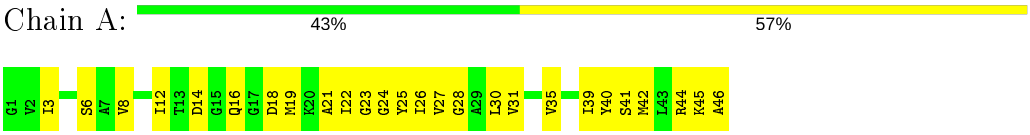
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: COAT PROTEIN B

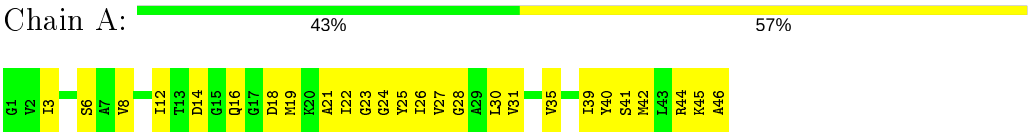
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: COAT PROTEIN B

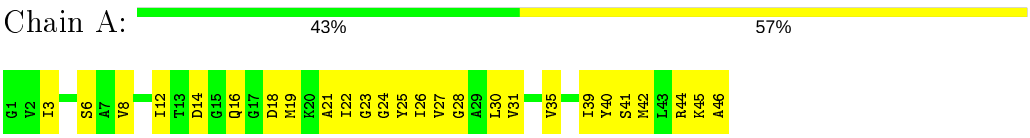
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: COAT PROTEIN B

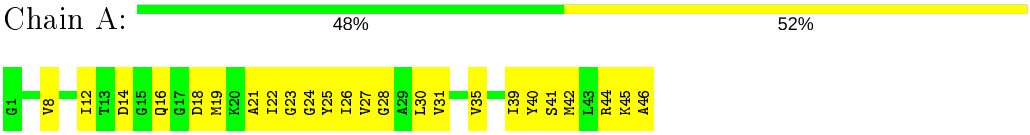
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: COAT PROTEIN B

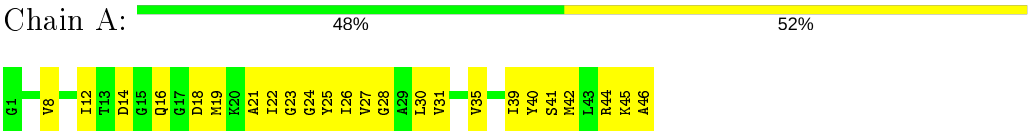
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: COAT PROTEIN B

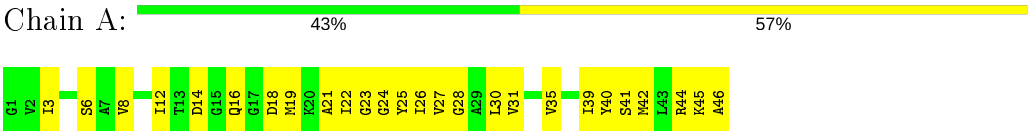
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: COAT PROTEIN B

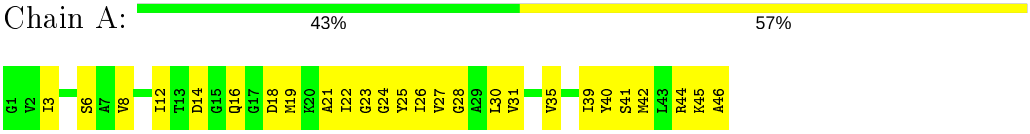
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: COAT PROTEIN B

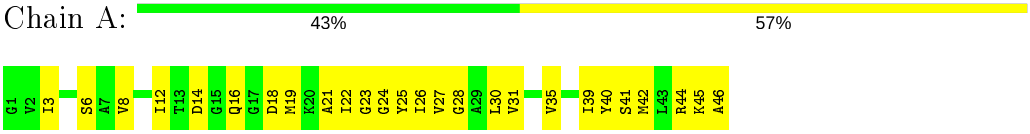
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: COAT PROTEIN B

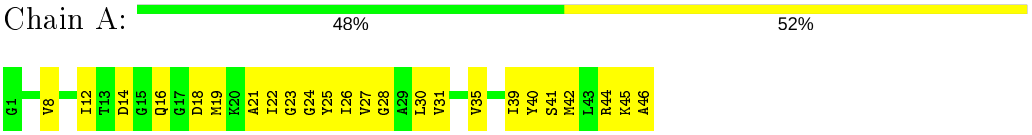
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: COAT PROTEIN B

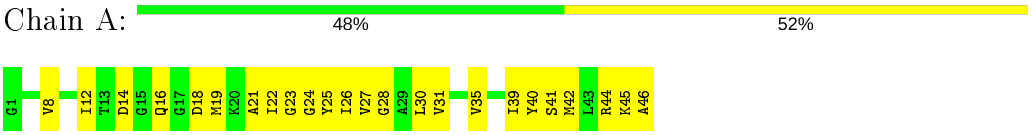
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: COAT PROTEIN B

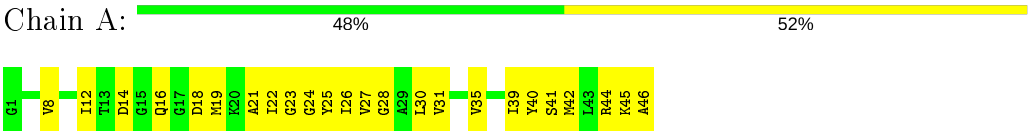
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: COAT PROTEIN B

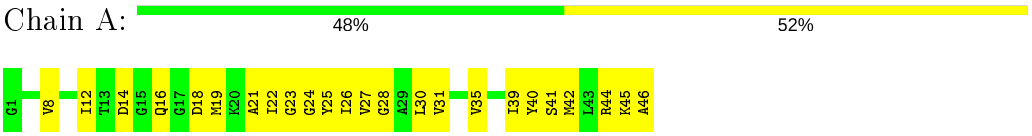
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: COAT PROTEIN B

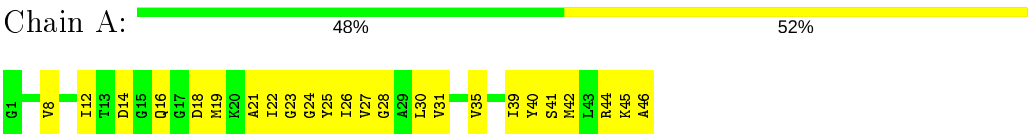
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: COAT PROTEIN B

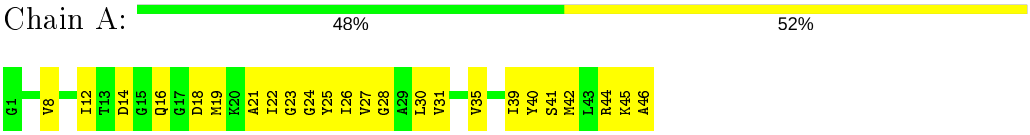
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: COAT PROTEIN B

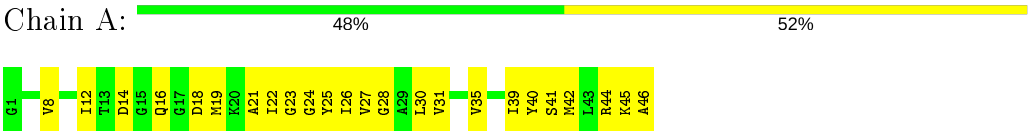
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: COAT PROTEIN B

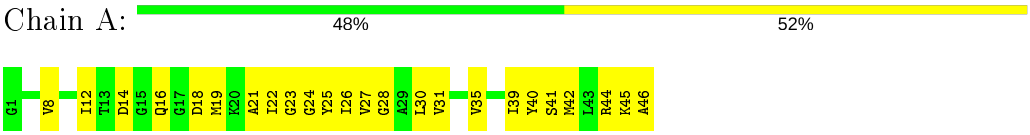
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: COAT PROTEIN B

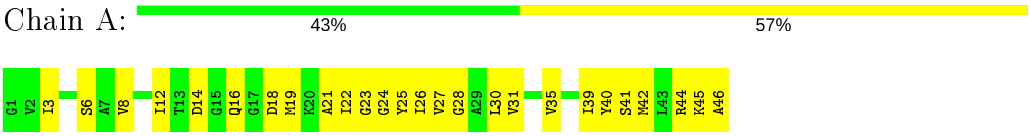
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: COAT PROTEIN B

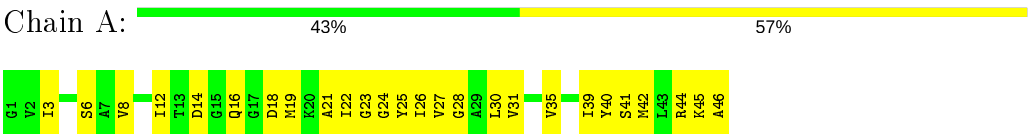
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: COAT PROTEIN B

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONSTRUCTION OF BACTERIOPHAGE MODEL BASED ON THE SOLID STATE NMR STRUCTURE OF THE MAJOR COAT PROTEIN MONOMER.*

Of the 116 calculated structures, 27 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
MATLAB SCRIPTS 6.5, SCWRL	refinement	2.95 (BLUE HORIZON MODIFIED)
FELIX	structure solution	2000.1
XWINNMR	structure solution	
MATLAB SCRIPT	structure solution	6.5

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	321	345	343	36±7
All	All	8482	8970	8975	982

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:MET:O	1:A:46:ALA:O	1.18	1.62	3	26
1:A:14:ASP:O	1:A:18:ASP:OD2	1.02	1.77	12	26
1:A:35:VAL:O	1:A:39:ILE:HG12	0.96	1.60	14	26
1:A:12:ILE:O	1:A:16:GLN:HB3	0.95	1.62	20	26
1:A:8:VAL:CG1	1:A:12:ILE:CG1	0.82	2.58	20	26
1:A:41:SER:O	1:A:45:LYS:CB	0.82	2.27	21	26
1:A:8:VAL:CG1	1:A:12:ILE:HG13	0.78	2.09	2	26
1:A:8:VAL:HG13	1:A:12:ILE:CG1	0.77	2.10	23	26
1:A:14:ASP:O	1:A:18:ASP:CG	0.76	2.24	25	26
1:A:12:ILE:O	1:A:16:GLN:CB	0.74	2.35	4	26
1:A:8:VAL:O	1:A:12:ILE:HG12	0.72	1.84	23	26
1:A:8:VAL:HG12	1:A:12:ILE:HG13	0.71	1.62	3	26
1:A:41:SER:O	1:A:45:LYS:N	0.68	2.26	17	26
1:A:24:GLY:O	1:A:28:GLY:N	0.66	2.29	22	26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:O	1:A:12:ILE:CG1	0.62	2.47	26	26
1:A:41:SER:O	1:A:45:LYS:HB2	0.62	1.95	7	26
1:A:8:VAL:HG12	1:A:12:ILE:CG1	0.62	2.23	27	26
1:A:8:VAL:CG1	1:A:12:ILE:HG12	0.62	2.25	13	26
1:A:31:VAL:O	1:A:35:VAL:HG23	0.62	1.95	20	26
1:A:8:VAL:HG13	1:A:12:ILE:HG12	0.59	1.74	15	26
1:A:24:GLY:HA2	1:A:27:VAL:HG12	0.59	1.75	8	13
1:A:41:SER:O	1:A:45:LYS:HB3	0.57	2.00	18	26
1:A:8:VAL:O	1:A:12:ILE:CB	0.57	2.53	23	26
1:A:8:VAL:O	1:A:12:ILE:N	0.55	2.37	2	26
1:A:40:TYR:O	1:A:44:ARG:N	0.55	2.38	27	26
1:A:16:GLN:O	1:A:19:MET:CB	0.54	2.56	4	26
1:A:35:VAL:O	1:A:39:ILE:CG1	0.54	2.49	24	26
1:A:12:ILE:O	1:A:16:GLN:N	0.54	2.41	19	26
1:A:22:ILE:O	1:A:26:ILE:HG13	0.52	2.05	11	26
1:A:23:GLY:O	1:A:27:VAL:HG23	0.52	2.05	4	13
1:A:22:ILE:O	1:A:26:ILE:CG1	0.51	2.59	26	26
1:A:24:GLY:CA	1:A:27:VAL:HG12	0.49	2.38	2	13
1:A:26:ILE:O	1:A:30:LEU:HG	0.48	2.09	3	26
1:A:23:GLY:O	1:A:27:VAL:HG12	0.47	2.10	8	13
1:A:8:VAL:O	1:A:12:ILE:HB	0.46	2.11	5	26
1:A:16:GLN:O	1:A:19:MET:HB3	0.46	2.11	7	26
1:A:22:ILE:HG22	1:A:26:ILE:HD12	0.46	1.88	4	26
1:A:21:ALA:O	1:A:25:TYR:CB	0.43	2.67	2	26
1:A:24:GLY:HA2	1:A:27:VAL:CG1	0.42	2.44	2	10
1:A:40:TYR:O	1:A:44:ARG:CB	0.42	2.68	2	26
1:A:3:ILE:HA	1:A:6:SER:HB2	0.41	1.92	27	10

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	44/46 (96%)	43±0 (98±0%)	1±0 (2±0%)	0±0 (0±0%)	100	100
All	All	1188/1242 (96%)	1161 (98%)	27 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	32/32 (100%)	31±6 (96±19%)	0±0 (0±0%)	100	100
All	All	832/864 (96%)	832 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided