



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:30 PM BST

PDB ID : 1YJT
Title : Solution structure of the Cu(I) form of the sixth soluble domain A69P mutant of Menkes protein
Authors : Banci, L.; Bertini, I.; Cantini, F.; Migliardi, M.; Rosato, A.; Wang, S.
Deposited on : 2005-01-15

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

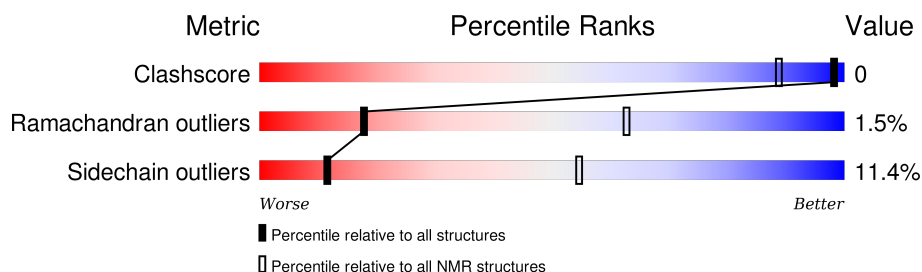
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 49%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	75	

2 Ensemble composition and analysis ⓘ

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:5-A:72 (68)	0.36	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1167 atoms, of which 593 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-transporting ATPase 1.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1166	363	593	98	107	5	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q04656
A	69	PRO	ALA	ENGINEERED	UNP Q04656
A	74	ILE	-	CLONING ARTIFACT	UNP Q04656
A	75	GLU	-	CLONING ARTIFACT	UNP Q04656

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

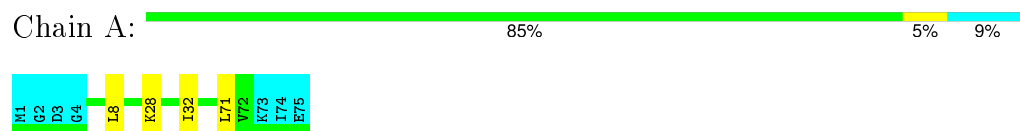
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

4 Residue-property plots

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: Copper-transporting ATPase 1

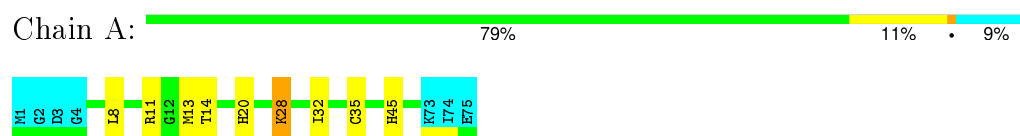


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

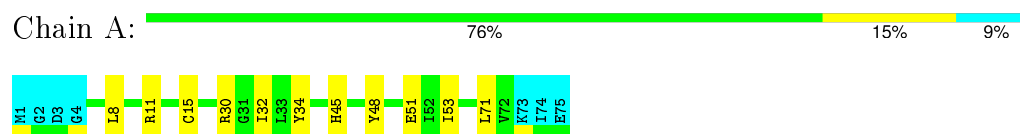
4.2.1 Score per residue for model 1

- Molecule 1: Copper-transporting ATPase 1



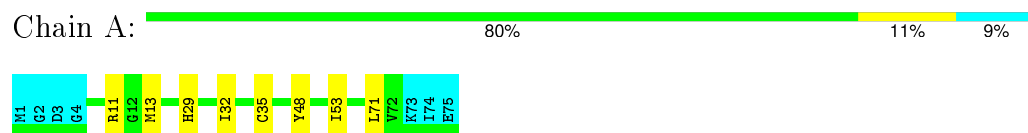
4.2.2 Score per residue for model 2

- Molecule 1: Copper-transporting ATPase 1



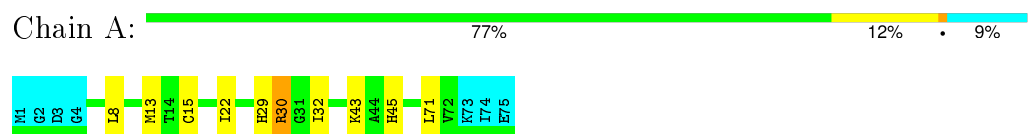
4.2.3 Score per residue for model 3

- Molecule 1: Copper-transporting ATPase 1



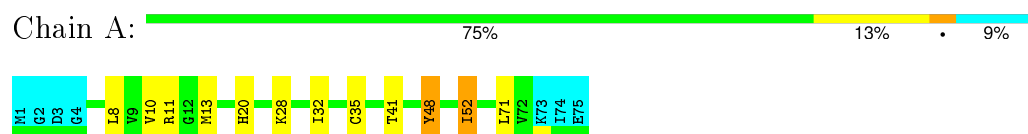
4.2.4 Score per residue for model 4

- Molecule 1: Copper-transporting ATPase 1



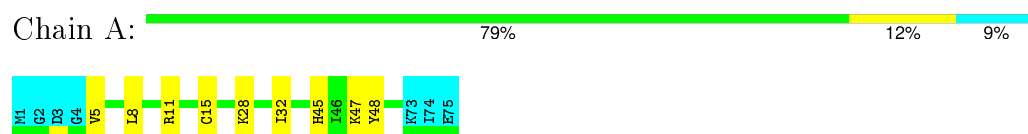
4.2.5 Score per residue for model 5

- Molecule 1: Copper-transporting ATPase 1



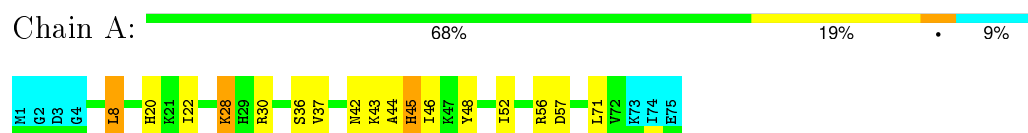
4.2.6 Score per residue for model 6

- Molecule 1: Copper-transporting ATPase 1



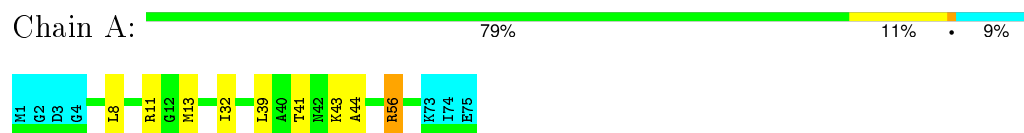
4.2.7 Score per residue for model 7

- Molecule 1: Copper-transporting ATPase 1



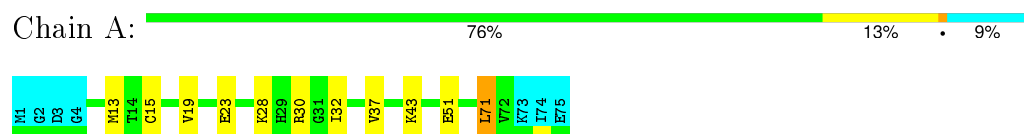
4.2.8 Score per residue for model 8

- Molecule 1: Copper-transporting ATPase 1



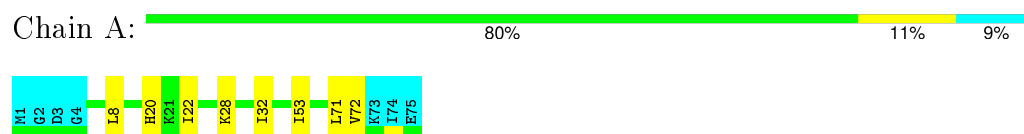
4.2.9 Score per residue for model 9

- Molecule 1: Copper-transporting ATPase 1



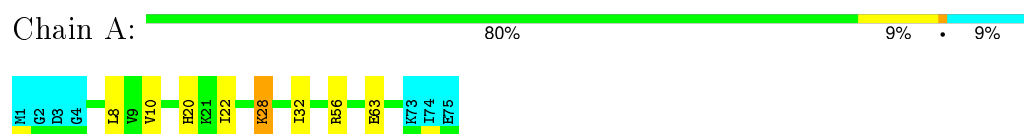
4.2.10 Score per residue for model 10

- Molecule 1: Copper-transporting ATPase 1



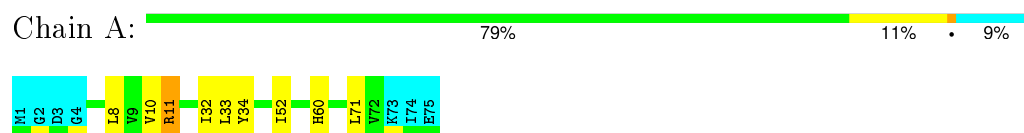
4.2.11 Score per residue for model 11

- Molecule 1: Copper-transporting ATPase 1



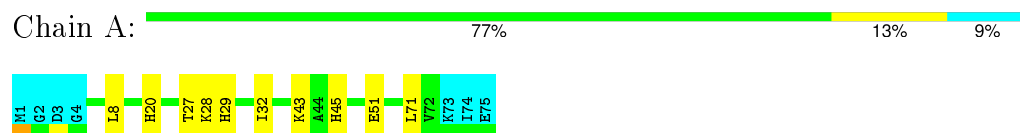
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Copper-transporting ATPase 1



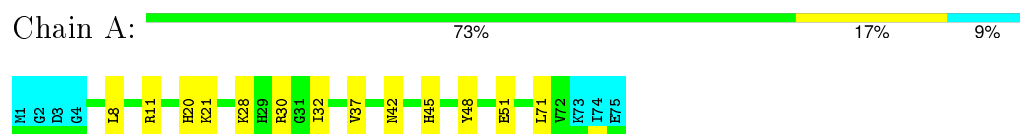
4.2.13 Score per residue for model 13

- Molecule 1: Copper-transporting ATPase 1



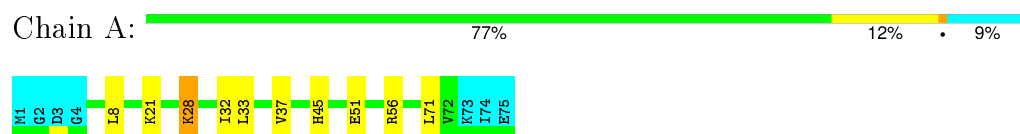
4.2.14 Score per residue for model 14

- Molecule 1: Copper-transporting ATPase 1



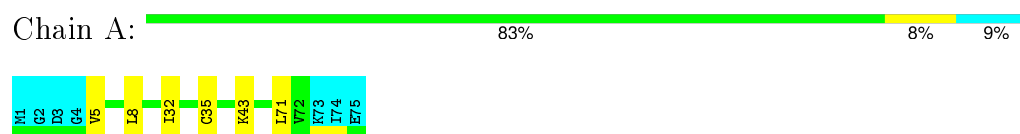
4.2.15 Score per residue for model 15

- Molecule 1: Copper-transporting ATPase 1



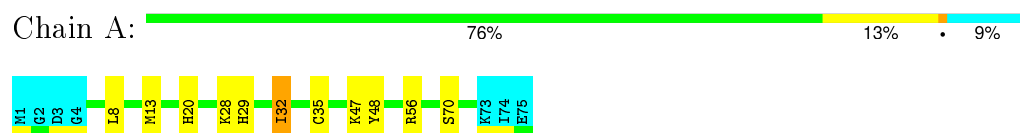
4.2.16 Score per residue for model 16

- Molecule 1: Copper-transporting ATPase 1



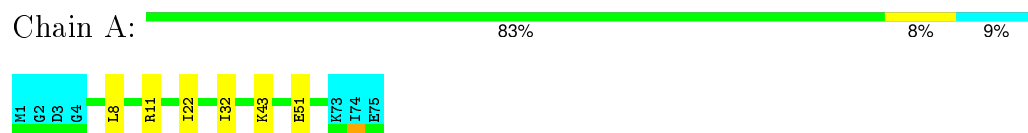
4.2.17 Score per residue for model 17

- Molecule 1: Copper-transporting ATPase 1



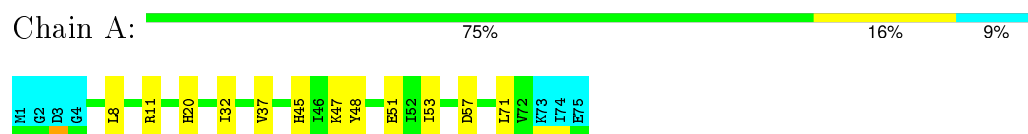
4.2.18 Score per residue for model 18

- Molecule 1: Copper-transporting ATPase 1



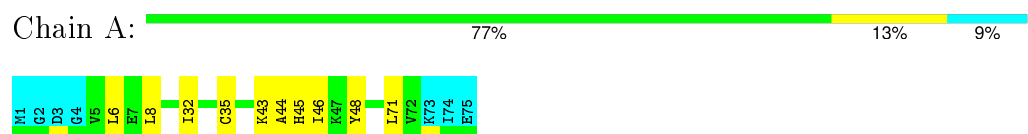
4.2.19 Score per residue for model 19

- Molecule 1: Copper-transporting ATPase 1



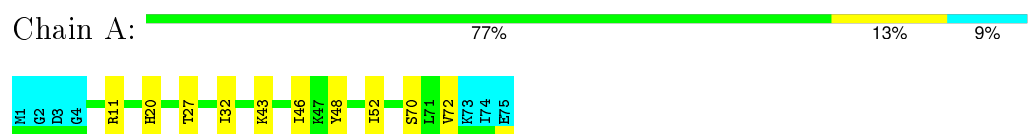
4.2.20 Score per residue for model 20

- Molecule 1: Copper-transporting ATPase 1



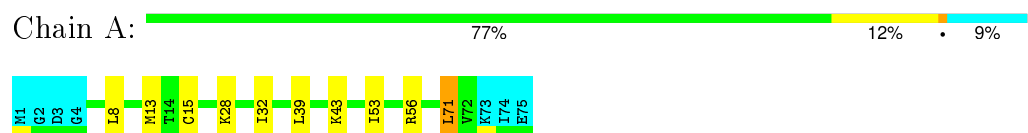
4.2.21 Score per residue for model 21

- Molecule 1: Copper-transporting ATPase 1



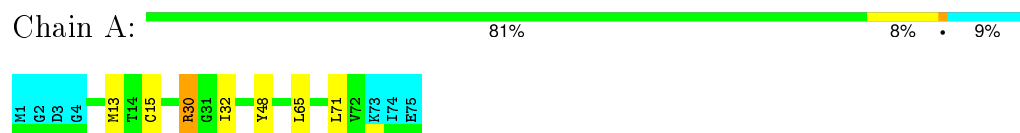
4.2.22 Score per residue for model 22

- Molecule 1: Copper-transporting ATPase 1



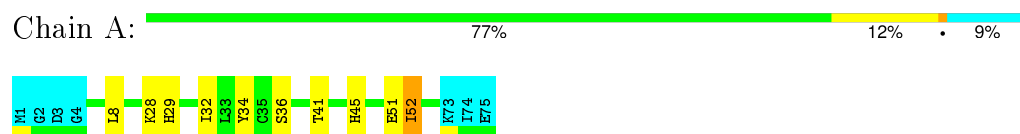
4.2.23 Score per residue for model 23

- Molecule 1: Copper-transporting ATPase 1



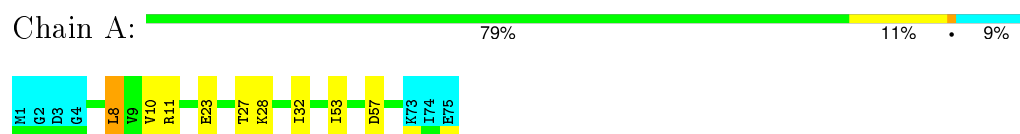
4.2.24 Score per residue for model 24

- Molecule 1: Copper-transporting ATPase 1



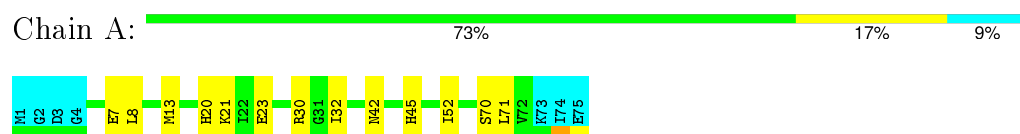
4.2.25 Score per residue for model 25

- Molecule 1: Copper-transporting ATPase 1



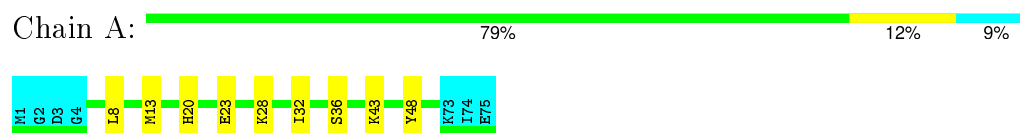
4.2.26 Score per residue for model 26

- Molecule 1: Copper-transporting ATPase 1



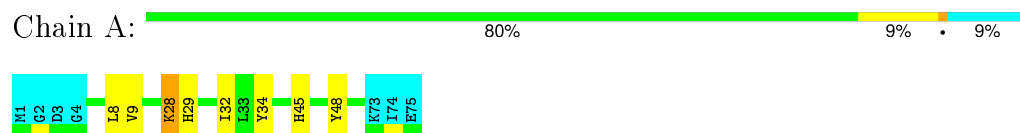
4.2.27 Score per residue for model 27

- Molecule 1: Copper-transporting ATPase 1



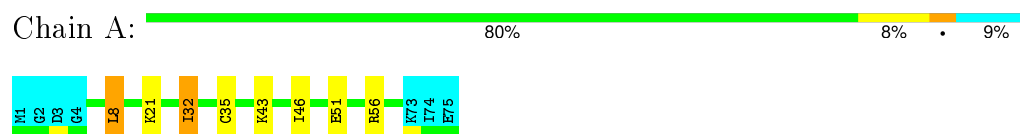
4.2.28 Score per residue for model 28

- Molecule 1: Copper-transporting ATPase 1



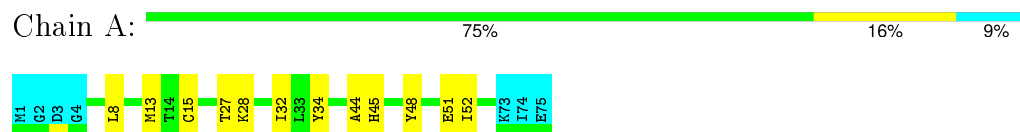
4.2.29 Score per residue for model 29

- Molecule 1: Copper-transporting ATPase 1



4.2.30 Score per residue for model 30

- Molecule 1: Copper-transporting ATPase 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics coupled with simulated annealing followed by restrained energy minimization*.

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
AMBER	refinement	5.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6482
Number of chemical shift lists	1
Total number of shifts	546
Number of shifts mapped to atoms	546
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

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: CU1

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	0.50±0.01	0±0/532 (0.0±0.0%)	0.90±0.02	0±0/722 (0.0±0.0%)
All	All	0.50	0/15960 (0.0%)	0.90	1/21660 (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	0.0±0.0	1.7±1.1
All	All	0	52

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	ARG	NE-CZ-NH2	-5.24	117.68	120.30	12	1

There are no chirality outliers.

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	48	TYR	Sidechain	14
1	A	35	CYS	Peptide	7
1	A	56	ARG	Sidechain	6
1	A	45	HIS	Sidechain	6
1	A	11	ARG	Sidechain	6
1	A	29	HIS	Sidechain,Peptide	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	34	TYR	Sidechain	4
1	A	44	ALA	Peptide	2
1	A	30	ARG	Sidechain	2
1	A	43	LYS	Peptide	1

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	522	542	542	0±1
All	All	15690	16260	16260	15

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:HIS:NE2	1:A:32:ILE:HD12	0.54	2.17	17	1
1:A:8:LEU:HD21	1:A:46:ILE:HD13	0.52	1.82	7	2
1:A:23:GLU:CG	1:A:37:VAL:HG12	0.51	2.36	9	1
1:A:71:LEU:H	1:A:71:LEU:HD22	0.49	1.67	5	1
1:A:44:ALA:HB1	1:A:46:ILE:CD1	0.47	2.39	20	1
1:A:45:HIS:C	1:A:46:ILE:HD12	0.45	2.31	7	1
1:A:71:LEU:H	1:A:71:LEU:HD23	0.45	1.71	22	1
1:A:37:VAL:HG23	1:A:44:ALA:HB2	0.44	1.89	7	1
1:A:22:ILE:HB	1:A:37:VAL:HG11	0.42	1.89	7	1
1:A:71:LEU:HD23	1:A:71:LEU:H	0.42	1.74	7	1
1:A:19:VAL:HG13	1:A:37:VAL:HG13	0.42	1.90	9	1
1:A:8:LEU:HD23	1:A:8:LEU:N	0.41	2.31	25	1
1:A:46:ILE:HD12	1:A:46:ILE:N	0.41	2.31	21	1
1:A:32:ILE:HD11	1:A:46:ILE:HG23	0.40	1.92	29	1

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	68/75 (91%)	58±2 (85±3%)	9±2 (14±3%)	1±1 (2±1%)	18	63
All	All	2040/2250 (91%)	1726 (85%)	283 (14%)	31 (2%)	18	63

All 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	28	LYS	14
1	A	30	ARG	5
1	A	27	THR	3
1	A	52	ILE	2
1	A	51	GLU	2
1	A	71	LEU	2
1	A	22	ILE	1
1	A	5	VAL	1
1	A	72	VAL	1

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	60/65 (92%)	53±2 (89±3%)	7±2 (11±3%)	11	54
All	All	1800/1950 (92%)	1594 (89%)	206 (11%)	11	54

All 40 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	32	ILE	29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	8	LEU	26
1	A	71	LEU	14
1	A	13	MET	12
1	A	20	HIS	12
1	A	43	LYS	11
1	A	45	HIS	8
1	A	28	LYS	8
1	A	51	GLU	7
1	A	15	CYS	7
1	A	52	ILE	7
1	A	53	ILE	6
1	A	11	ARG	6
1	A	21	LYS	4
1	A	10	VAL	4
1	A	22	ILE	3
1	A	41	THR	3
1	A	36	SER	3
1	A	23	GLU	3
1	A	37	VAL	3
1	A	57	ASP	3
1	A	70	SER	3
1	A	42	ASN	3
1	A	33	LEU	2
1	A	56	ARG	2
1	A	39	LEU	2
1	A	30	ARG	2
1	A	65	LEU	1
1	A	29	HIS	1
1	A	60	HIS	1
1	A	5	VAL	1
1	A	63	GLU	1
1	A	27	THR	1
1	A	14	THR	1
1	A	48	TYR	1
1	A	6	LEU	1
1	A	72	VAL	1
1	A	7	GLU	1
1	A	34	TYR	1
1	A	9	VAL	1

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](#)

Of 1 ligands modelled in this entry, 1 is 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

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 48% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6482

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	546
Number of shifts mapped to atoms	546
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	69	0.64 ± 0.31	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 49%, i.e. 406 atoms were assigned a chemical shift out of a possible 821. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	195/334 (58%)	131/133 (98%)	0/136 (0%)	64/65 (98%)
Sidechain	199/434 (46%)	198/253 (78%)	0/167 (0%)	1/14 (7%)

Continued on next page...

	Total	¹H	¹³C	¹⁵N
Aromatic	12/53 (23%)	12/29 (41%)	0/20 (0%)	0/4 (0%)
Overall	406/821 (49%)	341/415 (82%)	0/323 (0%)	65/83 (78%)

	Total	¹H	¹³C	¹⁵N
Backbone	210/369 (57%)	141/147 (96%)	0/150 (0%)	69/72 (96%)
Sidechain	213/475 (45%)	212/277 (77%)	0/183 (0%)	1/15 (7%)
Aromatic	12/53 (23%)	12/29 (41%)	0/20 (0%)	0/4 (0%)
Overall	435/897 (48%)	365/453 (81%)	0/353 (0%)	70/91 (77%)

7.1.5 Random Coil Index (RCI) plots

Random coil index (RCI) for chain A:

