Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 11:45 am BST

PDB ID	:	6PQM
Title	:	Structural Basis for Client Recognition and Activity of Hsp40 Chaperones
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Deposited on	:	2019-07-09

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:

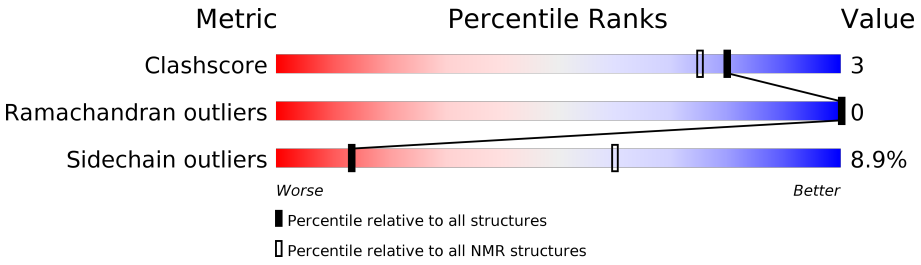
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)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

The overall completeness of chemical shifts assignment is 85%.

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	94	69% 7% 23%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:168-A:173, A:191-A:256 (72)	0.18	9

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1348 atoms, of which 679 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alkaline phosphatase,Chaperone protein DnaJ 2 fusion.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1348	414	679	120	131	4	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	MET	-	initiating methionine	UNP P00634
A	180	GLY	-	linker	UNP P00634
A	181	SER	-	linker	UNP P00634
A	182	GLY	-	linker	UNP P00634
A	183	GLY	-	linker	UNP P00634
A	184	SER	-	linker	UNP P00634
A	185	GLY	-	linker	UNP P00634
A	186	GLY	-	linker	UNP P00634
A	187	SER	-	linker	UNP P00634
A	188	GLY	-	linker	UNP P00634
A	189	GLY	-	linker	UNP P00634
A	190	SER	-	linker	UNP P00634

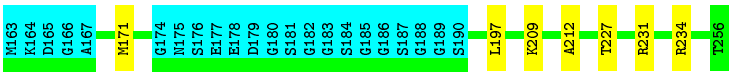
4 Residue-property plots

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: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

Chain A:



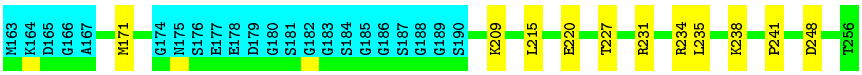
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

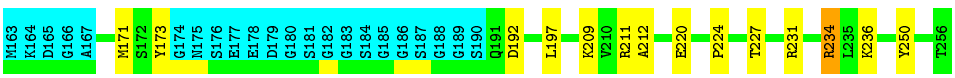
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

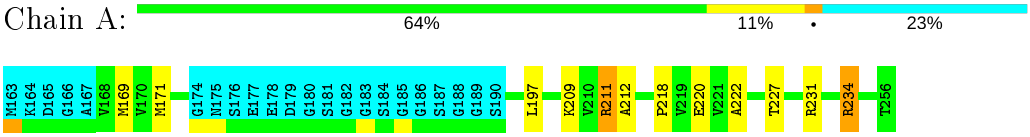
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

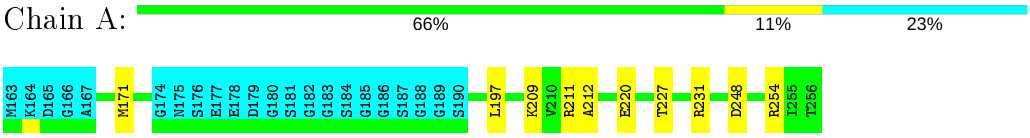
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

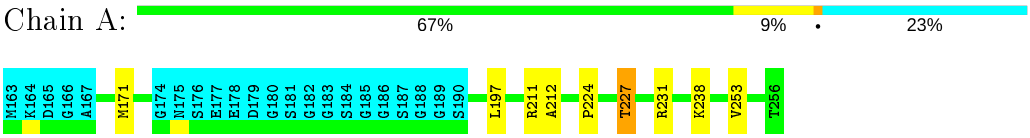
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

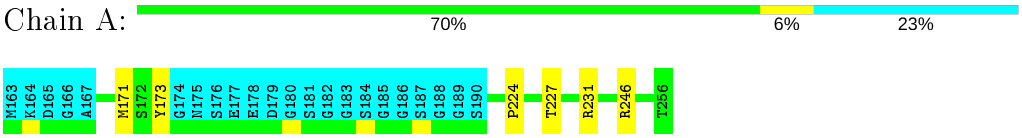
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

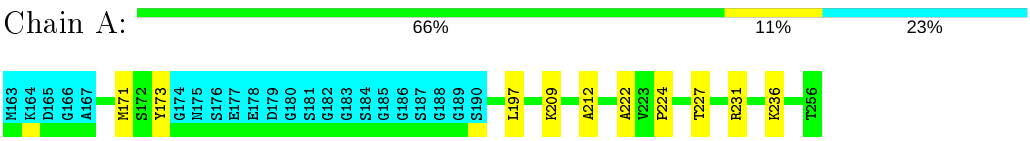
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

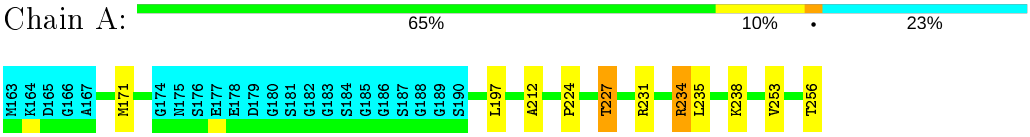
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

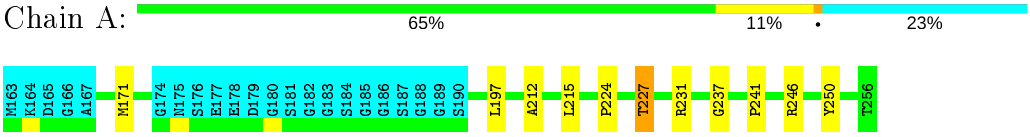
Chain A:



4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

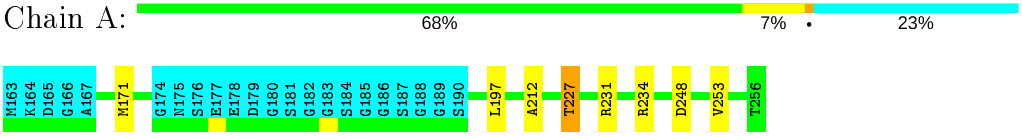
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

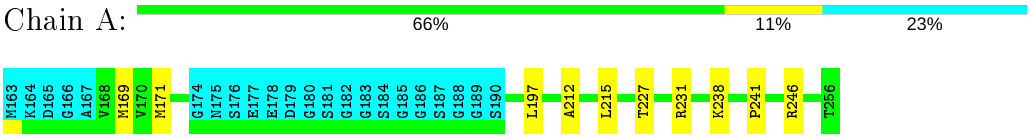
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

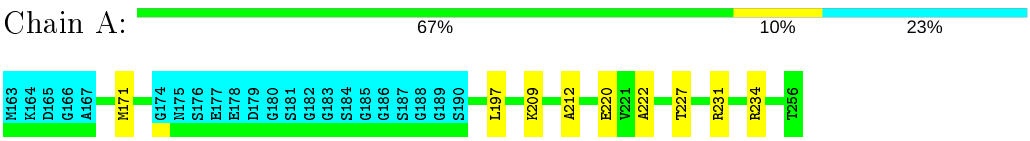
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

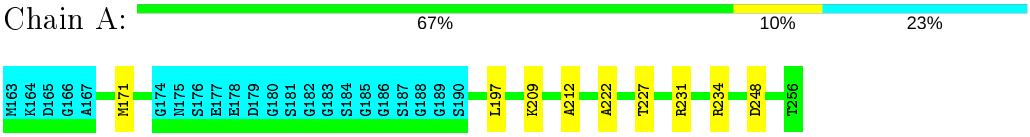
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

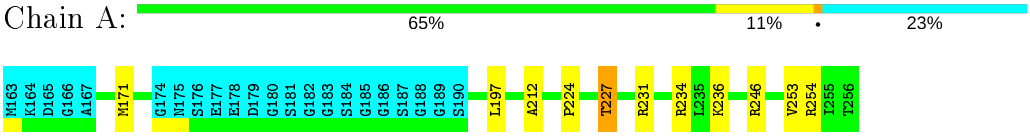
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

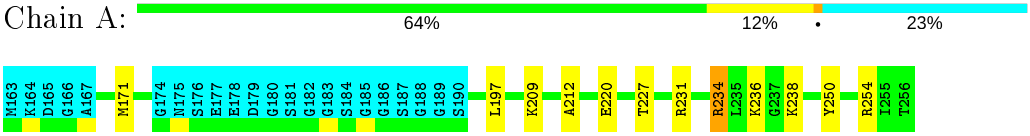
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

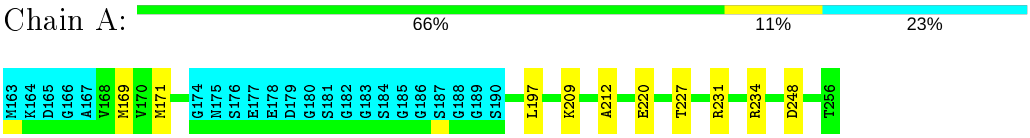
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

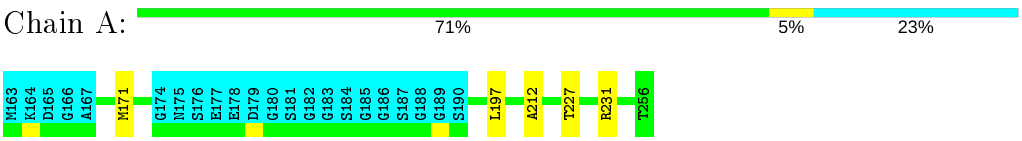
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

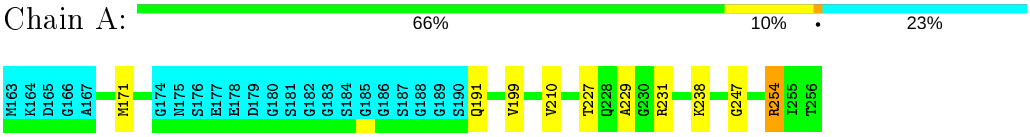
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

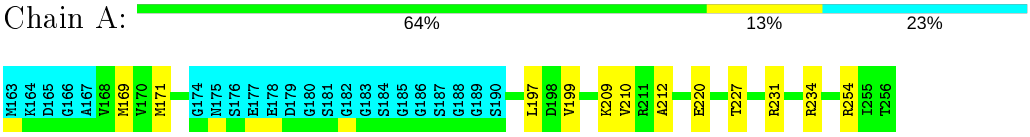
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

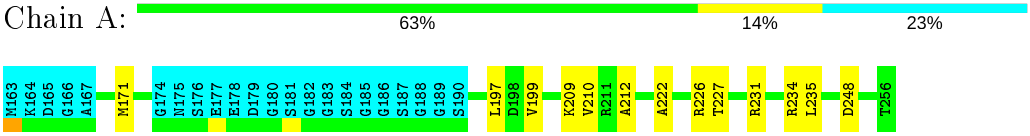
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CNS	refinement	
CYANA	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	949
Number of shifts mapped to atoms	949
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	539	572	572	3±1
All	All	10780	11440	11440	59

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LEU:HD13	1:A:212:ALA:HB2	0.56	1.78	19	17
1:A:234:ARG:HD3	1:A:236:LYS:HE2	0.48	1.84	15	2
1:A:234:ARG:H	1:A:234:ARG:HD2	0.46	1.71	8	1
1:A:197:LEU:HD11	1:A:210:VAL:HG23	0.45	1.88	19	1
1:A:224:PRO:HG2	1:A:227:THR:HB	0.45	1.87	9	4
1:A:173:TYR:HB2	1:A:224:PRO:HG3	0.45	1.88	7	1
1:A:209:LYS:HD3	1:A:220:GLU:HB3	0.44	1.89	16	8
1:A:227:THR:HG23	1:A:253:VAL:HG11	0.44	1.90	14	4
1:A:235:LEU:HB3	1:A:238:LYS:HB2	0.44	1.90	8	2
1:A:215:LEU:HD21	1:A:241:PRO:HD3	0.43	1.89	11	3
1:A:199:VAL:HG22	1:A:210:VAL:HG21	0.43	1.90	19	3
1:A:211:ARG:HE	1:A:218:PRO:HB3	0.43	1.73	3	1
1:A:173:TYR:HB2	1:A:224:PRO:HB3	0.42	1.90	2	2
1:A:229:ALA:HB1	1:A:254:ARG:HH21	0.42	1.73	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:LYS:HA	1:A:222:ALA:HA	0.42	1.91	7	5
1:A:235:LEU:O	1:A:248:ASP:HB2	0.42	2.14	20	1
1:A:191:GLN:HB3	1:A:247:GLY:HA3	0.41	1.91	18	1
1:A:234:ARG:H	1:A:234:ARG:HD3	0.41	1.75	3	1
1:A:237:GLY:HA2	1:A:246:ARG:HH11	0.41	1.76	9	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	71/94 (76%)	66±0 (93±1%)	5±0 (7±1%)	0±0 (0±0%)	100	100
All	All	1420/1880 (76%)	1324 (93%)	96 (7%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	56/68 (82%)	51±1 (91±2%)	5±1 (9±2%)	13	60
All	All	1120/1360 (82%)	1020 (91%)	100 (9%)	13	60

All 14 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	231	ARG	20
1	A	227	THR	20
1	A	171	MET	20

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Mol	Chain	Res	Type	Models (Total)
1	A	234	ARG	11
1	A	254	ARG	5
1	A	248	ASP	5
1	A	211	ARG	4
1	A	238	LYS	4
1	A	250	TYR	3
1	A	246	ARG	3
1	A	236	LYS	2
1	A	226	ARG	1
1	A	256	THR	1
1	A	192	ASP	1

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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *E415-D430_CBD2.bmrb*

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	949
Number of shifts mapped to atoms	949
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	90	0.05 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	75	0.13 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	68	2.76 ± 0.15	Should be applied
^{15}N	79	-0.64 ± 0.29	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 85%, i.e. 734 atoms were assigned a chemical shift out of a possible 865. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	312/346 (90%)	127/137 (93%)	124/144 (86%)	61/65 (94%)
Sidechain	390/486 (80%)	232/285 (81%)	158/177 (89%)	0/24 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	32/33 (97%)	16/17 (94%)	16/16 (100%)	0/0 (—%)
Overall	734/865 (85%)	375/439 (85%)	298/337 (88%)	61/89 (69%)

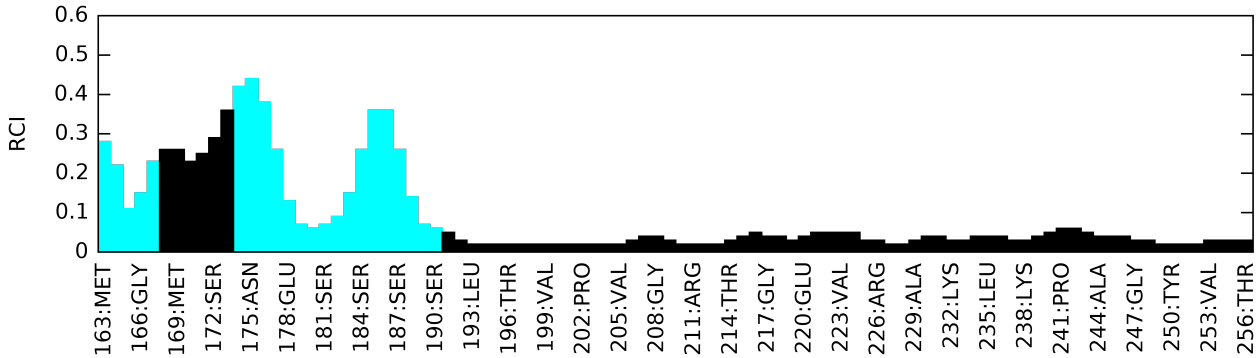
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 868 atoms were assigned a chemical shift out of a possible 1042. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	401/456 (88%)	164/181 (91%)	158/188 (84%)	79/87 (91%)
Sidechain	435/553 (79%)	259/325 (80%)	176/202 (87%)	0/26 (0%)
Aromatic	32/33 (97%)	16/17 (94%)	16/16 (100%)	0/0 (—%)
Overall	868/1042 (83%)	439/523 (84%)	350/406 (86%)	79/113 (70%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: