Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:46 AM BST

PDB ID	:	5HP0
Title	:	Solution Structure of TAZ2-p53AD2
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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 (i) symbol.

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

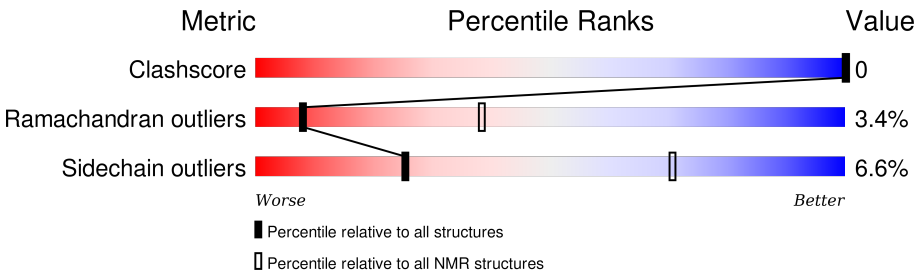
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 83%.

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	122	62% 13% 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:1768-A:1809, A:1813-A:1851, A:3043-A:3053 (92)	0.15	11

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1880 atoms, of which 932 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CREB-binding protein,Cellular tumor antigen p53 fusion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1877	573	932	182	174	16	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2001	GLY	-	linker	UNP P45481
A	2002	SER	-	linker	UNP P45481
A	2003	GLY	-	linker	UNP P45481
A	2004	SER	-	linker	UNP P45481
A	2005	GLY	-	linker	UNP P45481

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

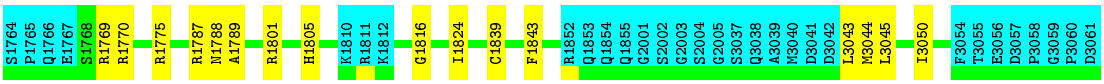
4 Residue-property plots (i)

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: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A:



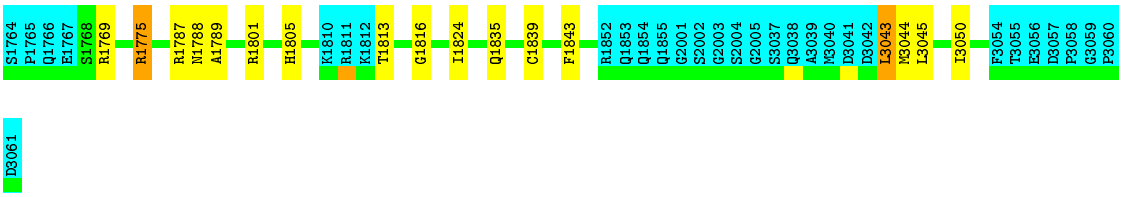
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

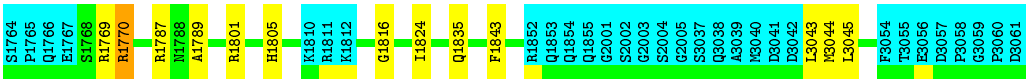
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A: 62% 13% 25%

S1764 P1765 Q1766 E1767 S1768 R1769 R1775 R1787 N1788 A1789 R1801 H1805 K1810 R1811 K1812 T1813 G1816 I1824 C1839 F1843 R1852 Q1853 Q1854 Q1855 G2001 S2002 G2003 S2004 G2005 S3037 Q3038 A3039 M3040 D3041 D3042 L3043 M3044 L3045 I3050 F3054 T3055 E3056 D3057 P3058 G3059 P3060 D3061

4.2.4 Score per residue for model 4

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A: 67% 8% 25%

S1764 P1765 Q1766 E1767 R1770 R1787 N1788 A1789 R1801 H1805 K1810 R1811 K1812 G1816 I1824 R1852 Q1853 Q1854 Q1855 G2001 S2002 G2003 S2004 G2005 S3037 Q3038 A3039 M3040 D3041 D3042 L3045 I3050 F3054 T3055 E3056 D3057 P3058 G3059 P3060 D3061

4.2.5 Score per residue for model 5

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A: 63% 12% 25%

S1764 P1765 Q1766 E1767 S1768 R1769 R1770 R1787 N1788 A1789 R1801 H1805 K1810 R1811 K1812 G1816 I1824 Q1835 C1839 F1843 R1852 Q1853 Q1854 Q1855 G2001 S2002 G2003 S2004 G2005 S3037 Q3038 A3039 M3040 D3041 D3042 L3043 M3044 L3045 I3050 F3054 T3055 E3056 D3057 P3058 G3059 P3060 D3061

4.2.6 Score per residue for model 6

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A: 65% 11% 25%

S1764 P1765 Q1766 E1767 R1775 R1787 N1788 A1789 R1801 H1805 K1810 R1811 K1812 G1816 I1824 A1825 L1826 R1852 Q1853 Q1854 Q1855 G2001 S2002 G2003 S2004 G2005 S3037 Q3038 A3039 M3040 D3041 D3042 L3043 M3044 L3045 I3050 F3054 T3055 E3056 D3057 P3058 G3059 P3060 D3061

4.2.7 Score per residue for model 7

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

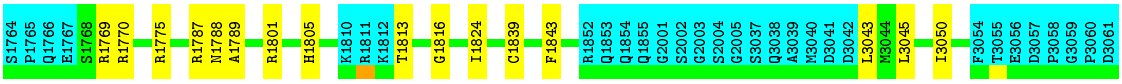
Chain A: 64% 11% • 25%

S1764 P1765 Q1766 E1767 S1768 R1769 R1770 R1775 R1787 N1788 A1789 R1801 H1805 K1810 R1811 K1812 G1816 I1824 C1839 R1852 Q1853 Q1854 Q1855 G2001 S2002 G2003 S2004 G2005 S3037 Q3038 A3039 M3040 D3041 D3042 L3043 M3044 L3045 I3050 F3054 T3055 E3056 D3057 P3058 G3059 P3060 D3061

4.2.8 Score per residue for model 8

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

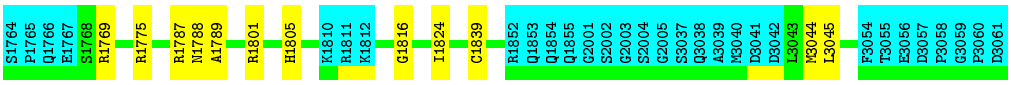
Chain A: 62% 13% 25%



4.2.9 Score per residue for model 9

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

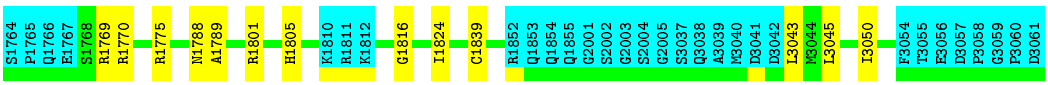
Chain A: 66% 10% 25%



4.2.10 Score per residue for model 10

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

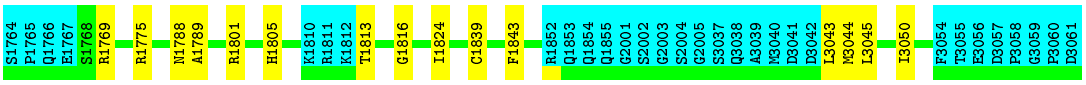
Chain A: 65% 11% 25%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

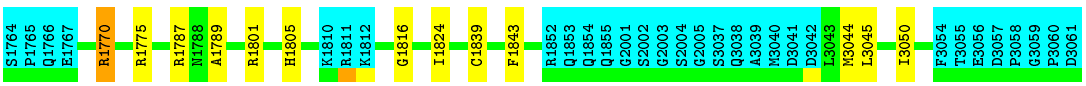
Chain A: 63% 12% 25%



4.2.12 Score per residue for model 12

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

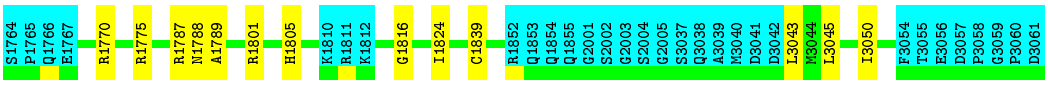
Chain A: 65% 10% • 25%



4.2.13 Score per residue for model 13

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

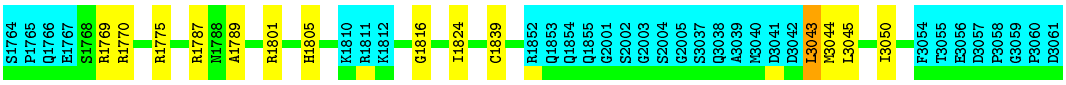
Chain A: 65% 11% 25%



4.2.14 Score per residue for model 14

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

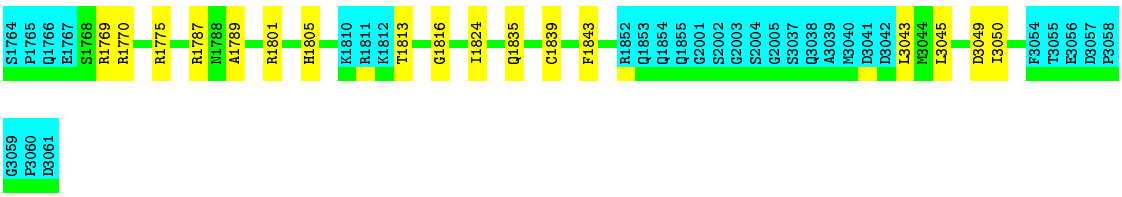
Chain A: 64% 11% • 25%



4.2.15 Score per residue for model 15

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

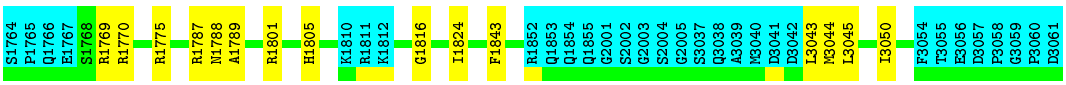
Chain A: 61% 14% 25%



4.2.16 Score per residue for model 16

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

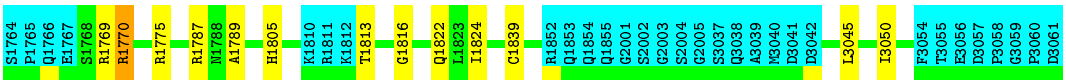
Chain A: 63% 12% 25%



4.2.17 Score per residue for model 17

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

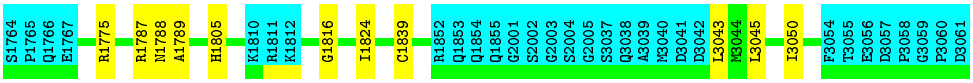
Chain A: 65% 10% • 25%



4.2.18 Score per residue for model 18

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

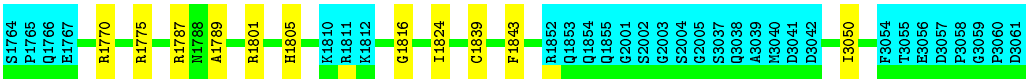
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

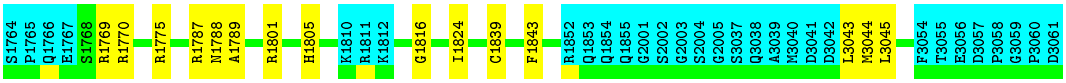
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 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
AMBER	refinement	12

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)	5hp0_cs.str
Number of chemical shift lists	1
Total number of shifts	1329
Number of shifts mapped to atoms	1329
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.60±0.00	0±0/732 (0.0±0.0%)	1.06±0.02	4±1/986 (0.5±0.1%)
All	All	0.60	0/14640 (0.0%)	1.06	89/19720 (0.5%)

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	1.0±0.0
All	All	0	20

There are no bond-length outliers.

All 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	1787	ARG	NE-CZ-NH2	7.83	124.21	120.30	13	16
1	A	1801	ARG	NE-CZ-NH2	7.28	123.94	120.30	19	16
1	A	1787	ARG	NE-CZ-NH1	6.77	123.69	120.30	8	2
1	A	1775	ARG	NE-CZ-NH2	6.60	123.60	120.30	13	13
1	A	1769	ARG	NE-CZ-NH2	6.35	123.47	120.30	9	14
1	A	1770	ARG	NE-CZ-NH1	6.27	123.44	120.30	4	3
1	A	1770	ARG	NE-CZ-NH2	6.22	123.41	120.30	14	10
1	A	1801	ARG	NE-CZ-NH1	5.99	123.29	120.30	20	2
1	A	1775	ARG	NE-CZ-NH1	5.68	123.14	120.30	1	4
1	A	1843	PHE	CB-CG-CD1	-5.30	117.09	120.80	15	5
1	A	1843	PHE	CB-CG-CD2	-5.24	117.14	120.80	8	4

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	1805	HIS	Sidechain	20

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
All	All	14420	14580	14540	-

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 -.

There are no clashes.

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	92/122 (75%)	84±1 (92±1%)	5±1 (5±1%)	3±1 (3±1%)	8 38
All	All	1840/2440 (75%)	1685 (92%)	93 (5%)	62 (3%)	8 38

All 5 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	1816	GLY	20
1	A	1789	ALA	20
1	A	3043	LEU	15
1	A	1813	THR	6
1	A	3044	MET	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	85/110 (77%)	79±1 (93±1%)	6±1 (7±1%)	25	71
All	All	1700/2200 (77%)	1588 (93%)	112 (7%)	25	71

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	1824	ILE	20
1	A	3045	LEU	19
1	A	3050	ILE	17
1	A	1839	CYS	16
1	A	1788	ASN	13
1	A	3044	MET	10
1	A	1770	ARG	5
1	A	1835	GLN	4
1	A	3043	LEU	2
1	A	1843	PHE	2
1	A	3049	ASP	1
1	A	1822	GLN	1
1	A	1826	LEU	1
1	A	1775	ARG	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 3 ligands modelled in this entry, 3 are 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 (i)

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: 5hp0_cs.str

Chemical shift list name: *p53ad2_corrected_shifts.str*

7.1.1 Bookkeeping (i)

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	1329
Number of shifts mapped to atoms	1329
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	118	-0.39 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	111	0.34 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	105	-0.47 ± 0.21	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 960 atoms were assigned a chemical shift out of a possible 1161. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	349/450 (78%)	175/179 (98%)	91/184 (49%)	83/87 (95%)
Sidechain	563/645 (87%)	357/386 (92%)	194/223 (87%)	12/36 (33%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	48/66 (73%)	25/35 (71%)	22/23 (96%)	1/8 (12%)
Overall	960/1161 (83%)	557/600 (93%)	307/430 (71%)	96/131 (73%)

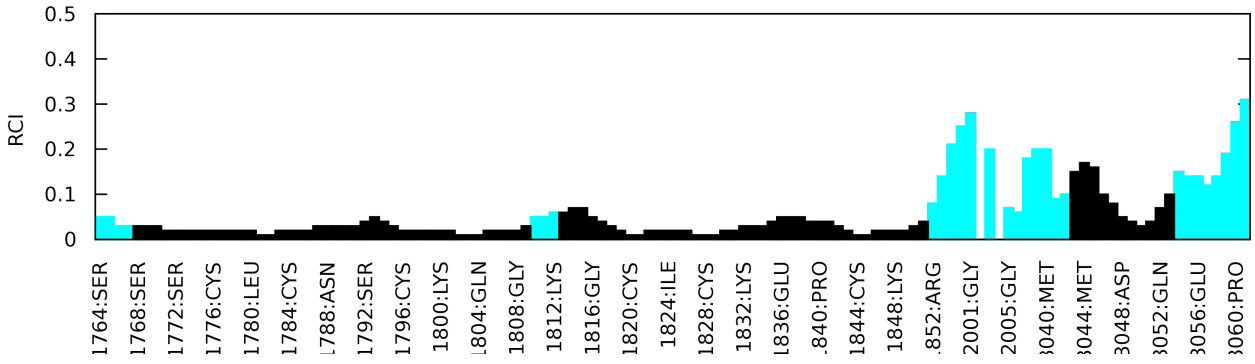
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1222 atoms were assigned a chemical shift out of a possible 1512. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	447/594 (75%)	224/236 (95%)	118/244 (48%)	105/114 (92%)
Sidechain	718/843 (85%)	460/506 (91%)	242/288 (84%)	16/49 (33%)
Aromatic	57/75 (76%)	30/40 (75%)	26/27 (96%)	1/8 (12%)
Overall	1222/1512 (81%)	714/782 (91%)	386/559 (69%)	122/171 (71%)

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: