



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:03 PM BST

PDB ID : 2CH0  
Title : SOLUTION STRUCTURE OF THE HUMAN MAN1 C-TERMINAL DOMAIN (RESIDUES 655-775)  
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Deposited on : 2006-03-10

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

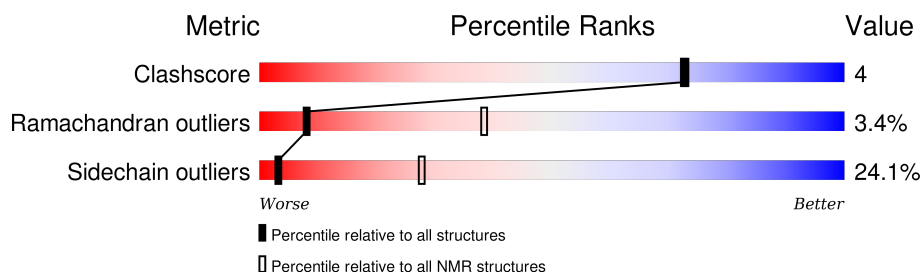
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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  $\geq 3$ , 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	133	<div> <div>41%</div> <div>18%</div> <div>•</div> <div>38%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:18-A:100 (83)	0.62	7

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 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2225 atoms, of which 1107 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INNER NUCLEAR MEMBRANE PROTEIN MAN1.

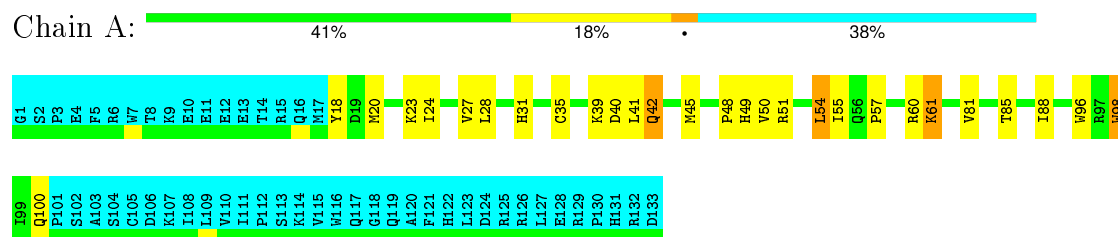
Mol	Chain	Residues	Atoms						Trace
1	A	133	Total	C	H	N	O	S	0
			2225	702	1107	212	198	6	

## 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: INNER NUCLEAR MEMBRANE PROTEIN MAN1

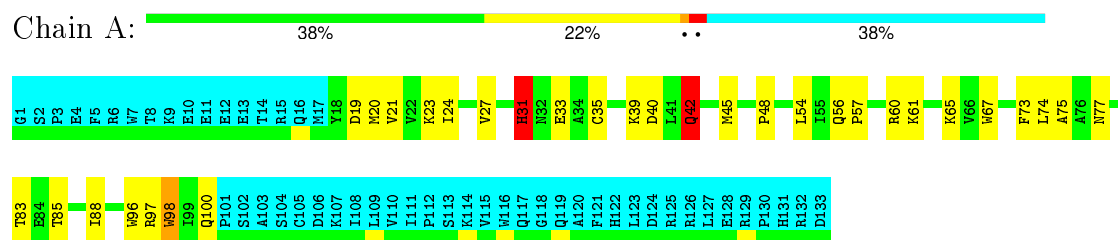


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

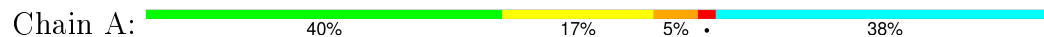
#### 4.2.1 Score per residue for model 1

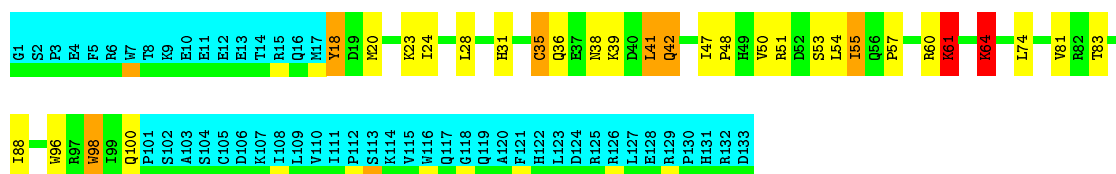
- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



#### 4.2.2 Score per residue for model 2

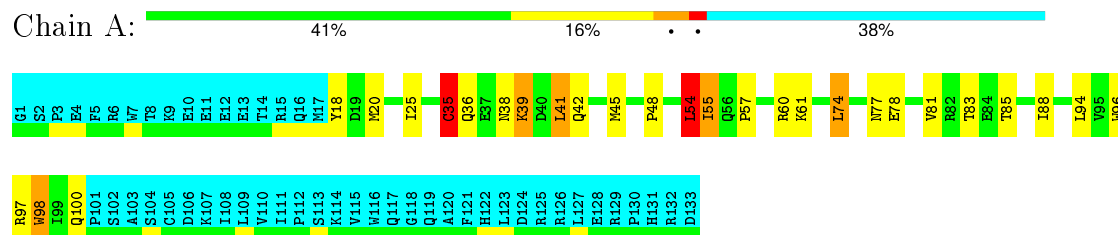
- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1





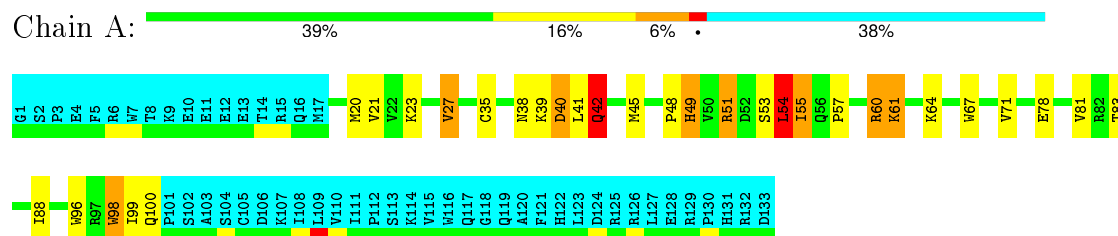
### 4.2.3 Score per residue for model 3

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



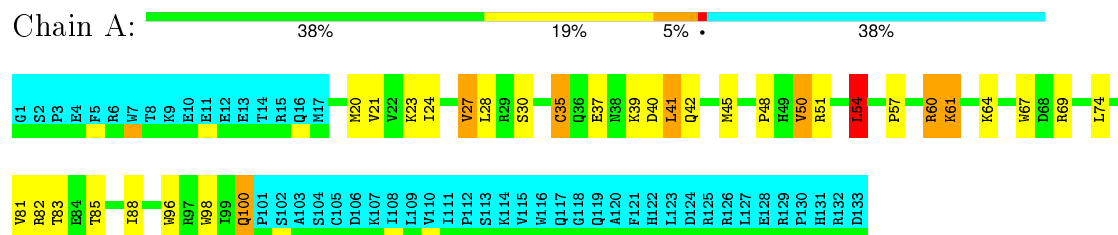
### 4.2.4 Score per residue for model 4

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



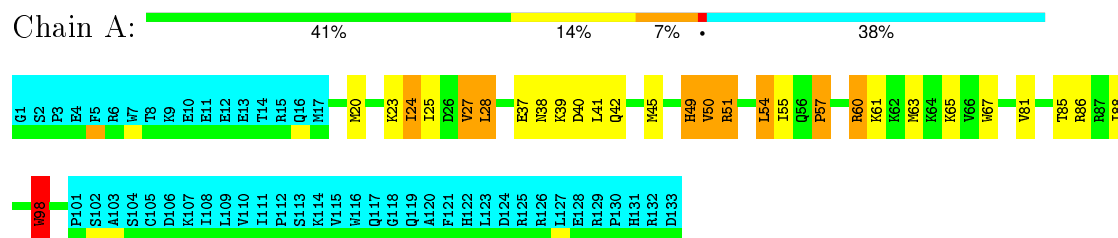
### 4.2.5 Score per residue for model 5

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



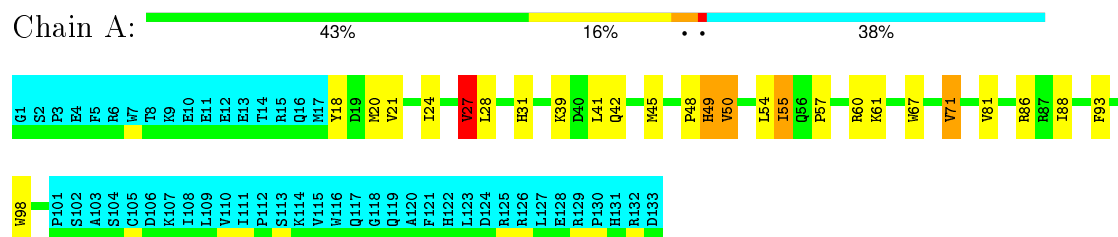
### 4.2.6 Score per residue for model 6

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



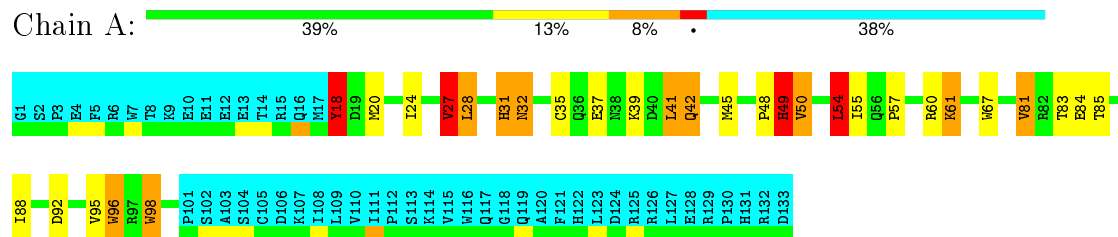
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



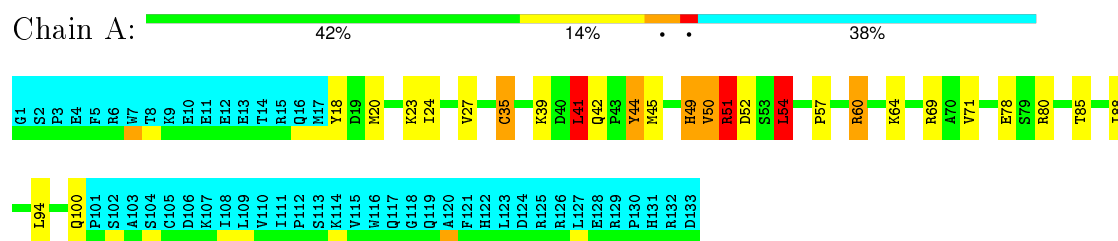
#### 4.2.8 Score per residue for model 8

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



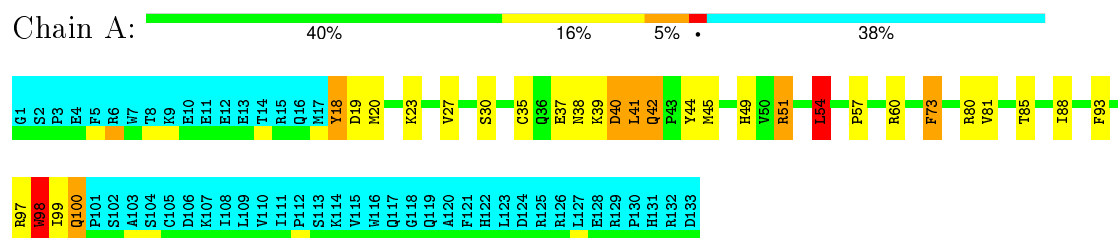
#### 4.2.9 Score per residue for model 9

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



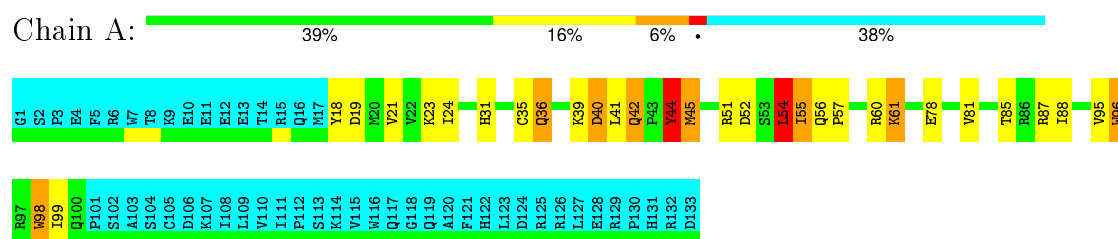
### 4.2.10 Score per residue for model 10

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



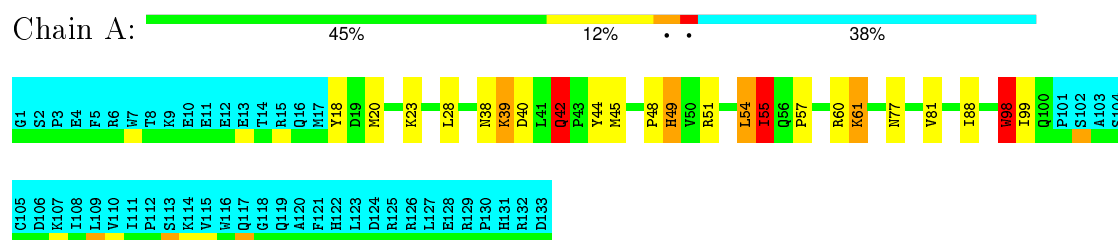
### 4.2.11 Score per residue for model 11

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



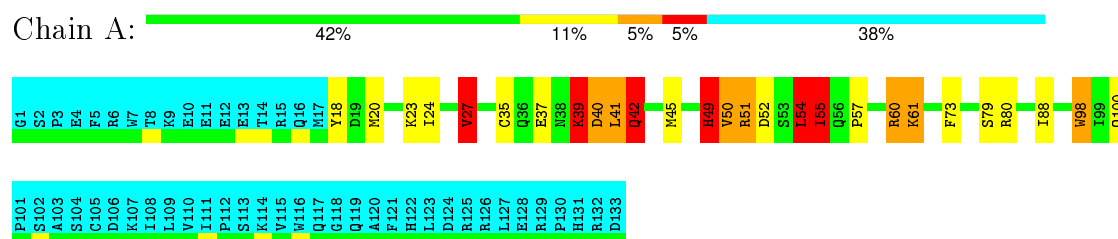
### 4.2.12 Score per residue for model 12

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



### 4.2.13 Score per residue for model 13

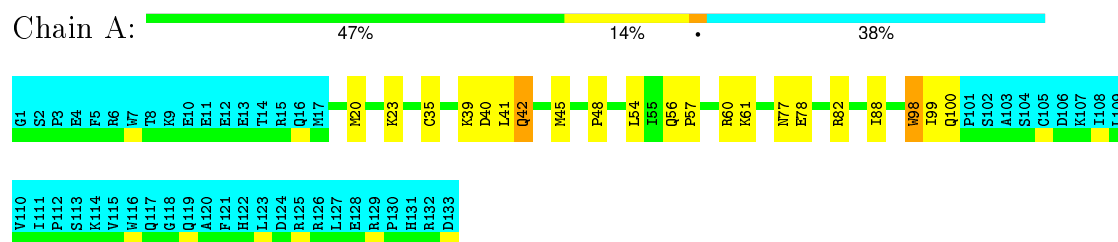
- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1





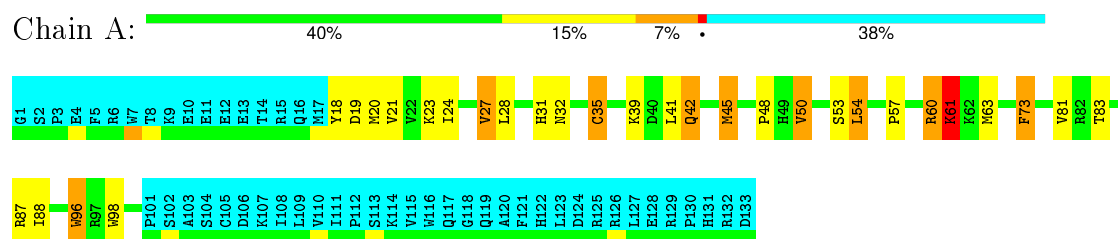
## 4.2.14 Score per residue for model 14

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



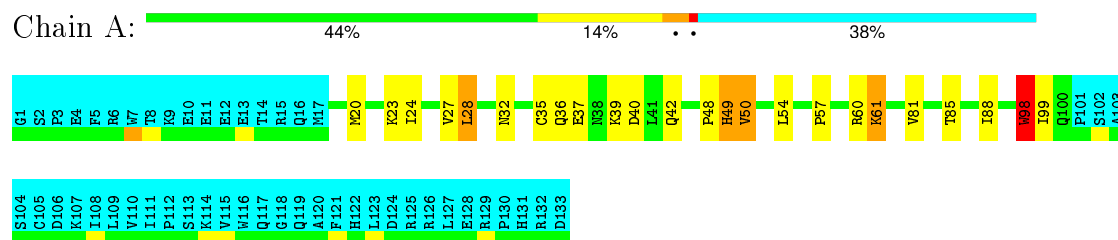
## 4.2.15 Score per residue for model 15

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



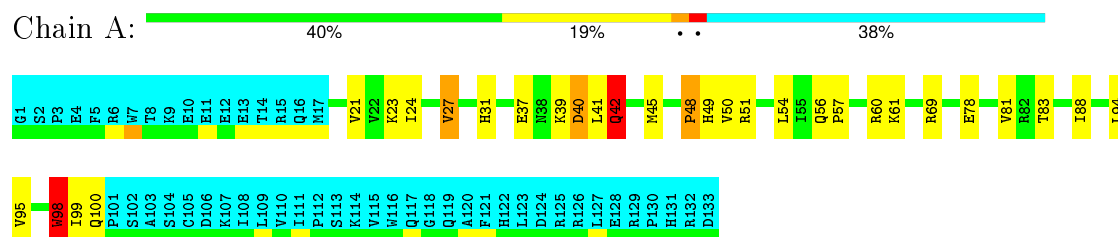
## 4.2.16 Score per residue for model 16

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



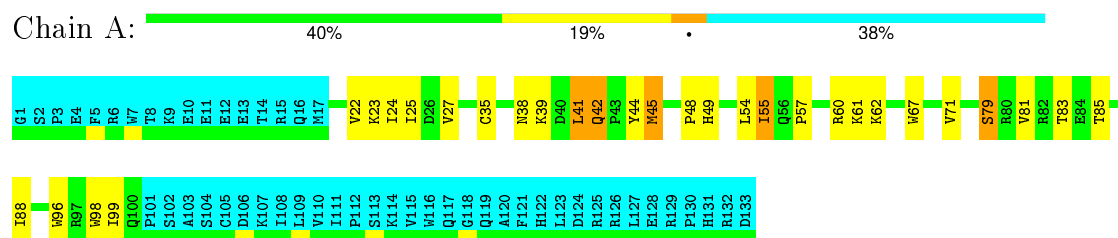
## 4.2.17 Score per residue for model 17

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



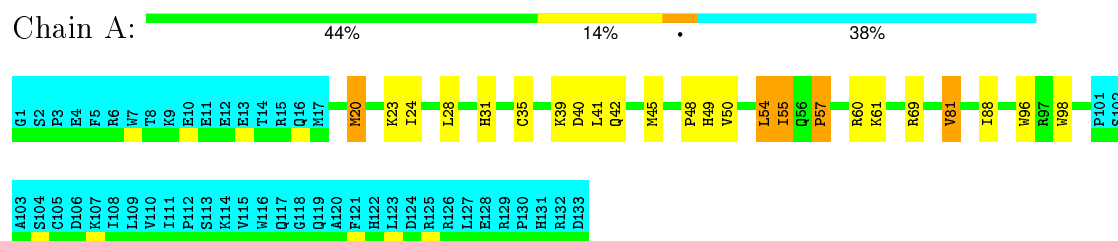
### 4.2.18 Score per residue for model 18

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



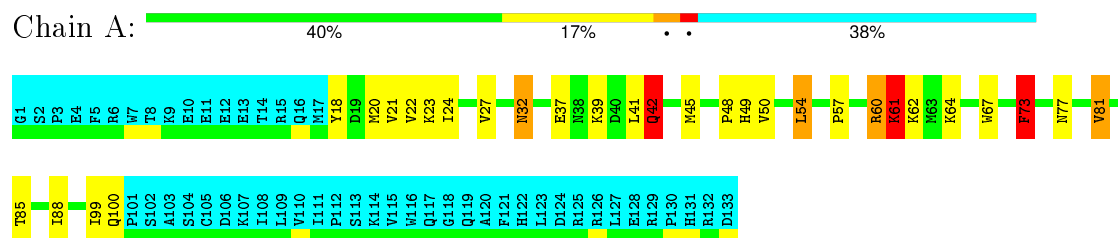
### 4.2.19 Score per residue for model 19

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



### 4.2.20 Score per residue for model 20

- Molecule 1: INNER NUCLEAR MEMBRANE PROTEIN MAN1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *BACK CALCULATED DATA AGREE WITH EXPERIMENTAL NOESY SPECTRUM, STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY, STRUCTURES WITH FAVORABLE NON-BOND ENERGY, STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS, STRUCTURES WITH THE LOWEST ENERGY*.

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

Software name	Classification	Version
CNS 1.0	refinement	
XWINNMR 2.5	structure solution	
NMRPIPE 2.0	structure solution	
FELIX 2000.1	structure solution	
CNS 1.0	structure solution	

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 6919
Number of chemical shift lists	1
Total number of shifts	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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

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	1.14±0.02	0±0/715 (0.0±0.0%)	1.62±0.06	10±3/968 (1.1±0.3%)
All	All	1.15	0/14300 (0.0%)	1.62	206/19360 (1.1%)

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	0.1±0.3	1.1±1.2
All	All	2	23

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	98	TRP	CB-CG-CD2	-17.75	103.52	126.60	2	6
1	A	18	TYR	CB-CG-CD1	9.55	126.73	121.00	8	2
1	A	98	TRP	CB-CG-CD1	-9.47	114.69	127.00	6	4
1	A	73	PHE	CB-CG-CD1	9.22	127.26	120.80	20	3
1	A	35	CYS	CA-CB-SG	8.81	129.86	114.00	3	3
1	A	20	MET	CG-SD-CE	8.80	114.28	100.20	5	2
1	A	61	LYS	CB-CA-C	8.42	127.24	110.40	5	16
1	A	27	VAL	CA-CB-CG2	8.06	122.99	110.90	7	6
1	A	41	LEU	C-N-CA	7.92	141.51	121.70	10	15
1	A	18	TYR	CB-CG-CD2	-7.69	116.39	121.00	8	2
1	A	18	TYR	N-CA-C	7.42	131.05	111.00	3	4
1	A	73	PHE	CB-CG-CD2	-7.34	115.66	120.80	10	2
1	A	54	LEU	CB-CG-CD2	7.33	123.46	111.00	20	8
1	A	27	VAL	CA-CB-CG1	7.30	121.85	110.90	8	6
1	A	44	TYR	N-CA-CB	-7.27	97.51	110.60	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	40	ASP	N-CA-C	-7.20	91.57	111.00	17	2
1	A	49	HIS	N-CA-CB	7.09	123.36	110.60	4	1
1	A	79	SER	N-CA-CB	7.06	121.08	110.50	18	1
1	A	45	MET	CG-SD-CE	6.94	111.30	100.20	13	2
1	A	54	LEU	CB-CA-C	-6.88	97.14	110.20	9	1
1	A	81	VAL	CA-CB-CG2	6.74	121.01	110.90	20	1
1	A	44	TYR	CB-CG-CD1	-6.70	116.98	121.00	9	1
1	A	52	ASP	C-N-CA	6.56	138.10	121.70	11	3
1	A	63	MET	N-CA-CB	6.45	122.21	110.60	6	2
1	A	48	PRO	N-CA-CB	6.38	110.96	103.30	1	13
1	A	42	GLN	CA-C-N	6.37	134.94	117.10	12	6
1	A	49	HIS	CA-CB-CG	6.32	124.35	113.60	6	3
1	A	48	PRO	CA-C-N	6.31	131.07	117.20	15	10
1	A	55	ILE	CA-CB-CG1	6.29	122.95	111.00	13	7
1	A	38	ASN	C-N-CA	6.28	137.40	121.70	4	6
1	A	40	ASP	C-N-CA	6.24	137.30	121.70	10	2
1	A	54	LEU	CA-CB-CG	6.17	129.50	115.30	11	2
1	A	98	TRP	N-CA-C	6.17	127.66	111.00	12	4
1	A	27	VAL	CG1-CB-CG2	-6.16	101.05	110.90	8	3
1	A	45	MET	CA-CB-CG	6.15	123.76	113.30	5	2
1	A	54	LEU	N-CA-CB	5.99	122.39	110.40	13	2
1	A	21	VAL	CB-CA-C	5.96	122.72	111.40	1	1
1	A	31	HIS	CA-CB-CG	5.95	123.71	113.60	1	1
1	A	48	PRO	CB-CA-C	5.80	126.51	112.00	19	7
1	A	40	ASP	CB-CA-C	5.75	121.91	110.40	4	1
1	A	42	GLN	N-CA-CB	5.75	120.94	110.60	15	1
1	A	53	SER	CB-CA-C	-5.66	99.34	110.10	2	1
1	A	93	PHE	CB-CG-CD1	5.64	124.75	120.80	10	2
1	A	98	TRP	CG-CD2-CE3	-5.63	128.83	133.90	2	2
1	A	31	HIS	C-N-CA	5.63	135.78	121.70	8	1
1	A	50	VAL	CA-CB-CG2	5.58	119.26	110.90	7	1
1	A	100	GLN	N-CA-CB	5.54	120.57	110.60	4	1
1	A	36	GLN	CB-CG-CD	5.54	125.99	111.60	11	1
1	A	51	ARG	CB-CG-CD	5.50	125.91	111.60	9	1
1	A	98	TRP	CE2-CD2-CG	-5.47	102.92	107.30	2	1
1	A	71	VAL	CG1-CB-CG2	-5.43	102.21	110.90	7	1
1	A	50	VAL	CB-CA-C	5.42	121.69	111.40	5	2
1	A	27	VAL	N-CA-CB	5.41	123.41	111.50	4	2
1	A	74	LEU	CB-CA-C	-5.41	99.93	110.20	1	1
1	A	42	GLN	CB-CA-C	5.36	121.11	110.40	14	1
1	A	64	LYS	N-CA-CB	5.33	120.20	110.60	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	ALA	CB-CA-C	5.27	118.01	110.10	1	1
1	A	96	TRP	CB-CG-CD2	-5.22	119.82	126.60	11	1
1	A	45	MET	CA-C-N	5.17	131.58	117.10	15	2
1	A	54	LEU	C-N-CA	5.17	134.62	121.70	5	1
1	A	48	PRO	O-C-N	-5.16	114.45	122.70	3	1
1	A	42	GLN	CA-C-O	-5.15	109.28	120.10	12	2
1	A	32	ASN	CB-CA-C	5.13	120.67	110.40	20	1
1	A	71	VAL	CA-CB-CG1	5.13	118.59	110.90	7	2
1	A	44	TYR	CB-CG-CD2	5.11	124.07	121.00	9	1
1	A	55	ILE	N-CA-CB	5.11	122.55	110.80	11	1
1	A	27	VAL	CB-CA-C	-5.08	101.75	111.40	7	1
1	A	49	HIS	CB-CA-C	-5.07	100.27	110.40	12	2
1	A	61	LYS	N-CA-CB	5.06	119.72	110.60	3	1
1	A	55	ILE	N-CA-C	-5.05	97.37	111.00	6	3
1	A	74	LEU	CB-CG-CD1	5.01	119.52	111.00	3	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	61	LYS	CA	1
1	A	98	TRP	CA	1

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	44	TYR	Sidechain	5
1	A	18	TYR	Sidechain	5
1	A	49	HIS	Sidechain	5
1	A	42	GLN	Peptide	4
1	A	31	HIS	Sidechain	3
1	A	39	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	698	701	701	6±3
All	All	13960	14020	14020	118

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:HG11	1:A:53:SER:HB3	0.79	1.53	15	2
1:A:81:VAL:HG22	1:A:98:TRP:HB2	0.74	1.60	18	3
1:A:49:HIS:CE1	1:A:50:VAL:HG12	0.72	2.19	6	2
1:A:81:VAL:HG12	1:A:98:TRP:HB3	0.70	1.63	17	4
1:A:27:VAL:HG21	1:A:50:VAL:HB	0.66	1.67	16	3
1:A:51:ARG:O	1:A:54:LEU:HD22	0.65	1.91	10	4
1:A:49:HIS:CE1	1:A:50:VAL:CG1	0.64	2.79	7	2
1:A:24:ILE:HD11	1:A:54:LEU:HA	0.63	1.70	8	1
1:A:81:VAL:HG22	1:A:98:TRP:CB	0.60	2.25	18	3
1:A:31:HIS:CE1	1:A:42:GLN:HB2	0.60	2.31	8	1
1:A:24:ILE:O	1:A:27:VAL:HG22	0.57	1.98	16	5
1:A:54:LEU:HD21	1:A:60:ARG:O	0.57	2.00	6	3
1:A:51:ARG:HA	1:A:54:LEU:HD22	0.56	1.77	6	1
1:A:81:VAL:HG13	1:A:98:TRP:CE3	0.54	2.37	15	1
1:A:45:MET:HB3	1:A:49:HIS:CG	0.54	2.37	7	2
1:A:50:VAL:HG13	1:A:96:TRP:CZ3	0.53	2.39	8	2
1:A:24:ILE:HG21	1:A:67:TRP:CH2	0.52	2.39	6	4
1:A:60:ARG:HD3	1:A:61:LYS:H	0.52	1.65	4	4
1:A:18:TYR:CD1	1:A:73:PHE:CD2	0.52	2.98	20	1
1:A:24:ILE:HG21	1:A:67:TRP:CZ3	0.51	2.41	20	1
1:A:54:LEU:HD22	1:A:54:LEU:H	0.51	1.66	8	1
1:A:35:CYS:SG	1:A:100:GLN:HB3	0.51	2.46	10	1
1:A:81:VAL:HG12	1:A:96:TRP:CD1	0.51	2.41	3	1
1:A:54:LEU:O	1:A:55:ILE:HD13	0.50	2.07	3	1
1:A:81:VAL:HG23	1:A:98:TRP:CE3	0.50	2.41	19	1
1:A:81:VAL:HG12	1:A:98:TRP:CG	0.49	2.42	2	2
1:A:24:ILE:HG21	1:A:67:TRP:CZ2	0.49	2.42	18	1
1:A:35:CYS:HB2	1:A:98:TRP:CZ2	0.49	2.42	2	1
1:A:51:ARG:HG2	1:A:67:TRP:CD1	0.49	2.42	5	1
1:A:81:VAL:HA	1:A:98:TRP:HB3	0.49	1.84	4	4
1:A:67:TRP:CE2	1:A:71:VAL:CG2	0.49	2.96	4	2
1:A:24:ILE:O	1:A:27:VAL:HG12	0.48	2.08	13	2
1:A:31:HIS:O	1:A:35:CYS:HB2	0.47	2.10	15	2
1:A:67:TRP:O	1:A:71:VAL:HG23	0.47	2.09	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TYR:CE1	1:A:73:PHE:CG	0.47	3.03	20	1
1:A:45:MET:SD	1:A:81:VAL:HG11	0.47	2.50	12	1
1:A:49:HIS:CD2	1:A:50:VAL:HG12	0.46	2.45	8	2
1:A:45:MET:SD	1:A:49:HIS:CD2	0.46	3.08	18	1
1:A:81:VAL:HG13	1:A:98:TRP:CH2	0.46	2.45	8	1
1:A:81:VAL:CG2	1:A:98:TRP:CE3	0.46	2.99	16	2
1:A:81:VAL:CG1	1:A:98:TRP:CE3	0.45	3.00	15	1
1:A:24:ILE:HG21	1:A:67:TRP:HH2	0.45	1.70	6	1
1:A:28:LEU:HA	1:A:31:HIS:CE1	0.45	2.45	2	1
1:A:24:ILE:HD12	1:A:51:ARG:HH11	0.45	1.71	11	1
1:A:61:LYS:HA	1:A:64:LYS:HB3	0.45	1.87	4	3
1:A:27:VAL:HG23	1:A:28:LEU:HD13	0.45	1.87	6	2
1:A:35:CYS:HB2	1:A:100:GLN:HG3	0.44	1.87	9	1
1:A:81:VAL:HG13	1:A:97:ARG:C	0.44	2.32	3	1
1:A:54:LEU:HD23	1:A:60:ARG:O	0.44	2.12	9	1
1:A:51:ARG:HG3	1:A:54:LEU:HD12	0.44	1.89	11	1
1:A:35:CYS:SG	1:A:100:GLN:HG3	0.44	2.52	9	1
1:A:27:VAL:HG13	1:A:28:LEU:HD13	0.44	1.88	8	1
1:A:32:ASN:ND2	1:A:98:TRP:CE2	0.43	2.83	15	1
1:A:45:MET:CB	1:A:49:HIS:CD2	0.43	3.02	7	1
1:A:81:VAL:HG12	1:A:98:TRP:CB	0.43	2.44	6	1
1:A:41:LEU:CD1	1:A:41:LEU:H	0.43	2.27	9	1
1:A:31:HIS:HB2	1:A:98:TRP:CZ2	0.42	2.49	1	1
1:A:51:ARG:O	1:A:64:LYS:HB2	0.42	2.14	2	1
1:A:81:VAL:HG23	1:A:98:TRP:CD2	0.42	2.49	19	1
1:A:42:GLN:CB	1:A:98:TRP:CZ3	0.42	3.03	17	1
1:A:35:CYS:HB2	1:A:100:GLN:HB3	0.41	1.91	5	1
1:A:80:ARG:O	1:A:98:TRP:CZ3	0.41	2.73	13	1
1:A:27:VAL:HG11	1:A:53:SER:CB	0.41	2.42	4	1
1:A:54:LEU:C	1:A:55:ILE:HD13	0.41	2.36	12	2
1:A:81:VAL:HG12	1:A:98:TRP:HB2	0.41	1.93	6	1
1:A:67:TRP:CZ2	1:A:71:VAL:HG22	0.41	2.51	18	1
1:A:35:CYS:SG	1:A:98:TRP:CZ2	0.41	3.14	3	1
1:A:32:ASN:ND2	1:A:98:TRP:CZ2	0.41	2.89	8	1
1:A:48:PRO:O	1:A:51:ARG:HB3	0.41	2.16	17	1
1:A:35:CYS:HA	1:A:41:LEU:HD23	0.41	1.93	8	1
1:A:27:VAL:HG11	1:A:50:VAL:HB	0.41	1.92	13	1
1:A:44:TYR:CE2	1:A:95:VAL:HG11	0.41	2.51	11	1
1:A:35:CYS:SG	1:A:98:TRP:CD1	0.40	3.07	1	1
1:A:81:VAL:CG1	1:A:98:TRP:CG	0.40	3.04	2	1
1:A:18:TYR:N	1:A:18:TYR:CD1	0.40	2.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:MET:CE	1:A:49:HIS:CE1	0.40	3.04	7	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	83/133 (62%)	73±2 (88±2%)	7±1 (9±2%)	3±1 (3±1%)	8	38
All	All	1660/2660 (62%)	1457 (88%)	147 (9%)	56 (3%)	8	38

All 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	42	GLN	20
1	A	57	PRO	20
1	A	78	GLU	6
1	A	19	ASP	4
1	A	39	LYS	3
1	A	41	LEU	1
1	A	40	ASP	1
1	A	79	SER	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	76/122 (62%)	58±3 (76±4%)	18±3 (24±4%)	3	28
All	All	1520/2440 (62%)	1154 (76%)	366 (24%)	3	28

All 57 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	39	LYS	20
1	A	54	LEU	20
1	A	60	ARG	20
1	A	88	ILE	20
1	A	23	LYS	17
1	A	20	MET	16
1	A	45	MET	11
1	A	85	THR	11
1	A	98	TRP	11
1	A	40	ASP	11
1	A	50	VAL	10
1	A	55	ILE	10
1	A	61	LYS	10
1	A	96	TRP	9
1	A	99	ILE	9
1	A	35	CYS	9
1	A	100	GLN	9
1	A	83	THR	9
1	A	37	GLU	8
1	A	42	GLN	8
1	A	41	LEU	8
1	A	49	HIS	8
1	A	28	LEU	8
1	A	21	VAL	7
1	A	51	ARG	6
1	A	77	ASN	5
1	A	81	VAL	5
1	A	56	GLN	4
1	A	24	ILE	4
1	A	73	PHE	4
1	A	18	TYR	4
1	A	36	GLN	4
1	A	69	ARG	4
1	A	27	VAL	4
1	A	94	LEU	3
1	A	25	ILE	3
1	A	32	ASN	3
1	A	74	LEU	3
1	A	82	ARG	2
1	A	65	LYS	2
1	A	57	PRO	2

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Mol	Chain	Res	Type	Models (Total)
1	A	80	ARG	2
1	A	86	ARG	2
1	A	22	VAL	2
1	A	62	LYS	2
1	A	64	LYS	2
1	A	95	VAL	2
1	A	97	ARG	2
1	A	30	SER	2
1	A	87	ARG	2
1	A	31	HIS	1
1	A	38	ASN	1
1	A	79	SER	1
1	A	47	ILE	1
1	A	33	GLU	1
1	A	84	GLU	1
1	A	92	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 61% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6919

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	95	$-0.31 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	87	$0.21 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	90	$-0.18 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	89	$0.17 \pm 0.52$	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 77%, i.e. 869 atoms were assigned a chemical shift out of a possible 1126. 12 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	366/407 (90%)	148/162 (91%)	148/166 (89%)	70/79 (89%)
Sidechain	448/628 (71%)	283/370 (76%)	159/218 (73%)	6/40 (15%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	55/91 (60%)	29/48 (60%)	23/37 (62%)	3/6 (50%)
Overall	869/1126 (77%)	460/580 (79%)	330/421 (78%)	79/125 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 1091 atoms were assigned a chemical shift out of a possible 1801. 12 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	461/649 (71%)	187/258 (72%)	185/266 (70%)	89/125 (71%)
Sidechain	563/1005 (56%)	360/596 (60%)	197/345 (57%)	6/64 (9%)
Aromatic	67/147 (46%)	36/78 (46%)	27/59 (46%)	4/10 (40%)
Overall	1091/1801 (61%)	583/932 (63%)	409/670 (61%)	99/199 (50%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	96	TRP	CZ3	131.45	129.20 – 113.60	6.4
1	A	47	ILE	HG12	-1.23	3.27 – -0.73	-6.2
1	A	67	TRP	CZ3	113.32	129.20 – 113.60	-5.2

#### 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:

