



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:57 AM BST

PDB ID : 2M0G  
Title : Structure, phosphorylation and U2AF65 binding of the Nterminal Domain of splicing factor 1 during 3 splice site Recognition  
Authors : Madl, T.; Sattler, M.; Zhang, Y.; Bagdiul, I.; Kern, T.; Kang, H.; Zou, P.; Maeusbacher, N.; Sieber, S.A.; Kraemer, A.  
Deposited on : 2012-10-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
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

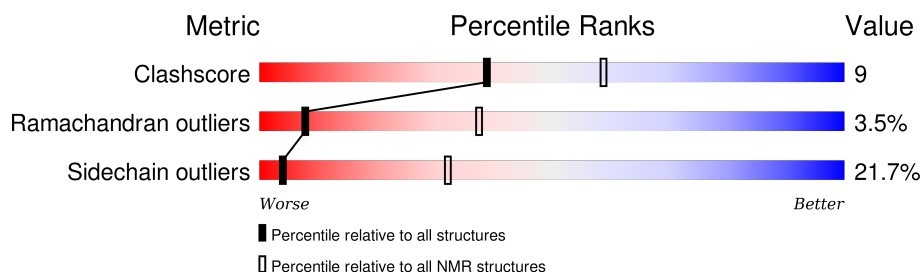
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 34%.

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	145	
2	B	104	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 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:12-A:26, B:374-B:474 (116)	0.07	1
2	A:44-A:70, A:96-A:129 (61)	0.07	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 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 5, 7, 8
2	1, 6, 10
Single-model clusters	9

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4004 atoms, of which 1999 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Splicing factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	145	Total	C	H	N	O	S	0
			2355	727	1187	214	221	6	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	CYS	SER	ENGINEERED MUTATION	UNP Q15637

- Molecule 2 is a protein called Splicing factor U2AF 65 kDa subunit.

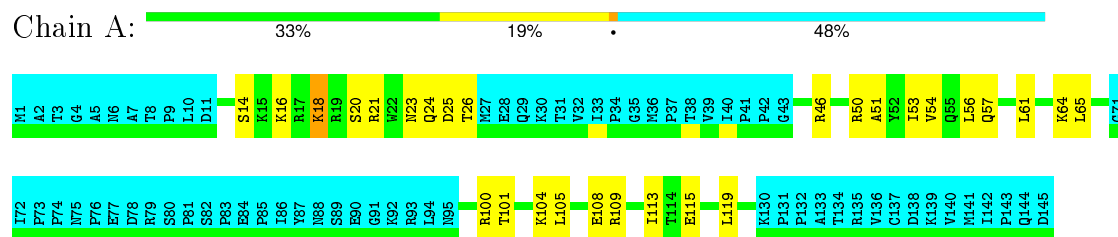
Mol	Chain	Residues	Atoms						Trace
2	B	104	Total	C	H	N	O	S	0
			1649	529	812	137	163	8	

## 4 Residue-property plots

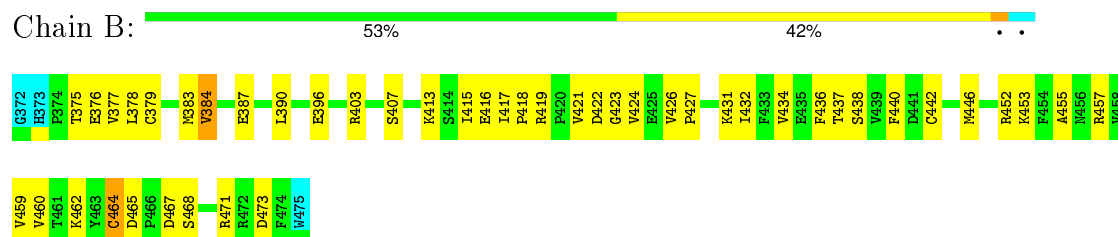
### 4.1 Average score per residue in the NMR ensemble

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: Splicing factor 1



- Molecule 2: Splicing factor U2AF 65 kDa subunit

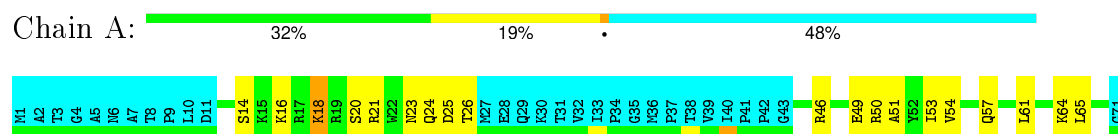


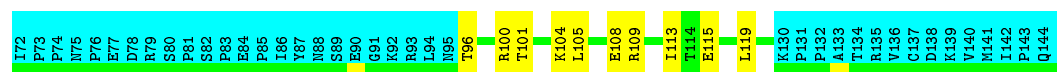
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Splicing factor 1





### • Molecule 2: Splicing factor U2AF 65 kDa subunit

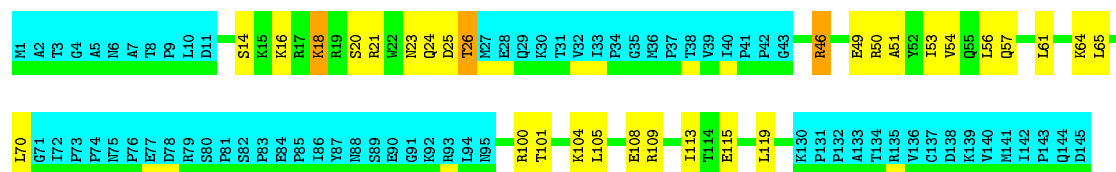
Chain B: 55% 40%



## 4.2.2 Score per residue for model 2

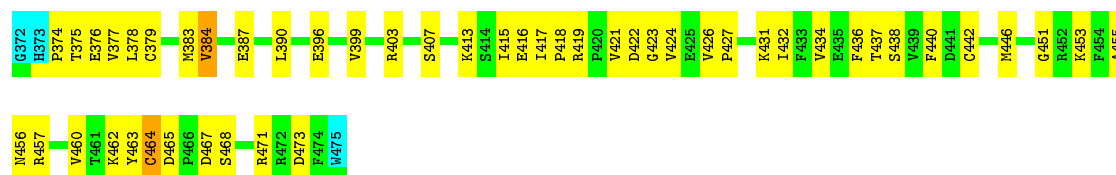
### • Molecule 1: Splicing factor 1

Chain A: 32% 19% 48%



### • Molecule 2: Splicing factor U2AF 65 kDa subunit

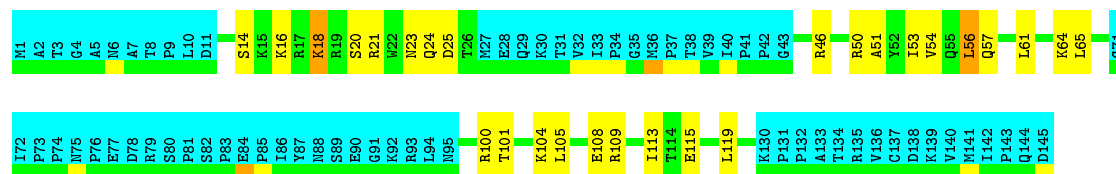
Chain B: 50% 45%



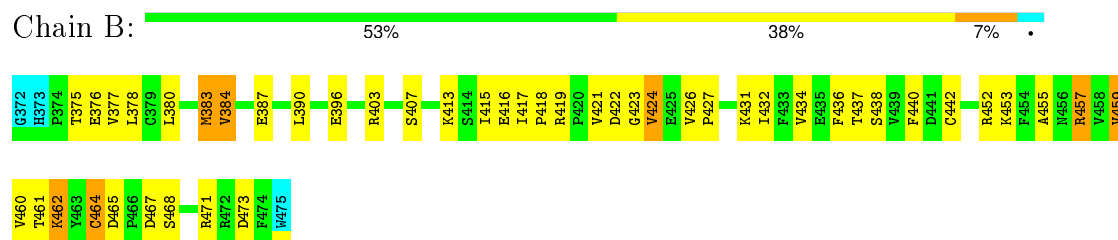
## 4.2.3 Score per residue for model 3

### • Molecule 1: Splicing factor 1

Chain A: 34% 17% 48%

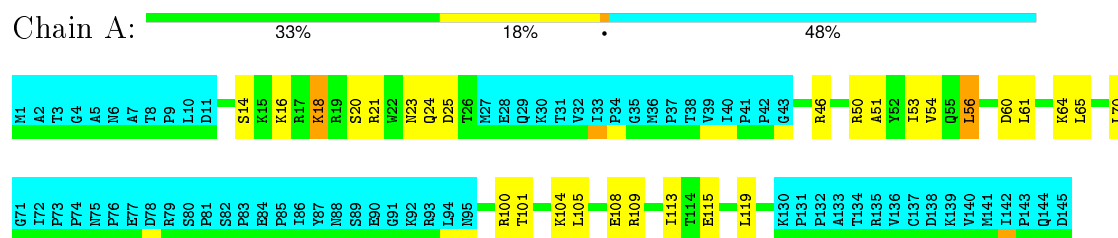


### • Molecule 2: Splicing factor U2AF 65 kDa subunit

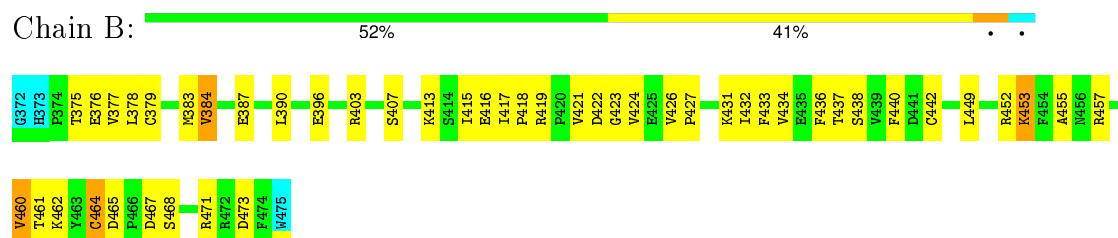


#### 4.2.4 Score per residue for model 4

- Molecule 1: Splicing factor 1

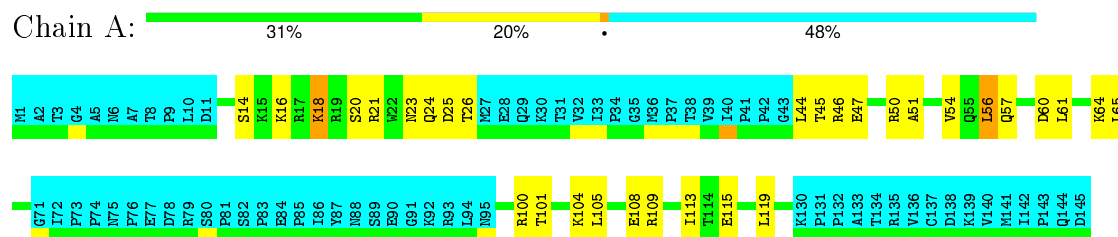


- Molecule 2: Splicing factor U2AF 65 kDa subunit

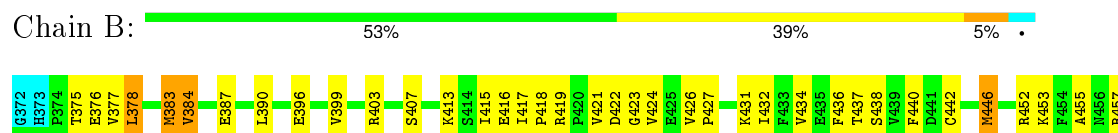


#### 4.2.5 Score per residue for model 5

- Molecule 1: Splicing factor 1



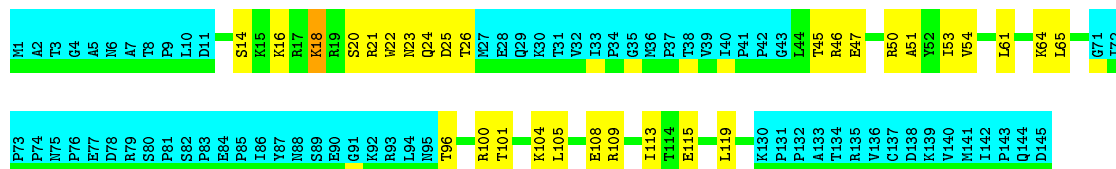
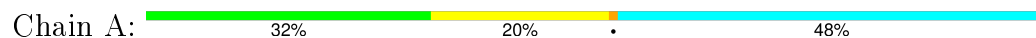
- Molecule 2: Splicing factor U2AF 65 kDa subunit



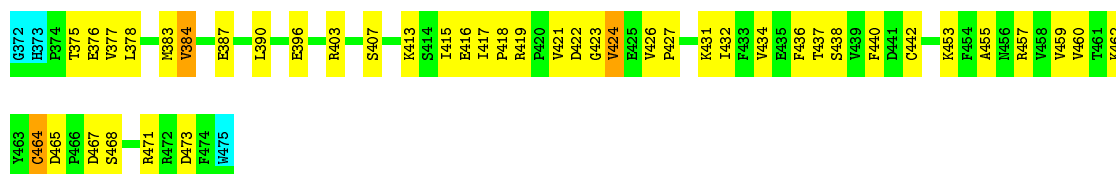


#### 4.2.6 Score per residue for model 6

- Molecule 1: Splicing factor 1

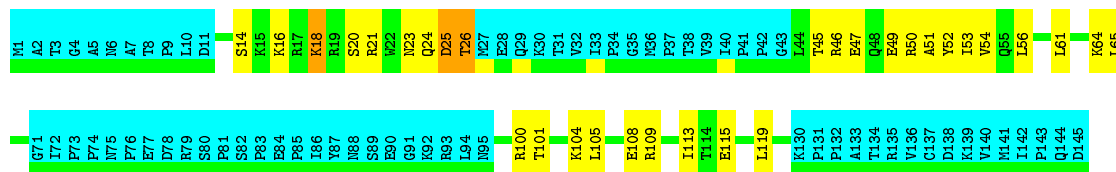
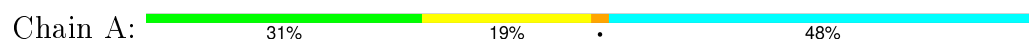


- Molecule 2: Splicing factor U2AF 65 kDa subunit

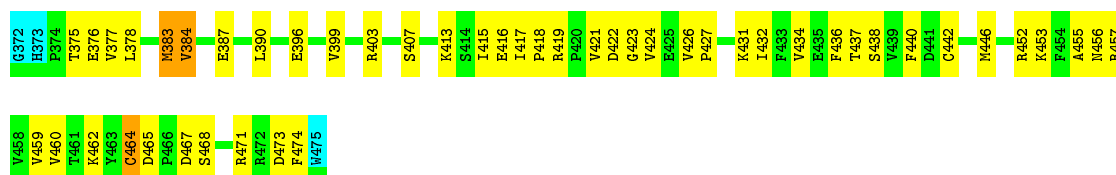


#### 4.2.7 Score per residue for model 7

- Molecule 1: Splicing factor 1

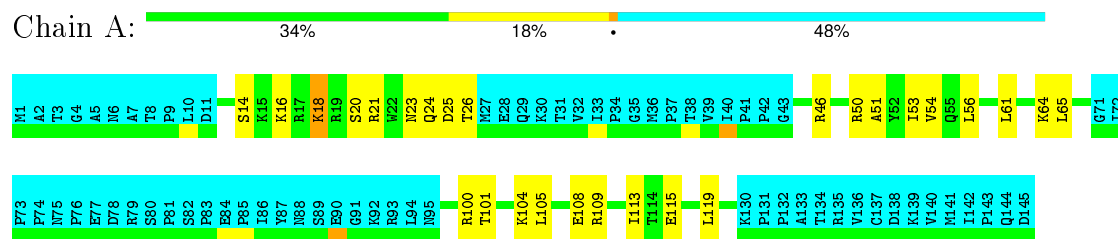


- Molecule 2: Splicing factor U2AF 65 kDa subunit

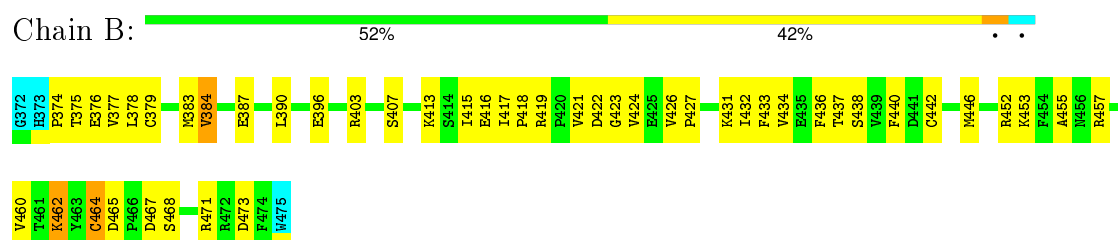


### 4.2.8 Score per residue for model 8

- Molecule 1: Splicing factor 1

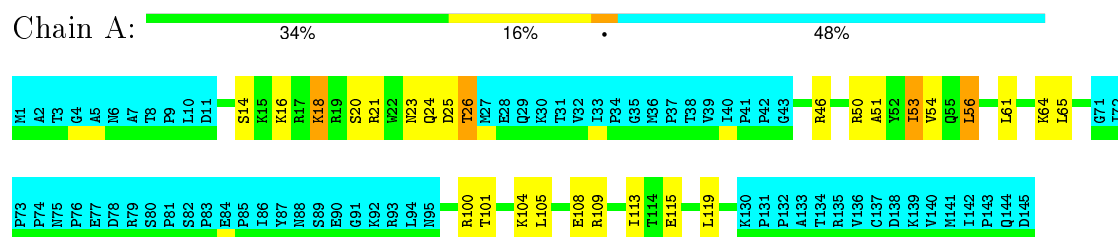


- Molecule 2: Splicing factor U2AF 65 kDa subunit

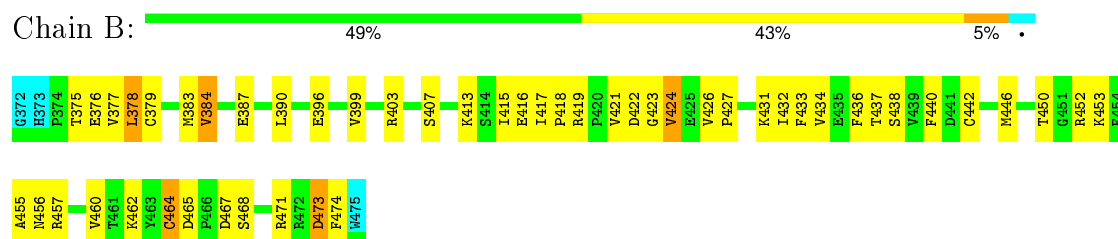


### 4.2.9 Score per residue for model 9

- Molecule 1: Splicing factor 1

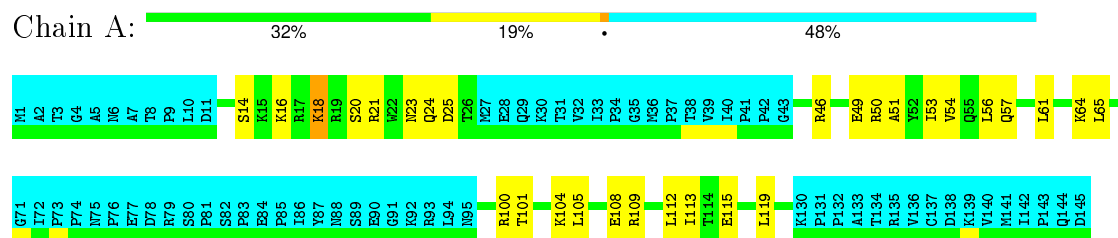


- Molecule 2: Splicing factor U2AF 65 kDa subunit

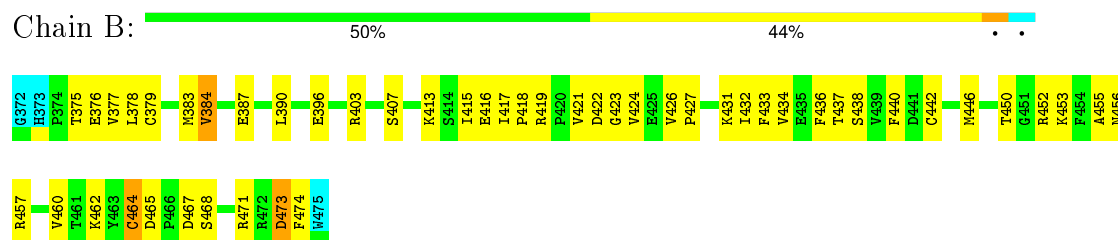


### 4.2.10 Score per residue for model 10

- Molecule 1: Splicing factor 1



● Molecule 2: Splicing factor U2AF 65 kDa subunit



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
ARIA	structure solution	2.1
CYANA	structure solution	3.0
ARIA	refinement	2.1
CYANA	refinement	3.0

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)	2m0g_cs.str
Number of chemical shift lists	1
Total number of shifts	1253
Number of shifts mapped to atoms	1253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

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	655	668	667	10±1
2	B	808	789	788	18±1
All	All	14630	14570	14550	276

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:417:ILE:HG23	2:B:432:ILE:HG21	0.85	1.48	10	10
2:B:417:ILE:HG23	2:B:432:ILE:CG2	0.69	2.18	6	10
2:B:426:VAL:N	2:B:427:PRO:HD2	0.62	2.09	6	10
2:B:383:MET:HB3	2:B:459:VAL:HG12	0.61	1.70	5	3
1:A:101:THR:O	1:A:105:LEU:HG	0.61	1.96	9	10
1:A:53:ILE:O	1:A:56:LEU:HG	0.59	1.98	2	3
1:A:53:ILE:HG12	2:B:460:VAL:HG22	0.58	1.75	9	1
1:A:53:ILE:HA	1:A:56:LEU:HD23	0.56	1.76	9	3
1:A:53:ILE:HG23	2:B:460:VAL:HG21	0.54	1.80	10	4
2:B:384:VAL:HG21	2:B:432:ILE:HG23	0.54	1.80	8	10
2:B:426:VAL:N	2:B:427:PRO:CD	0.54	2.71	1	10
1:A:53:ILE:O	1:A:57:GLN:HG2	0.52	2.04	2	1
2:B:449:LEU:HB2	2:B:461:THR:HG21	0.52	1.82	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:THR:HB	1:A:47:GLU:OE1	0.51	2.05	6	3
1:A:115:GLU:O	1:A:119:LEU:HG	0.51	2.06	8	10
1:A:46:ARG:O	1:A:49:GLU:HG2	0.51	2.06	2	1
1:A:56:LEU:HG	1:A:57:GLN:N	0.51	2.20	5	2
2:B:413:LYS:HG3	2:B:437:THR:HG22	0.50	1.84	1	10
2:B:446:MET:O	2:B:450:THR:HG23	0.48	2.08	10	2
2:B:377:VAL:HG22	2:B:464:CYS:O	0.47	2.10	9	10
2:B:423:GLY:HA2	2:B:426:VAL:HG23	0.46	1.88	5	10
1:A:50:ARG:O	1:A:54:VAL:HG22	0.46	2.11	4	10
2:B:449:LEU:CB	2:B:461:THR:HG21	0.46	2.41	4	1
2:B:417:ILE:HG12	2:B:432:ILE:HB	0.46	1.88	9	10
1:A:22:TRP:CZ3	2:B:459:VAL:HG11	0.45	2.46	6	1
2:B:417:ILE:CD1	2:B:432:ILE:HD12	0.45	2.41	2	10
2:B:418:PRO:HD2	2:B:432:ILE:HG22	0.45	1.89	5	10
1:A:109:ARG:O	1:A:113:ILE:HG12	0.45	2.12	6	10
1:A:51:ALA:HA	1:A:54:VAL:HG22	0.45	1.89	3	10
2:B:417:ILE:HG12	2:B:432:ILE:HD12	0.44	1.90	4	10
1:A:61:LEU:O	1:A:64:LYS:HB3	0.44	2.13	5	10
2:B:473:ASP:O	2:B:474:PHE:HB2	0.44	2.13	10	2
1:A:25:ASP:O	1:A:26:THR:CB	0.44	2.66	7	1
1:A:100:ARG:O	1:A:104:LYS:HB2	0.42	2.15	3	10
2:B:378:LEU:HD21	2:B:446:MET:HB3	0.42	1.89	5	2
2:B:415:ILE:HG23	2:B:434:VAL:HG12	0.42	1.91	7	10
1:A:25:ASP:O	1:A:26:THR:HB	0.42	2.15	7	1
1:A:104:LYS:O	1:A:108:GLU:HG2	0.42	2.15	3	10
2:B:421:VAL:H	2:B:424:VAL:HB	0.42	1.75	8	10
2:B:446:MET:SD	2:B:463:TYR:CE2	0.42	3.13	2	1
1:A:22:TRP:HZ3	2:B:459:VAL:HG11	0.41	1.75	6	1
2:B:421:VAL:N	2:B:424:VAL:HB	0.41	2.31	8	10
2:B:379:CYS:HA	2:B:433:PHE:HB3	0.41	1.93	9	4
1:A:53:ILE:O	1:A:57:GLN:HG3	0.41	2.16	1	1
1:A:57:GLN:HB3	1:A:112:LEU:CD1	0.41	2.46	10	1
2:B:379:CYS:HB3	2:B:462:LYS:HG3	0.40	1.93	2	1
2:B:399:VAL:HG22	2:B:417:ILE:HD12	0.40	1.94	2	4
2:B:380:LEU:HD23	2:B:461:THR:HG22	0.40	1.94	3	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	76/145 (52%)	69±1 (91±1%)	4±1 (6±1%)	2±0 (3±1%)	8	40
2	B	101/104 (97%)	89±1 (88±1%)	9±1 (9±1%)	4±0 (4±0%)	7	35
All	All	1770/2490 (71%)	1580 (89%)	128 (7%)	62 (4%)	8	37

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)
2	B	383	MET	10
2	B	455	ALA	10
1	A	24	GLN	10
1	A	18	LYS	10
2	B	376	GLU	10
2	B	452	ARG	8
1	A	96	THR	2
1	A	26	THR	2

### 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	72/132 (55%)	62±1 (86±1%)	10±1 (14±1%)	8	47
2	B	93/95 (98%)	68±1 (73±1%)	25±1 (27±1%)	2	22
All	All	1650/2270 (73%)	1292 (78%)	358 (22%)	4	32

All 47 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)
2	B	387	GLU	10
2	B	390	LEU	10
1	A	14	SER	10
2	B	457	ARG	10
2	B	467	ASP	10
1	A	18	LYS	10
2	B	416	GLU	10
2	B	422	ASP	10
2	B	453	LYS	10
2	B	436	PHE	10
1	A	23	ASN	10
2	B	442	CYS	10
2	B	473	ASP	10
2	B	471	ARG	10
2	B	403	ARG	10
1	A	25	ASP	10
2	B	440	PHE	10
2	B	465	ASP	10
2	B	378	LEU	10
2	B	438	SER	10
1	A	65	LEU	10
2	B	396	GLU	10
1	A	21	ARG	10
2	B	419	ARG	10
2	B	468	SER	10
1	A	20	SER	10
1	A	16	LYS	10
2	B	431	LYS	10
2	B	407	SER	10
1	A	46	ARG	10
2	B	375	THR	10
2	B	464	CYS	10
2	B	384	VAL	10
1	A	56	LEU	5
2	B	462	LYS	4
2	B	446	MET	3
2	B	424	VAL	3
1	A	26	THR	3
1	A	70	LEU	2
2	B	459	VAL	1
1	A	52	TYR	1
2	B	474	PHE	1
1	A	53	ILE	1

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Mol	Chain	Res	Type	Models (Total)
2	B	460	VAL	1
1	A	60	ASP	1
1	A	44	LEU	1
2	B	374	PRO	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](#)

There are no ligands in this entry.

### 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 34% for the well-defined parts and 33% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2m0g\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

#### 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	1253
Number of shifts mapped to atoms	1253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	212	$-0.01 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	160	$0.88 \pm 0.11$	Should be applied
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	197	$-0.13 \pm 0.19$	None needed ( $< 0.5$ ppm)

#### 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 34%, i.e. 796 atoms were assigned a chemical shift out of a possible 2327. 28 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	490/865 (57%)	174/344 (51%)	160/354 (45%)	156/167 (93%)
Sidechain	300/1314 (23%)	98/773 (13%)	196/466 (42%)	6/75 (8%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	6/148 (4%)	5/78 (6%)	0/65 (0%)	1/5 (20%)
Overall	796/2327 (34%)	277/1195 (23%)	356/885 (40%)	163/247 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 1045 atoms were assigned a chemical shift out of a possible 3179. 31 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	645/1197 (54%)	236/474 (50%)	212/498 (43%)	197/225 (88%)
Sidechain	392/1806 (22%)	132/1069 (12%)	250/643 (39%)	10/94 (11%)
Aromatic	8/176 (5%)	6/92 (7%)	0/76 (0%)	2/8 (25%)
Overall	1045/3179 (33%)	374/1635 (23%)	462/1217 (38%)	209/327 (64%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

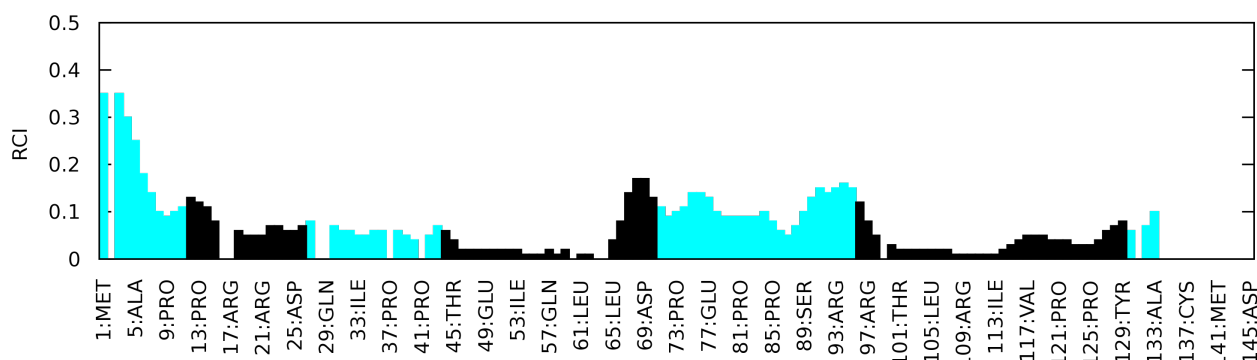
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	382	ASN	HB2	8.88	4.36 – 1.26	19.6

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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:



Random coil index (RCI) for chain B:

