



Full wwPDB NMR Structure Validation Report ⓘ

Nov 29, 2022 – 12:20 pm GMT

PDB ID : 6Z29
BMRB ID : 34517
Title : Structure of eIF4G1 (37-49) - PUB1 RRM3 chimera in solution
Authors : Chaves-Arquero, B.; Martinez-Lumbreras, S.; Perez-Canadillas, J.M.
Deposited on : 2020-05-15

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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 : 2.31.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

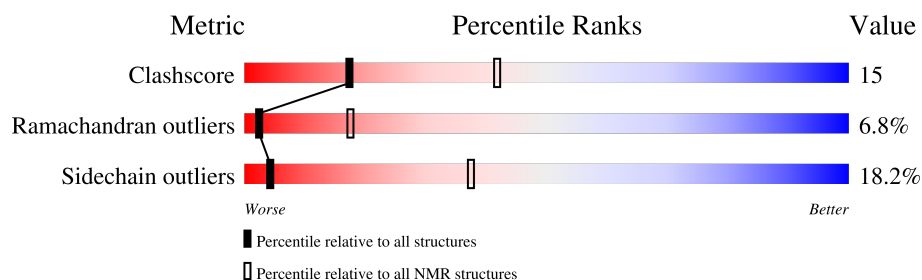
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	116	<div> <div>37%</div> <div>33%</div> <div>•</div> <div>28%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 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:324-A:372, A:378-A:411 (83)	0.42	1

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1812 atoms, of which 891 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1.

Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1812	591	891	162	165	3	

There are 2 discrepancies between the modelled and reference sequences:

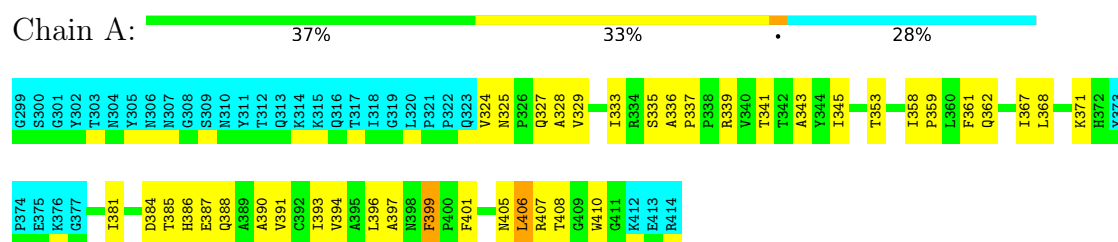
Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLY	-	expression tag	UNP P39935
A	300	SER	-	expression tag	UNP P39935

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

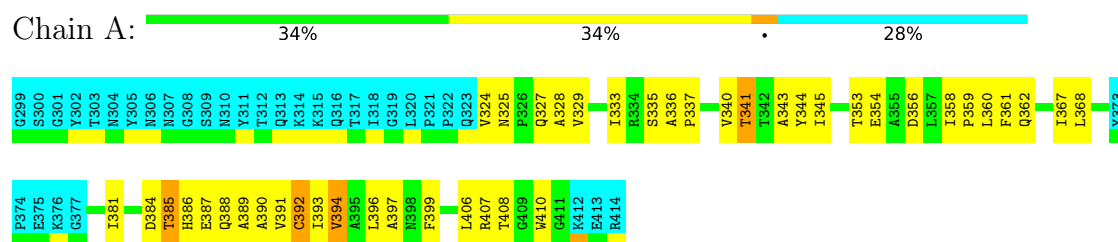


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

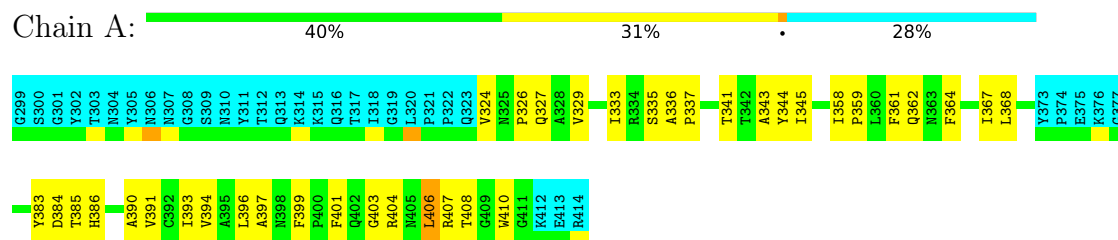
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



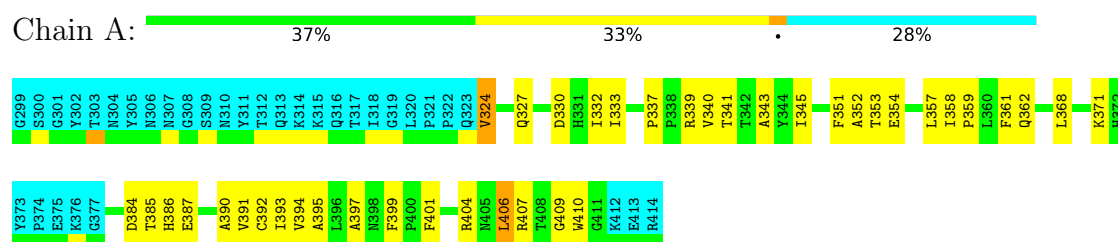
4.2.2 Score per residue for model 2

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



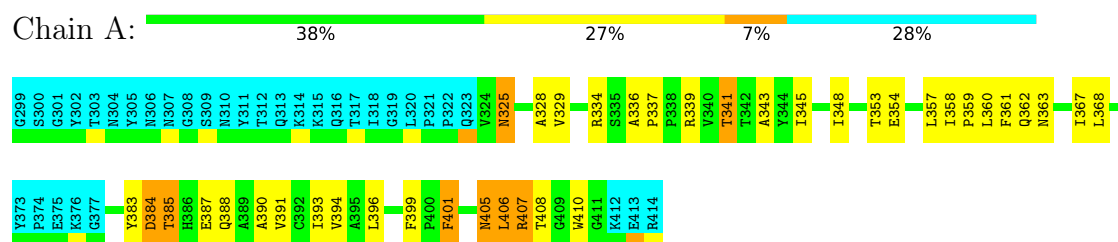
4.2.3 Score per residue for model 3

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



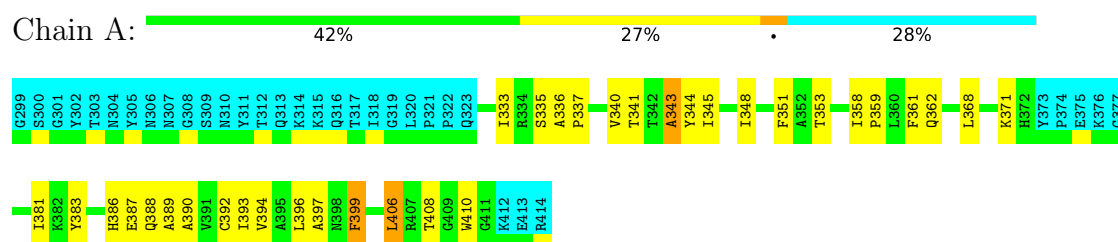
4.2.4 Score per residue for model 4

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



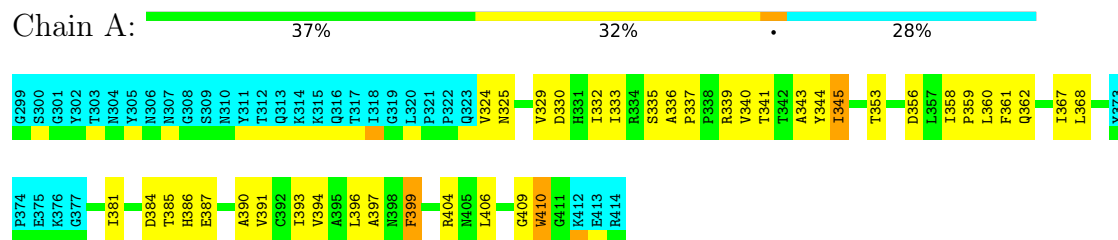
4.2.5 Score per residue for model 5

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



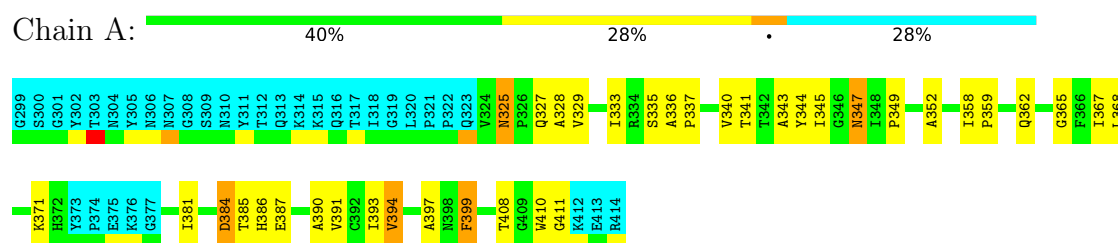
4.2.6 Score per residue for model 6

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



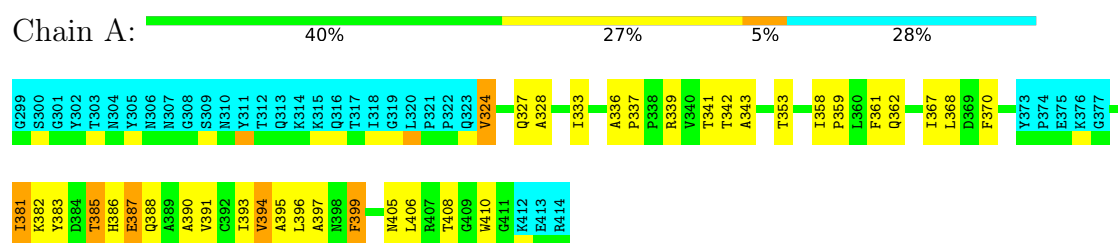
4.2.7 Score per residue for model 7

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



4.2.8 Score per residue for model 8

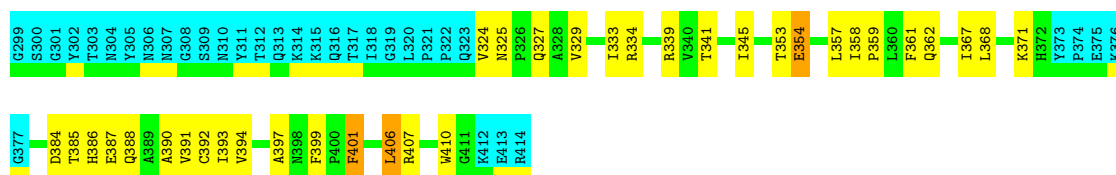
- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



4.2.9 Score per residue for model 9

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

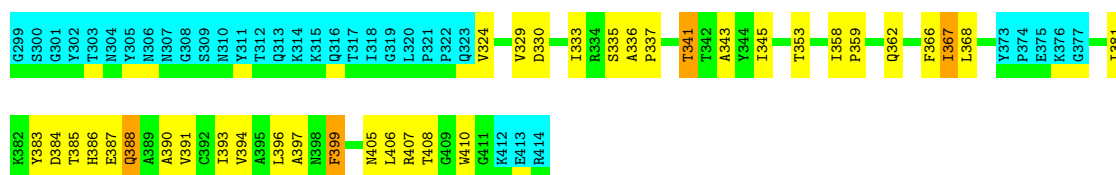




4.2.10 Score per residue for model 10

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

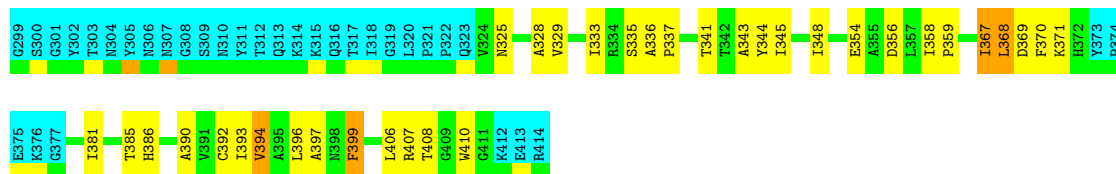
Chain A: 41% 28% 28%



4.2.11 Score per residue for model 11

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

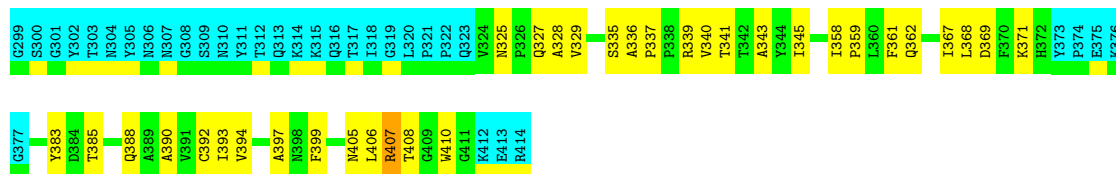
Chain A: 41% 27% 28%



4.2.12 Score per residue for model 12

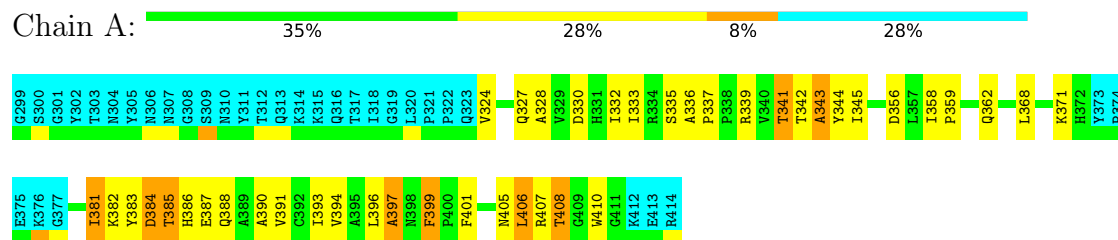
- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

Chain A: 42% 28% 28%



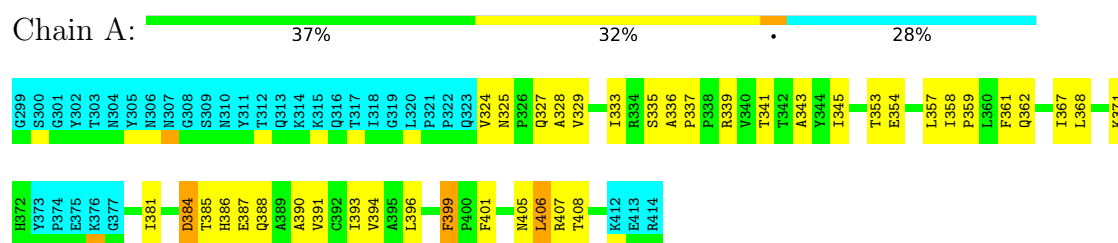
4.2.13 Score per residue for model 13

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



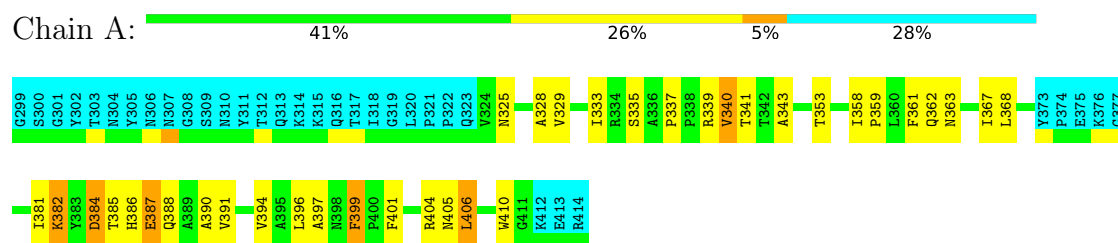
4.2.14 Score per residue for model 14

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



4.2.15 Score per residue for model 15

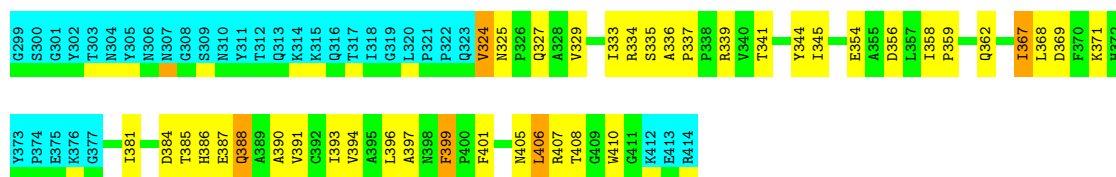
- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



4.2.16 Score per residue for model 16

- Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

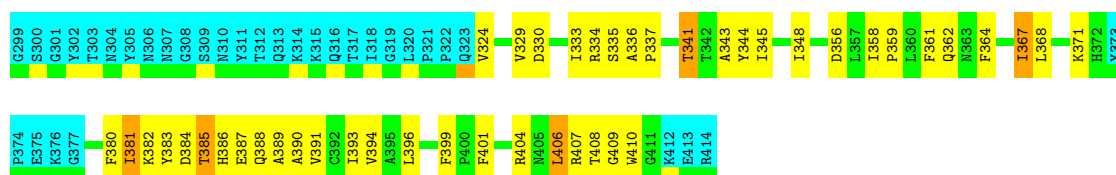




4.2.17 Score per residue for model 17

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

Chain A: 33% 34% 28%



4.2.18 Score per residue for model 18

- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

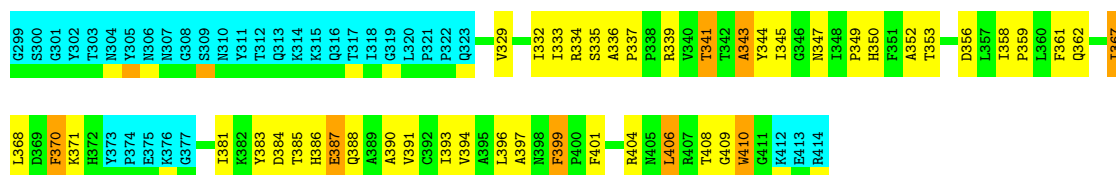
Chain A: 40% 25% 6% 28%



4.2.19 Score per residue for model 19

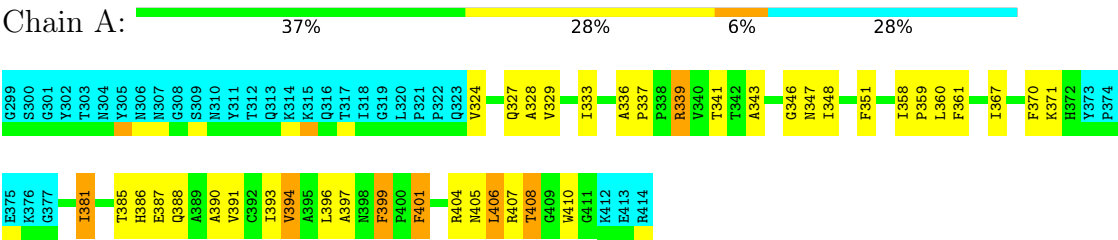
- Molecule 1: Eukaryotic initiation factor 4F subunit p150, Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1

Chain A: 32% 33% 7% 28%



4.2.20 Score per residue for model 20

● Molecule 1: Eukaryotic initiation factor 4F subunit p150,Nuclear and cytoplasmic polyadenylated RNA-binding protein PUB1



5 Refinement protocol and experimental data overview

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

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
CYANA	structure calculation	
Amber	refinement	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1232
Number of shifts mapped to atoms	1232
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	659	641	641	20±4
All	All	13180	12820	12820	396

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:ILE:HG22	1:A:348:ILE:HD11	0.94	1.36	5	4
1:A:324:VAL:HG21	1:A:391:VAL:HG13	0.82	1.52	20	2
1:A:329:VAL:HG22	1:A:394:VAL:HG21	0.76	1.54	15	8
1:A:367:ILE:HG23	1:A:381:ILE:HG23	0.75	1.57	14	5
1:A:360:LEU:HD21	1:A:396:LEU:HD21	0.75	1.58	4	2
1:A:333:ILE:HG23	1:A:386:HIS:CD2	0.68	2.23	2	17
1:A:345:ILE:HG21	1:A:406:LEU:HD23	0.68	1.66	13	1
1:A:328:ALA:O	1:A:394:VAL:HG11	0.67	1.90	7	10
1:A:387:GLU:O	1:A:391:VAL:HG23	0.66	1.91	18	16
1:A:344:TYR:O	1:A:345:ILE:HD13	0.64	1.91	13	7
1:A:325:ASN:O	1:A:329:VAL:HG13	0.63	1.93	16	1
1:A:401:PHE:CB	1:A:406:LEU:HD21	0.63	2.24	15	3
1:A:343:ALA:HB3	1:A:381:ILE:HG12	0.62	1.69	17	1
1:A:368:LEU:HD11	1:A:384:ASP:CA	0.62	2.25	1	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:358:ILE:N	1:A:359:PRO:HD2	0.61	2.11	7	20
1:A:401:PHE:HB2	1:A:406:LEU:HD21	0.61	1.72	20	7
1:A:357:LEU:HD22	1:A:361:PHE:CE1	0.61	2.29	3	1
1:A:396:LEU:HD22	1:A:399:PHE:CG	0.61	2.29	13	9
1:A:390:ALA:HB2	1:A:410:TRP:CZ2	0.61	2.31	11	19
1:A:405:ASN:C	1:A:406:LEU:HD23	0.61	2.17	15	6
1:A:357:LEU:HD22	1:A:361:PHE:CE2	0.60	2.31	9	1
1:A:325:ASN:O	1:A:329:VAL:HG23	0.60	1.97	15	7
1:A:345:ILE:HG23	1:A:407:ARG:O	0.60	1.95	10	3
1:A:324:VAL:HG11	1:A:394:VAL:CG1	0.60	2.27	13	1
1:A:361:PHE:HB3	1:A:367:ILE:HD11	0.60	1.72	17	2
1:A:329:VAL:HG11	1:A:391:VAL:HG22	0.59	1.74	9	7
1:A:390:ALA:HA	1:A:393:ILE:HD12	0.59	1.73	19	7
1:A:336:ALA:HB1	1:A:340:VAL:HG11	0.59	1.75	5	3
1:A:343:ALA:HB3	1:A:381:ILE:HG13	0.58	1.74	18	4
1:A:332:ILE:HG22	1:A:410:TRP:NE1	0.58	2.14	3	4
1:A:343:ALA:HB2	1:A:389:ALA:HB1	0.58	1.74	17	3
1:A:368:LEU:HD11	1:A:384:ASP:HA	0.58	1.75	9	11
1:A:329:VAL:O	1:A:333:ILE:HD12	0.57	1.99	9	1
1:A:329:VAL:CG2	1:A:394:VAL:HG21	0.56	2.29	14	4
1:A:367:ILE:C	1:A:368:LEU:HD23	0.56	2.20	10	1
1:A:324:VAL:HG21	1:A:395:ALA:HB2	0.56	1.76	3	1
1:A:367:ILE:HG23	1:A:381:ILE:CG2	0.55	2.31	10	4
1:A:396:LEU:HD22	1:A:399:PHE:CB	0.55	2.31	19	2
1:A:393:ILE:O	1:A:397:ALA:HB2	0.55	2.01	13	1
1:A:393:ILE:HG23	1:A:408:THR:HB	0.55	1.77	10	16
1:A:368:LEU:HD21	1:A:384:ASP:HB2	0.55	1.77	19	3
1:A:324:VAL:HG22	1:A:391:VAL:HG13	0.54	1.78	8	1
1:A:324:VAL:HG11	1:A:395:ALA:HB2	0.53	1.80	8	1
1:A:333:ILE:HG23	1:A:386:HIS:NE2	0.53	2.19	16	8
1:A:361:PHE:CB	1:A:367:ILE:HD11	0.52	2.35	19	6
1:A:345:ILE:HD11	1:A:392:CYS:SG	0.52	2.44	9	7
1:A:324:VAL:HG13	1:A:395:ALA:HA	0.52	1.80	18	1
1:A:360:LEU:HD21	1:A:396:LEU:CD2	0.52	2.31	4	2
1:A:341:THR:HG22	1:A:385:THR:O	0.52	2.05	10	7
1:A:354:GLU:HA	1:A:357:LEU:HD12	0.52	1.81	4	3
1:A:361:PHE:HB2	1:A:367:ILE:HD11	0.51	1.82	15	8
1:A:333:ILE:HD11	1:A:387:GLU:CG	0.51	2.35	19	1
1:A:358:ILE:N	1:A:359:PRO:CD	0.51	2.73	4	18
1:A:349:PRO:HG2	1:A:352:ALA:HB2	0.51	1.82	7	2
1:A:324:VAL:CG2	1:A:391:VAL:HG13	0.50	2.36	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:ILE:HG21	1:A:406:LEU:HD13	0.50	1.83	19	1
1:A:341:THR:HG22	1:A:385:THR:C	0.50	2.27	8	1
1:A:330:ASP:HA	1:A:333:ILE:HD12	0.49	1.83	17	3
1:A:406:LEU:HD23	1:A:406:LEU:N	0.49	2.22	16	5
1:A:337:PRO:HG2	1:A:340:VAL:HG23	0.49	1.83	15	3
1:A:344:TYR:C	1:A:345:ILE:HD12	0.49	2.28	17	2
1:A:367:ILE:O	1:A:368:LEU:HD23	0.49	2.07	10	1
1:A:345:ILE:HG21	1:A:361:PHE:CZ	0.49	2.43	5	1
1:A:344:TYR:C	1:A:345:ILE:HD13	0.48	2.29	6	2
1:A:343:ALA:HB3	1:A:381:ILE:HD12	0.48	1.85	11	2
1:A:358:ILE:HB	1:A:359:PRO:HD3	0.48	1.86	11	18
1:A:340:VAL:HG21	1:A:411:GLY:O	0.48	2.09	7	1
1:A:345:ILE:HD13	1:A:408:THR:HG22	0.48	1.86	19	1
1:A:360:LEU:HD22	1:A:401:PHE:CE2	0.47	2.45	20	1
1:A:336:ALA:HB1	1:A:337:PRO:HD2	0.47	1.85	7	16
1:A:357:LEU:HD21	1:A:401:PHE:CE2	0.47	2.45	14	1
1:A:406:LEU:N	1:A:406:LEU:HD23	0.47	2.25	5	3
1:A:345:ILE:CG2	1:A:406:LEU:HD23	0.47	2.38	13	1
1:A:399:PHE:CD1	1:A:399:PHE:C	0.47	2.87	7	1
1:A:380:PHE:C	1:A:381:ILE:HD13	0.47	2.30	17	1
1:A:390:ALA:HA	1:A:393:ILE:HD13	0.47	1.87	14	4
1:A:368:LEU:HD21	1:A:384:ASP:HB3	0.46	1.87	17	1
1:A:345:ILE:O	1:A:348:ILE:HD11	0.46	2.11	4	1
1:A:345:ILE:CD1	1:A:408:THR:HG22	0.46	2.40	19	1
1:A:396:LEU:HD22	1:A:399:PHE:CD1	0.46	2.46	6	2
1:A:399:PHE:CD2	1:A:399:PHE:C	0.46	2.90	19	1
1:A:368:LEU:HD12	1:A:382:LYS:O	0.45	2.11	8	2
1:A:360:LEU:HD21	1:A:399:PHE:CE1	0.45	2.46	6	1
1:A:367:ILE:HG12	1:A:381:ILE:HG21	0.45	1.88	10	1
1:A:333:ILE:HD11	1:A:387:GLU:HG3	0.44	1.89	19	1
1:A:368:LEU:HD11	1:A:384:ASP:CB	0.44	2.43	16	1
1:A:396:LEU:O	1:A:397:ALA:C	0.44	2.56	13	1
1:A:332:ILE:HG22	1:A:410:TRP:HE1	0.44	1.71	19	1
1:A:368:LEU:HD21	1:A:384:ASP:CB	0.44	2.43	19	1
1:A:364:PHE:CE1	1:A:396:LEU:HD11	0.43	2.48	17	2
1:A:324:VAL:CG1	1:A:395:ALA:HB2	0.43	2.43	8	1
1:A:328:ALA:C	1:A:394:VAL:HG21	0.43	2.34	13	1
1:A:396:LEU:HD22	1:A:406:LEU:HD12	0.42	1.91	17	1
1:A:336:ALA:HB1	1:A:340:VAL:CG1	0.42	2.44	5	1
1:A:329:VAL:HG22	1:A:394:VAL:CG2	0.42	2.36	15	1
1:A:337:PRO:O	1:A:340:VAL:HG12	0.41	2.15	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:407:ARG:O	1:A:408:THR:HG23	0.41	2.15	12	1
1:A:345:ILE:CG2	1:A:348:ILE:HD11	0.41	2.45	17	1
1:A:353:THR:O	1:A:354:GLU:CB	0.41	2.68	14	1
1:A:324:VAL:HG21	1:A:391:VAL:CG1	0.40	2.46	9	1
1:A:396:LEU:HD22	1:A:399:PHE:HB2	0.40	1.93	19	1
1:A:358:ILE:HG22	1:A:359:PRO:N	0.40	2.32	5	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	83/116 (72%)	59±3 (71±3%)	18±3 (22±3%)	6±2 (7±3%)	2	17
All	All	1660/2320 (72%)	1178 (71%)	369 (22%)	113 (7%)	2	17

All 25 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	397	ALA	17
1	A	343	ALA	12
1	A	335	SER	11
1	A	383	TYR	10
1	A	339	ARG	10
1	A	406	LEU	8
1	A	324	VAL	7
1	A	367	ILE	6
1	A	409	GLY	4
1	A	388	GLN	4
1	A	370	PHE	4
1	A	347	ASN	3
1	A	410	TRP	2
1	A	342	THR	2
1	A	408	THR	2
1	A	371	LYS	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	403	GLY	1
1	A	352	ALA	1
1	A	365	GLY	1
1	A	366	PHE	1
1	A	340	VAL	1
1	A	368	LEU	1
1	A	346	GLY	1
1	A	348	ILE	1
1	A	351	PHE	1

6.3.2 Protein sidechains ⓘ

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	69/97 (71%)	56±2 (82±3%)	13±2 (18±3%)	4	37
All	All	1380/1940 (71%)	1129 (82%)	251 (18%)	4	37

All 37 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	399	PHE	20
1	A	341	THR	19
1	A	362	GLN	18
1	A	385	THR	17
1	A	394	VAL	15
1	A	388	GLN	14
1	A	327	GLN	11
1	A	407	ARG	11
1	A	371	LYS	11
1	A	353	THR	10
1	A	406	LEU	10
1	A	381	ILE	9
1	A	401	PHE	8
1	A	356	ASP	7
1	A	384	ASP	7
1	A	404	ARG	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	325	ASN	6
1	A	334	ARG	6
1	A	405	ASN	5
1	A	354	GLU	4
1	A	387	GLU	4
1	A	369	ASP	4
1	A	324	VAL	3
1	A	363	ASN	3
1	A	339	ARG	3
1	A	335	SER	3
1	A	382	LYS	3
1	A	351	PHE	2
1	A	368	LEU	2
1	A	330	ASP	2
1	A	392	CYS	1
1	A	345	ILE	1
1	A	347	ASN	1
1	A	366	PHE	1
1	A	367	ILE	1
1	A	350	HIS	1
1	A	370	PHE	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 monosaccharides in this entry.

6.6 Ligand geometry ⓘ

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 79% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *cif4g1_37-49-Pub1R3_new_CS.str*

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	1232
Number of shifts mapped to atoms	1232
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	113	-0.08 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	0.06 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	105	0.27 ± 0.21	None needed (< 0.5 ppm)
^{15}N	105	0.82 ± 0.48	None needed (imprecise)

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 79%, i.e. 815 atoms were assigned a chemical shift out of a possible 1030. 3 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	390/403 (97%)	157/160 (98%)	157/166 (95%)	76/77 (99%)
Sidechain	372/499 (75%)	254/293 (87%)	105/183 (57%)	13/23 (57%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	53/128 (41%)	52/70 (74%)	0/53 (0%)	1/5 (20%)
Overall	815/1030 (79%)	463/523 (89%)	262/402 (65%)	90/105 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1101 atoms were assigned a chemical shift out of a possible 1438. 3 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	537/562 (96%)	214/223 (96%)	218/232 (94%)	105/107 (98%)
Sidechain	495/716 (69%)	341/424 (80%)	133/255 (52%)	21/37 (57%)
Aromatic	69/160 (43%)	68/86 (79%)	0/69 (0%)	1/5 (20%)
Overall	1101/1438 (77%)	623/733 (85%)	351/556 (63%)	127/149 (85%)

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
1	A	336	ALA	HB1	-0.09	2.61 – 0.11	-5.8
1	A	336	ALA	HB2	-0.09	2.61 – 0.11	-5.8
1	A	336	ALA	HB3	-0.09	2.61 – 0.11	-5.8
1	A	338	PRO	HA	2.56	6.05 – 2.75	-5.6
1	A	393	ILE	HD11	-0.91	2.13 – -0.77	-5.5
1	A	393	ILE	HD12	-0.91	2.13 – -0.77	-5.5
1	A	393	ILE	HD13	-0.91	2.13 – -0.77	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

