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Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:35 am GMT

PDB ID	:	4UQT
Title	:	RRM-peptide structure in RES complex
Authors	:	Tripsianes, K.; Friberg, A.; Barrandon, C.; Seraphin, B.; Sattler, M.
Deposited on	:	2014-06-25

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

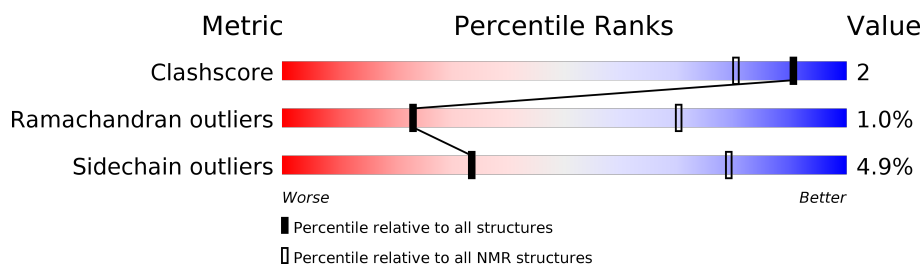|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		1.0%
Sidechain outliers		4.9%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	93	75% • 18% •
2	B	39	49% 13% 28% 10%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:31-A:64, A:72-A:109, B:226-B:234 (81)	0.16	19
2	B:240-B:254 (15)	0.46	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2006 atoms, of which 985 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U2 SNRNP COMPONENT IST3.

Mol	Chain	Residues	Atoms					Trace
1	A	89	Total	C	H	N	O	0
			1425	457	702	123	143	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	EXPRESSION TAG	UNP P40565
A	22	ALA	-	EXPRESSION TAG	UNP P40565
A	23	MET	-	EXPRESSION TAG	UNP P40565
A	24	GLY	-	EXPRESSION TAG	UNP P40565

- Molecule 2 is a protein called PRE-MRNA-SPLICING FACTOR CWC26.

Mol	Chain	Residues	Atoms						Trace
2	B	35	Total	C	H	N	O	S	0
			581	187	283	57	53	1	

There are 4 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
B	218	GLY	-	EXPRESSION TAG	UNP P46947
B	219	ALA	-	EXPRESSION TAG	UNP P46947
B	220	MET	-	EXPRESSION TAG	UNP P46947
B	221	GLY	-	EXPRESSION TAG	UNP P46947

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: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
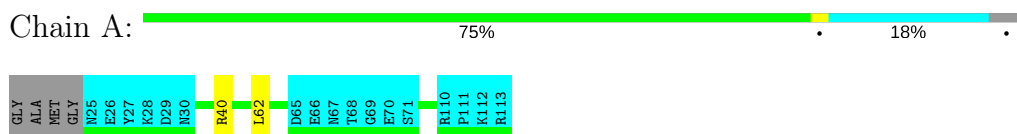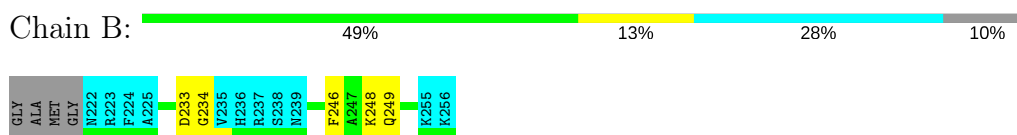
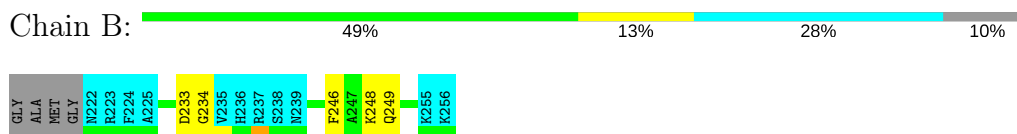## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1
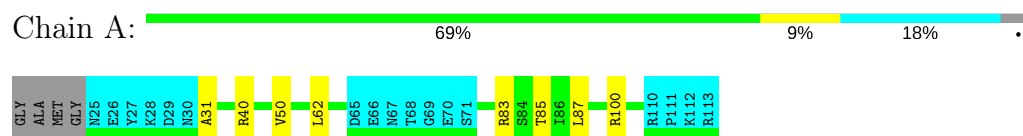
• Molecule 1: U2 SNRNP COMPONENT IST3
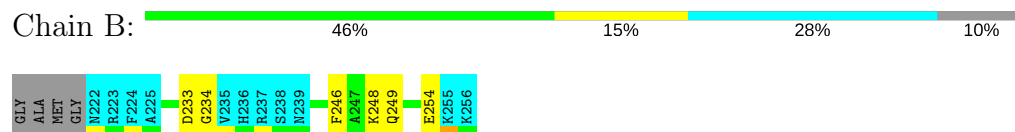
Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
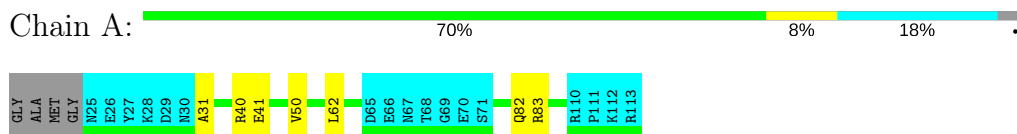
4.2.2 Score per residue for model 2

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
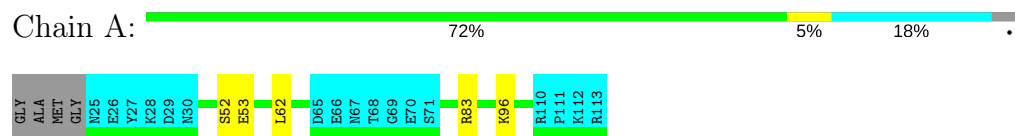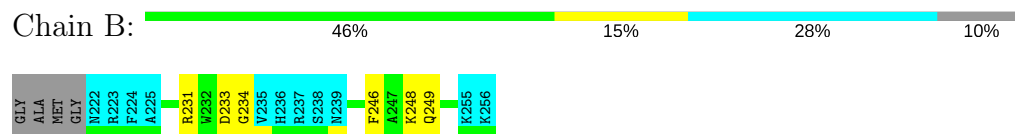
4.2.4 Score per residue for model 4

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
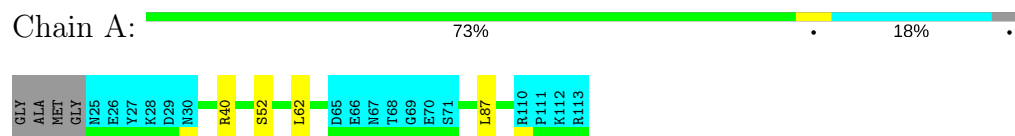
4.2.5 Score per residue for model 5

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

71% 6% 18% •

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 V50 P57 L62 D65 E66 N67 T68 G69 E70 S71 L77 N91 K96 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

41% 21% 28% 10%
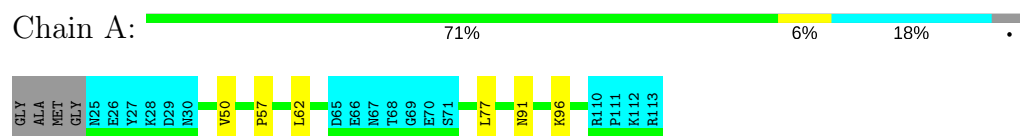
GLY ALA MET GLY N222 R223 F224 A225 D233 G234 V235 H236 R237 S238 N239 G240 K244 W245 F246 A247 K248 Q249 E254 K255 K256
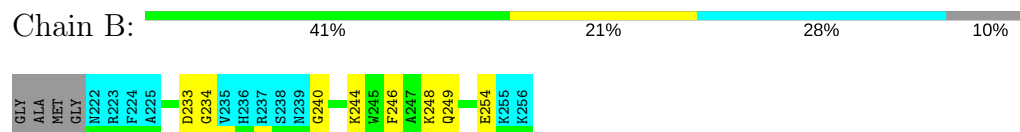
4.2.6 Score per residue for model 6

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

68% 10% 18% •

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 V50 L62 S63 R64 D65 E66 N67 T68 G69 E70 S71 Q72 D81 Q82 R83 S84 T85 I86 L87 A88 V89 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

46% 15% 28% 10%
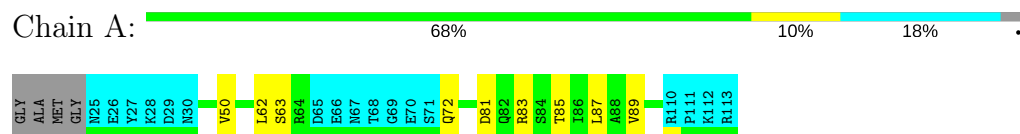
GLY ALA MET GLY N222 R223 F224 A225 D233 G234 V235 H236 R237 S238 N239 F246 A247 K248 Q249 E254 K255 K256
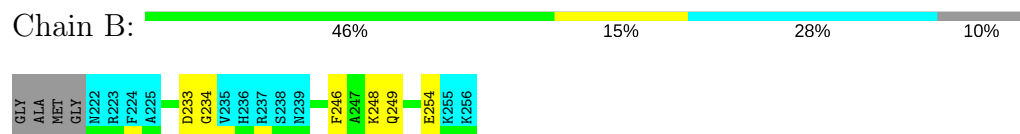
4.2.7 Score per residue for model 7

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

74% • 18% •

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 R40 L62 D65 E66 N67 T68 G69 E70 S71 R83 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

46% 15% 28% 10%
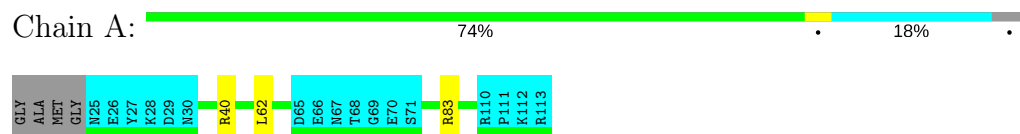
GLY ALA MET GLY N222 R223 F224 A225 D233 G234 V235 H236 R237 S238 N239 W245 F246 A247 K248 Q249 K255 K256
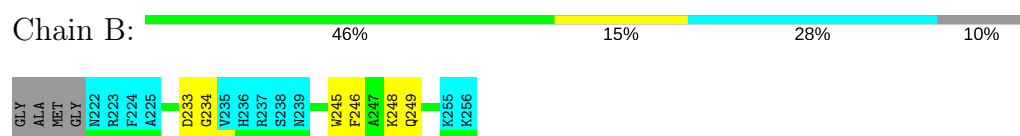
4.2.8　Score per residue for model 8

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:　　71%　　6%　　18%　　•

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 I35 R40 S52 L62 D65 E66 N67 T68 G69 E70 S71 K96 I104 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:　　41%　　21%　　28%　　10%
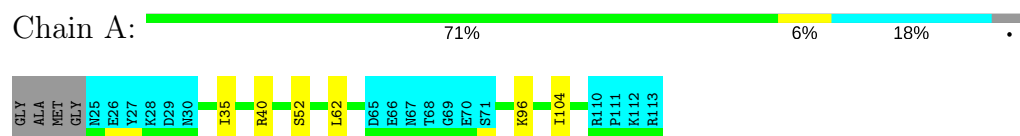
GLY ALA MET GLY N222 R223 F224 A225 R231 W232 D233 G234 V235 H236 R237 S238 N239 G240 K244 W245 F246 A247 K248 Q249 K255 K256
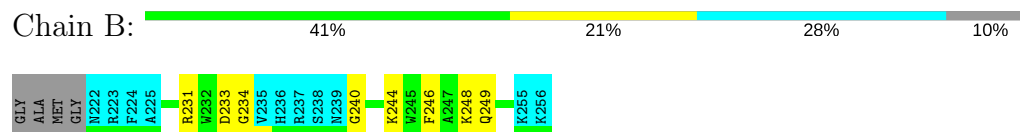
4.2.9　Score per residue for model 9

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:　　71%　　6%　　18%　　•

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 R40 E41 L62 D65 E66 N67 T68 G69 E70 S71 L87 K96 H106 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:　　44%　　18%　　28%　　10%
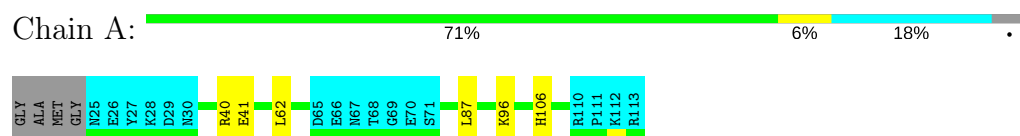
GLY ALA MET GLY N222 R223 F224 A225 D233 G234 V235 H236 R237 S238 N239 G240 K244 W245 F246 A247 K248 Q249 K255 K256
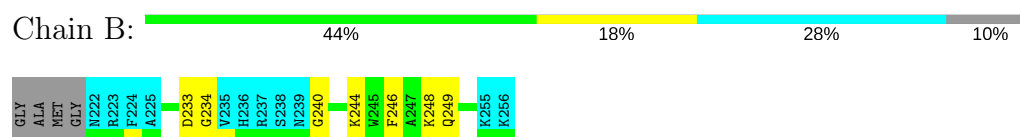
4.2.10　Score per residue for model 10

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:　　71%　　5%　　•　　18%　　•

GLY ALA MET GLY N25 E26 Y27 K28 D29 N30 R40 E41 L62 D65 E66 N67 T68 G69 E70 S71 R83 L87 K96 R110 P111 K112 R113

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:　　46%　　15%　　28%　　10%
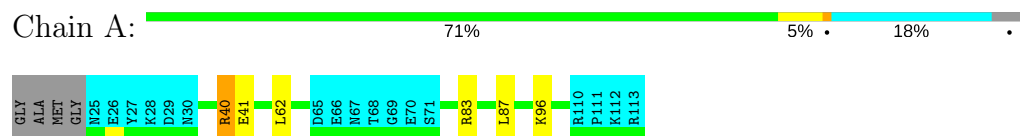
GLY ALA MET GLY N222 R223 F224 A225 D233 G234 V235 H236 R237 S238 N239 F246 A247 K248 Q249 N250 K255 K256
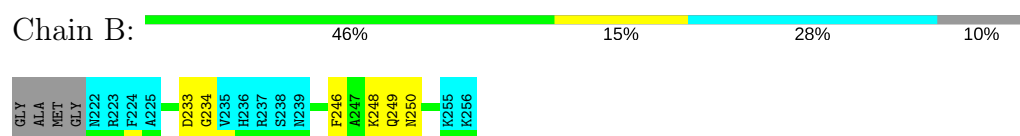
4.2.11 Score per residue for model 11

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

4.2.12 Score per residue for model 12
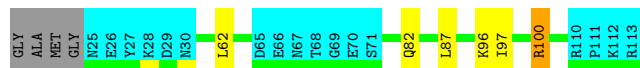
• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

4.2.13 Score per residue for model 13

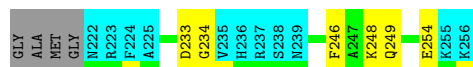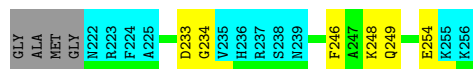• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:

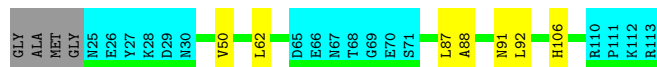### 4.2.16 Score per residue for model 16

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
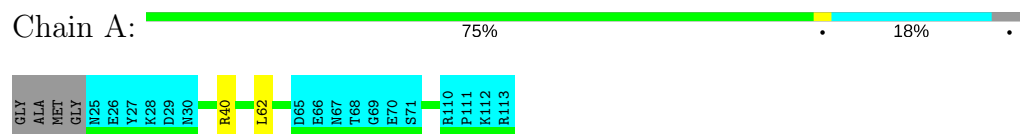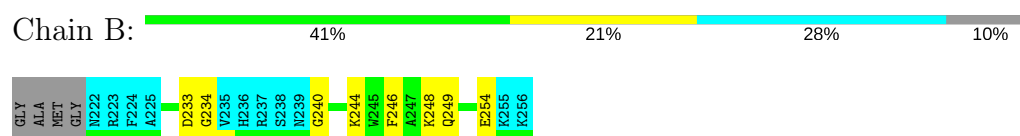
4.2.17 Score per residue for model 17

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26
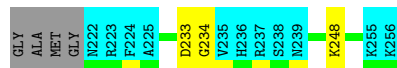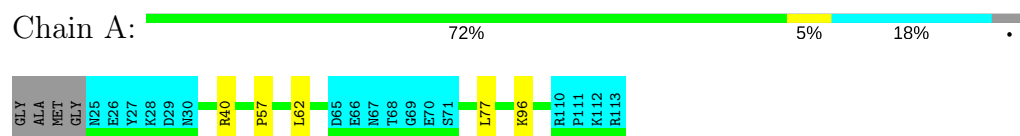
Chain B:
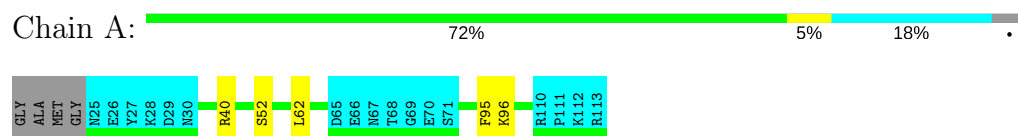
4.2.18 Score per residue for model 18

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
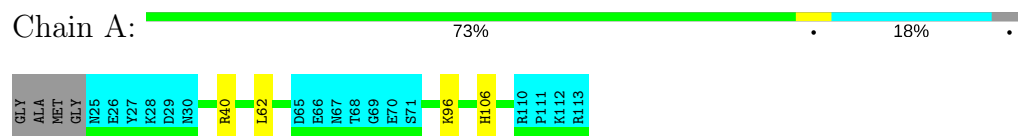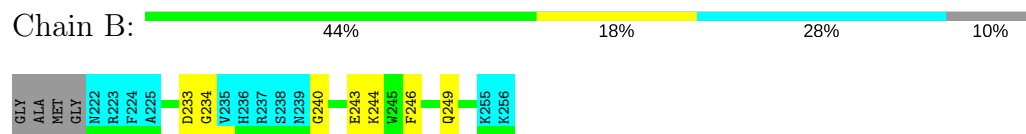
4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
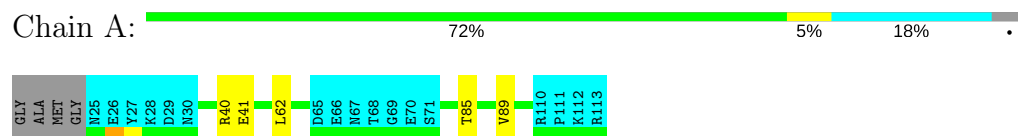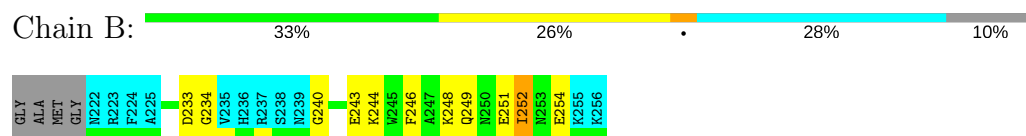
4.2.20 Score per residue for model 20

• Molecule 1: U2 SNRNP COMPONENT IST3

Chain A:

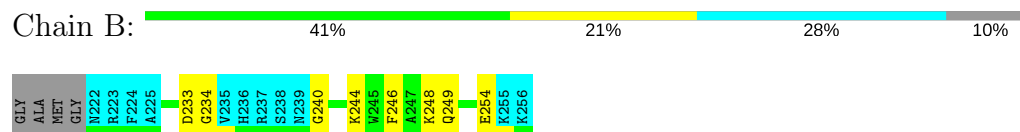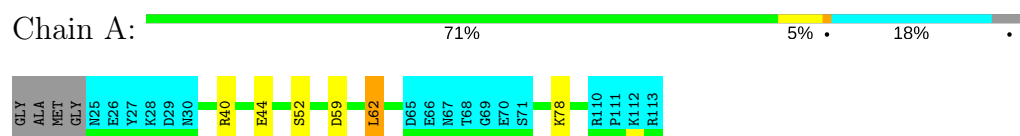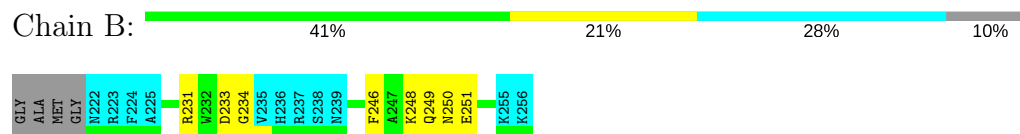• Molecule 2: PRE-MRNA-SPLICING FACTOR CWC26

Chain B:
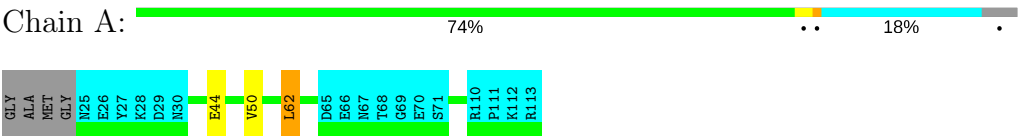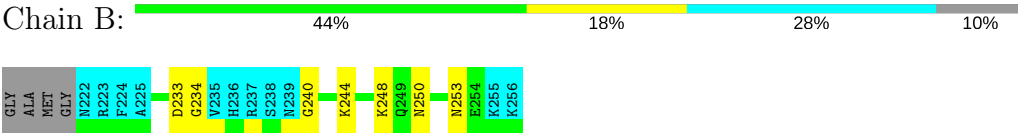
5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY.*

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

Software name	Classification	Version
CNS	refinement	
CCPNMR ANALYSIS	structure solution	2.1
CYANA	structure solution	
CNS	structure solution	
TALOS	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)	4uqt_cs.str
Number of chemical shift lists	1
Total number of shifts	1420
Number of shifts mapped to atoms	1420
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 ⓘ

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	579	573	573	1±1
2	B	202	182	182	2±1
All	All	15620	15100	15100	57

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:246:PHE:O	2:B:249:GLN:HG2	0.62	1.94	7	13
2:B:240:GLY:O	2:B:243:GLU:HG2	0.53	2.03	18	2
1:A:81:ASP:OD1	1:A:83:ARG:HG2	0.52	2.04	6	1
2:B:240:GLY:O	2:B:244:LYS:HG2	0.50	2.05	20	8
1:A:52:SER:OG	2:B:231:ARG:HB2	0.49	2.06	15	5
2:B:248:LYS:O	2:B:251:GLU:HG2	0.47	2.09	4	1
2:B:251:GLU:HB3	2:B:254:GLU:HB2	0.47	1.86	19	1
1:A:40:ARG:HD2	1:A:41:GLU:N	0.46	2.26	10	4
1:A:63:SER:OG	1:A:72:GLN:HB2	0.45	2.12	6	1
1:A:59:ASP:HB3	1:A:78:LYS:HG2	0.44	1.87	15	1
2:B:246:PHE:HA	2:B:249:GLN:NE2	0.44	2.27	9	1
2:B:252:ILE:HD13	2:B:252:ILE:H	0.44	1.72	19	1
1:A:40:ARG:HD2	1:A:40:ARG:C	0.43	2.33	12	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:97:ILE:HB	1:A:100:ARG:HH21	0.43	1.74	11	1
1:A:57:PRO:HB3	1:A:77:LEU:HD21	0.42	1.92	14	2
1:A:88:ALA:O	1:A:92:LEU:HB2	0.42	2.15	13	1
1:A:35:ILE:HG23	1:A:104:ILE:CD1	0.41	2.45	8	1
1:A:44:GLU:CG	1:A:62:LEU:HB2	0.41	2.45	15	2
1:A:31:ALA:HA	1:A:85:THR:HG21	0.41	1.93	2	1
1:A:31:ALA:HB2	1:A:82:GLN:NE2	0.41	2.30	1	1
2:B:240:GLY:O	2:B:244:LYS:HE2	0.41	2.16	9	1
2:B:246:PHE:HA	2:B:249:GLN:HG2	0.41	1.93	15	1
1:A:85:THR:O	1:A:89:VAL:HG23	0.40	2.16	19	2
2:B:246:PHE:HA	2:B:249:GLN:CD	0.40	2.36	11	1
2:B:245:TRP:O	2:B:248:LYS:HG3	0.40	2.16	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	72/93 (77%)	71±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
2	B	24/39 (62%)	22±1 (92±3%)	1±1 (4±3%)	1±0 (4±1%)	6	33
All	All	1920/2640 (73%)	1867 (97%)	34 (2%)	19 (1%)	23	70

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	234	GLY	19

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	61/78 (78%)	59±1 (96±2%)	3±1 (4±2%)	40	84
2	B	20/31 (65%)	19±1 (93±4%)	1±1 (7±4%)	21	67
All	All	1620/2180 (74%)	1541 (95%)	79 (5%)	33	79

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	62	LEU	20
2	B	248	LYS	18
1	A	96	LYS	9
1	A	40	ARG	7
1	A	83	ARG	5
2	B	254	GLU	5
1	A	106	HIS	4
2	B	250	ASN	3
1	A	100	ARG	2
1	A	91	ASN	2
2	B	253	ASN	1
2	B	251	GLU	1
2	B	252	ILE	1
1	A	53	GLU	1

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6   Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: 4uqt_cs.str

Chemical shift list name: *assigned_chem_shift_list*

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	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	123	-0.13 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	110	-0.09 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	117	-0.25 ± 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 83%, i.e. 998 atoms were assigned a chemical shift out of a possible 1208. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	375/476 (79%)	188/190 (99%)	95/192 (49%)	92/94 (98%)
Sidechain	505/599 (84%)	312/349 (89%)	185/221 (84%)	8/29 (28%)

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W O R L D W I D E
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PROTEIN DATA BANK

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	118/133 (89%)	61/70 (87%)	55/60 (92%)	2/3 (67%)
Overall	998/1208 (83%)	561/609 (92%)	335/473 (71%)	102/126 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1277 atoms were assigned a chemical shift out of a possible 1594. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	481/614 (78%)	241/245 (98%)	123/248 (50%)	117/121 (97%)
Sidechain	657/823 (80%)	413/483 (86%)	231/290 (80%)	13/50 (26%)
Aromatic	139/157 (89%)	72/83 (87%)	65/70 (93%)	2/4 (50%)
Overall	1277/1594 (80%)	726/811 (90%)	419/608 (69%)	132/175 (75%)

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.
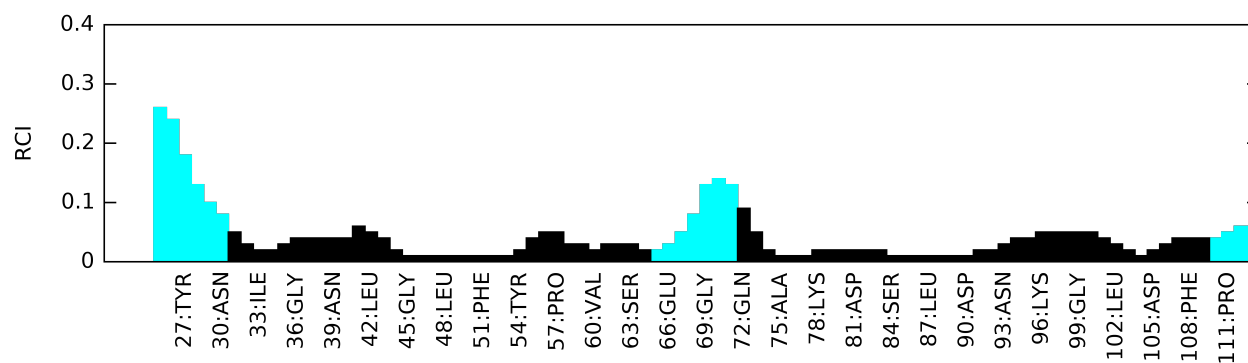
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	223	ARG	HD2	1.08	4.27 − 1.97	-8.9
1	A	53	GLU	HG2	0.45	3.33 − 1.23	-8.7
1	A	53	GLU	HG3	0.45	3.31 − 1.21	-8.6
2	B	223	ARG	HG2	-0.49	2.92 − 0.22	-7.6
1	A	84	SER	HB3	1.77	5.25 − 2.45	-7.4
2	B	237	ARG	HB2	-0.09	3.15 − 0.45	-7.0
1	A	53	GLU	HB2	0.61	3.08 − 0.98	-6.8
1	A	90	ASP	HB2	0.94	4.07 − 1.37	-6.6
1	A	53	GLU	HB3	0.61	3.10 − 0.90	-6.3
2	B	223	ARG	HB2	0.15	3.15 − 0.45	-6.1
1	A	78	LYS	HB3	0.18	3.10 − 0.40	-5.8
2	B	223	ARG	HG3	-0.08	3.00 − 0.10	-5.6
2	B	234	GLY	H	4.62	11.63 − 5.03	-5.6
1	A	53	GLU	HA	2.15	6.30 − 2.20	-5.1
2	B	223	ARG	HB3	0.36	3.17 − 0.37	-5.0

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: