wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:16 PM BST

PDB ID	:	5AN9
EMDB ID:	:	EMD-3145
Title	:	Mechanism of eIF6 release from the nascent 60S ribosomal subunit
Authors	:	Weis, F.; Giudice, E.; Churcher, M.; Jin, L.; Hilcenko, C.; Wong, C.C.; Traynor, D.; Kay, R.R.; Warren, A.J.
Deposited on	:	2015-09-06
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

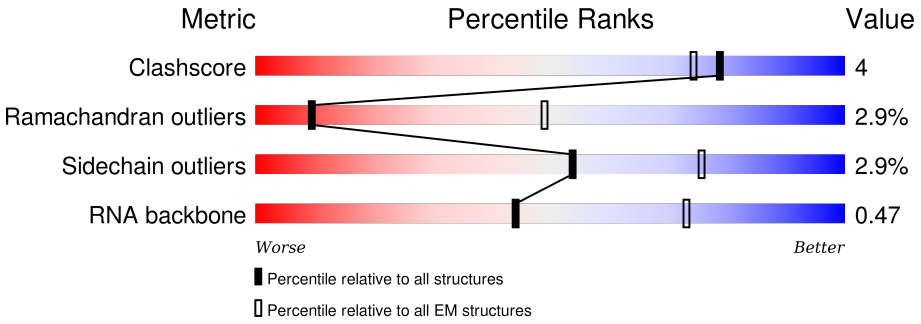
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	398	82% 15% •
2	B	188	88% 12%
3	C	205	97% •
4	D	166	96% • •
5	E	136	85% 15% •
6	F	217	86% 13%
7	G	69	91% 9%
8	H	52	83% 13% • •

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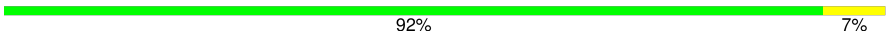
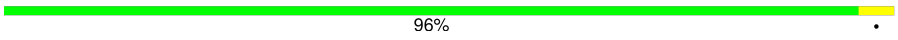
Mol	Chain	Length	Quality of chain
9	I	224	
10	J	250	
11	N	3741	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 39693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	398	Total	C	N	O	S	0	0
			3176	2018	599	547	12		

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	188	Total	C	N	O	S	0	0
			1491	944	264	277	6		

- Molecule 3 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	205	Total	C	N	O	S	0	0
			1571	998	271	294	8		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1245	790	220	228	7		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	136	Total	C	N	O	S	0	0
			1017	640	188	181	8		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	217	Total	C	N	O	S	0	0
			1721	1079	332	297	13		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	69	Total	C	N	O	S	0	0
			586	378	105	99	4		

- Molecule 8 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	52	Total	C	N	O	S	0	0
			427	269	88	64	6		

- Molecule 9 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	224	Total	C	N	O	S	0	0
			1686	1048	290	338	10		

- Molecule 10 is a protein called RIBOSOME MATURATION PROTEIN SBDS.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	250	Total	C	N	O	S	0	0
			2015	1272	352	380	11		

- Molecule 11 is a RNA chain called 26S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	1162	Total	C	N	O	P	0	0
			24758	11082	4431	8087	1158		

There is a discrepancy between the modelled and reference sequences:

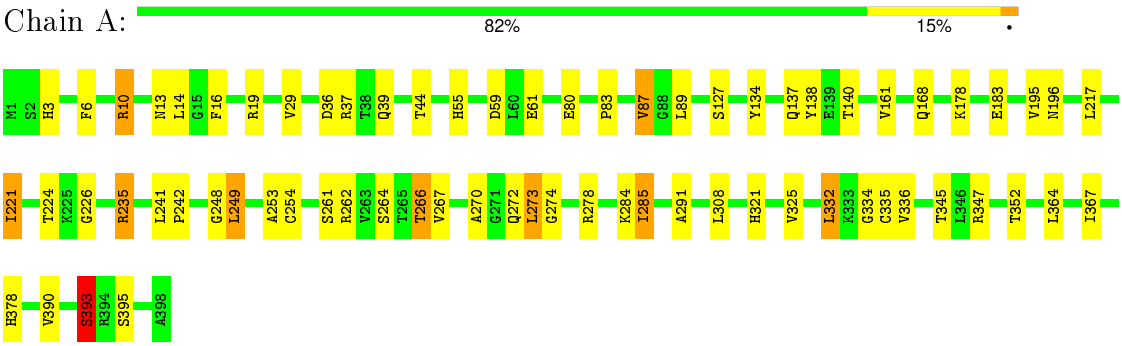
Chain	Residue	Modelled	Actual	Comment	Reference
N	3119	C	G	CONFLICT	GB FR733594.

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

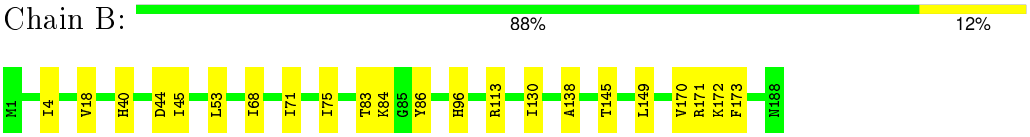
- Molecule 1: 60S RIBOSOMAL PROTEIN L3

Chain A:



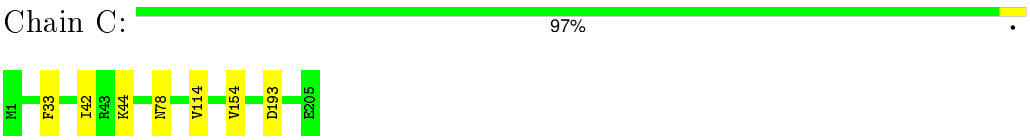
- Molecule 2: 60S RIBOSOMAL PROTEIN L9

Chain B:



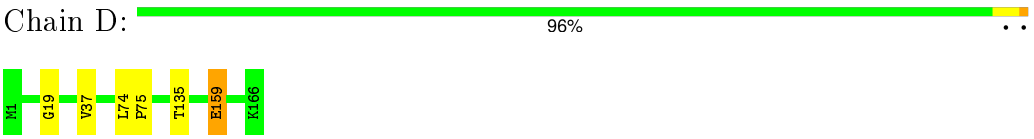
- Molecule 3: 60S ACIDIC RIBOSOMAL PROTEIN P0

Chain C:



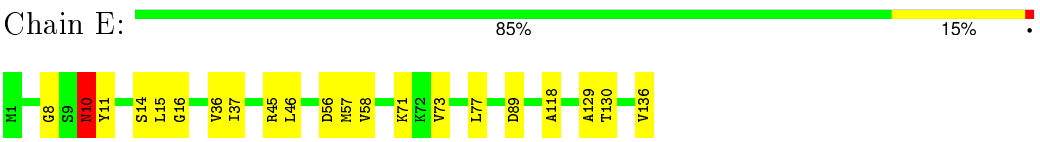
- Molecule 4: 60S RIBOSOMAL PROTEIN L12

Chain D:



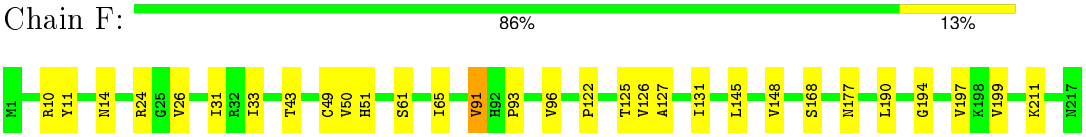
- Molecule 5: 60S RIBOSOMAL PROTEIN L23

Chain E:



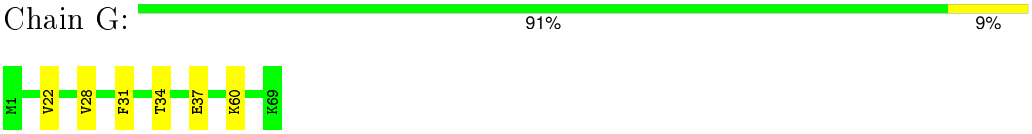
• Molecule 6: 60S RIBOSOMAL PROTEIN L10

Chain F:



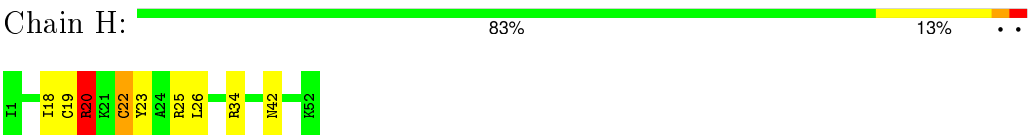
• Molecule 7: 60S RIBOSOMAL PROTEIN L24

Chain G:



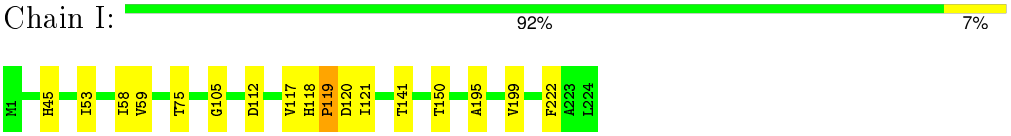
• Molecule 8: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain H:



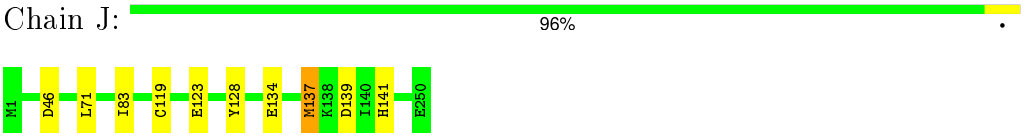
• Molecule 9: EUKARYOTIC TRANSLATION INITIATION FACTOR 6

Chain I:



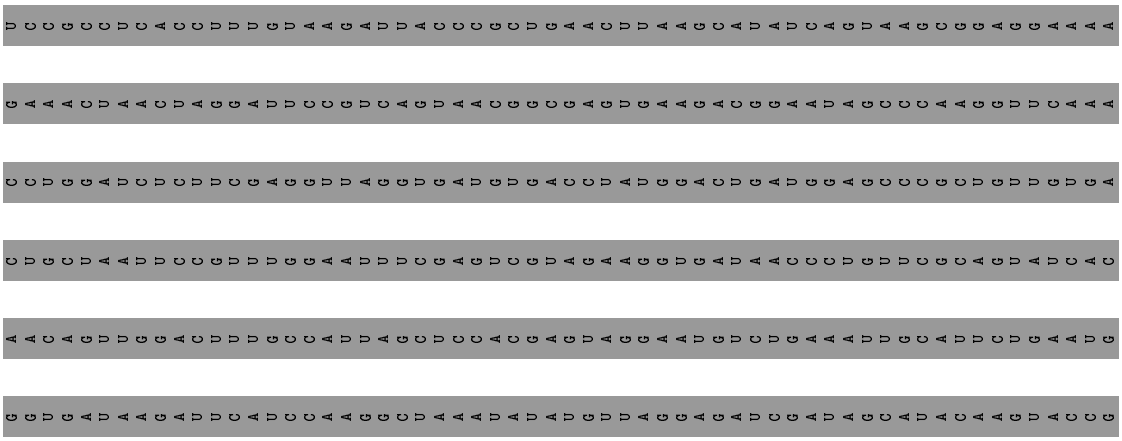
• Molecule 10: RIBOSOME MATURATION PROTEIN SBDS

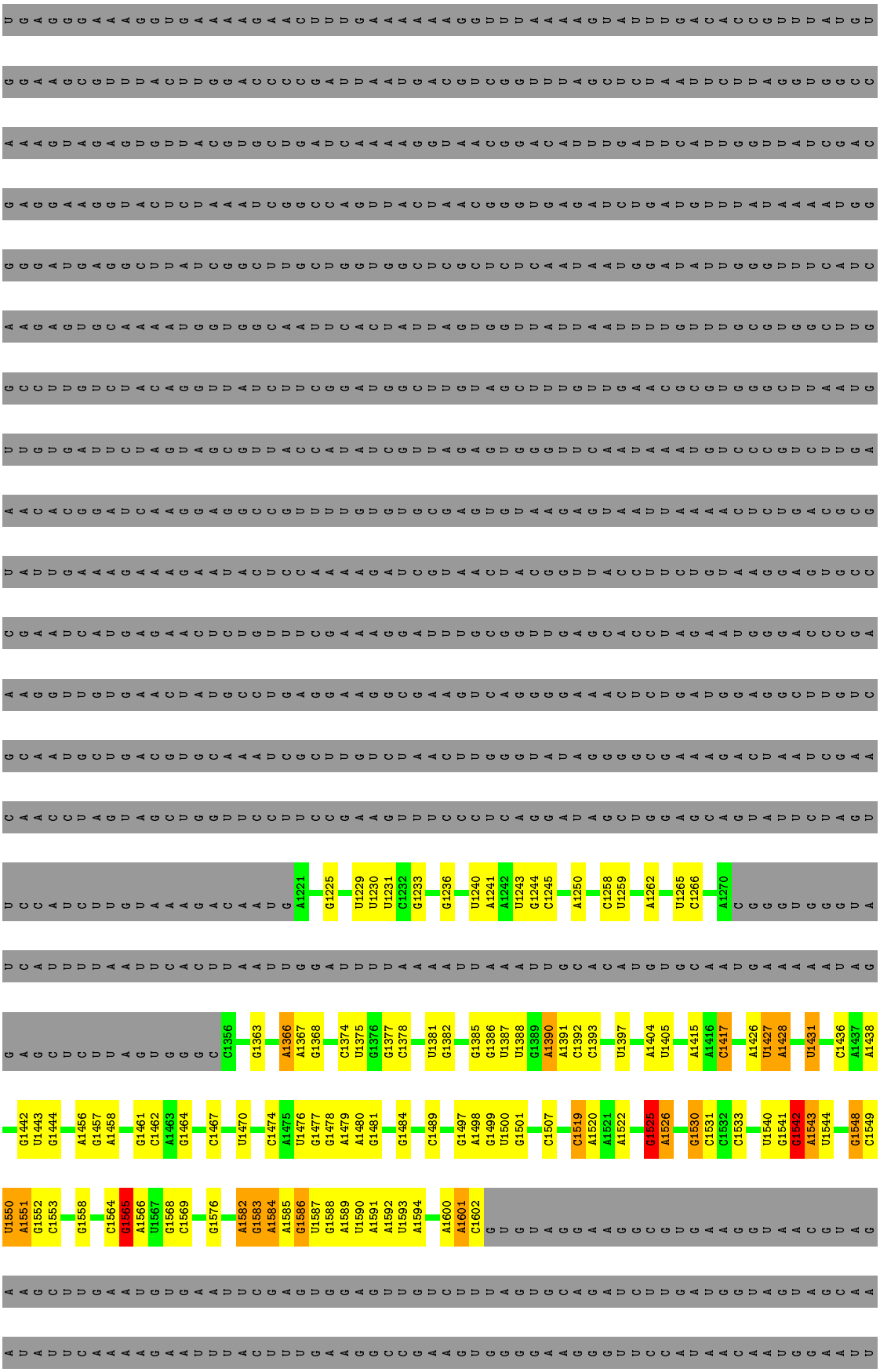
Chain J:

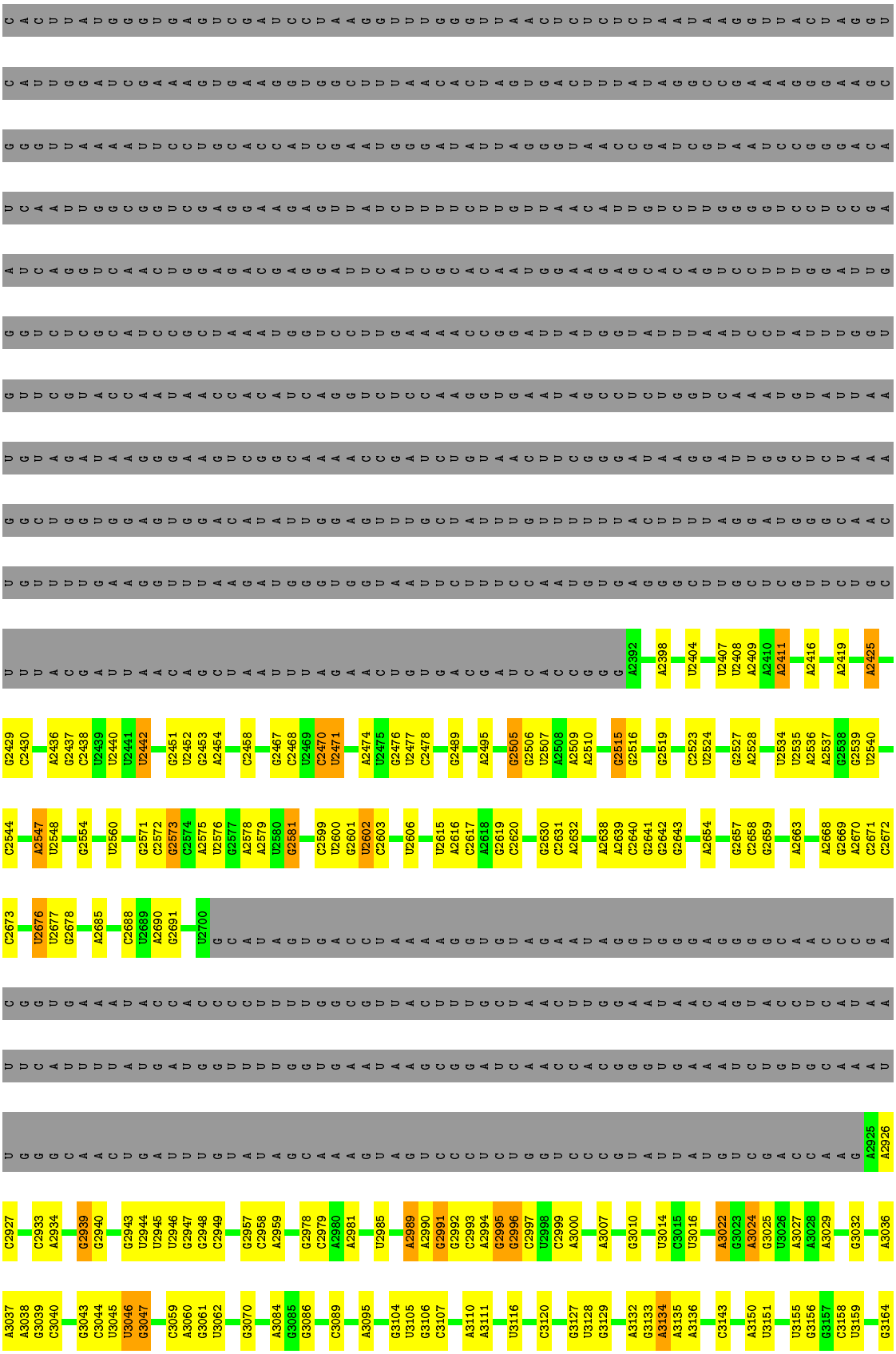


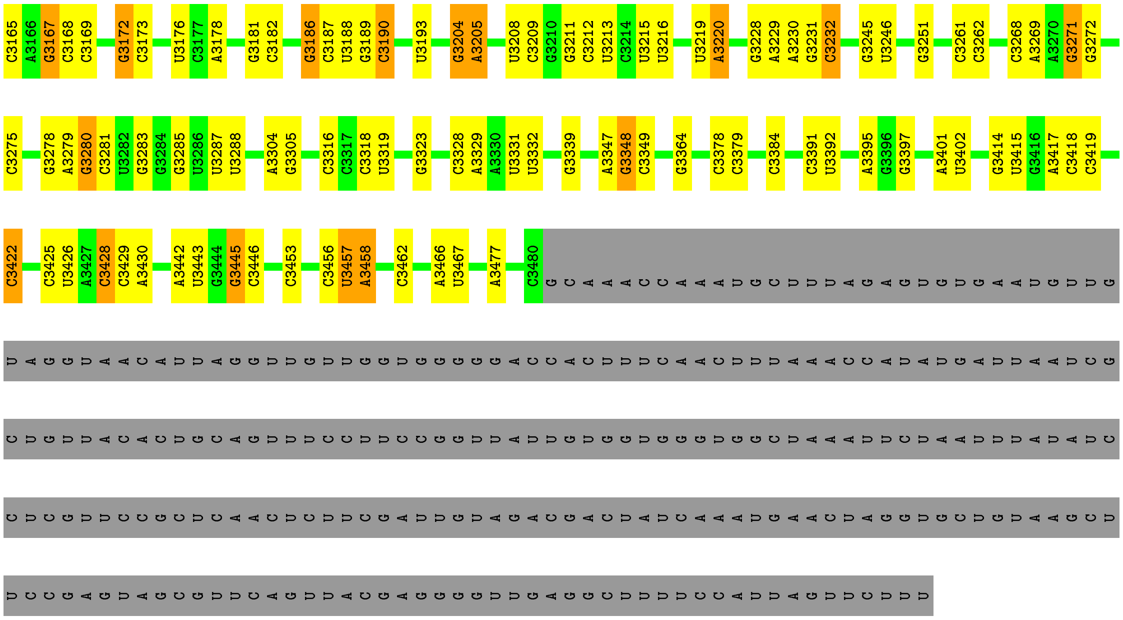
• Molecule 11: 26S RIBOSOMAL RNA

Chain N:








C3165 A3166 G3167 C3168 C3169 G3172 C3173 U3176 C3177 A3178 G3181 C3182 G3186 C3187 U3188 G3189 C3190 U3193 G3204 A3205 U3208 C3209 G3210 G3211 C3212 U3213 C3214 U3215 U3216 U3219 A3220 G3228 A3229 A3230 G3231 C3232 G3245 U3246 G3251 C3261 C3262 C3268 A3269 A3270 G3271 G3272
C3275 G3278 A3279 G3280 C3281 U3282 G3283 G3284 G3285 U3286 U3287 U3288 A3304 G3305 C3316 C3317 C3318 U3319 G3323 C3328 A3329 A3330 U3331 U3332 G3339 A3347 G3348 C3349 G3364 C3378 C3379 C3384 C3391 U3392 A3395 G3396 G3397 A3401 U3402 G3414 U3415 G3416 A3417 C3418 C3419
C3422 C3425 U3426 A3427 C3428 C3429 A3430 A3442 U3443 G3444 G3445 C3446 C3453 C3456 U3457 A3458 C3462 A3466 U3467 A3477 C3480 G C A A A C C A A A U G C U U U A G A G U G U G A A U G U U G
U A G G U A A C A U U A G G U U G U U G G U G G G G G A C C A C U U U C A A C U U U A A A C C A U A U G A U U A A U C G
C U G U U A C A C U G C A G U U U C C U U C C G G U U A U U G U G G U G G G U G G C U A A A U U C U A A U U U A U A U C
C U C G U U C C G C U C A A C U C U U C G A U U G U A G A C G A C U A U C A A A U G A A C U A G G U G C U G U A A G C U
U C C G A G U A G C G G U U C A G U U A C G G A G G G G U U G A G G C U U U U C C A U U A G U U C U U U

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.45	0/3241	0.78	1/4339 (0.0%)
10	J	0.38	0/2038	0.64	0/2727
11	N	0.35	0/27702	0.74	7/43160 (0.0%)
2	B	0.37	0/1510	0.68	0/2030
3	C	0.38	0/1592	0.57	0/2142
4	D	0.37	0/1265	0.58	0/1702
5	E	0.36	0/1032	0.69	0/1386
6	F	0.38	0/1752	0.70	0/2345
7	G	0.44	0/600	0.67	0/801
8	H	0.39	0/433	0.77	0/571
9	I	0.37	0/1706	0.62	0/2325
All	All	0.36	0/42871	0.72	8/63528 (0.0%)

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 outliers	#Planarity outliers
1	A	0	2
5	E	0	1
9	I	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	2995	G	C2'-C3'-O3'	8.84	128.96	109.50
11	N	1582	A	C2'-C3'-O3'	7.68	126.41	109.50
11	N	1565	G	C4'-C3'-O3'	6.44	125.88	113.00
11	N	1519	C	C2'-C3'-O3'	6.32	123.81	113.70
11	N	2515	G	C2'-C3'-O3'	6.02	123.33	113.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PHE	Peptide
1	A	393	SER	Peptide
5	E	10	ASN	Peptide
9	I	118	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3176	0	3319	26	0
2	B	1491	0	1555	8	0
3	C	1571	0	1657	1	0
4	D	1245	0	1338	1	0
5	E	1017	0	1076	11	0
6	F	1721	0	1778	14	0
7	G	586	0	601	2	0
8	H	427	0	483	5	0
9	I	1686	0	1685	7	0
10	J	2015	0	2112	2	0
11	N	24758	0	12487	174	0
All	All	39693	0	28091	238	0

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.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:CD1	1:A:332:LEU:HD23	2.24	0.68
11:N:1415:A:N3	11:N:1564:C:O2'	2.26	0.67
6:F:96:VAL:HG12	6:F:125:THR:HG22	1.78	0.64
6:F:14:ASN:ND2	11:N:1363:G:OP2	2.29	0.64
5:E:36:VAL:HG13	5:E:58:VAL:HG13	1.79	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 EM 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	396/398 (100%)	328 (83%)	50 (13%)	18 (4%)	3 21
2	B	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	12 48
3	C	203/205 (99%)	185 (91%)	15 (7%)	3 (2%)	13 49
4	D	164/166 (99%)	142 (87%)	17 (10%)	5 (3%)	5 33
5	E	134/136 (98%)	114 (85%)	13 (10%)	7 (5%)	2 18
6	F	215/217 (99%)	188 (87%)	21 (10%)	6 (3%)	6 34
7	G	67/69 (97%)	62 (92%)	4 (6%)	1 (2%)	13 49
8	H	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	4 24
9	I	222/224 (99%)	199 (90%)	17 (8%)	6 (3%)	6 35
10	J	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	16 54
All	All	1885/1905 (99%)	1659 (88%)	172 (9%)	54 (3%)	9 34

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
2	B	138	ALA
5	E	46	LEU
9	I	119	PRO
1	A	285	ILE

5.3.2 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 EM 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	337/337 (100%)	317 (94%)	20 (6%)	24 63
2	B	168/168 (100%)	162 (96%)	6 (4%)	42 76
3	C	172/172 (100%)	169 (98%)	3 (2%)	68 86
4	D	139/139 (100%)	138 (99%)	1 (1%)	88 94
5	E	108/108 (100%)	104 (96%)	4 (4%)	41 76
6	F	180/180 (100%)	176 (98%)	4 (2%)	60 84
7	G	65/65 (100%)	64 (98%)	1 (2%)	72 88
8	H	48/48 (100%)	44 (92%)	4 (8%)	14 47
9	I	190/190 (100%)	189 (100%)	1 (0%)	92 95
10	J	228/228 (100%)	224 (98%)	4 (2%)	66 85
All	All	1635/1635 (100%)	1587 (97%)	48 (3%)	54 80

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	113	ARG
3	C	42	ILE
10	J	119	CYS
2	B	130	ILE
2	B	171	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	114	ASN
2	B	135	ASN
4	D	103	ASN
2	B	40	HIS
3	C	164	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	N	1158/3741 (30%)	216 (18%)	36 (3%)

5 of 216 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	N	1225	G
11	N	1229	U
11	N	1230	U
11	N	1231	U
11	N	1233	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	N	2515	G
11	N	2575	A
11	N	3429	C
11	N	2547	A
11	N	2995	G

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.