



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 23, 2017 – 12:13 AM EDT

PDB ID : 2X7N
EMDB ID: : EMD-1705
Title : Mechanism of eIF6s anti-association activity
Authors : Gartmann, M.; Blau, M.; Armache, J.-P.; Mielke, T.; Topf, M.; Beckmann, R.
Deposited on : unknown
Resolution : 11.80 Å(reported)
Based on PDB ID : 1G62

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

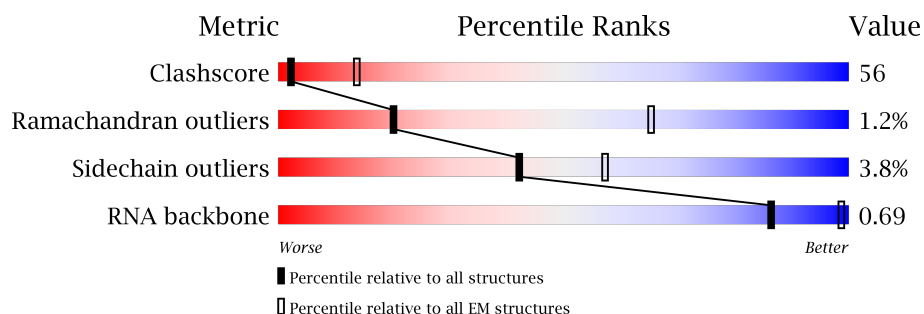
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	28	<div> <div>43%</div> <div>54%</div> <div>.</div> </div>
2	B	224	<div> <div>62%</div> <div>36%</div> <div>.</div> </div>
3	C	132	<div> <div>32%</div> <div>57%</div> <div>8%</div> <div>.</div> </div>
4	D	56	<div> <div>36%</div> <div>63%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3737 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 RNA chain called SARCIN-RICIN LOOP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	28	Total	C	N	O	P	0	0
			600	267	112	193	28		

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1693	1051	293	342	7		

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	132	Total	C	N	O	S	0	0
			982	617	184	174	7		

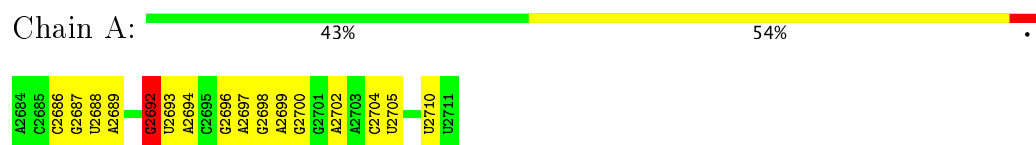
- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	56	Total	C	N	O	S	0	0
			462	298	88	75	1		

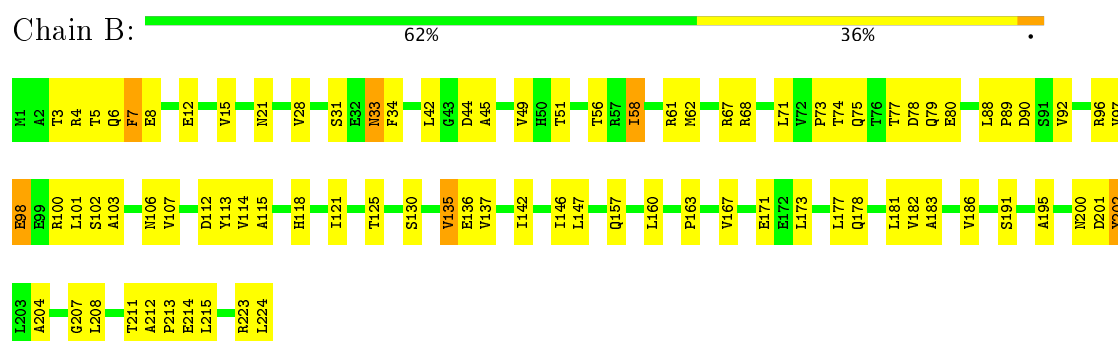
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

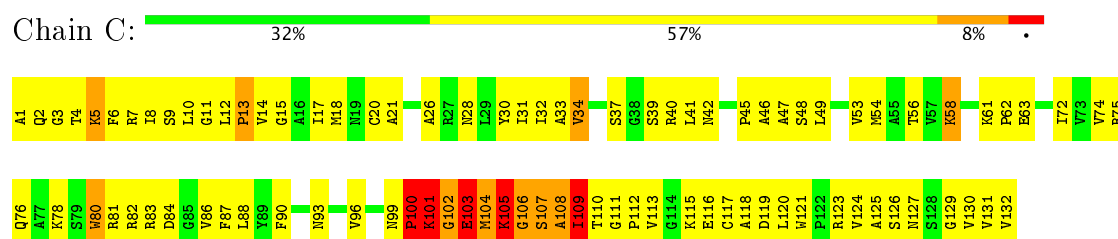
- Molecule 1: SARCIN-RICIN LOOP



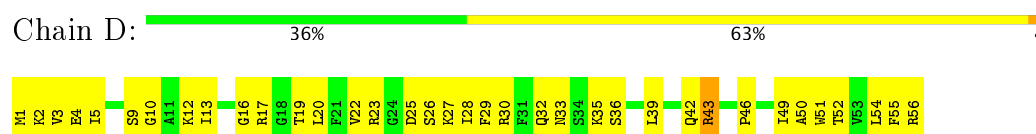
- Molecule 2: EUKARYOTIC TRANSLATION INITIATION FACTOR 6



- Molecule 3: 60S RIBOSOMAL PROTEIN L23



- Molecule 4: 60S RIBOSOMAL PROTEIN L24-A



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	38900	Depositor
Image detector	KODAK SO-163 FILM	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	0.38	0/671	0.73	2/1043 (0.2%)
2	B	0.45	1/1714 (0.1%)	0.70	1/2331 (0.0%)
3	C	1.70	13/996 (1.3%)	2.62	42/1336 (3.1%)
4	D	1.05	0/472	1.09	0/628
All	All	1.00	14/3853 (0.4%)	1.48	45/5338 (0.8%)

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	1	0
3	C	1	9
All	All	2	9

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	100	PRO	CA-C	22.20	1.97	1.52
3	C	100	PRO	N-CD	19.60	1.75	1.47
3	C	100	PRO	C-O	-11.76	0.99	1.23
3	C	109	ILE	C-N	11.25	1.59	1.34
3	C	105	LYS	N-CA	-8.39	1.29	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	PRO	O-C-N	-36.17	64.83	122.70
3	C	100	PRO	CA-C-O	-30.93	45.97	120.20
3	C	109	ILE	CA-C-N	-24.72	62.82	117.20
3	C	101	LYS	O-C-N	-22.09	85.65	123.20
3	C	103	GLU	O-C-N	-19.42	91.62	122.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2692	G	C1'
3	C	109	ILE	CB

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	100	PRO	Peptide
3	C	101	LYS	Mainchain
3	C	103	GLU	Mainchain,Peptide
3	C	105	LYS	Mainchain
3	C	34	VAL	Mainchain

5.2 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 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	600	0	301	18	0
2	B	1693	0	1688	160	0
3	C	982	0	1034	231	0
4	D	462	0	484	98	0
All	All	3737	0	3507	406	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 56.

The worst 5 of 406 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)
2:B:102:SER:HA	3:C:129:GLY:CA	1.38	1.49
2:B:102:SER:CA	3:C:129:GLY:CA	1.93	1.46
2:B:75:GLN:NE2	4:D:26:SER:HB3	1.30	1.39
2:B:75:GLN:HE22	4:D:26:SER:CB	1.34	1.37
2:B:75:GLN:NE2	4:D:26:SER:O	1.61	1.32

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 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	
2	B	222/224 (99%)	208 (94%)	13 (6%)	1 (0%)	32	74
3	C	128/132 (97%)	115 (90%)	9 (7%)	4 (3%)	5	37
4	D	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	404/412 (98%)	375 (93%)	24 (6%)	5 (1%)	20	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	37	SER
3	C	101	LYS
3	C	105	LYS
2	B	58	ILE
3	C	13	PRO

5.3.2 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 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	
2	B	192/192 (100%)	187 (97%)	5 (3%)	51	75
3	C	102/102 (100%)	95 (93%)	7 (7%)	18	51
4	D	49/49 (100%)	48 (98%)	1 (2%)	60	82
All	All	343/343 (100%)	330 (96%)	13 (4%)	42	67

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5	LYS
3	C	42	ASN
3	C	105	LYS
2	B	186	VAL
3	C	103	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
2	B	83	HIS
3	C	2	GLN
2	B	79	GLN
2	B	178	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	27/28 (96%)	0	1 (3%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2692	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	99:ASN	C	100:PRO	N	2.18