



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J16
EMDB ID: : EMD-2010
Title : Models of ribosome-bound Dom34p and Rli1p and their ribosomal binding partners
Authors : Becker, T.; Franckenberg, S.; Wickles, S.; Shoemaker, C.J.; Anger, A.M.; Armache, J.-P.; Sieber, H.; Ungewickell, C.; Berninghausen, O.; Daberkow, I.; Karcher, A.; Thomm, M.; Hopfner, K.-P.; Green, R.; Beckmann, R.
Deposited on : 2011-12-12
Resolution : 7.20 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 : 1.7.1 (RC1), CSD as537be (2016)
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

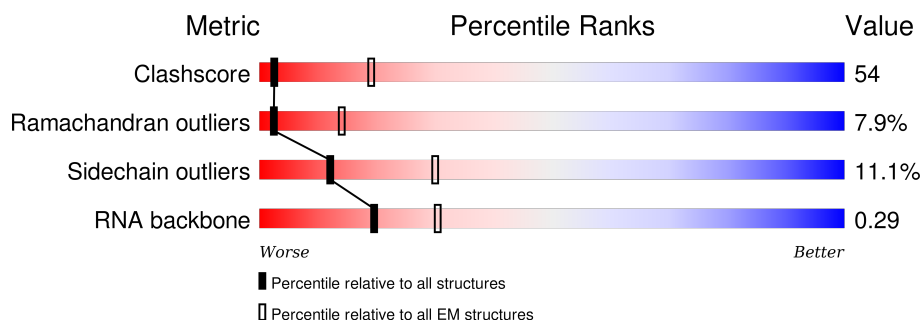
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	386	50% 34% 11% 5%
2	B	608	32% 60% 7% .
3	J	233	. 34% 44% 18%
4	K	155	. 26% 49% 24%
5	L	75	. 41% 41% 15%
6	F	191	52% 35% 12% .
7	E	63	48% 29% 10% . 13%
8	G	312	40% 15% 5% . 36%

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Mol	Chain	Length	Quality of chain
9	C	236	
10	H	165	
11	I	137	
12	D	135	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	MG	B	701	-	-	X	-
14	ATP	B	702	-	-	X	-
15	SF4	B	703	-	-	X	-
15	SF4	B	704	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26208 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 Dom34p.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	386	Total	C	N	O	S	0	0
			3097	1996	483	603	15		

- Molecule 2 is a protein called Rli1p.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	608	Total	C	N	O	S	0	0
			4804	3065	831	884	24		

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	233	Total	C	N	O	P	0	0
			4942	2222	899	1598	223		

- Molecule 4 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	155	Total	C	N	O	P	0	0
			3286	1476	591	1069	150		

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	75	Total	C	N	O	P	0	0
			1595	712	280	529	74		

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	191	Total	C	N	O	S	0	0
			1519	963	274	278	4		

- Molecule 7 is a protein called 40S ribosomal protein S30E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	55	Total	C	N	O	S	0	0
			440	277	90	72	1		

- Molecule 8 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	199	Total	C	N	O	S	0	0
			1541	986	268	282	5		

- Molecule 9 is a protein called 40S ribosomal protein S6E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	138	Total	C	N	O	S	0	0
			1037	651	190	194	2		

- Molecule 11 is a protein called 40S ribosomal protein S24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	136	Total	C	N	O	S	0	0
			1004	628	189	180	7		

- Molecule 12 is a protein called 40S ribosomal protein S24-A.

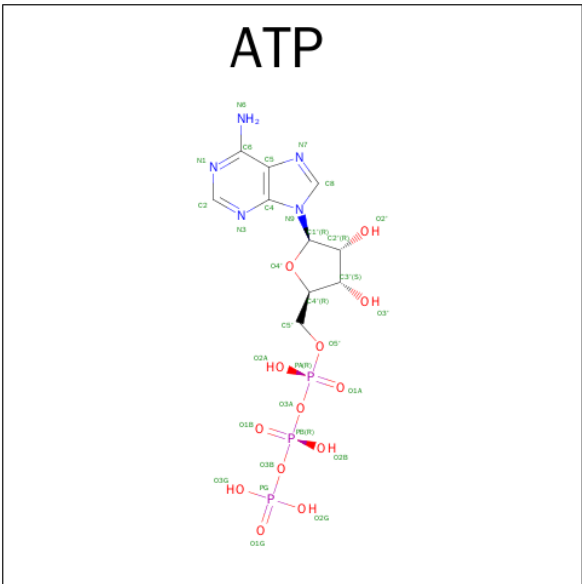
Mol	Chain	Residues	Atoms				AltConf	Trace
12	D	134	Total	C	N	O	0	0
			1074	676	208	190		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total	Mg	0
			1	1	

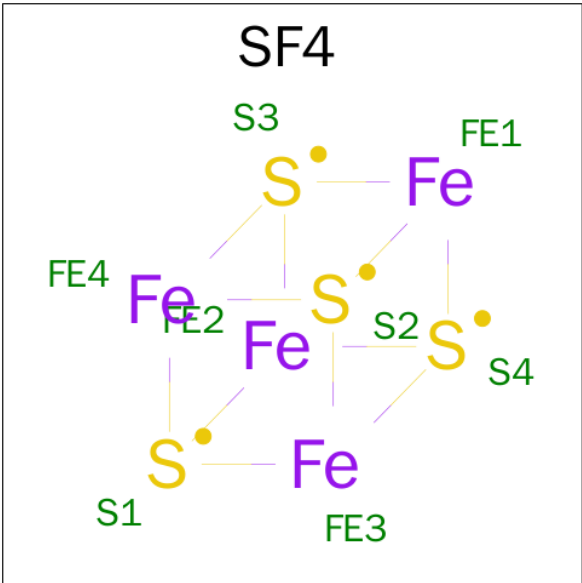
- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	Fe	S	0
			16	8	8	
15	B	1	Total	Fe	S	0
			16	8	8	

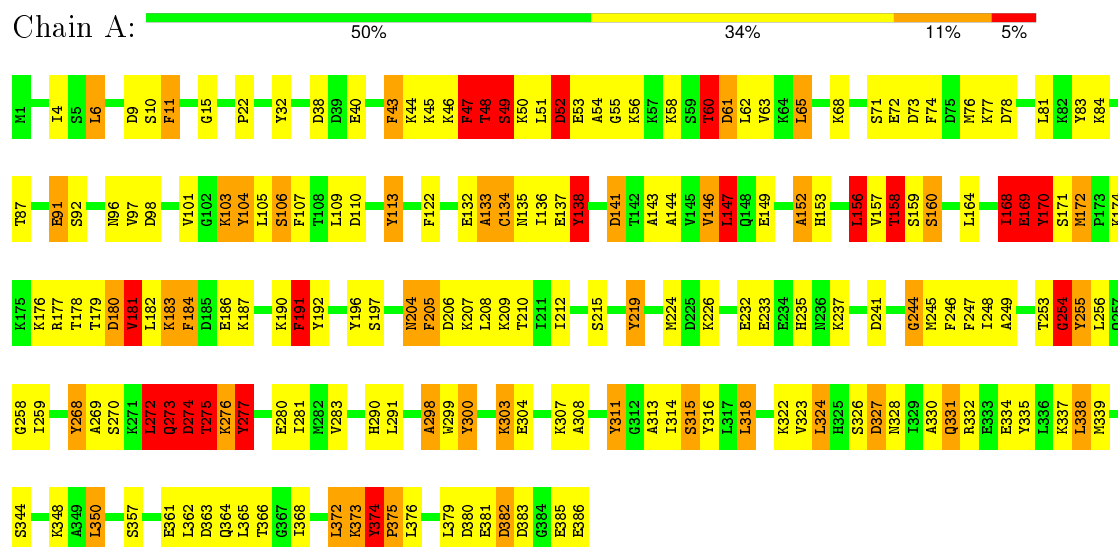
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total	O	0
			1	1	

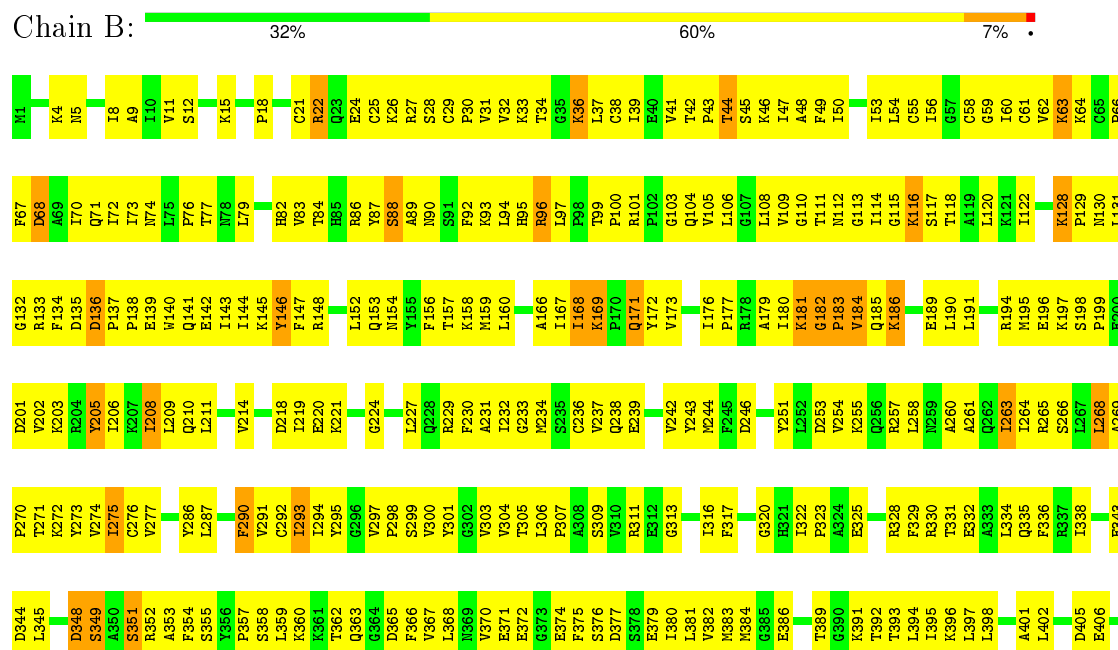
3 Residue-property plots

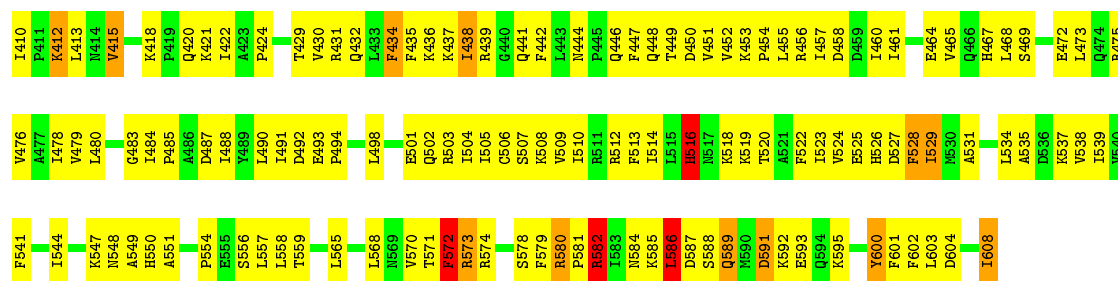
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Dom34p

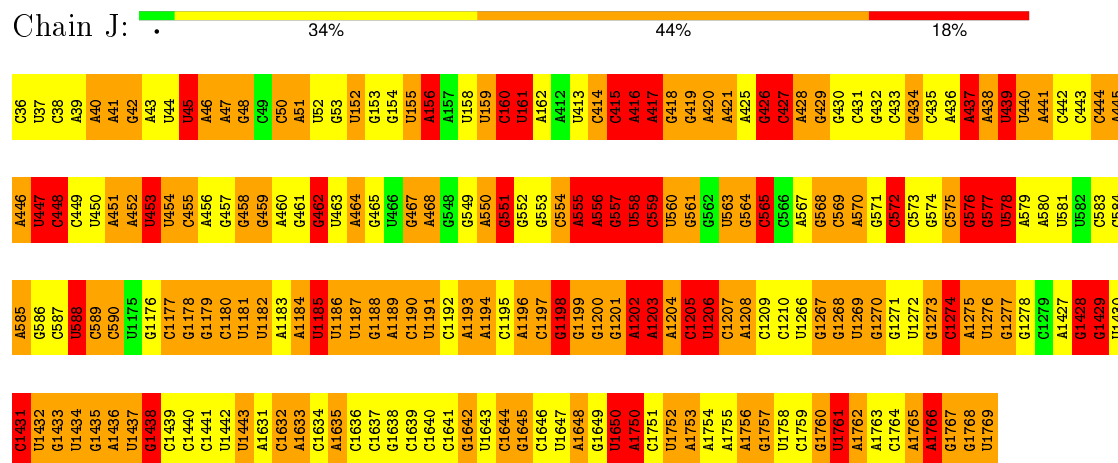


• Molecule 2: Rli1p

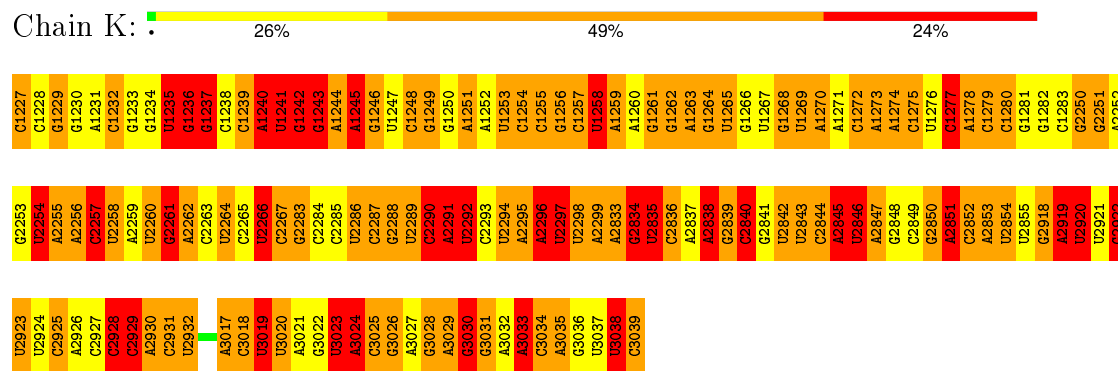




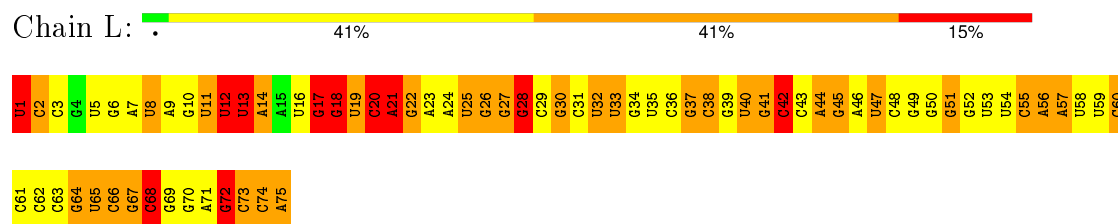
• Molecule 3: 28S ribosomal RNA



• Molecule 4: 18S ribosomal RNA

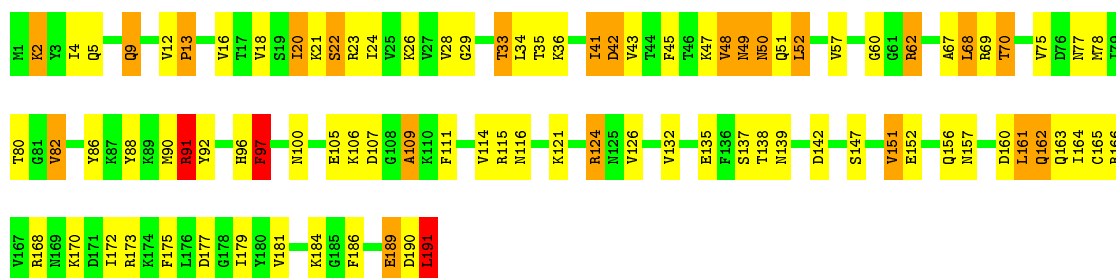


• Molecule 5: P-site tRNA



• Molecule 6: 60S ribosomal protein L6





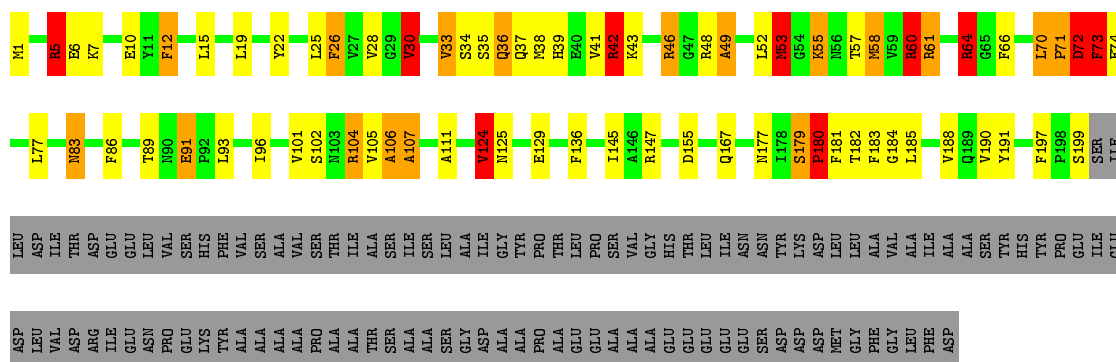
- Molecule 7: 40S ribosomal protein S30E

Chain E: 48% 29% 10% 13%



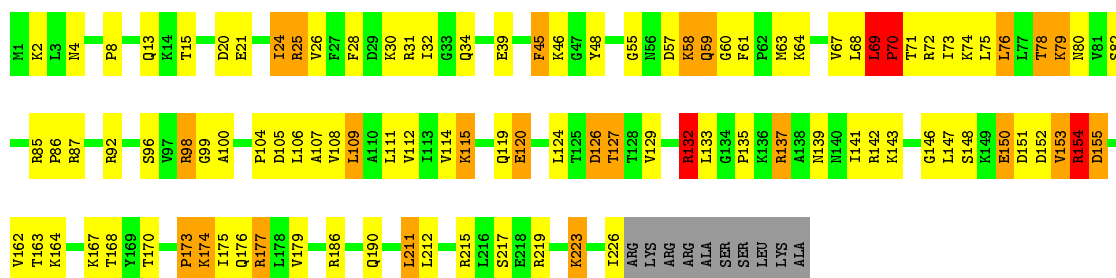
- Molecule 8: 60S ribosomal protein L10

Chain G: 40% 15% 5% 36%



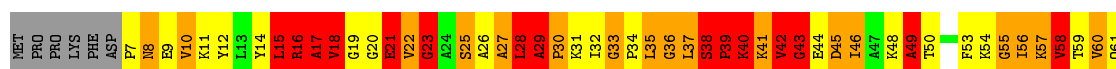
- Molecule 9: 40S ribosomal protein S6E

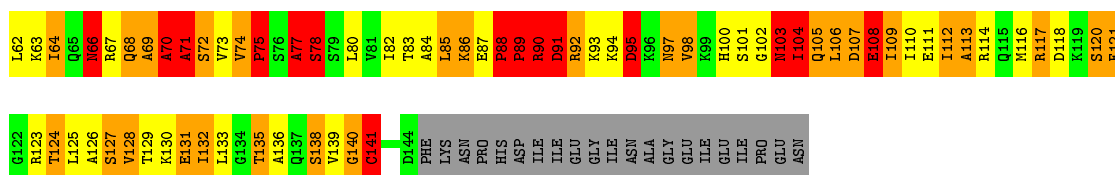
Chain C: 52% 32% 10%



- Molecule 10: 60S ribosomal protein L11

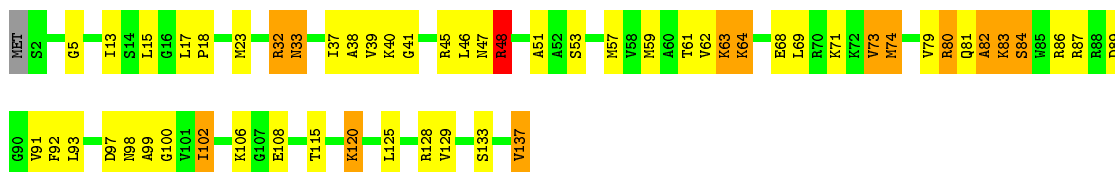
Chain H: 12% 27% 27% 18% 16%





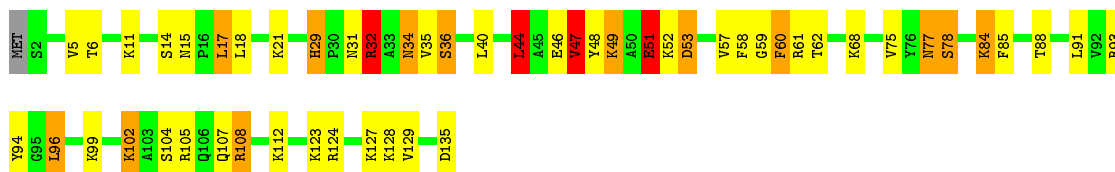
- Molecule 11: 40S ribosomal protein S24E

Chain I: 58% 31% 9% ..



- Molecule 12: 40S ribosomal protein S24-A

Chain D: 60% 27% 10% ..



4 Experimental information

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	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, ATP

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	1.68	20/3149 (0.6%)	2.15	114/4230 (2.7%)
10	H	2.17	9/1048 (0.9%)	2.61	95/1408 (6.7%)
11	I	1.01	2/1019 (0.2%)	1.04	4/1369 (0.3%)
12	D	0.68	1/1088 (0.1%)	0.87	4/1449 (0.3%)
2	B	0.99	6/4893 (0.1%)	1.18	19/6603 (0.3%)
3	J	1.80	184/5523 (3.3%)	2.28	379/8591 (4.4%)
4	K	1.79	103/3671 (2.8%)	2.46	282/5709 (4.9%)
5	L	2.52	94/1781 (5.3%)	2.58	165/2775 (5.9%)
6	F	1.03	3/1540 (0.2%)	1.12	9/2073 (0.4%)
7	E	0.95	1/447 (0.2%)	1.29	7/595 (1.2%)
8	G	1.73	17/1568 (1.1%)	2.33	55/2119 (2.6%)
9	C	0.70	2/1844 (0.1%)	0.84	2/2464 (0.1%)
All	All	1.58	442/27571 (1.6%)	1.99	1135/39385 (2.9%)

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	18
10	H	0	13
12	D	0	1
2	B	0	4
3	J	0	25
4	K	0	20
5	L	0	5
6	F	0	2
7	E	0	2
8	G	0	13
All	All	0	103

The worst 5 of 442 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	88	PRO	CG-CD	50.97	3.18	1.50
5	L	41	G	C2'-C1'	-21.76	1.29	1.53
8	G	5	ARG	C-O	-20.62	0.84	1.23
5	L	22	G	C2'-C1'	-15.84	1.35	1.53
8	G	72	ASP	C-O	-15.71	0.93	1.23

The worst 5 of 1135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2845	A	N1-C6-N6	40.71	143.02	118.60
4	K	2845	A	C6-N1-C2	39.69	142.41	118.60
4	K	2845	A	C5-C6-N1	-35.84	99.78	117.70
8	G	5	ARG	O-C-N	-35.31	66.20	122.70
10	H	88	PRO	N-CD-CG	-34.39	51.62	103.20

There are no chirality outliers.

5 of 103 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Sidechain
1	A	113	TYR	Sidechain
1	A	158	THR	Peptide
1	A	170	TYR	Sidechain
1	A	48	THR	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	3097	0	3156	158	0
2	B	4804	0	4938	988	0
3	J	4942	0	2531	522	0
4	K	3286	0	1680	563	0
5	L	1595	0	808	24	0
6	F	1519	0	1587	73	0
7	E	440	0	488	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1541	0	1584	83	0
9	C	1820	0	1916	115	0
10	H	1037	0	1107	283	0
11	I	1004	0	1048	93	0
12	D	1074	0	1132	22	0
13	B	1	0	0	2	0
14	B	31	0	12	40	0
15	B	16	0	0	24	0
16	B	1	0	0	0	0
All	All	26208	0	21987	2612	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 54.

The worst 5 of 2612 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)
10:H:85:LEU:CD2	10:H:87:GLU:H	1.02	1.62
2:B:56:ILE:HG12	15:B:703:SF4:S3	1.41	1.60
8:G:43:LYS:HG2	10:H:121:PHE:CD1	1.31	1.58
8:G:107:ALA:HB3	8:G:183:PHE:CE2	1.36	1.57
10:H:85:LEU:CD2	10:H:86:LYS:H	1.10	1.56

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	384/386 (100%)	289 (75%)	50 (13%)	45 (12%)	0 9
2	B	606/608 (100%)	561 (93%)	29 (5%)	16 (3%)	7 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	189/191 (99%)	167 (88%)	16 (8%)	6 (3%)	5	41
7	E	53/63 (84%)	42 (79%)	7 (13%)	4 (8%)	1	21
8	G	197/312 (63%)	170 (86%)	15 (8%)	12 (6%)	2	26
9	C	224/236 (95%)	190 (85%)	22 (10%)	12 (5%)	2	29
10	H	136/165 (82%)	47 (35%)	35 (26%)	54 (40%)	0	0
11	I	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	26	71
12	D	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	1	14
All	All	2055/2233 (92%)	1696 (82%)	196 (10%)	163 (8%)	2	19

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	15	GLY
1	A	46	LYS
1	A	48	THR
1	A	56	LYS

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	
1	A	348/348 (100%)	318 (91%)	30 (9%)	13	47
2	B	537/537 (100%)	517 (96%)	20 (4%)	41	73
6	F	171/171 (100%)	133 (78%)	38 (22%)	1	9
7	E	48/54 (89%)	40 (83%)	8 (17%)	3	19
8	G	167/254 (66%)	161 (96%)	6 (4%)	42	74
9	C	193/201 (96%)	154 (80%)	39 (20%)	1	11
10	H	112/136 (82%)	96 (86%)	16 (14%)	4	25
11	I	104/105 (99%)	88 (85%)	16 (15%)	3	22
12	D	112/113 (99%)	86 (77%)	26 (23%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1792/1919 (93%)	1593 (89%)	199 (11%)	12	34

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	26	LYS
9	C	78	THR
12	D	57	VAL
7	E	29	LYS
8	G	89	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	463	GLN
6	F	96	HIS
10	H	137	GLN
2	B	589	GLN
6	F	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	J	224/233 (96%)	113 (50%)	26 (11%)
4	K	149/155 (96%)	86 (57%)	13 (8%)
5	L	74/75 (98%)	26 (35%)	10 (13%)
All	All	447/463 (96%)	225 (50%)	49 (10%)

5 of 225 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	J	40	A
3	J	41	A
3	J	42	G
3	J	45	U
3	J	46	A

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	J	1756	A
4	K	1264	G
5	L	44	A
3	J	1765	A
4	K	1272	C

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	ATP	B	702	13	26,33,33	2.11	7 (26%)	26,52,52	3.46	12 (46%)
15	SF4	B	703	2	0,12,12	0.00	-	0,24,24	0.00	-
15	SF4	B	704	2	0,12,12	0.00	-	0,24,24	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	B	702	13	-	0/18/38/38	0/3/3/3
15	SF4	B	703	2	-	0/0/48/48	0/6/5/5
15	SF4	B	704	2	-	0/0/48/48	0/6/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	702	ATP	O5'-C5'	-4.41	1.27	1.44
14	B	702	ATP	PA-O5'	-2.79	1.47	1.59
14	B	702	ATP	PB-O2B	-2.76	1.43	1.55
14	B	702	ATP	C3'-C4'	-2.10	1.47	1.53
14	B	702	ATP	C8-N7	-2.06	1.30	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	702	ATP	O5'-PA-O1A	-6.24	83.69	109.21
14	B	702	ATP	C5'-C4'-C3'	-5.07	95.59	115.20
14	B	702	ATP	O2B-PB-O3A	-4.37	86.54	105.27
14	B	702	ATP	N3-C2-N1	-3.30	126.28	128.87
14	B	702	ATP	C1'-N9-C4	-3.04	123.41	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	702	ATP	40	0
15	B	703	SF4	18	0
15	B	704	SF4	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.