



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:46 PM BST

PDB ID : 4V4V
EMDB ID: : EMD-1056
Title : Structure of a pre-translocational E. coli ribosome obtained by fitting atomic models for RNA and protein components into cryo-EM map EMD-1056
Authors : Mitra, K.; Frank, J.
Deposited on : 2006-05-09
Resolution : 15.00 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

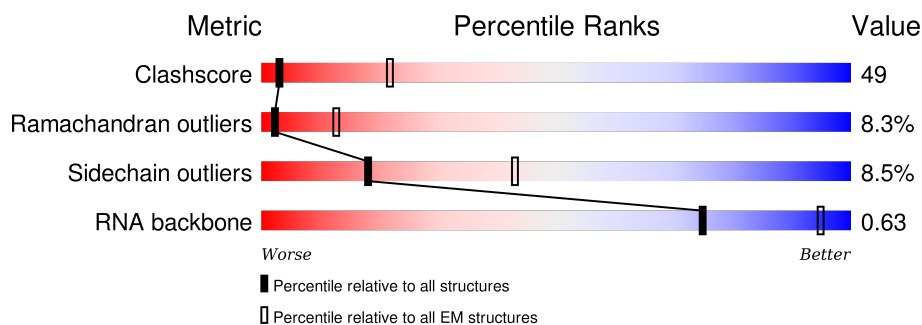
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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.



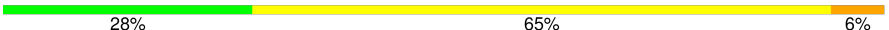


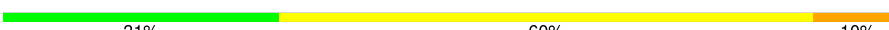
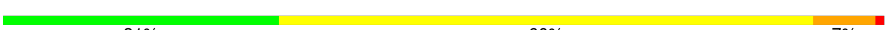
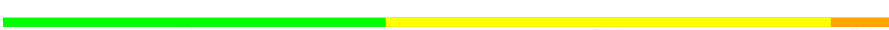




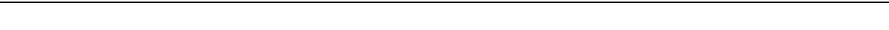

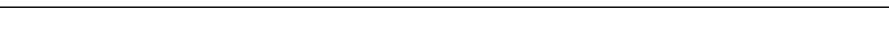
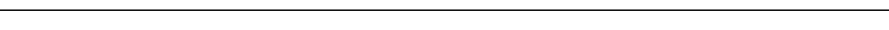


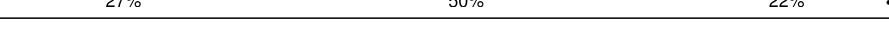




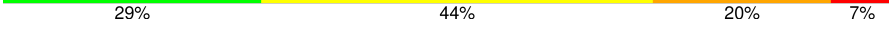


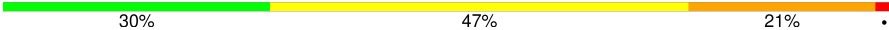
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	AA	1488	<div> <div>38%</div> <div>43%</div> <div>18%</div> <div>.</div> </div>
2	AU	76	<div> <div>41%</div> <div>36%</div> <div>24%</div> </div>
2	AV	76	<div> <div>36%</div> <div>45%</div> <div>20%</div> </div>
2	AW	76	<div> <div>37%</div> <div>43%</div> <div>20%</div> </div>
3	AB	236	<div> <div>45%</div> <div>51%</div> <div>.</div> </div>
4	AC	206	<div> <div>42%</div> <div>49%</div> <div>9%</div> </div>
5	AD	204	<div> <div>38%</div> <div>59%</div> <div>.</div> </div>
6	AE	148	<div> <div>41%</div> <div>55%</div> <div>..</div> </div>


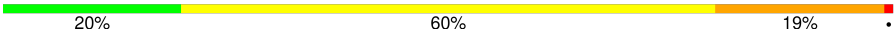
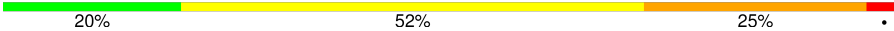



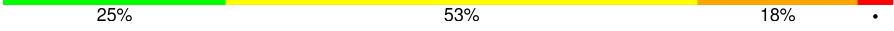



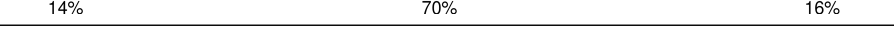
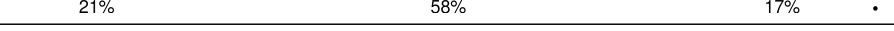





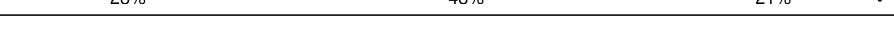

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Mol	Chain	Length	Quality of chain
7	AF	95	
8	AG	137	
9	AH	127	
10	AI	126	
11	AJ	96	
12	AK	116	
13	AL	101	
14	AM	115	
15	AN	61	
16	AO	86	
17	AP	78	
18	AQ	79	
19	AR	69	
20	AS	87	
21	AT	83	
22	B0	2740	
23	B9	108	
24	B2	222	
25	B3	119	
25	B5	119	
26	BA	227	
27	BB	209	
28	BC	198	
29	BD	177	
30	BE	167	

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Mol	Chain	Length	Quality of chain
31	BF	149	 68% 30% .
32	BG	139	 20% 60% 19% .
33	BH	142	 20% 52% 25% .
34	BI	122	 50% 41% 9%
35	BJ	140	 21% 45% 31% .
36	BK	131	 49% 40% 10% .
37	BL	114	 25% 53% 18% .
38	BM	113	 53% 42% 5%
39	BN	114	 11% 48% 38% .
40	BO	115	 8% 57% 30% 5%
41	BQ	106	 14% 70% 16%
42	BR	92	 21% 58% 17% .
43	BS	99	 45% 43% 11% .
44	BT	94	 52% 43% 5%
45	BU	84	 20% 52% 24% .
46	BW	60	 33% 63% .
47	BX	56	 36% 59% 5%
48	BZ	29	 28% 48% 21% .
49	B1	52	 35% 38% 27%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 141668 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1488	Total	C	N	O	P	0	0
			31924	14238	5854	10345	1487		

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AU	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		
2	AV	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		
2	AW	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 3 is a protein called 30S ribosomal subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	236	Total	C	N	O	S	0	0
			1847	1165	328	346	8		

- Molecule 4 is a protein called 30S ribosomal subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 5 is a protein called 30S ribosomal subunit protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	204	Total	C	N	O	S	0	0
			1638	1023	314	297	4		

- Molecule 6 is a protein called 30S ribosomal subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	148	Total	C	N	O	S	0	0
			1093	679	208	200	6		

- Molecule 7 is a protein called 30S ribosomal subunit protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	95	Total	C	N	O	S	0	0
			784	495	143	140	6		

- Molecule 8 is a protein called 30S ribosomal subunit protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	137	Total	C	N	O	S	0	0
			1079	671	204	200	4		

- Molecule 9 is a protein called 30S ribosomal subunit protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	127	Total	C	N	O	S	0	0
			968	610	171	181	6		

- Molecule 10 is a protein called 30S ribosomal subunit protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AI	126	Total	C	N	O	S	0	0
			1014	630	204	177	3		

- Molecule 11 is a protein called 30S ribosomal subunit protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AJ	96	Total	C	N	O	S	0	0
			773	484	148	140	1		

- Molecule 12 is a protein called 30S ribosomal subunit protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AK	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 13 is a protein called 30S ribosomal subunit protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AL	101	Total	C	N	O	S	0	0
			787	486	159	138	4		

- Molecule 14 is a protein called 30S ribosomal subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	115	Total	C	N	O	S	0	0
			892	552	179	158	3		

- Molecule 15 is a protein called 30S ribosomal subunit protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AN	61	Total	C	N	O	S	0	0
			500	310	108	80	2		

- Molecule 16 is a protein called 30S ribosomal subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AO	86	Total	C	N	O	S	0	0
			697	430	139	127	1		

- Molecule 17 is a protein called 30S ribosomal subunit protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AP	78	Total	C	N	O	S	0	0
			622	390	122	109	1		

- Molecule 18 is a protein called 30S ribosomal subunit protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AQ	79	Total	C	N	O	S	0	0
			640	405	119	113	3		

- Molecule 19 is a protein called 30S ribosomal subunit protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	69	Total	C	N	O	S	0	0
			576	362	112	101	1		

- Molecule 20 is a protein called 30S ribosomal subunit protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	87	Total	C	N	O	S	0	0
			695	443	132	118	2		

- Molecule 21 is a protein called 30S ribosomal subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AT	83	Total	C	N	O	S	0	0
			649	401	134	111	3		

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B0	2740	Total	C	N	O	P	0	0
			58824	26239	10826	19019	2740		

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B9	108	Total	C	N	O	P	0	0
			2310	1030	423	750	107		

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B2	222	Total	C	N	O	S	0	0
			1652	1031	301	314	6		

- Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B3	119	Total	C	N	O	S	0	0
			845	531	137	174	3		
25	B5	119	Total	C	N	O	S	0	0
			845	531	137	174	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	227	Total	C	N	O	S	0	0
			1733	1064	352	311	6		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	198	Total	C	N	O	S	0	0
			1531	960	280	287	4		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	177	Total	C	N	O	S	0	0
			1415	902	250	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BE	167	Total	C	N	O	S	0	0
			1253	789	228	234	2		

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BF	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	139	Total	C	N	O	S	0	0
			1019	644	177	192	6		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	122	Total	C	N	O	S	0	0
			939	588	180	166	5		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	140	Total	C	N	O	S	0	0
			1017	632	200	184	1		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	131	Total	C	N	O	S	0	0
			1036	661	200	171	4		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	114	Total	C	N	O	S	0	0
			908	564	184	156	4		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	BM	113	Total	C	N	O	0	0
			864	534	174	156		

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	115	Total	C	N	O	0	0
			937	598	190	149		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	106	Total	C	N	O	S	0	0
			825	512	162	149	2		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	92	Total	C	N	O	S	0	0
			717	455	132	129	1		

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	99	Total	C	N	O	S	0	0
			762	480	143	139			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BW	60	Total	C	N	O	S	0	0
			495	305	96	92	2		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BX	56	Total	C	N	O	S	0	0
			435	272	84	77	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	BZ	29	Total	C	N	O	0	0
			234	145	47	42		

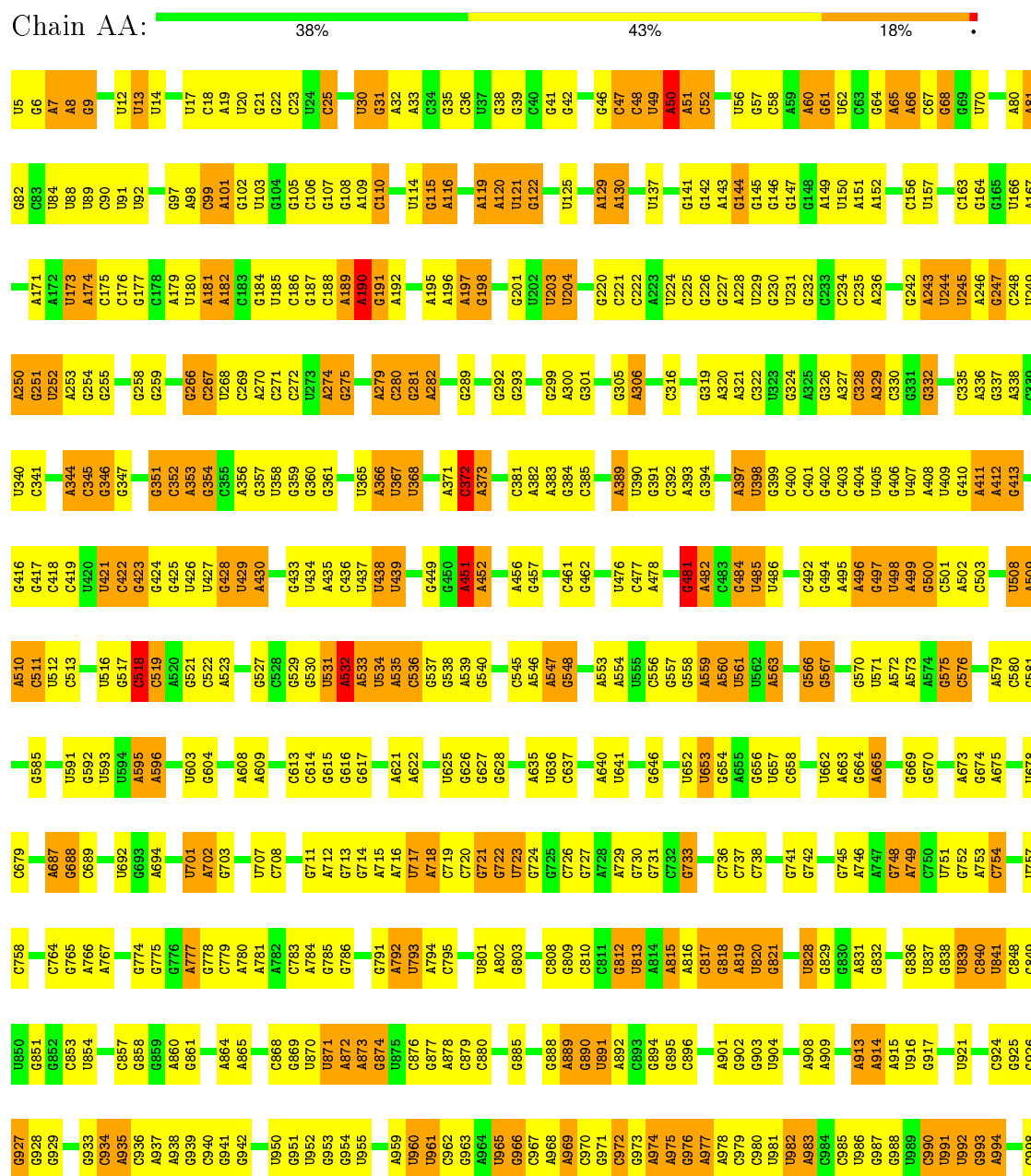
- Molecule 49 is a protein called 50S ribosomal protein L33.

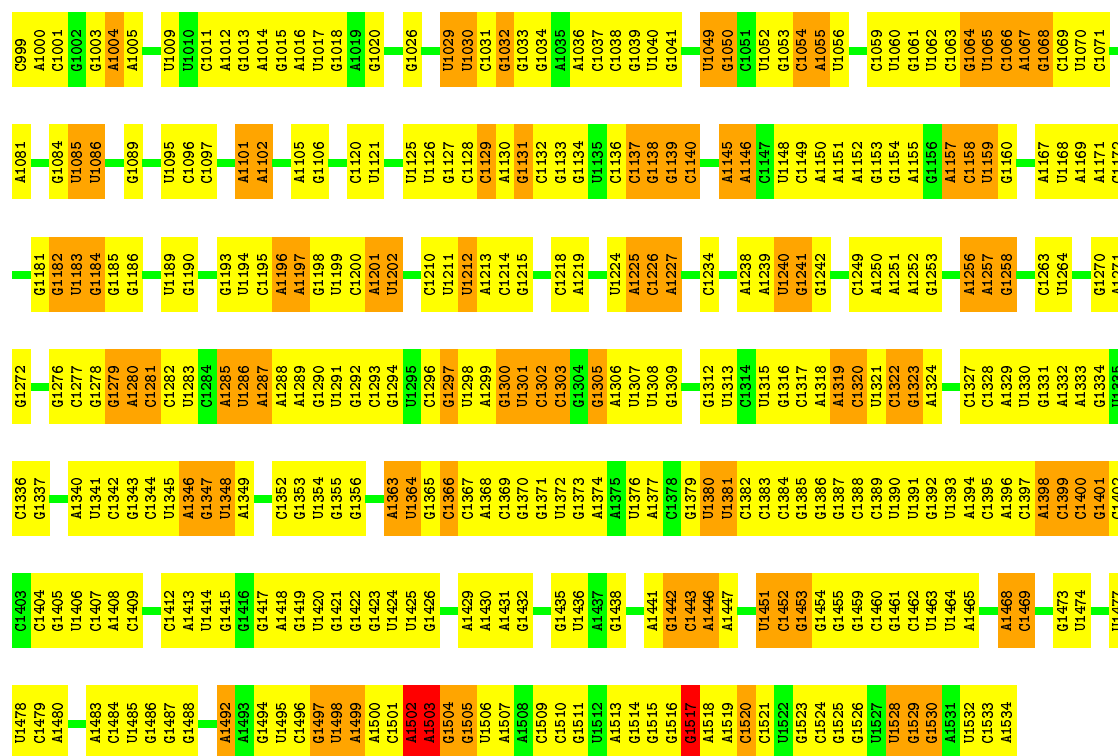
Mol	Chain	Residues	Atoms				AltConf	Trace
49	B1	52	Total	C	N	O	0	0
			424	272	78	74		

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.

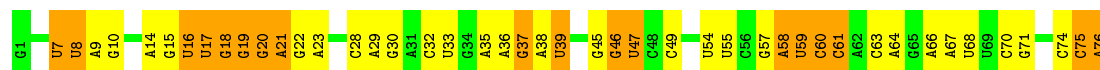
• Molecule 1: 16S ribosomal RNA





- Molecule 2: tRNA

Chain AU: 41% 36% 24%



- Molecule 2: tRNA

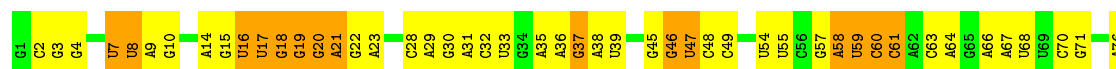
Chain AV: 36% 45% 20%



C74
C75
A76

- Molecule 2: tRNA

Chain AW: 37% 43% 20%

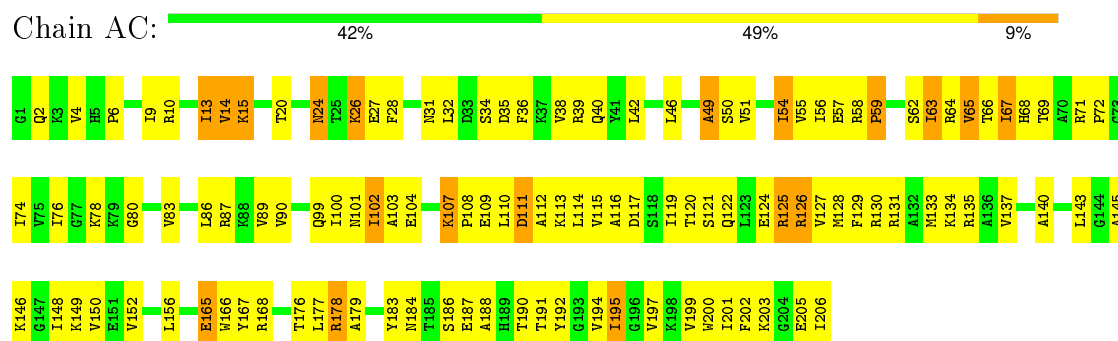


- Molecule 3: 30S ribosomal subunit protein S2

Chain AB: 45% 51% 4%



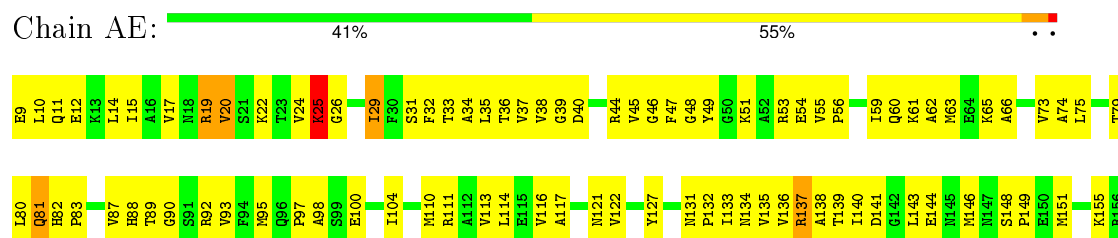
• Molecule 4: 30S ribosomal subunit protein S3



• Molecule 5: 30S ribosomal subunit protein S4

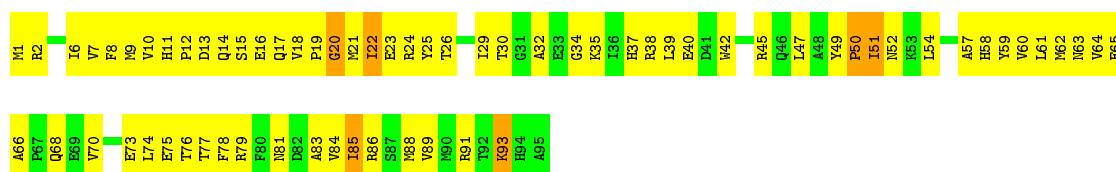


• Molecule 6: 30S ribosomal subunit protein S5



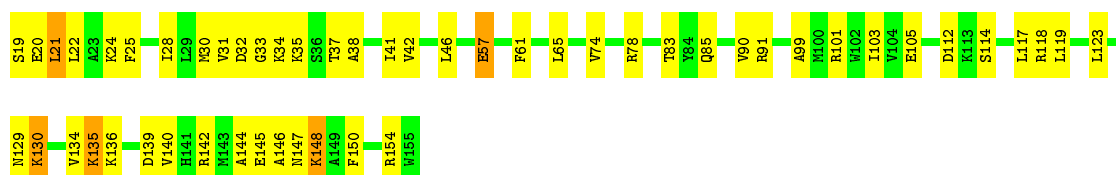
• Molecule 7: 30S ribosomal subunit protein S6





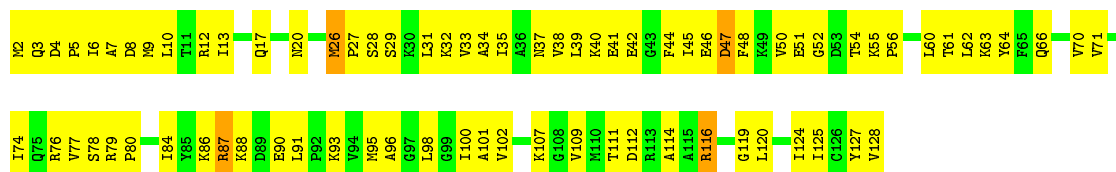
• Molecule 8: 30S ribosomal subunit protein S7

Chain AG: 62% 34%



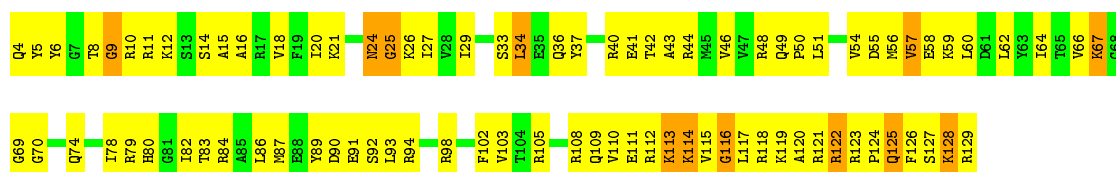
• Molecule 9: 30S ribosomal subunit protein S8

Chain AH: 39% 58%



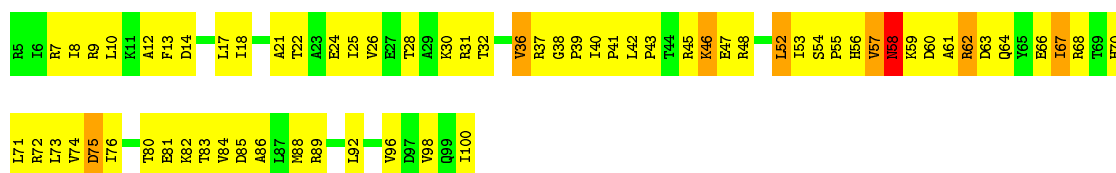
• Molecule 10: 30S ribosomal subunit protein S9

Chain AI: 31% 60% 10%



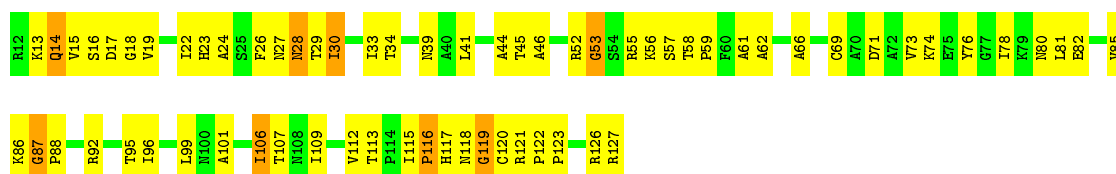
• Molecule 11: 30S ribosomal subunit protein S10

Chain AJ: 31% 60% 7%



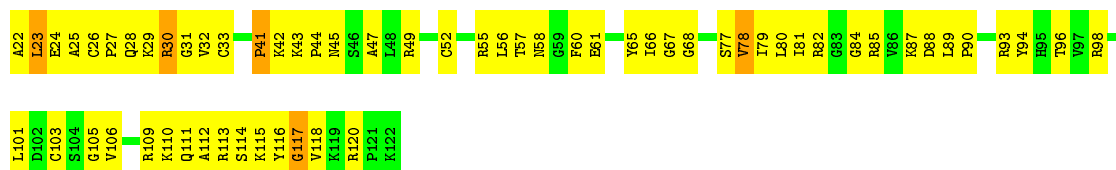
• Molecule 12: 30S ribosomal subunit protein S11

Chain AK: 43% 50% 7%



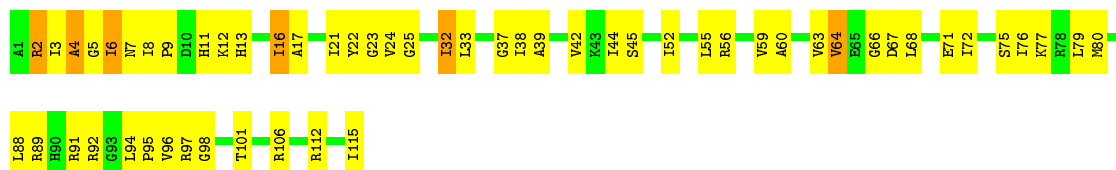
- Molecule 13: 30S ribosomal subunit protein S12

Chain AL: 40% 55% 5%



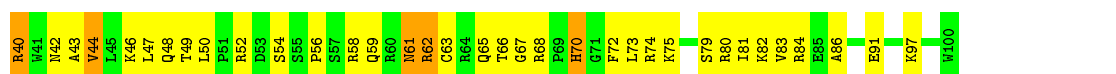
- Molecule 14: 30S ribosomal subunit protein S13

Chain AM: 51% 43% 5%



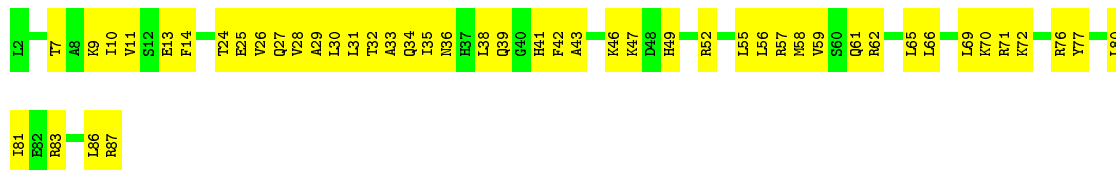
- Molecule 15: 30S ribosomal subunit protein S14

Chain AN: 43% 49% 8%



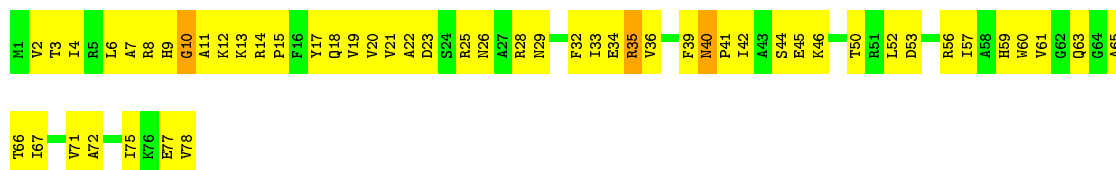
- Molecule 16: 30S ribosomal subunit protein S15

Chain AO: 44% 56%

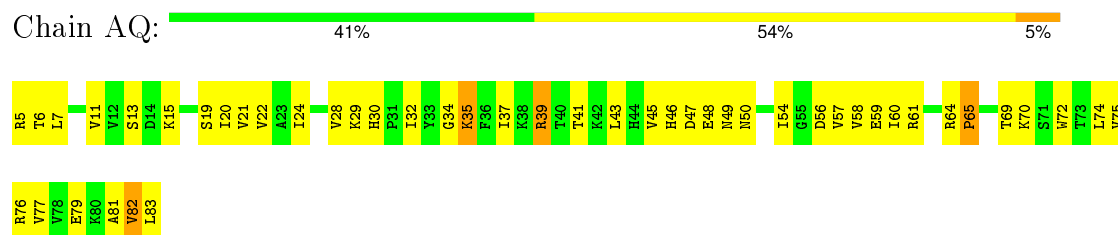


- Molecule 17: 30S ribosomal subunit protein S16

Chain AP: 32% 64%



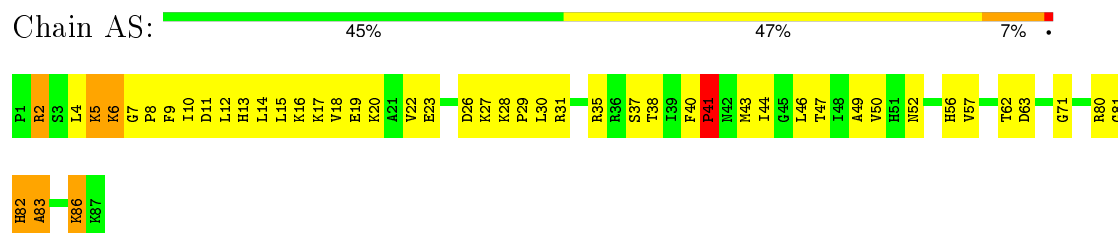
- Molecule 18: 30S ribosomal subunit protein S17



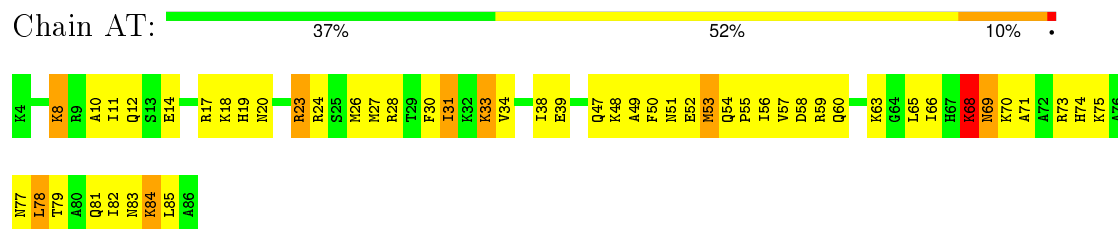
- Molecule 19: 30S ribosomal subunit protein S18



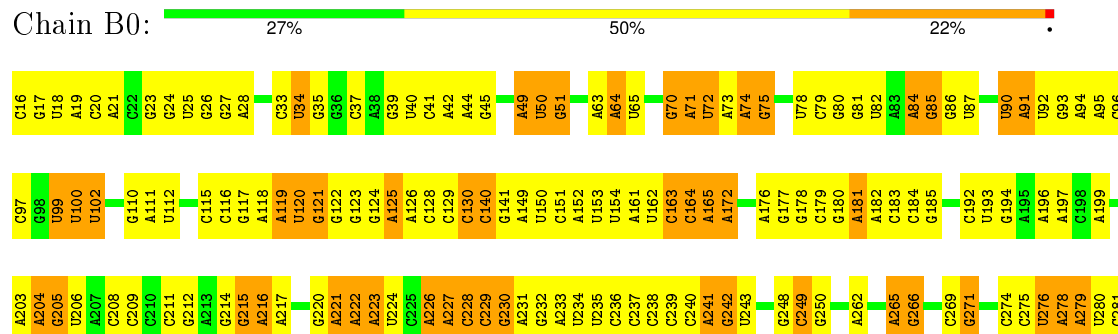
- Molecule 20: 30S ribosomal subunit protein S19



- Molecule 21: 30S ribosomal subunit protein S20

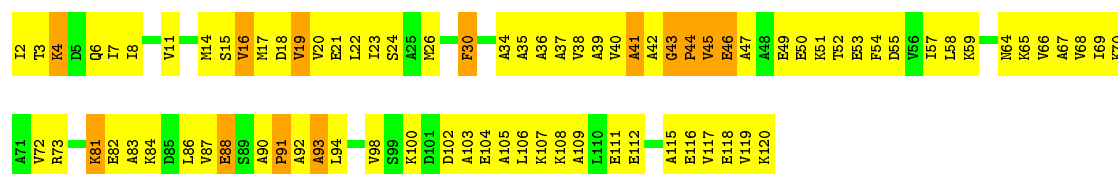


- Molecule 22: 23S ribosomal RNA



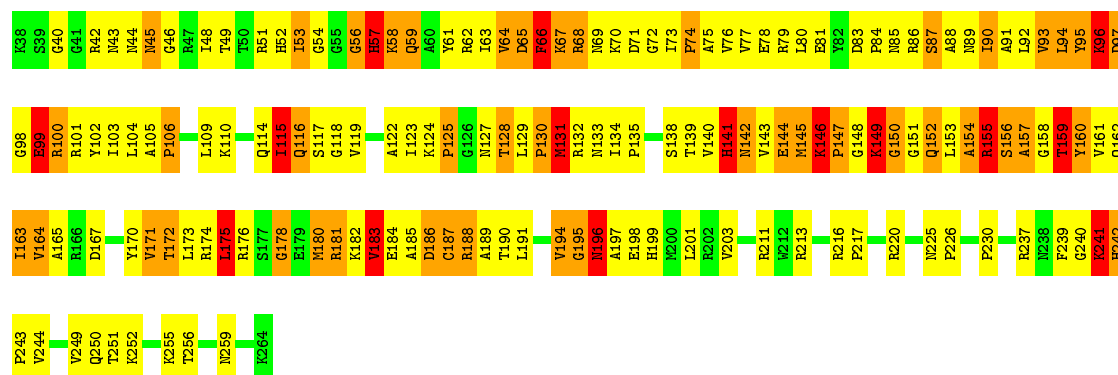
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U1402	G1331	G1266	G1200	G1124	G1055	A989	U913	U942	G769	G709	U641	U571	U499	C418	C351	U284
G1403	G1332	U1267	U1201	G1125	G1056	G988	G917	G943	G770	U709	U641	U571	G500	U419	A352	G285
C1404	G1333	A1268	G1202	A1126	A1057	A990	A918	A844	G771	U710	A644	A572	A501	C420	C353	U286
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U1408	U1340	U1273	U1209	U1130	U1061	G994	A925	U850	G775	U714	G649	U576	A506	C358	U357	U290
G1409	U1341	U1274	G1210	U1132	G1062	A996	G926	C951	G776	A715	G650	U580	G506	A432	U358	G291
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	U2402	U2335	U2478	U2394	U2253	U2253	U2173	C2046	U1979	U1913	G1756	A1665	C1595	C1515	C1515
	U2403	U2336	U2479	U2395	U2254	U2254	C2174	G2047	G1980	A1914	G1757	A1666	A1596	A1516	A1516
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	U2419	U2352	U2495	U2411	U2270	U2270	U2190								
	U2420	U2353	U2496	U2412	U2271	U2271	U2191								
	U2421	U2354	U2497	U2413	U2272	U2272	U2192								
	U2422	U2355	U2498	U2414	U2273	U2273	U2193								
	U2423	U2356	U2499	U2415	U2274	U2274	U2194								
	U2424	U2357	U2500	U2416	U2275	U2275	U2195								
	U2425	U2358	U2501	U2417	U2276	U2276	U2196								
	U2426	U2359	U2502	U2418	U2277	U2277	U2197								
	U2427	U2360	U2503	U2419	U2278	U2278	U2198								
	U2428	U2361	U2504	U2420	U2279	U2279	U2199								
	U2429	U2362	U2505	U2421	U2280	U2280	U2200								
	U2430	U2363	U2506	U2422	U2281	U2281	U2201								
	U2431	U2364		U2423	U2282	U2282	U2202								
	U2432	U2365		U2434	U2283	U2283	U2203								
	U2433	U2366		U2435	U2284	U2284	U2204								
	U2434	U2367		U2436	U2285	U2285	U2205								
	U2435	U2368		U2437	U2286	U2286	U2206								
	U2436	U2369		U2438	U2287	U2287	U2207								
	U2437	U2370		U2439	U2288	U2288	U2208								
	U2438	U2371		U2440	U2289	U2289	U2209								
	U2439	U2372		U2441	U2290	U2290	U2210								
	U2440	U2373		U2442	U2291	U2291	U2211								
	U2441	U2374		U2443	U2292	U2292	U2212								
	U2442	U2375		U2444	U2293	U2293	U2213								
	U2443	U2376		U2445	U2294	U2294	U2214								
	U2444	U2377		U2446	U2295	U2295	U2215								
	U2445	U2378		U2447	U2296	U2296	U2216								
	U2446	U2379		U2448	U2297	U2297	U2217								



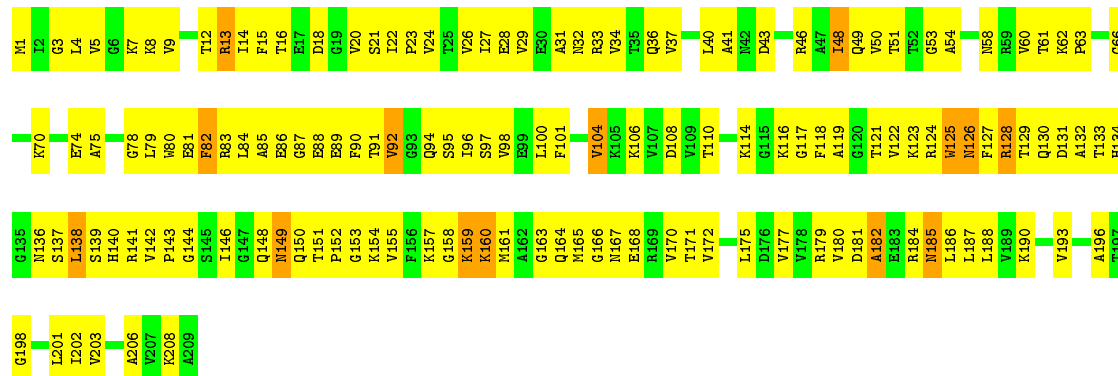
• Molecule 26: 50S ribosomal protein L2

Chain BA: 29% 44% 20% 7%



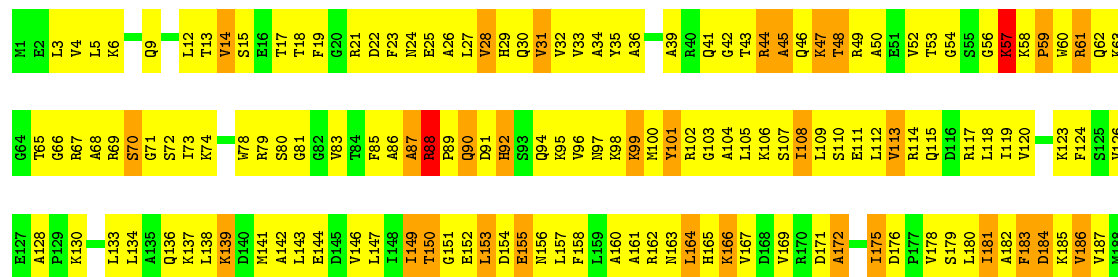
• Molecule 27: 50S ribosomal protein L3

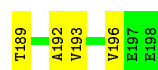
Chain BB: 31% 62% 7%



• Molecule 28: 50S ribosomal protein L4

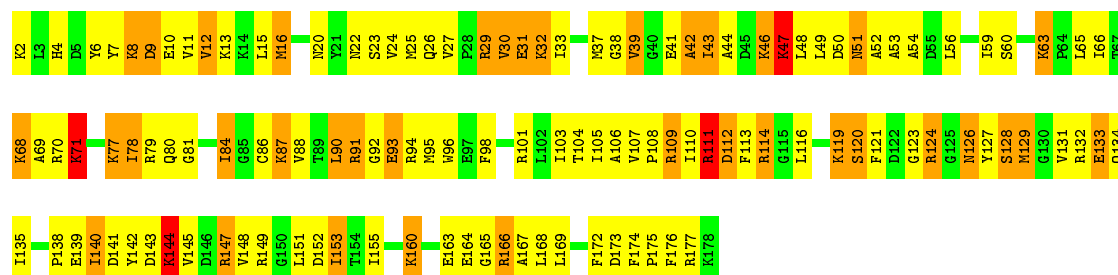
Chain BC: 23% 61% 15%





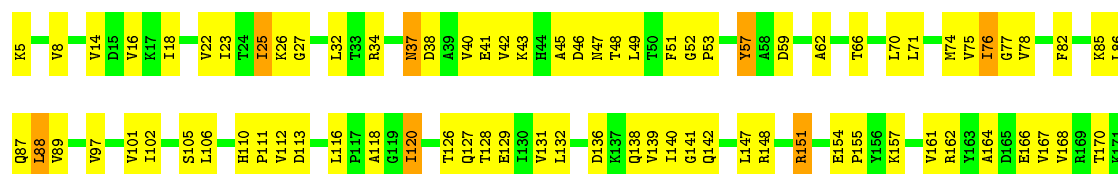
- Molecule 29: 50S ribosomal protein L5

Chain BD: 30% 47% 21%



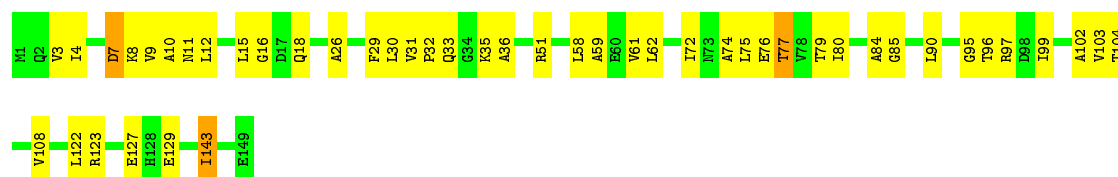
- Molecule 30: 50S ribosomal protein L6

Chain BE: 52% 44%



- Molecule 31: 50S ribosomal protein L9

Chain BF: 68% 30%



- Molecule 32: 50S ribosomal protein L11

Chain BG: 20% 60% 19%



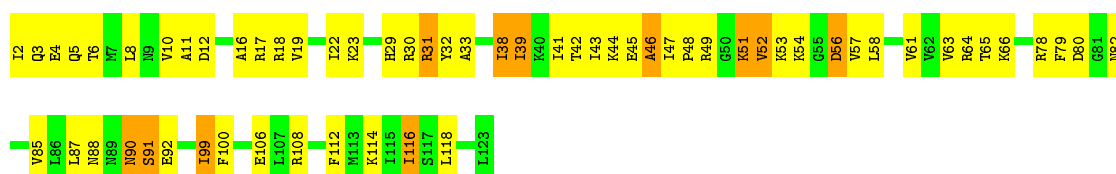
- Molecule 33: 50S ribosomal protein L13

Chain BH: 

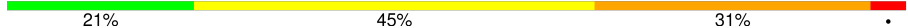


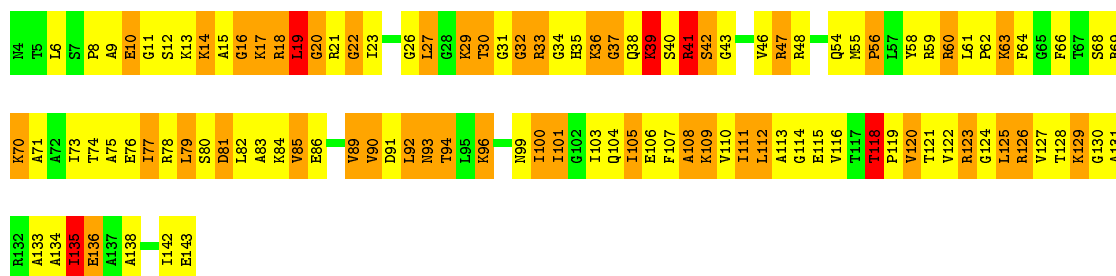
- Molecule 34: 50S ribosomal protein L14

Chain BI: 



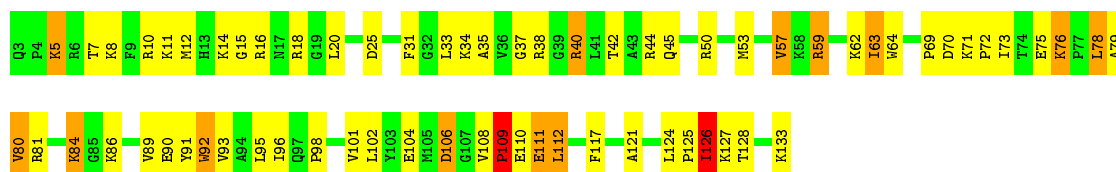
- Molecule 35: 50S ribosomal protein L15

Chain BJ: 



- Molecule 36: 50S ribosomal protein L16

Chain BK: 



- Molecule 37: 50S ribosomal protein L17

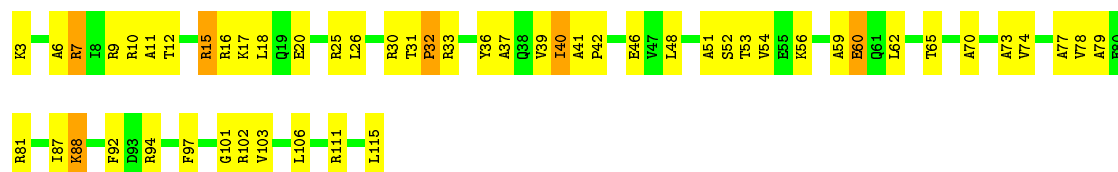
Chain BL: 





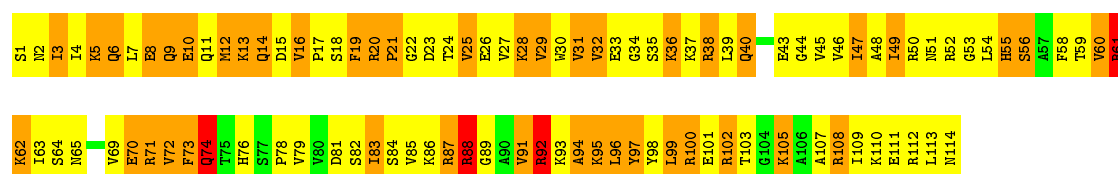
- Molecule 38: 50S ribosomal protein L18

Chain BM: 53% 42% 5%



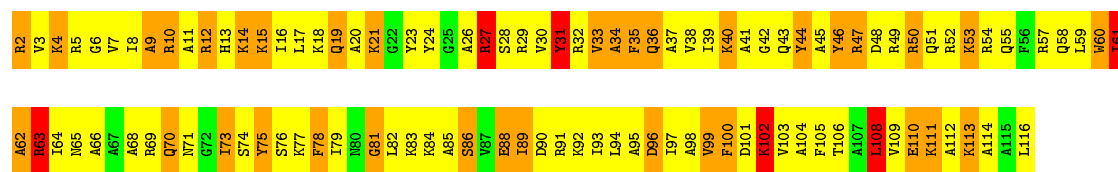
- Molecule 39: 50S ribosomal protein L19

Chain BN: 11% 48% 38%



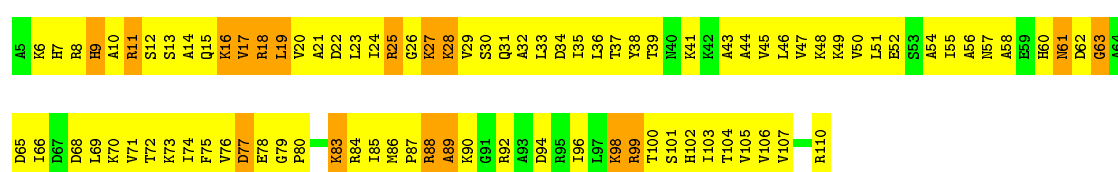
- Molecule 40: 50S RIBOSOMAL PROTEIN L20

Chain BO: 8% 57% 30%



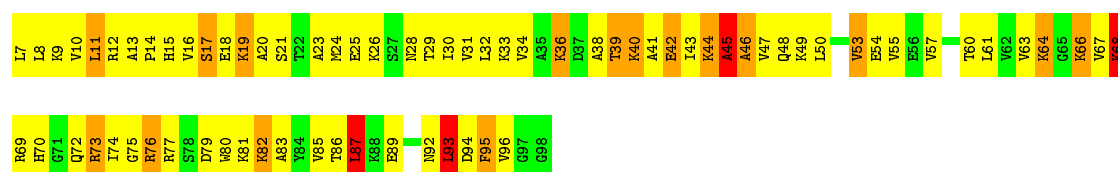
- Molecule 41: 50S ribosomal protein L22

Chain BQ: 14% 70% 16%

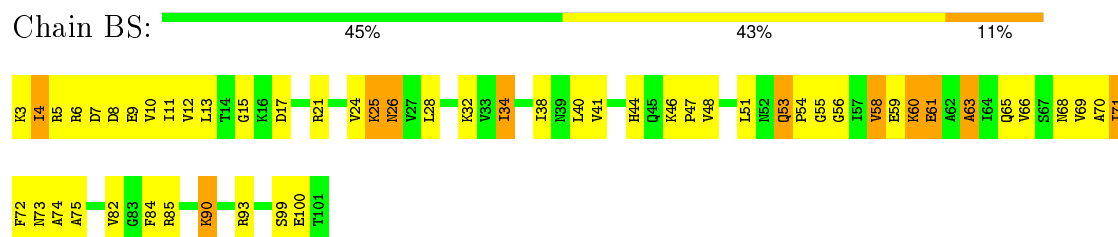


- Molecule 42: 50S ribosomal protein L23

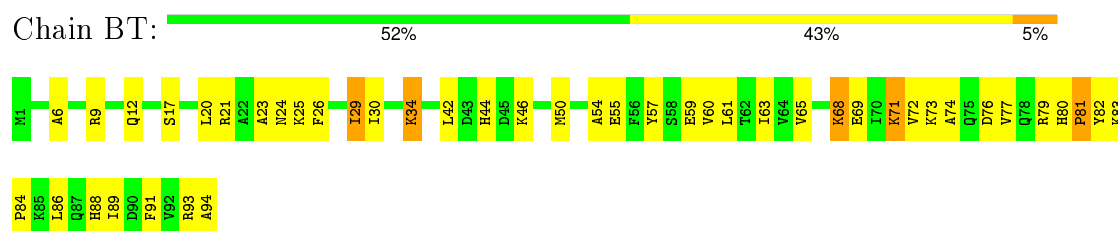
Chain BR: 21% 58% 17%



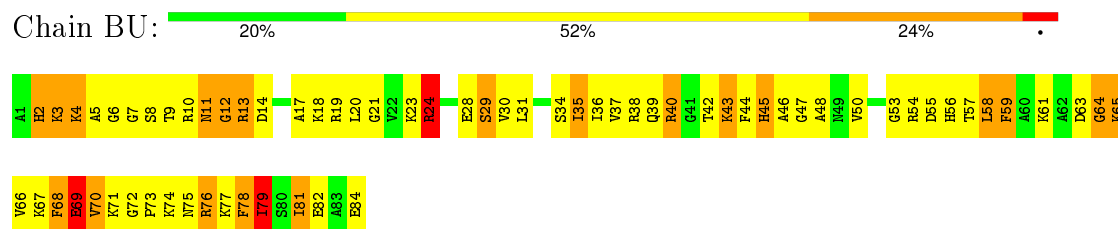
- Molecule 43: 50S ribosomal protein L24



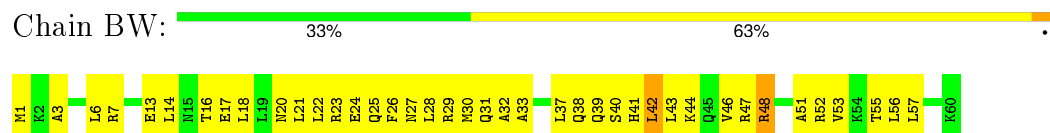
- Molecule 44: 50S ribosomal protein L25



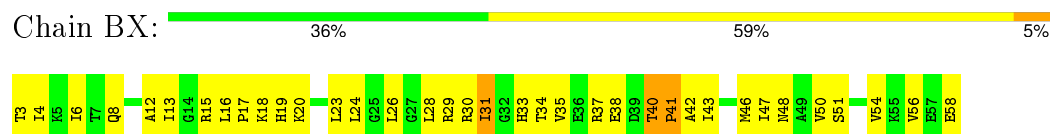
- Molecule 45: 50S ribosomal protein L27



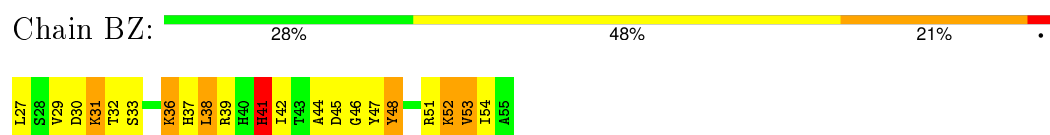
- Molecule 46: 50S ribosomal protein L29



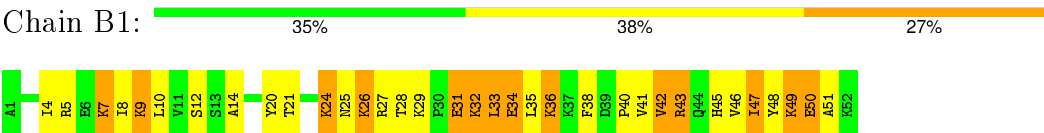
- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



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	CTF correction of 3D-maps by Wiener filtration	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	1.1	Depositor
Maximum defocus (nm)	3.8	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 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	AA	0.31	12/35745 (0.0%)	0.67	10/55764 (0.0%)
10	AI	0.24	0/1026	0.49	1/1364 (0.1%)
11	AJ	0.23	0/783	0.52	0/1058
12	AK	0.25	0/886	0.46	0/1195
13	AL	0.22	0/799	0.46	0/1070
14	AM	0.22	0/900	0.48	0/1201
15	AN	0.25	0/510	0.42	0/679
16	AO	0.23	0/705	0.42	0/942
17	AP	0.26	0/632	0.49	0/848
18	AQ	0.24	0/649	0.47	0/870
19	AR	0.25	0/585	0.40	0/782
2	AU	1.35	6/1814 (0.3%)	2.20	9/2827 (0.3%)
2	AV	0.20	0/1814	0.66	0/2827
2	AW	0.20	0/1814	0.65	0/2827
20	AS	0.25	0/712	0.48	0/955
21	AT	0.26	0/655	0.40	0/866
22	B0	0.41	28/65882 (0.0%)	0.71	50/102783 (0.0%)
23	B9	0.21	0/2583	0.66	0/4028
24	B2	0.46	2/1665 (0.1%)	0.56	1/2240 (0.0%)
25	B3	0.43	0/846	0.67	1/1135 (0.1%)
25	B5	0.23	0/845	0.48	0/1132
26	BA	0.55	2/1759 (0.1%)	0.90	9/2356 (0.4%)
27	BB	0.27	0/1582	0.54	0/2122
28	BC	0.26	0/1549	0.57	0/2082
29	BD	0.26	0/1438	0.54	0/1927
3	AB	0.25	0/1877	0.42	0/2523
30	BE	0.23	0/1273	0.46	0/1725
31	BF	0.24	0/1120	0.47	0/1509
32	BG	0.26	0/1032	0.69	1/1388 (0.1%)
33	BH	0.38	0/1152	0.80	5/1551 (0.3%)
34	BI	0.23	0/948	0.50	0/1269
35	BJ	0.27	0/1025	0.69	0/1363
36	BK	0.26	0/1055	0.52	0/1409
37	BL	0.26	0/920	0.72	2/1229 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BM	0.22	0/873	0.43	0/1170
39	BN	0.28	0/929	0.60	0/1242
4	AC	0.23	0/1652	0.44	0/2225
40	BO	1.30	6/949 (0.6%)	3.63	12/1261 (1.0%)
41	BQ	0.24	0/832	0.69	1/1113 (0.1%)
42	BR	0.25	0/723	0.67	1/965 (0.1%)
43	BS	0.26	0/769	0.50	0/1023
44	BT	0.25	0/766	0.44	0/1025
45	BU	0.28	0/642	0.62	0/848
46	BW	0.23	0/496	0.45	0/658
47	BX	0.24	0/439	0.50	0/587
48	BZ	0.25	0/238	0.53	0/316
49	B1	0.27	0/431	0.51	0/572
5	AD	0.22	0/1660	0.41	0/2220
6	AE	0.24	0/1106	0.44	0/1488
7	AF	0.24	0/802	0.49	0/1081
8	AG	0.23	0/1093	0.42	0/1467
9	AH	0.23	0/978	0.45	0/1311
All	All	0.39	56/153958 (0.0%)	0.75	103/230418 (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	AA	3	0
2	AU	0	1
22	B0	5	12
23	B9	0	1
26	BA	0	1
40	BO	0	1
All	All	8	16

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AU	39	U	C5-C6	32.23	1.63	1.34
22	B0	1499	U	N3-C4	30.48	1.65	1.38
22	B0	2131	U	N3-C4	28.17	1.63	1.38
22	B0	2136	G	C2-N3	26.30	1.53	1.32
2	AU	39	U	N1-C6	25.41	1.60	1.38

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	BO	100	PHE	CZ-CE2-CD2	-70.55	35.44	120.10
40	BO	100	PHE	CD1-CE1-CZ	-68.43	37.99	120.10
2	AU	39	U	N3-C4-C5	-67.79	73.93	114.60
40	BO	100	PHE	CE1-CZ-CE2	-53.38	23.91	120.00
2	AU	39	U	N1-C2-N3	-50.81	84.42	114.90

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	190	A	C1'
1	AA	1502	A	C1'
1	AA	1503	A	C1'
22	B0	301	G	C1'
22	B0	1593	G	C1'

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AU	39	U	Sidechain
22	B0	1417	U	Sidechain
22	B0	1418	G	Sidechain
22	B0	611	C	Sidechain
22	B0	884	U	Sidechain

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	AA	31924	0	16068	1365	0
2	AU	1622	0	820	98	0
2	AV	1622	0	821	63	0
2	AW	1622	0	821	61	0
3	AB	1847	0	1855	113	0
4	AC	1625	0	1699	163	0
5	AD	1638	0	1702	148	0
6	AE	1093	0	1132	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AF	784	0	776	98	0
8	AG	1079	0	1108	48	0
9	AH	968	0	1021	101	0
10	AI	1014	0	1064	148	0
11	AJ	773	0	812	137	0
12	AK	870	0	878	118	0
13	AL	787	0	825	86	0
14	AM	892	0	954	68	0
15	AN	500	0	526	54	0
16	AO	697	0	716	52	0
17	AP	622	0	637	75	0
18	AQ	640	0	678	52	0
19	AR	576	0	599	53	0
20	AS	695	0	725	107	0
21	AT	649	0	697	79	0
22	B0	58824	0	29589	4577	0
23	B9	2310	0	1173	65	0
24	B2	1652	0	1729	250	0
25	B3	845	0	880	418	0
25	B5	845	0	879	165	0
26	BA	1733	0	1766	956	0
27	BB	1565	0	1612	294	0
28	BC	1531	0	1593	456	0
29	BD	1415	0	1451	191	0
30	BE	1253	0	1289	79	0
31	BF	1111	0	1146	40	0
32	BG	1019	0	1076	168	0
33	BH	1129	0	1162	326	0
34	BI	939	0	1011	79	0
35	BJ	1017	0	1086	330	0
36	BK	1036	0	1109	91	0
37	BL	908	0	946	216	0
38	BM	864	0	902	61	0
39	BN	917	0	965	265	0
40	BO	937	0	1008	276	0
41	BQ	825	0	886	176	0
42	BR	717	0	773	166	0
43	BS	762	0	809	91	0
44	BT	753	0	780	39	0
45	BU	634	0	656	204	0
46	BW	495	0	530	53	0
47	BX	435	0	470	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BZ	234	0	235	49	0
49	B1	424	0	461	60	0
All	All	141668	0	94906	11577	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 49.

The worst 5 of 11577 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)
26:BA:155:ARG:CD	26:BA:155:ARG:NE	1.68	1.53
22:B0:1499:U:N3	26:BA:155:ARG:CD	1.67	1.52
22:B0:1083:U:C5'	25:B3:85:ASP:H	1.29	1.45
22:B0:2127:G:H3'	22:B0:2166:U:C5'	1.47	1.45
22:B0:2127:G:C8	22:B0:2166:U:H5''	1.52	1.42

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	
3	AB	230/236 (98%)	192 (84%)	27 (12%)	11 (5%)	3	32
4	AC	204/206 (99%)	159 (78%)	33 (16%)	12 (6%)	2	27
5	AD	202/204 (99%)	180 (89%)	18 (9%)	4 (2%)	9	51
6	AE	146/148 (99%)	139 (95%)	5 (3%)	2 (1%)	14	58
7	AF	93/95 (98%)	81 (87%)	8 (9%)	4 (4%)	3	34
8	AG	135/137 (98%)	126 (93%)	8 (6%)	1 (1%)	26	71
9	AH	125/127 (98%)	114 (91%)	10 (8%)	1 (1%)	24	69
10	AI	124/126 (98%)	101 (82%)	14 (11%)	9 (7%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AJ	94/96 (98%)	75 (80%)	13 (14%)	6 (6%)	2	25
12	AK	114/116 (98%)	96 (84%)	10 (9%)	8 (7%)	1	22
13	AL	99/101 (98%)	76 (77%)	18 (18%)	5 (5%)	2	30
14	AM	111/115 (96%)	100 (90%)	7 (6%)	4 (4%)	4	38
15	AN	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	23
16	AO	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
17	AP	76/78 (97%)	69 (91%)	6 (8%)	1 (1%)	15	60
18	AQ	77/79 (98%)	69 (90%)	6 (8%)	2 (3%)	7	45
19	AR	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
20	AS	85/87 (98%)	67 (79%)	12 (14%)	6 (7%)	1	22
21	AT	81/83 (98%)	68 (84%)	11 (14%)	2 (2%)	7	46
24	B2	216/222 (97%)	174 (81%)	29 (13%)	13 (6%)	2	26
25	B3	114/119 (96%)	90 (79%)	12 (10%)	12 (10%)	1	12
25	B5	113/119 (95%)	87 (77%)	16 (14%)	10 (9%)	1	17
26	BA	217/227 (96%)	121 (56%)	47 (22%)	49 (23%)	0	2
27	BB	199/209 (95%)	157 (79%)	30 (15%)	12 (6%)	2	26
28	BC	194/198 (98%)	127 (66%)	41 (21%)	26 (13%)	0	7
29	BD	173/177 (98%)	94 (54%)	51 (30%)	28 (16%)	0	5
30	BE	165/167 (99%)	147 (89%)	16 (10%)	2 (1%)	16	61
31	BF	143/149 (96%)	121 (85%)	17 (12%)	5 (4%)	4	39
32	BG	135/139 (97%)	80 (59%)	37 (27%)	18 (13%)	0	7
33	BH	140/142 (99%)	78 (56%)	37 (26%)	25 (18%)	0	4
34	BI	120/122 (98%)	96 (80%)	19 (16%)	5 (4%)	3	34
35	BJ	136/140 (97%)	70 (52%)	33 (24%)	33 (24%)	0	2
36	BK	129/131 (98%)	97 (75%)	25 (19%)	7 (5%)	2	29
37	BL	110/114 (96%)	68 (62%)	25 (23%)	17 (16%)	0	5
38	BM	111/113 (98%)	91 (82%)	16 (14%)	4 (4%)	4	38
39	BN	112/114 (98%)	46 (41%)	38 (34%)	28 (25%)	0	2
40	BO	111/115 (96%)	65 (59%)	28 (25%)	18 (16%)	0	5
41	BQ	104/106 (98%)	73 (70%)	25 (24%)	6 (6%)	2	27
42	BR	88/92 (96%)	43 (49%)	31 (35%)	14 (16%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BS	95/99 (96%)	71 (75%)	16 (17%)	8 (8%)	1	18
44	BT	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	3	34
45	BU	82/84 (98%)	37 (45%)	29 (35%)	16 (20%)	0	3
46	BW	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	11	55
47	BX	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
48	BZ	27/29 (93%)	11 (41%)	10 (37%)	6 (22%)	0	2
49	B1	50/52 (96%)	28 (56%)	13 (26%)	9 (18%)	0	4
All	All	5494/5639 (97%)	4152 (76%)	884 (16%)	458 (8%)	2	18

5 of 458 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	14	HIS
3	AB	225	SER
4	AC	14	VAL
4	AC	126	ARG
9	AH	47	ASP

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	
3	AB	195/195 (100%)	189 (97%)	6 (3%)	47	77
4	AC	170/170 (100%)	162 (95%)	8 (5%)	32	68
5	AD	172/172 (100%)	170 (99%)	2 (1%)	78	90
6	AE	112/112 (100%)	106 (95%)	6 (5%)	27	64
7	AF	83/83 (100%)	79 (95%)	4 (5%)	31	67
8	AG	112/112 (100%)	107 (96%)	5 (4%)	34	69
9	AH	103/103 (100%)	99 (96%)	4 (4%)	39	72
10	AI	104/104 (100%)	99 (95%)	5 (5%)	31	67
11	AJ	84/84 (100%)	79 (94%)	5 (6%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AK	89/89 (100%)	87 (98%)	2 (2%)	60	83
13	AL	85/85 (100%)	84 (99%)	1 (1%)	78	90
14	AM	93/93 (100%)	90 (97%)	3 (3%)	46	76
15	AN	52/52 (100%)	50 (96%)	2 (4%)	40	73
16	AO	74/74 (100%)	74 (100%)	0	100	100
17	AP	63/63 (100%)	61 (97%)	2 (3%)	46	76
18	AQ	73/73 (100%)	71 (97%)	2 (3%)	52	79
19	AR	60/60 (100%)	59 (98%)	1 (2%)	68	87
20	AS	75/75 (100%)	73 (97%)	2 (3%)	52	79
21	AT	63/63 (100%)	54 (86%)	9 (14%)	4	25
24	B2	172/172 (100%)	165 (96%)	7 (4%)	37	71
25	B3	83/83 (100%)	76 (92%)	7 (8%)	14	48
25	B5	83/83 (100%)	79 (95%)	4 (5%)	31	67
26	BA	176/176 (100%)	147 (84%)	29 (16%)	3	19
27	BB	164/164 (100%)	160 (98%)	4 (2%)	57	82
28	BC	163/163 (100%)	153 (94%)	10 (6%)	23	60
29	BD	149/149 (100%)	123 (83%)	26 (17%)	2	17
30	BE	130/130 (100%)	123 (95%)	7 (5%)	27	64
31	BF	114/114 (100%)	113 (99%)	1 (1%)	84	93
32	BG	108/108 (100%)	87 (81%)	21 (19%)	2	12
33	BH	116/116 (100%)	96 (83%)	20 (17%)	2	17
34	BI	103/103 (100%)	97 (94%)	6 (6%)	25	61
35	BJ	99/99 (100%)	73 (74%)	26 (26%)	0	5
36	BK	104/104 (100%)	91 (88%)	13 (12%)	6	30
37	BL	94/94 (100%)	76 (81%)	18 (19%)	2	13
38	BM	83/83 (100%)	78 (94%)	5 (6%)	24	60
39	BN	99/99 (100%)	73 (74%)	26 (26%)	0	5
40	BO	89/89 (100%)	64 (72%)	25 (28%)	0	3
41	BQ	89/89 (100%)	77 (86%)	12 (14%)	5	27
42	BR	77/77 (100%)	65 (84%)	12 (16%)	3	21
43	BS	82/82 (100%)	77 (94%)	5 (6%)	23	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BT	78/78 (100%)	75 (96%)	3 (4%)	40	73
45	BU	62/62 (100%)	49 (79%)	13 (21%)	1	9
46	BW	55/55 (100%)	53 (96%)	2 (4%)	42	74
47	BX	47/47 (100%)	44 (94%)	3 (6%)	22	58
48	BZ	24/24 (100%)	18 (75%)	6 (25%)	1	6
49	B1	46/46 (100%)	37 (80%)	9 (20%)	1	12
All	All	4551/4551 (100%)	4162 (92%)	389 (8%)	18	48

5 of 389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	BG	94	LYS
35	BJ	39	LYS
45	BU	11	ASN
32	BG	116	MET
33	BH	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
21	AT	51	ASN
27	BB	36	GLN
45	BU	45	HIS
21	AT	77	ASN
26	BA	127	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1488 (99%)	249 (16%)	95 (6%)
2	AU	75/76 (98%)	16 (21%)	7 (9%)
2	AV	75/76 (98%)	15 (20%)	7 (9%)
2	AW	75/76 (98%)	14 (18%)	7 (9%)
22	B0	2739/2740 (99%)	580 (21%)	182 (6%)
23	B9	107/108 (99%)	23 (21%)	6 (5%)
All	All	4558/4564 (99%)	897 (19%)	304 (6%)

5 of 897 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G
1	AA	32	A

5 of 304 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	B0	387	U
22	B0	865	C
22	B0	2490	G
22	B0	474	G
22	B0	627	A

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
27	BB	4
26	BA	4
25	B5	3

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Mol	Chain	Number of breaks
3	AB	2
31	BF	2
25	B3	2
24	B2	2
40	BO	1
42	BR	1
37	BL	1
29	BD	1
43	BS	1
35	BJ	1
32	BG	1
28	BC	1
14	AM	1

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	52:THR	C	53:GLU	N	8.77
1	B5	51:LYS	C	52:THR	N	8.07
1	BA	60:ALA	C	61:TYR	N	8.05
1	B3	53:GLU	C	54:PHE	N	7.33
1	BB	167:ASN	C	168:GLU	N	7.32