



wwPDB EM Map/Model Validation Report ⓘ

May 19, 2016 – 06:54 PM EDT

PDB ID : 4D5Y
EMDB ID: : EMD-2810
Title : Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors : Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on : 2014-11-07
Resolution : 9.00 Å(reported)
Based on PDB ID : 4CXD

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) : rb-20027457

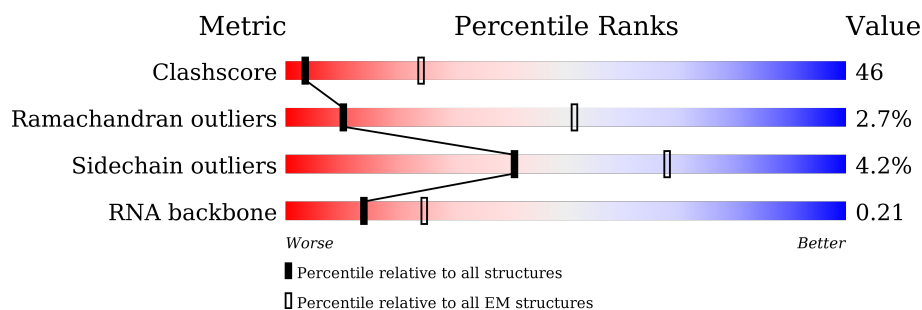
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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.






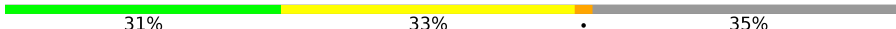


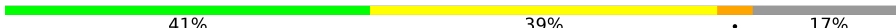










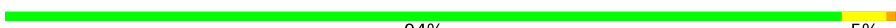







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	257	57% 38% . .
2	B	403	57% 36% 5% .
3	C	427	45% 35% 5% . 15%
4	D	297	55% 40% . .
5	E	288	23% 28% . 45%
6	F	248	52% 40% . 6%
7	G	266	50% 35% . . 12%
8	H	192	56% 41% .

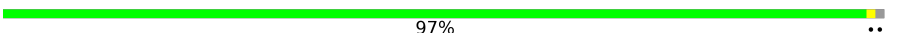

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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	215	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	159	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

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Mol	Chain	Length	Quality of chain
34	i	105	 83% 8% • 8%
35	j	97	 84% • 12%
36	k	70	 97% ••
37	l	51	 94% ••
38	m	128	 38% • 59%
39	n	25	 100%
40	o	106	 93% 7%
41	p	92	 93% 5% •
42	t	137	 86% 7% • 5%
43	u	210	 92% 8%
44	2	5025	 7% 28% 36% • 28%
45	3	194	 7% 38% 35% • 19%
46	4	119	 13% 34% 52% •

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 136495 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 UL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	1
			1888	1183	388	311	6		

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN UL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	396	Total	C	N	O	S	0	1
			3190	2030	601	545	14		

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN UL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	364	Total	C	N	O	S	0	1
			2889	1817	578	480	14		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN UL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	290	Total	C	N	O	S	0	0
			2361	1489	431	427	14		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN EL6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	158	Total	C	N	O	0	0
			1286	834	238	214		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN UL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	234	Total	C	N	O	S	0	0
			1949	1252	376	312	9		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN EL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	235	Total	C	N	O	S	0	1
			1881	1197	363	317	4		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN UL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1535	965	286	278	6		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN UL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	196	Total	C	N	O	S	0	0
			1604	1022	308	262	12		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN UL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN EL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	200	Total	C	N	O	S	0	1
			1617	1013	335	265	4		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN EL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	140	Total	C	N	O	S	0	1
			1139	730	219	183	7		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN EL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	204	Total	C	N	O	S	0	0
			1708	1077	360	266	5		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	196	Total	C	N	O	S	0	1
			1607	1034	316	252	5		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN UL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	1
			1234	771	241	213	9		

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN EL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	184	Total	C	N	O	S	0	0
			1493	933	311	244	5		

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN UL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	183	Total	C	N	O	S	0	1
			1526	943	331	242	10		

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN EL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	173	Total	C	N	O	S	0	0
			1438	916	280	232	10		

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN EL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN EL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	102	Total	C	N	O	S	0	1
			827	529	146	150	2		

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN UL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	128	Total	C	N	O	S	0	0
			963	610	181	167	5		

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	64	Total	C	N	O	S	0	1
			529	337	104	85	3		

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN UL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			975	624	183	167	1		

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN UL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	128	Total	C	N	O	S	0	1
			1065	668	217	177	3		

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN EL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	136	Total	C	N	O	S	0	0
			1114	719	209	182	4		

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN UL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1161	736	237	185	3		

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN EL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	69	Total	C	N	O	S	0	1
			560	344	123	90	3		

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN EL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	104	Total	C	N	O	S	0	1
			802	508	142	145	7		

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN EL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	109	Total	C	N	O	S	0	0
			904	570	174	158	2		

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN EL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	1
			1053	664	219	165	5		

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN EL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	107	Total	C	N	O	S	0	0
			865	550	172	140	3		

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN EL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	115	Total	C	N	O	S	0	1
			907	566	188	147	6		

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN UL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN EL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	97	Total	C	N	O	S	0	1
			783	488	168	122	5		

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN EL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	85	Total	C	N	O	S	0	1
			690	423	153	109	5		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN EL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN EL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			428	266	90	66	6		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	106	Total	C	N	O	S	0	0
			870	547	176	140	7		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN EL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			707	445	136	119	7		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN EL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	130	Total	C	N	O	S	0	1
			1043	646	220	172	5		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN UL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	210	Total	C	N	O	S	0	0
			1621	990	278	347	6		

- Molecule 44 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	3616	Total	C	N	O	P	0	0
			77488	34508	14153	25212	3615		

- Molecule 45 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	157	Total	C	N	O	P	0	0
			3334	1489	587	1102	156		

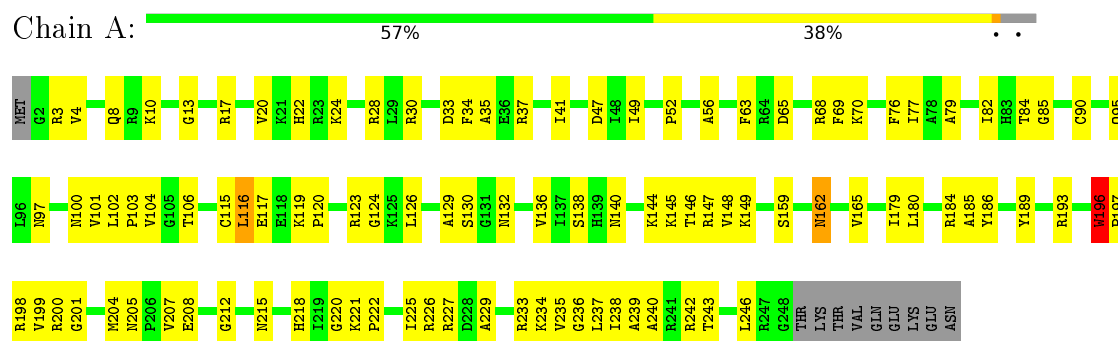
- Molecule 46 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

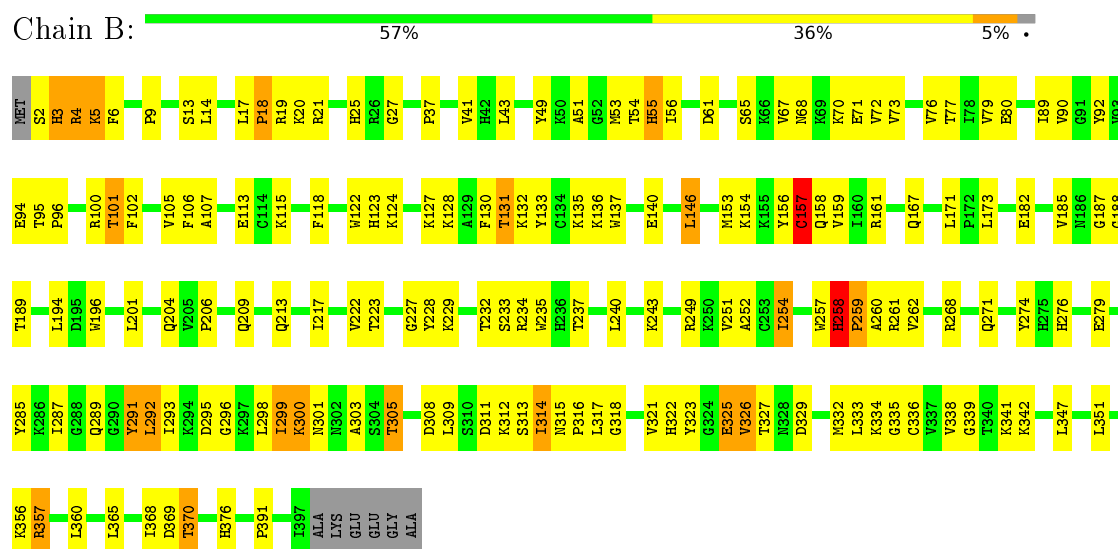
3 Residue-property plots

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.

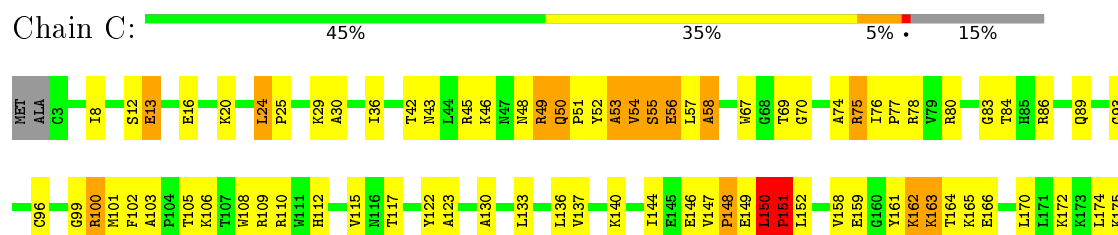
• Molecule 1: 60S RIBOSOMAL PROTEIN UL2

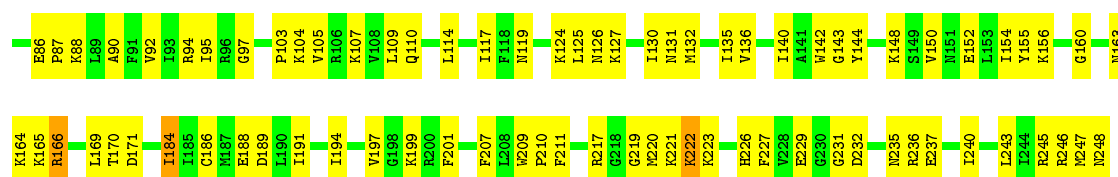


• Molecule 2: 60S RIBOSOMAL PROTEIN UL3



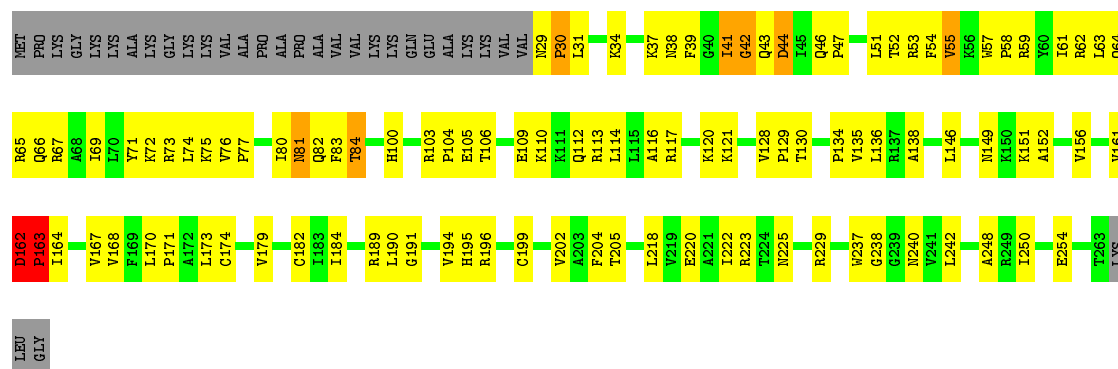
• Molecule 3: 60S RIBOSOMAL PROTEIN UL4





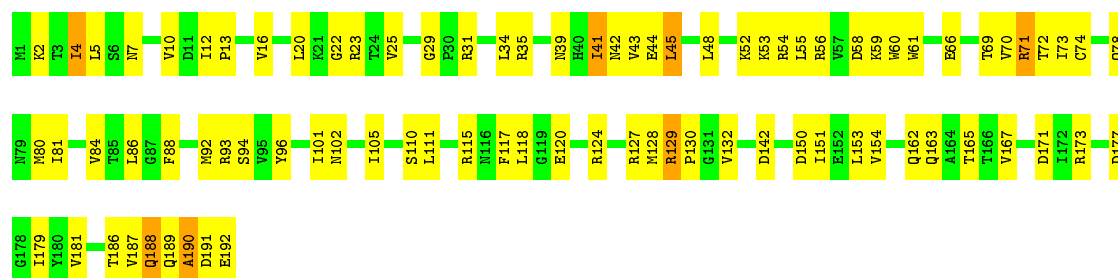
• Molecule 7: 60S RIBOSOMAL PROTEIN EL8

Chain G: 50% 35% 12%



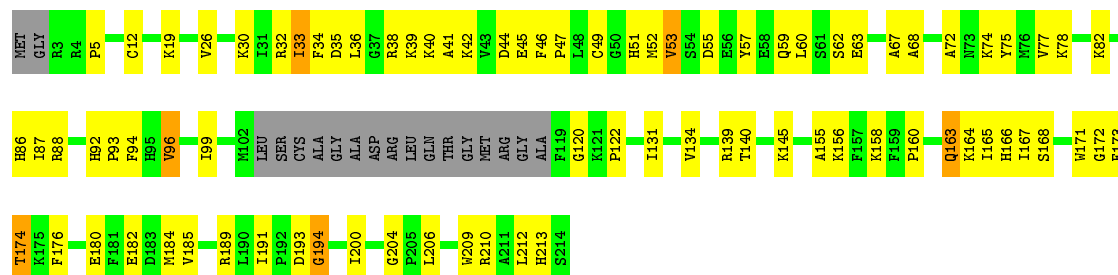
• Molecule 8: 60S RIBOSOMAL PROTEIN UL6

Chain H: 56% 41% 3%



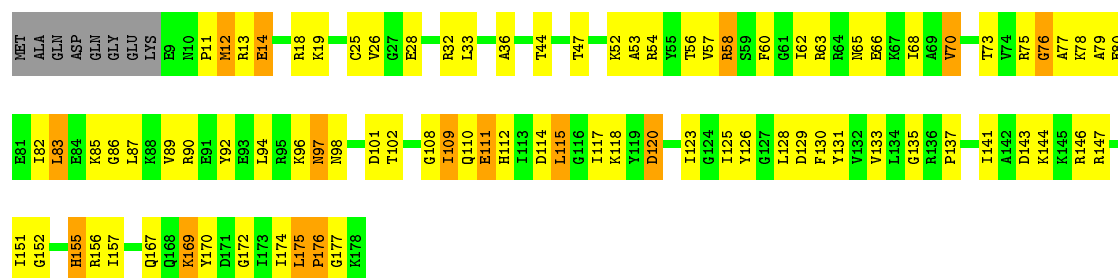
• Molecule 9: 60S RIBOSOMAL PROTEIN UL16

Chain I: 53% 36% 8%



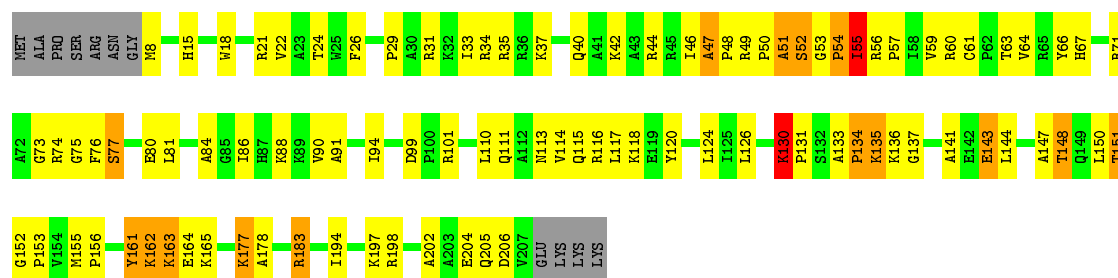
• Molecule 10: 60S RIBOSOMAL PROTEIN UL5

Chain J: 47% 40% 8%



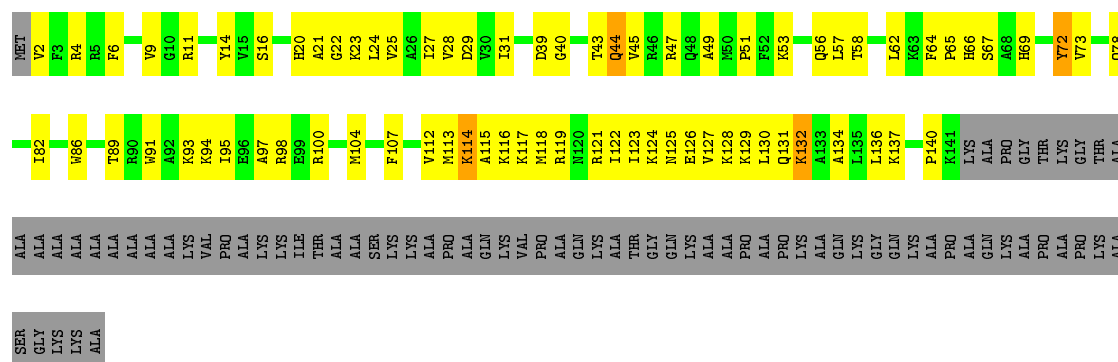
• Molecule 11: 60S RIBOSOMAL PROTEIN EL13

Chain L: 50% 37% 7% 5%



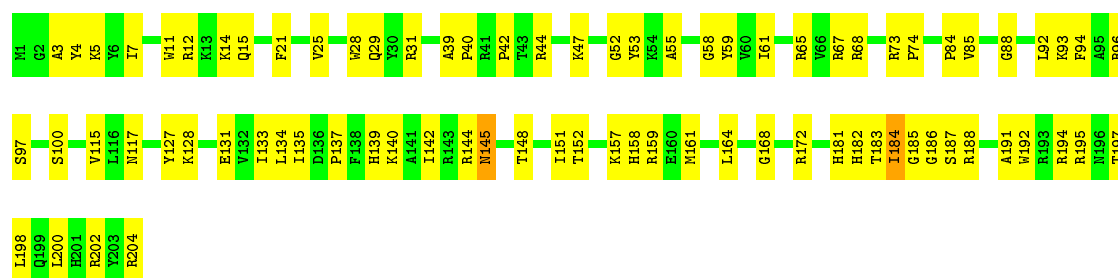
• Molecule 12: 60S RIBOSOMAL PROTEIN EL14

Chain M: 31% 33% 35%



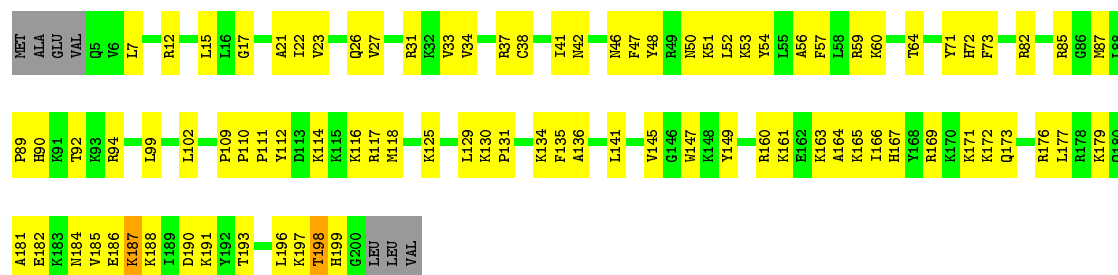
• Molecule 13: 60S RIBOSOMAL PROTEIN EL15

Chain N: 61% 38%



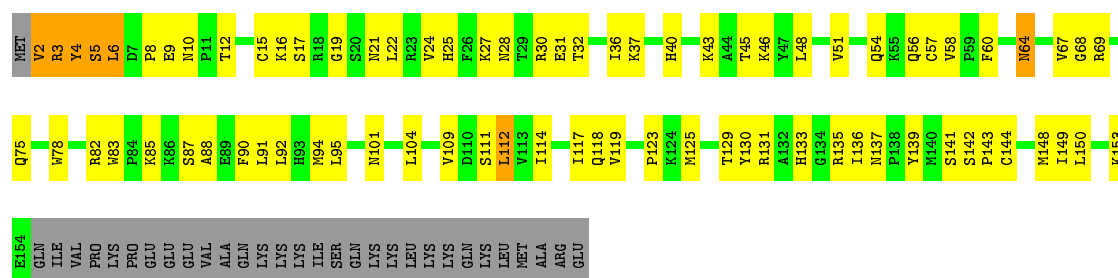
• Molecule 14: 60S RIBOSOMAL PROTEIN UL13

Chain 0:  53% 42% ..



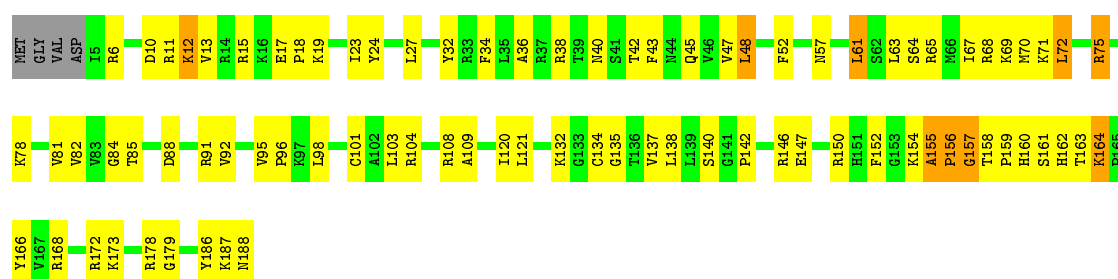
• Molecule 15: 60S RIBOSOMAL PROTEIN UL22

Chain P:  41% 39% 1% 17%



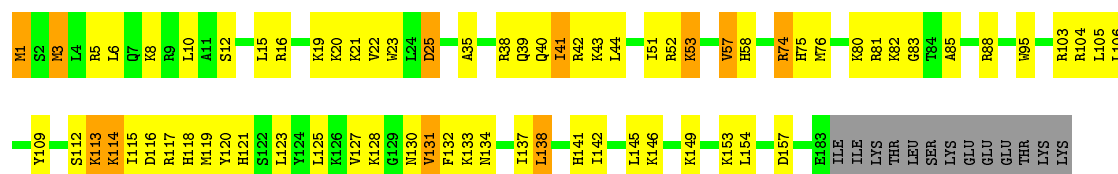
- Molecule 16: 60S RIBOSOMAL PROTEIN EL18

Chain Q:  53% 40% 5%



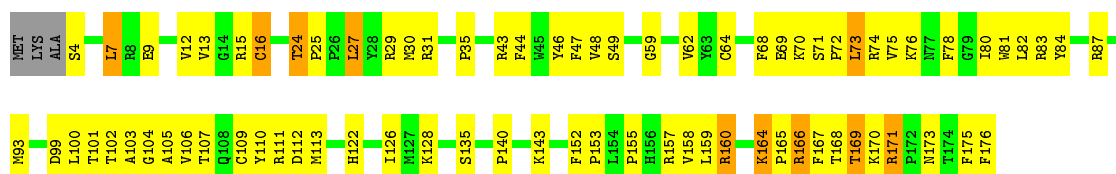
• Molecule 17: 60S RIBOSOMAL PROTEIN UL19

Chain R: 57% 31% 6% 7%



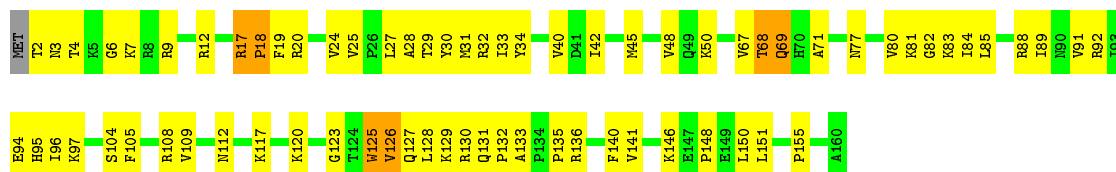
• Molecule 18: 60S RIBOSOMAL PROTEIN EL20

Chain S: 54% 39% 6%



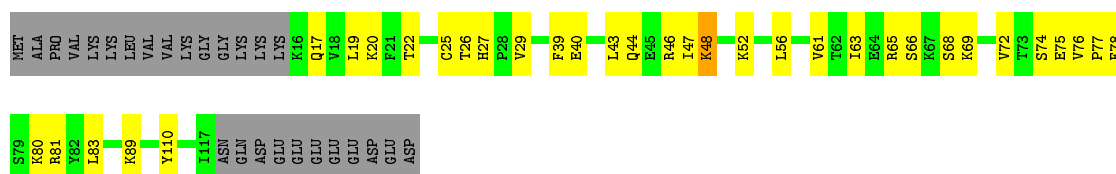
• Molecule 19: 60S RIBOSOMAL PROTEIN EL21

Chain T: 55% 41% . .



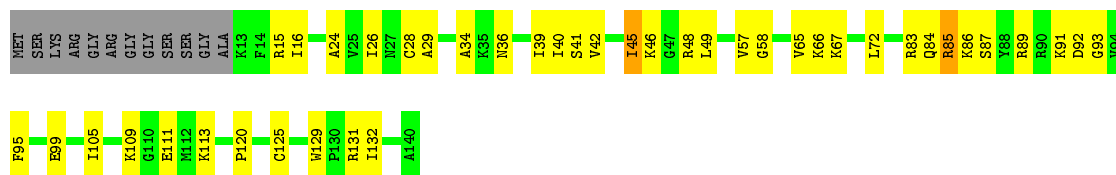
• Molecule 20: 60S RIBOSOMAL PROTEIN EL22

Chain U: 53% 26% . 20%



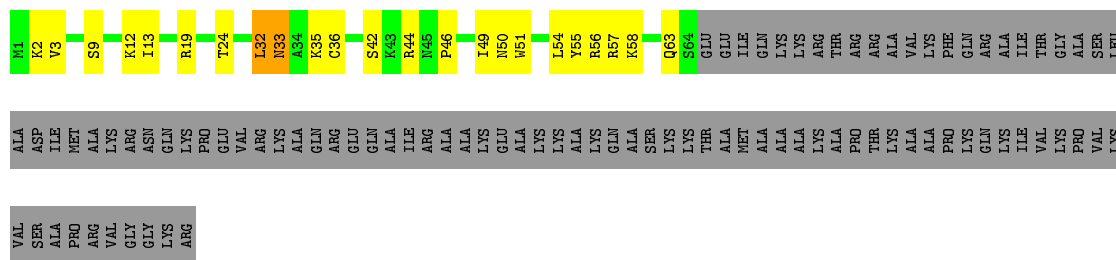
• Molecule 21: 60S RIBOSOMAL PROTEIN UL14

Chain V: 61% 29% . 9%



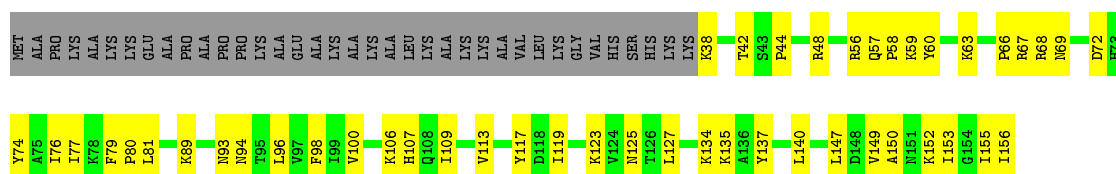
• Molecule 22: 60S RIBOSOMAL PROTEIN EL24

Chain W: 26% 13% . 59%

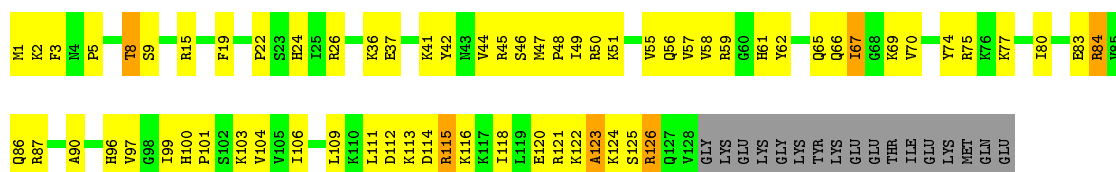


• Molecule 23: 60S RIBOSOMAL PROTEIN UL23

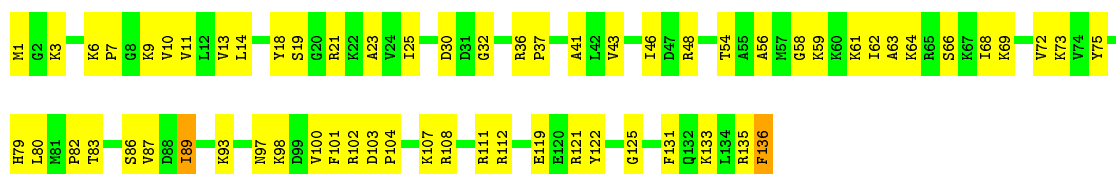
Chain X: 46% 30% 24%



• Molecule 24: 60S RIBOSOMAL PROTEIN UL24



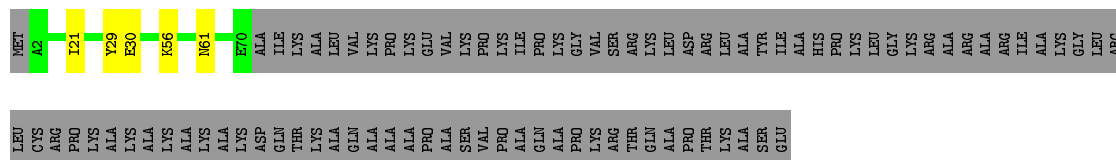
• Molecule 25: 60S RIBOSOMAL PROTEIN EL27



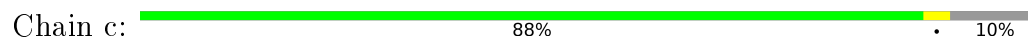
• Molecule 26: 60S RIBOSOMAL PROTEIN UL15



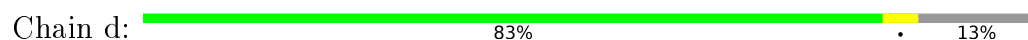
• Molecule 27: 60S RIBOSOMAL PROTEIN EL29

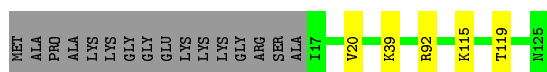


• Molecule 28: 60S RIBOSOMAL PROTEIN EL30



● Molecule 29: 60S RIBOSOMAL PROTEIN EL31





- Molecule 30: 60S RIBOSOMAL PROTEIN EL32

Chain e: 90% • 5%



- Molecule 31: 60S RIBOSOMAL PROTEIN EL33

Chain f: 86% 10% ••



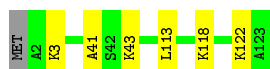
- Molecule 32: 60S RIBOSOMAL PROTEIN EL34

Chain g: 87% 10% ••



- Molecule 33: 60S RIBOSOMAL PROTEIN UL29

Chain h: 94% 5% •



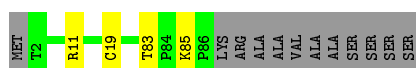
- Molecule 34: 60S RIBOSOMAL PROTEIN EL36

Chain i: 83% 8% • 8%



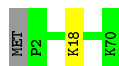
- Molecule 35: 60S RIBOSOMAL PROTEIN EL37

Chain j: 84% • 12%



- Molecule 36: 60S RIBOSOMAL PROTEIN EL38

Chain k: 97% ••



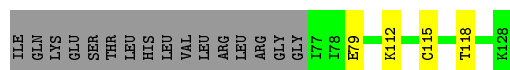
- Molecule 37: 60S RIBOSOMAL PROTEIN EL39

Chain l:  94%



- Molecule 38: 60S RIBOSOMAL PROTEIN EL40

Chain m:  38% 59%



- Molecule 39: 60S RIBOSOMAL PROTEIN EL41

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 60S RIBOSOMAL PROTEIN EL44

Chain o:  93% 7%



- Molecule 41: 60S RIBOSOMAL PROTEIN EL43

Chain p:  93% 5%



- Molecule 42: 60S RIBOSOMAL PROTEIN EL28

Chain t:  86% 7% 5%



- Molecule 43: 60S RIBOSOMAL PROTEIN UL1

Chain u:  92% 8%



- Molecule 44: 28S Ribosomal RNA

Chain 2: 7% 28% 36% 28%

C1	G2	C3	G4	A5	C6	C7	U8	C9	A10	G11	C12	A13	U14	G15	C16	A17	C18	G19	U20	C21	G22	C23	G24	A25	C26	G27	C28	A29	G30	C31	U32	G33	A34	C35	U36	G37	A38	C39	G40	C41	A42	U43	G44	A45	U46	C47	G48	U49	C50	A51	G52	C53	A54	G55	C56	A57	G58	C59	A60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A61	A62	G63	G64	A65	C66	C67	U68	A69	C70	G71	C72	A73	G74	C75	A76	G77	U78	C79	G80	C81	U82	C83	A84	G85	U86	A87	C88	G89	A90	C91	U92	G93	A94	C95	U96	G97	A98	C99	G100	A101	C102	G103	A104	U105	C106	G107	A108	C109	G110	C111	G112	A113	C114	G115	C116	A117	G118	C119	U120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A121	U122	C123	G124	C125	A126	G127	C128	U129	C130	G131	C132	A133	G134	C135	U136	G137	C138	A139	G140	C141	U142	G143	A144	C145	U146	G147	C148	A149	G150	C151	U152	G153	A154	C155	U156	G157	A158	C159	G160	U161	C162	G163	A164	C165	U166	G167	C168	A169	C170	G171	C172	A173	G174	C175	U176	G177	C178	A179	C180	U181																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C182	G183	U184	C185	A186	G187	C188	U189	G190	C191	A192	C193	G194	A195	C196	U197	G198	C199	U200	A201	C202	U203	G204	A205	C206	U207	G208	A209	C210	G211	C212	A213	C214	G215	A216	C217	U218	C219	G220	U221	C222	A223	G224	C225	U226	G227	A228	C229	U230	G231	C232	A233	G234	C235	U236	G237	A238	C239	G240	U241																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C242	G243	C244	G245	C246	U247	G248	C249	U250	C251	A252	C253	G254	C255	U256	C257	G258	C259	U260	G261	C262	U263	G264	C265	U266	C267	G268	C269	A270	G271	C272	A273	C274	G275	U276	C277	A278	C279	G280	U281	C282	A283	G284	C285	U286	A287	C288	U289	C290	A291	G292	C293	U294	C295	U296	A297	C298	G299	C300	U301																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G302	C303	U304	G305	C306	U307	A308	C309	G310	C311	U312	C313	G314	A315	U316	C317	G318	A319	C320	U321	G322	A323	C324	U325	G326	C327	A328	C329	G330	C331	U332	G333	A334	C335	U336	G337	A338	C339	U340	C341	G342	C343	A344	U345	C346	G347	U348	C349	A350	G351	C352	A353	C354	U355	G356	C357	A358	C359	U360	G361	C362																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A363	C364	G365	C366	A367	C368	U369	G370	C371	U372	G373	A374	C375	U376	G377	C378	A379	C380	U381	G382	C383	U384	G385	A386	C387	G388	C389	G390	A391	C392	U393	G394	C395	U396	C397	A398	C399	U400	A401	C402	G403	A404	U405	C406	U407	A408	C409	U410	A411	C412	U413	A414	C415	U416	A417	C418	U419	A420	C421	U422																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U423	A424	C425	G426	C427	A428	U429	G430	C431	U432	G433	A434	C435	U436	C437	G438	A439	C440	U441	C442	A443	U444	G445	C446	U447	G448	C449	U450	C451	A452	C453	U454	G455	C456	U457	A458	C459	U460	A461	C462	U463	G464	C465	U466	G467	C468	U469	A470	C471	U472	G473	C474	U475	A476	C477	U478	G479	C480	U481	G482	U483																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G484	U485	C486	G487	C488	U489	G490	C491	U492	G493	C494	U495	A500	U501	C502	U503	G504	C505	U506	C507	G508	C509	U510	C511	G512	C513	U514	C515	G516	C517	U518	C519	G520	C521	U522	G523	C524	U525	C526	G527	C528	U529	C530	G531	C532	U533	C534	U535	G536	C537	U538	C539	G540	C541	U542	C543	U544	G545	C546	U547	C548	G549	C550	U551	C552	G553	C554	U555	C556	G557	C558	U559	C560	G561	C562	U563	G564	C565	U566	G567	C568	U569	C570	G571	C572	U573	C574	U575	G576	C577	U578	C579	G580	C581	U582	C583	G584	C585	U586	C587	G588	C589	U590	C591	G592	C593	U594	C595	G596	C597	U598	C599	G600	C601	U602	C603	G604	C605	U606	C607	G608	C609	U610	C611	G612	C613	U614	C615	G616	C617	U618	C619	G620	C621	U622	C623	G624	C625	U626	C627	G628	C629	U630	C631	G632	C633	U634	C635	G636	C637	U638	C639	G640	C641	U642	C643	G644	C645	U646	C647	G648	C649	U650	C651	G652	C653	U654	C655	G656	C657	U658	C659	G660	C661	U662	C663	G664	C665	U666	G667	C668	U669	C670	G671	C672	U673	C674	U675	G676	C677	U678	C679	G680	C681	U682	C683	G684	C685	U686	C687	G688	C689	U690	C691	G692	C693	U694	C695	G696	C697	U698	C699	G700	C701	U702	G703	C704	U705	C706	G707	C708	U709	G710	C711	U712	G713	C714	U715	G716	C717	U718	C719	G720	C721	U722	G723	C724	U725	G726	C727	U728	G729	C730	U731	C732	G733	C734	U735	G736	C737	U738	C739	G740	C741	U742	G743	C744	U745	G746	C747	U748	C749	G750	C751	U752	C753	G754	C755	U756	C757	G758	C759	U760	C761	G762	C763	U764	C765	G766	C767	U768	C769	G770	C771	U772	C773	G774	C775	U776	C777	G778	C779	U780	C781	G782	C783	U784	C785	G786	C787	U788	C789	G790	C791	U792	C793	G794	C795	U796	C797	G798	C799	U800	C801	G802	C803	U804	C805	G806	C807	U808	C809	G810	C811	U812	C813	G814	C815	U816	C817	G818	C819	U820	C821	G822	C823	U824	C825	G826	C827	U828	C829	G830	C831	U832	C833	G834	C835	U836	C837	G838	C839	U840	C841	G842	C843	U844	C845	G846	C847	U848	C849	G850	C851	U852	C853	G854	C855	U856	C857	G858	C859	U860	C861	G862	C863	U864	C865	G866	C867	U868	C869	G870	C871	U872	C873	G874	C875	U876	C877	G878	C879	U880	C881	G882	C883	U884	C885	G886	C887	U888	C889	G890	C891	U892	C893	G894	C895	U896	C896	G897	C898	U899	C899	G900	C901	U902	C903	G904	C905	U906	C907	G908	C909	U910	C910	G911	C912	U913	C914	G915	C916	U917	C918	G919	C920	U921	C921	G922	C923	U924	C925	G926	C927	U928	C929	G930	C931	U932	C933	G934	C935	U936	C937	G938	C939	U940	C941	G942	C943	U944	C945	G946	C947	U948	C949	G950	C951	U952	C953	G954	C955	U956	C956	G957	C958	U959	C959	G960	C961	U962	C963	G964	C965	U966	C967	G968	C969	U970	C971	G972	C973	U974	C975	G976	C977	U978	C979	G980	C981	U982	C983	G984	C985	U986	C987	G988	C989	U990	C991	G992	C993	U994	C995	G996	C997	U998	C999	G1000	C1001	U1002	C1003	G1004	C1005	U1006	C1007	G1008	C1009	U1010	C1011	G1012	C1013	U1014	C1015	G1016	C1017	U1018	C1019	G1020	C1021	U1022	C1023	G1024	C1025	U1026	C1027	G1028	C1029	U1030	C1031	G1032	C1033	U1034	C1035	G1036	C1037	U1038	C1039	G1040	C1041	U1042	C1043	G1044	C1045	U1046	C1047	G1048	C1049	U1050	C1051	G1052	C1053	U1054	C1055	G1056	C1057	U1058	C1059	G1060	C1061	U1062	C1063	G1064	C1065	U1066	C1067	G1068	C1069	U1070	C1071	G1072	C1073	U1074	C1075	G1076	C1077	U1078	C1079	G1080	C1081	U1082	C1083	G1084	C1085	U1086	C1087	G1088	C1089	U1090	C1091	G1092	C1093	U1094	C1095	G1096	C1097	U1098	C1099	G1100	C1101	U1102	C1103	G1104	C1105	U1106	C1107	G1108	C1109	U1110	C1111	G1112	C1113	U1114	C1115	G1116	C1117	U1118	C1119	G1120	C1121	U1122	C1123	G1124	C1125	U1126	C1127	G1128	C1129	U1130	C1131	G1132	C1133	U1134	C1135	G1136	C1137	U1138	C1139	G1140	C1141	U1142	C1143	G1144	C1145	U1146	C1147	G1148	C1149	U1150	C1151	G1152	C1153	U1154	C1155	G1156	C1157	U1158	C1159	G1160	C1161	U1162	C1163	G1164	C1165	U1166	C1167	G1168	C1169	U1170	C1171	G1172	C1173	U1174	C1175	G1176	C1177	U1178	C1179	G1180	C1181	U1182	C1183	G1184	C1185	U1186	C1187	G1188	C1189	U1190	C1191	G1192	C1193	U1194	C1195	G1196	C1197	U1198	C1199	G1200	C1201	U1202	C1203	G1204	C1205	U1206	C1207	G1208	C1209	U1210	C1211	G1212	C1213	U1214	C1215	G1216	C1217	U1218	C1219	G1220	C1221	U1222	C1223	G1224	C1225	U1226	C1227	G1228	C1229	U1230	C1231	G1232	C1233	U1234	C1235	G1236	C1237	U1238	C1239	G1240	C1241	U1242	C1243	G1244	C1245	U1246	C1247	G1248	C1249	U1250	C1251	G1252	C1253	U1254	C1255	G1256	C1257	U1258	C1259	G1260	C1261	U1262	C1263	G1264	C1265	U1266	C1267	G1268	C1269	U1270	C1271	G1272	C1273	U1274	C1275	G1276	C1277	U1278	C1279	G1280	C1281	U1282	C1283	G1284	C1285	U1286	C1287	G1288	C1289	U1290	C1291	G1292	C1293	U1294	C1295	G1296	C1297	U1298	C1299	G1300	C1301	U1302	C1303	G1304	C1305	U1306	C1307	G1308	C1309	U1310	C1311	G1312	C1313	U1314	C1315	G1316	C1317	U1318	C1319	G1320	C1321	U1322	C1323	G1324	C1325	U1326	C1327	G1328	C1329	U1330	C1331	G1332	C1333	U1334	C1335	U1336	G1337	C1338	U1339	C1340	G1341	C1342	U1343	C1344	G1345	C1346	U1347	C1348	G1349	C1350	U1351	C1352	G1353	C1354	U1355	C1356	G1357	C1358	U1359	C1360	G1361	C1362	U1363	C1364	G1365	C1366	U1367	C1368	G1369	C1370	U1371	C1372	G1373	C1374	U1375	C1376	G1377	C1378	U1379	C1380	G1381	C1382	U1383	C1384	G1385	C1386	U1387	C1388	G1389	C1390	U1391	C1392	G1393	C1394	U1395	C1396	G1397	C1398	U1399	C1400	G140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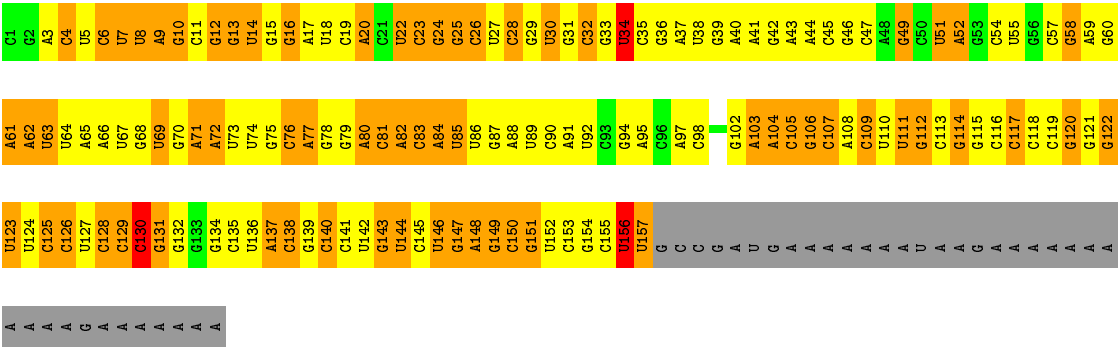
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A	G1895	G1831	U1771	U1709	G1649	G1588	G1529	C1465	G1404	C1343	G1281	G1221	C1160		C
C	U1896	G1832	A1772	C1710	U1650	C1589		G1466	G1405	U1344	U1282	G1222	C1161		C
U	G1897	G1833	A1773	G1712	U1651	G1590	C1530	G1467	G1406		A1283	G1223	C1162		C
C	C1898	G1834	A1774	G1713	U1652	G1591	G1531	G1468	A1407		C1284	G1224	C1163		U
G	C1899	U1775	G1713	C1683	C1684	A1592	A1532		U1408		C1285	G1225	A1164		C
A	G1900	G1776	A1714	C1694	C1695	A1593	A1533		C1409		C1286	G1226	G1165		C
A	C1837	G1777	A1715	C1654	C1655	C1594	G1534		C1410		U1227	G1227	U1166		U
U	U1838	G1778	A1716	U1656	U1657	U1595	C1535		C1411		C1288	G1228			G1044
U	G1839	U1779	A1717	C1657	C1658	U1596	C1536		C1412		C1289	G1229			G1045
C	U1840	A1780	G1718	A1658	G1659	G1597	A1537				C1290	G1230			G1046
G		A1781	G1719	G1659	G1660	U1598	G1538		G1415		G1291	C1231			G1047
G	C1906	G1782	G1720	U1599	G1661	U1599	A1539		C1416		A1292	C1232			G1048
A	A1845	A1783	A1721	A1600	A1662		G1540		C1417		G				G1049
A	U1908	A1784			U1662		G1541		U1418		A				G1050
U	C1847	G1785	A1725	G1603	G1663	G1604	A1541		U1419		C1293	G			C1056
C	C1848	C1786	A1726	G1605	G1664	G1606	A1542		C1420		C1295	A			C1057
C	A1849	C1787	U1727	G1606	C1665	G1607	A1543		U1421		G1296	G			C1051
C	G1856	C1788	U1728	C1607	U1666	C1608	A1544		C1422		U1297	A			G1053
G	C1913	G1789	A1728	C1608	U1667	G1609	C1546		C1423		C1298	G1238			G1054
C	A1851	G1790	G1729	G1608	G1668	A1547	U1546		U1424		U1300	G1239			A1067
U	C1852	C1791	A1730	G1609	C1669	U1548	U1548		G1425		G1301	G1240			C1061
A	U1854	U1792	G1731	A1610	G1670	G1549	G1550		U1426		A1302	G1241			C1062
C	G1855	C1793	G1732	A1611	G1671	G1551	G1551		C1427		A1303	G1242			U1063
G	G1856	G1794	U1733	G1612	U1672	U1552	U1551		G1428		A1304	G1243			C1065
A	C1857	C1795	U1734	A1613	C1673	G1553	C1553		C1429		A1305	G1244			C1066
G	U1858	G1796	U1735	G1614	U	G1554	G1554		U1430		A1306	G1245			C1067
A	C1859	G1797	U1736	A1615	C	U1555	A1554		C1431		C1307	G1246			C1068
U	U1860	G1798	G1737	A1616	C	U1556	U1555		G1432		G1308	G1247			G1069
U	G1861	C1799	G1738	A1617	C	U1557	G1556		A1433			G1248			C1070
U	C1862	G1800	G1739	A1618	A	G1558	G1563		G1434			G1249			C1071
U	U1925	U1801	G1740	G1619	G	C1559	C1564		U1435			G1250			G1074
A	C1865	G1802	C1741	A1620	A	C1560	G1565		G1436		A1312	G1251			A1075
A	U1927	A1866	C1742	A1621	C	U1561	G1566		U1437		A1313	G1252			C1076
C	U1928	A1804	G1743	A1622	C	U1562	U1567		C1438		G1315	G1253			C1077
C	G1929	G1805	A1744	C1623	C	A1561	C1568		A1439		A1322	G1254			G1078
A	U1930	A1806	A1745	C1624	G	U1562	U1570		C1440		A1323	G1255			C1079
U	U1931	C1807	A1746	A1625	A	C1563	C1569		U1441		A1324	G1256			U1080
U	C1870	G1808	C1747	G1626	C	U1566	U1570		C1442		G1318	G1257			C1081
C	C1933	C1872	G1748	C1627	G	U1567	U1571		C1443		G1319	G1258			U1082
A	U1934	A1810	A1749	C1628	C	U1568	U1572		G1444		U1321	G1259			C1083
C	U1935	A1811	U1750	A1629	A	C1569	C1573		U1445		A1325	G1260			C1084
C	A1936	G1812	C1751	G1630	C	C1570	U1575		C1446		G1326	G1261			C1085
C		G1813	U1752	U1631	C	U1570	U1576		C1447		G1327	G1262			C1086
C		G1814	C1753	A1632	C	U1571	U1577		C1448		A1202	G1263			U1087
C	G1939	A1815	A1754	G1633	C	A1572	C1577		G1449		G1203	G1264			C1088
C2000	C2001	A1940	A1755	C1634	C	C1573	G1574		U1450		U1205	G1265			U1089
C2002	G2002	C1941	U1756	U1635	C	G1574	U1575		C1451		U1206	G1266			C1090
A2003	A2004	A1942	C1757	G1636	C	U1575	U1576		U1452		C1267	G1267			C1091
A2004	U2005	G1943	U1758	G1637	C	G1576	G1577		C1453		C1269	G1268			C1092
U2005	C2006	C1944	U1759	U1638	A	U1577	C1578		G1454		G1270	G1269			C1093
C2006	A2007	A1945	U1760	U1639	C	A1578	U1579		C1455		G1271	G1270			C1094
C2007		G	U1761	G1640	C	U1580	U1580		C1456		C1272	G1271			U1157
C2008	C2009	A2008	G1762	A1641	C	U1580	U1581		C1457		G1273	G1272			
C2009	U2010	U2010	U1763	C1642	C	U1581	U1582		G1458		A1274	G1273			
A2011	A2011	C1889	C1825	U1643	C	U1582	C1582		C1459		G1275	G1274			
G2012	G2012	U1826	A1766	C1644	C	U1583	G1583		C1460		G1276	G1275			
C2013	C2013	U1827	U1704	C1645	C	U1584	G1584		G1461		G1277	G1276			
C2014	C2014	C1768	U1706	G1646	C	U1585	U1585		G1462		G1278	G1277			

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

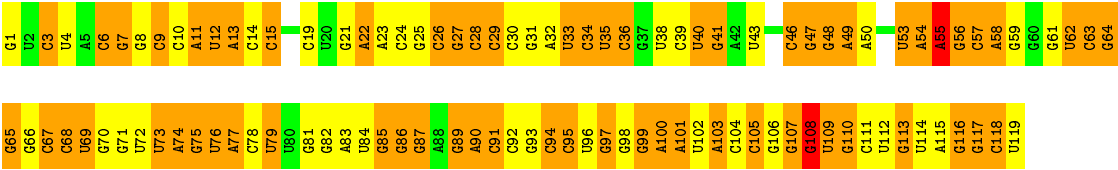



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G5017	G4949	C	U4824	A4704	A4643	C4582	U4458	U4398	A4338	C4278	A4216	G4152
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G5019	G4951	C	G4826	C4706	U4645	A4584	U4460	G4400	A4340	G4280	C4218	U4154
U5020	G4952	C	G4827	U4707	C4646	C4585	U4461	A4401	A4341	U4281	C4219	G4155
U5021	G4953	C	G4828	C4708	A4647	U4586	U4462	U4402	G4342	G4282	U4220	G4156
U5022	U4957	A	G4829	G4709	U4648	C4587	U4463	U4403	U4343	A4283	C4221	G4157
G	G4958	C	G4830	C4710	U4649	U4588	U4464	U4404	U4344	A4284	C4222	G4158
U	G4959	C	G4831	U4711	G4650	U4589	A4467	U4405	A4345	G4285	C4223	C4159
C	C4960	G	G4832	U4712	A4651	G4590	U4468	U4406	C4346	G4286	G4224	G4160
	U4961	C	G4833	G4713	G4591	U4529	U4469	C4407	C4347	C4287	U4225	G4161
	G4962	C	G4834	G4714	U4592	G4530	U4470	G4408	A4348	G4288	G4226	U4162
	C4963	C	C4835	C4715	G4652	A4531	A4471	A4409	C4349	G4289	G4227	A4163
		C	U4836	C4716	U4656	U4594	U4472	U4410	A4350	G4290	A4228	A4164
		C	U4837	U4717	U4657	G4595	U4473	G4411	A4351	G4291	G4229	A4165
		C	C4838	C4718	C4658	U4596	G4474	U4412	G4352	C4292	C4230	A4166
		C	G4839	G4719	U4659	G4535	G4475	U4413	G4353	C4293	C4231	C4167
		C	U4840	G4720	A4660	U4598	G4476	G4414	A4354	U4294	G4232	U4168
		C	C4841	A4721	U4661	G4599	A4477	G4415	A4355	C4295	A4233	G4169
		G	C4842	U4722	G4662	C4600	U4478	C4416	A4356	A4296	A4234	U4170
		G	G4843	A4723	U4663	U4601	U4479	U4417	A4357	G4297	G4235	
		G	U4844	G4724	C4664	U4602	G4480	C4418	C4358	G4298	G4236	
		A	G4845	C4725	A4665	G4603	U4481	U4419	U4359	A4299	G4237	
		C	G4846	C4726	G4666	C4604	G4482	U4420	G4360	U4300	C4238	
		G	A4847	G4727	A4667	C4605	A4483	C4421	G4361	C4301	A4239	
		C	A4848	G4728	U4668	U4606	G4484	C4422	C4362	C4302	A4240	
		C	A4849	U4729	U4669	G4607	U4485	U4423	C4363	U4303	A4241	
		C	C4850	C4730	C4670	A4608	U4486	A4424	A4364	U4304	G4242	
		C	G4851	C4731	C4671	G4609	G4487	U4425	G4365	C4305	A4180	
		C	G4852	C4732	C4672	U4610	G4488	C4426	U4366	U4306	C4243	
		U	G4853	C4733	G4673	A4611	G4489	A4427	G4367	C4307	U4245	
		G	G4854	C4734	C4674	A4549	U4490	U4428	A4368	U4308	C4246	
		C	C4855	G4735	C4675	U4550	U4491	U4429	C4369	A4309	G4247	
		C	G4856	C4736	C4676	U4551	U4492	G4430	G4370	C4310	C4248	
		C	C4857	C4737	A4677	A4615	U4493	U4431	G4371	U4311	U4249	
		C	G4858	U4738	G4678	A4616	G4494	G4432	C4372	U4312	G4251	
		C	G4859	G4739	G4679	U4617	U4495	A4433	C4373	U4313	G4252	
		C	C4860	U4740	C4680	G4618	C4496	A4434	A4374	U4314	A4253	
		C4800	C4741	G4681			U4497	G4435	A4375	U4315	C4254	
		C4801					U4498	A4436	G4376	G4317	U4255	
		C4802					U4499	A4437	G4377	U4318	U4256	
		C4803					G4500	G4438	G4378	U4319	G4257	
		G4804					G4501	A4439	G4379	A4320	A4258	
		C4805					U4502	A4440	U4380	U4321	U4259	
		G4806					A4504	U4441	C4381	U4322	U4260	
		C4807					G4505	U4442	A4382	A4323	U4261	
		C4808					U4506	G4443	U4383	U4324	U4262	
		G4809					C4507	C4444	A4384	G4325	C4263	
		G4810					U4508	C4445	G4385	C4326	A4264	
		G4811					A4509	C4446	C4386	A4327	G4265	
		A4812					G4510	A4447	G4387	G4328	U4266	
		C4813					U4511	G4448	A4388	A4329	C4267	
		C4814					U4512	G4449	C4389	G4330	G4268	
		G4815					C4513	C4450	G4390	G4331	A4270	
		C4816					U4514	G4451	C4392	U4332	G4271	
		G4817					A4515	U4452	G4393	G4333	A4272	
		C4818					U4516	U4453	C4394	U4334	C4273	
		U4819					U4517	U4454	U4395			
		C4820					U4518					
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		C					U4610					
	</											



● Molecule 46: 5S Ribosomal RNA

Chain 4: 13% 34% 52%



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	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	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	A	0.44	0/1926	0.67	0/2583
10	J	0.49	0/1385	0.71	0/1852
11	L	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
12	M	0.49	0/1162	0.70	0/1556
13	N	0.43	0/1753	0.65	0/2348
14	O	0.44	0/1639	0.69	0/2193
15	P	0.44	0/1260	0.70	0/1691
16	Q	0.45	0/1517	0.74	0/2026
17	R	0.41	0/1542	0.64	0/2037
18	S	0.45	0/1478	0.73	0/1985
19	T	0.46	0/1325	0.72	0/1770
2	B	0.45	0/3258	0.73	2/4361 (0.0%)
20	U	0.47	0/841	0.71	0/1128
21	V	0.43	0/977	0.63	0/1312
22	W	0.43	0/542	0.59	0/722
23	X	0.41	0/992	0.67	0/1334
24	Y	0.47	0/1082	0.72	1/1441 (0.1%)
25	Z	0.47	0/1137	0.79	0/1517
26	a	0.45	0/1190	0.71	0/1591
27	b	0.45	0/570	0.72	0/752
28	c	0.46	0/813	0.70	0/1091
29	d	0.45	0/919	0.67	0/1238
3	C	0.47	0/2943	0.73	1/3953 (0.0%)
30	e	0.45	0/1071	0.68	0/1428
31	f	0.50	0/884	0.81	0/1185
32	g	0.48	0/917	0.74	0/1222
33	h	0.38	0/1022	0.64	0/1351
34	i	0.43	0/793	0.75	0/1048
35	j	0.49	0/704	0.76	0/931
36	k	0.43	0/574	0.73	0/761
37	l	0.40	0/453	0.61	0/599
38	m	0.42	0/434	0.70	0/575
39	n	0.40	0/240	0.50	0/305
4	D	0.49	1/2406 (0.0%)	0.70	1/3221 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	o	0.46	0/884	0.74	0/1166
41	p	0.40	0/717	0.61	0/953
42	t	0.48	0/1058	0.75	0/1416
43	u	0.45	0/1638	0.69	1/2222 (0.0%)
44	2	0.41	22/86672 (0.0%)	0.81	41/135198 (0.0%)
45	3	0.36	0/3723	0.79	1/5800 (0.0%)
46	4	0.38	0/2836	0.82	3/4421 (0.1%)
5	E	0.52	0/1311	0.73	0/1763
6	F	0.45	0/1985	0.68	0/2644
7	G	0.46	0/1914	0.72	0/2578
8	H	0.43	0/1554	0.69	0/2089
9	I	0.42	0/1642	0.67	0/2194
All	All	0.43	25/147330 (0.0%)	0.77	54/217756 (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
44	2	0	34
45	3	0	2
All	All	0	36

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1701	C	C5'-C4'	18.32	1.73	1.51
44	2	1673	C	C3'-O3'	15.33	1.63	1.42
44	2	1701	C	O5'-C5'	14.40	1.67	1.44
44	2	1673	C	O3'-P	14.19	1.78	1.61
44	2	1701	C	P-O5'	13.52	1.73	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	1701	C	O4'-C4'-C3'	-15.18	88.82	104.00
2	B	258	HIS	C-N-CD	-13.98	89.84	120.60
44	2	1701	C	O4'-C1'-N1	12.32	118.06	108.20
44	2	1701	C	C4'-C3'-O3'	12.21	137.41	113.00
44	2	1701	C	C2'-C3'-O3'	-10.63	86.10	109.50

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	2	1	C	Sidechain
44	2	115	C	Sidechain
44	2	121	A	Sidechain
44	2	149	U	Sidechain
44	2	2	G	Sidechain

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	1888	0	1983	135	0
2	B	3190	0	3327	164	0
3	C	2889	0	3064	277	0
4	D	2361	0	2385	157	0
5	E	1286	0	1398	171	0
6	F	1949	0	2093	134	0
7	G	1881	0	2018	136	0
8	H	1535	0	1611	94	0
9	I	1604	0	1652	60	0
10	J	1362	0	1399	89	0
11	L	1617	0	1725	120	0
12	M	1139	0	1204	134	0
13	N	1708	0	1761	97	0
14	O	1607	0	1745	127	0
15	P	1234	0	1263	91	0
16	Q	1493	0	1612	119	0
17	R	1526	0	1682	75	0
18	S	1438	0	1472	85	0
19	T	1297	0	1366	115	0
20	U	827	0	852	29	0
21	V	963	0	1026	42	0
22	W	529	0	541	27	0
23	X	975	0	1053	64	0
24	Y	1065	0	1145	102	0
25	Z	1114	0	1194	62	0
26	a	1161	0	1213	0	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	560	0	590	0	0
28	c	802	0	845	0	0
29	d	904	0	947	0	0
30	e	1053	0	1144	0	0
31	f	865	0	904	0	0
32	g	907	0	1002	0	0
33	h	1014	0	1148	0	0
34	i	783	0	862	0	0
35	j	690	0	719	0	0
36	k	568	0	637	0	0
37	l	443	0	483	0	0
38	m	428	0	466	0	0
39	n	239	0	289	0	0
40	o	870	0	943	0	0
41	p	707	0	760	0	0
42	t	1043	0	1120	0	0
43	u	1621	0	1555	0	0
44	2	77488	0	39153	7461	0
45	3	3334	0	1693	313	0
46	4	2538	0	1286	273	0
All	All	136495	0	98330	9536	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 46.

The worst 5 of 9536 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)
44:2:1673:C:C3'	44:2:1673:C:O3'	1.63	1.46
44:2:1701:C:C5'	44:2:1701:C:O5'	1.67	1.39
44:2:3910:G:O2'	44:2:3911:A:H5'	1.22	1.34
1:A:196:TRP:HB3	1:A:197:PRO:CD	1.62	1.25
20:U:29:VAL:O	44:2:4022:C:O2'	186.30	1.23

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	
1	A	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	16	61
2	B	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	4	38
3	C	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	3	35
4	D	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	11	55
5	E	156/288 (54%)	141 (90%)	8 (5%)	7 (4%)	3	33
6	F	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	11	55
7	G	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	4	36
8	H	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	12	56
9	I	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	12	56
10	J	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	22
11	L	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	2	28
12	M	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	14	58
13	N	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	13	57
14	O	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	13	57
15	P	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	9	51
16	Q	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	5	40
17	R	181/196 (92%)	174 (96%)	4 (2%)	3 (2%)	11	55
18	S	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	4	39
19	T	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	10	52
20	U	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
21	V	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	12	56
22	W	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
23	X	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
24	Y	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	7	47
25	Z	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	5	40
27	b	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	2	26
28	c	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	9	51
29	d	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	21	67
30	e	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	7	47
31	f	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	3	32
32	g	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	4	39
33	h	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	7	46
34	i	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	2	25
35	j	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	7	47
36	k	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	13	57
37	l	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	9	50
38	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	51
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	10	52
41	p	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	5	40
42	t	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	2	29
43	u	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	14	58
All	All	6479/7422 (87%)	6102 (94%)	200 (3%)	177 (3%)	10	45

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	196	TRP
2	B	4	ARG
2	B	5	LYS
2	B	157	CYS

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	189/199 (95%)	184 (97%)	5 (3%)	54	80
2	B	344/349 (99%)	326 (95%)	18 (5%)	29	65
3	C	302/348 (87%)	284 (94%)	18 (6%)	24	60
4	D	244/250 (98%)	237 (97%)	7 (3%)	50	78
5	E	143/252 (57%)	135 (94%)	8 (6%)	26	62
6	F	203/215 (94%)	196 (97%)	7 (3%)	44	75
7	G	199/223 (89%)	192 (96%)	7 (4%)	43	74
8	H	171/171 (100%)	164 (96%)	7 (4%)	37	71
9	I	170/181 (94%)	161 (95%)	9 (5%)	28	64
10	J	143/149 (96%)	137 (96%)	6 (4%)	36	70
11	L	167/177 (94%)	156 (93%)	11 (7%)	21	57
12	M	118/161 (73%)	114 (97%)	4 (3%)	44	75
13	N	172/172 (100%)	170 (99%)	2 (1%)	78	90
14	O	168/174 (97%)	166 (99%)	2 (1%)	78	90
15	P	133/163 (82%)	126 (95%)	7 (5%)	28	64
16	Q	162/165 (98%)	157 (97%)	5 (3%)	47	77
17	R	161/175 (92%)	150 (93%)	11 (7%)	20	57
18	S	155/157 (99%)	148 (96%)	7 (4%)	34	69
19	T	139/140 (99%)	134 (96%)	5 (4%)	42	74
20	U	91/115 (79%)	88 (97%)	3 (3%)	45	76
21	V	100/107 (94%)	99 (99%)	1 (1%)	82	92
22	W	55/126 (44%)	52 (94%)	3 (6%)	27	63
23	X	107/133 (80%)	105 (98%)	2 (2%)	65	86
24	Y	119/135 (88%)	115 (97%)	4 (3%)	44	75
25	Z	118/118 (100%)	112 (95%)	6 (5%)	29	66
26	a	120/121 (99%)	116 (97%)	4 (3%)	45	76
27	b	58/126 (46%)	57 (98%)	1 (2%)	68	87
28	c	88/97 (91%)	87 (99%)	1 (1%)	80	91
29	d	100/110 (91%)	96 (96%)	4 (4%)	38	71
30	e	115/121 (95%)	112 (97%)	3 (3%)	54	80
31	f	87/89 (98%)	79 (91%)	8 (9%)	11	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	98/100 (98%)	88 (90%)	10 (10%)	9	37
33	h	109/110 (99%)	106 (97%)	3 (3%)	51	78
34	i	82/89 (92%)	76 (93%)	6 (7%)	17	54
35	j	71/80 (89%)	69 (97%)	2 (3%)	51	78
36	k	64/65 (98%)	64 (100%)	0	100	100
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	84
38	m	48/116 (41%)	45 (94%)	3 (6%)	22	59
39	n	24/24 (100%)	24 (100%)	0	100	100
40	o	94/94 (100%)	89 (95%)	5 (5%)	28	64
41	p	74/75 (99%)	72 (97%)	2 (3%)	52	79
42	t	113/121 (93%)	106 (94%)	7 (6%)	23	60
43	u	177/177 (100%)	163 (92%)	14 (8%)	15	51
All	All	5642/6318 (89%)	5403 (96%)	239 (4%)	41	70

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	N	31	ARG
17	R	138	LEU
42	t	20	ARG
15	P	2	VAL
16	Q	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	180	GLN
18	S	117	HIS
38	m	87	GLN
15	P	54	GLN
16	Q	162	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	2	3605/5025 (71%)	2046 (56%)	325 (9%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	3	156/194 (80%)	81 (51%)	6 (3%)
46	4	118/119 (99%)	68 (57%)	9 (7%)
All	All	3879/5338 (72%)	2195 (56%)	340 (8%)

5 of 2195 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	2	2	G
44	2	3	C
44	2	5	A
44	2	6	C
44	2	8	U

5 of 340 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	2006	C
44	2	2561	G
44	2	4867	G
44	2	2034	G
44	2	2371	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 ⓘ

There are no chain breaks in this entry.