



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:50 PM BST

PDB ID : 4V69
EMDB ID: : EMD-5036
Title : Ternary complex-bound E.coli 70S ribosome.
Authors : Villa, E.; Sengupta, J.; Trabuco, L.G.; LeBarron, J.; Baxter, W.T.; Shaikh, T.R.; Grassucci, R.A.; Nissen, P.; Ehrenberg, M.; Schulten, K.; Frank, J.
Deposited on : 2008-12-11
Resolution : 6.70 Å(reported)
Based on PDB ID : 2i2u, 2i2v, 2j00, 1ob2

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

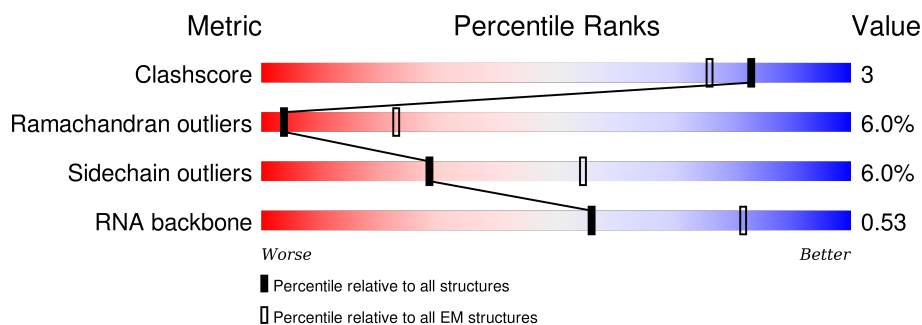
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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.














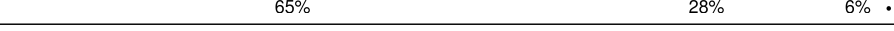

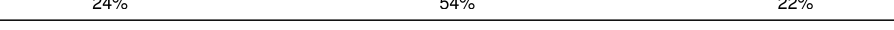
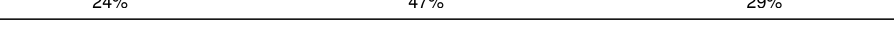




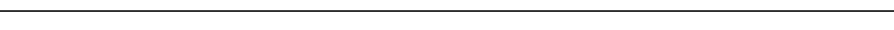

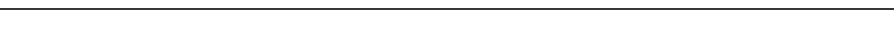
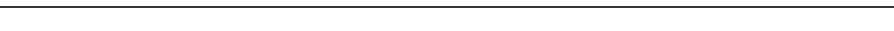


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	AJ	98	66% 26% 7% .
2	AK	117	69% 26% ..
3	AL	123	67% 26% 7% .
4	AM	113	58% 28% 13%
5	AN	96	58% 28% 13% .
6	AO	88	65% 27% 6% .
7	AP	80	65% 29% 6%
8	AQ	80	74% 18% 9%









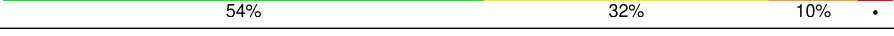

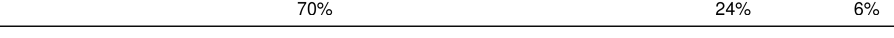
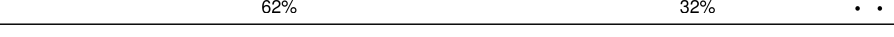

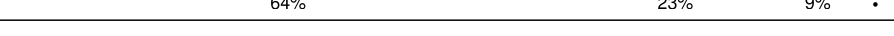


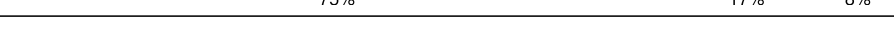

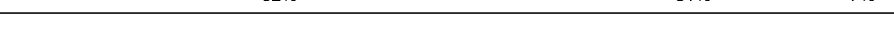






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AR	55	 67% 22% 11%
10	AS	79	 65% 27% 9%
11	AT	85	 76% 20% .
12	AU	51	 59% 29% 12%
13	AB	218	 70% 23% 7%
14	AC	206	 70% 24% 5% .
15	AD	205	 62% 26% 10% .
16	AE	150	 68% 29% .
17	AF	100	 69% 25% 5% .
18	AG	150	 60% 33% 6% .
19	AH	129	 68% 27% 5%
20	AI	127	 65% 28% 6% .
21	AA	1530	 36% 47% 17%
22	AY	76	 24% 54% 22%
23	AW	76	 24% 47% 29%
24	AX	11	 55% 27% 18%
25	AZ	393	 64% 28% 7% .
26	AV	77	 . 38% 48% 13%
27	B5	234	 74% 22% . .
28	BI	141	 67% 28% . .
29	BJ	142	 65% 24% 8% .
30	BK	121	 67% 27% 6%
31	BL	143	 66% 28% 5% .
32	BM	136	 71% 23% 5% .
33	BN	120	 63% 29% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	BO	116	
35	BP	114	
36	BQ	117	
37	BR	103	
38	BS	110	
39	BT	93	
40	BU	102	
41	BV	94	
42	BW	79	
43	BX	77	
44	BY	63	
45	BC	271	
46	BZ	58	
47	B0	56	
48	B1	50	
49	B2	46	
50	B3	64	
51	B4	38	
52	BD	209	
53	BE	201	
54	BF	178	
55	BG	176	
56	BH	149	
57	BB	2903	
58	BA	117	

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 152250 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 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	113	Total	C	N	O	S	0	0
			877	541	177	156	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	SER	DELETION	UNP P0AG59
AN	?	-	ASP	DELETION	UNP P0AG59
AN	?	-	GLU	DELETION	UNP P0AG59

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	ASP	DELETION	UNP P0AG59

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	80	Total	C	N	O	S	0	0
			639	400	126	112	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AR	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 12 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AU	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 13 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AB	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 14 is a protein called 30S ribosomal protein S3.

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

- Molecule 15 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	150	Total	C	N	O	S	0	0
			1175	730	226	215	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32832	14642	6024	10636	1530		

- Molecule 22 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AY	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 23 is a RNA chain called P-site tRNA fMet (Unmodified bases except for Thymine 54).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0
			232	106	44	72	10		

- Molecule 25 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AZ	393	Total	C	N	O	S	0	0
			3035	1918	523	581	13		

- Molecule 26 is a RNA chain called E-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	77	Total	C	N	O	P	0	0
			1645	733	297	538	77		

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 29 is a protein called 50S ribosomal protein L13.

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

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BK	121	Total	C	N	O	S	0	0
			931	582	179	165	5		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BN	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 35 is a protein called 50S ribosomal protein L19.

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

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BT	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BU	102	Total	C	N	O		
			780	492	146	142	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BW	79	Total	C	N	O	S		
			596	367	120	108	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BC	271	Total	C	N	O	S		
			2083	1288	423	365	7	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L3.

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

- Molecule 53 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 56 is a protein called 50S ribosomal protein L9.

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

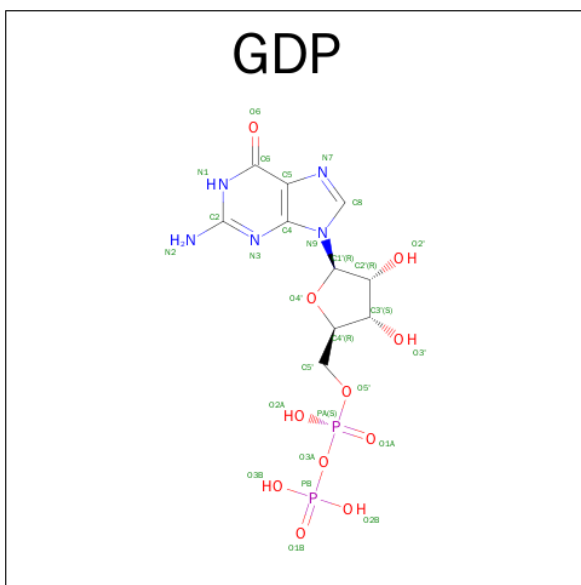
- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BB	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BA	117	Total	C	N	O	P	0	0
			2508	1116	459	816	117		

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

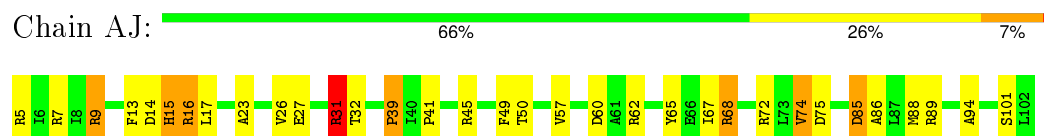


Mol	Chain	Residues	Atoms					AltConf
59	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	

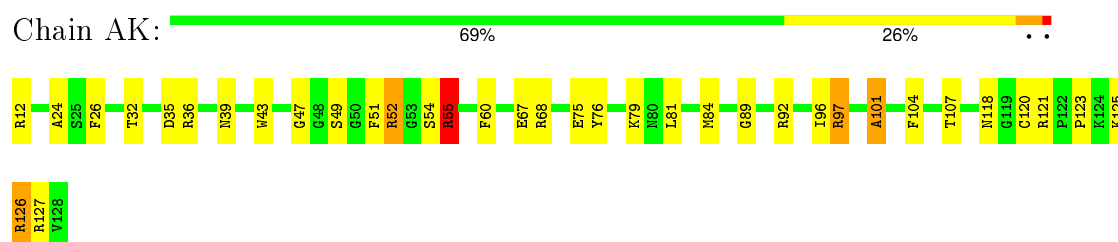
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

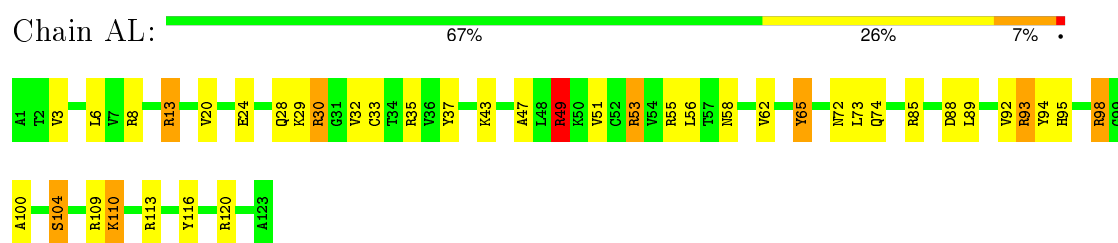
- Molecule 1: 30S ribosomal protein S10



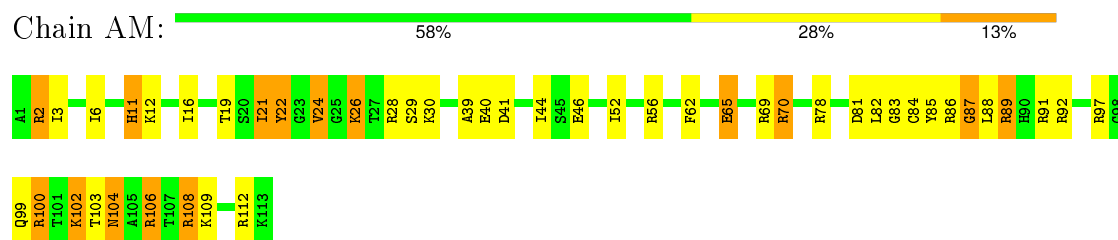
- Molecule 2: 30S ribosomal protein S11



- Molecule 3: 30S ribosomal protein S12

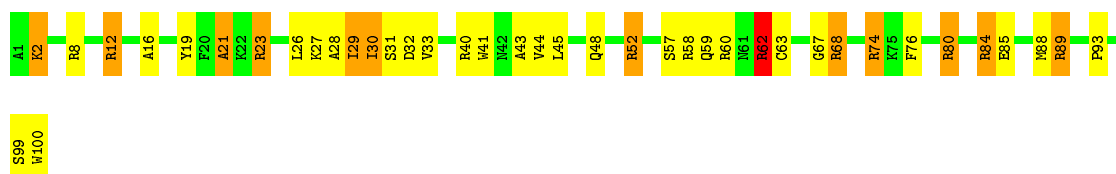


- Molecule 4: 30S ribosomal protein S13



- Molecule 5: 30S ribosomal protein S14





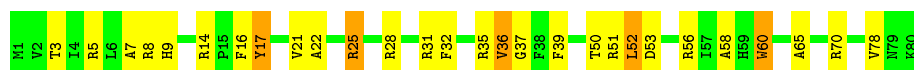
- Molecule 6: 30S ribosomal protein S15

Chain AO: 65% 27% 6% .



- Molecule 7: 30S ribosomal protein S16

Chain AP: 65% 29% 6%



- Molecule 8: 30S ribosomal protein S17

Chain AQ: 74% 18% 9%



- Molecule 9: 30S ribosomal protein S18

Chain AR: 67% 22% 11%



- Molecule 10: 30S ribosomal protein S19

Chain AS: 65% 27% 9%



- Molecule 11: 30S ribosomal protein S20

Chain AT: 76% 20%



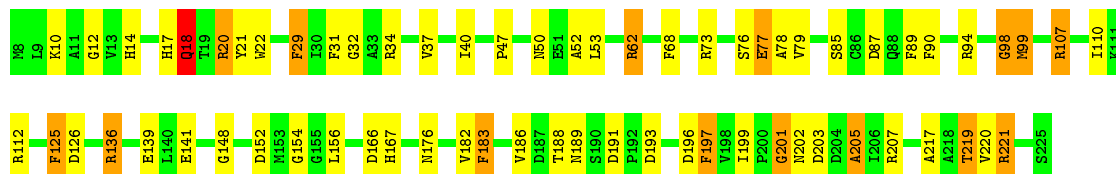
- Molecule 12: 30S ribosomal protein S21

Chain AU: 59% 29% 12%



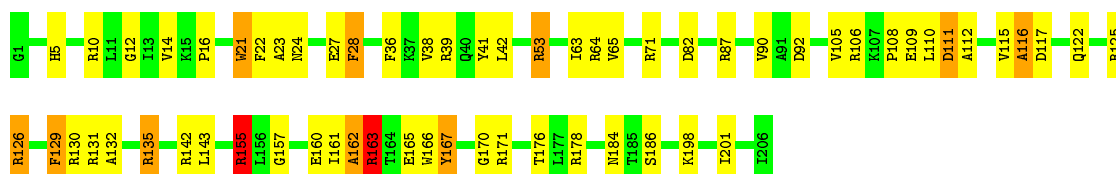
- Molecule 13: 30S ribosomal protein S2

Chain AB: 70% 23% 7%



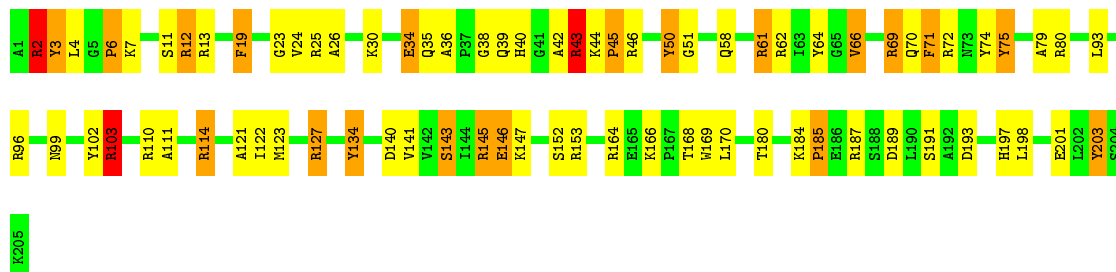
- Molecule 14: 30S ribosomal protein S3

Chain AC: 70% 24% 5%



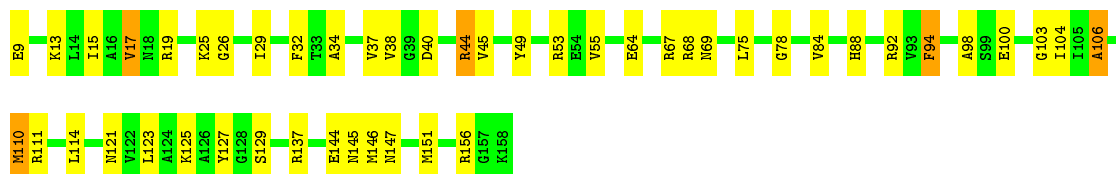
- Molecule 15: 30S ribosomal protein S4

Chain AD: 62% 26% 10%



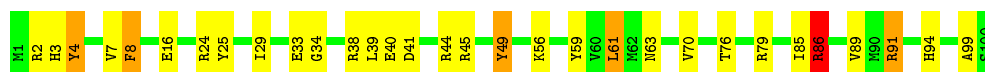
- Molecule 16: 30S ribosomal protein S5

Chain AE: 68% 29% 3%



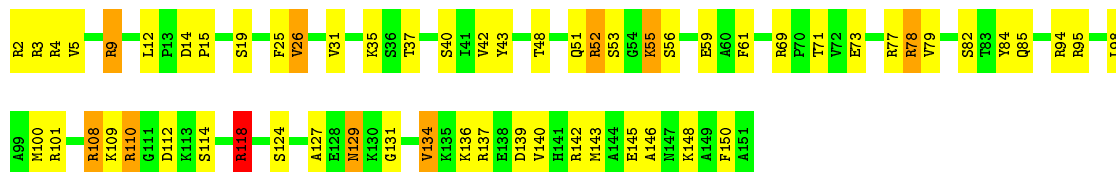
- Molecule 17: 30S ribosomal protein S6

Chain AF: 69% 25% 5%



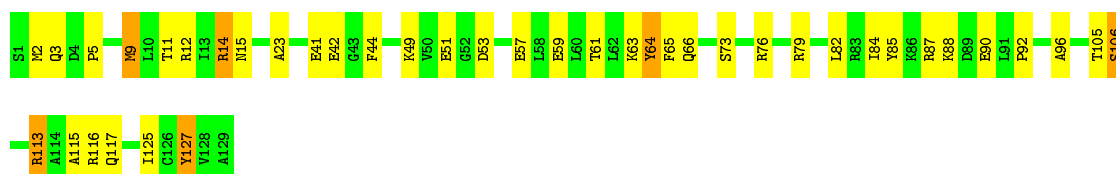
- Molecule 18: 30S ribosomal protein S7

Chain AG: 60% 33% 6%



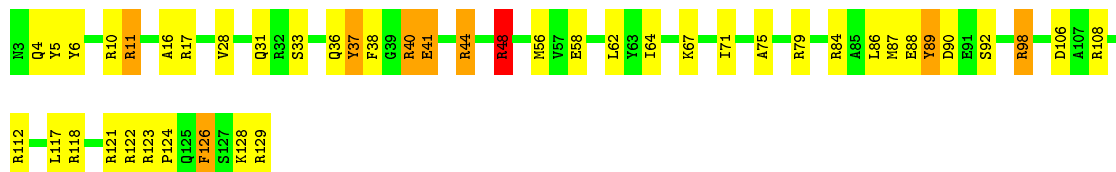
- Molecule 19: 30S ribosomal protein S8

Chain AH: 68% 27% 5%



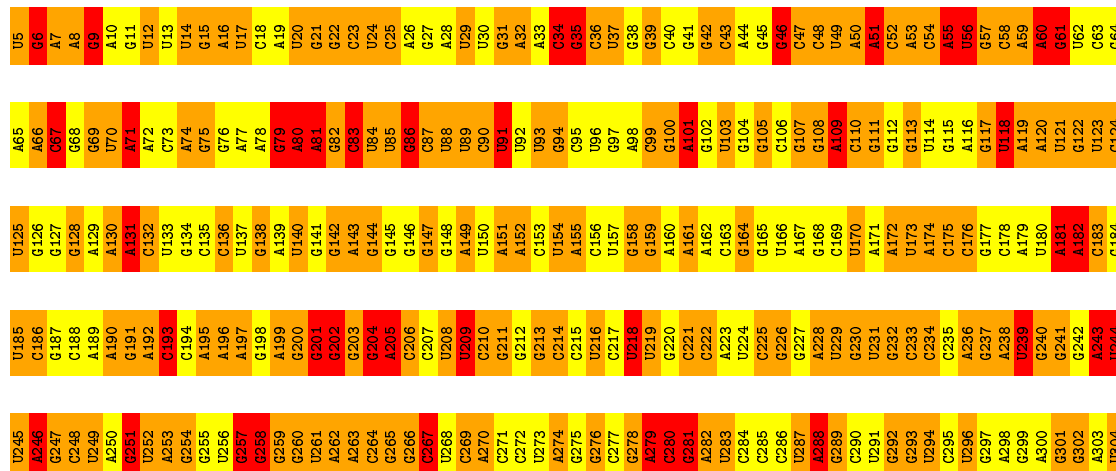
- Molecule 20: 30S ribosomal protein S9

Chain AI: 65% 28% 6%

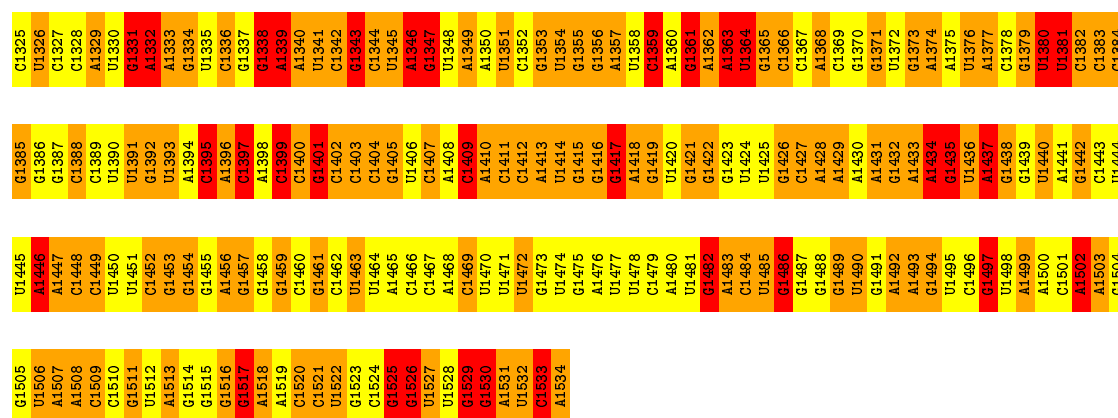


- Molecule 21: 16S rRNA

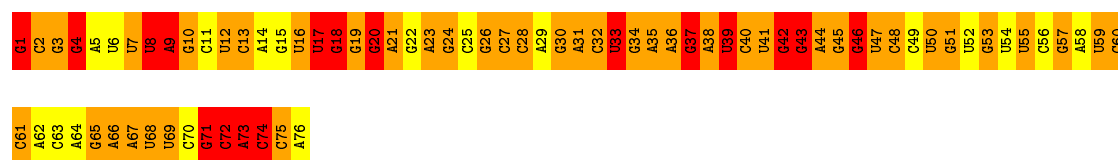
Chain AA: 36% 47% 17%



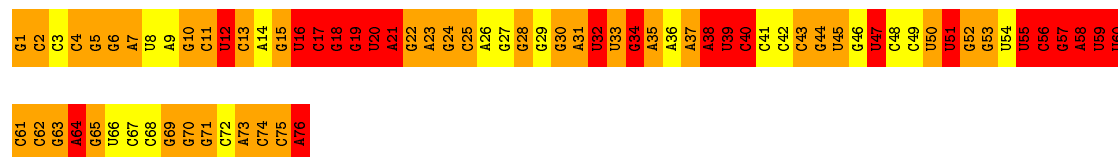
C1265	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725	A665	U605	C545	U485	G425	U365	G305
G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G786	G726	G666	G606	A546	U486	U426	A366	A306
G1267	C1207	G1087	G1087	C1027	G967	A907	G847	A787	G727	G667	A607	A547	A367	U427	G307	C308
G1268	G1208	U1148	G1088	G1028	A968	A908	G848	U788	A728	G668	A608	A548	U368	G428	U368	C308
G1269	C1209	C1149	G1089	U1029	A969	A909	G849	U789	A729	G669	A609	C549	C369	U429	G309	A309
G1270	G1210	A1150	U1090	U1030	C970	C910	U850	A790	G730	G670	U610	U550	C370	A430	C370	G310
U1211	U1211	A1151	U1091	C1031	G971	U911	G851	G791	G731	G671	C611	U551	A371	A431	A371	C311
G1272	U1212	A1152	A1092	G1032	C972	C912	G852	A792	G732	U672	C612	U552	C372	A432	C372	C312
C1273	G1213	G1153	A1093	G1033	G973	A913	C853	U793	G733	A673	C613	A553	A373	A433	A373	A313
A1274	C1214	A1154	U1094	G1034	A974	A914	U854	A794	G734	G674	C614	U554	A374	U434	A374	C314
A1275	G1215	A1155	U1095	A1035	A975	A915	U855	C795	G735	A675	C615	U555	U375	A435	U375	A315
G1276	A1216	G1156	C1096	A1036	G976	U916	C856	G796	G736	G676	G616	C556	A376	A436	G376	G316
C1277	C1217	A1157	C1097	C1037	A977	G917	C857	C797	G737	U677	C617	U557	G377	U437	G377	U317
G1278	C1218	C1158	C1098	C1038	A978	A918	G858	U798	G738	U678	C618	U558	A498	U438	G378	G318
G1279	A1219	U1159	G1099	G1039	C979	A919	G859	G799	G739	C679	U619	A559	A499	U439	C379	G319
A1280	G1220	C1160	C1100	U1040	C980	A920	A860	G800	U740	C680	C620	A560	G380	C440	G380	A320
C1281	G1221	C1161	A1101	U1041	U981	U921	G861	U801	G741	A681	A621	U561	C381	A441	C381	A321
G1282	G1222	C1162	A1102	A1042	U982	G922	C862	A802	G742	A682	A622	U562	A382	G442	A382	C322
U1283	C1223	A1163	C1103	G1043	A983	A923	U863	G803	A743	G683	C623	A563	C503	C443	A383	U323
C1284	U1224	G1164	G1104	A1044	C984	C924	A864	U804	G744	U684	C624	C564	C504	G444	G384	G324
A1285	A1225	U1165	A1105	C1045	C985	G925	A865	C805	G745	U685	U625	U565	G505	G445	C385	A325
U1286	C1226	G1166	G1106	A1046	U986	G926	G866	C806	A746	U686	G626	U566	G506	G446	C386	G326
A1287	A1227	A1167	G1107	G1047	G987	G927	G867	A807	A747	U687	G627	U567	C507	G447	U387	A327
A1288	G1228	U1168	G1108	G1048	G988	G928	C868	G808	G748	G688	G628	U568	U508	A448	G388	C328
A1289	A1229	A1169	C1109	U1049	U989	G929	G869	G809	A749	C689	A629	C569	A509	G449	A389	A329
G1290	C1230	A1170	A1110	G1050	C990	C930	U870	C910	G750	G690	A630	G570	A510	G450	U390	C330
U1291	G1231	C1171	A1111	C1051	U991	C931	U871	C911	U751	G691	C631	U571	C391	A451	G391	G331
G1292	C1232	A1172	U1112	U1052	U992	C932	A872	G912	G752	U692	A632	U572	C392	A452	C392	G332
C1293	G1233	G1173	C1113	G1053	G993	G933	A873	U913	A753	G693	G633	C513	A393	G453	A393	U333
G1294	A1234	U1174	C1114	C1054	A994	C934	G874	A814	G754	A694	C634	A514	G394	G454	G394	C334
U1295	U1235	G1175	U1115	A1055	C995	A935	U875	A815	G755	A695	A635	G515	C395	G455	C395	C335
C1296	A1236	A1176	U1116	U1056	A996	C936	C876	A816	G756	A696	U636	U516	C396	A456	C396	A336
G1297	C1237	G1177	A1117	G1057	U997	G937	G877	C917	U757	U697	C637	G517	A397	G457	A397	G337
U1298	A1238	G1178	U1118	G1058	C998	A938	A878	G918	G758	G698	U638	C518	U398	A458	U398	A338
A1299	C1239	A1179	C1119	C1059	C999	G939	C879	A819	A759	C699	G639	A519	G399	U459	C399	C339
G1300	U1240	A1180	C1120	U1060	A1000	C940	C880	U820	G760	A640	A640	C520	C400	A460	C400	U340
U1301	G1241	G1181	U1121	G1061	C1001	G941	G881	G821	G761	U641	U641	G521	C401	A461	C401	C341
C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	U822	U762	A642	A642	C522	G402	G462	G402	C342
C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	C823	G763	C643	C643	A523	C403	U463	C403	U343
G1304	G1244	G1184	G1124	A1064	A1004	G944	U884	G824	G764	U644	U644	G524	G404	U464	G404	A344
G1305	C1245	U1185	U1125	U1065	A1005	G945	G885	A825	G765	G645	G645	C525	U405	A465	U405	C345
A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	C826	A766	C586	G646	C526	G406	A466	G406	G346
U1307	U1247	G1187	G1127	A1067	U1007	G947	G887	U827	A767	U647	C647	G527	U407	U467	U407	C347
U1308	C1248	A1188	C1128	G1068	U1008	C948	G888	U828	A768	G648	A648	G528	A408	A468	A408	C348
G1309	G1249	U1189	C1129	C1069	U1009	A949	A889	G829	G768	U649	A649	G529	U409	C469	U409	A349
G1310	A1250	G1190	A1130	U1070	G1010	U950	G890	G830	C770	G650	G650	U590	G410	C470	G410	G350
A1311	A1251	A1191	G1131	C1071	G951	G951	U891	A831	G771	C651	C651	U591	A411	U471	A411	G351
G1312	G1252	C1192	C1132	A1072	A1012	U952	A892	G832	U772	U652	U652	G592	A412	U472	A412	C352
U1313	C1253	G1193	G1133	U1073	G1013	G953	C893	G833	G773	G713	U653	U593	G413	U473	G413	A353
C1314	A1254	U1194	G1134	G1074	A1014	G954	G894	U834	G774	G714	G654	U594	A414	G474	A414	G354
U1315	G1255	C1195	U1135	U1075	G1015	U955	G895	U835	G775	A715	A655	A595	A415	C475	A415	C355
A1316	A1256	A1196	C1136	A1076	U956	A1016	C896	G836	G776	A716	G656	A596	A356	U476	A356	A356
C1317	G1257	G1197	C1137	G1077	U957	U957	C897	U837	A777	U717	U657	G597	G417	C477	G417	G357
A1318	C1258	U1198	G1138	U1078	A958	A958	G898	G838	G778	A718	C658	U598	C418	A478	C418	U358
A1319	C1259	U1199	C1139	G1079	A959	U960	G899	C839	C779	G719	U659	C599	A419	U479	A419	G359
G1320	U1260	C1140	U1080	A1080	G1020	U960	A900	C840	A780	C720	C660	A600	U420	U480	U420	G360
U1321	A1261	A1201	A1021	A1081	U861	U861	A901	C841	A781	G721	G661	G601	U421	G481	U421	G361
C1322	C1262	U1202	A1022	A1082	A1022	C962	G902	U842	A782	G722	U662	A602	C422	A482	C422	G362
G1323	G1263	G1143	G1023	U1083	G963	G963	G903	U843	A783	G723	A663	U603	C423	C483	C423	A363
A1324	U1264	A1204	G1144	G1084	G1024	A964	U904	G844	A784	G724	G664	G604	G424	G484	G424	A364



- Molecule 22: A/T-site tRNA Phe



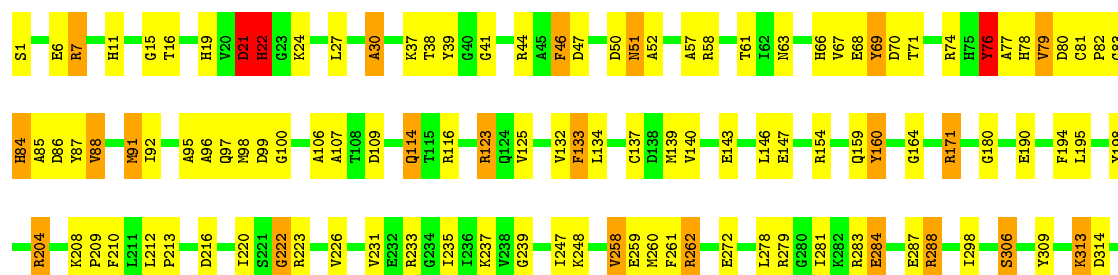
- Molecule 23: P-site tRNA fMet (Unmodified bases except for Thymine 54)



- Molecule 24: mRNA

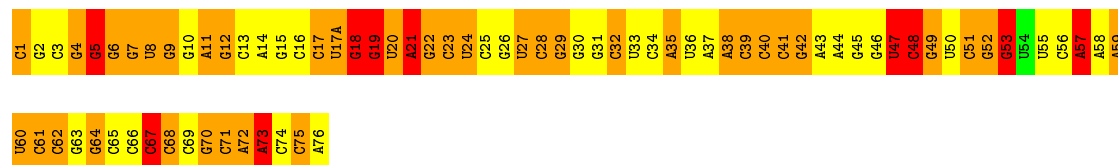


- Molecule 25: Elongation factor Tu

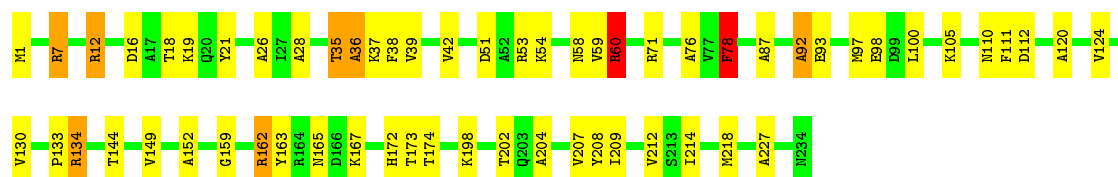




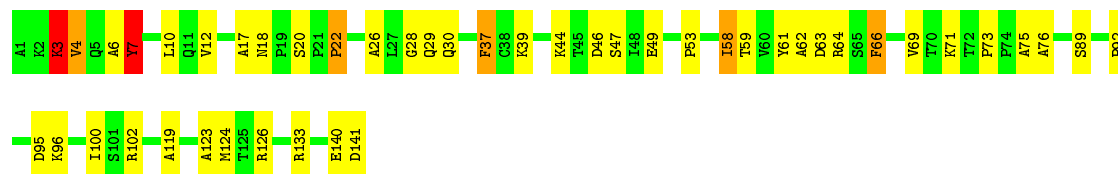
• Molecule 26: E-site tRNA Phe



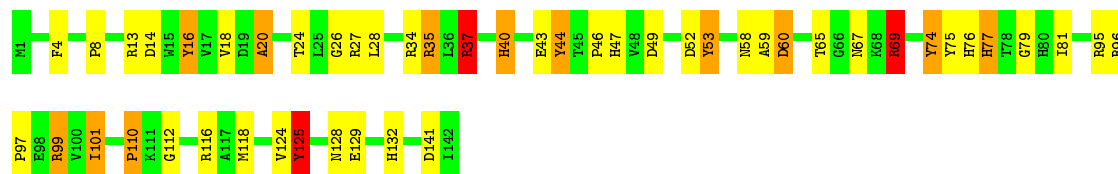
• Molecule 27: 50S ribosomal protein L1



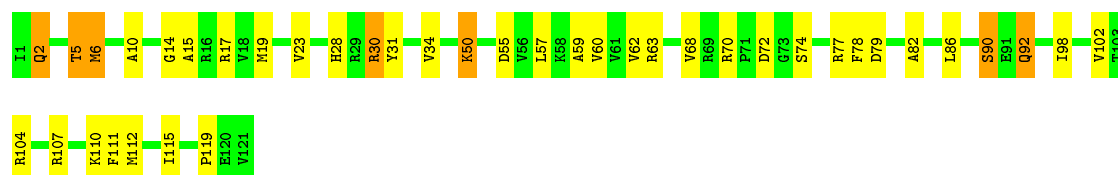
• Molecule 28: 50S ribosomal protein L11



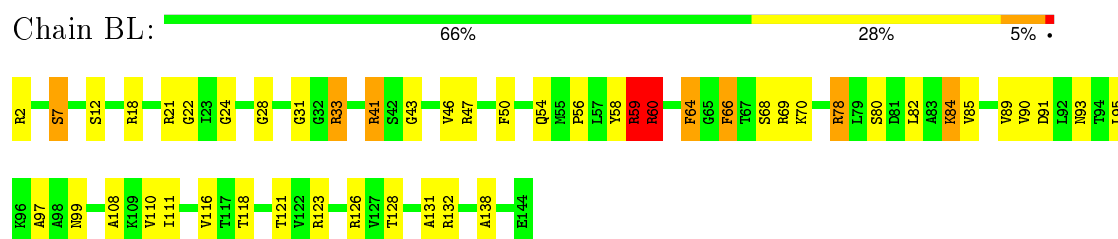
• Molecule 29: 50S ribosomal protein L13



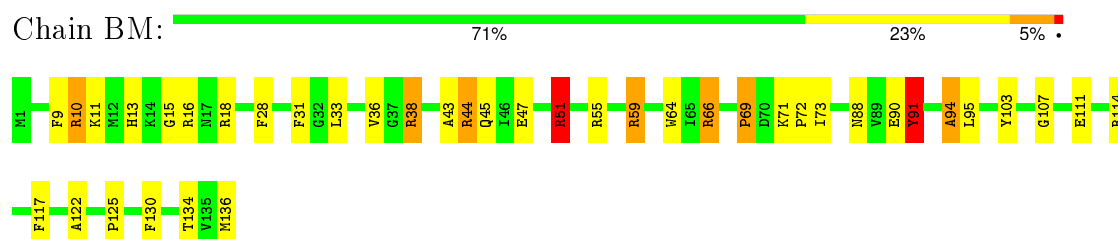
• Molecule 30: 50S ribosomal protein L14



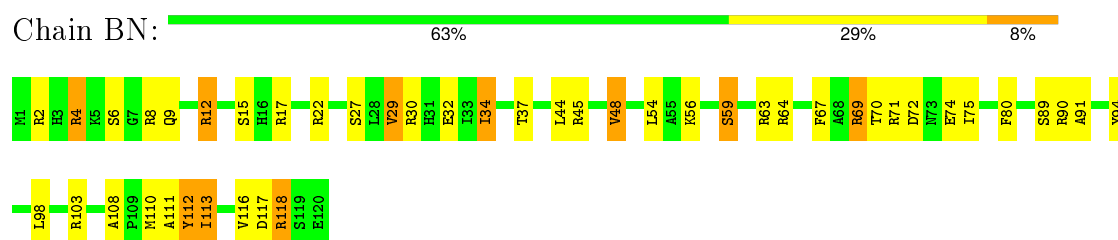
- Molecule 31: 50S ribosomal protein L15



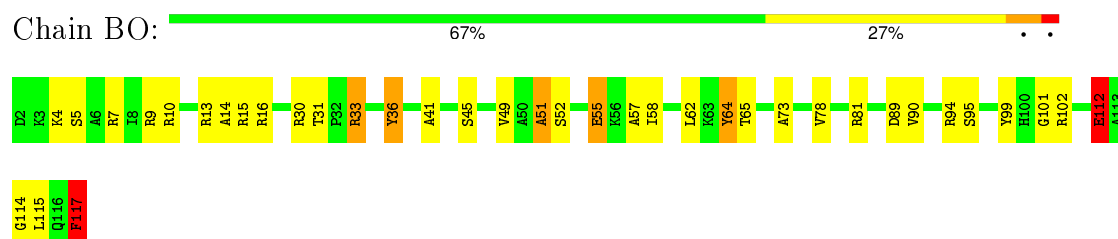
- Molecule 32: 50S ribosomal protein L16



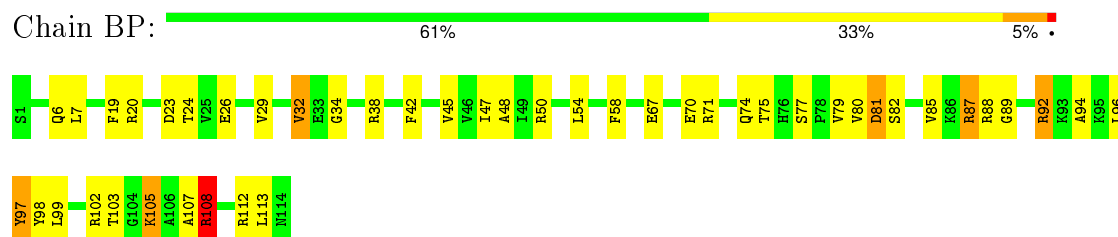
- Molecule 33: 50S ribosomal protein L17



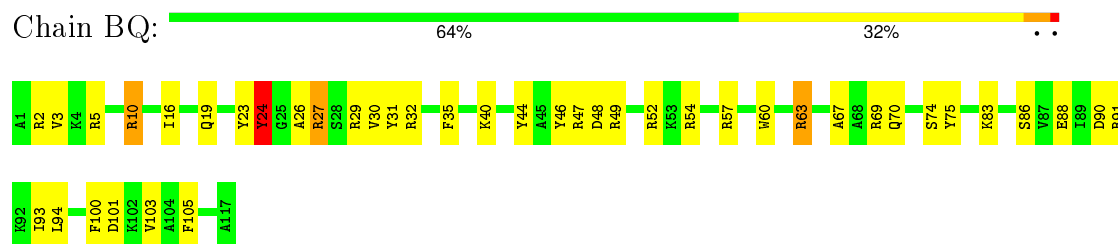
- Molecule 34: 50S ribosomal protein L18



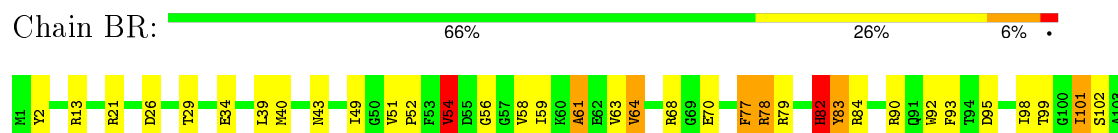
- Molecule 35: 50S ribosomal protein L19



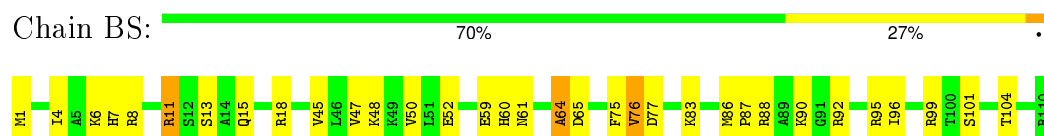
- Molecule 36: 50S ribosomal protein L20



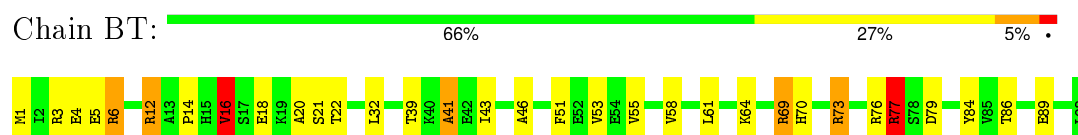
- Molecule 37: 50S ribosomal protein L21



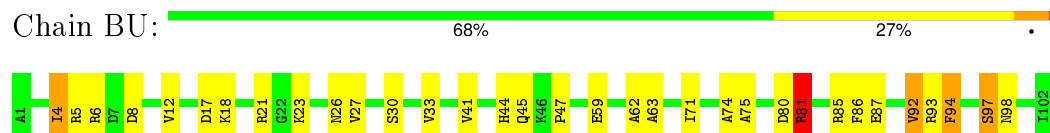
- Molecule 38: 50S ribosomal protein L22



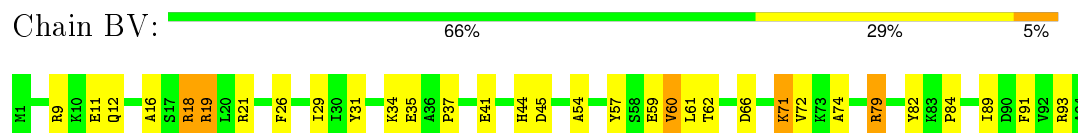
- Molecule 39: 50S ribosomal protein L23



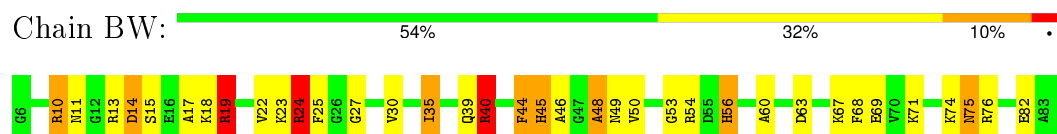
- Molecule 40: 50S ribosomal protein L24



- Molecule 41: 50S ribosomal protein L25

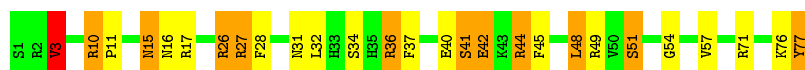


- Molecule 42: 50S ribosomal protein L27



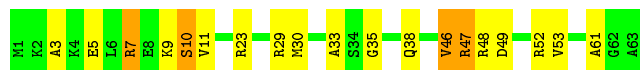
- Molecule 43: 50S ribosomal protein L28

Chain BX: 



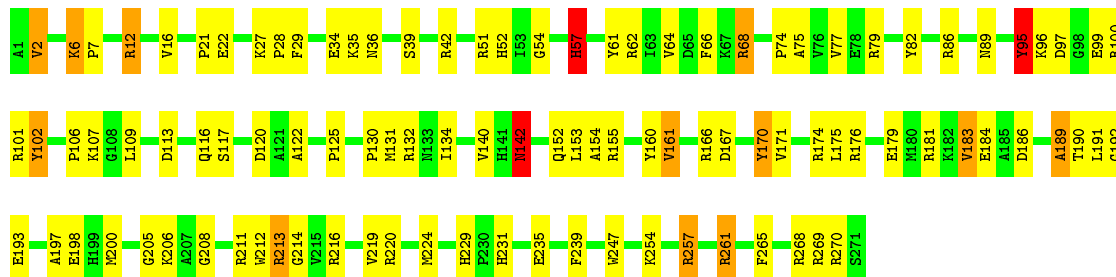
- Molecule 44: 50S ribosomal protein L29

Chain BY: 



- Molecule 45: 50S ribosomal protein L2

Chain BC: 



- Molecule 46: 50S ribosomal protein L30

Chain BZ: 



- Molecule 47: 50S ribosomal protein L32

Chain B0: 



- Molecule 48: 50S ribosomal protein L33

Chain B1: 

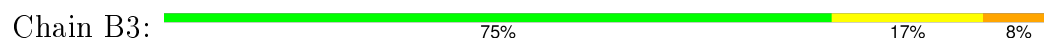


- Molecule 49: 50S ribosomal protein L34

Chain B2: 



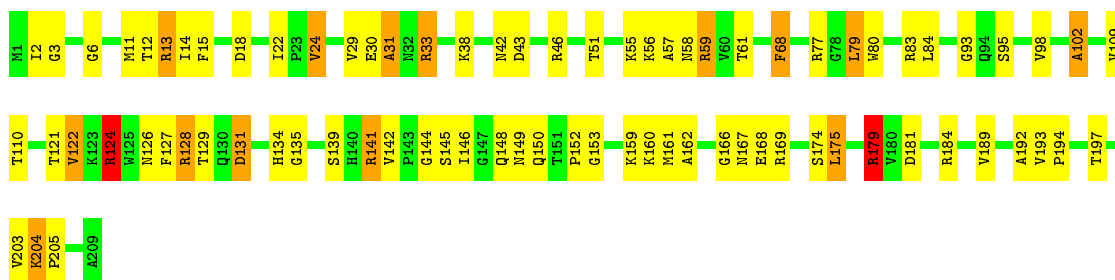
- Molecule 50: 50S ribosomal protein L35



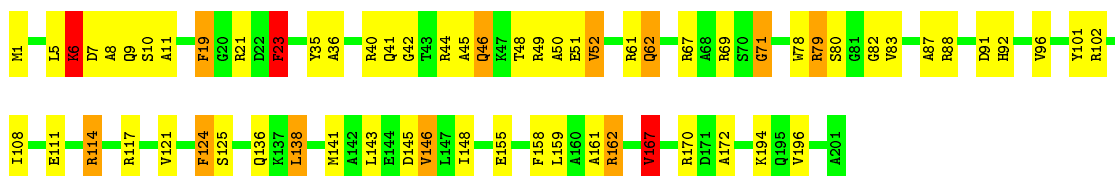
- Molecule 51: 50S ribosomal protein L36



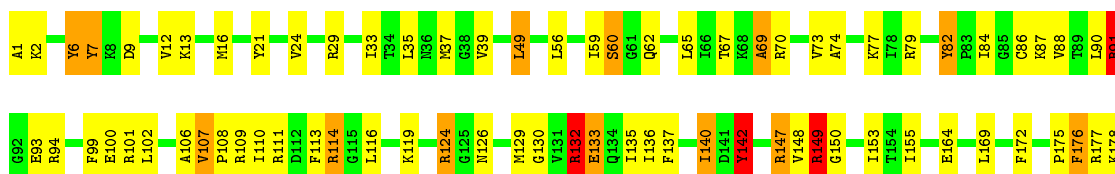
- Molecule 52: 50S ribosomal protein L3



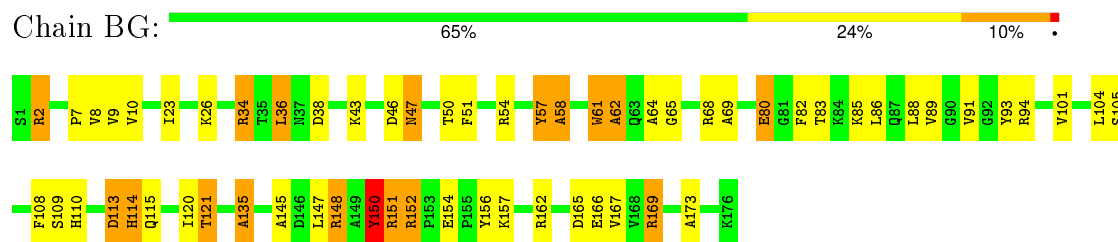
- Molecule 53: 50S ribosomal protein L4



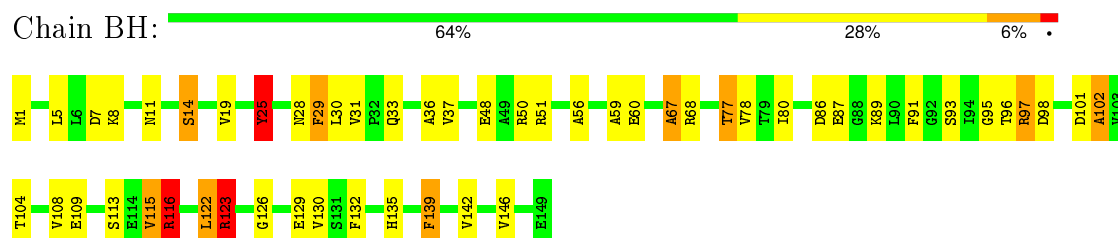
- Molecule 54: 50S ribosomal protein L5



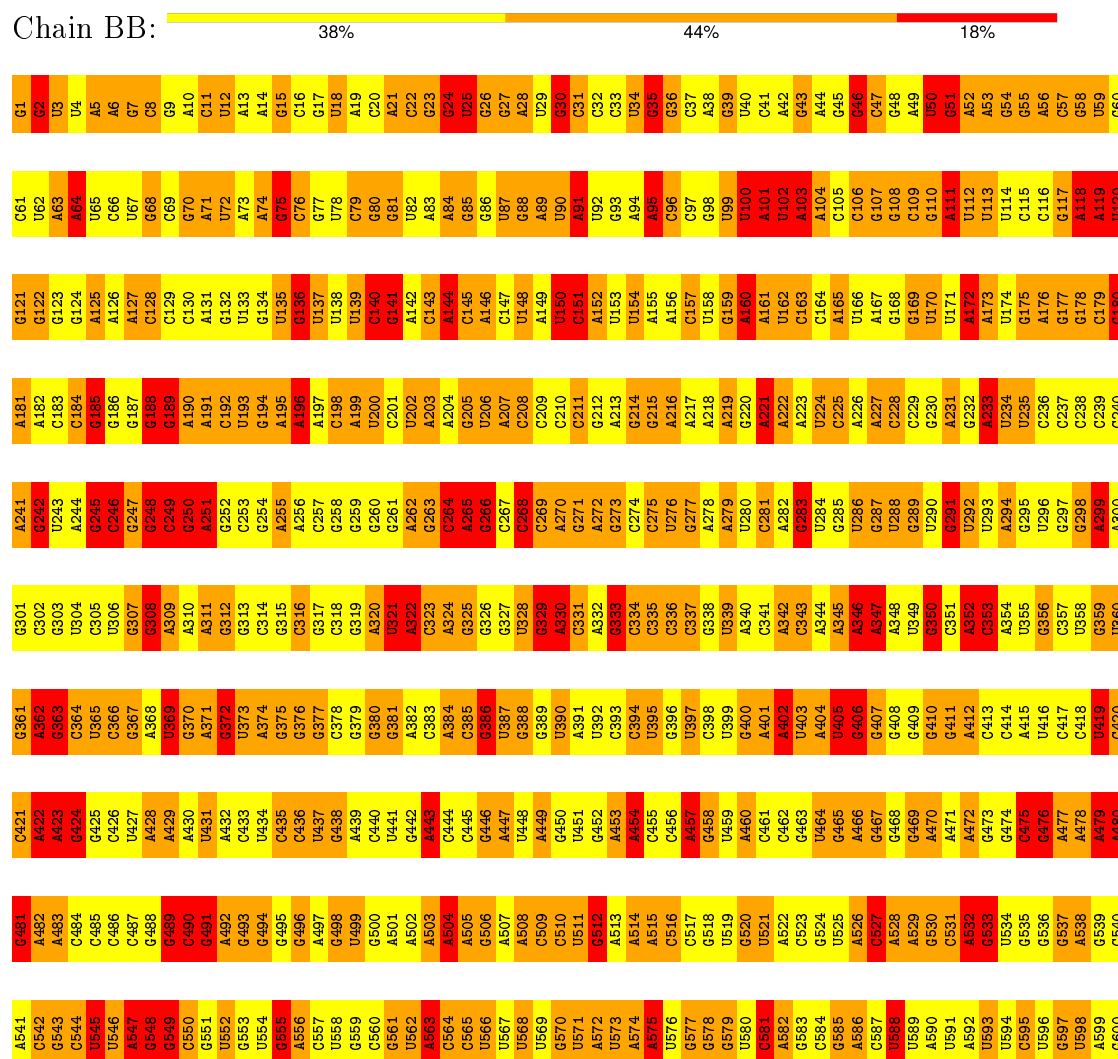
- Molecule 55: 50S ribosomal protein L6



• Molecule 56: 50S ribosomal protein L9



• Molecule 57: 23S ribosomal RNA



A1502	U1442	G1382	A1322	A1262	G1202	A1142	U1082	A1021	C961	C901	G841	A781	A721	A661	C601
A1503	U1443	A1383	C1323	U1263	U1203	A1143	U1083	G1022	G962	C902	U842	A782	A722	G662	A602
A1504	G1444	A1384	G1324	A1264	A1204	A1144	A1084	U1023	U963	C903	G843	A783	C723	G663	A603
A1505	G1445	A1385	U1325	A1265	A1205	C1145	A1085	G1024	C964	C904	A844	G784	U724	G664	A604
U1506	G1446	A1386	U1326	G1266	G1206	C1146	A1086	G1025	C965	A905	A845	G785	G725	U665	G605
C1507	C1447	A1387	A1327	U1267	G1207	A1147	G1087	G1026	G966	U906	U846	C786	G726	A666	U606
A1508	G1448	A1388	A1328	A1268	C1208	U1148	A1088	A1027	U967	C907	U847	C787	A727	U667	U607
A1509	G1449	G1389	U1329	A1269	U1209	G1149	A1089	A1028	C968	C908	C848	A788	G728	U668	A608
G1510	G1450	U1390	C1330	C1270	G1210	C1150	A1090	A1029	G969	A909	A849	A789	G729	G669	A609
G1511	G1451	U1391	G1331	G1271	C1211	A1151	G1091	C1030	U970	A910	U850	U790	A730	A670	C610
C1512	C1452	A1392	G1332	A1272	G1212	C1152	C1092	G1031	G971	A911	C851	C791	C731	C671	C611
U1513	A1453	G1393	G1333	U1273	C1213	G1153	G1093	A1032	A972	G912	U852	A792	G732	C672	G612
G1514	C1454	U1394	G1334	A1274	U1214	G1154	U1094	U1033	A973	U913	C853	A793	G733	G673	A613
A1515	G1455	A1395	C1335	A1275	G1215	A1155	A1095	G1034	G974	G914	C854	A794	A734	G674	A614
G1516	U1456	U1396	A1336	A1276	G1216	A1156	A1096	U1035	A975	C915	G855	C795	A735	A675	U615
G1517	U1457	G1337	G1337	G1277	U1217	G1157	U1097	G1036	G976	G916	U856	C796	G736	A676	A616
C1518	U1458	C1398	C1338	C1278	G1218	C1158	A1098	G1037	G977	A917	G857	G797	C737	U617	G617
G1519	G1459	G1399	G1339	G1279	U1219	U1159	G1099	G1038	G978	A918	G858	G798	G738	C678	G618
U1520	U1460	U1400	U1340	G1280	G1220	G1160	C1100	A1039	A979	U919	G859	G799	A739	C679	G619
G1521	G1461	G1401	G1341	G1281	C1221	C1161	U1101	A1040	A980	A920	U860	A800	C740	C680	G620
A1522	A1462	U1402	U1342	U1282	U1222	G1162	U1102	G1041	A981	C921	A861	G801	U741	G681	A621
C1523	G1463	A1403	G1343	G1283	G1223	G1163	A1103	G1042	C982	C922	G862	A802	A742	G682	G622
G1524	G1464	C1404	A1344	A1284	C1164	C1164	C1104	C1043	A983	G923	A863	U803	A743	U683	C623
A1525	G1465	U1405	C1345	A1285	G1225	A1165	U1105	C1044	A984	G924	G864	A804	U744	G684	C624
C1526	U1466	U1406	G1346	A1286	G1226	G1166	G1106	C1045	C985	A925	C865	G805	G745	A685	G625
G1527	U1467	G1407	A1347	A1287	G1227	C1167	G1107	A1046	C986	G926	A866	C806	U746	U686	A626
A1528	U1468	C1408	C1348	G1288	G1228	G1168	U1108	G1047	C987	A927	C867	U807	U747	C687	A627
G1529	A1469	U1409	C1349	C1289	G1229	A1169	A988	A1048	A988	A928	G868	G808	G748	U688	G628
G1530	A1470	G1410	C1350	G1290	A1230	C1170	G989	C1049	U989	U929	G869	G809	A749	A689	G629
C1531	G1471	U1411	C1351	C1291	U1231	G1171	A1050	A1050	A990	G930	U870	U840	A750	G690	G630
A1532	C1472	U1412	U1352	G1292	G1232	C1172	G1112	G1051	C991	U931	U871	U811	A751	C691	A631
C1533	G1473	A1413	A1353	C1293	C1233	U1173	G1113	C1052	C992	U932	U872	C812	A752	C692	A632
U1534	U1474	A1414	A1354	U1294	U1234	U1174	C1114	A1053	G993	A933	C873	U813	A753	A693	A633
A1535	G1475	U1415	G1355	G1295	G1235	A1175	G1115	A1054	C994	U934	C874	C814	U754	U694	C634
C1536	U1476	G1416	G1356	C1296	G1236	U1176	G1116	G1055	C995	G935	G875	C815	U755	G695	C635
G1537	A1477	C1417	C1357	C1297	A1237	G1177	C1117	G1056	A996	A936	C876	C816	A756	G696	G636
G1538	G1478	G1418	G1358	C1298	G1238	C1178	C1118	A1057	G997	C937	A877	C817	G757	G697	A637
U1539	G1479	A1419	A1359	G1299	G1239	G1179	U1119	U1058	C998	G938	A878	G818	C758	C698	G638
G1540	U1480	A1420	G1360	G1300	U1240	U1180	G1120	G1059	U999	G939	G879	A819	G759	A699	U639
C1541	U1481	G1421	G1361	A1301	C1241	U1181	C1121	U1060	A1000	G940	G880	A820	G760	G700	C640
U1542	G1482	G1422	A1362	A1302	U1242	U1182	G1122	U1061	A1001	A941	G881	A821	A761	G701	U641
G1543	G1483	G1423	C1363	G1303	C1243	U1183	C1123	G1062	G1002	G942	G882	G822	U762	U702	U642
A1544	U1484	G1424	A1364	A1304	U1244	U1184	G1124	G1063	G1003	A943	G883	C823	G763	U703	A643
A1545	U1485	G1425	A1365	C1305	G1245	G1185	G1125	C1064	U1004	G944	U884	U824	A764	G704	G644
G1546	U1486	G1426	A1366	C1306	A1246	G1186	A1126	A1067	C1005	A945	C885	A825	C765	A705	C645
A1548	U1487	A1427	A1367	A1307	U1247	G1187	A1127	G1068	C1007	G946	A886	U826	U766	A706	U646
C1549	G1488	C1428	G1368	A1308	G1248	U1188	G1128	A1069	C947	A947	U887	U827	U767	G707	G647
U1550	G1489	G1429	G1369	G1309	U1249	A1189	A1129	C889	C948	C948	C889	U828	G768	G708	G648
C1551	A1490	G1430	C1370	G1310	G1250	G1190	U1130	A1070	A1009	G949	C890	A829	U769	U709	G649
A1552	G1491	A1431	G1371	G1311	C1251	G1191	U1131	G1071	G950	G950	C890	G830	G770	U710	C650
G1553	G1492	G1432	U1372	U1312	G1252	G1192	U1132	C1072	G951	C951	G891	G831	G771	G711	G651
A1554	C1493	A1433	A1373	U1313	A1253	G1193	A1133	A1073	U1012	G952	A892	U832	C772	G712	U652
U1555	A1494	A1434	G1374	C1314	U1254	A1194	A1134	G1074	C953	G953	C893	A833	G773	G713	U653
G1556	A1495	G1435	U1375	C1315	U1255	G1195	C1135	C1075	A1014	G954	U894	G834	U774	U714	A654
A1557	U1496	G1436	G1376	U1316	G1256	C1196	G1136	C1076	U1015	U955	U895	C835	G775	A715	A655
C1557	U1497	G1437	G1377	G1317	C1257	G1197	G1137	A1077	G956	G956	A896	G836	G776	A716	G656
G1558	C1498	U1438	A1378	U1318	U1258	U1198	G1138	U1078	C957	C957	C897	C837	G777	C717	U657
U1559	U1499	A1439	U1379	C1319	G1259	U1199	G1139	C1079	U1018	U958	C898	U838	G778	C718	U658
G1560	G1500	U1440	G1380	C1320	A1260	C1140	U1139	U1079	U1019	A959	A899	U839	U779	C719	G659
C1561	G1501	G1441	G1381	A1321	C1261	U1201	U1141	U1081	A1020	A960	A900	C840	G780	U720	C660

C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521
U2402	C2403	U2404	C2405	C2406	C2407	U2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	U2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461
C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281
C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221
C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161
A2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101
U1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041
G1922	U1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	U1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981
G1862	G1863	U1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921
A1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861
G1682	U1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741
U1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801
G1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681
U1562	U1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621




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	Correction of reconstruction of each defocus group	Depositor
Microscope	FEI Polara 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	4520	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	Kodak SO163 Film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP

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	AJ	1.80	12/797 (1.5%)	1.89	19/1077 (1.8%)
10	AS	1.77	6/653 (0.9%)	1.98	15/877 (1.7%)
11	AT	1.70	8/671 (1.2%)	1.88	12/888 (1.4%)
12	AU	1.95	8/431 (1.9%)	2.14	13/570 (2.3%)
13	AB	1.69	20/1736 (1.2%)	2.01	42/2338 (1.8%)
14	AC	1.76	18/1652 (1.1%)	1.95	34/2225 (1.5%)
15	AD	1.79	20/1665 (1.2%)	2.02	46/2227 (2.1%)
16	AE	1.75	12/1119 (1.1%)	2.03	28/1504 (1.9%)
17	AF	1.80	5/836 (0.6%)	1.98	19/1128 (1.7%)
18	AG	1.83	15/1188 (1.3%)	2.09	34/1591 (2.1%)
19	AH	1.72	10/989 (1.0%)	2.00	24/1326 (1.8%)
2	AK	1.83	17/893 (1.9%)	2.02	24/1205 (2.0%)
20	AI	1.77	10/1034 (1.0%)	2.01	29/1375 (2.1%)
21	AA	3.42	4975/36763 (13.5%)	3.74	8350/57350 (14.6%)
22	AY	4.00	354/1814 (19.5%)	4.28	526/2827 (18.6%)
23	AW	5.13	269/1809 (14.9%)	3.87	451/2819 (16.0%)
24	AX	3.54	39/260 (15.0%)	3.68	65/403 (16.1%)
25	AZ	1.79	30/3091 (1.0%)	2.04	97/4182 (2.3%)
26	AV	3.50	261/1814 (14.4%)	3.81	416/2825 (14.7%)
27	B5	1.66	6/1748 (0.3%)	2.01	42/2355 (1.8%)
28	BI	1.69	5/1046 (0.5%)	2.02	30/1410 (2.1%)
29	BJ	1.75	9/1152 (0.8%)	1.97	27/1551 (1.7%)
3	AL	1.73	7/969 (0.7%)	1.96	24/1300 (1.8%)
30	BK	1.76	6/940 (0.6%)	2.06	30/1258 (2.4%)
31	BL	1.85	17/1054 (1.6%)	2.05	30/1403 (2.1%)
32	BM	1.83	16/1093 (1.5%)	2.20	29/1460 (2.0%)
33	BN	1.87	16/974 (1.6%)	2.12	35/1301 (2.7%)
34	BO	1.87	15/902 (1.7%)	2.04	26/1209 (2.2%)
35	BP	1.78	6/929 (0.6%)	2.00	27/1242 (2.2%)
36	BQ	1.78	14/960 (1.5%)	2.16	38/1278 (3.0%)
37	BR	1.86	14/829 (1.7%)	2.09	25/1107 (2.3%)
38	BS	1.71	14/864 (1.6%)	1.97	19/1156 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BT	1.61	3/745 (0.4%)	2.03	23/994 (2.3%)
4	AM	1.83	12/885 (1.4%)	2.12	35/1181 (3.0%)
40	BU	1.72	5/788 (0.6%)	1.96	14/1051 (1.3%)
41	BV	1.70	7/766 (0.9%)	1.99	27/1025 (2.6%)
42	BW	1.85	15/603 (2.5%)	2.15	22/797 (2.8%)
43	BX	1.85	11/635 (1.7%)	1.98	18/848 (2.1%)
44	BY	1.67	5/510 (1.0%)	1.93	14/677 (2.1%)
45	BC	1.78	22/2122 (1.0%)	2.01	50/2852 (1.8%)
46	BZ	1.64	4/453 (0.9%)	1.99	11/605 (1.8%)
47	B0	1.78	2/450 (0.4%)	2.04	14/599 (2.3%)
48	B1	1.75	2/417 (0.5%)	1.91	8/554 (1.4%)
49	B2	1.87	7/380 (1.8%)	2.44	22/498 (4.4%)
5	AN	1.84	13/786 (1.7%)	2.19	27/1046 (2.6%)
50	B3	1.63	5/513 (1.0%)	1.85	10/676 (1.5%)
51	B4	1.88	3/303 (1.0%)	1.98	8/397 (2.0%)
52	BD	1.71	15/1586 (0.9%)	2.02	39/2134 (1.8%)
53	BE	1.71	13/1571 (0.8%)	1.99	42/2113 (2.0%)
54	BF	1.75	12/1444 (0.8%)	2.09	40/1937 (2.1%)
55	BG	1.76	21/1343 (1.6%)	2.07	37/1816 (2.0%)
56	BH	1.65	10/1122 (0.9%)	2.01	37/1515 (2.4%)
57	BB	3.38	9332/69800 (13.4%)	3.73	15942/108892 (14.6%)
58	BA	3.35	371/2804 (13.2%)	3.76	649/4371 (14.8%)
6	AO	1.75	9/724 (1.2%)	1.94	16/966 (1.7%)
7	AP	1.90	14/649 (2.2%)	2.07	22/870 (2.5%)
8	AQ	1.80	10/658 (1.5%)	1.95	11/881 (1.2%)
9	AR	1.81	5/463 (1.1%)	2.10	16/621 (2.6%)
All	All	3.03	16162/165195 (9.8%)	3.37	27780/246683 (11.3%)

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	AJ	0	3
10	AS	0	1
11	AT	0	3
12	AU	0	5
13	AB	0	4
14	AC	0	5
15	AD	0	9
16	AE	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
17	AF	0	2
18	AG	0	4
19	AH	0	4
2	AK	0	4
20	AI	0	6
21	AA	0	713
22	AY	0	40
23	AW	3	39
24	AX	0	3
25	AZ	0	8
26	AV	0	37
27	B5	1	7
28	BI	0	3
29	BJ	0	9
3	AL	0	7
30	BK	0	1
31	BL	0	8
32	BM	0	4
33	BN	0	3
34	BO	0	4
35	BP	0	2
36	BQ	0	4
37	BR	0	6
38	BS	0	1
39	BT	0	2
4	AM	0	5
40	BU	0	2
41	BV	0	4
42	BW	0	3
43	BX	0	3
44	BY	0	2
45	BC	0	9
46	BZ	0	3
47	B0	0	4
48	B1	0	2
49	B2	0	1
5	AN	0	5
50	B3	0	2
51	B4	0	1
52	BD	0	5
53	BE	0	7
54	BF	0	9

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
55	BG	0	5
56	BH	0	3
57	BB	0	1349
58	BA	0	56
6	AO	0	5
7	AP	0	3
8	AQ	0	1
9	AR	0	4
All	All	4	2445

The worst 5 of 16162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	63	G	N9-C8	84.56	1.97	1.37
23	AW	63	G	N7-C5	78.06	1.86	1.39
23	AW	63	G	C5-C4	69.51	1.87	1.38
23	AW	63	G	N9-C4	65.35	1.90	1.38
23	AW	63	G	C8-N7	61.20	1.67	1.30

The worst 5 of 27780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	523	A	N1-C6-N6	27.08	134.85	118.60
57	BB	2097	A	N1-C6-N6	26.55	134.53	118.60
57	BB	725	G	N1-C6-O6	26.46	135.78	119.90
57	BB	2274	A	N1-C6-N6	26.21	134.33	118.60
58	BA	9	G	N1-C6-O6	25.88	135.43	119.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	AW	17	C	C1'
23	AW	47	U	C1'
23	AW	70	G	C3'
27	B5	37	LYS	CA

5 of 2445 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AJ	16	ARG	Sidechain
1	AJ	68	ARG	Sidechain
1	AJ	9	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	AK	26	PHE	Sidechain
2	AK	55	ARG	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	AJ	787	0	828	4	0
2	AK	877	0	887	1	0
3	AL	955	0	1019	9	0
4	AM	877	0	937	8	0
5	AN	774	0	828	9	0
6	AO	716	0	742	8	0
7	AP	639	0	656	2	0
8	AQ	649	0	691	3	0
9	AR	456	0	478	4	0
10	AS	638	0	665	7	0
11	AT	665	0	714	1	0
12	AU	426	0	449	0	0
13	AB	1705	0	1732	9	0
14	AC	1625	0	1699	7	0
15	AD	1643	0	1710	17	0
16	AE	1106	0	1148	6	0
17	AF	818	0	808	6	0
18	AG	1175	0	1230	10	0
19	AH	979	0	1034	4	0
20	AI	1022	0	1070	4	0
21	AA	32832	0	16503	179	0
22	AY	1622	0	812	11	0
23	AW	1619	0	822	22	0
24	AX	232	0	120	2	0
25	AZ	3035	0	3049	17	0
26	AV	1645	0	834	6	0
27	B5	1733	0	1823	10	0
28	BI	1032	0	1088	4	0
29	BJ	1129	0	1162	8	0
30	BK	931	0	1003	5	0
31	BL	1045	0	1117	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BM	1074	0	1157	1	0
33	BN	961	0	1000	5	0
34	BO	892	0	923	2	0
35	BP	917	0	965	5	0
36	BQ	947	0	1022	4	0
37	BR	816	0	839	3	0
38	BS	857	0	922	3	0
39	BT	739	0	807	4	0
40	BU	780	0	834	5	0
41	BV	753	0	780	3	0
42	BW	596	0	610	5	0
43	BX	625	0	655	3	0
44	BY	509	0	543	1	0
45	BC	2083	0	2157	16	0
46	BZ	449	0	491	0	0
47	B0	444	0	461	6	0
48	B1	410	0	440	4	0
49	B2	377	0	418	3	0
50	B3	504	0	574	3	0
51	B4	302	0	343	0	0
52	BD	1565	0	1616	16	0
53	BE	1552	0	1619	7	0
54	BF	1420	0	1460	10	0
55	BG	1323	0	1374	7	0
56	BH	1111	0	1148	4	0
57	BB	62321	0	31298	323	0
58	BA	2508	0	1268	8	0
59	AZ	28	0	12	0	0
All	All	152250	0	103394	772	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 3.

The worst 5 of 772 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)
23:AW:63:G:C4	23:AW:63:G:C5	1.87	1.59
23:AW:63:G:C8	23:AW:63:G:N7	1.67	1.56
23:AW:63:G:N7	23:AW:63:G:C5	1.86	1.43
23:AW:63:G:C4	23:AW:63:G:N9	1.90	1.40
23:AW:63:G:C8	23:AW:63:G:N9	1.97	1.31

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	AJ	96/98 (98%)	77 (80%)	11 (12%)	8 (8%)	1	18
2	AK	115/117 (98%)	90 (78%)	18 (16%)	7 (6%)	2	26
3	AL	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	7	46
4	AM	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	17
5	AN	94/96 (98%)	67 (71%)	18 (19%)	9 (10%)	1	15
6	AO	86/88 (98%)	73 (85%)	8 (9%)	5 (6%)	2	27
7	AP	78/80 (98%)	61 (78%)	14 (18%)	3 (4%)	4	37
8	AQ	78/80 (98%)	62 (80%)	13 (17%)	3 (4%)	4	37
9	AR	53/55 (96%)	43 (81%)	10 (19%)	0	100	100
10	AS	77/79 (98%)	55 (71%)	17 (22%)	5 (6%)	1	25
11	AT	83/85 (98%)	73 (88%)	8 (10%)	2 (2%)	7	47
12	AU	49/51 (96%)	35 (71%)	10 (20%)	4 (8%)	1	18
13	AB	216/218 (99%)	166 (77%)	37 (17%)	13 (6%)	2	26
14	AC	204/206 (99%)	168 (82%)	26 (13%)	10 (5%)	3	31
15	AD	203/205 (99%)	161 (79%)	28 (14%)	14 (7%)	1	23
16	AE	148/150 (99%)	118 (80%)	21 (14%)	9 (6%)	2	26
17	AF	98/100 (98%)	79 (81%)	15 (15%)	4 (4%)	3	35
18	AG	148/150 (99%)	122 (82%)	18 (12%)	8 (5%)	2	29
19	AH	127/129 (98%)	96 (76%)	26 (20%)	5 (4%)	4	36
20	AI	125/127 (98%)	102 (82%)	21 (17%)	2 (2%)	12	56
25	AZ	391/393 (100%)	319 (82%)	52 (13%)	20 (5%)	2	30
27	B5	232/234 (99%)	195 (84%)	31 (13%)	6 (3%)	7	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BI	139/141 (99%)	121 (87%)	11 (8%)	7 (5%)	3	31
29	BJ	140/142 (99%)	116 (83%)	11 (8%)	13 (9%)	1	16
30	BK	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	3	34
31	BL	141/143 (99%)	118 (84%)	16 (11%)	7 (5%)	3	31
32	BM	134/136 (98%)	101 (75%)	26 (19%)	7 (5%)	2	30
33	BN	118/120 (98%)	97 (82%)	17 (14%)	4 (3%)	5	40
34	BO	114/116 (98%)	100 (88%)	8 (7%)	6 (5%)	2	29
35	BP	112/114 (98%)	87 (78%)	15 (13%)	10 (9%)	1	17
36	BQ	115/117 (98%)	99 (86%)	14 (12%)	2 (2%)	11	55
37	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	3	31
38	BS	108/110 (98%)	85 (79%)	15 (14%)	8 (7%)	1	21
39	BT	91/93 (98%)	64 (70%)	19 (21%)	8 (9%)	1	17
40	BU	100/102 (98%)	79 (79%)	13 (13%)	8 (8%)	1	19
41	BV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	8	49
42	BW	77/79 (98%)	56 (73%)	10 (13%)	11 (14%)	0	6
43	BX	75/77 (97%)	60 (80%)	10 (13%)	5 (7%)	1	24
44	BY	61/63 (97%)	47 (77%)	11 (18%)	3 (5%)	3	31
45	BC	269/271 (99%)	201 (75%)	43 (16%)	25 (9%)	1	16
46	BZ	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
47	B0	54/56 (96%)	43 (80%)	9 (17%)	2 (4%)	4	37
48	B1	48/50 (96%)	44 (92%)	2 (4%)	2 (4%)	3	34
49	B2	44/46 (96%)	32 (73%)	11 (25%)	1 (2%)	8	48
50	B3	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	3	32
51	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	44
52	BD	207/209 (99%)	152 (73%)	39 (19%)	16 (8%)	1	20
53	BE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	25
54	BF	176/178 (99%)	129 (73%)	28 (16%)	19 (11%)	0	11
55	BG	174/176 (99%)	137 (79%)	23 (13%)	14 (8%)	1	19
56	BH	147/149 (99%)	107 (73%)	23 (16%)	17 (12%)	0	9
All	All	6242/6344 (98%)	4971 (80%)	897 (14%)	374 (6%)	4	26

5 of 374 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AJ	67	ILE
3	AL	24	GLU
4	AM	3	ILE
4	AM	29	SER
4	AM	99	GLN

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	AJ	86/86 (100%)	82 (95%)	4 (5%)	32	68
2	AK	90/90 (100%)	87 (97%)	3 (3%)	45	76
3	AL	103/103 (100%)	98 (95%)	5 (5%)	31	66
4	AM	91/91 (100%)	85 (93%)	6 (7%)	21	57
5	AN	79/79 (100%)	78 (99%)	1 (1%)	76	89
6	AO	76/76 (100%)	74 (97%)	2 (3%)	54	80
7	AP	65/65 (100%)	63 (97%)	2 (3%)	47	77
8	AQ	74/74 (100%)	67 (90%)	7 (10%)	11	41
9	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
10	AS	70/70 (100%)	67 (96%)	3 (4%)	35	70
11	AT	65/65 (100%)	65 (100%)	0	100	100
12	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
13	AB	180/180 (100%)	172 (96%)	8 (4%)	35	69
14	AC	170/170 (100%)	158 (93%)	12 (7%)	18	55
15	AD	172/172 (100%)	163 (95%)	9 (5%)	29	65
16	AE	113/113 (100%)	106 (94%)	7 (6%)	23	60
17	AF	87/87 (100%)	81 (93%)	6 (7%)	19	56
18	AG	123/123 (100%)	115 (94%)	8 (6%)	21	58
19	AH	104/104 (100%)	95 (91%)	9 (9%)	13	45
20	AI	105/105 (100%)	97 (92%)	8 (8%)	16	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AZ	325/326 (100%)	303 (93%)	22 (7%)	20	57
27	B5	181/181 (100%)	170 (94%)	11 (6%)	23	60
28	BI	109/109 (100%)	100 (92%)	9 (8%)	14	48
29	BJ	116/116 (100%)	107 (92%)	9 (8%)	16	51
30	BK	102/102 (100%)	94 (92%)	8 (8%)	16	51
31	BL	102/102 (100%)	100 (98%)	2 (2%)	63	85
32	BM	109/109 (100%)	100 (92%)	9 (8%)	14	48
33	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
34	BO	86/86 (100%)	83 (96%)	3 (4%)	43	74
35	BP	99/99 (100%)	92 (93%)	7 (7%)	18	55
36	BQ	89/89 (100%)	86 (97%)	3 (3%)	44	75
37	BR	84/84 (100%)	78 (93%)	6 (7%)	18	55
38	BS	93/93 (100%)	89 (96%)	4 (4%)	35	70
39	BT	80/80 (100%)	72 (90%)	8 (10%)	9	38
40	BU	83/83 (100%)	72 (87%)	11 (13%)	5	28
41	BV	78/78 (100%)	75 (96%)	3 (4%)	40	73
42	BW	59/59 (100%)	53 (90%)	6 (10%)	9	37
43	BX	67/67 (100%)	60 (90%)	7 (10%)	9	36
44	BY	55/55 (100%)	53 (96%)	2 (4%)	42	74
45	BC	216/216 (100%)	205 (95%)	11 (5%)	29	66
46	BZ	48/48 (100%)	44 (92%)	4 (8%)	14	48
47	B0	47/47 (100%)	42 (89%)	5 (11%)	8	36
48	B1	45/45 (100%)	42 (93%)	3 (7%)	20	57
49	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
50	B3	51/51 (100%)	49 (96%)	2 (4%)	39	72
51	B4	34/34 (100%)	34 (100%)	0	100	100
52	BD	164/164 (100%)	150 (92%)	14 (8%)	13	48
53	BE	165/165 (100%)	157 (95%)	8 (5%)	31	67
54	BF	149/149 (100%)	139 (93%)	10 (7%)	20	57
55	BG	137/137 (100%)	126 (92%)	11 (8%)	15	50
56	BH	114/114 (100%)	107 (94%)	7 (6%)	23	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5170/5171 (100%)	4858 (94%)	312 (6%)	28 60

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BI	73	PRO
33	BN	29	VAL
54	BF	91	ARG
29	BJ	18	VAL
30	BK	68	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
25	AZ	11	HIS
25	AZ	329	GLN
52	BD	148	GLN
25	AZ	19	HIS
25	AZ	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1530 (99%)	281 (18%)	42 (2%)
22	AY	75/76 (98%)	20 (26%)	5 (6%)
23	AW	75/76 (98%)	24 (32%)	6 (8%)
24	AX	10/11 (90%)	3 (30%)	0
26	AV	76/77 (98%)	14 (18%)	0
57	BB	2902/2903 (99%)	491 (16%)	63 (2%)
58	BA	116/117 (99%)	19 (16%)	4 (3%)
All	All	4783/4790 (99%)	852 (17%)	120 (2%)

5 of 852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	14	U

5 of 120 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	BB	241	A
57	BB	973	A
57	BB	2402	U
57	BB	329	G
57	BB	789	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	5MU	AV	54	26	13,22,23	2.08	4 (30%)	16,32,35	4.79	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	5MU	AV	54	26	-	0/3/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AV	54	5MU	O2'-C2'	-2.45	1.37	1.43
26	AV	54	5MU	C2'-C1'	-2.14	1.50	1.53
26	AV	54	5MU	O4'-C1'	4.33	1.47	1.41
26	AV	54	5MU	C4-N3	4.49	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AV	54	5MU	C5-C4-N3	-12.11	115.18	125.35
26	AV	54	5MU	O4'-C1'-N1	3.47	114.70	108.10
26	AV	54	5MU	C4-N3-C2	14.19	127.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GDP	AZ	401	-	24,30,30	1.88	7 (29%)	26,47,47	2.90	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	AZ	401	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AZ	401	GDP	O3'-C3'	-2.14	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AZ	401	GDP	C2'-C1'	-2.01	1.50	1.53
59	AZ	401	GDP	PA-O2A	-2.01	1.46	1.55
59	AZ	401	GDP	C4-N3	2.26	1.39	1.35
59	AZ	401	GDP	C2-N1	2.56	1.40	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AZ	401	GDP	C5-C6-N1	-9.11	111.61	123.52
59	AZ	401	GDP	N3-C2-N1	-5.48	120.10	127.56
59	AZ	401	GDP	O3'-C3'-C2'	2.25	119.11	111.86
59	AZ	401	GDP	N2-C2-N3	3.07	123.47	117.72
59	AZ	401	GDP	C1'-N9-C4	4.60	131.94	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.