



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:13 PM BST

PDB ID : 3JCE
EMDB ID: : EMD-6550
Title : Structure of Escherichia coli EF4 in pretranslocational ribosomes (Pre EF4)
Authors : Zhang, D.; Yan, K.; Liu, G.; Song, G.; Luo, J.; Shi, Y.; Cheng, E.; Wu, S.;
Jiang, T.; Low, J.; Gao, N.; Qin, Y.
Deposited on : 2015-12-01
Resolution : 3.20 Å(reported)
Based on PDB ID : 4V9O

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>

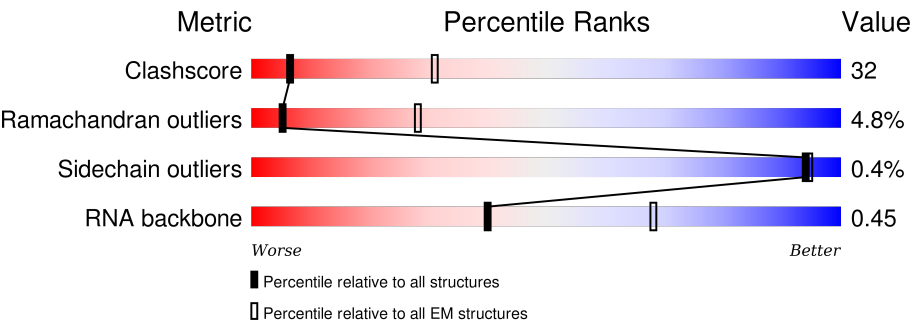
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





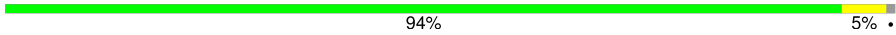


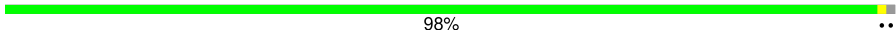
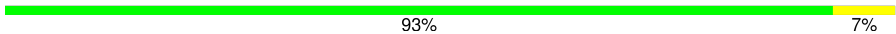



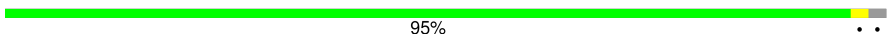














Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	a	1533	<div><div>80%20%</div></div>
2	c	233	<div><div>86%12%</div></div>
3	d	206	<div><div>96%</div></div>
4	e	167	<div><div>87%10%</div></div>
5	f	135	<div><div>70%5%24%</div></div>
6	g	179	<div><div>82%16%</div></div>
7	h	130	<div><div>98%</div></div>
8	i	130	<div><div>95%</div></div>


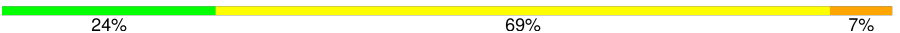
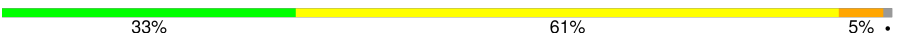


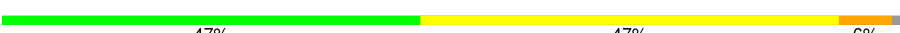
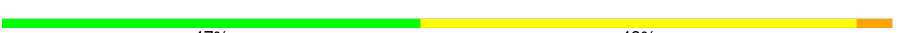




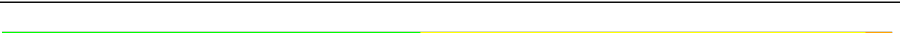





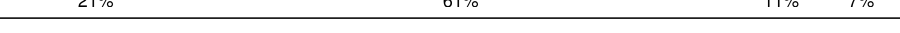







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Mol	Chain	Length	Quality of chain
9	j	103	
10	k	129	
11	l	124	
12	m	118	
13	n	101	
14	o	89	
15	p	82	
16	q	84	
17	r	75	
18	s	92	
19	t	87	
20	u	71	
21	b	241	
22	0	57	
23	1	55	
24	2	46	
25	3	65	
26	4	38	
27	5	234	
28	A	2904	
29	B	120	
30	C	273	
31	D	209	
32	E	201	
33	F	179	

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Mol	Chain	Length	Quality of chain
34	G	177	
35	H	149	
36	I	142	
37	J	142	
38	K	123	
39	L	144	
40	M	136	
41	N	127	
42	O	117	
43	P	115	
44	Q	118	
45	R	103	
46	S	110	
47	T	100	
48	U	104	
49	V	94	
50	W	85	
51	X	78	
52	Y	63	
53	Z	59	
54	6	76	
55	7	15	
56	8	77	
57	x	599	
58	9	76	

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 154017 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called EF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a RNA chain called RNA (2903-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	2903	Total	C	N	O	P	0	0
			62320	27801	11467	20149	2903		

- Molecule 29 is a RNA chain called RNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a RNA chain called PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	76	Total	C	N	O	P	0	0
			1633	732	291	534	76		

- Molecule 55 is a RNA chain called RNA (5'-R(P*CP*AP*UP*AP*UP*GP*UP*UP*CP*A P*AP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	15	Total	C	N	O	P	0	0
			320	144	59	102	15		

- Molecule 56 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

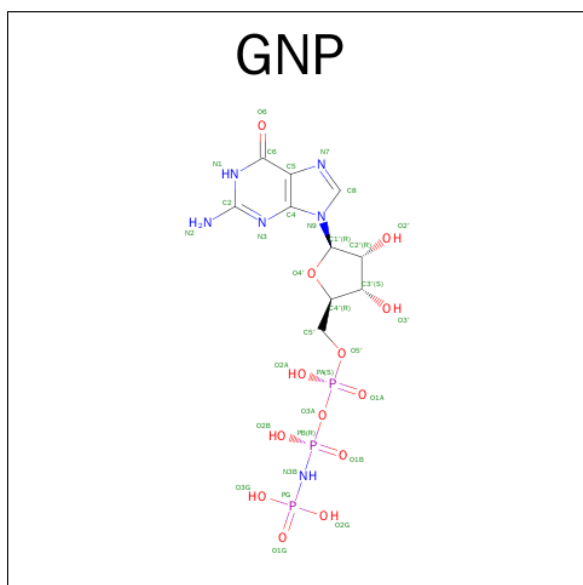
- Molecule 57 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	586	Total	C	N	O	S	0	0
			4573	2885	792	875	21		

- Molecule 58 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	9	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

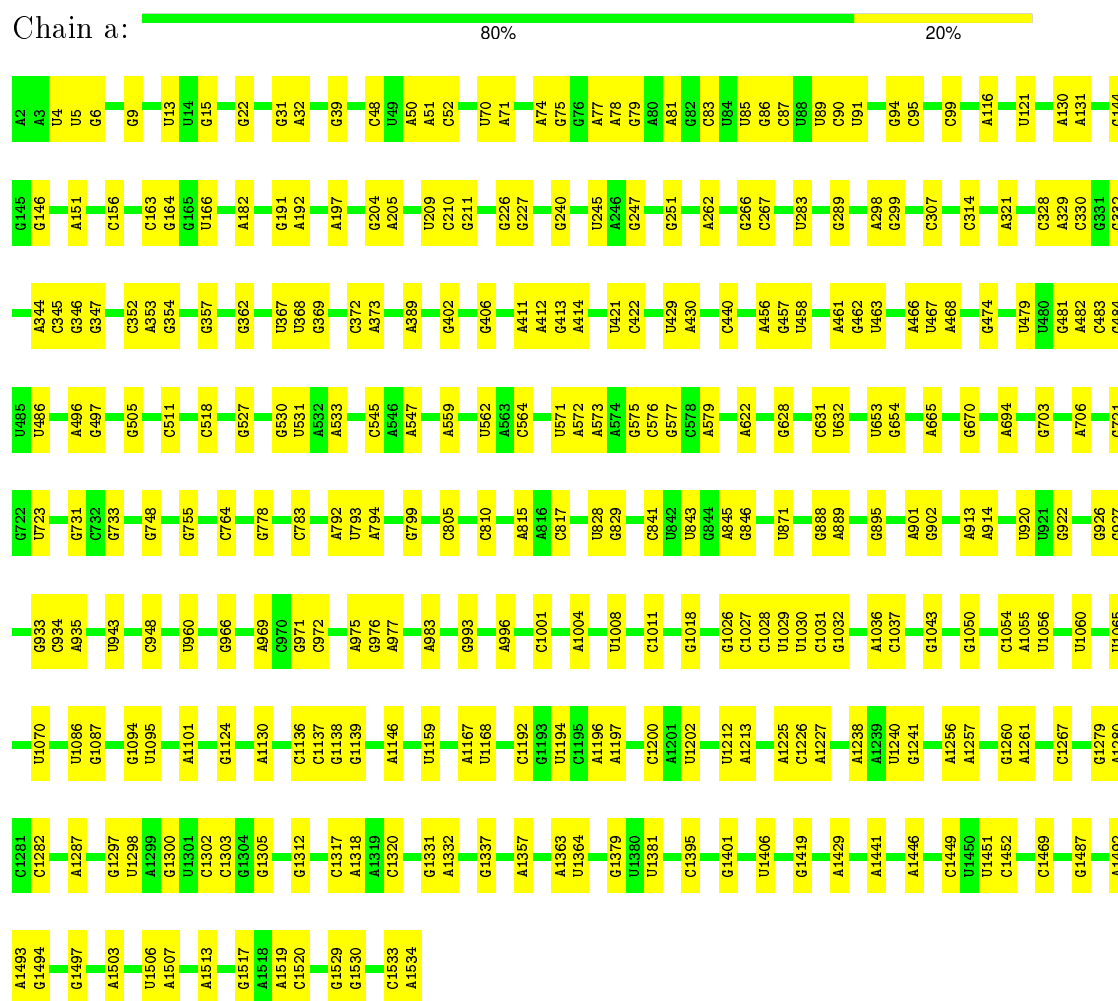
- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



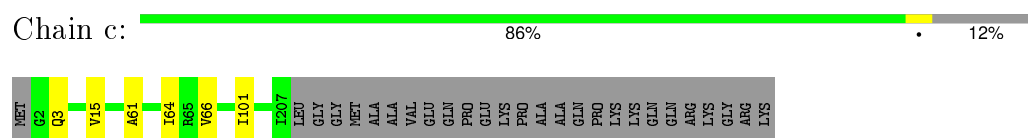
3 Residue-property plots

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: EF4



- Molecule 2: 30S ribosomal protein S3




- Molecule 3: 30S ribosomal protein S4

Chain d:  96%



- Molecule 4: 30S ribosomal protein S5

Chain e:  87% 10%




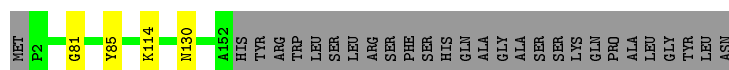
- Molecule 5: 30S ribosomal protein S6

Chain f:  70% 5% 24%



- Molecule 6: 30S ribosomal protein S7

Chain g:  82% 16%



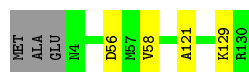
- Molecule 7: 30S ribosomal protein S8

Chain h:  98%




- Molecule 8: 30S ribosomal protein S9

Chain i:  95%




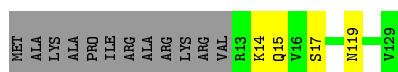
- Molecule 9: 30S ribosomal protein S10

Chain j:  86% 9% 5%



- Molecule 10: 30S ribosomal protein S11

Chain k:  88% 9%



- Molecule 11: 30S ribosomal protein S12

Chain l: 94% 5%



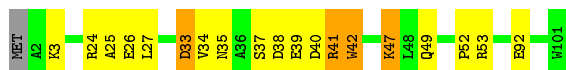
- Molecule 12: 30S ribosomal protein S13

Chain m: 92%



- Molecule 13: 30S ribosomal protein S14

Chain n: 80% 15%



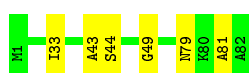
- Molecule 14: 30S ribosomal protein S15

Chain o: 98%



- Molecule 15: 30S ribosomal protein S16

Chain p: 93% 7%



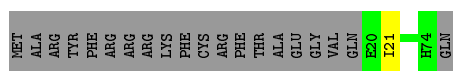
- Molecule 16: 30S ribosomal protein S17

Chain q: 93% 5%




- Molecule 17: 30S ribosomal protein S18

Chain r: 72% 27%



- Molecule 18: 30S ribosomal protein S19

Chain s:  82% 14%



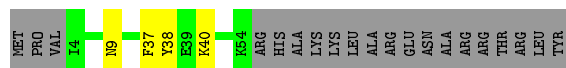
- Molecule 19: 30S ribosomal protein S20

Chain t:  95%




- Molecule 20: 30S ribosomal protein S21

Chain u:  66% 6% 28%



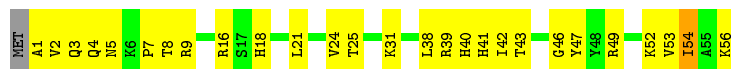
- Molecule 21: 30S ribosomal protein S2

Chain b:  88% 10%

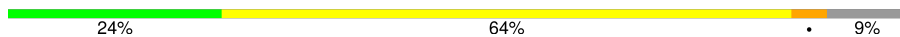


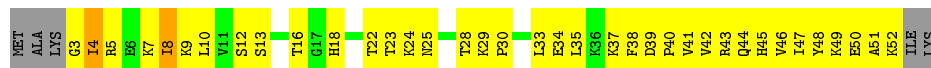
- Molecule 22: 50S ribosomal protein L32

Chain 0:  51% 46%



- Molecule 23: 50S ribosomal protein L33

Chain 1:  24% 64% 9%



- Molecule 24: 50S ribosomal protein L34

Chain 2:  70% 30%

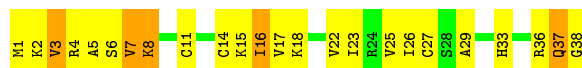


- Molecule 25: 50S ribosomal protein L35

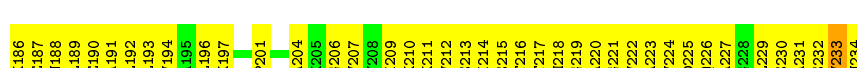
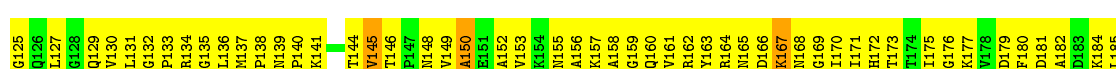
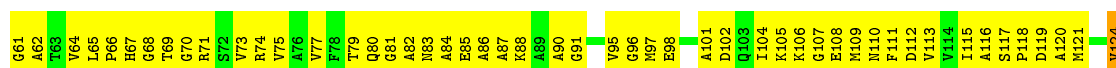
Chain 3:  51% 45%



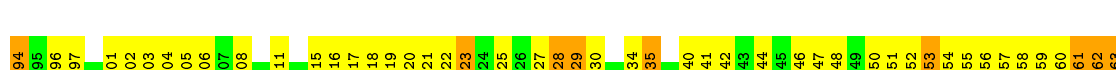
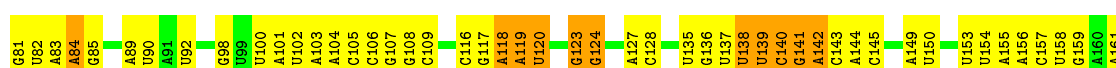
- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L1



- Molecule 28: RNA (2903-MER)



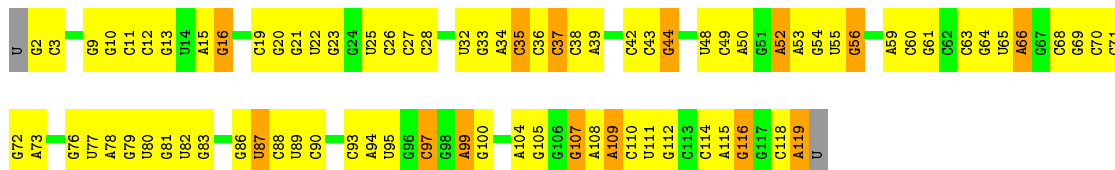
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G1622	A1551	G1491	U1409	C1319	G1236	G1160	U1094	A1028	C961	C888	A819	G745	U591	A527
A1626	A1553	G1492	U1411	C1320	A1095	G1162	A1096	C1030	G962	C890	A821	U746	U594	A528
G1627	G1554	C1493	U1412	A1322	G1238	G1163	U1097	G1031	G966	G891	U824	U747	C595	G530
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U1629	U1495	A1495	C1414	G1324	C1243	U1168	G1099	U1033	A972	C893	A826	A749	G597	A532
A1630	U1496	U1415	G1325	A1244	G1245	C1169	U1101	G1036	A973	U894	U827	A750	U598	G533
G1631	U1497	G1416	U1326	A1326	G1246	C1170	G1102	G1037	G974	A896	U828	A751	A599	U534
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C1564	A1501	G1421	G1332	U1263	U1263	U1174	G1106	C1044	G978	A900	U832	G760	G604	A538
G1665	A1502	G1422	G1336	A1265	A1265	U1175	G1107	C1045	A979	C901	A833	A761	U686	G539
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G1649	G1514	G1436	A1353	U1372	G1197	U1186	U1120	G1058	C992	C915	C851	G778	G624	G553
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G1661	G1524	U1460	U1379	U1293	G1207	U1194	U1131	G1074	C1007	A933	G859	C786	A633	G561
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A1697	A1535	G1478	C1398	G1306	G1218	U1205	A1142	A1080	U1013	A943	G875	A727	G648	A574
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A1684	A1540	U1481	U1386	U1307	G1223	U1210	U1151	A1085	A1020	C948	G881	G732	U653	G585
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G2902	U2655	U2739	U2655	U2572	U2505	U2430	C2358	C2296	G2222	G2156	C2099	C2018	C1929	U1846	U1765
U2899	U2656	U2740	U2656	U2573	U2506	U2431	C2359	C2297	G2223	C2157	C2099	C2019	C1930	G1847	G1766
A2893	U2657	U2741	U2657	U2574	U2507	U2432	C2360	C2298	G2224	A2159	C2099	C2020	C1931	A1848	G1767
G2903	U2658	U2742	U2658	U2575	U2508	U2433	C2361	C2299	G2225	U2160	C2099	C2021	C1932	A1849	
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U2899	U2669	U2753	U2669	U2586	U2519	U2444	C2372	C2310	U2237	C2171	C2099	C2032	C1943		
A2893	U2670	U2754	U2670	U2587	U2520	U2445	C2373	C2311	U2238	C2172	C2099	C2033	C1944		
G2904	U2671	U2755	U2671	U2588	U2521	U2446	C2374	C2312	U2239	C2173	C2099	C2034	C1945		
U2899	U2672	U2756	U2672	U2589	U2522	U2447	C2375	C2313	U2240	C2174	C2099	C2035	C1946		
A2893	U2673	U2757	U2673	U2590	U2523	U2448	C2376	C2314	U2241	C2175	C2099	C2036	C1947		
G2904	U2674	U2758	U2674	U2591	U2524	U2449	C2377	C2315	U2242	C2176	C2099	C2037	C1948		
U2899	U2675	U2759	U2675	U2592	U2525	U2450	C2378	C2316	U2243	C2177	C2099	C2038	C1949		
A2893	U2676	U2760	U2676	U2593	U2526	U2451	C2379	C2317	U2244	C2178	C2099	C2039	C1950		
G2904	U2677	U2761	U2677	U2594	U2527	U2452	C2380	C2318	U2245	C2179	C2099	C2040	C1951		
U2899	U2678	U2762	U2678	U2595	U2528	U2453	C2381	C2319	U2246	C2180	C2099	C2041	C1952		
A2893	U2679	U2763	U2679	U2596	U2529	U2454	C2382	C2320	U2247	C2181	C2099	C2042	C1953		
G2904	U2680	U2764	U2680	U2597	U2530	U2455	C2383	C2321	U2248	C2182	C2099	C2043	C1954		
U2899	U2681	U2765	U2681	U2598	U2531	U2456	C2384	C2322	U2249	C2183	C2099	C2044	C1955		
A2893	U2682	U2766	U2682	U2599	U2532	U2457	C2385	C2323	U2250	C2184	C2099	C2045	C1956		
G2904	U2683	U2767	U2683	U2600	U2533	U2458	C2386	C2324	U2251	C2185	C2099	C2046	C1957		
U2899	U2684	U2768	U2684	U2601	U2534	U2459	C2387	C2325	U2252	C2186	C2099	C2047	C1958		
A2893	U2685	U2769	U2685	U2602	U2535	U2460	C2388	C2326	U2253	C2187	C2099	C2048	C1959	</	



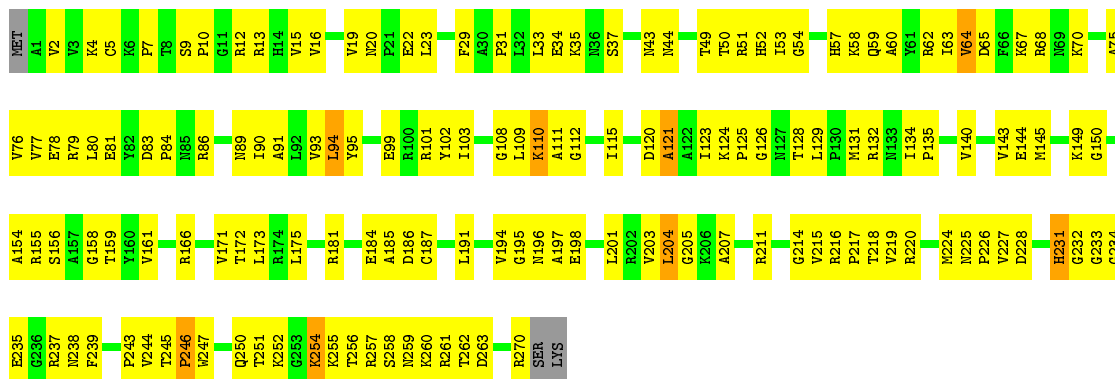
• Molecule 29: RNA (118-MER)

Chain B: 30% 57% 12%



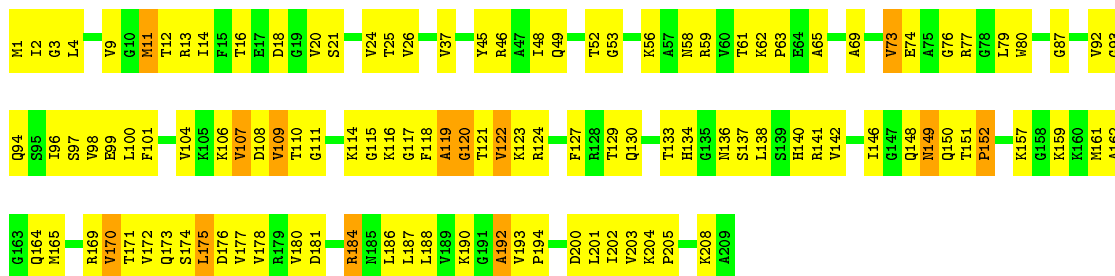
• Molecule 30: 50S ribosomal protein L2

Chain C: 44% 52%



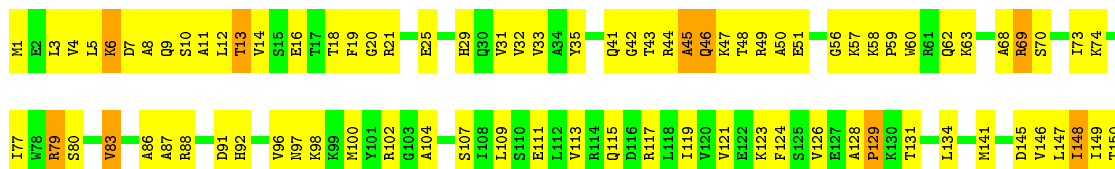
• Molecule 31: 50S ribosomal protein L3

Chain D: 45% 49% 6%



• Molecule 32: 50S ribosomal protein L4

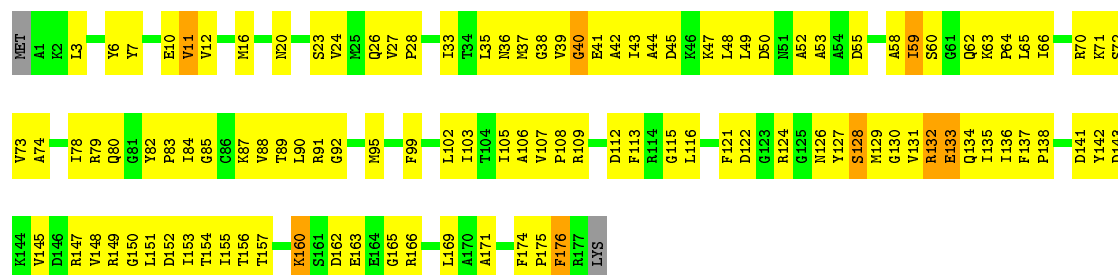
Chain E: 43% 52% 5%





• Molecule 33: 50S ribosomal protein L5

Chain F: 36% 58%



• Molecule 34: 50S ribosomal protein L6

Chain G: 35% 60%



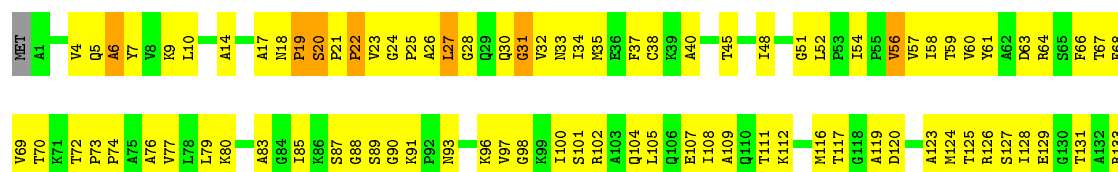
• Molecule 35: 50S ribosomal protein L9

Chain H: 24% 69% 7%



• Molecule 36: 50S ribosomal protein L11

Chain I: 33% 61% 5%



S134
M135
G136
L137
V138
V139
E140
D141

• Molecule 37: 50S ribosomal protein L13

Chain J: 45% 51%

H1 H2 T3 F4 K7 T10 V11 K12 R13 D14 H15 Y16 V17 V18 G26 A29 T30 L32 R35 L36 R37 G38 K39 H40 K41 K42 K43 K44 T45 P46 K47 V48 D49 T50 G51 D52 Y53 I54 I55 V56 L57 M58 A59 V64 T65 K68 R69 T70 D71 R72 V73 T74

Y75 H80 I81 G82 G83 I84 T88 F89 E90 E91 R96 P97 E98 R99 I103 A104 V105 P110 K111 G112 P113 L114 G115 R116 A117 M118 F119 K120 K121 L122 K123 V124 Y125 A126 E129 H132 Q135 Q136 P137 L140 D141 I142

• Molecule 38: 50S ribosomal protein L14

Chain K: 45% 51%

H1 I2 Q3 E4 Q5 T6 M7 L8 N9 V10 A11 D12 H13 S14 G15 A16 R17 R18 R19 M20 C21 I22 R23 V24 L25 V35 G36 I39 K40 I41 I42 I43 K44 E45 A46 I47 P48 R49 G50 K51 D56 V61 V62 V63 R64 T65 G68 V69 R70 P71 P72 D73 V76 I77

R78 F79 N82 A83 G84 V85 L86 L87 E92 Q93 P94 R98 V103 T104 R105 R106 L107 R108 S109 E110 M113 L118 A119 V122 L120

• Molecule 39: 50S ribosomal protein L15

Chain L: 47% 47% 6%

MET R2 L3 N4 T5 L6 S7 P8 K14 L19 G20 R21 G22 G26 L27 G28 K29 T30 G31 G32 R33 K36 G37 Q38 K39 S40 R41 R47 Q54 P55 P56 L57 R60 L61 P62 P66 P67 S68 R69 K70 A71 T74 I77 R78 L79 S80 D81 L82 A83 R84

V85 E86 V89 V90 N93 T94 L95 K96 I100 I101 I105 E106 F107 A108 K109 V110 I111 L112 A113 T117 T118 P119 V120 K121 V122 R123 G124 L125 R126 V127 G130 I135 A138 K141 I142 E143 E144

• Molecule 40: 50S ribosomal protein L16

Chain M: 47% 49%

M1 L2 P3 K8 F9 R10 H13 K14 L20 A21 G22 G23 T24 D25 V26 S27 F28 G29 S30 F31 G32 A35 V36 G37 R40 L41 T42 A43 R44 Q45 I46 E47 R50 M53 A56 R59 K62 I63 W64 I65 R66 V67 V68 P69 D70 K71 P72 I73 T74

P77 M82 K86 G87 V93 A94 L95 I96 O97 P98 L102 Y103 E104 M105 D106 G107 V108 P109 E110 F111 L112 A113 R114 F117 A120 K123 L124 P125 I126 K127 T128 V131 T132 K133 T134 V135 M136

• Molecule 41: 50S ribosomal protein L17

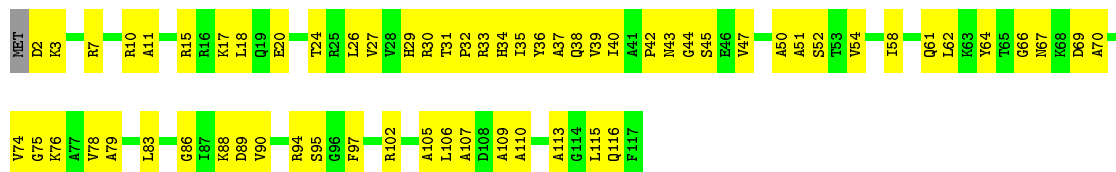
Chain N: 49% 44% 6%

H1 R2 R12 R17 N20 F21 N24 A25 G26 S27 L28 V29 R31 E32 R33 T36 T37 P38 P39 R40 A41 A42 E43 E44 V48 E49 F50 L51 A55 V56 D57 D58 S59 N62 R63 F67 A68 R69 T70 T71 D72 I73 E74 I75 V76 A77 K78 L79 F80 N81



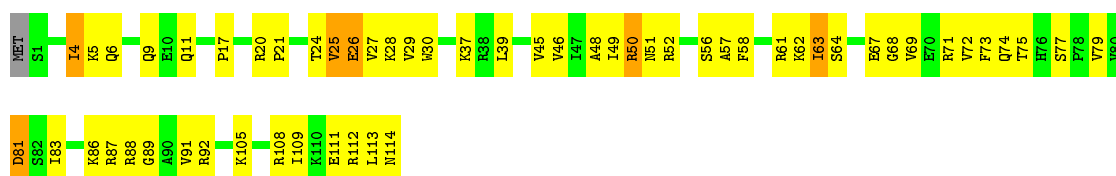
• Molecule 42: 50S ribosomal protein L18

Chain O: 45% 54%



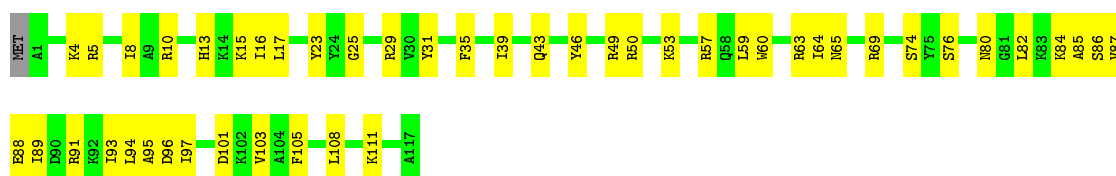
• Molecule 43: 50S ribosomal protein L19

Chain P: 50% 43% 5%



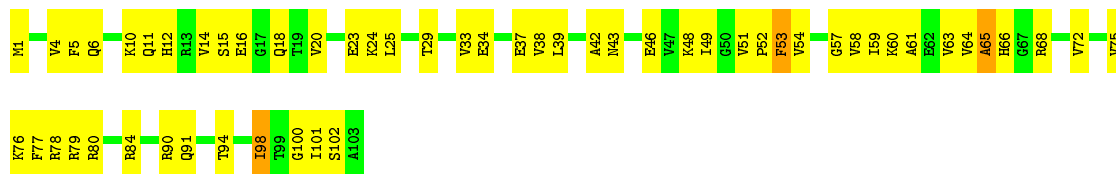
• Molecule 44: 50S ribosomal protein L20

Chain Q: 59% 40%



• Molecule 45: 50S ribosomal protein L21

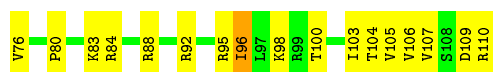
Chain R: 47% 50%



• Molecule 46: 50S ribosomal protein L22

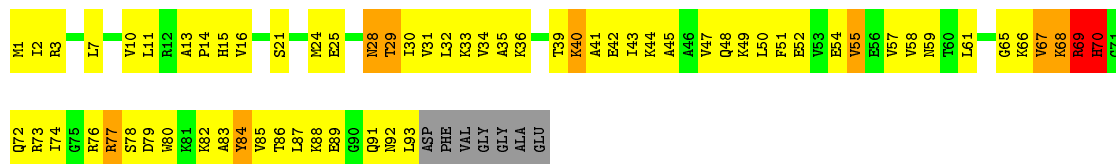
Chain S: 47% 51%





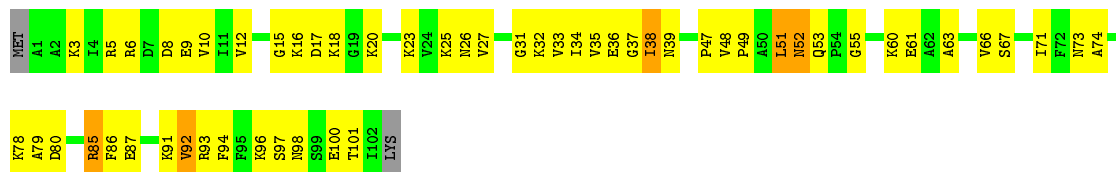
• Molecule 47: 50S ribosomal protein L23

Chain T: 27% 56% 8% 7%



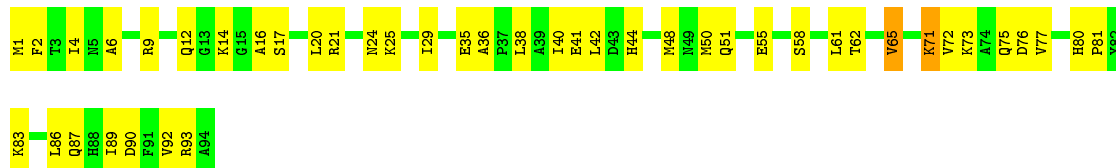
• Molecule 48: 50S ribosomal protein L24

Chain U: 45% 48% 5%



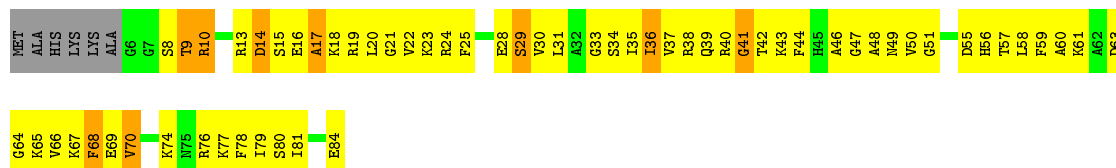
• Molecule 49: 50S ribosomal protein L25

Chain V: 53% 45% 2%



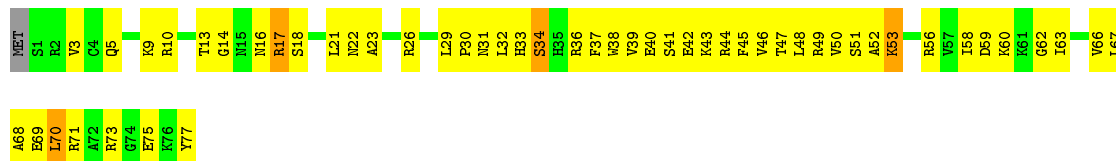
• Molecule 50: 50S ribosomal protein L27

Chain W: 21% 61% 11% 7%

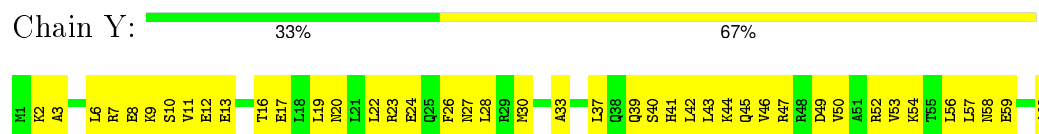


• Molecule 51: 50S ribosomal protein L28

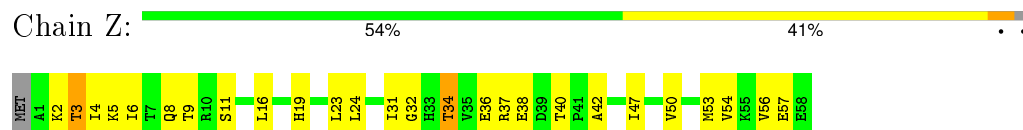
Chain X: 32% 62% 5%



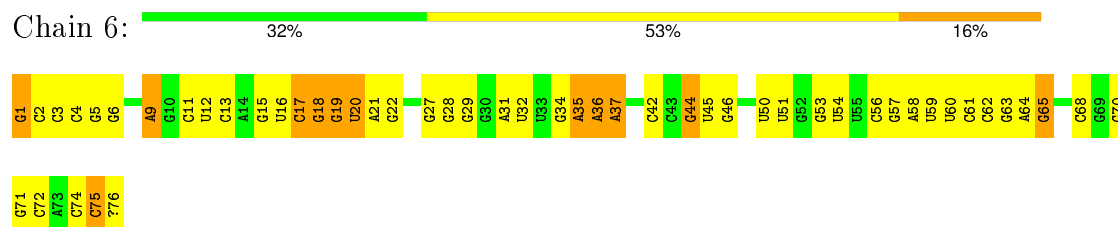
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30



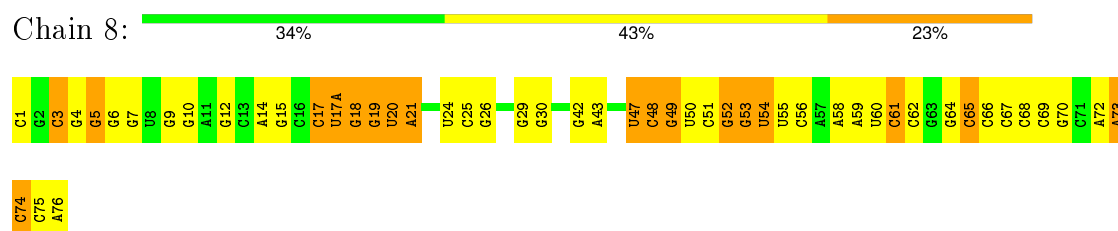
- Molecule 54: PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER



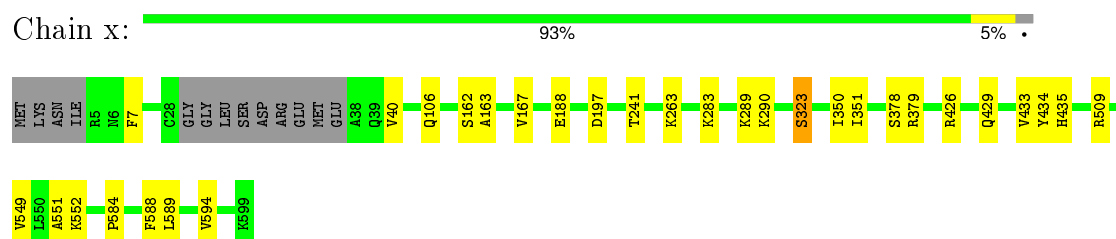
- Molecule 55: RNA (5'-R(P*CP*AP*UP*AP*UP*GP*UP*UP*CP*AP*AP*AP*GP*AP*A)-3')



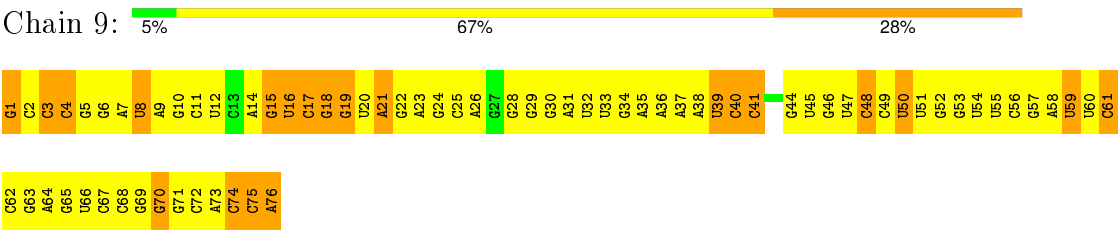
- Molecule 56: RNA (77-MER)



- Molecule 57: Elongation factor 4



● Molecule 58: RNA (76-MER)



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG, F3O

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	0.73	0/36834	0.79	0/57462
10	k	0.43	0/893	0.54	0/1205
11	l	0.46	0/969	0.55	0/1300
12	m	0.38	0/892	0.55	0/1193
13	n	0.37	0/817	0.52	0/1088
14	o	0.43	0/722	0.50	0/964
15	p	0.36	0/659	0.47	0/884
16	q	0.42	0/657	0.54	0/881
17	r	0.43	0/462	0.49	0/621
18	s	0.36	0/652	0.50	0/877
19	t	0.37	0/671	0.46	0/888
2	c	0.42	0/1651	0.52	0/2225
20	u	0.38	0/430	0.53	0/570
21	b	0.35	0/1735	0.51	0/2338
22	0	0.48	0/450	0.54	0/599
23	1	0.44	0/416	0.52	0/554
24	2	0.52	0/380	0.57	0/498
25	3	0.45	0/513	0.58	0/676
26	4	0.45	0/303	0.58	0/397
27	5	0.24	0/1748	0.53	0/2355
28	A	0.84	0/69799	0.81	2/108892 (0.0%)
29	B	0.63	0/2828	0.74	0/4410
3	d	0.38	0/1665	0.50	0/2227
30	C	0.52	0/2115	0.58	0/2844
31	D	0.48	0/1586	0.56	0/2134
32	E	0.43	0/1571	0.54	0/2113
33	F	0.37	0/1434	0.47	0/1926
34	G	0.37	0/1343	0.51	0/1816
35	H	0.30	0/1122	0.57	0/1515
36	I	0.28	0/1046	0.50	0/1410
37	J	0.50	0/1152	0.58	0/1551
38	K	0.49	0/947	0.58	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	L	0.45	0/1054	0.57	0/1403
4	e	0.46	0/1118	0.56	0/1504
40	M	0.49	0/1093	0.61	0/1460
41	N	0.48	0/973	0.56	0/1301
42	O	0.38	0/902	0.48	0/1209
43	P	0.45	0/929	0.56	0/1242
44	Q	0.57	0/960	0.55	0/1278
45	R	0.48	0/829	0.54	0/1107
46	S	0.48	0/864	0.57	0/1156
47	T	0.40	0/744	0.57	0/994
48	U	0.37	0/787	0.54	0/1051
49	V	0.40	0/766	0.49	0/1025
5	f	0.37	0/851	0.53	0/1150
50	W	0.47	0/603	0.64	0/797
51	X	0.47	0/635	0.56	0/848
52	Y	0.41	0/510	0.51	0/677
53	Z	0.41	0/453	0.58	0/605
54	6	0.63	1/1788 (0.1%)	0.78	0/2784
55	7	0.64	0/358	0.92	2/555 (0.4%)
56	8	0.64	0/1832	0.76	0/2855
57	x	0.39	0/4646	0.52	0/6285
58	9	0.40	1/1813 (0.1%)	0.79	0/2823
6	g	0.37	0/1195	0.49	0/1602
7	h	0.43	0/989	0.52	0/1326
8	i	0.39	0/1034	0.56	0/1375
9	j	0.37	0/796	0.51	0/1077
All	All	0.70	2/166984 (0.0%)	0.74	4/249170 (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
11	l	0	1
20	u	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	9	1	G	OP3-P	-10.74	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	1	G	OP3-P	-10.67	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	323	C	N1-C2-O2	5.44	122.17	118.90
55	7	21	C	C2-N1-C1'	5.24	124.56	118.80
55	7	21	C	N1-C2-O2	5.22	122.03	118.90
28	A	2689	U	C2-N1-C1'	-5.05	111.64	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	l	23	ALA	Peptide
20	u	37	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32895	0	16553	0	0
2	c	1624	0	1696	0	0
3	d	1643	0	1707	0	0
4	e	1105	0	1148	0	0
5	f	832	0	824	0	0
6	g	1181	0	1238	0	0
7	h	979	0	1031	0	0
8	i	1022	0	1070	0	0
9	j	786	0	828	0	0
10	k	877	0	887	0	0
11	l	955	0	1016	0	0
12	m	883	0	941	0	0
13	n	805	0	843	0	0
14	o	714	0	734	0	0
15	p	649	0	666	0	0
16	q	648	0	691	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	r	455	0	478	0	0
18	s	637	0	665	0	0
19	t	665	0	714	0	0
20	u	425	0	449	0	0
21	b	1704	0	1732	0	0
22	0	444	0	461	39	0
23	1	409	0	440	53	0
24	2	377	0	418	16	0
25	3	504	0	574	34	0
26	4	302	0	340	40	0
27	5	1733	0	1824	393	0
28	A	62320	0	31344	2129	0
29	B	2529	0	1281	94	0
30	C	2076	0	2152	168	0
31	D	1565	0	1616	144	0
32	E	1552	0	1619	134	0
33	F	1410	0	1447	127	0
34	G	1323	0	1374	155	0
35	H	1111	0	1148	235	0
36	I	1032	0	1088	163	0
37	J	1129	0	1162	114	0
38	K	938	0	1012	76	0
39	L	1045	0	1117	97	0
40	M	1074	0	1157	81	0
41	N	960	0	1000	59	0
42	O	892	0	923	83	0
43	P	917	0	965	86	0
44	Q	947	0	1022	100	0
45	R	816	0	839	93	0
46	S	857	0	922	61	0
47	T	738	0	807	100	0
48	U	779	0	834	53	0
49	V	753	0	780	47	0
50	W	596	0	610	121	0
51	X	625	0	655	63	0
52	Y	509	0	543	45	0
53	Z	449	0	491	33	0
54	6	1633	0	830	51	0
55	7	320	0	162	18	0
56	8	1640	0	837	50	0
57	x	4573	0	4619	0	0
58	9	1623	0	821	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	x	32	0	13	0	0
60	x	1	0	0	0	0
All	All	154017	0	105158	4944	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 32.

The worst 5 of 4944 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)
50:W:37:VAL:HG12	50:W:38:ARG:HG3	1.19	1.17
35:H:90:LEU:HD11	35:H:146:VAL:HG23	1.27	1.15
42:O:51:ALA:HB3	42:O:78:VAL:HG12	1.25	1.14
31:D:119:ALA:HB1	31:D:124:ARG:HB2	1.24	1.13
31:D:184:ARG:HG2	31:D:186:LEU:HD13	1.26	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	204/233 (88%)	182 (89%)	16 (8%)	6 (3%)	6	36
3	d	203/206 (98%)	180 (89%)	16 (8%)	7 (3%)	5	31
4	e	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	6	39
5	f	100/135 (74%)	84 (84%)	9 (9%)	7 (7%)	1	10
6	g	149/179 (83%)	134 (90%)	11 (7%)	4 (3%)	6	39
7	h	127/130 (98%)	114 (90%)	11 (9%)	2 (2%)	12	54
8	i	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	5	33
9	j	96/103 (93%)	76 (79%)	11 (12%)	9 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	115/129 (89%)	102 (89%)	9 (8%)	4 (4%)	4	31
11	l	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	27
12	m	112/118 (95%)	101 (90%)	6 (5%)	5 (4%)	3	24
13	n	98/101 (97%)	70 (71%)	15 (15%)	13 (13%)	0	1
14	o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	60
15	p	80/82 (98%)	66 (82%)	8 (10%)	6 (8%)	1	9
16	q	78/84 (93%)	62 (80%)	14 (18%)	2 (3%)	7	40
17	r	53/75 (71%)	50 (94%)	2 (4%)	1 (2%)	10	50
18	s	77/92 (84%)	68 (88%)	5 (6%)	4 (5%)	2	19
19	t	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	7	43
20	u	49/71 (69%)	39 (80%)	7 (14%)	3 (6%)	2	15
21	b	216/241 (90%)	189 (88%)	20 (9%)	7 (3%)	5	33
22	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	10	50
23	1	48/55 (87%)	41 (85%)	6 (12%)	1 (2%)	9	46
24	2	44/46 (96%)	43 (98%)	0	1 (2%)	8	44
25	3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	5	33
26	4	36/38 (95%)	25 (69%)	5 (14%)	6 (17%)	0	1
27	5	232/234 (99%)	190 (82%)	34 (15%)	8 (3%)	5	31
30	C	268/273 (98%)	228 (85%)	28 (10%)	12 (4%)	3	24
31	D	207/209 (99%)	169 (82%)	23 (11%)	15 (7%)	1	10
32	E	199/201 (99%)	171 (86%)	14 (7%)	14 (7%)	1	10
33	F	175/179 (98%)	146 (83%)	21 (12%)	8 (5%)	3	23
34	G	174/177 (98%)	140 (80%)	21 (12%)	13 (8%)	1	9
35	H	147/149 (99%)	114 (78%)	22 (15%)	11 (8%)	1	9
36	I	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	1	13
37	J	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	3	25
38	K	120/123 (98%)	100 (83%)	14 (12%)	6 (5%)	3	21
39	L	141/144 (98%)	115 (82%)	17 (12%)	9 (6%)	2	13
40	M	134/136 (98%)	112 (84%)	15 (11%)	7 (5%)	2	19
41	N	118/127 (93%)	104 (88%)	10 (8%)	4 (3%)	5	31
42	O	114/117 (97%)	104 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	P	112/115 (97%)	93 (83%)	13 (12%)	6 (5%)	2	19
44	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
45	R	101/103 (98%)	81 (80%)	15 (15%)	5 (5%)	3	21
46	S	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	6	37
47	T	91/100 (91%)	61 (67%)	18 (20%)	12 (13%)	0	1
48	U	100/104 (96%)	81 (81%)	11 (11%)	8 (8%)	1	7
49	V	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	8	45
50	W	77/85 (91%)	49 (64%)	17 (22%)	11 (14%)	0	1
51	X	75/78 (96%)	64 (85%)	7 (9%)	4 (5%)	2	19
52	Y	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
53	Z	56/59 (95%)	51 (91%)	3 (5%)	2 (4%)	4	30
57	x	582/599 (97%)	496 (85%)	58 (10%)	28 (5%)	3	22
All	All	6442/6818 (94%)	5465 (85%)	667 (10%)	310 (5%)	5	22

5 of 310 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	125	VAL
5	f	98	GLU
5	f	101	PRO
9	j	57	VAL
9	j	61	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	170/190 (90%)	170 (100%)	0	100	100
3	d	172/173 (99%)	172 (100%)	0	100	100
4	e	113/126 (90%)	113 (100%)	0	100	100
5	f	89/116 (77%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	g	124/147 (84%)	124 (100%)	0	100	100
7	h	104/105 (99%)	104 (100%)	0	100	100
8	i	105/107 (98%)	105 (100%)	0	100	100
9	j	86/90 (96%)	86 (100%)	0	100	100
10	k	90/99 (91%)	90 (100%)	0	100	100
11	l	103/104 (99%)	103 (100%)	0	100	100
12	m	92/96 (96%)	92 (100%)	0	100	100
13	n	83/84 (99%)	73 (88%)	10 (12%)	6	28
14	o	76/77 (99%)	76 (100%)	0	100	100
15	p	65/65 (100%)	65 (100%)	0	100	100
16	q	74/78 (95%)	74 (100%)	0	100	100
17	r	48/65 (74%)	48 (100%)	0	100	100
18	s	70/79 (89%)	70 (100%)	0	100	100
19	t	65/66 (98%)	65 (100%)	0	100	100
20	u	44/61 (72%)	44 (100%)	0	100	100
21	b	180/199 (90%)	180 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	44 (98%)	1 (2%)	60	87
24	2	38/38 (100%)	38 (100%)	0	100	100
25	3	51/52 (98%)	51 (100%)	0	100	100
26	4	34/34 (100%)	34 (100%)	0	100	100
27	5	181/181 (100%)	181 (100%)	0	100	100
30	C	215/218 (99%)	215 (100%)	0	100	100
31	D	164/164 (100%)	164 (100%)	0	100	100
32	E	165/165 (100%)	165 (100%)	0	100	100
33	F	148/150 (99%)	148 (100%)	0	100	100
34	G	137/138 (99%)	137 (100%)	0	100	100
35	H	114/114 (100%)	114 (100%)	0	100	100
36	I	109/110 (99%)	109 (100%)	0	100	100
37	J	116/116 (100%)	116 (100%)	0	100	100
38	K	103/104 (99%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	L	102/103 (99%)	102 (100%)	0	100	100
40	M	109/109 (100%)	109 (100%)	0	100	100
41	N	100/103 (97%)	100 (100%)	0	100	100
42	O	86/87 (99%)	86 (100%)	0	100	100
43	P	99/100 (99%)	99 (100%)	0	100	100
44	Q	89/90 (99%)	89 (100%)	0	100	100
45	R	84/84 (100%)	84 (100%)	0	100	100
46	S	93/93 (100%)	93 (100%)	0	100	100
47	T	80/84 (95%)	74 (92%)	6 (8%)	17	55
48	U	83/85 (98%)	83 (100%)	0	100	100
49	V	78/78 (100%)	78 (100%)	0	100	100
50	W	59/63 (94%)	59 (100%)	0	100	100
51	X	67/68 (98%)	67 (100%)	0	100	100
52	Y	55/55 (100%)	55 (100%)	0	100	100
53	Z	48/49 (98%)	48 (100%)	0	100	100
57	x	500/511 (98%)	496 (99%)	4 (1%)	86	96
All	All	5352/5570 (96%)	5331 (100%)	21 (0%)	94	98

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	n	47	LYS
47	T	66	LYS
57	x	106	GLN
13	n	42	TRP
57	x	323	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
32	E	165	HIS
37	J	40	HIS
57	x	407	HIS
34	G	21	GLN
34	G	110	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1532/1533 (99%)	302 (19%)	0
28	A	2902/2904 (99%)	566 (19%)	24 (0%)
29	B	117/120 (97%)	18 (15%)	0
54	6	74/76 (97%)	15 (20%)	3 (4%)
55	7	14/15 (93%)	7 (50%)	1 (7%)
56	8	76/77 (98%)	20 (26%)	0
58	9	75/76 (98%)	24 (32%)	2 (2%)
All	All	4790/4801 (99%)	952 (19%)	30 (0%)

5 of 952 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	13	U

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1020	A
28	A	1847	A
55	7	20	U
28	A	1584	U
28	A	1905	C

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
54	F3O	6	76	54	29,35,37	1.11	1 (3%)	31,49,54	2.15	6 (19%)

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
54	F3O	6	76	54	-	0/14/36/38	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	76	F3O	O3'-C	4.84	1.45	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	6	76	F3O	N3-C2-N1	-9.62	121.31	128.87
54	6	76	F3O	C3'-O3'-C	-3.35	112.54	118.06
54	6	76	F3O	O3'-C-O	-2.46	119.12	123.88
54	6	76	F3O	C4'-O4'-C1'	2.32	112.10	109.64
54	6	76	F3O	C3'-C2'-C1'	2.65	105.82	100.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	6	76	F3O	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	GNP	x	701	60	29,34,34	1.97	7 (24%)	29,54,54	2.65	7 (24%)

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	GNP	x	701	60	-	0/13/38/38	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	x	701	GNP	PB-O3A	-5.91	1.51	1.59
59	x	701	GNP	PB-O2B	-3.23	1.48	1.56
59	x	701	GNP	PG-O2G	-2.26	1.50	1.56
59	x	701	GNP	PG-O3G	-2.24	1.50	1.56
59	x	701	GNP	C8-N7	-2.11	1.30	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	701	GNP	C5-C6-N1	-8.93	111.85	123.52
59	x	701	GNP	PA-O3A-PB	-3.63	119.55	132.71
59	x	701	GNP	O3G-PG-O1G	-2.99	105.70	113.58
59	x	701	GNP	N3-C2-N1	-2.70	123.88	127.56
59	x	701	GNP	O3G-PG-O2G	2.39	114.62	107.67

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.