



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 01:43 AM EDT

PDB ID : 5UYL
EMDB ID : EMD-8616
Title : 70S ribosome bound with cognate ternary complex base-paired to A site codon (Structure II)
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2017-02-24
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

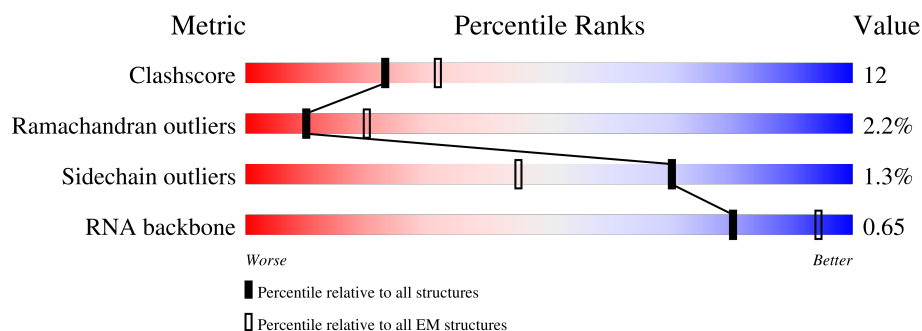
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	04	271	68% 30% .
2	05	209	67% 33%
3	06	201	71% 27% .
4	07	177	61% 38% .
5	08	176	70% 28% .
6	09	149	61% 38% .
7	10	131	46% 49% 5%


























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Mol	Chain	Length	Quality of chain
8	11	141	
9	12	142	
10	13	122	
11	14	143	
12	15	136	
13	16	120	
14	17	116	
15	18	114	
16	19	117	
17	20	103	
18	21	110	
19	22	93	
20	23	102	
21	24	94	
22	25	75	
23	26	77	
24	27	63	
25	28	58	
26	29	66	
27	30	56	
28	31	50	
29	32	46	
30	33	64	
31	34	38	
32	B	218	

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Mol	Chain	Length	Quality of chain
33	C	206	
34	D	205	
35	E	157	
36	F	100	
37	G	151	
38	H	129	
39	I	127	
40	J	98	
41	K	116	
42	L	123	
43	M	114	
44	N	100	
45	O	88	
46	P	82	
47	Q	80	
48	R	65	
49	S	79	
50	T	85	
51	U	65	
52	03	234	
53	A	1539	
54	01	2903	
55	02	120	
56	W	77	
56	X	77	

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Mol	Chain	Length	Quality of chain
57	V	18	<div><div></div><div>72%</div><div>22%</div><div>6%</div></div>
58	Y	76	<div><div></div><div>43%</div><div>46%</div><div>11%</div></div>
59	Z	392	<div><div></div><div>33%</div><div>63%</div><div>..</div></div>

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153753 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	04	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	07	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	10	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	13	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	16	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

- Molecule 33 is a protein called 30S ribosomal protein S3.

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

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

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

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	G	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

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

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	R	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

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

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	03	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	01	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	02	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

- Molecule 56 is a RNA chain called tRNAfMet.

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

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 58 is a RNA chain called tRNAPhe.

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

- Molecule 59 is a protein called Elongation factor Tu 2.

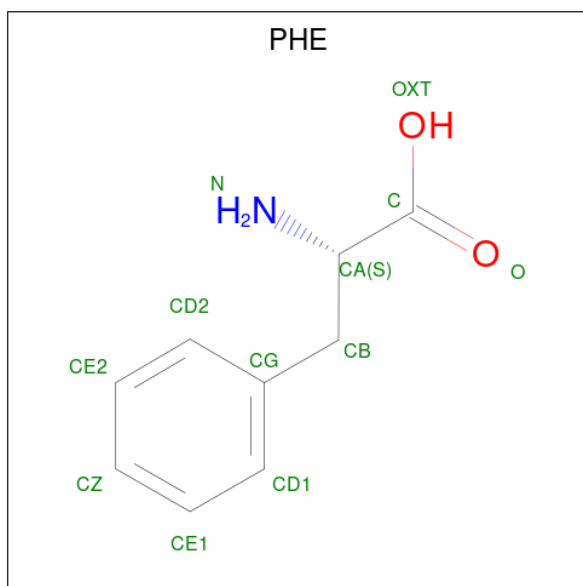
Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	392	Total	C	N	O	S	0	0
			3029	1915	521	580	13		

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



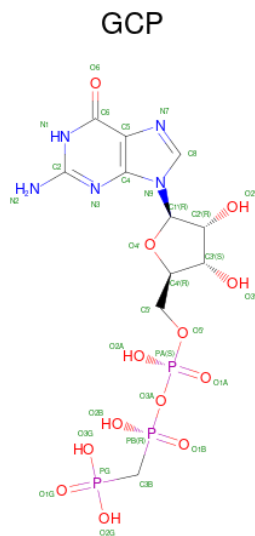
Mol	Chain	Residues	Atoms					AltConf
60	W	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
61	Y	1	Total	C	N	O		0
			11	9	1	1		

- Molecule 62 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

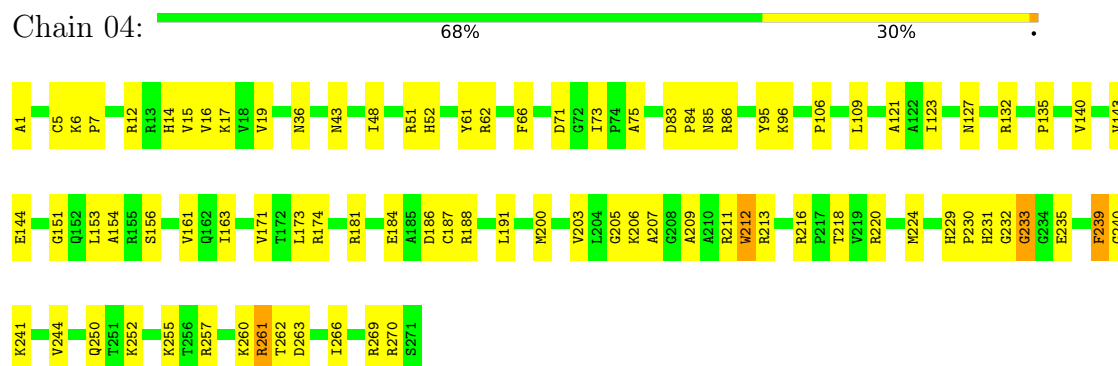


Mol	Chain	Residues	Atoms					AltConf
62	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	

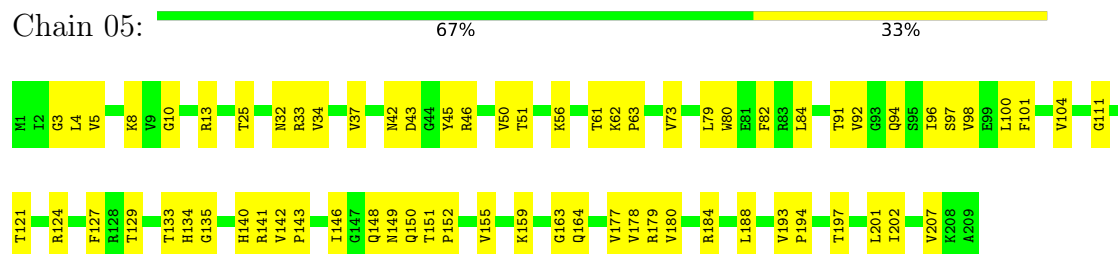
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

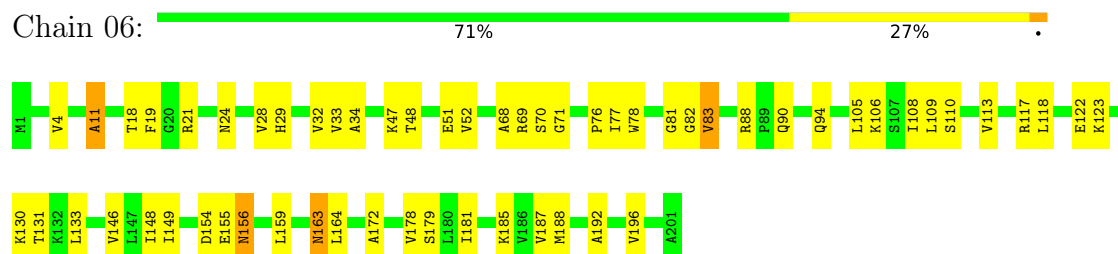
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

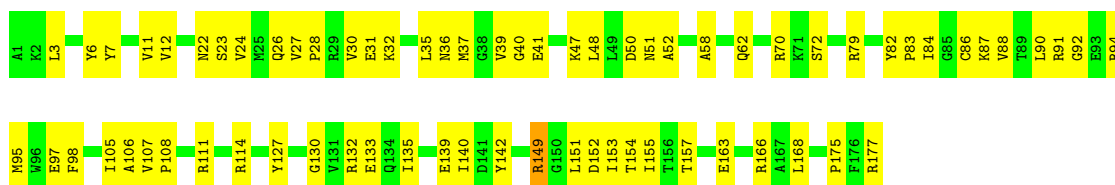


- Molecule 3: 50S ribosomal protein L4



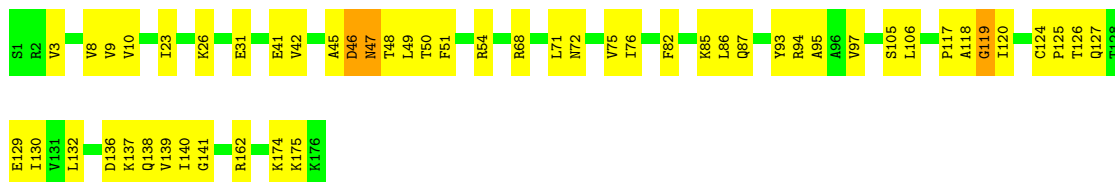
- Molecule 4: 50S ribosomal protein L5





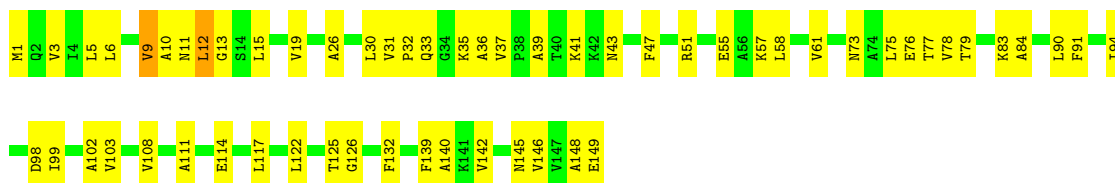
• Molecule 5: 50S ribosomal protein L6

Chain 08: 70% 28% .



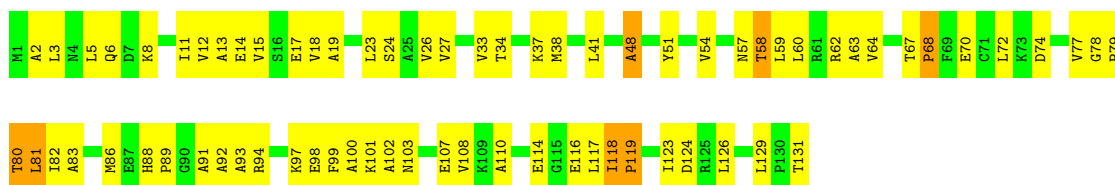
• Molecule 6: 50S ribosomal protein L9

Chain 09: 61% 38% .



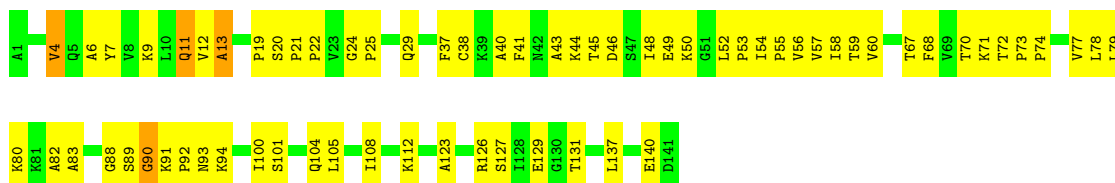
• Molecule 7: 50S ribosomal protein L10

Chain 10: 46% 49% 5% .



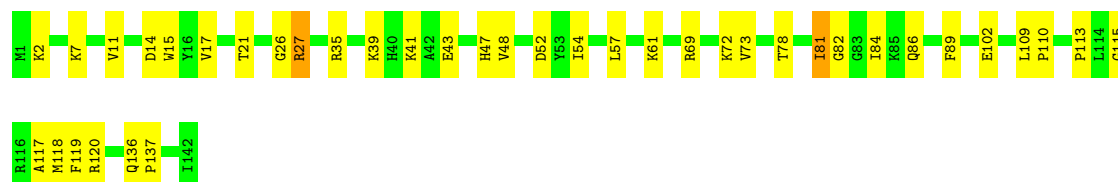
• Molecule 8: 50S ribosomal protein L11

Chain 11: 52% 45% .



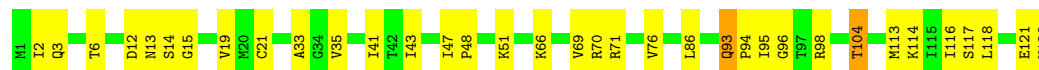
• Molecule 9: 50S ribosomal protein L13

Chain 12: 73% 26% .



- Molecule 10: 50S ribosomal protein L14

Chain 13: 71% 27% .



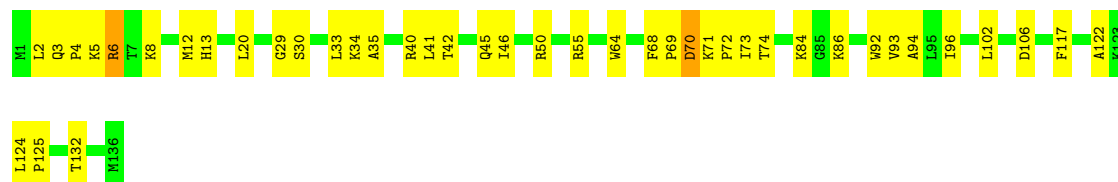
- Molecule 11: 50S ribosomal protein L15

Chain 14: 69% 29% .



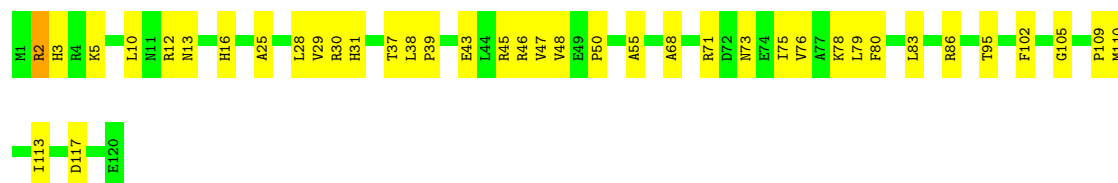
- Molecule 12: 50S ribosomal protein L16

Chain 15: 69% 29% .



- Molecule 13: 50S ribosomal protein L17

Chain 16: 68% 32% .



- Molecule 14: 50S ribosomal protein L18

Chain 17: 72% 28%




- Molecule 15: 50S ribosomal protein L19

Chain 18:  68% 32%



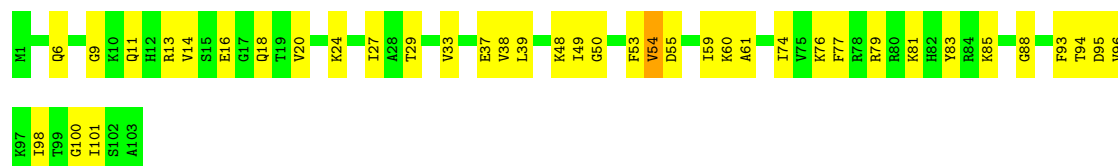
- Molecule 16: 50S ribosomal protein L20

Chain 19:  76% 22% .



- Molecule 17: 50S ribosomal protein L21

Chain 20:  62% 37% .



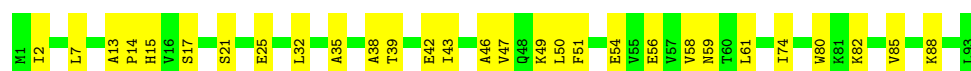
- Molecule 18: 50S ribosomal protein L22

Chain 21:  68% 31% .



- Molecule 19: 50S ribosomal protein L23

Chain 22:  69% 31%



- Molecule 20: 50S ribosomal protein L24

Chain 23:  68% 29% .

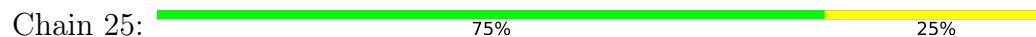


- Molecule 21: 50S ribosomal protein L25

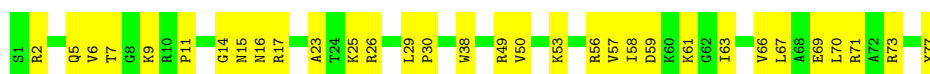
Chain 24:  65% 34% .



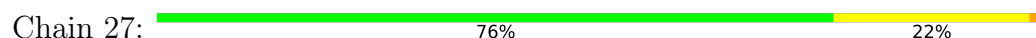
- Molecule 22: 50S ribosomal protein L27



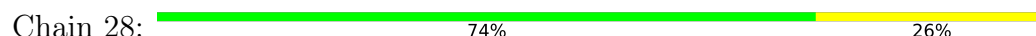
- Molecule 23: 50S ribosomal protein L28



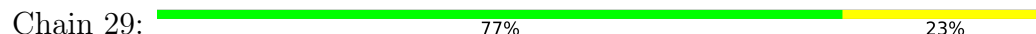
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



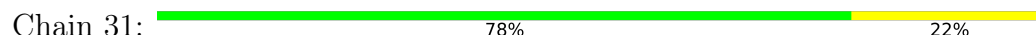
- Molecule 26: 50S ribosomal protein L31

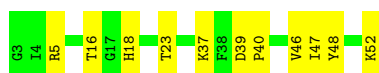


- Molecule 27: 50S ribosomal protein L32

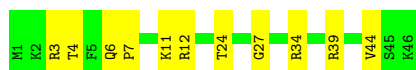
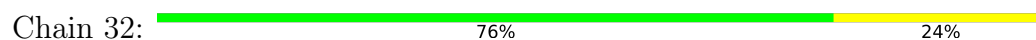


- Molecule 28: 50S ribosomal protein L33

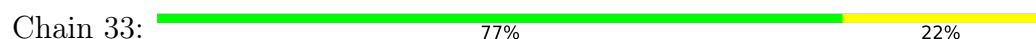




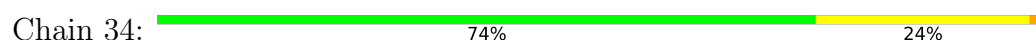
- Molecule 29: 50S ribosomal protein L34



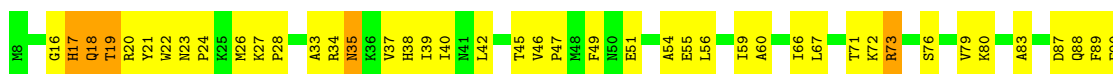
- Molecule 30: 50S ribosomal protein L35



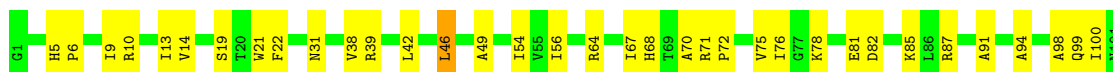
- Molecule 31: 50S ribosomal protein L36



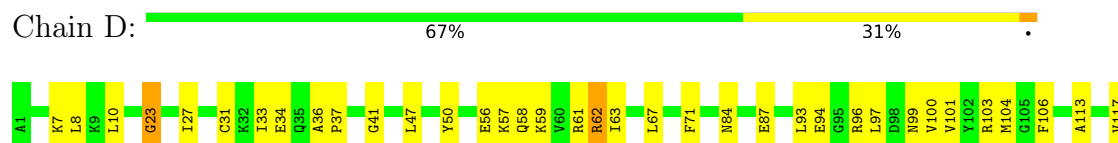
- Molecule 32: 30S ribosomal protein S2



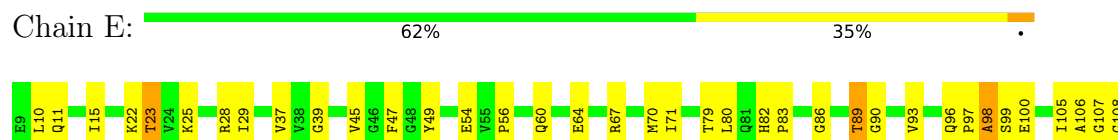
- Molecule 33: 30S ribosomal protein S3



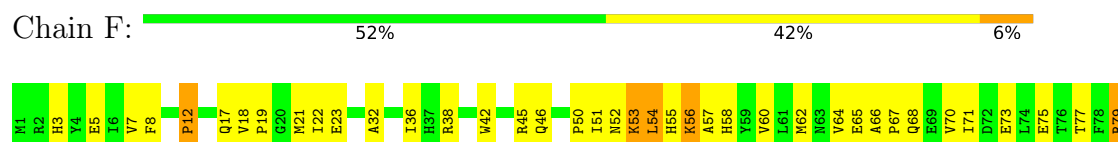
- Molecule 34: 30S ribosomal protein S4



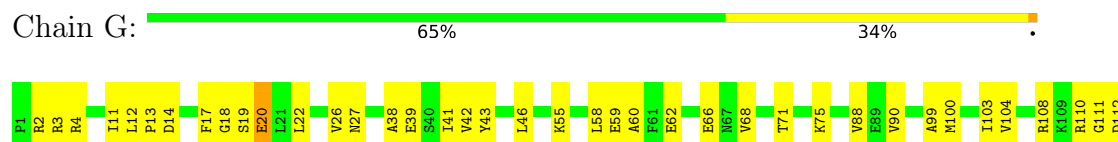
- Molecule 35: 30S ribosomal protein S5



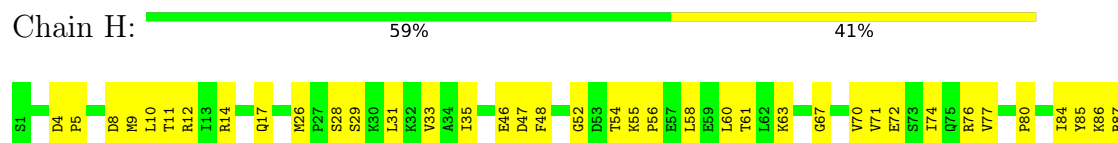
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

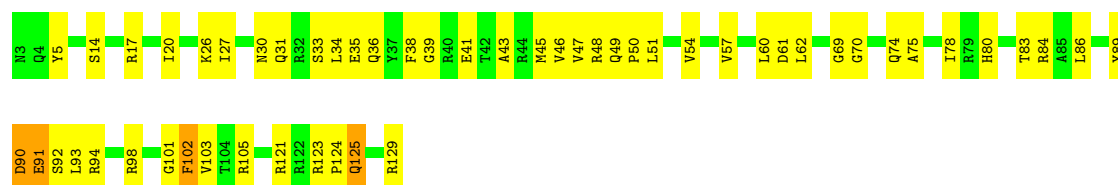


- Molecule 38: 30S ribosomal protein S8



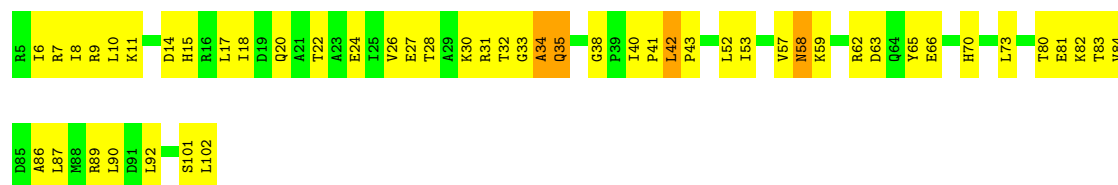
- Molecule 39: 30S ribosomal protein S9

Chain I:  58% 39%



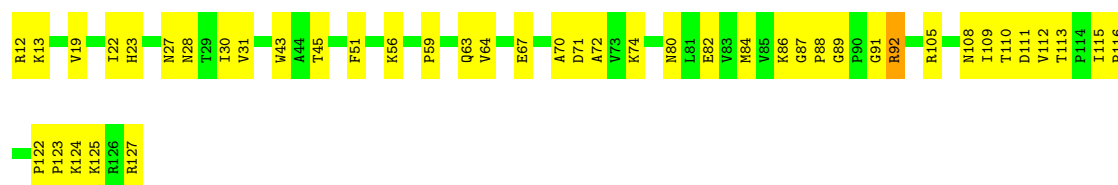
- Molecule 40: 30S ribosomal protein S10

Chain J:  49% 47%



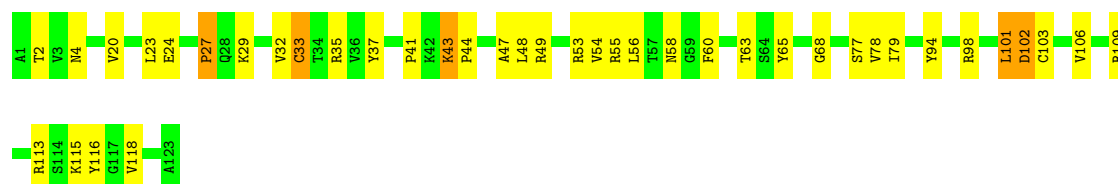
- Molecule 41: 30S ribosomal protein S11

Chain K:  62% 37%



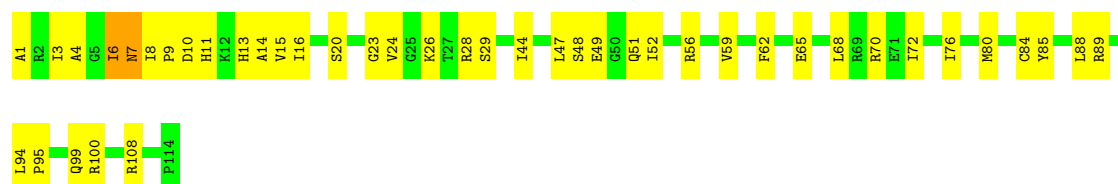
- Molecule 42: 30S ribosomal protein S12

Chain L:  67% 28%



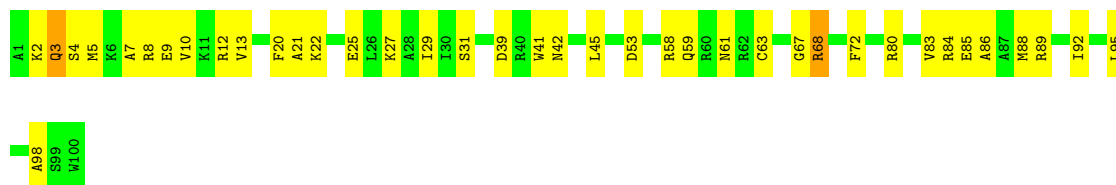
- Molecule 43: 30S ribosomal protein S13

Chain M:  62% 36%



- Molecule 44: 30S ribosomal protein S14

Chain N:  61% 37%



- Molecule 45: 30S ribosomal protein S15

Chain O:  70% 28%



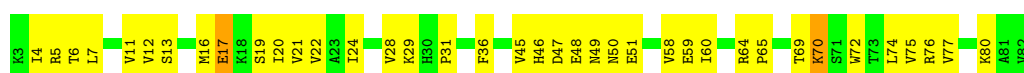
- Molecule 46: 30S ribosomal protein S16

Chain P:  62% 35%



- Molecule 47: 30S ribosomal protein S17

Chain Q:  52% 45%



- Molecule 48: 30S ribosomal protein S18

Chain R:  55% 35% 8%



- Molecule 49: 30S ribosomal protein S19

Chain S:  54% 44%



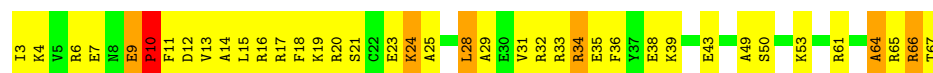
- Molecule 50: 30S ribosomal protein S20

Chain T:  71% 28%




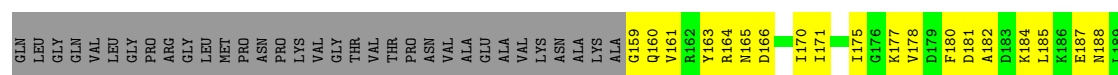
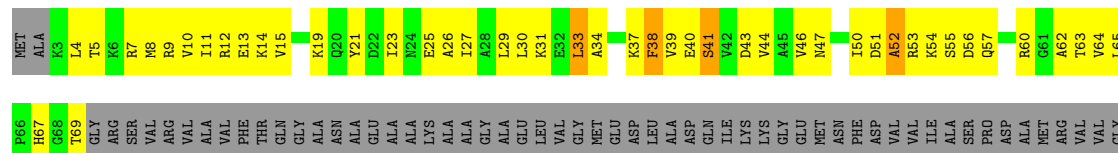
- Molecule 51: 30S ribosomal protein S21

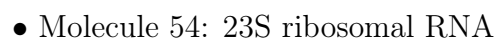
Chain U:  40% 49% 9%



- Molecule 52: 50S ribosomal protein L1

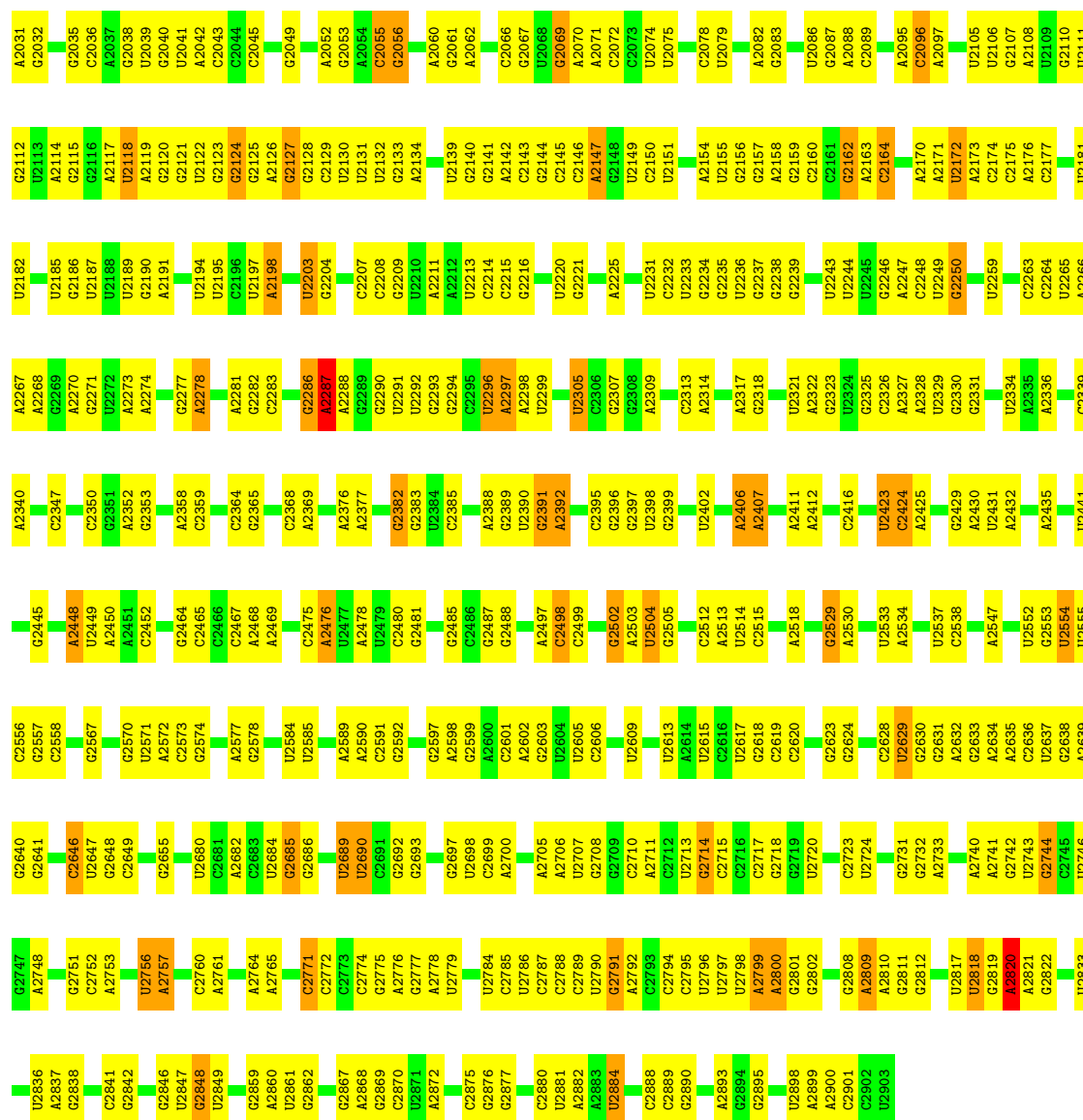
Chain 03:  20% 35% 43%





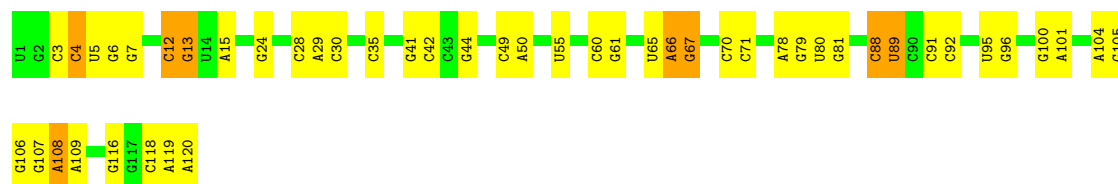
G446	G329	C225	U138	G1
U451	A330	A226	U139	C8
C455	G333	A227	C140	G9
G456	A340	C228	G141	A10
A457	G356	C229	A142	C11
A460	C353	G232	A144	U12
C461	A354	A233	C145	C16
U464	U355	U234	A146	G17
G465	G357	C239	C147	G17
G466	U358	C240	U148	C20
G467	G361	A241	A149	A21
A477	A362	C242	A152	G27
G481	G363	U243	A155	U34
C490	C364	A244	A156	G35
A491	U365	G245	C157	G45
A492	G366	G248	U158	C46
C493	A371	C249	A161	A49
A495	G372	A255	U162	U50
U499	U373	A256	C163	G51
G500	G381	C257	C164	C57
A504	G389	G264	G168	G57
G506	U390	A265	G169	G58
U507	G388	G276	A172	A63
A508	G389	C275	A173	G68
G512	C394	C281	G176	C69
C517	U395	A282	G177	G70
U518	G400	G283	A181	A71
G520	A404	G287	A182	A74
A528	U405	U288	C183	G75
G529	G406	A294	G186	G85
C531	G411	G295	G187	C96
A532	C414	U296	G189	C97
G533	A415	G297	A195	U100
U534	C421	G301	A196	A101
G535	A422	C302	A197	U102
C536	G423	G303	C198	C116
U537	G424	A310	G205	G117
A538	U437	A311	C211	A118
G539	C438	G312	G212	A119
C540	A439	U321	A213	U120
A541	G440	A322	G214	G121
C542	U441	C323	C215	C128
G543	G442	G326	A216	C129
U544	C445	G327	A221	C130
		U328	C222	A131

C1924	A1829	C1732	A1597	G1482	A1378	A1287	U1181	G1093	A1020	U826	U741	A633	U545
C1830	C1830	U1736	A1598	G1483	U1379	G1288	G1182	A1096	A1021	U827	U742	C634	U546
G1831	G1831	G1737	A1603	U1486	A1383	C1295	U1183	U1097	G1022	U828	A743	G635	A547
C1837	C1837	A1738	A1603	U1487	A1383	G1296	G1186	A1098	U1023	A829	G744	G636	G548
G1842	G1842	G1740	A1608	U1490	C1386	C1297	G1187	G1099	U1023	G830	U745	A637	G549
C1843	C1843	A1744	G1611	A1491	A1387	G1300	G1190	A1103	G1026	U832	U746	G638	G553
A1847	A1847	A1745	A1616	G1491	G1388	A1301	G1191	C1104	A1027	A833	C747	C640	U554
A1936	A1936	A1746	A1616	C1498	G1389	A1301	G1191	U1105	U1033	G834	C748	U641	U555
G1849	G1849	U1747	A1634	C1499	U1394	A1307	C1196	G1106	U1033	U839	A749	C645	C557
G1850	G1850	C1748	A1634	G1500	U1395	A1308	G1197	U1105	U1033	C840	A752	U646	U558
U1943	U1943	G1753	A1637	U1506	U1397	G1310	U1203	G1110	G1037	A845	U755	C560	G559
U1944	U1944	A1754	A1637	C1507	U1397	G1311	U1203	G1111	G1038	U846	U756	C561	C560
U1955	U1955	A1745	A1616	A1508	U1409	G1314	G1206	G1112	A1039	U847	U757	U562	G561
C1967	C1967	U1758	A1646	A1509	G1410	C1315	G1212	U1113	A1040	C848	U766	A563	A563
U1956	U1956	A1759	U1647	A1510	U1411	C1316	A1213	C1114	A1041	A849	U767	A654	U566
G1857	G1857	C1760	U1648	A1515	U1412	U1317	G1222	G1115	G1042	A851	G768	A655	U567
A1858	A1858	C1761	U1648	A1515	U1412	U1317	U1222	G1116	G1043	C851	U769	A656	U568
A1866	A1866	C1762	G1651	A1522	G1416	U1318	U1223	U1119	C1044	U852	G770	U657	U569
G1867	G1867	U1765	G1653	U1523	A1419	C1319	U1224	G1120	A1046	C853	G771	U658	G570
C1868	C1868	G1766	G1653	U1524	A1420	C1320	U1225	G1121	G1047	G854	G772	C772	G571
C1870	C1870	A1773	G1659	A1525	G1421	A1321	G1225	G1122	G1047	G855	U773	G662	U571
A1871	A1871	C1774	G1660	C1526	G1421	U1326	G1236	C1123	C1053	G856	G776	U573	A572
A1872	A1872	U1775	A1664	A1532	C1428	A1327	A1237	G1124	A1054	G857	G776	A574	U573
G1873	G1873	G1776	A1664	A1532	G1429	A1328	A1238	U1130	G1055	G858	G780	A575	A574
U1991	U1991	U1777	A1665	U1533	G1430	A1329	G1238	G1131	G1056	U860	A781	C672	U576
U1993	U1993	U1778	G1666	U1534	A1431	C1330	G1245	U1132	A1057	A861	A782	C673	G577
A1877	A1877	U1779	A1535	U1535	A1434	G1331	G1245	U1133	U1060	G862	A783	G674	G578
C1878	C1878	A1780	C1536	C1537	G1435	G1332	G1248	C1135	U1061	A863	A784	A675	G579
C1879	C1879	U1781	G1537	G1537	G1435	A1336	U1249	U1141	U1062	G864	G785	A676	U580
U1880	U1880	A1789	G1538	G1538	G1436	A1337	C1251	A1142	G1063	G865	A788	A677	C581
C1881	C1881	G1790	A1677	U1539	C1437	G1337	C1252	A1143	U1064	G866	C796	U686	A582
A1791	A1791	A1791	G1540	G1540	U1438	G1338	G1253	C1145	A1070	G867	G797	C687	G583
A1794	A1794	C1795	C1547	C1547	U1440	A1342	A1254	U1148	U1065	G869	C798	U687	U588
C1795	C1795	U1796	A1548	A1548	G1441	C1345	U1255	G1149	U1066	C873	G799	G695	U593
G1797	G1797	U1797	A1549	A1549	U1442	C1345	G1256	A1143	A1067	G874	G800	U720	U594
U1798	U1798	U1798	U1554	U1554	U1443	A1354	C1257	A1144	G1068	C876	A801	U703	C595
G1799	G1799	U1799	G1555	G1555	U1444	A1354	U1258	C1145	A1069	A877	G802	G704	U598
C1800	C1800	C1800	U1555	U1555	G1445	G1355	G1259	U1148	G1071	A878	A802	A705	A599
A1801	A1801	A1801	G1560	G1560	G1446	G1356	G1266	A1149	A1077	C885	G805	G708	U599
A1806	A1806	C1806	U1563	U1563	U1447	C1357	U1267	G1156	U1078	C886	C806	A603	A603
C1807	C1807	U1807	C1564	C1564	G1448	G1358	A1268	A1157	C1079	A886	U807	U720	A609
A1808	A1808	A1808	C1565	C1565	C1454	G1360	A1269	G1157	A1080	U887	G808	A721	C610
A1809	A1809	A1809	A1566	A1566	C1461	C1362	G1270	G1170	U1081	C888	U809	G729	C611
A1810	A1810	A1810	A1566	A1566	C1461	C1362	G1271	G1171	U1082	C889	U810	U724	U615
A1811	A1811	A1811	A1569	A1569	U1468	G1363	A1272	C1172	A1084	C890	U811	G725	A616
C1816	C1816	C1816	A1579	A1579	A1469	C1364	C1278	U1173	A1085	A896	C812	G726	G617
A1912	A1912	A1912	A1580	A1580	A1470	A1365	G1279	U1174	A1086	C897	U813	A727	U616
A1913	A1913	U1817	G1581	G1581	G1471	A1366	C1280	A1175	G1087	C898	C814	G728	G617
U2026	U2026	U1818	G1581	G1581	C1472	G1368	U1282	A1176	A1088	A899	C817	G729	A627
G2027	G2027	U1917	U1594	U1594	G1475	G1369	G1283	G1177	A1089	A900	C818	A730	G628
U2028	U2028	A1918	C1595	C1595	U1476	G1370	A1284	C1178	A1090	C901	A819	G736	G628
A2030	A2030	U1827	C1730	C1730	U1476	G1371	A1286	U1180	G1092	G907	A825	C737	C737



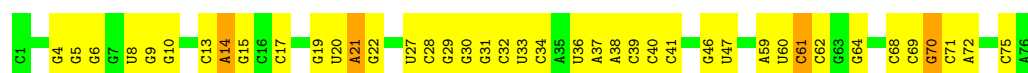
• Molecule 55: 5S ribosomal RNA

Chain 02: 60% 33% 7%



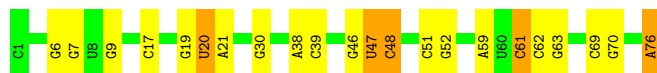
• Molecule 56: tRNA^{fMet}

Chain X: 47% 48% 5%



- Molecule 56: tRNA^{fMet}

Chain W:  71% 22% 6%



- Molecule 57: mRNA

Chain V:  72% 22% 6%



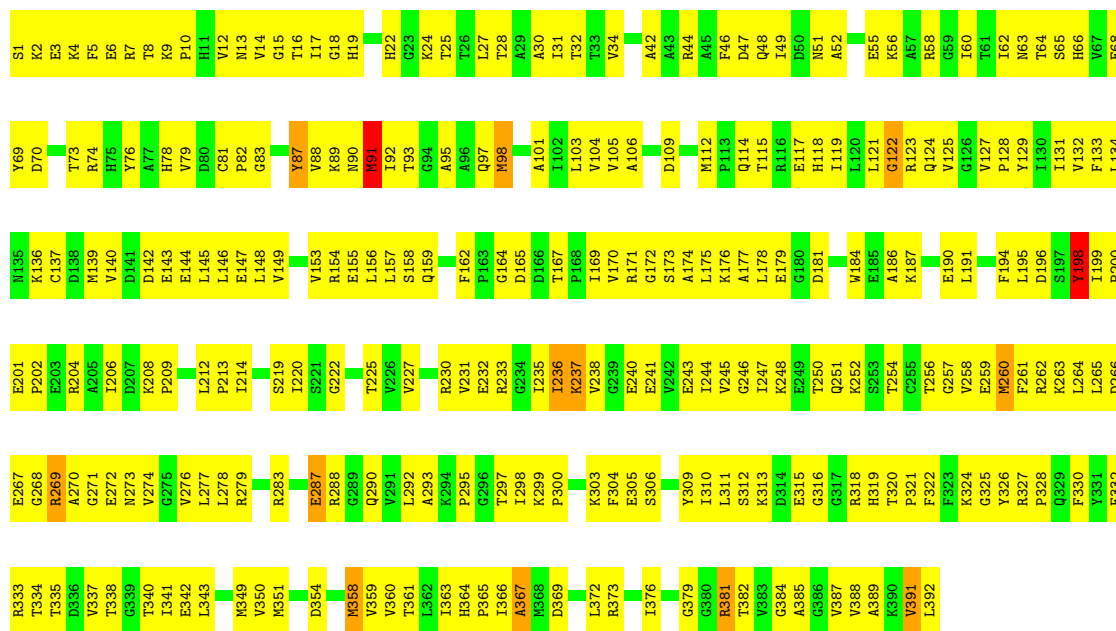
- Molecule 58: tRNA^{Phe}

Chain Y:  43% 46% 11%



- Molecule 59: Elongation factor Tu 2

Chain Z:  33% 63% 4%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	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: FME, GCP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	04	0.34	0/2122	0.61	0/2852
2	05	0.37	0/1586	0.57	0/2134
3	06	0.35	0/1571	0.59	1/2113 (0.0%)
4	07	0.38	0/1435	0.56	0/1926
5	08	0.34	0/1343	0.59	1/1816 (0.1%)
6	09	0.40	0/1122	0.64	0/1515
7	10	0.46	0/1002	0.74	2/1350 (0.1%)
8	11	0.42	0/1046	0.64	0/1410
9	12	0.35	0/1152	0.58	0/1551
10	13	0.35	0/948	0.60	0/1268
11	14	0.34	0/1054	0.62	0/1403
12	15	0.39	0/1093	0.57	0/1460
13	16	0.37	0/974	0.56	0/1301
14	17	0.33	0/902	0.53	0/1209
15	18	0.35	0/929	0.58	0/1242
16	19	0.39	0/960	0.52	0/1278
17	20	0.38	0/829	0.66	1/1107 (0.1%)
18	21	0.32	0/864	0.59	0/1156
19	22	0.34	0/745	0.55	0/994
20	23	0.38	0/788	0.62	0/1051
21	24	0.38	0/766	0.55	0/1025
22	25	0.39	0/582	0.54	0/769
23	26	0.36	0/635	0.56	0/848
24	27	0.35	0/510	0.58	0/677
25	28	0.33	0/453	0.56	0/605
26	29	0.42	0/532	0.57	0/709
27	30	0.31	0/450	0.52	0/599
28	31	0.38	0/417	0.52	0/554
29	32	0.41	0/380	0.60	0/498
30	33	0.35	0/513	0.61	0/676
31	34	0.30	0/303	0.54	0/397
32	B	0.41	1/1736 (0.1%)	0.67	2/2338 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	C	0.36	0/1652	0.57	0/2225
34	D	0.35	0/1665	0.60	0/2227
35	E	0.35	0/1170	0.62	0/1573
36	F	0.37	0/836	0.70	0/1128
37	G	0.34	0/1196	0.58	0/1602
38	H	0.34	0/989	0.62	1/1326 (0.1%)
39	I	0.37	0/1034	0.66	0/1375
40	J	0.37	0/797	0.65	0/1077
41	K	0.37	0/886	0.60	0/1195
42	L	0.36	0/969	0.72	1/1300 (0.1%)
43	M	0.31	0/893	0.57	0/1193
44	N	0.36	0/817	0.53	0/1088
45	O	0.35	0/722	0.55	0/964
46	P	0.37	0/659	0.62	0/884
47	Q	0.36	0/658	0.65	0/881
48	R	0.41	0/545	0.67	0/731
49	S	0.39	0/653	0.59	0/877
50	T	0.34	0/671	0.54	0/888
51	U	0.44	0/551	0.70	1/728 (0.1%)
52	03	1.71	1/1033 (0.1%)	0.83	0/1387
53	A	0.44	0/36963	0.69	7/57662 (0.0%)
54	01	0.45	0/69796	0.68	9/108888 (0.0%)
55	02	0.37	0/2872	0.69	0/4479
56	W	0.42	0/1832	0.68	0/2855
56	X	0.62	0/1832	0.71	0/2855
57	V	0.50	0/436	0.67	0/679
58	Y	0.57	0/1809	0.70	0/2819
59	Z	1.75	6/3085 (0.2%)	0.77	0/4173
All	All	0.50	8/166763 (0.0%)	0.67	26/248890 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	160	LEU	C-N	5.97	1.47	1.34
59	Z	91	MET	SD-CE	5.73	2.10	1.77
59	Z	287	GLU	CB-CG	5.66	1.62	1.52
59	Z	287	GLU	CG-CD	5.54	1.60	1.51
59	Z	260	MET	SD-CE	5.31	2.07	1.77

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	160	LEU	O-C-N	-8.61	108.92	122.70
17	20	50	GLY	N-CA-C	-6.51	96.82	113.10
53	A	1301	U	N1-C1'-C2'	6.23	122.09	114.00
54	01	301	G	N9-C1'-C2'	6.21	122.07	114.00
32	B	160	LEU	CA-C-N	6.06	130.52	117.20

There are no chirality outliers.

There are no planarity outliers.

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	04	2083	0	2157	73	0
2	05	1565	0	1616	47	0
3	06	1552	0	1619	49	0
4	07	1411	0	1447	64	0
5	08	1323	0	1374	34	0
6	09	1111	0	1148	37	0
7	10	989	0	1025	62	0
8	11	1032	0	1088	63	0
9	12	1129	0	1162	30	0
10	13	939	0	1012	27	0
11	14	1045	0	1117	34	0
12	15	1074	0	1157	38	0
13	16	961	0	1000	30	0
14	17	892	0	923	20	0
15	18	917	0	965	33	0
16	19	947	0	1022	31	0
17	20	816	0	839	29	0
18	21	857	0	922	23	0
19	22	739	0	807	20	0
20	23	780	0	834	22	0
21	24	753	0	780	28	0
22	25	575	0	592	18	0
23	26	625	0	655	19	0
24	27	509	0	543	9	0
25	28	449	0	491	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	29	523	0	524	17	0
27	30	444	0	461	21	0
28	31	410	0	440	7	0
29	32	377	0	418	10	0
30	33	504	0	574	13	0
31	34	302	0	343	9	0
32	B	1705	0	1732	92	0
33	C	1625	0	1699	49	0
34	D	1643	0	1710	50	0
35	E	1157	0	1199	47	0
36	F	818	0	808	39	0
37	G	1182	0	1240	40	0
38	H	979	0	1034	46	0
39	I	1022	0	1070	38	0
40	J	787	0	828	44	0
41	K	870	0	878	36	0
42	L	955	0	1019	26	0
43	M	884	0	944	35	0
44	N	805	0	847	34	0
45	O	714	0	737	17	0
46	P	649	0	666	26	0
47	Q	649	0	691	29	0
48	R	536	0	552	24	0
49	S	638	0	665	31	0
50	T	665	0	714	20	0
51	U	545	0	579	44	0
52	03	1026	0	1092	121	0
53	A	33012	0	16618	454	0
54	01	62317	0	31346	855	0
55	02	2568	0	1303	34	0
56	W	1640	0	836	15	0
56	X	1640	0	837	28	0
57	V	388	0	196	4	0
58	Y	1619	0	821	38	0
59	Z	3029	0	3043	291	0
60	W	10	0	10	3	0
61	Y	11	0	8	3	0
62	Z	32	0	14	0	0
All	All	153753	0	104791	3217	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 12.

The worst 5 of 3217 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)
59:Z:112:MET:CE	59:Z:112:MET:SD	2.02	1.47
59:Z:358:MET:SD	59:Z:358:MET:CE	2.05	1.45
52:03:218:MET:CE	52:03:218:MET:SD	2.05	1.44
56:W:76:A:O3'	60:W:101:FME:C	1.63	1.43
59:Z:260:MET:CE	59:Z:260:MET:SD	2.07	1.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	04	269/271 (99%)	233 (87%)	33 (12%)	3 (1%)	14	53
2	05	207/209 (99%)	184 (89%)	23 (11%)	0	100	100
3	06	199/201 (99%)	175 (88%)	22 (11%)	2 (1%)	15	55
4	07	175/177 (99%)	154 (88%)	20 (11%)	1 (1%)	25	64
5	08	174/176 (99%)	155 (89%)	13 (8%)	6 (3%)	3	31
6	09	147/149 (99%)	117 (80%)	26 (18%)	4 (3%)	5	35
7	10	129/131 (98%)	97 (75%)	22 (17%)	10 (8%)	1	11
8	11	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3	29
9	12	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	61
10	13	120/122 (98%)	101 (84%)	17 (14%)	2 (2%)	9	45
11	14	141/143 (99%)	112 (79%)	23 (16%)	6 (4%)	2	24
12	15	134/136 (98%)	115 (86%)	18 (13%)	1 (1%)	22	61
13	16	118/120 (98%)	102 (86%)	14 (12%)	2 (2%)	9	45
14	17	114/116 (98%)	106 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	18	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
16	19	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
17	20	101/103 (98%)	83 (82%)	16 (16%)	2 (2%)	7	41
18	21	108/110 (98%)	95 (88%)	11 (10%)	2 (2%)	8	42
19	22	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
20	23	100/102 (98%)	83 (83%)	14 (14%)	3 (3%)	4	33
21	24	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
22	25	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
23	26	75/77 (97%)	66 (88%)	9 (12%)	0	100	100
24	27	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	9	46
25	28	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
26	29	64/66 (97%)	51 (80%)	13 (20%)	0	100	100
27	30	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
28	31	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	40
29	32	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
30	33	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	46
31	34	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	34
32	B	216/218 (99%)	180 (83%)	30 (14%)	6 (3%)	5	34
33	C	204/206 (99%)	187 (92%)	16 (8%)	1 (0%)	29	68
34	D	203/205 (99%)	167 (82%)	31 (15%)	5 (2%)	5	36
35	E	155/157 (99%)	133 (86%)	15 (10%)	7 (4%)	2	23
36	F	98/100 (98%)	75 (76%)	18 (18%)	5 (5%)	2	20
37	G	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	12	50
38	H	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	59
39	I	125/127 (98%)	98 (78%)	22 (18%)	5 (4%)	3	26
40	J	96/98 (98%)	78 (81%)	10 (10%)	8 (8%)	1	10
41	K	114/116 (98%)	92 (81%)	19 (17%)	3 (3%)	5	35
42	L	121/123 (98%)	95 (78%)	18 (15%)	8 (7%)	1	16
43	M	112/114 (98%)	95 (85%)	14 (12%)	3 (3%)	5	35
44	N	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	15	55
45	O	86/88 (98%)	74 (86%)	11 (13%)	1 (1%)	13	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	P	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	5	36
47	Q	78/80 (98%)	61 (78%)	11 (14%)	6 (8%)	1	12
48	R	63/65 (97%)	50 (79%)	7 (11%)	6 (10%)	0	8
49	S	77/79 (98%)	66 (86%)	9 (12%)	2 (3%)	5	35
50	T	83/85 (98%)	75 (90%)	7 (8%)	1 (1%)	13	51
51	U	63/65 (97%)	41 (65%)	15 (24%)	7 (11%)	0	6
52	03	130/234 (56%)	107 (82%)	22 (17%)	1 (1%)	19	59
59	Z	390/392 (100%)	329 (84%)	55 (14%)	6 (2%)	10	47
All	All	6366/6574 (97%)	5449 (86%)	776 (12%)	141 (2%)	10	39

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	06	83	VAL
5	08	46	ASP
5	08	47	ASN
5	08	119	GLY
6	09	9	VAL

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	04	216/216 (100%)	210 (97%)	6 (3%)	43	72
2	05	164/164 (100%)	164 (100%)	0	100	100
3	06	165/165 (100%)	163 (99%)	2 (1%)	71	87
4	07	148/148 (100%)	148 (100%)	0	100	100
5	08	137/137 (100%)	137 (100%)	0	100	100
6	09	114/114 (100%)	111 (97%)	3 (3%)	46	74
7	10	100/100 (100%)	100 (100%)	0	100	100
8	11	109/109 (100%)	108 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	12	116/116 (100%)	114 (98%)	2 (2%)	60	82
10	13	103/103 (100%)	102 (99%)	1 (1%)	76	88
11	14	102/102 (100%)	101 (99%)	1 (1%)	76	88
12	15	109/109 (100%)	107 (98%)	2 (2%)	59	81
13	16	100/100 (100%)	98 (98%)	2 (2%)	55	79
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	99 (100%)	0	100	100
16	19	89/89 (100%)	87 (98%)	2 (2%)	52	77
17	20	84/84 (100%)	84 (100%)	0	100	100
18	21	93/93 (100%)	91 (98%)	2 (2%)	52	77
19	22	80/80 (100%)	79 (99%)	1 (1%)	69	86
20	23	83/83 (100%)	82 (99%)	1 (1%)	71	87
21	24	78/78 (100%)	77 (99%)	1 (1%)	69	86
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	65 (97%)	2 (3%)	41	71
24	27	55/55 (100%)	54 (98%)	1 (2%)	59	81
25	28	48/48 (100%)	48 (100%)	0	100	100
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	45 (100%)	0	100	100
29	32	38/38 (100%)	38 (100%)	0	100	100
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	34 (100%)	0	100	100
32	B	180/180 (100%)	178 (99%)	2 (1%)	73	88
33	C	170/170 (100%)	166 (98%)	4 (2%)	49	75
34	D	172/172 (100%)	168 (98%)	4 (2%)	50	76
35	E	119/119 (100%)	118 (99%)	1 (1%)	81	91
36	F	87/87 (100%)	85 (98%)	2 (2%)	50	76
37	G	124/124 (100%)	124 (100%)	0	100	100
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	J	86/86 (100%)	86 (100%)	0	100	100
41	K	89/89 (100%)	88 (99%)	1 (1%)	73	88
42	L	103/103 (100%)	102 (99%)	1 (1%)	76	88
43	M	92/92 (100%)	90 (98%)	2 (2%)	52	77
44	N	83/83 (100%)	82 (99%)	1 (1%)	71	87
45	O	76/76 (100%)	76 (100%)	0	100	100
46	P	65/65 (100%)	63 (97%)	2 (3%)	40	71
47	Q	74/74 (100%)	74 (100%)	0	100	100
48	R	56/56 (100%)	53 (95%)	3 (5%)	22	57
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	65 (100%)	0	100	100
51	U	55/55 (100%)	51 (93%)	4 (7%)	14	46
52	03	110/181 (61%)	106 (96%)	4 (4%)	35	67
59	Z	324/325 (100%)	314 (97%)	10 (3%)	40	71
All	All	5285/5357 (99%)	5214 (99%)	71 (1%)	70	86

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	03	25	GLU
52	03	41	SER
59	Z	237	LYS
19	22	32	LEU
18	21	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
34	D	139	ASN
42	L	4	ASN
36	F	17	GLN
39	I	80	HIS
45	O	36	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	160 (10%)	9 (0%)
54	01	2902/2903 (99%)	358 (12%)	16 (0%)
55	02	119/120 (99%)	11 (9%)	2 (1%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	13 (17%)	0
57	V	17/18 (94%)	2 (11%)	0
58	Y	75/76 (98%)	14 (18%)	0
All	All	4803/4810 (99%)	565 (11%)	27 (0%)

5 of 565 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G
53	A	22	G
53	A	31	G
53	A	32	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	1020	A
54	01	1130	U
54	01	2756	U
54	01	1111	A
54	01	1475	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	$\# Z > 2$
62	GCP	Z	401	-	27,34,34	2.31	11 (40%)	34,54,54	3.88	17 (50%)
60	FME	W	101	-	8,9,10	0.82	0	7,9,11	1.33	1 (14%)
61	PHE	Y	101	58	10,11,12	1.01	0	10,13,15	0.34	0

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
62	GCP	Z	401	-	-	9/15/38/38	0/3/3/3
60	FME	W	101	-	-	3/7/9/11	-
61	PHE	Y	101	58	-	1/5/6/8	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	Z	401	GCP	O4'-C1'	5.13	1.48	1.41
62	Z	401	GCP	PB-O3A	-3.96	1.53	1.58
62	Z	401	GCP	C2'-C1'	3.96	1.59	1.53
62	Z	401	GCP	C5-C6	3.81	1.47	1.41
62	Z	401	GCP	C2-N2	3.72	1.41	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Z	401	GCP	C1'-N9-C4	12.96	149.41	126.64
62	Z	401	GCP	C5-C6-N1	-9.02	111.10	123.43
62	Z	401	GCP	C2-N1-C6	7.33	127.57	115.93
62	Z	401	GCP	O1G-PG-C3B	-7.29	95.52	111.24
62	Z	401	GCP	O4'-C1'-C2'	-4.93	99.72	106.93

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

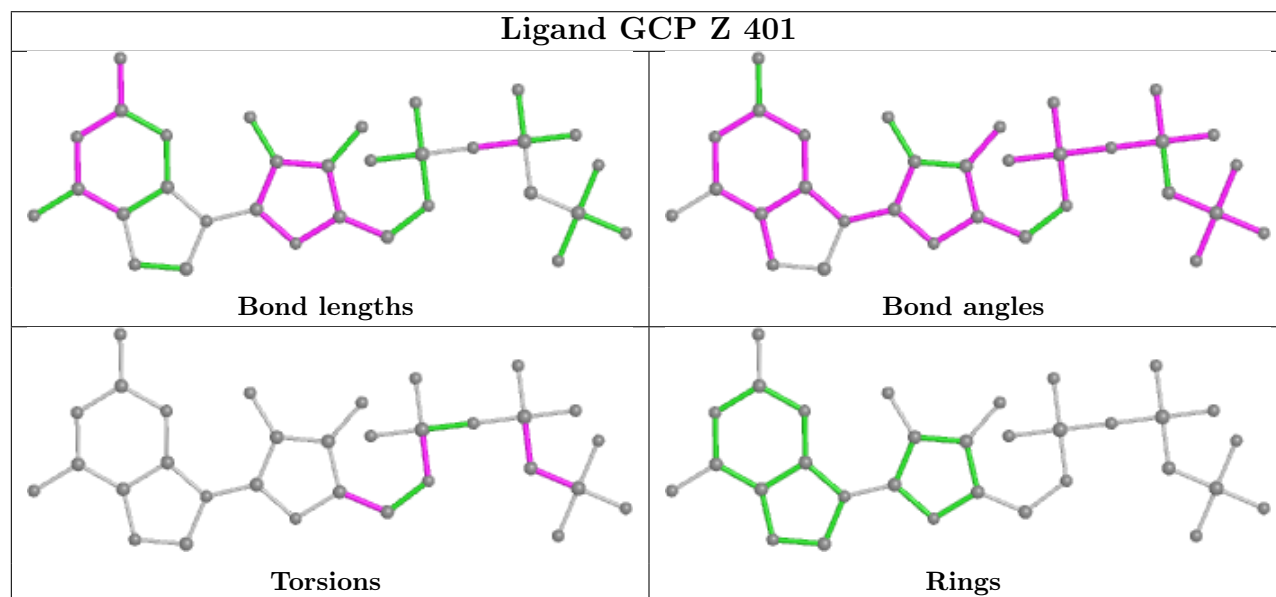
Mol	Chain	Res	Type	Atoms
60	W	101	FME	O1-CN-N-CA
60	W	101	FME	O-C-CA-CB
61	Y	101	PHE	O-C-CA-CB
62	Z	401	GCP	PB-C3B-PG-O1G
62	Z	401	GCP	PB-C3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	W	101	FME	3	0
61	Y	101	PHE	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8616. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.