



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 02:42 AM EDT

PDB ID : 5UYN
EMDB ID : EMD-8618
Title : 70S ribosome bound with near-cognate ternary complex not base-paired to A site codon (Structure I-nc)
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2017-02-24
Resolution : 4.00 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

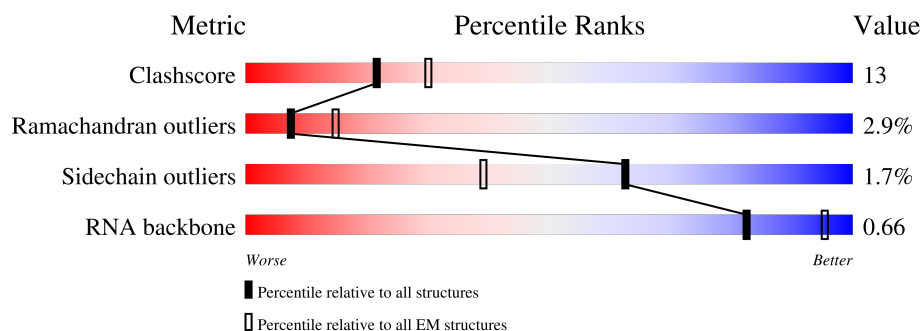
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	65% 34% .
2	05	209	59% 40%
3	06	201	60% 38% .
4	07	177	45% 55%
5	08	176	62% 37% .
6	09	149	55% 43% .
7	10	131	49% 46% 5%







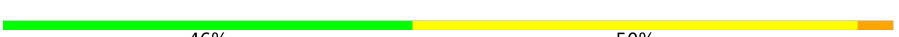



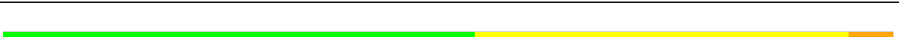


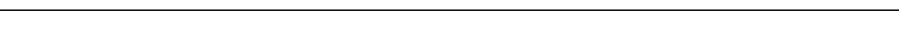
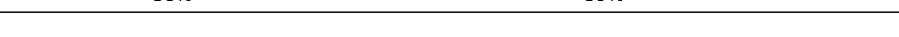
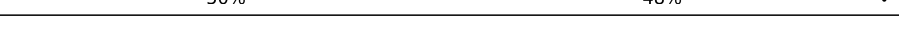



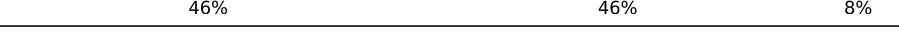
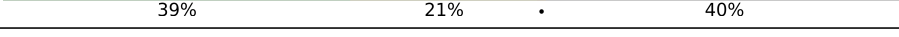




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Mol	Chain	Length	Quality of chain
8	11	141	 43%52% . .
9	12	142	 61%38% .
10	13	122	 62%37% .
11	14	143	 69%29% .
12	15	136	 57%42% ..
13	16	120	 62%36% .
14	17	116	 63%37%
15	18	114	 59%39% .
16	19	117	 56%44%
17	20	103	 50%48% .
18	21	110	 60%36% .
19	22	93	 65%34% .
20	23	102	 62%37% .
21	24	94	 61%38% .
22	25	75	 76%24%
23	26	77	 62%38%
24	27	63	 56%43% .
25	28	58	 78%22%
26	29	66	 71%29%
27	30	56	 57%43%
28	31	50	 64%34% .
29	32	46	 59%41%
30	33	64	 52%47% .
31	34	38	 47%47% 5%
32	B	218	 53%43% .




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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	223	
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	17	 76% 18% 6%
58	Y	76	 34% 47% 18%
59	Z	392	 54% 44% .

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153717 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
			917	574	179	163	1	0

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

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

- 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
			816	516	153	145	2	0

- 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
			857	532	166	156	3	0

- 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
			739	466	139	132	2	0

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

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

- 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
			1027	645	186	194	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	17	Total	C	N	O	P	0	0
			373	168	79	110	16		

- Molecule 58 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	76	Total	C	N	O	P	S	0	0
			1618	723	282	536	76	1		

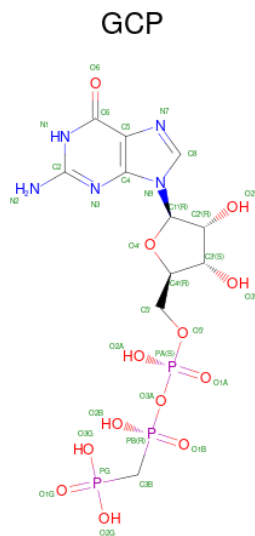
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	34	U8U	-	insertion	GB 558570689

- 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 PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

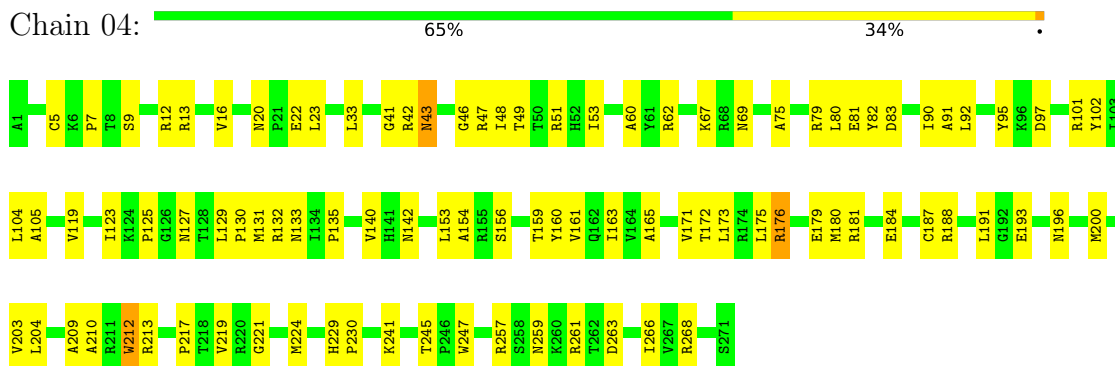


Mol	Chain	Residues	Atoms					AltConf
60	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	

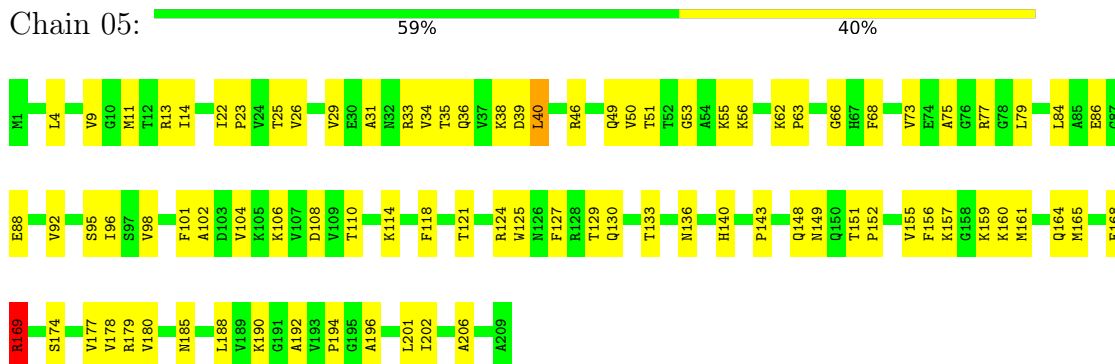
3 Residue-property plots

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.

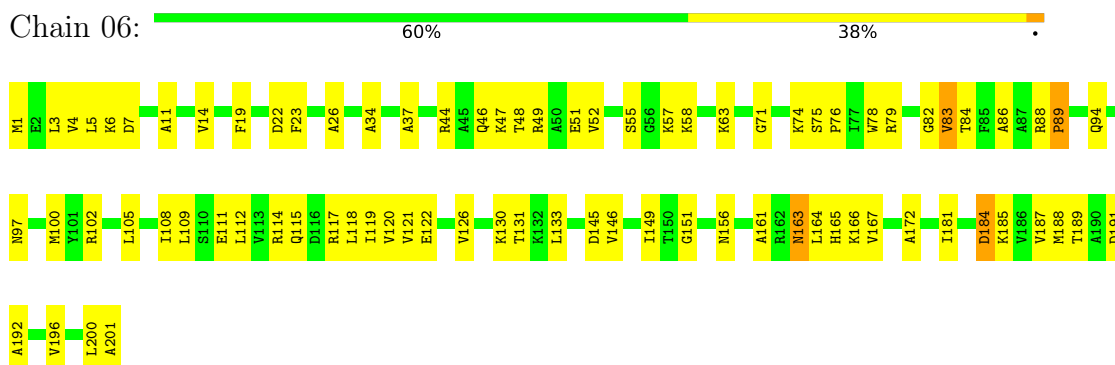
- Molecule 1: 50S ribosomal protein L2



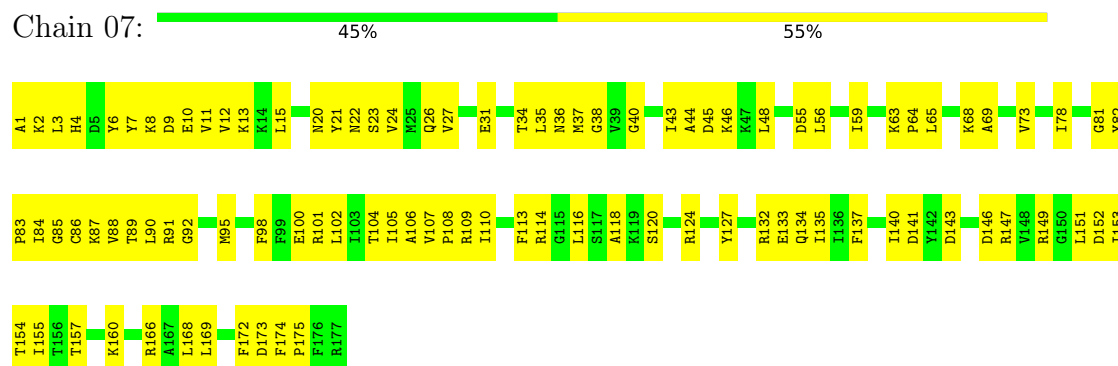
- Molecule 2: 50S ribosomal protein L3



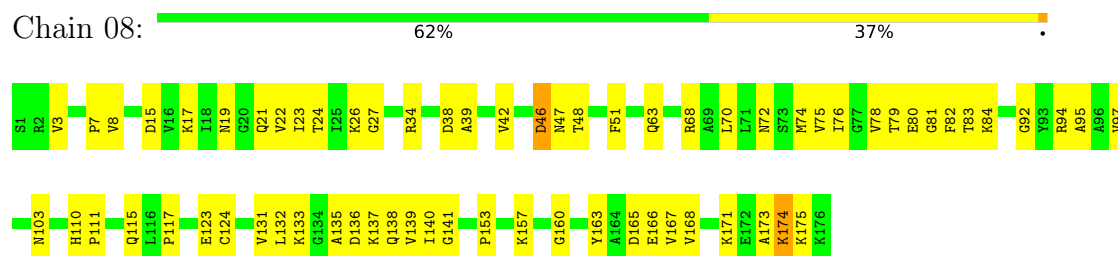
- Molecule 3: 50S ribosomal protein L4



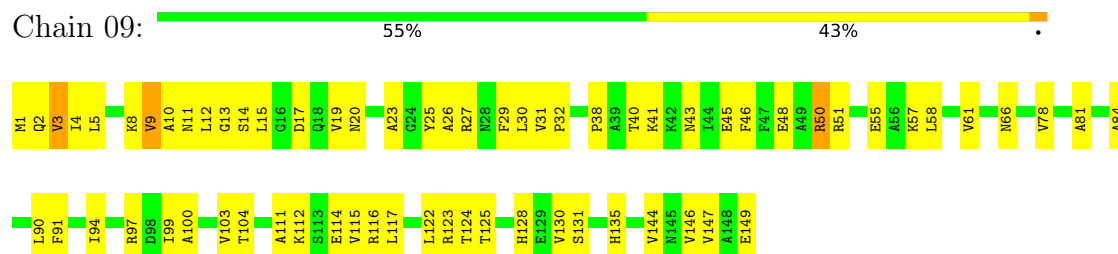
- Molecule 4: 50S ribosomal protein L5



- Molecule 5: 50S ribosomal protein L6



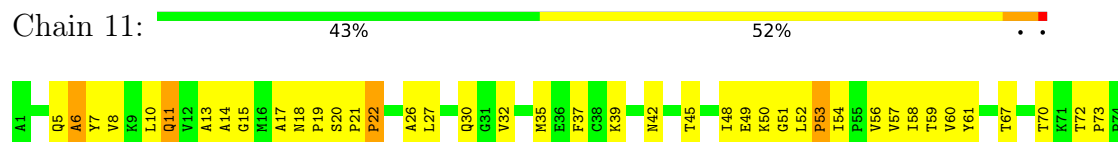
- Molecule 6: 50S ribosomal protein L9

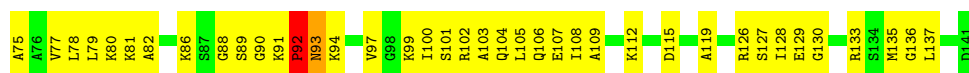


- Molecule 7: 50S ribosomal protein L10



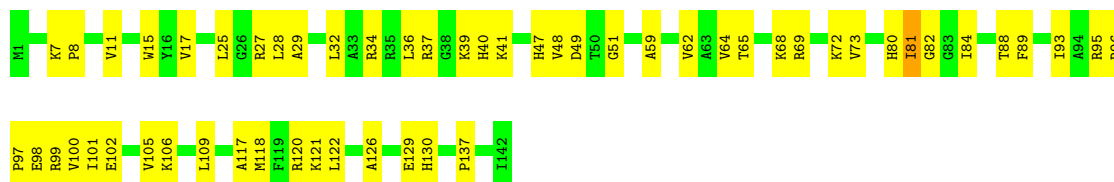
- Molecule 8: 50S ribosomal protein L11





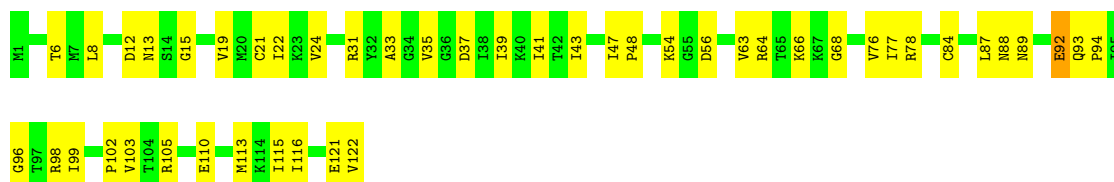
• Molecule 9: 50S ribosomal protein L13

Chain 12: 61% 38%



• Molecule 10: 50S ribosomal protein L14

Chain 13: 62% 37%



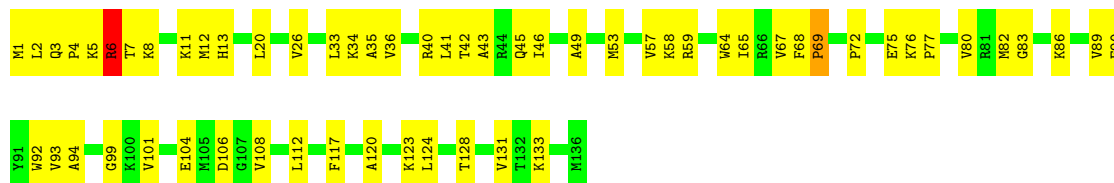
• Molecule 11: 50S ribosomal protein L15

Chain 14: 69% 29%



• Molecule 12: 50S ribosomal protein L16

Chain 15: 57% 42%



• Molecule 13: 50S ribosomal protein L17

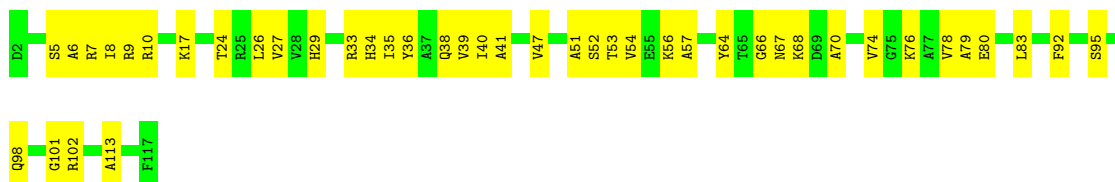
Chain 16: 62% 36%





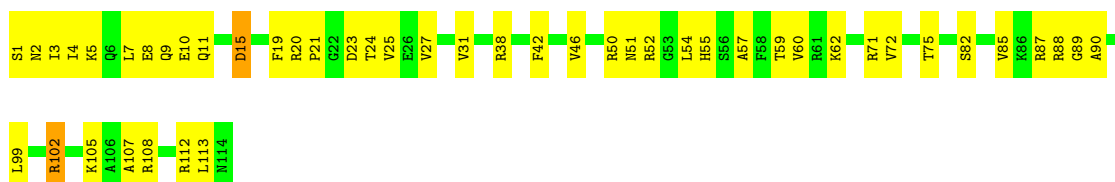
- Molecule 14: 50S ribosomal protein L18

Chain 17: 63% 37%



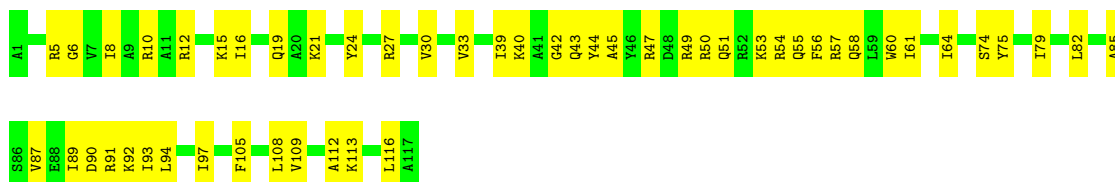
- Molecule 15: 50S ribosomal protein L19

Chain 18: 59% 39%



- Molecule 16: 50S ribosomal protein L20

Chain 19: 56% 44%



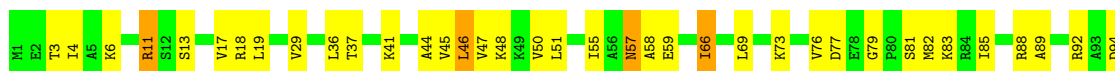
- Molecule 17: 50S ribosomal protein L21

Chain 20: 50% 48%



- Molecule 18: 50S ribosomal protein L22

Chain 21: 60% 36%





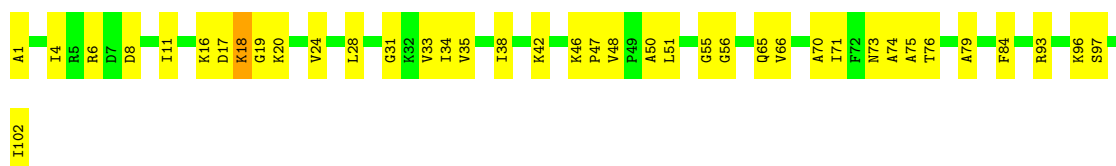
- Molecule 19: 50S ribosomal protein L23

Chain 22: 65% 34%



- Molecule 20: 50S ribosomal protein L24

Chain 23: 62% 37%



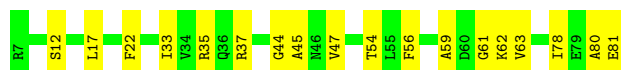
- Molecule 21: 50S ribosomal protein L25

Chain 24: 61% 38%



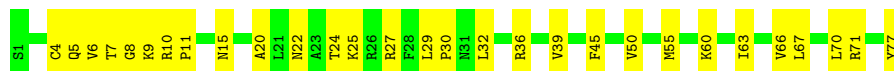
- Molecule 22: 50S ribosomal protein L27

Chain 25: 76% 24%



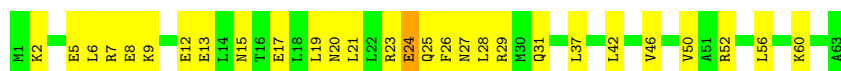
- Molecule 23: 50S ribosomal protein L28

Chain 26: 62% 38%




- Molecule 24: 50S ribosomal protein L29

Chain 27: 56% 43%



- Molecule 25: 50S ribosomal protein L30

Chain 28:  78% 22%



- Molecule 26: 50S ribosomal protein L31

Chain 29:  71% 29%



- Molecule 27: 50S ribosomal protein L32

Chain 30:  57% 43%



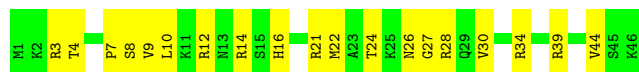
- Molecule 28: 50S ribosomal protein L33

Chain 31:  64% 34%



- Molecule 29: 50S ribosomal protein L34

Chain 32:  59% 41%



- Molecule 30: 50S ribosomal protein L35

Chain 33:  52% 47%



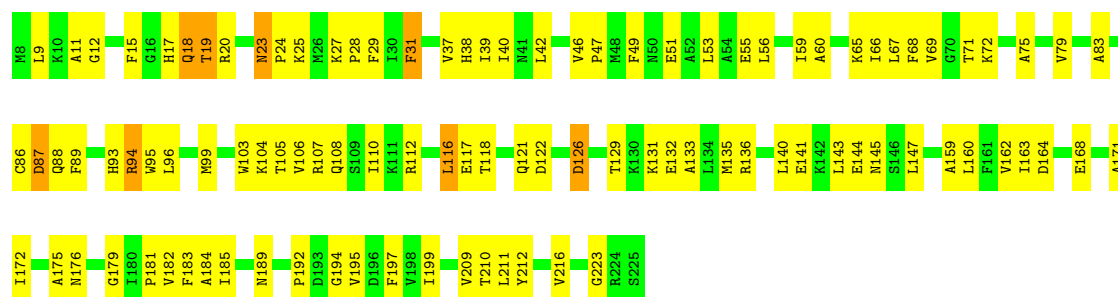
- Molecule 31: 50S ribosomal protein L36

Chain 34:  47% 47% 5%



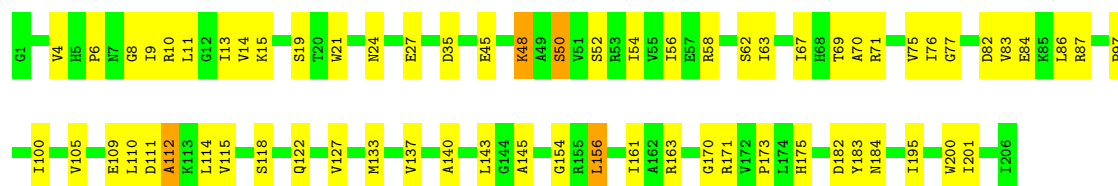
- Molecule 32: 30S ribosomal protein S2

Chain B: 



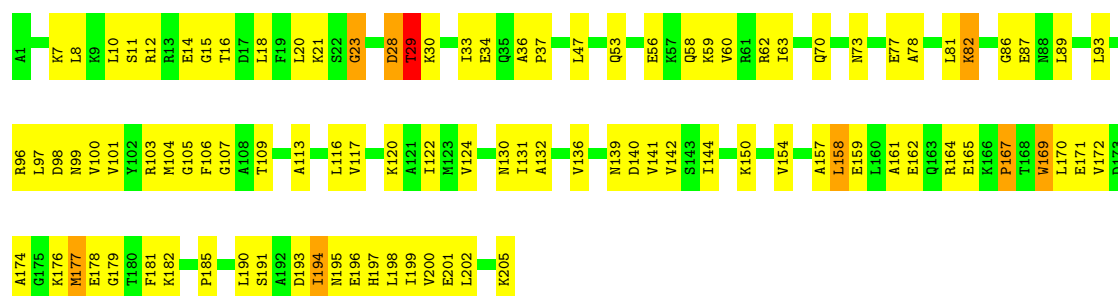
- Molecule 33: 30S ribosomal protein S3

Chain C: 



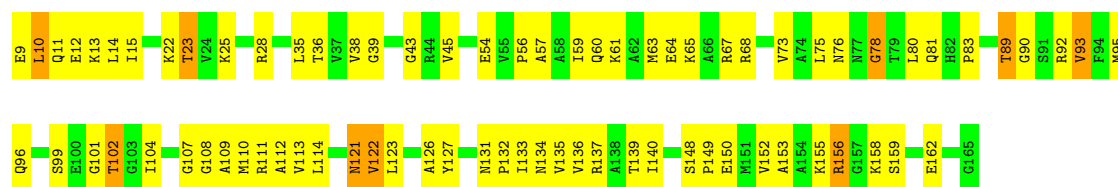
- Molecule 34: 30S ribosomal protein S4

Chain D: 



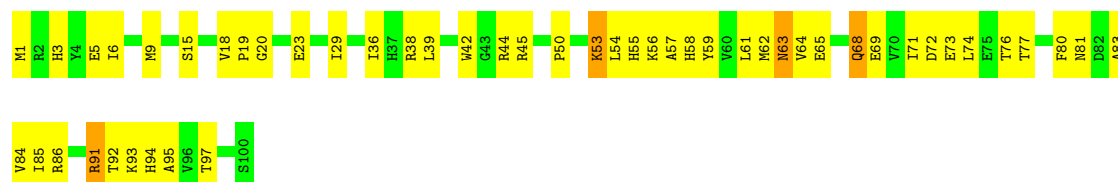
- Molecule 35: 30S ribosomal protein S5

Chain E: 



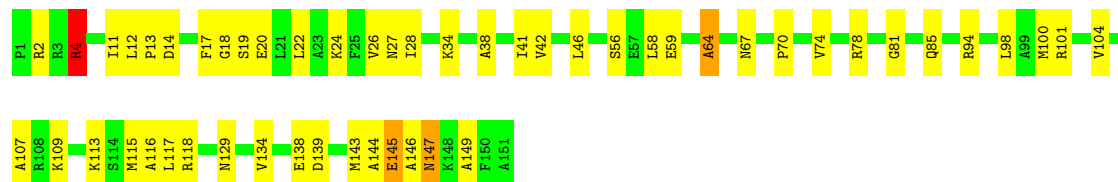
- Molecule 36: 30S ribosomal protein S6

Chain F: 



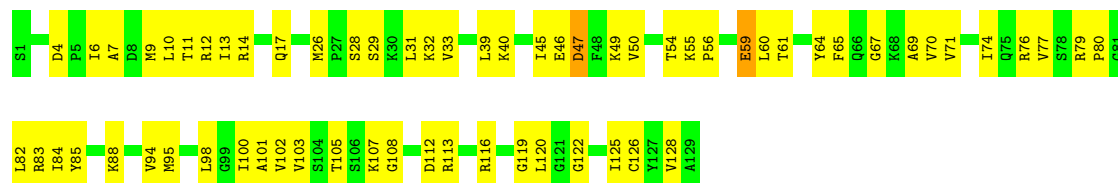
- Molecule 37: 30S ribosomal protein S7

Chain G: 66% 32% ..



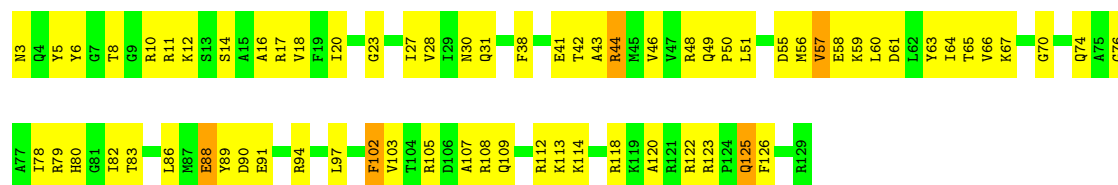
- Molecule 38: 30S ribosomal protein S8

Chain H: 50% 48% .



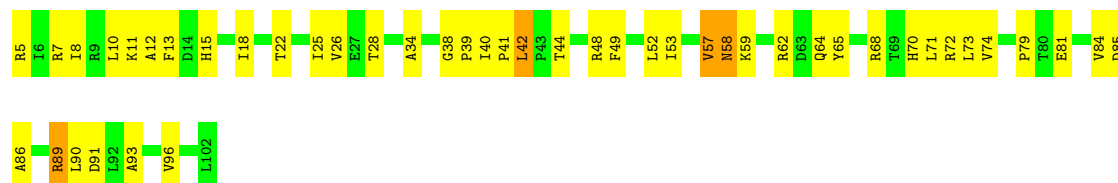
- Molecule 39: 30S ribosomal protein S9

Chain I: 46% 50% .



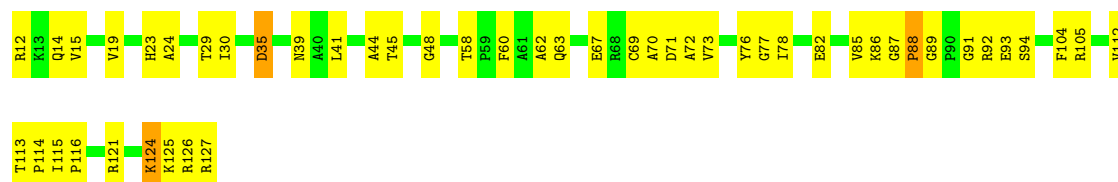
- Molecule 40: 30S ribosomal protein S10

Chain J: 53% 43% .

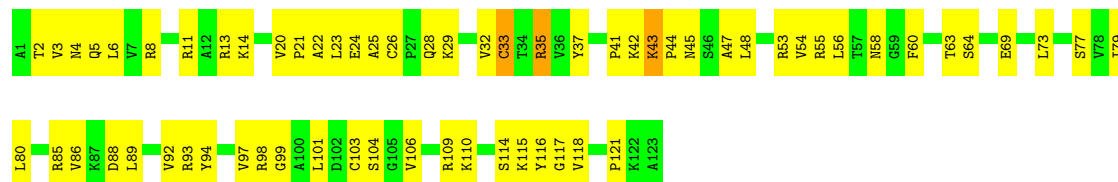


- Molecule 41: 30S ribosomal protein S11

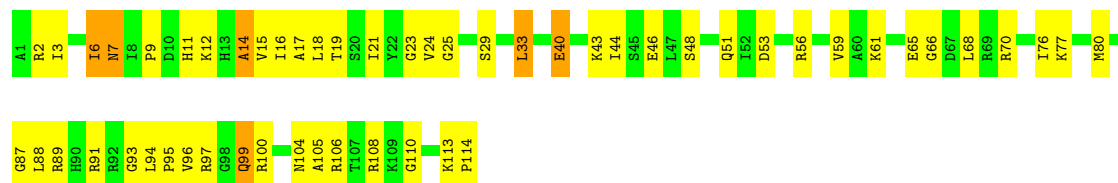
Chain K: 58% 40% .



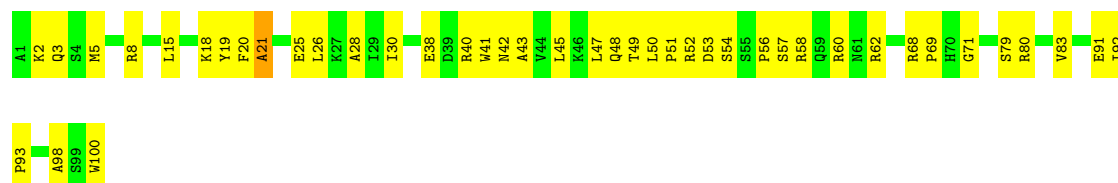
• Molecule 42: 30S ribosomal protein S12



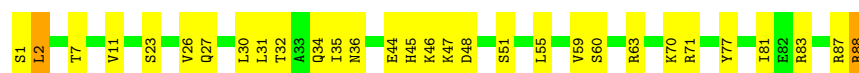
• Molecule 43: 30S ribosomal protein S13



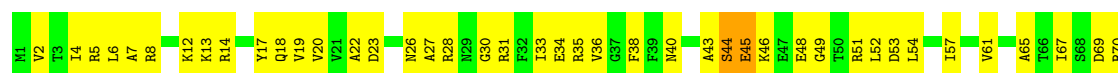
• Molecule 44: 30S ribosomal protein S14



• Molecule 45: 30S ribosomal protein S15



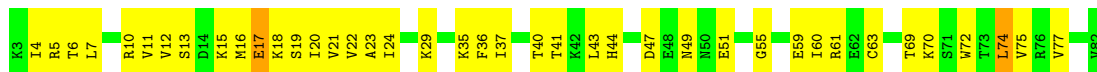
• Molecule 46: 30S ribosomal protein S16





- Molecule 47: 30S ribosomal protein S17

Chain Q: 50% 48%



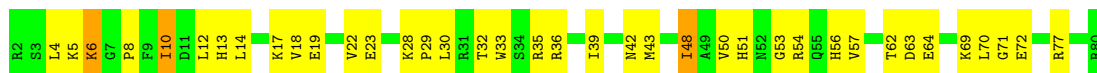
- Molecule 48: 30S ribosomal protein S18

Chain R: 46% 49% 5%



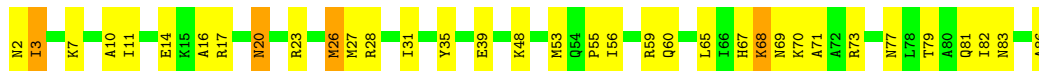
- Molecule 49: 30S ribosomal protein S19

Chain S: 52% 44%



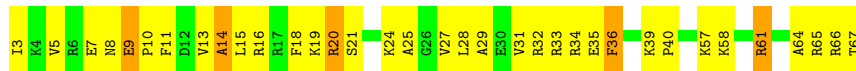
- Molecule 50: 30S ribosomal protein S20

Chain T: 59% 36% 5%



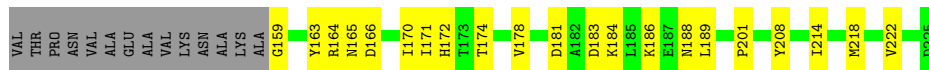
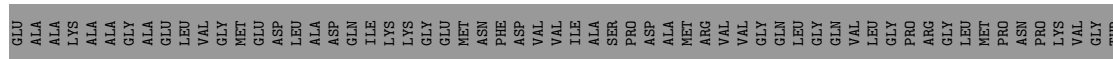
- Molecule 51: 30S ribosomal protein S21

Chain U: 46% 46% 8%



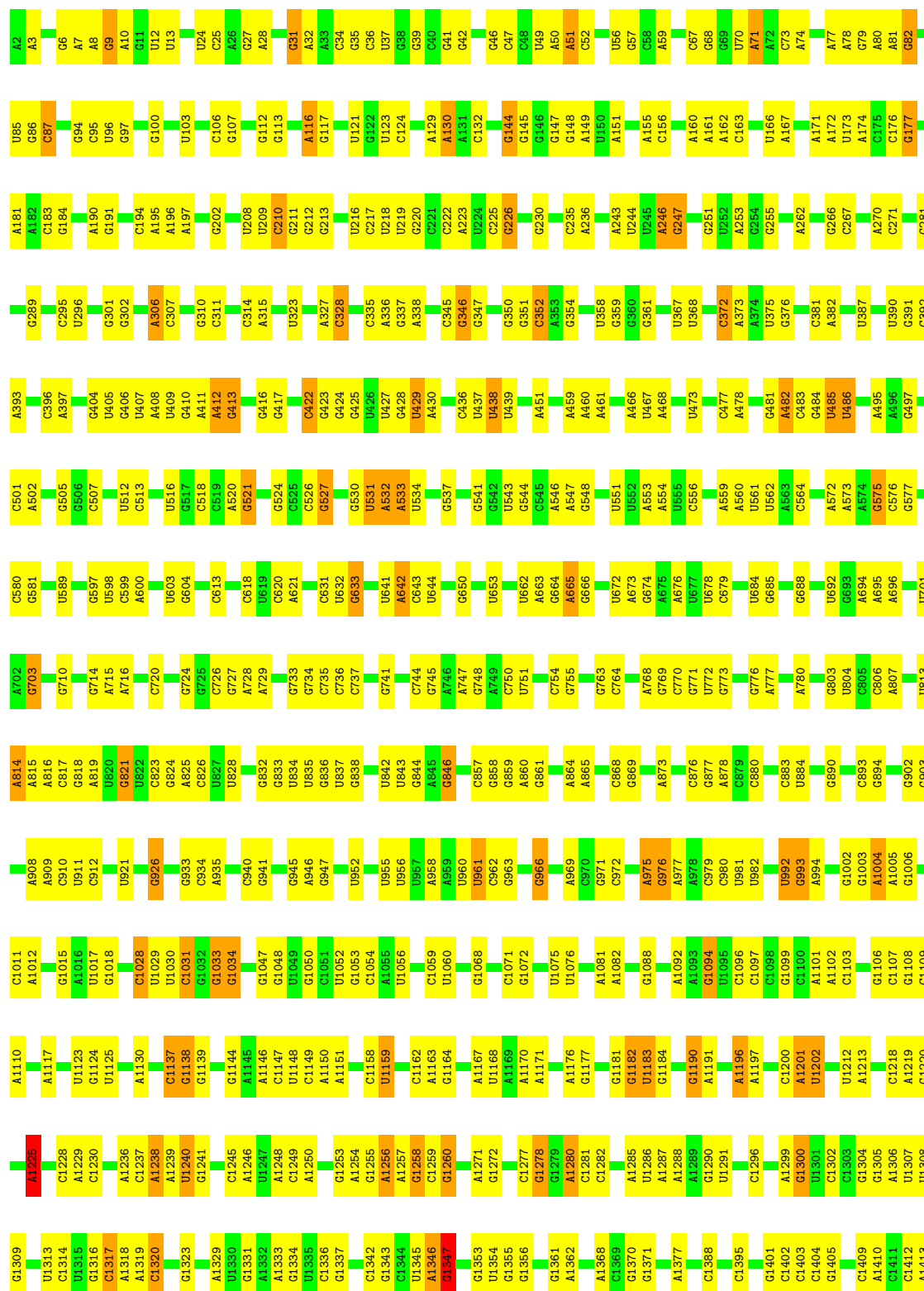
- Molecule 52: 50S ribosomal protein L1

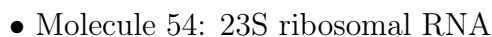
Chain 03: 39% 21% 40%



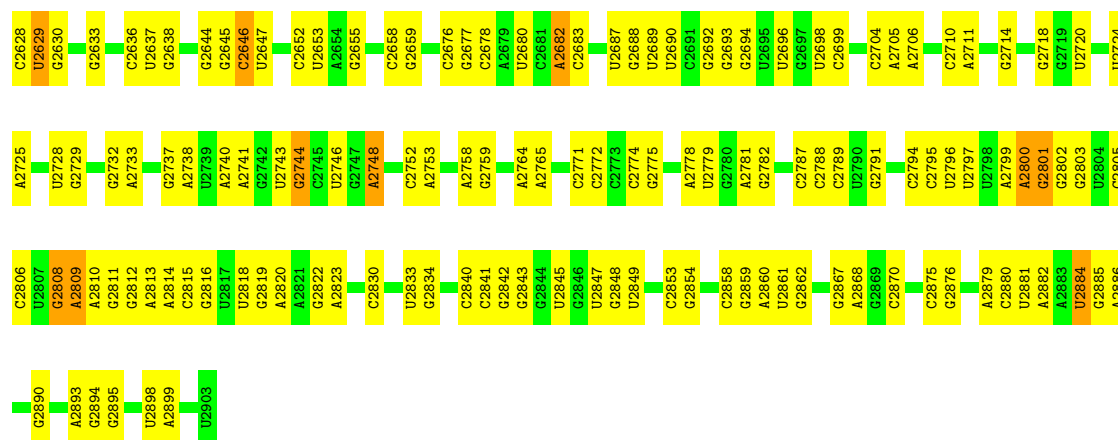
• Molecule 53: 16S ribosomal RNA

Chain A:  58% 36% 5%



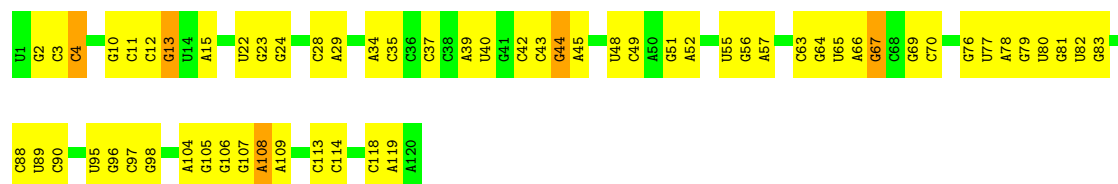


G2529	A2530	U2533	A2534	U2537	C2538	G2543	G2544	A2547	G2553	U2554	C2556	G2557	A2564	A2565	A2566	G2567	A2577	U2580	G2581	U2584	U2585	U2586	A2587	G2588	A2589	A2590	C2591	G2592	G2597	A2602	U2605	C2606	U2609	U2613	A2614	U2615	C2616	U2617	G2618	C2619	G2626	G2627									
G2444	G2445	A2448	C2452	G2455	C2456	U2457	C2466	C2467	A2468	A2469	G2470	C2475	A2476	U2477	U2478	U2479	A2480	G2481	G2484	G2485	U2492	G2493	G2494	G2495	C2496	A2497	C2498	C2499	U2500	G2501	G2502	A2503	U2504	G2505	G2508	U2511	U2514	C2515	A2516	G2517	A2518	U2519	C2520	C2521	U2522	G2526	C2527	U2528			
G2355	U2356	G2357	A2358	C2359	C2364	G2365	G2370	G2371	U2372	G2373	C2374	G2375	A2376	A2377	C2380	A2381	G2382	U2383	U2384	C2385	G2389	U2390	A2392	U2393	C2394	C2395	U2402	C2403	A2411	A2412	G2413	U2419	C2420	G2421	U2434	A2435	C2437	G2438	G2439	A2440	U2441	C2442	C2443								
G2277	A2278	C2283	G2286	U2287	A2288	G2292	G2293	U2296	A2297	A2298	U2299	U2302	A2311	G2312	G2313	U2314	G2315	G2316	A2322	G2323	U2324	G2325	C2326	A2327	A2328	U2329	G2330	C2331	C2332	U2334	A2335	C2339	A2340	G2341	U2342	U2343	U2344	G2345	A2346	C2347	U2348	G2349	C2350	G2351	C2354						
G2191	U2192	G2193	U2194	U2195	C2196	A2198	A2199	U2203	G2204	A2205	C2206	C2207	U2210	A2211	A2212	U2213	C2214	C2215	G2216	U2220	G2221	A2225	G2230	U2231	C2232	U2233	G2234	G2239	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2250	U2259	C2260	C2261	U2262	C2263	C2264	U2265	A2266	A2267	A2268	G2269	A2270	G2271		
A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	A2126	G2127	G2128	C2129	U2130	U2131	U2132	A2134	G2141	A2142	C2145	C2146	A2147	A2154	U2155	G2156	U2157	A2158	G2159	C2160	C2161	G2162	A2163	C2164	A2170	A2171	U2172	A2173	C2174	A2176	U2180	U2181	U2182	A2183	A2184	U2185	G2186	U2187	U2188	A2189	G2190
G2034	C2035	U2038	G2039	A2040	A2041	G2042	C2043	C2048	G2049	A2052	C2055	G2056	G2057	A2060	C2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	C2073	U2074	U2075	C2091	U2092	G2093	A2094	A2095	U2105	A2106	U2107	U2108	U2109	G2110	U2111	C2112	U2113								
U1898	A1899	A1900	A1901	C1902	G1906	G1907	A1913	C1924	C1925	G1929	G1930	C1931	A1938	C1941	C1942	U1955	U1956	G1957	C1958	U1963	C1967	A1970	U1971	C1972	A1981	U1982	U1991	G1992	U1993	C1997	G2002	C2006	U2011	G2012	A2013	A2014	U2017	A2020	C2021	U2022	C2023										
C1800	A1801	A1802	C1803	A1804	A1805	C1806	G1807	A1808	A1809	A1810	G1811	G1812	G1813	C1816	G1817	U1818	A1819	U1820	U1825	G1826	G1828	A1829	C1830	G1831	C1837	G1842	U1856	G1857	A1858	U1859	G1860	A1866	G1869	C1870	A1871	A1872	G1873	A1877	G1878	C1879	U1880	U1881	U1882	U1883	G1884	A1885	C1889	C1894			
A1705	C1706	U1709	G1710	A1711	G1715	U1716	A1717	G1718	U1719	U1720	G1721	U1729	G1730	G1731	C1732	U1736	G1737	G1738	A1744	A1745	A1746	C1748	A1755	U1756	A1757	U1758	A1759	C1760	A1761	A1762	G1763	C1764	U1765	G1766	U1769	A1773	G1774	U1775	G1776	G1681	G1682	U1683	G1684	A1689	G1695	G1696	G1697	C1704			
U1594	C1595	A1603	G1606	C1607	A1608	A1609	G1611	A1610	G1611	C1612	A1616	G1628	A1637	C1638	G1639	A1640	A1641	G1642	G1645	U1647	U1648	U1653	U1654	A1655	C1656	U1662	G1663	A1664	A1665	G1666	G1674	C1675	A1676	G1681	G1682	U1683	G1684	A1689	G1695	G1696	G1697	C1704									
U1484	U1485	U1486	A1490	C1493	A1494	C1498	A1504	A1505	U1506	C1507	G1524	A1525	G1527	C1533	U1534	A1535	C1536	U1537	G1538	A1539	G1540	G1555	G1560	C1561	U1562	U1563	C1564	C1565	A1569	A1570	A1571	A1572	A1579	A1580	G1581	U1582	A1583	U1584	G1587												
G1389	C1390	A1395	C1398	C1414	U1415	G1416	G1417	G1418	A1419	A1420	G1424	G1425	G1426	A1427	G1432	A1433	A1434	G1435	G1436	C1437	A1438	A1439	U1440	U1441	U1442	U1443	G1444	G1449	G1450	C1451	G1452	A1453	C1454	G1455	C1461	C1462	G1463	G1465	U1466	U1467	U1468	A1469	A1470	U1474	G1475	U1476	G1482	G1483			
A1287	G1288	C1289	C1297	C1298	G1299	A1300	G1301	G1306	G1309	C1315	U1316	G1317	U1318	C1319	G1320	A1321	U1326	A1327	A1328	U1329	C1330	G1340	U1341	U1345	G1356	C1357	G1358	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1372	A1373	C1376	G1377	A1378	U1379	G1380	A1383	C1386	A1387	G1388				
G1177	C1178	G1179	U1180	U1181	C1182	U1183	U1184	G1185	G1186	G1187	G1190	G1191	C1196	G1197	U1203	A1204	G1205	G1206	C1211	A1212	A1213	G1218	U1219	U1222	G1223	U1224	G1225	G1236	G1239	U1240	C1243	A1245	G1250	C1251	G1252	A1253	G1256	A1265	A1268	A1269	C1270	G1271	A1272	C1278	G1279						



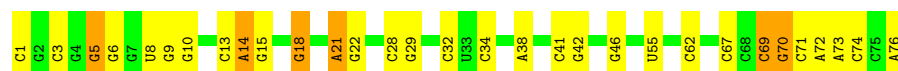
• Molecule 55: 5S ribosomal RNA

Chain 02: 49% 47%



• Molecule 56: tRNA^{fMet}

Chain X: 60% 32% 8%



• Molecule 56: tRNA^{fMet}

Chain W: 74% 21% 5%



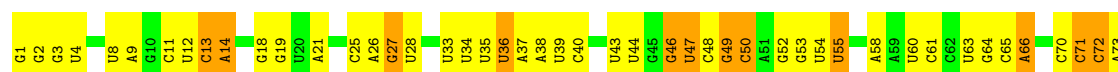
• Molecule 57: mRNA

Chain V: 76% 18% 6%



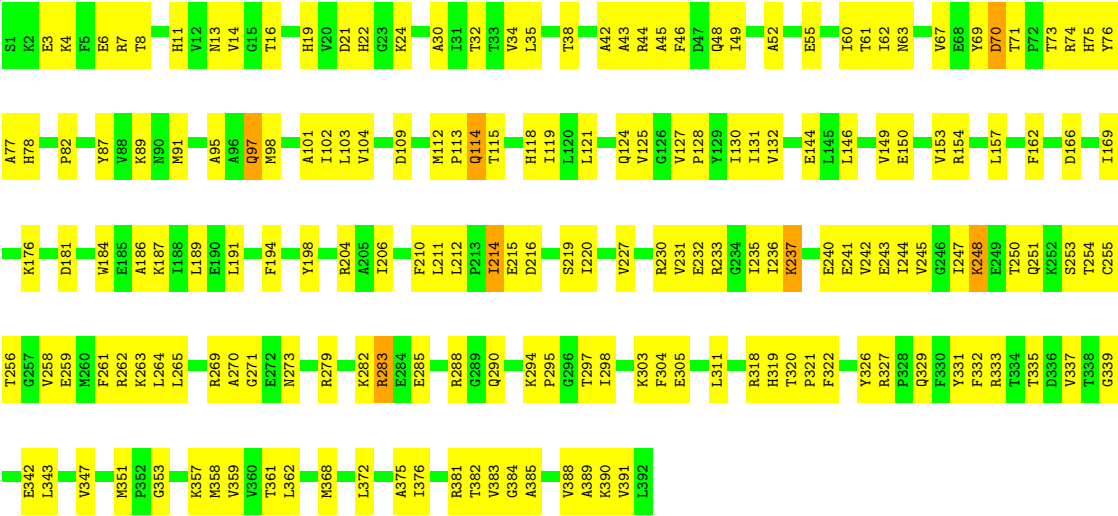
• Molecule 58: tRNA^{Lys}

Chain Y: 34% 47% 18%





● Molecule 59: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4629	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U8U, 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	0.30	0/2122	0.54	0/2852
2	05	0.31	0/1586	0.55	0/2134
3	06	0.31	0/1571	0.56	0/2113
4	07	0.35	0/1435	0.54	0/1926
5	08	0.32	0/1343	0.59	0/1816
6	09	0.36	0/1122	0.61	0/1515
7	10	0.39	0/1002	0.66	0/1350
8	11	0.37	0/1046	0.64	0/1410
9	12	0.33	0/1152	0.55	0/1551
10	13	0.31	0/948	0.55	0/1268
11	14	0.32	0/1054	0.58	0/1403
12	15	0.34	0/1093	0.54	0/1460
13	16	0.33	0/974	0.55	0/1301
14	17	0.31	0/902	0.50	0/1209
15	18	0.32	0/929	0.56	0/1242
16	19	0.34	0/960	0.48	0/1278
17	20	0.34	0/829	0.62	0/1107
18	21	0.30	0/864	0.56	0/1156
19	22	0.32	0/745	0.55	0/994
20	23	0.33	0/788	0.60	1/1051 (0.1%)
21	24	0.33	0/766	0.56	0/1025
22	25	0.33	0/582	0.52	0/769
23	26	0.32	0/635	0.51	0/848
24	27	0.31	0/510	0.56	0/677
25	28	0.31	0/453	0.51	0/605
26	29	0.34	0/532	0.57	0/709
27	30	0.30	0/450	0.52	0/599
28	31	0.37	0/417	0.58	0/554
29	32	0.32	0/380	0.48	0/498
30	33	0.31	0/513	0.54	0/676
31	34	0.29	0/303	0.52	0/397
32	B	0.35	0/1736	0.60	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	C	0.33	0/1652	0.52	0/2225
34	D	0.34	0/1665	0.57	0/2227
35	E	0.33	0/1170	0.57	0/1573
36	F	0.34	0/836	0.56	0/1128
37	G	0.32	0/1196	0.57	0/1602
38	H	0.32	0/989	0.59	0/1326
39	I	0.34	0/1034	0.60	0/1375
40	J	0.32	0/797	0.60	0/1077
41	K	0.33	0/886	0.53	0/1195
42	L	0.32	0/969	0.64	0/1300
43	M	0.31	0/893	0.54	0/1193
44	N	0.33	0/817	0.53	0/1088
45	O	0.31	0/722	0.52	0/964
46	P	0.33	0/659	0.57	0/884
47	Q	0.34	0/658	0.57	0/881
48	R	0.37	0/545	0.59	0/731
49	S	0.35	0/653	0.56	0/877
50	T	0.31	0/671	0.50	0/888
51	U	0.38	0/551	0.62	0/728
52	03	0.35	0/1034	0.62	0/1387
53	A	0.38	0/36963	0.68	5/57662 (0.0%)
54	01	0.38	0/69796	0.68	6/108888 (0.0%)
55	02	0.40	0/2872	0.67	0/4479
56	W	0.42	0/1832	0.67	0/2855
56	X	0.46	0/1832	0.69	0/2855
57	V	0.43	0/421	0.70	0/657
58	Y	0.53	1/1780 (0.1%)	0.70	0/2767
59	Z	0.36	0/3085	0.60	0/4173
All	All	0.37	1/166720 (0.0%)	0.65	12/248816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	1	G	OP3-P	-7.14	1.52	1.61

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	01	1178	C	N1-C1'-C2'	6.88	122.94	114.00
54	01	1130	U	C2'-C3'-O3'	5.71	122.83	113.70
54	01	1818	U	N1-C1'-C2'	5.64	121.33	114.00
53	A	438	U	C2'-C3'-O3'	5.54	122.56	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	23	96	LYS	N-CA-C	-5.41	96.39	111.00

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	83	0
2	05	1565	0	1616	71	0
3	06	1552	0	1619	70	0
4	07	1411	0	1447	81	0
5	08	1323	0	1374	46	0
6	09	1111	0	1148	53	0
7	10	989	0	1025	51	0
8	11	1032	0	1088	71	0
9	12	1129	0	1162	45	0
10	13	939	0	1012	32	0
11	14	1045	0	1117	40	0
12	15	1074	0	1157	50	0
13	16	961	0	1000	39	0
14	17	892	0	923	31	0
15	18	917	0	965	42	0
16	19	947	0	1022	47	0
17	20	816	0	839	44	0
18	21	857	0	922	32	0
19	22	739	0	807	22	0
20	23	780	0	834	29	0
21	24	753	0	780	31	0
22	25	575	0	592	14	0
23	26	625	0	655	25	0
24	27	509	0	543	21	0
25	28	449	0	491	9	0
26	29	523	0	524	15	0
27	30	444	0	461	23	0
28	31	410	0	440	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	32	377	0	418	20	0
30	33	504	0	574	27	0
31	34	302	0	343	25	0
32	B	1705	0	1732	82	0
33	C	1625	0	1699	59	0
34	D	1643	0	1710	74	0
35	E	1157	0	1199	70	0
36	F	818	0	808	41	0
37	G	1182	0	1240	40	0
38	H	979	0	1034	52	0
39	I	1022	0	1070	57	0
40	J	787	0	828	37	0
41	K	870	0	878	43	0
42	L	955	0	1019	60	0
43	M	884	0	944	51	0
44	N	805	0	847	40	0
45	O	714	0	737	25	0
46	P	649	0	666	51	0
47	Q	649	0	691	34	0
48	R	536	0	552	36	0
49	S	638	0	665	37	0
50	T	665	0	714	34	0
51	U	545	0	579	32	0
52	03	1027	0	1092	41	0
53	A	33012	0	16618	461	0
54	01	62317	0	31346	876	0
55	02	2568	0	1303	55	0
56	W	1640	0	837	11	0
56	X	1640	0	837	19	0
57	V	373	0	187	2	0
58	Y	1618	0	821	37	0
59	Z	3029	0	3043	152	0
60	Z	32	0	14	1	0
All	All	153717	0	104765	3363	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 13.

The worst 5 of 3363 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)
54:01:45:G:H5''	54:01:46:G:H5'	1.37	1.06
12:15:45:GLN:HE21	54:01:2485:G:H5''	1.26	1.00
3:06:76:PRO:HA	3:06:82:GLY:HA2	1.45	0.94
54:01:1045:C:H5'	54:01:1046:A:H5'	1.49	0.93
6:09:12:LEU:HD22	6:09:19:VAL:HG11	1.51	0.93

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%)	229 (85%)	37 (14%)	3 (1%)	14	51
2	05	207/209 (99%)	173 (84%)	30 (14%)	4 (2%)	8	40
3	06	199/201 (99%)	177 (89%)	19 (10%)	3 (2%)	10	45
4	07	175/177 (99%)	147 (84%)	26 (15%)	2 (1%)	14	51
5	08	174/176 (99%)	152 (87%)	18 (10%)	4 (2%)	6	37
6	09	147/149 (99%)	117 (80%)	22 (15%)	8 (5%)	2	21
7	10	129/131 (98%)	93 (72%)	26 (20%)	10 (8%)	1	14
8	11	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	1	18
9	12	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	46
10	13	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	3	25
11	14	141/143 (99%)	112 (79%)	23 (16%)	6 (4%)	2	25
12	15	134/136 (98%)	120 (90%)	10 (8%)	4 (3%)	4	32
13	16	118/120 (98%)	100 (85%)	16 (14%)	2 (2%)	9	43
14	17	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	8	41
15	18	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5	34
16	19	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	17	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	20	101/103 (98%)	78 (77%)	21 (21%)	2 (2%)	7	40
18	21	108/110 (98%)	92 (85%)	15 (14%)	1 (1%)	17	55
19	22	91/93 (98%)	72 (79%)	17 (19%)	2 (2%)	6	37
20	23	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	26
21	24	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	14	51
22	25	73/75 (97%)	61 (84%)	12 (16%)	0	100	100
23	26	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
24	27	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	44
25	28	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
26	29	64/66 (97%)	44 (69%)	20 (31%)	0	100	100
27	30	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
28	31	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	39
29	32	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
30	33	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	4	31
31	34	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	20
32	B	216/218 (99%)	174 (81%)	35 (16%)	7 (3%)	4	31
33	C	204/206 (99%)	186 (91%)	15 (7%)	3 (2%)	10	45
34	D	203/205 (99%)	167 (82%)	28 (14%)	8 (4%)	3	26
35	E	155/157 (99%)	123 (79%)	21 (14%)	11 (7%)	1	16
36	F	98/100 (98%)	79 (81%)	11 (11%)	8 (8%)	1	13
37	G	149/151 (99%)	124 (83%)	20 (13%)	5 (3%)	3	30
38	H	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	36
39	I	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	3	26
40	J	96/98 (98%)	67 (70%)	22 (23%)	7 (7%)	1	15
41	K	114/116 (98%)	89 (78%)	20 (18%)	5 (4%)	2	24
42	L	121/123 (98%)	85 (70%)	28 (23%)	8 (7%)	1	17
43	M	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	3	28
44	N	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	7	40
45	O	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	29
46	P	80/82 (98%)	62 (78%)	14 (18%)	4 (5%)	2	22
47	Q	78/80 (98%)	63 (81%)	13 (17%)	2 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R	63/65 (97%)	52 (82%)	8 (13%)	3 (5%)	2	23
49	S	77/79 (98%)	64 (83%)	11 (14%)	2 (3%)	5	34
50	T	83/85 (98%)	75 (90%)	6 (7%)	2 (2%)	6	36
51	U	63/65 (97%)	38 (60%)	21 (33%)	4 (6%)	1	18
52	03	130/223 (58%)	105 (81%)	23 (18%)	2 (2%)	10	45
59	Z	390/392 (100%)	337 (86%)	49 (13%)	4 (1%)	15	53
All	All	6366/6563 (97%)	5298 (83%)	882 (14%)	186 (3%)	7	32

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	06	83	VAL
3	06	184	ASP
5	08	46	ASP
5	08	174	LYS
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	65
2	05	164/164 (100%)	161 (98%)	3 (2%)	59	77
3	06	165/165 (100%)	163 (99%)	2 (1%)	71	84
4	07	148/148 (100%)	146 (99%)	2 (1%)	67	81
5	08	137/137 (100%)	135 (98%)	2 (2%)	65	80
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	100 (100%)	0	100	100
8	11	109/109 (100%)	107 (98%)	2 (2%)	59	77
9	12	116/116 (100%)	116 (100%)	0	100	100
10	13	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	14	102/102 (100%)	100 (98%)	2 (2%)	55	73
12	15	109/109 (100%)	108 (99%)	1 (1%)	78	88
13	16	100/100 (100%)	98 (98%)	2 (2%)	55	73
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	97 (98%)	2 (2%)	55	73
16	19	89/89 (100%)	89 (100%)	0	100	100
17	20	84/84 (100%)	82 (98%)	2 (2%)	49	69
18	21	93/93 (100%)	90 (97%)	3 (3%)	39	62
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	68
20	23	83/83 (100%)	82 (99%)	1 (1%)	71	84
21	24	78/78 (100%)	78 (100%)	0	100	100
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	67 (100%)	0	100	100
24	27	55/55 (100%)	55 (100%)	0	100	100
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%)	46 (98%)	1 (2%)	53	72
28	31	45/45 (100%)	44 (98%)	1 (2%)	52	71
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%)	177 (98%)	3 (2%)	60	78
33	C	170/170 (100%)	168 (99%)	2 (1%)	71	84
34	D	172/172 (100%)	165 (96%)	7 (4%)	30	57
35	E	119/119 (100%)	116 (98%)	3 (2%)	47	68
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	122 (98%)	2 (2%)	62	79
38	H	104/104 (100%)	103 (99%)	1 (1%)	76	86
39	I	105/105 (100%)	103 (98%)	2 (2%)	57	75
40	J	86/86 (100%)	85 (99%)	1 (1%)	71	84
41	K	89/89 (100%)	86 (97%)	3 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	L	103/103 (100%)	102 (99%)	1 (1%)	76	86
43	M	92/92 (100%)	89 (97%)	3 (3%)	38	62
44	N	83/83 (100%)	82 (99%)	1 (1%)	71	84
45	O	76/76 (100%)	74 (97%)	2 (3%)	46	67
46	P	65/65 (100%)	64 (98%)	1 (2%)	65	80
47	Q	74/74 (100%)	72 (97%)	2 (3%)	44	66
48	R	56/56 (100%)	55 (98%)	1 (2%)	59	77
49	S	70/70 (100%)	67 (96%)	3 (4%)	29	56
50	T	65/65 (100%)	62 (95%)	3 (5%)	27	54
51	U	55/55 (100%)	53 (96%)	2 (4%)	35	61
52	03	110/174 (63%)	109 (99%)	1 (1%)	78	88
59	Z	324/325 (100%)	313 (97%)	11 (3%)	37	61
All	All	5285/5350 (99%)	5196 (98%)	89 (2%)	62	78

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	K	124	LYS
49	S	42	ASN
43	M	7	ASN
46	P	45	GLU
51	U	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
25	28	8	GLN
50	T	69	ASN
34	D	53	GLN
50	T	51	ASN
59	Z	124	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	150 (9%)	7 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	01	2902/2903 (99%)	348 (11%)	12 (0%)
55	02	119/120 (99%)	11 (9%)	1 (0%)
56	W	76/77 (98%)	8 (10%)	0
56	X	76/77 (98%)	14 (18%)	0
57	V	16/17 (94%)	2 (12%)	0
58	Y	74/76 (97%)	22 (29%)	0
All	All	4801/4809 (99%)	555 (11%)	20 (0%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G
53	A	31	G
53	A	32	A
53	A	39	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	1378	A
54	01	2391	G
55	02	88	C
54	01	2808	G
53	A	1347	G

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
58	U8U	Y	34	58	19,24,25	1.33	2 (10%)	23,34,37	1.04	3 (13%)

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
58	U8U	Y	34	58	-	2/9/28/29	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	34	U8U	C6-N1	3.80	1.44	1.38
58	Y	34	U8U	C4-C5	3.02	1.51	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Y	34	U8U	C2'-C1'-N1	2.52	120.36	113.22
58	Y	34	U8U	O4-C4-C5	-2.29	121.56	124.96
58	Y	34	U8U	C5-C6-N1	2.04	125.64	122.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Y	34	U8U	N-C-C5-C4
58	Y	34	U8U	N-C-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	GCP	Z	401	-	27,34,34	1.89	7 (25%)	34,54,54	3.96	18 (52%)

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
60	GCP	Z	401	-	-	9/15/38/38	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)
60	Z	401	GCP	PB-O3A	-4.11	1.53	1.58
60	Z	401	GCP	C5-C6	3.93	1.48	1.41
60	Z	401	GCP	O4'-C1'	3.79	1.46	1.41
60	Z	401	GCP	C6-N1	3.48	1.39	1.33
60	Z	401	GCP	C2'-C1'	2.58	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z	401	GCP	C1'-N9-C4	13.76	150.81	126.64
60	Z	401	GCP	C5-C6-N1	-8.56	111.72	123.43
60	Z	401	GCP	O1G-PG-C3B	-7.40	95.29	111.24
60	Z	401	GCP	C2-N1-C6	6.56	126.35	115.93
60	Z	401	GCP	O4'-C1'-C2'	-5.67	98.65	106.93

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	Z	401	GCP	PB-C3B-PG-O1G
60	Z	401	GCP	PB-C3B-PG-O2G
60	Z	401	GCP	PG-C3B-PB-O1B
60	Z	401	GCP	C5'-O5'-PA-O3A

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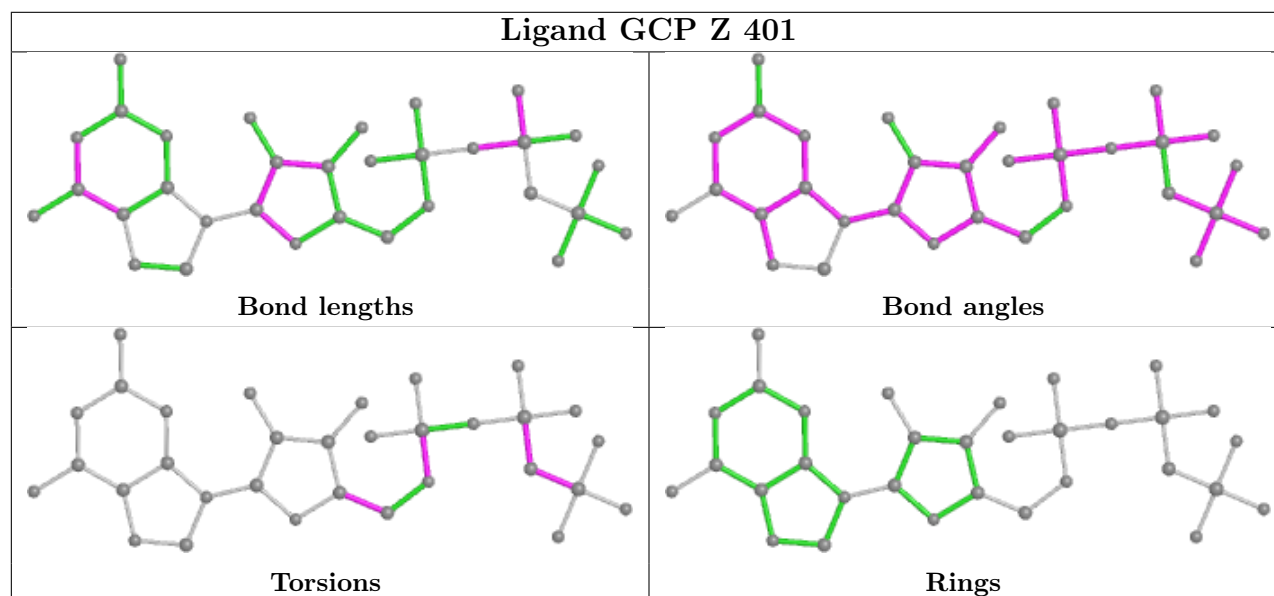
Mol	Chain	Res	Type	Atoms
60	Z	401	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	Z	401	GCP	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8618. 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.