



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:30 PM BST

PDB ID : 3J81
EMDB ID: : EMD-2763
Title : CryoEM structure of a partial yeast 48S preinitiation complex
Authors : Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.
Deposited on : 2014-08-29
Resolution : 4.00 Å(reported)
Based on PDB ID : 3V11, 3U5C, 3U5B

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

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

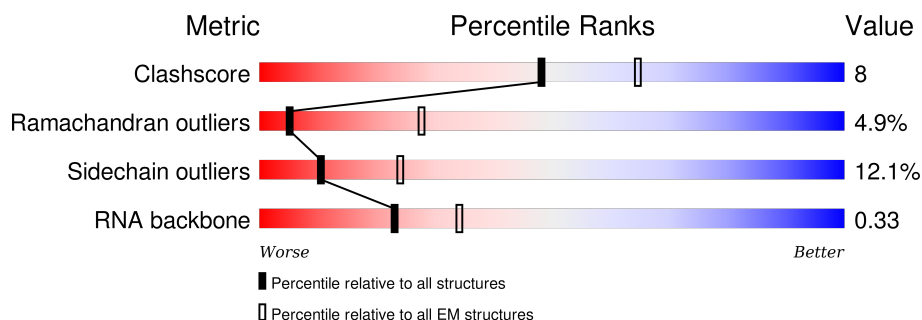
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.













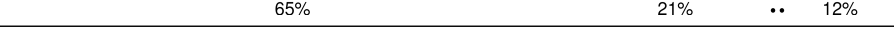
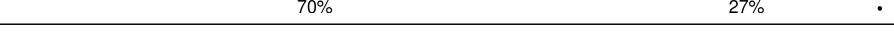
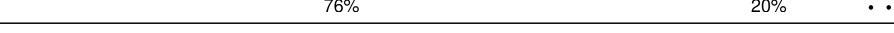


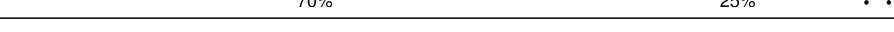









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	2	1799	34% 51% 14% .
2	A	254	54% 23% . 19%
3	B	255	61% 20% . 16%
4	C	259	58% 23% . 16%
5	D	237	62% 30% . 6%
6	E	261	71% 26% .
7	F	227	55% 31% 5% 9%
8	G	236	72% 19% . .









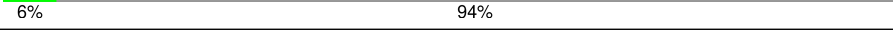
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Mol	Chain	Length	Quality of chain
9	H	190	
10	I	201	
11	J	188	
12	K	106	
13	L	156	
14	M	134	
15	N	151	
16	O	137	
17	P	140	
18	Q	143	
19	R	136	
20	S	146	
21	T	144	
22	U	117	
23	V	87	
24	W	130	
25	X	145	
26	Y	135	
27	Z	108	
28	a	119	
29	b	82	
30	c	67	
31	f	150	
32	g	326	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	h	25	
36	1	75	
37	3	25	
38	i	153	
39	j	300	
40	m	108	
41	k	527	
42	l	285	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 83760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	207	Total	C	N	O	S	0	0
			1625	1040	286	297	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1727	1092	314	318	3		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 9 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	119	Total	C	N	O	S	0	0
			943	604	171	163	5		

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	106	Total	C	N	O	S	0
			845	540	152	152	1	0

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	87	Total	C	N	O	S	0
			687	424	126	135	2	0

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	129	Total	C	N	O	S	0
			1021	651	187	180	3	0

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	144	Total	C	N	O	S	0
			1119	708	218	191	2	0

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	70	Total	C	N	O	S	0
			558	355	104	98	1	0

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 31 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 32 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S	0	0
			433	271	88	73	1		

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	74	Total	C	N	O	P	0	0
			1584	706	291	513	74		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	22	Total	C	N	O	P	0	0
			447	201	62	162	22		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	252	Total	C	N	O	S	0	0
			2025	1294	336	386	9		

- Molecule 40 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 41 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	365	Total	C	N	O	0	0
			1798	1068	365	365		

- Molecule 42 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	17	Total	C	N	O	0	0
			84	50	17	17		

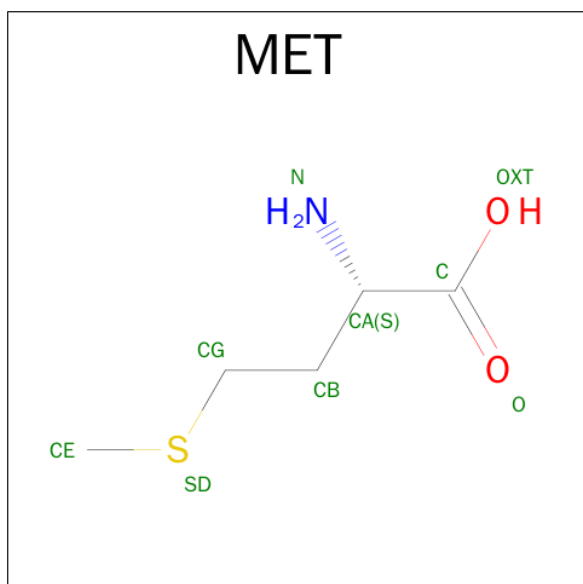
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	G	1	Total	Mg	0
			1	1	
43	2	80	Total	Mg	0
			80	80	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	b	1	Total	Zn	0
			1	1	
44	a	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	

- Molecule 45 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).

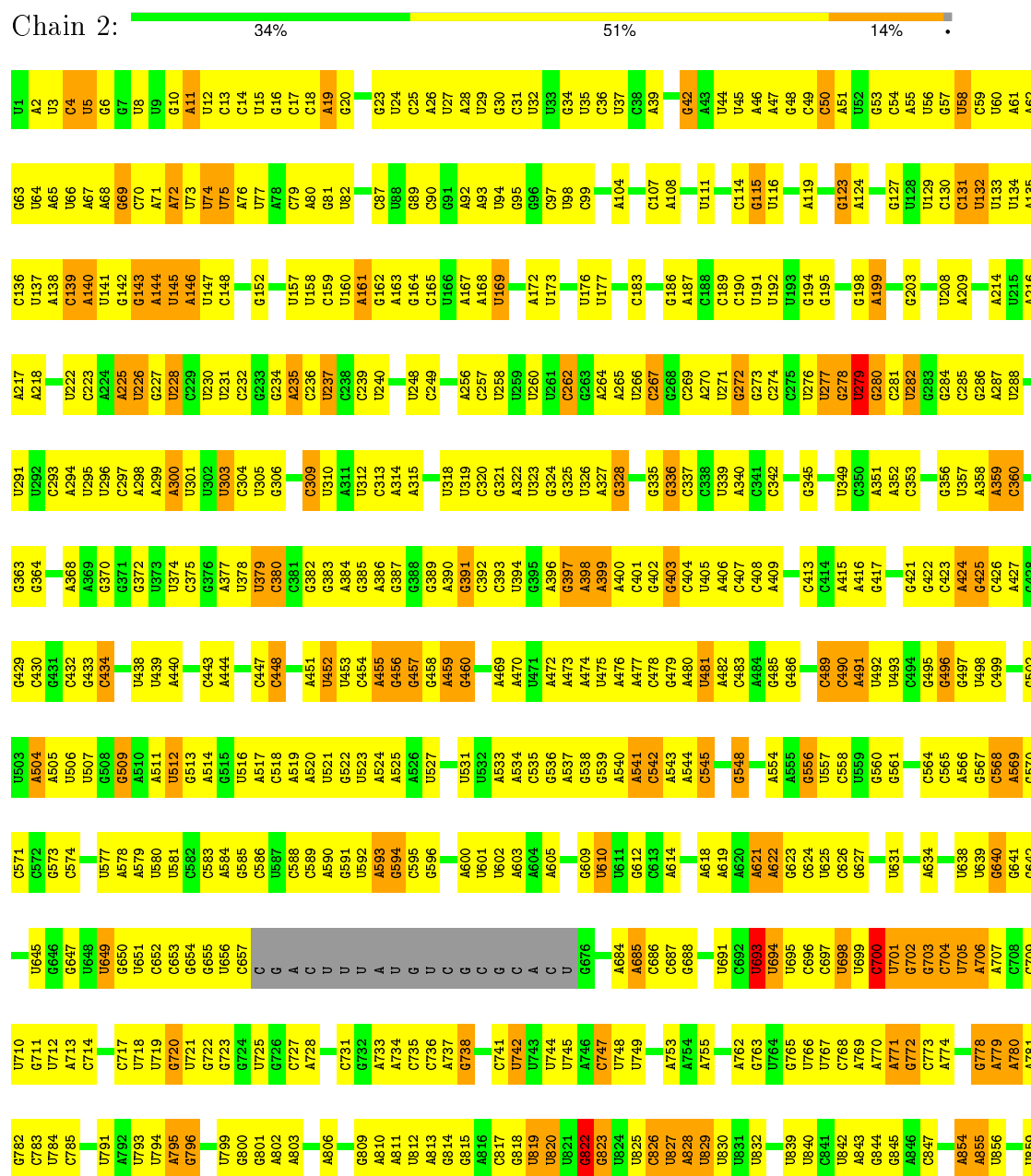


Mol	Chain	Residues	Atoms					AltConf
45	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

3 Residue-property plots

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

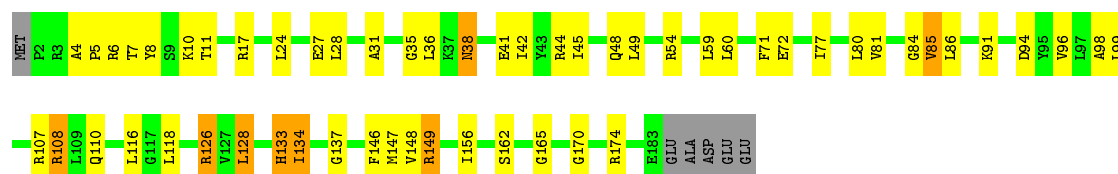
• Molecule 1: 18S rRNA



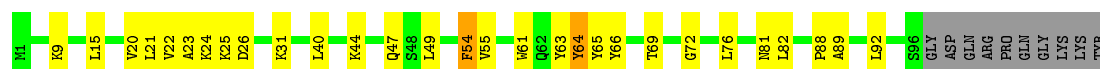
- Molecule 2: uS2

Response	Percentage
Yes	54%
No	23%
Don't know	1%
No answer	19%

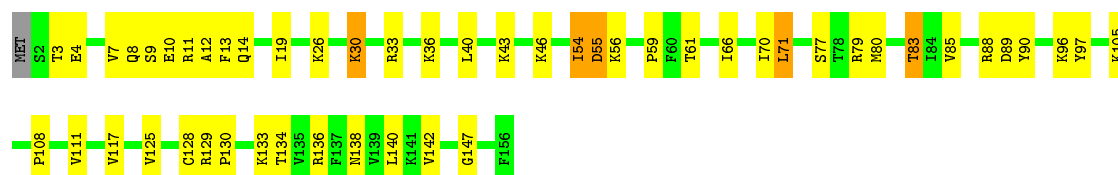


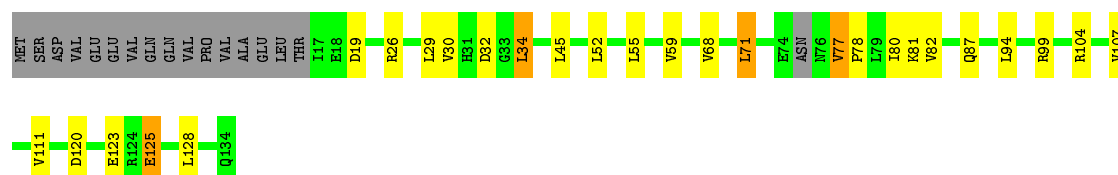
- Molecule 12: eS10



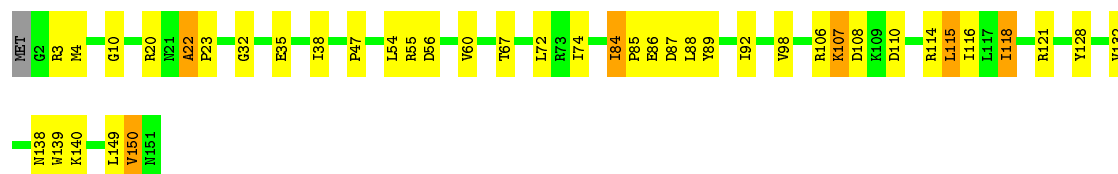
- Molecule 13: uS17



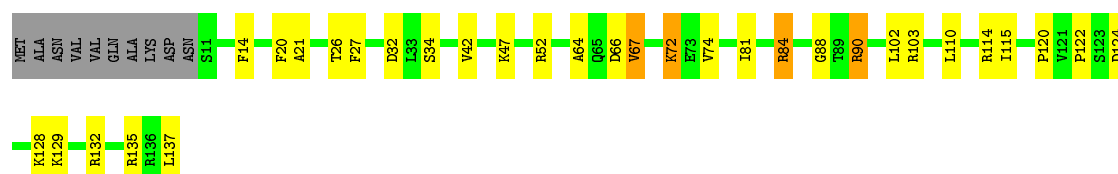
- Molecule 14: eS12



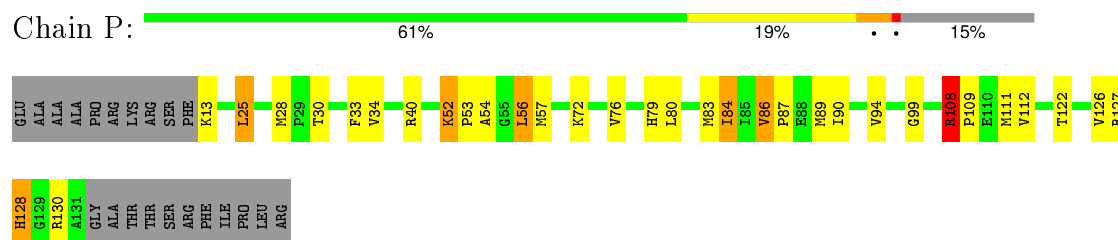
- Molecule 15: uS15



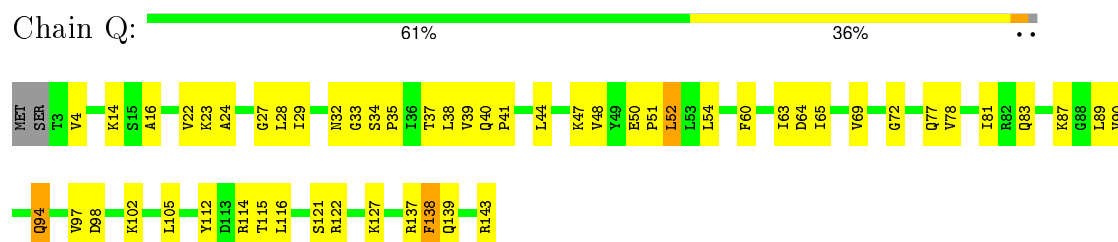
- Molecule 16: uS11



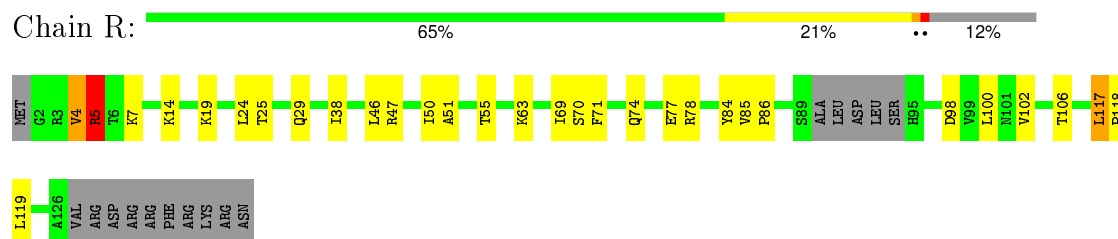
- Molecule 17: uS19



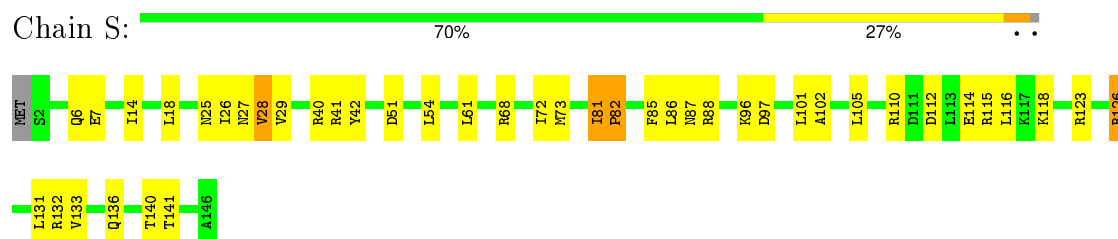
- Molecule 18: uS9



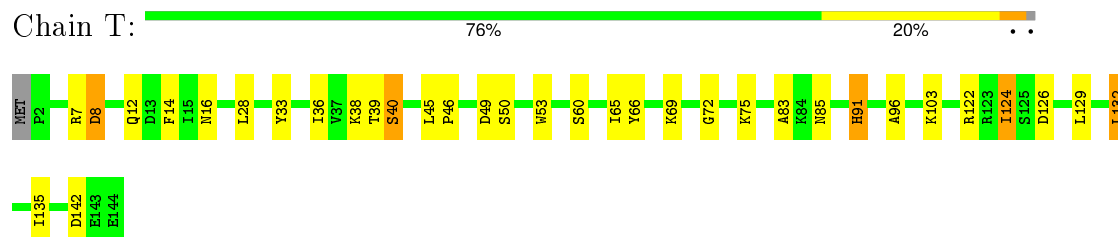
- Molecule 19: eS17



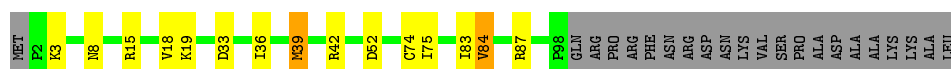
- Molecule 20: uS13



- Molecule 21: eS19

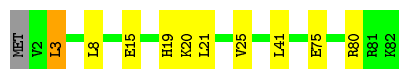


- Molecule 22: uS10



- Molecule 29: eS27

Chain b: 87% 11% ..



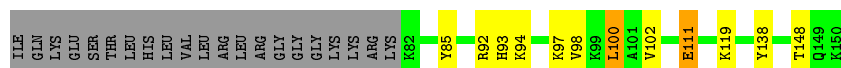
- Molecule 30: eS28

Chain c: 82% 10% 7%



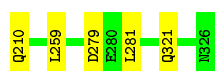
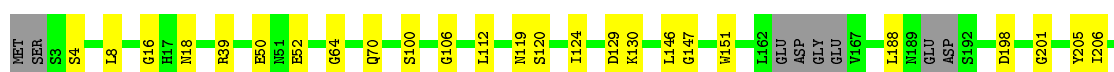
- Molecule 31: eS31

Chain f: 38% 7% 54%



- Molecule 32: RACK1

Chain g: 88% 9%



- Molecule 33: uS14

Chain d: 79% 16% 5%




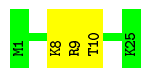
- Molecule 34: eS30

Chain e: 65% 21% 14%



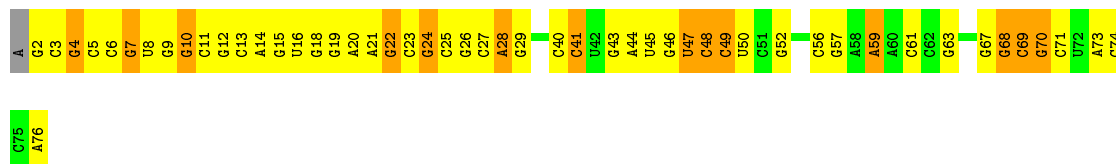
- Molecule 35: eL41

Chain h:  88% 12%

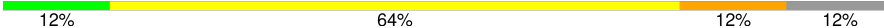


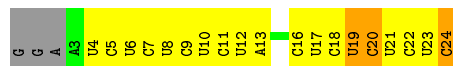
- Molecule 36: Met-tRNA_i

Chain 1:  31% 49% 19%



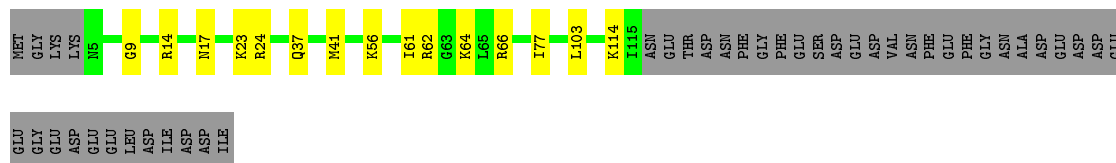
- Molecule 37: mRNA

Chain 3:  12% 64% 12% 12%



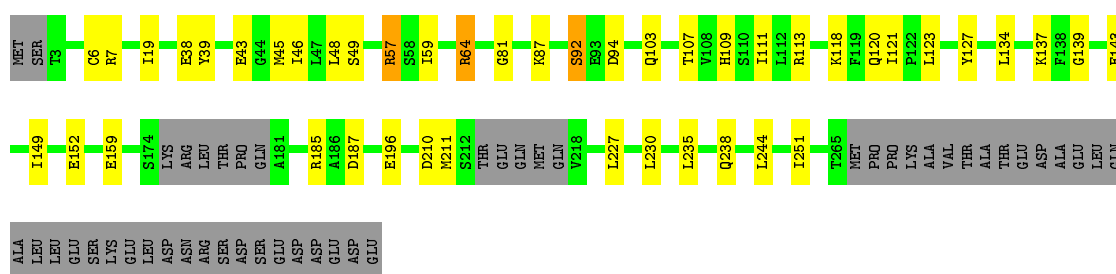
- Molecule 38: eIF1A

Chain i:  63% 10% 27%




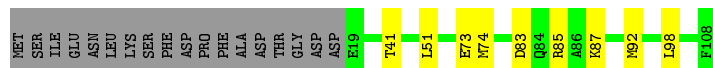
- Molecule 39: eIF2 alpha

Chain j:  69% 14% 16%



- Molecule 40: eIF1

Chain m:  75% 8% 17%



- Molecule 41: eIF2 gamma



MET	GLU	SER	GLU	GLU	GLU	GLU	GLU	GLU	PRO	SER	ILE	ILE	ASN	GLY	ASN	GLU	LEU	PRO	VAL	GLY	ASN	GLU	PRO	THR	GLU	VAL	ALA	GLN	GLU	THR	GLN	ASP	GLN	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
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• Molecule 42: eIF2 beta



PHE	PHE	LEU	SER	SER	ASP	MET	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP</
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	29698	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	2	0.25	0/42269	0.67	6/65862 (0.0%)
10	I	0.40	0/1519	0.66	1/2033 (0.0%)
11	J	0.41	0/1495	0.73	0/2001
12	K	0.47	0/831	0.72	0/1123
13	L	0.40	0/1276	0.64	0/1718
14	M	0.41	0/891	0.69	0/1201
15	N	0.42	0/1210	0.75	1/1628 (0.1%)
16	O	0.38	0/953	0.67	0/1279
17	P	0.41	0/962	0.69	1/1294 (0.1%)
18	Q	0.42	0/1125	0.70	1/1510 (0.1%)
19	R	0.41	0/969	0.70	0/1299
2	A	0.42	0/1665	0.73	1/2276 (0.0%)
20	S	0.40	0/1212	0.73	0/1629
21	T	0.39	0/1129	0.68	0/1520
22	U	0.39	0/857	0.66	0/1158
23	V	0.39	0/696	0.69	0/938
24	W	0.39	0/1039	0.69	0/1399
25	X	0.41	0/1137	0.71	0/1516
26	Y	0.38	0/1075	0.64	0/1433
27	Z	0.41	0/567	0.65	0/762
28	a	0.38	0/782	0.71	0/1047
29	b	0.38	0/619	0.66	0/837
3	B	0.40	0/1752	0.67	1/2360 (0.0%)
30	c	0.36	0/489	0.67	0/655
31	f	0.43	0/559	0.70	1/747 (0.1%)
32	g	0.40	0/2521	0.61	0/3431
33	d	0.44	0/457	0.65	0/607
34	e	0.42	0/440	0.69	0/586
35	h	0.35	0/234	0.79	0/300
36	1	0.25	0/1771	0.65	0/2760
37	3	0.28	0/493	0.71	0/761
38	i	0.38	0/894	0.67	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	j	0.41	0/2053	0.66	0/2762
4	C	0.39	0/1659	0.68	1/2252 (0.0%)
40	m	0.39	0/724	0.65	0/968
41	k	0.47	1/1791 (0.1%)	0.74	1/2480 (0.0%)
42	l	0.42	0/83	0.69	0/114
5	D	0.41	0/1769	0.69	0/2378
6	E	0.39	0/2122	0.66	2/2861 (0.1%)
7	F	0.41	0/1628	0.75	1/2198 (0.0%)
8	G	0.39	0/1835	0.66	2/2451 (0.1%)
9	H	0.40	0/1507	0.69	0/2028
All	All	0.34	1/89059 (0.0%)	0.67	20/129350 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	I	0	1
15	N	0	1
25	X	0	1
41	k	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	k	497	GLU	N-CA	5.42	1.57	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	k	497	GLU	N-CA-C	8.38	133.61	111.00
1	2	685	A	C2'-C3'-O3'	7.22	125.38	109.50
17	P	56	LEU	CA-CB-CG	5.95	128.98	115.30
1	2	1198	G	C2'-C3'-O3'	5.93	123.19	113.70
4	C	192	LEU	CA-CB-CG	5.91	128.90	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	I	183	TYR	Peptide
15	N	22	ALA	Peptide
25	X	63	GLN	Peptide
41	k	179	CYS	Peptide
41	k	495	ILE	Mainchain

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	2	37797	0	19016	520	0
2	A	1625	0	1642	25	0
3	B	1727	0	1797	24	0
4	C	1629	0	1710	32	0
5	D	1744	0	1826	37	0
6	E	2078	0	2157	28	0
7	F	1609	0	1679	34	0
8	G	1812	0	1911	26	0
9	H	1483	0	1579	16	0
10	I	1493	0	1515	17	0
11	J	1471	0	1554	23	0
12	K	809	0	810	9	0
13	L	1248	0	1311	22	0
14	M	885	0	917	12	0
15	N	1187	0	1251	12	0
16	O	942	0	979	13	0
17	P	943	0	989	11	0
18	Q	1105	0	1170	19	0
19	R	959	0	1006	13	0
20	S	1193	0	1217	17	0
21	T	1110	0	1124	16	0
22	U	845	0	913	14	0
23	V	687	0	682	14	0
24	W	1021	0	1056	18	0
25	X	1119	0	1198	19	0
26	Y	1061	0	1111	9	0
27	Z	558	0	585	5	0
28	a	770	0	821	0	0
29	b	609	0	631	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	487	0	528	0	0
31	f	546	0	559	0	0
32	g	2466	0	2406	0	0
33	d	446	0	436	0	0
34	e	433	0	470	0	0
35	h	233	0	284	0	0
36	1	1584	0	802	48	0
37	3	447	0	233	2	0
38	i	884	0	891	0	0
39	j	2025	0	2084	0	0
40	m	716	0	742	0	0
41	k	1798	0	822	0	0
42	l	84	0	33	0	0
43	2	80	0	0	0	0
43	G	1	0	0	0	0
44	a	1	0	0	0	0
44	b	1	0	0	0	0
44	f	1	0	0	0	0
45	k	8	0	8	0	0
All	All	83760	0	64455	956	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 8.

The worst 5 of 956 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)
36:1:7:G:H2'	36:1:49:C:OP2	1.59	1.02
1:2:1292:U:C4	1:2:1321:A:N1	2.33	0.97
1:2:71:A:H3'	1:2:72:A:H5''	1.45	0.95
1:2:1292:U:O4	1:2:1321:A:N1	2.02	0.92
1:2:1396:U:H3'	1:2:1397:C:H5'	1.52	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	205/254 (81%)	168 (82%)	26 (13%)	11 (5%)	2	30
3	B	213/255 (84%)	176 (83%)	23 (11%)	14 (7%)	1	25
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	3	33
5	D	221/237 (93%)	202 (91%)	13 (6%)	6 (3%)	6	47
6	E	258/261 (99%)	223 (86%)	25 (10%)	10 (4%)	4	38
7	F	204/227 (90%)	169 (83%)	24 (12%)	11 (5%)	2	30
8	G	224/236 (95%)	194 (87%)	24 (11%)	6 (3%)	6	47
9	H	182/190 (96%)	145 (80%)	23 (13%)	14 (8%)	1	20
10	I	184/201 (92%)	159 (86%)	21 (11%)	4 (2%)	8	52
11	J	180/188 (96%)	150 (83%)	21 (12%)	9 (5%)	3	32
12	K	94/106 (89%)	74 (79%)	12 (13%)	8 (8%)	1	17
13	L	153/156 (98%)	128 (84%)	16 (10%)	9 (6%)	2	28
14	M	113/134 (84%)	86 (76%)	21 (19%)	6 (5%)	2	31
15	N	148/151 (98%)	127 (86%)	11 (7%)	10 (7%)	1	24
16	O	125/137 (91%)	96 (77%)	24 (19%)	5 (4%)	4	37
17	P	117/140 (84%)	95 (81%)	15 (13%)	7 (6%)	2	27
18	Q	139/143 (97%)	115 (83%)	13 (9%)	11 (8%)	1	19
19	R	116/136 (85%)	101 (87%)	11 (10%)	4 (3%)	5	43
20	S	143/146 (98%)	119 (83%)	16 (11%)	8 (6%)	2	29
21	T	141/144 (98%)	129 (92%)	9 (6%)	3 (2%)	9	53
22	U	104/117 (89%)	88 (85%)	8 (8%)	8 (8%)	1	20
23	V	85/87 (98%)	69 (81%)	9 (11%)	7 (8%)	1	18
24	W	127/130 (98%)	107 (84%)	14 (11%)	6 (5%)	3	33
25	X	142/145 (98%)	111 (78%)	22 (16%)	9 (6%)	2	27
26	Y	132/135 (98%)	115 (87%)	13 (10%)	4 (3%)	5	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	68/108 (63%)	58 (85%)	9 (13%)	1 (2%)	13	58
28	a	95/119 (80%)	71 (75%)	17 (18%)	7 (7%)	1	21
29	b	79/82 (96%)	65 (82%)	11 (14%)	3 (4%)	4	39
30	c	60/67 (90%)	55 (92%)	4 (7%)	1 (2%)	11	56
31	f	67/150 (45%)	47 (70%)	14 (21%)	6 (9%)	1	17
32	g	312/326 (96%)	270 (86%)	32 (10%)	10 (3%)	5	44
33	d	51/56 (91%)	39 (76%)	10 (20%)	2 (4%)	4	38
34	e	52/63 (82%)	40 (77%)	8 (15%)	4 (8%)	1	20
35	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	90 (83%)	16 (15%)	3 (3%)	6	47
39	j	246/300 (82%)	213 (87%)	21 (8%)	12 (5%)	3	32
40	m	88/108 (82%)	80 (91%)	6 (7%)	2 (2%)	8	51
41	k	351/527 (67%)	270 (77%)	56 (16%)	25 (7%)	1	23
42	l	15/285 (5%)	11 (73%)	4 (27%)	0	100	100
All	All	5581/6684 (84%)	4660 (84%)	645 (12%)	276 (5%)	5	32

5 of 276 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	29	VAL
4	C	96	ARG
4	C	141	VAL
4	C	235	TRP
5	D	4	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	175/211 (83%)	145 (83%)	30 (17%)	2	19
3	B	196/228 (86%)	181 (92%)	15 (8%)	16	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	176/203 (87%)	154 (88%)	22 (12%)	6	32
5	D	185/196 (94%)	156 (84%)	29 (16%)	3	24
6	E	223/224 (100%)	197 (88%)	26 (12%)	7	35
7	F	174/194 (90%)	145 (83%)	29 (17%)	3	21
8	G	192/200 (96%)	174 (91%)	18 (9%)	11	45
9	H	164/170 (96%)	154 (94%)	10 (6%)	23	63
10	I	148/159 (93%)	130 (88%)	18 (12%)	6	33
11	J	153/158 (97%)	132 (86%)	21 (14%)	4	29
12	K	88/96 (92%)	75 (85%)	13 (15%)	4	26
13	L	136/137 (99%)	120 (88%)	16 (12%)	6	35
14	M	93/109 (85%)	86 (92%)	7 (8%)	17	56
15	N	127/128 (99%)	109 (86%)	18 (14%)	4	28
16	O	96/104 (92%)	84 (88%)	12 (12%)	6	32
17	P	101/117 (86%)	86 (85%)	15 (15%)	4	26
18	Q	117/119 (98%)	102 (87%)	15 (13%)	5	31
19	R	109/124 (88%)	99 (91%)	10 (9%)	11	46
20	S	128/129 (99%)	113 (88%)	15 (12%)	7	35
21	T	117/118 (99%)	103 (88%)	14 (12%)	6	33
22	U	96/107 (90%)	85 (88%)	11 (12%)	7	36
23	V	73/73 (100%)	61 (84%)	12 (16%)	3	21
24	W	110/111 (99%)	96 (87%)	14 (13%)	5	31
25	X	119/120 (99%)	103 (87%)	16 (13%)	5	30
26	Y	108/109 (99%)	97 (90%)	11 (10%)	9	41
27	Z	60/88 (68%)	57 (95%)	3 (5%)	30	68
28	a	82/100 (82%)	72 (88%)	10 (12%)	6	33
29	b	71/72 (99%)	63 (89%)	8 (11%)	7	37
30	c	54/59 (92%)	48 (89%)	6 (11%)	8	38
31	f	57/133 (43%)	50 (88%)	7 (12%)	6	33
32	g	265/272 (97%)	245 (92%)	20 (8%)	17	56
33	d	46/48 (96%)	39 (85%)	7 (15%)	3	25
34	e	47/55 (86%)	38 (81%)	9 (19%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	h	23/23 (100%)	20 (87%)	3 (13%)	5	31
38	i	93/130 (72%)	81 (87%)	12 (13%)	5	31
39	j	226/270 (84%)	190 (84%)	36 (16%)	3	23
40	m	77/96 (80%)	70 (91%)	7 (9%)	12	47
All	All	4505/4990 (90%)	3960 (88%)	545 (12%)	10	33

5 of 545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	136	ARG
18	Q	83	GLN
39	j	19	ILE
14	M	125	GLU
16	O	72	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	40	GLN
19	R	29	GLN
33	d	27	HIS
18	Q	74	HIS
18	Q	93	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	807 (45%)	139 (7%)
36	1	73/75 (97%)	34 (46%)	6 (8%)
37	3	21/25 (84%)	18 (85%)	6 (28%)
All	All	1872/1899 (98%)	859 (45%)	151 (8%)

5 of 859 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C

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Mol	Chain	Res	Type
1	2	5	U
1	2	8	U

5 of 151 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	810	A
1	2	1081	C
36	1	14	A
1	2	822	G
1	2	912	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 84 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	MET	k	601	-	5,7,8	0.42	0	4,7,9	0.95	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
45	MET	k	601	-	-	0/4/6/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.