



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:05 PM BST

PDB ID : 4V8T  
EMDB ID: : EMD-2169  
Title : Cryo-EM Structure of the 60S Ribosomal Subunit in Complex with Arx1 and Rei1  
Authors : Greber, B.J.; Boehringer, D.; Montellese, C.; Ban, N.  
Deposited on : 2012-08-07  
Resolution : 8.10 Å(reported)  
Based on PDB ID : 3U5H, 3U5I

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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

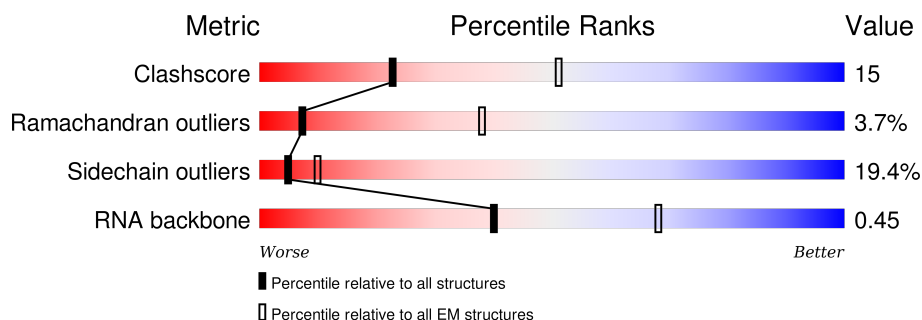
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.10 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.















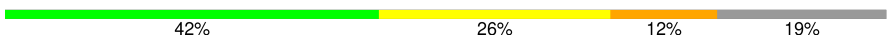












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	254	59% 29% 10% ..
2	B	387	58% 28% 11% .
3	C	362	54% 33% 11% .
4	D	297	59% 31% 8% ..
5	E	176	63% 18% 7% . 11%
6	F	244	60% 25% 6% . 9%
7	G	256	44% 32% 13% . 10%
8	H	191	50% 36% 13% .









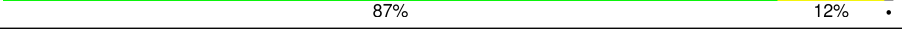

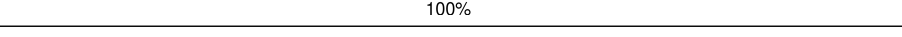
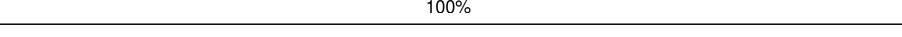
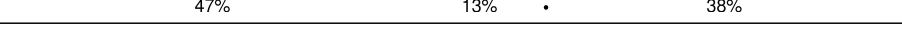
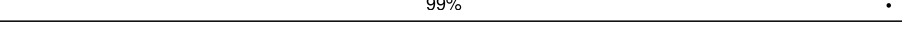

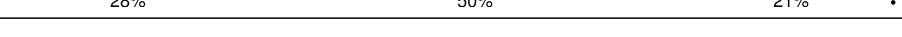

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Mol	Chain	Length	Quality of chain
9	I	221	
10	J	174	
11	K	155	
12	L	199	
13	M	138	
14	N	204	
15	O	219	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	W	155	
24	X	142	
25	Y	127	
26	Z	136	
27	a	149	
28	b	59	
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	

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Mol	Chain	Length	Quality of chain
34	h	120	
35	i	100	
36	j	88	
37	k	78	
38	l	51	
39	m	128	
40	n	25	
41	o	106	
42	p	92	
43	q	312	
44	r	47	
45	s	46	
46	t	614	
47	1	114	
48	5	3396	
49	7	121	
50	8	158	

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 130050 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 60S RIBOSOMAL PROTEIN L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	3	ALA	THR	CONFLICT	UNP Q3E757

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	150	Total	C	N	O		0	0
			750	450	150	150			

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	194	Total	C	N	O		0	0
			1548	965	316	267			

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	197	Total	C	N	O	S	197	0
			3119	2008	581	528	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	SER	VAL	MICROHETEROGENEITY	UNP P26784
O	4	GLN	GLU	MICROHETEROGENEITY	UNP P26784
O	11	ALA	GLY	MICROHETEROGENEITY	UNP P26784
O	13	ASP	GLY	MICROHETEROGENEITY	UNP P26784
O	16	LEU	VAL	MICROHETEROGENEITY	UNP P26784
O	22	THR	VAL	MICROHETEROGENEITY	UNP P26784
O	23	ILE	VAL	MICROHETEROGENEITY	UNP P26784
O	27	VAL	LEU	MICROHETEROGENEITY	UNP P26784
O	40	ALA	GLU	MICROHETEROGENEITY	UNP P26784
O	80	LEU	PHE	MICROHETEROGENEITY	UNP P26784
O	84	ILE	LEU	MICROHETEROGENEITY	UNP P26784
O	104	ILE	VAL	MICROHETEROGENEITY	UNP P26784
O	158	ASP	ALA	MICROHETEROGENEITY	UNP P26784
O	163	ARG	SER	MICROHETEROGENEITY	UNP P26784
O	179	SER	ALA	MICROHETEROGENEITY	UNP P26784
O	182	SER	ASN	MICROHETEROGENEITY	UNP P26784
O	184	ALA	THR	MICROHETEROGENEITY	UNP P26784
O	186	ALA	SER	MICROHETEROGENEITY	UNP P26784
O	196	ALA	SER	MICROHETEROGENEITY	UNP P26784
O	197	LEU	PHE	MICROHETEROGENEITY	UNP P26784

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	155	Total	C	N	O	0	0
			1227	764	238	225		

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L18-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L19-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	98	Total	C	N	O	0	0
			778	505	127	146		

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L24-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	135	Total	C	N	O	S	0	0
			1038	651	206	180	1		

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L41-A.

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

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 43 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	143	Total	C	N	O	S	0	0
			1077	687	192	195	3		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	199	UNK	SER	SEE REMARK 999	UNP P05317
q	200	UNK	SER	SEE REMARK 999	UNP P05317
q	201	UNK	ILE	SEE REMARK 999	UNP P05317
q	202	UNK	LEU	SEE REMARK 999	UNP P05317
q	203	UNK	ASP	SEE REMARK 999	UNP P05317
q	204	UNK	ILE	SEE REMARK 999	UNP P05317
q	205	UNK	THR	SEE REMARK 999	UNP P05317
q	206	UNK	ASP	SEE REMARK 999	UNP P05317
q	207	UNK	GLU	SEE REMARK 999	UNP P05317
q	208	UNK	GLU	SEE REMARK 999	UNP P05317
q	209	UNK	LEU	SEE REMARK 999	UNP P05317
q	210	UNK	VAL	SEE REMARK 999	UNP P05317
q	211	UNK	SER	SEE REMARK 999	UNP P05317
q	212	UNK	HIS	SEE REMARK 999	UNP P05317
q	213	UNK	PHE	SEE REMARK 999	UNP P05317
q	214	UNK	VAL	SEE REMARK 999	UNP P05317
q	215	UNK	SER	SEE REMARK 999	UNP P05317
q	216	UNK	ALA	SEE REMARK 999	UNP P05317
q	217	UNK	VAL	SEE REMARK 999	UNP P05317
q	218	UNK	SER	SEE REMARK 999	UNP P05317
q	219	UNK	THR	SEE REMARK 999	UNP P05317
q	220	UNK	ILE	SEE REMARK 999	UNP P05317
q	221	UNK	ALA	SEE REMARK 999	UNP P05317

- Molecule 44 is a protein called RIBOSOMAL PROTEIN P1 ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 45 is a protein called RIBOSOMAL PROTEIN P2 BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	46	Total	C	N	O	0	0
			230	138	46	46		

- Molecule 46 is a protein called PROBABLE METALLOPROTEASE ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	380	Total	C	N	O	S	0	0
			2938	1853	511	563	11		

- Molecule 47 is a RNA chain called ES27 OF THE 25S RRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
47	1	114	Total P 114 114	0	114

- Molecule 48 is a RNA chain called 25S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3150	Total	C	N	O	P	0	0
			67376	30095	12145	21987	3149		

- Molecule 49 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

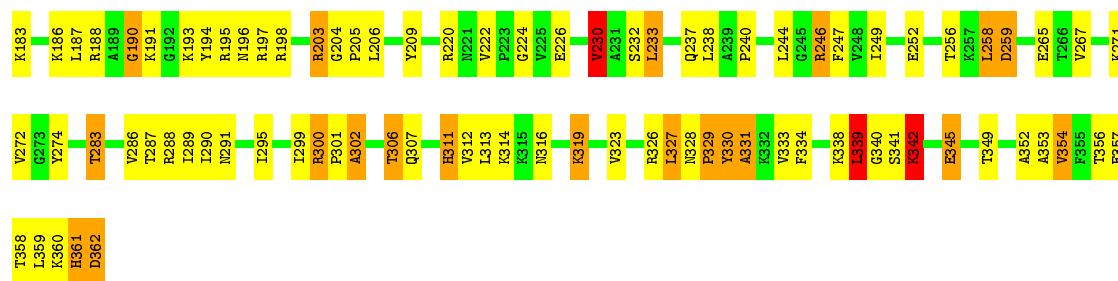
- Molecule 50 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

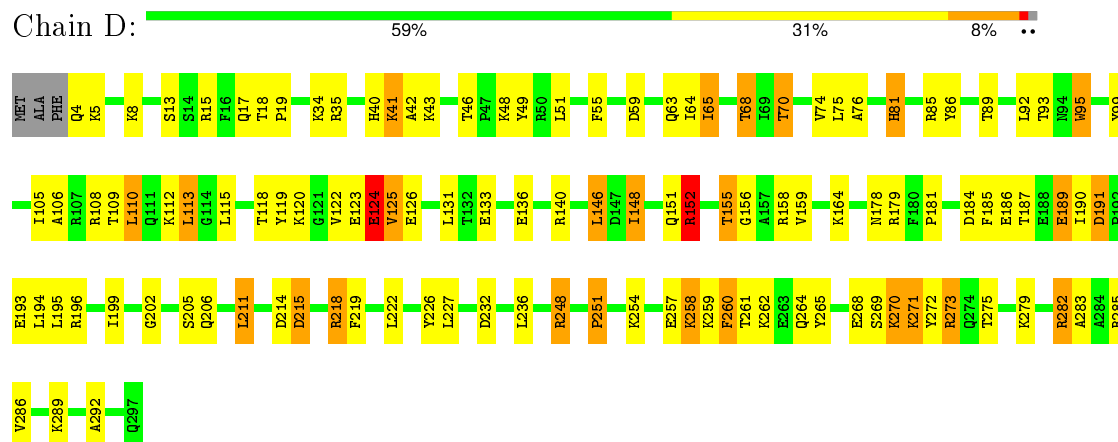
- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
51	p	1	Total Zn 1 1	0
51	o	1	Total Zn 1 1	0
51	j	1	Total Zn 1 1	0
51	m	1	Total Zn 1 1	0

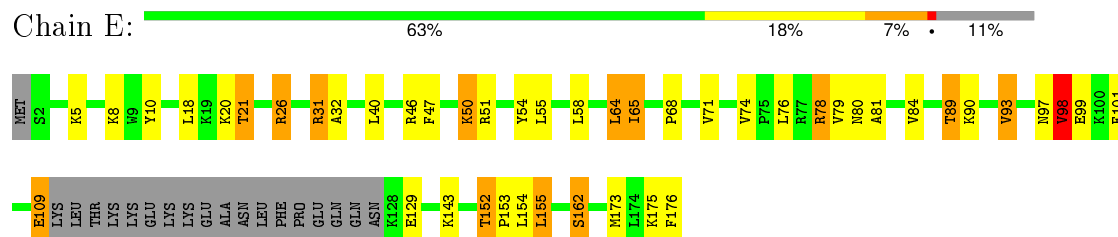




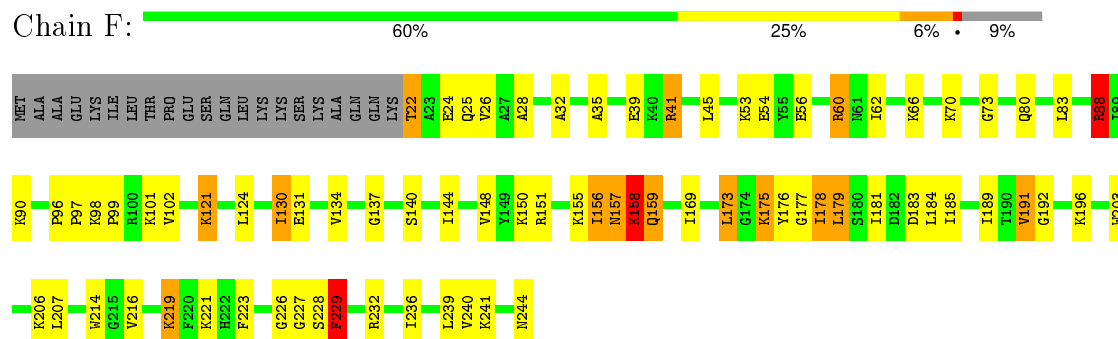
• Molecule 4: 60S RIBOSOMAL PROTEIN L5



• Molecule 5: 60S RIBOSOMAL PROTEIN L6-A

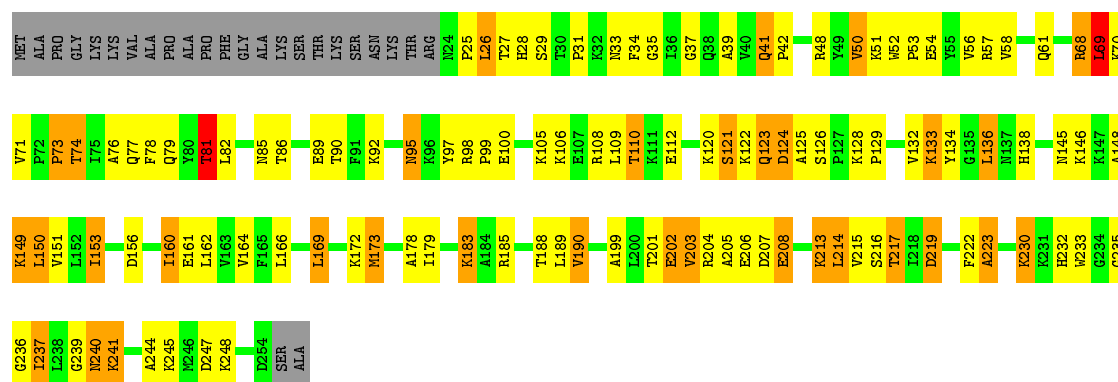


• Molecule 6: 60S RIBOSOMAL PROTEIN L7-A



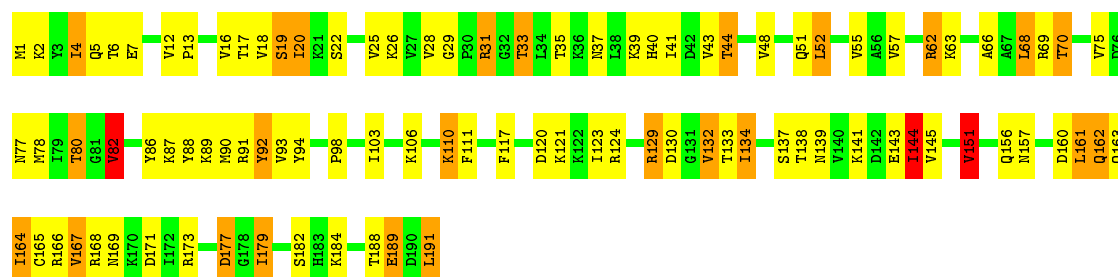
• Molecule 7: 60S RIBOSOMAL PROTEIN L8-A





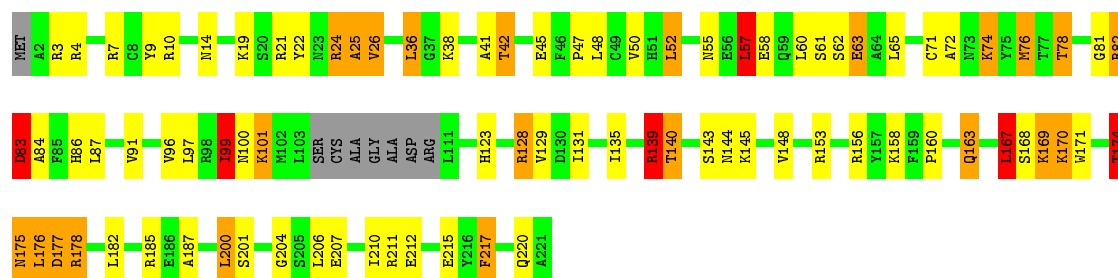
• Molecule 8: 60S RIBOSOMAL PROTEIN L9-A

Chain H: 50% 36% 13%



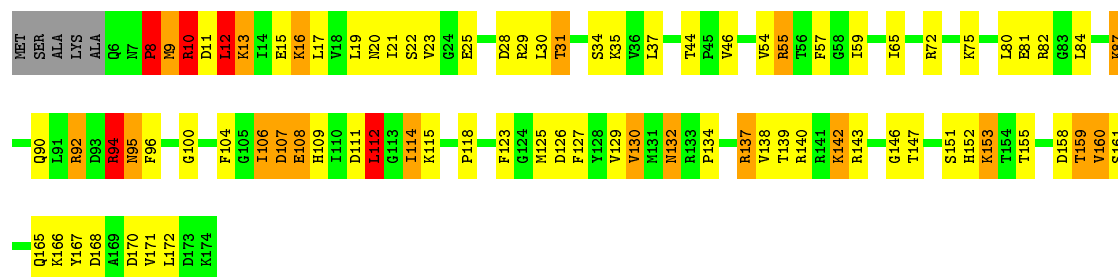
• Molecule 9: 60S RIBOSOMAL PROTEIN L10

Chain I: 57% 26% 10%




• Molecule 10: 60S RIBOSOMAL PROTEIN L11-B

Chain J: 49% 34% 11%



• Molecule 11: 60S RIBOSOMAL PROTEIN L12

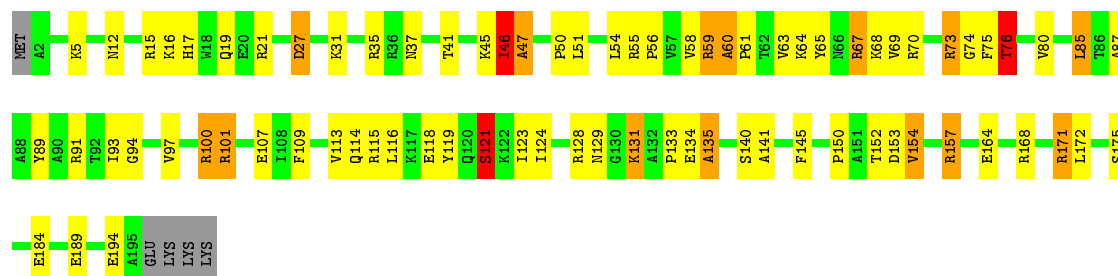


Chain K:  85% 12%



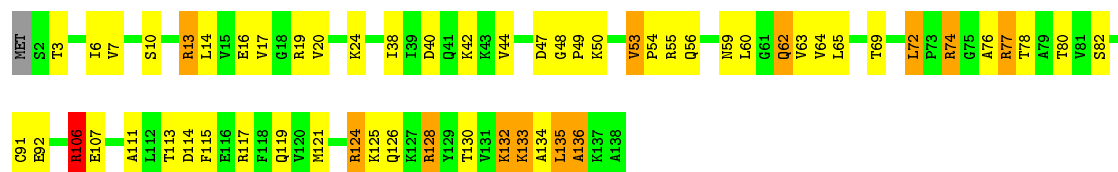
• Molecule 12: 60S RIBOSOMAL PROTEIN L13-A

Chain L:  58% 31% 7%



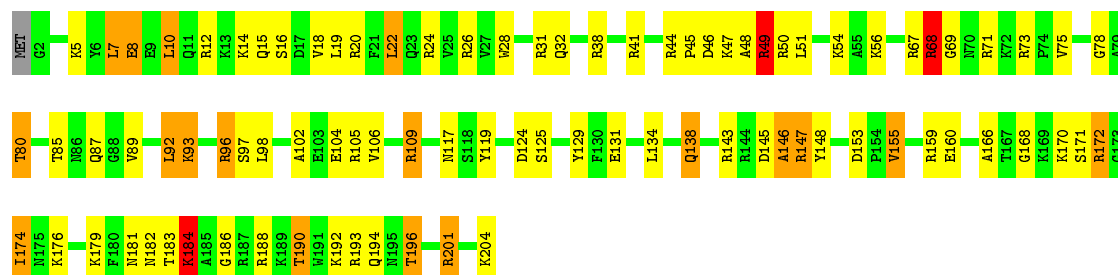
• Molecule 13: 60S RIBOSOMAL PROTEIN L14-A

Chain M:  57% 33% 9%



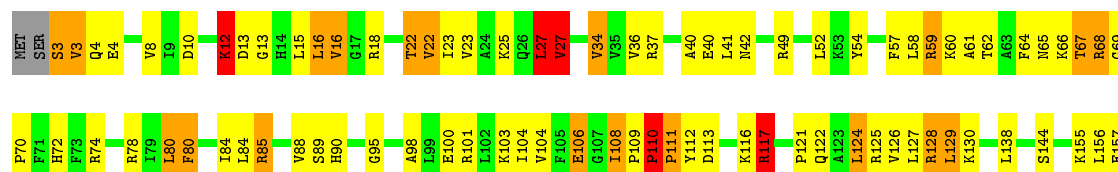
• Molecule 14: 60S RIBOSOMAL PROTEIN L15-A

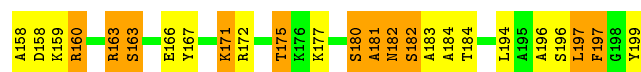
Chain N:  56% 33% 9%



• Molecule 15: 60S RIBOSOMAL PROTEIN L16-A

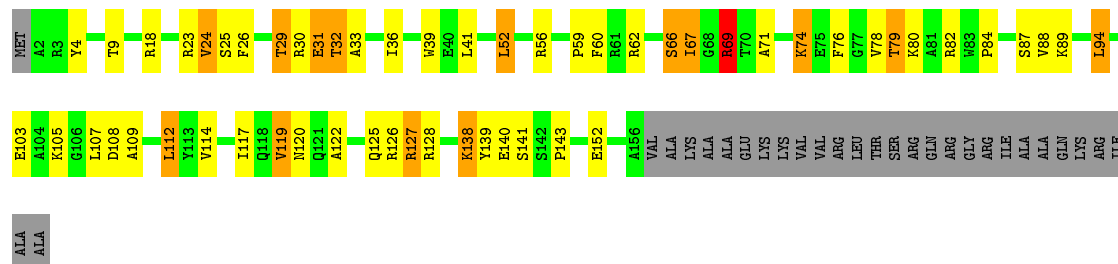
Chain O:  49% 34% 14%





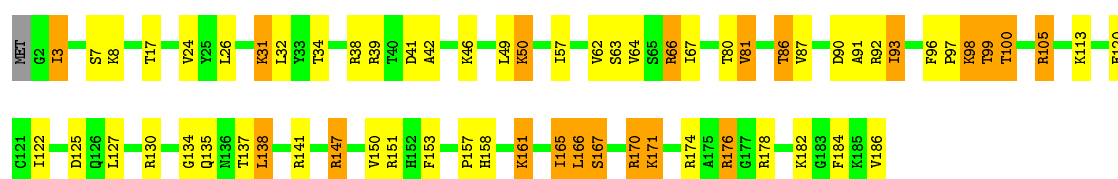
• Molecule 16: 60S RIBOSOMAL PROTEIN L17-A

Chain P: 54% 22% 8% 16%



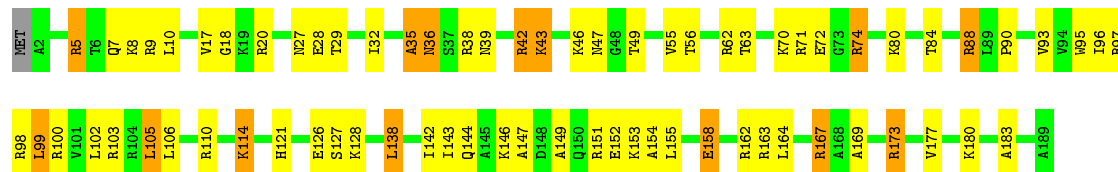
• Molecule 17: 60S RIBOSOMAL PROTEIN L18-B

Chain Q: 65% 24% 11%



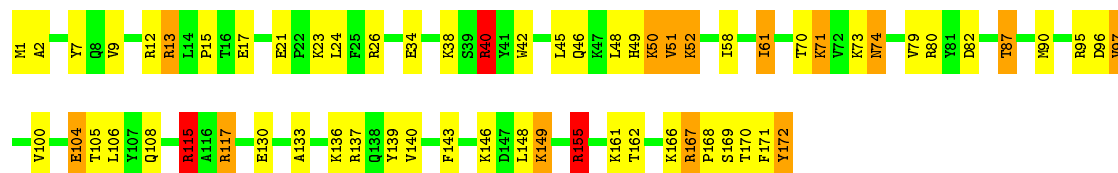
• Molecule 18: 60S RIBOSOMAL PROTEIN L19-B

Chain R: 61% 31% 7%



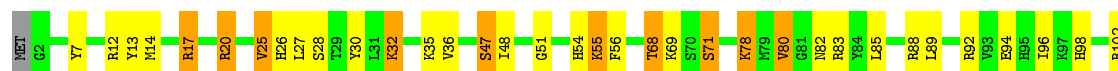
• Molecule 19: 60S RIBOSOMAL PROTEIN L20-A

Chain S: 63% 27% 8%



• Molecule 20: 60S RIBOSOMAL PROTEIN L21-A

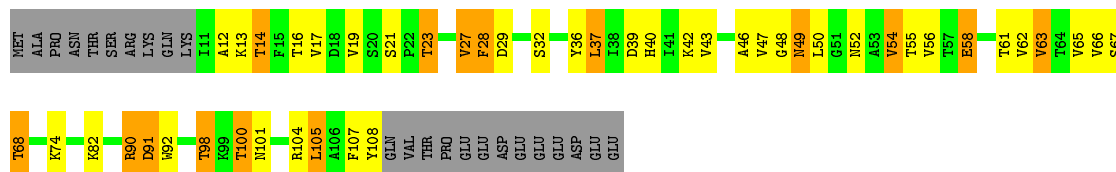
Chain T: 67% 21% 11%





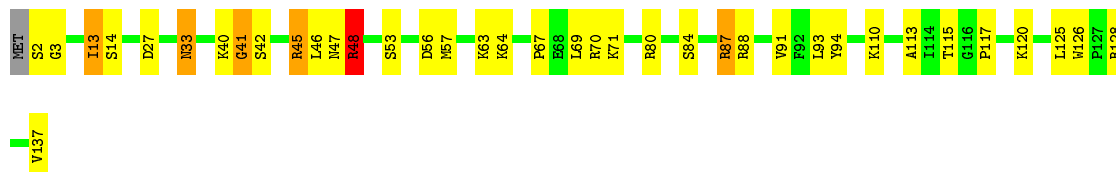
• Molecule 21: 60S RIBOSOMAL PROTEIN L22-A

Chain U: 42% 26% 12% 19%



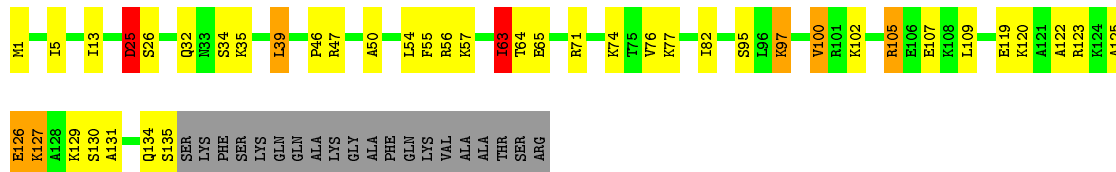
• Molecule 22: 60S RIBOSOMAL PROTEIN L23-A

Chain V: 72% 23% . .



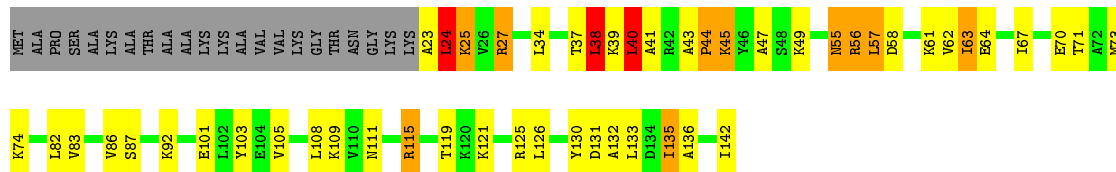
• Molecule 23: 60S RIBOSOMAL PROTEIN L24-A

Chain W: 59% 23% . . 13%



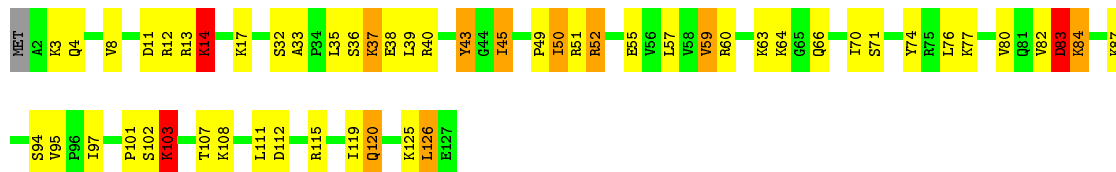
• Molecule 24: 60S RIBOSOMAL PROTEIN L25

Chain X: 49% 27% 7% . 15%



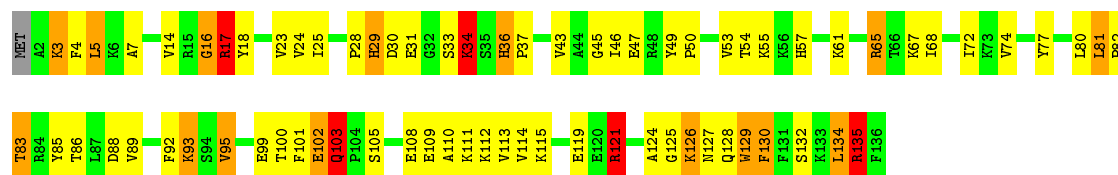
• Molecule 25: 60S RIBOSOMAL PROTEIN L26-A

Chain Y: 57% 33% 7% . .



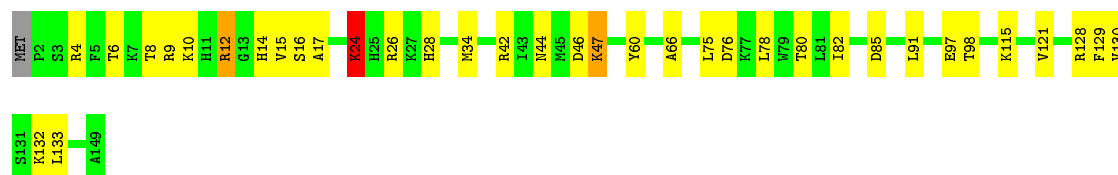
- Molecule 26: 60S RIBOSOMAL PROTEIN L27-A

Chain Z: 



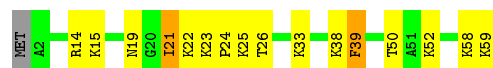
- Molecule 27: 60S RIBOSOMAL PROTEIN L28

Chain a: 




- Molecule 28: 60S RIBOSOMAL PROTEIN L29

Chain b: 



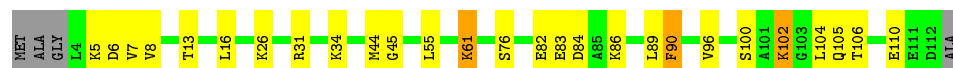
- Molecule 29: 60S RIBOSOMAL PROTEIN L32

Chain c: 



- Molecule 30: 60S RIBOSOMAL PROTEIN L31-A

Chain d: 




- Molecule 31: 60S RIBOSOMAL PROTEIN L30

Chain e: 



- Molecule 32: 60S RIBOSOMAL PROTEIN L33-A

Chain f: 



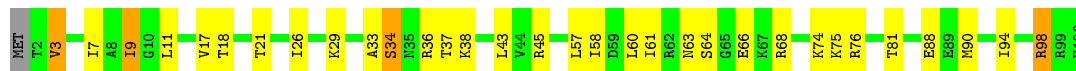
- Molecule 33: 60S RIBOSOMAL PROTEIN L34-A



- Molecule 34: 60S RIBOSOMAL PROTEIN L35-A



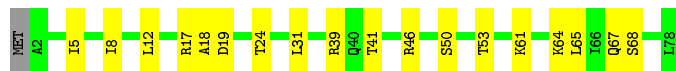
- Molecule 35: 60S RIBOSOMAL PROTEIN L36-A



- Molecule 36: 60S RIBOSOMAL PROTEIN L37-A



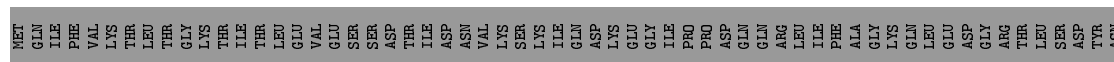
- Molecule 37: 60S RIBOSOMAL PROTEIN L38



- Molecule 38: 60S RIBOSOMAL PROTEIN L39

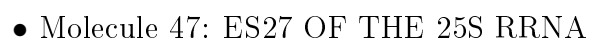


- Molecule 39: 60S RIBOSOMAL PROTEIN L40





Response	Percentage
Yes	47%
No	13%
Don't know	38%



99%



Frequency	Percentage
Daily	25%
Often	41%
Sometimes	21%
Rarely	6%
Never	7%

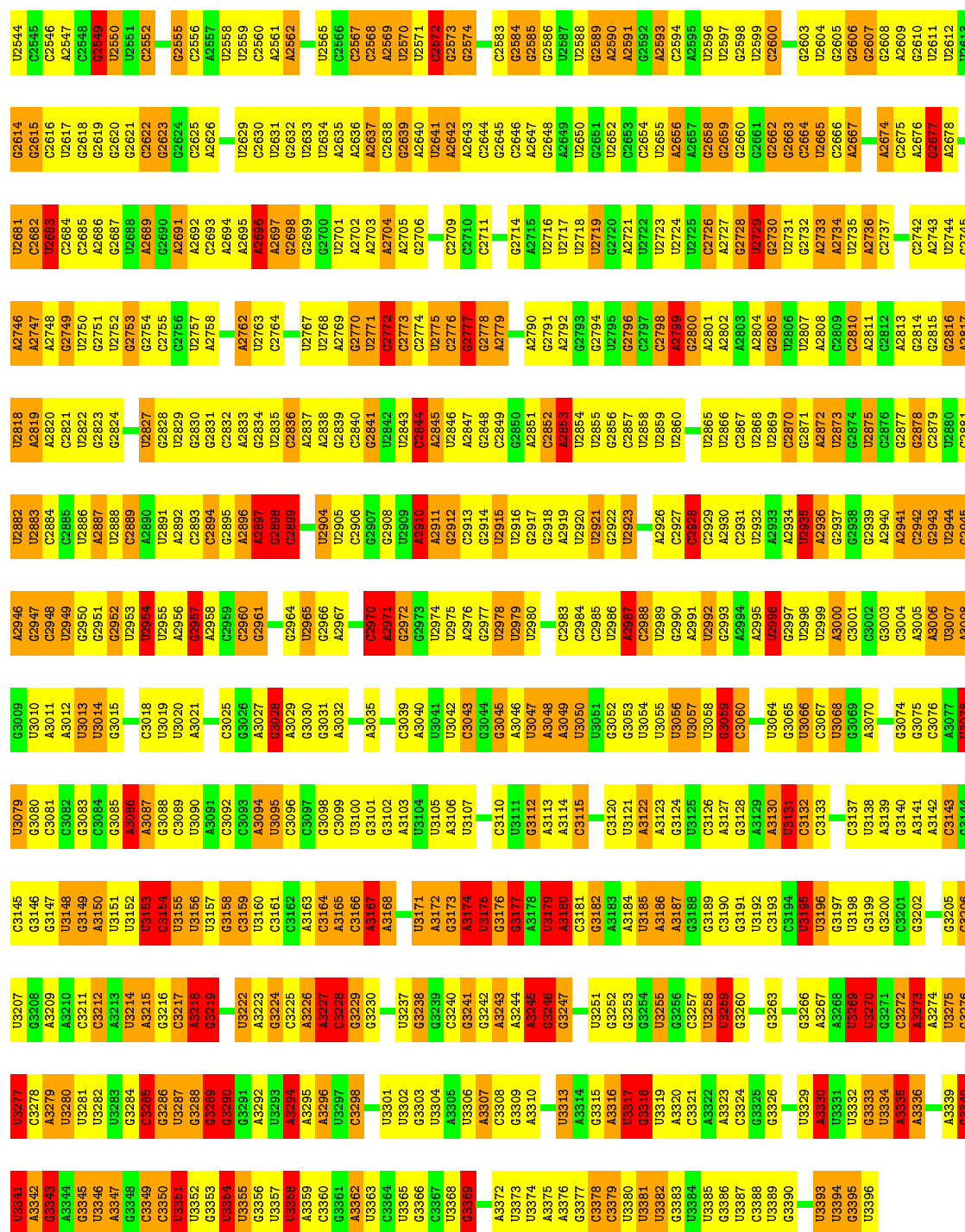




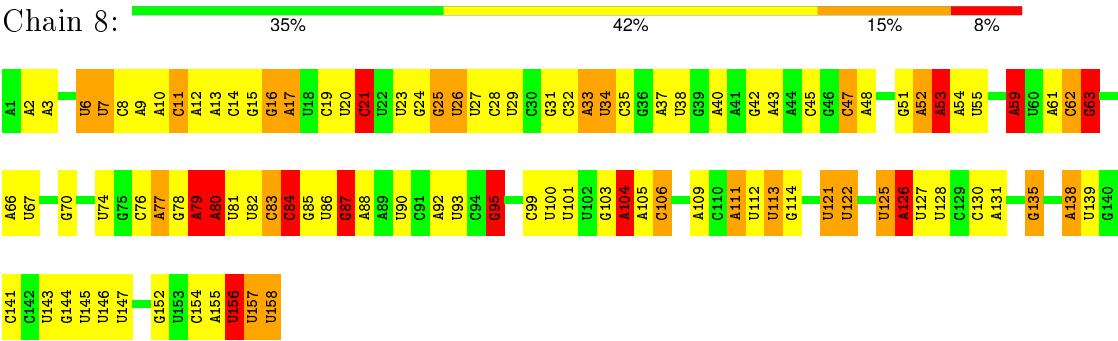



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM



● Molecule 50: 5.8S RIBOSOMAL RNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER FRAME	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	83000	Depositor
Image detector	GATAN ULTRASCAN 4000	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
10	J	0.81	1/1374 (0.1%)	0.99	3/1842 (0.2%)
12	L	0.82	0/1573	1.04	6/2113 (0.3%)
13	M	0.95	0/1074	1.01	4/1446 (0.3%)
14	N	0.83	0/1757	1.00	6/2354 (0.3%)
15	O	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
16	P	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
17	Q	0.89	1/1465 (0.1%)	1.12	8/1965 (0.4%)
18	R	0.78	1/1538 (0.1%)	0.87	3/2050 (0.1%)
19	S	1.02	0/1481	1.09	7/1990 (0.4%)
2	B	1.02	4/3146 (0.1%)	1.11	14/4228 (0.3%)
20	T	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
21	U	0.56	0/794	0.77	0/1076
22	V	0.98	0/1018	1.09	4/1369 (0.3%)
23	W	0.80	0/1052	0.90	1/1398 (0.1%)
24	X	0.72	0/974	0.86	0/1314
25	Y	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
26	Z	0.55	0/1118	0.83	2/1497 (0.1%)
27	a	0.95	2/1204 (0.2%)	1.14	9/1612 (0.6%)
28	b	0.91	0/473	1.14	1/629 (0.2%)
29	c	0.61	0/775	0.77	0/1040
3	C	0.87	0/2800	1.07	11/3790 (0.3%)
30	d	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
31	e	1.04	0/1041	1.27	12/1394 (0.9%)
32	f	1.12	1/868 (0.1%)	1.09	3/1168 (0.3%)
33	g	0.72	0/890	0.92	0/1189
34	h	0.67	0/974	0.79	0/1297
35	i	0.67	0/777	0.85	0/1033
36	j	0.87	0/696	1.04	3/923 (0.3%)
37	k	0.50	0/614	0.70	0/822
38	l	0.90	0/443	1.02	1/588 (0.2%)
39	m	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
4	D	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
40	n	0.90	0/234	1.15	1/300 (0.3%)
41	o	0.83	0/860	0.88	1/1136 (0.1%)
42	p	0.86	0/701	0.98	1/934 (0.1%)
43	q	0.54	0/977	0.75	1/1313 (0.1%)
46	t	5.64	18/2985 (0.6%)	4.15	194/4053 (4.8%)
48	5	1.46	609/75414 (0.8%)	1.88	3517/117575 (3.0%)
49	7	1.38	13/2883 (0.5%)	1.80	118/4491 (2.6%)
5	E	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
50	8	1.16	5/3746 (0.1%)	1.70	132/5832 (2.3%)
6	F	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
7	G	0.64	0/1795	0.81	1/2429 (0.0%)
8	H	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
9	I	0.92	1/1758 (0.1%)	1.08	11/2358 (0.5%)
All	All	1.49	681/138295 (0.5%)	1.70	4127/203388 (2.0%)

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
1	A	0	2
15	O	0	2
19	S	0	1
22	V	0	1
25	Y	0	1
26	Z	0	1
27	a	0	3
28	b	0	1
3	C	0	1
4	D	0	1
46	t	0	6
48	5	0	1
5	E	0	1
6	F	0	2
All	All	0	24

The worst 5 of 681 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	t	168	PRO	N-CD	120.75	3.16	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	t	545	PRO	N-CD	120.48	3.16	1.47
46	t	162	PRO	N-CD	120.12	3.16	1.47
46	t	172	PRO	N-CD	118.10	3.13	1.47
46	t	520	PRO	N-CD	117.23	3.12	1.47

The worst 5 of 4127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	t	81	LYS	O-C-N	-73.85	4.54	122.70
46	t	15	LYS	O-C-N	-50.53	41.85	122.70
46	t	544	ASN	O-C-N	-46.67	32.42	121.10
46	t	162	PRO	N-CA-CB	37.84	148.71	103.30
46	t	168	PRO	N-CA-CB	37.79	148.65	103.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Peptide
1	A	211	HIS	Peptide
3	C	91	GLY	Peptide
4	D	271	LYS	Peptide
5	E	129	GLU	Peptide

## 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	A	1912	0	1976	86	0
2	B	3075	0	3142	116	0
3	C	2748	0	2859	99	0
4	D	2359	0	2311	85	0
5	E	1248	0	1339	33	0
6	F	1791	0	1869	47	0
7	G	1763	0	1819	72	0
8	H	1518	0	1587	66	0
9	I	1722	0	1755	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1353	0	1383	56	0
11	K	750	0	185	11	0
12	L	1548	0	1613	45	0
13	M	1059	0	1154	40	0
14	N	1720	0	1779	63	0
15	O	3119	0	3302	94	0
16	P	1227	0	1236	32	0
17	Q	1441	0	1543	39	0
18	R	1521	0	1617	38	0
19	S	1445	0	1487	49	0
20	T	1276	0	1323	51	0
21	U	778	0	791	25	0
22	V	1003	0	1048	25	0
23	W	1038	0	1071	21	0
24	X	959	0	1020	27	0
25	Y	993	0	1081	28	0
26	Z	1092	0	1155	53	0
27	a	1173	0	1215	0	0
28	b	462	0	491	0	0
29	c	767	0	816	0	0
30	d	883	0	918	0	0
31	e	1020	0	1090	0	0
32	f	850	0	880	0	0
33	g	880	0	945	0	0
34	h	965	0	1067	0	0
35	i	770	0	846	0	0
36	j	681	0	683	0	0
37	k	608	0	671	0	0
38	l	436	0	475	0	0
39	m	417	0	455	0	0
40	n	233	0	284	0	0
41	o	847	0	915	0	0
42	p	694	0	734	0	0
43	q	1077	0	1012	0	0
44	r	235	0	50	0	0
45	s	230	0	49	0	0
46	t	2938	0	2993	0	0
47	1	114	0	0	2	0
48	5	67376	0	33833	1091	0
49	7	2579	0	1303	38	0
50	8	3353	0	1695	42	0
51	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	m	1	0	0	0	0
51	o	1	0	0	0	0
51	p	1	0	0	0	0
All	All	130050	0	94865	2209	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 15.

The worst 5 of 2209 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)
17:Q:171:LYS:CE	17:Q:171:LYS:NZ	1.67	1.55
20:T:82:ASN:HD21	47:1:2029:A:P	157.50	1.52
10:J:8:PRO:CG	10:J:8:PRO:CB	1.75	1.49
20:T:82:ASN:ND2	47:1:2029:A:P	157.87	1.25
2:B:296:THR:HG22	2:B:298:PHE:H	1.18	1.06

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	A	250/254 (98%)	213 (85%)	30 (12%)	7 (3%)	6	44
2	B	384/387 (99%)	341 (89%)	34 (9%)	9 (2%)	8	48
3	C	359/362 (99%)	306 (85%)	32 (9%)	21 (6%)	2	27
4	D	292/297 (98%)	267 (91%)	19 (6%)	6 (2%)	9	50
5	E	153/176 (87%)	134 (88%)	15 (10%)	4 (3%)	7	45
6	F	221/244 (91%)	201 (91%)	15 (7%)	5 (2%)	8	48
7	G	229/256 (90%)	181 (79%)	27 (12%)	21 (9%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	9	50
9	I	209/221 (95%)	175 (84%)	22 (10%)	12 (6%)	2	28
10	J	167/174 (96%)	135 (81%)	19 (11%)	13 (8%)	1	20
12	L	192/199 (96%)	161 (84%)	20 (10%)	11 (6%)	2	28
13	M	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	26	71
14	N	201/204 (98%)	182 (90%)	13 (6%)	6 (3%)	5	42
15	O	352/219 (161%)	324 (92%)	18 (5%)	10 (3%)	6	44
16	P	153/184 (83%)	142 (93%)	9 (6%)	2 (1%)	15	60
17	Q	183/186 (98%)	168 (92%)	9 (5%)	6 (3%)	5	40
18	R	186/189 (98%)	167 (90%)	16 (9%)	3 (2%)	12	56
19	S	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	30	74
20	T	157/160 (98%)	146 (93%)	9 (6%)	2 (1%)	15	60
21	U	96/121 (79%)	80 (83%)	13 (14%)	3 (3%)	5	42
22	V	134/137 (98%)	124 (92%)	8 (6%)	2 (2%)	13	57
23	W	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	2	26
24	X	118/142 (83%)	103 (87%)	7 (6%)	8 (7%)	1	23
25	Y	124/127 (98%)	107 (86%)	12 (10%)	5 (4%)	4	35
26	Z	133/136 (98%)	107 (80%)	13 (10%)	13 (10%)	1	14
27	a	146/149 (98%)	123 (84%)	18 (12%)	5 (3%)	5	40
28	b	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	1	17
29	c	98/105 (93%)	87 (89%)	8 (8%)	3 (3%)	5	42
30	d	107/113 (95%)	88 (82%)	13 (12%)	6 (6%)	2	28
31	e	125/130 (96%)	109 (87%)	10 (8%)	6 (5%)	3	32
32	f	104/107 (97%)	96 (92%)	5 (5%)	3 (3%)	6	43
33	g	110/121 (91%)	93 (84%)	13 (12%)	4 (4%)	4	38
34	h	117/120 (98%)	99 (85%)	14 (12%)	4 (3%)	5	40
35	i	97/100 (97%)	77 (79%)	13 (13%)	7 (7%)	1	22
36	j	85/88 (97%)	75 (88%)	8 (9%)	2 (2%)	7	47
37	k	75/78 (96%)	61 (81%)	10 (13%)	4 (5%)	2	29
38	l	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	9	50
39	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	n	23/25 (92%)	22 (96%)	0	1 (4%)	3	34
41	o	103/106 (97%)	90 (87%)	11 (11%)	2 (2%)	10	52
42	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
43	q	117/312 (38%)	93 (80%)	18 (15%)	6 (5%)	2	30
46	t	376/614 (61%)	354 (94%)	14 (4%)	8 (2%)	9	50
All	All	6846/7529 (91%)	6010 (88%)	585 (8%)	251 (4%)	7	38

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
2	B	129	ALA
2	B	140	ASP
2	B	347	SER
3	C	14	GLU

### 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	A	192/196 (98%)	154 (80%)	38 (20%)	1	12
2	B	321/323 (99%)	251 (78%)	70 (22%)	1	9
3	C	288/289 (100%)	222 (77%)	66 (23%)	1	7
4	D	243/245 (99%)	196 (81%)	47 (19%)	2	13
5	E	135/153 (88%)	115 (85%)	20 (15%)	4	24
6	F	187/205 (91%)	158 (84%)	29 (16%)	3	22
7	G	177/208 (85%)	138 (78%)	39 (22%)	1	9
8	H	171/171 (100%)	132 (77%)	39 (23%)	1	8
9	I	179/187 (96%)	142 (79%)	37 (21%)	1	10
10	J	147/150 (98%)	114 (78%)	33 (22%)	1	9
12	L	154/159 (97%)	124 (80%)	30 (20%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	108/109 (99%)	84 (78%)	24 (22%)	1	9
14	N	175/176 (99%)	143 (82%)	32 (18%)	2	14
15	O	323/179 (180%)	267 (83%)	56 (17%)	2	17
16	P	125/146 (86%)	103 (82%)	22 (18%)	2	16
17	Q	150/151 (99%)	123 (82%)	27 (18%)	2	15
18	R	153/154 (99%)	121 (79%)	32 (21%)	1	10
19	S	156/156 (100%)	123 (79%)	33 (21%)	1	9
20	T	136/137 (99%)	109 (80%)	27 (20%)	1	11
21	U	85/107 (79%)	62 (73%)	23 (27%)	0	4
22	V	104/105 (99%)	96 (92%)	8 (8%)	16	52
23	W	100/129 (78%)	85 (85%)	15 (15%)	3	23
24	X	104/118 (88%)	81 (78%)	23 (22%)	1	9
25	Y	109/110 (99%)	85 (78%)	24 (22%)	1	9
26	Z	115/116 (99%)	89 (77%)	26 (23%)	1	8
27	a	118/119 (99%)	95 (80%)	23 (20%)	2	12
28	b	46/47 (98%)	35 (76%)	11 (24%)	1	7
29	c	84/88 (96%)	69 (82%)	15 (18%)	2	15
30	d	94/97 (97%)	73 (78%)	21 (22%)	1	9
31	e	109/111 (98%)	89 (82%)	20 (18%)	2	14
32	f	90/91 (99%)	79 (88%)	11 (12%)	6	31
33	g	95/103 (92%)	71 (75%)	24 (25%)	1	6
34	h	103/105 (98%)	77 (75%)	26 (25%)	1	6
35	i	80/82 (98%)	51 (64%)	29 (36%)	0	1
36	j	70/71 (99%)	53 (76%)	17 (24%)	1	6
37	k	67/69 (97%)	53 (79%)	14 (21%)	1	10
38	l	45/46 (98%)	34 (76%)	11 (24%)	1	6
39	m	47/116 (40%)	34 (72%)	13 (28%)	0	4
40	n	23/23 (100%)	16 (70%)	7 (30%)	0	3
41	o	90/91 (99%)	74 (82%)	16 (18%)	2	16
42	p	71/72 (99%)	61 (86%)	10 (14%)	4	26
43	q	105/233 (45%)	76 (72%)	29 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	t	332/539 (62%)	330 (99%)	2 (1%)	90	95
All	All	5806/6282 (92%)	4687 (81%)	1119 (19%)	5	13

5 of 1119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	12[A]	LYS
18	R	98	ARG
38	l	21	ARG
15	O	74[A]	ARG
16	P	69	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	55	GLN
20	T	49	GLN
46	t	156	HIS
17	Q	9	GLN
21	U	40	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
47	1	0/114	-	-
48	5	3145/3396 (92%)	731 (23%)	129 (4%)
49	7	120/121 (99%)	18 (15%)	0
50	8	157/158 (99%)	32 (20%)	3 (1%)
All	All	3422/3789 (90%)	781 (22%)	132 (3%)

5 of 781 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
48	5	14	U
48	5	15	C
48	5	16	A
48	5	26	A
48	5	38	U

5 of 132 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	1554	U
48	5	1842	A
48	5	3269	U
48	5	1568	U
48	5	1724	U

## 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	K	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	52:UNK	C	54:UNK	N	3.86
1	K	23:UNK	C	28:UNK	N	3.48