



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2017 – 06:43 PM EDT

PDB ID : 5U9F  
EMDB ID: : EMD-8521  
Title : 3.2 Å cryo-EM ArfA-RF2 ribosome rescue complex (Structure II)  
Authors : Demo, G.; Svidritskiy, E.; Madireddy, R.; Diaz-Avalos, R.; Grant, T.; Grigorieff, N.; Sousa, D.; Korostelev, A.A.  
Deposited on : unknown  
Resolution : 3.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

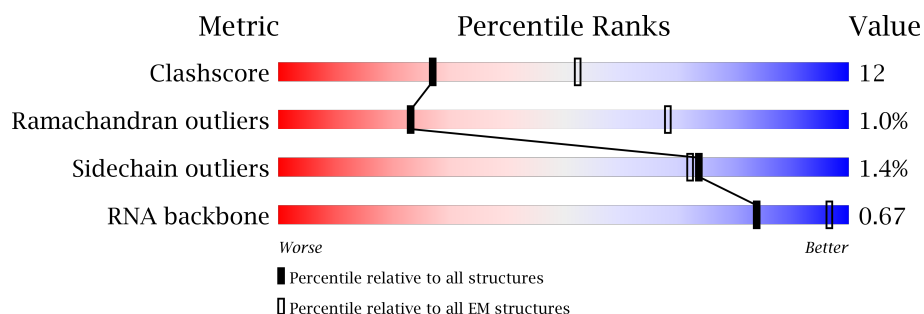
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1539	59% 36% 5%
2	01	2903	62% 34% 5%
3	02	119	55% 38% 8%
4	Y	72	40% 25% 35%
5	W	77	75% 22% .
5	X	77	52% 32% 16%
6	03	234	75% 19% 6%
7	04	273	67% 32% .












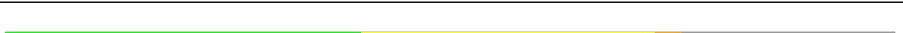













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Mol	Chain	Length	Quality of chain
8	05	209	
9	06	201	
10	07	179	
11	08	177	
12	09	149	
13	10	165	
14	11	142	
15	12	142	
16	13	123	
17	14	144	
18	15	136	
19	16	127	
20	17	117	
21	18	115	
22	19	118	
23	20	103	
24	21	110	
25	22	100	
26	23	104	
27	24	94	
28	25	85	
29	26	78	
30	27	63	
31	28	59	
32	29	70	

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Mol	Chain	Length	Quality of chain
33	30	57	
34	31	55	
35	32	46	
36	33	65	
37	34	38	
38	V	14	
39	Z	365	
40	B	241	
41	C	233	
42	D	206	
43	E	167	
44	F	131	
45	G	156	
46	H	130	
47	I	130	
48	J	103	
49	K	129	
50	L	124	
51	M	118	
52	N	101	
53	O	89	
54	P	82	
55	Q	84	
56	R	75	
57	S	92	

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Mol	Chain	Length	Quality of chain
58	T	87	<div><div></div><div>66%</div><div>32%</div><div></div></div>
59	U	71	<div><div></div><div>49%</div><div>38%</div><div>8%</div></div>

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 152819 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 16S ribosomal RNA.

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

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	01	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	1847	G	A	conflict	GB 2073407

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	02	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 4 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	47	Total	C	N	O	S	0	0
			377	233	78	65	1		

- Molecule 5 is a RNA chain called fMet-tRNA (P- and E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	77	Total	C	N	O	P	0	0
			1622	723	289	534	76		
5	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 6 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	03	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	04	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	07	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 13 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	10	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 14 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	13	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	16	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.



Mol	Chain	Residues	Atoms				AltConf	Trace
20	17	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	19	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	22	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	23	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	29	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	31	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 35 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 36 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 37 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 38 is a RNA chain called truncated mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	14	Total	C	N	O	P	0	0
			306	138	64	91	13		

- Molecule 39 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	361	Total	C	N	O	S	0	0
			2844	1748	503	583	10		

- Molecule 40 is a protein called 30S ribosomal protein S2.

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

- Molecule 41 is a protein called 30S ribosomal protein S3.

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

- Molecule 42 is a protein called 30S ribosomal protein S4.

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

- Molecule 43 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 44 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 45 is a protein called 30S ribosomal protein S7.

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

- Molecule 46 is a protein called 30S ribosomal protein S8.

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

- Molecule 47 is a protein called 30S ribosomal protein S9.

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

- Molecule 48 is a protein called 30S ribosomal protein S10.

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

- Molecule 49 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	K	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 50 is a protein called 30S ribosomal protein S12.

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

- Molecule 51 is a protein called 30S ribosomal protein S13.

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

- Molecule 52 is a protein called 30S ribosomal protein S14.

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

- Molecule 53 is a protein called 30S ribosomal protein S15.

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

- Molecule 54 is a protein called 30S ribosomal protein S16.

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

- Molecule 55 is a protein called 30S ribosomal protein S17.

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

- Molecule 56 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	R	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 57 is a protein called 30S ribosomal protein S19.

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

- Molecule 58 is a protein called 30S ribosomal protein S20.

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

- Molecule 59 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	U	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	17	1	Total	Mg	0
			1	1	
60	30	1	Total	Mg	0
			1	1	
60	I	1	Total	Mg	0
			1	1	
60	31	1	Total	Mg	0
			1	1	
60	W	3	Total	Mg	0
			3	3	
60	01	221	Total	Mg	0
			221	221	

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Mol	Chain	Residues	Atoms		AltConf
60	19	1	Total 1	Mg 1	0
60	V	1	Total 1	Mg 1	0
60	A	118	Total 118	Mg 118	0
60	02	6	Total 6	Mg 6	0
60	34	1	Total 1	Mg 1	0
60	X	5	Total 5	Mg 5	0

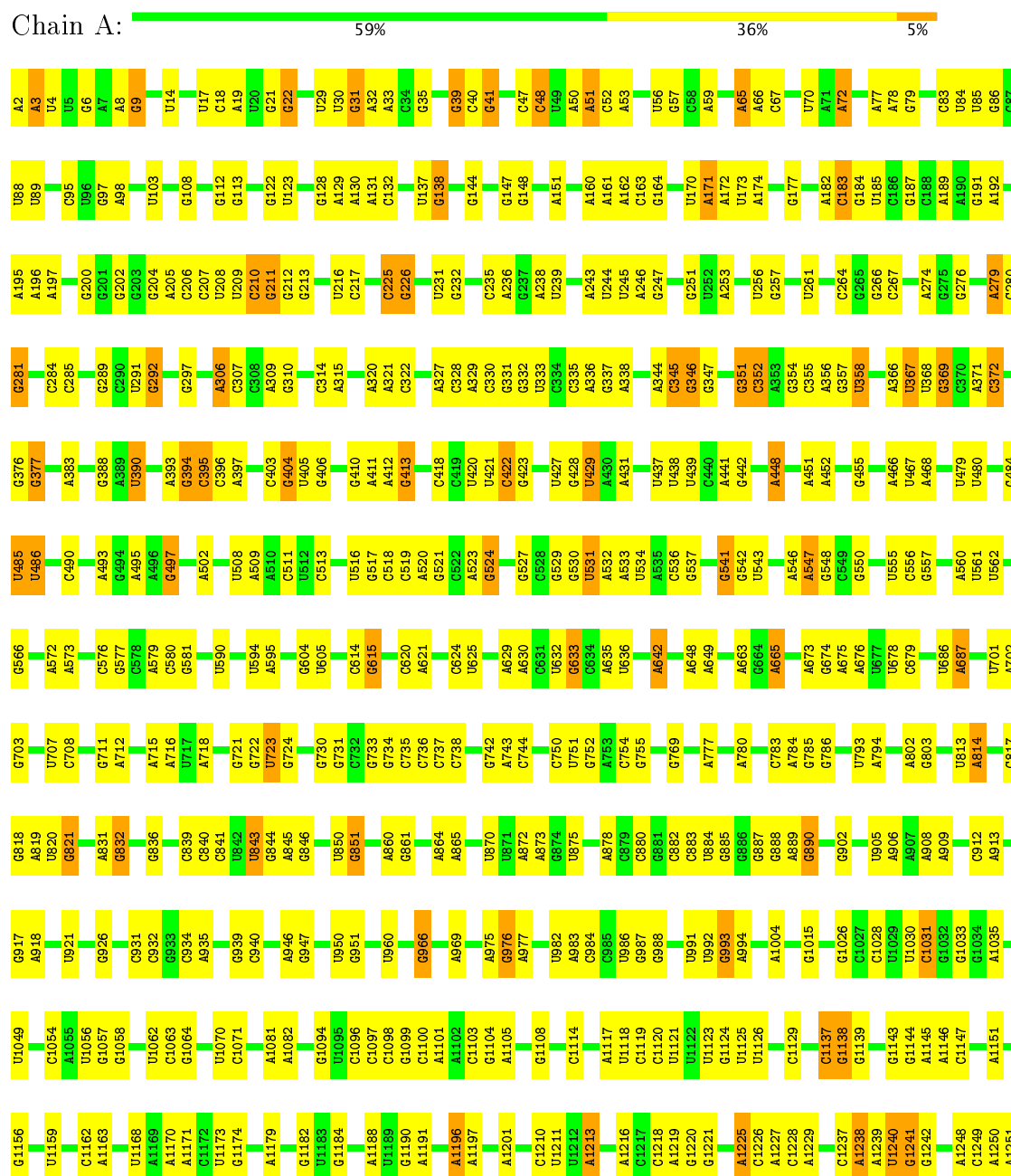
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	34	1	Total 1	Zn 1	0

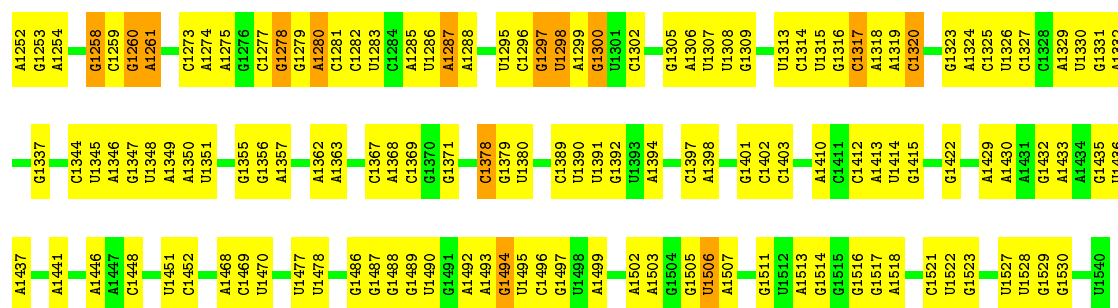
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 16S ribosomal RNA

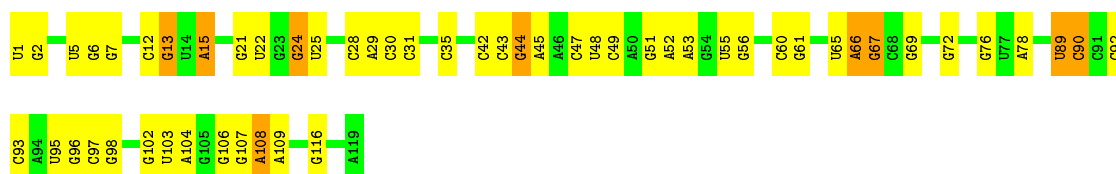




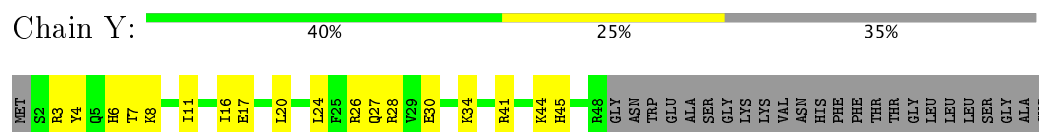




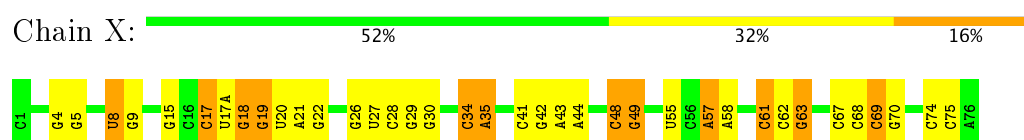
Response	Percentage
Yes	55%
No	38%
Don't know	8%



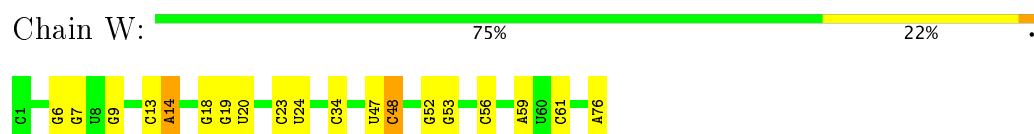
- Molecule 4: Alternative ribosome-rescue factor A



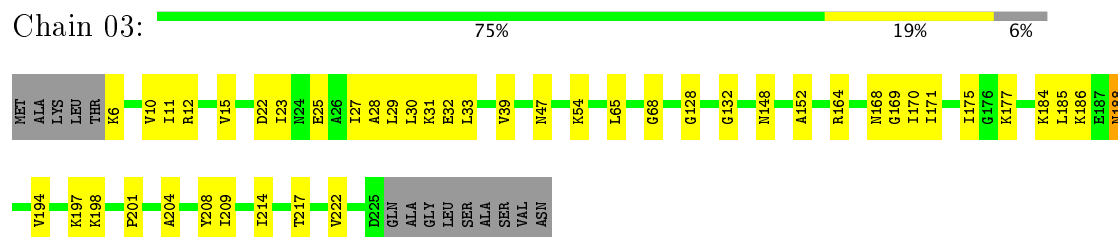
- Molecule 5: fMet-tRNA (P- and E-site)



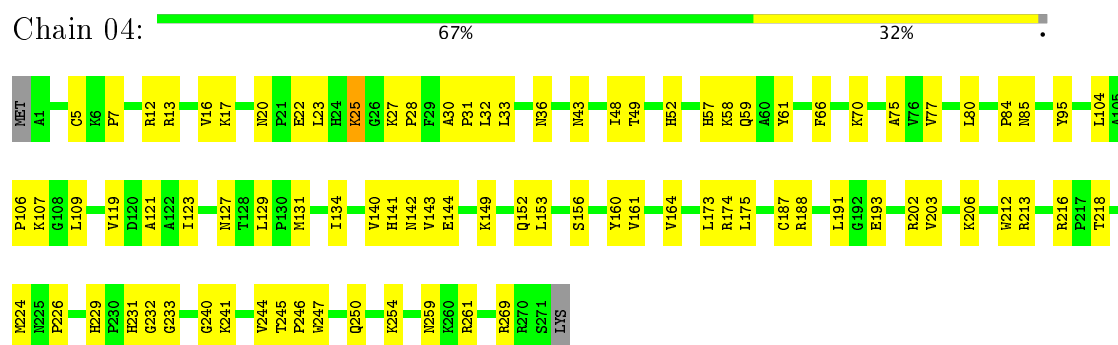
- Molecule 5: fMet-tRNA (P- and E-site)



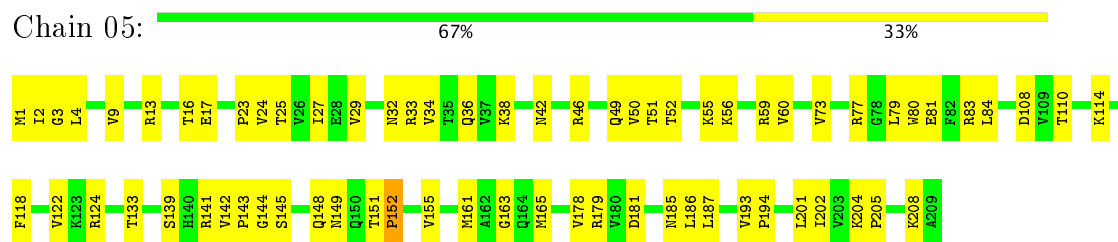
- Molecule 6: 50S ribosomal protein L1



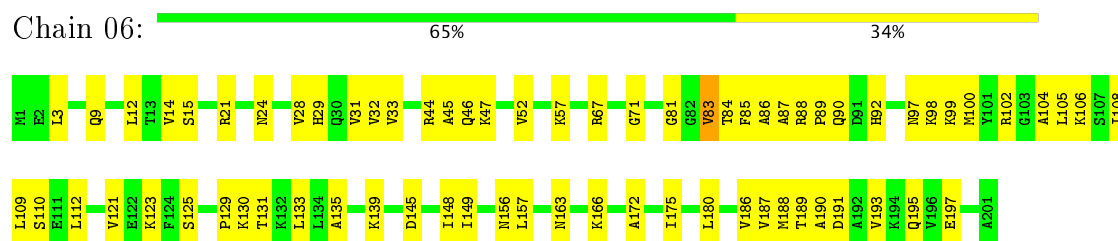
- Molecule 7: 50S ribosomal protein L2



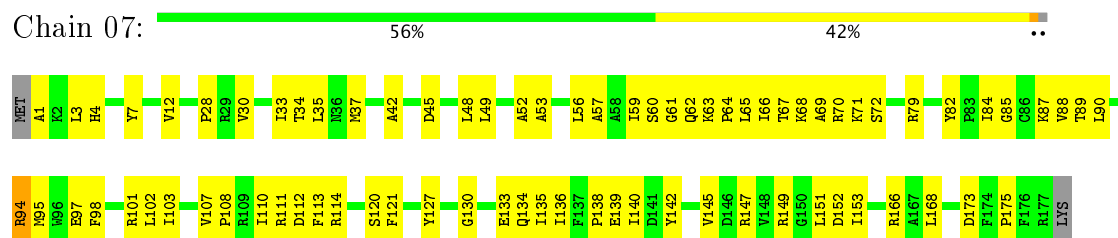
- Molecule 8: 50S ribosomal protein L3



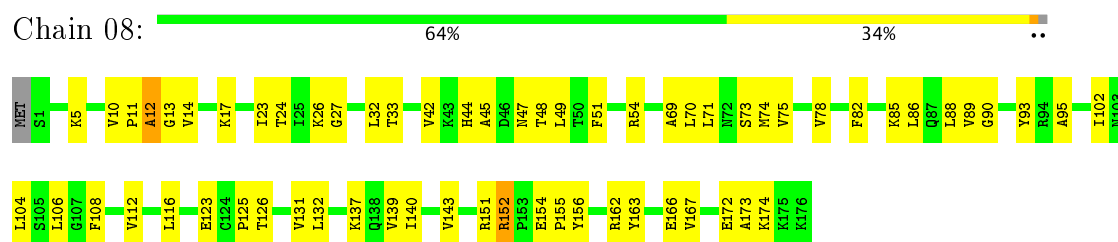
- Molecule 9: 50S ribosomal protein L4



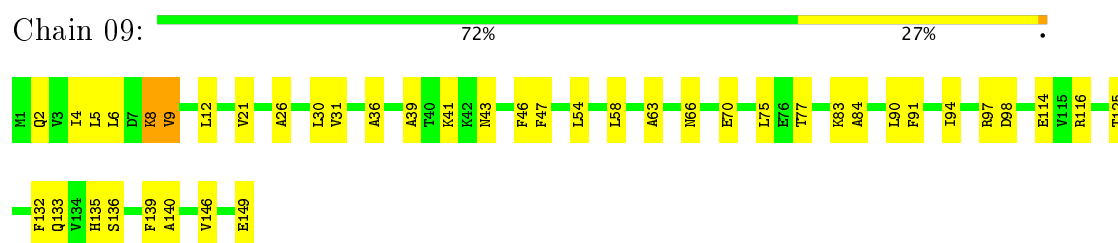
- Molecule 10: 50S ribosomal protein L5



- Molecule 11: 50S ribosomal protein L6

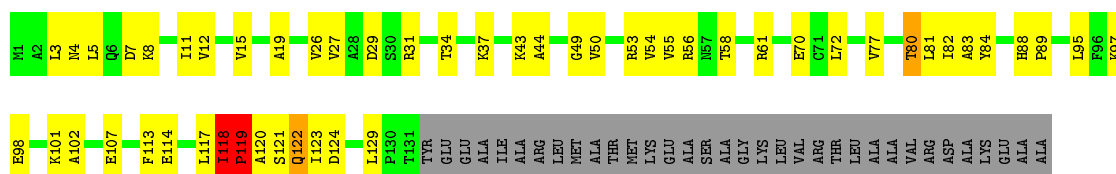


- Molecule 12: 50S ribosomal protein L9



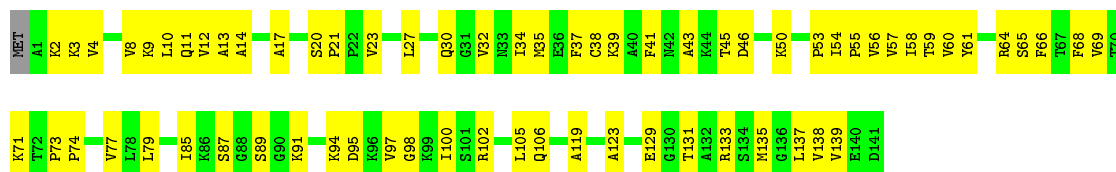
- Molecule 13: 50S ribosomal protein L10





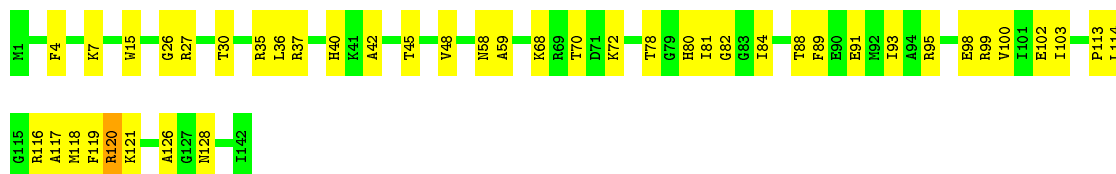
- Molecule 14: 50S ribosomal protein L11

Chain 11: 52% 47% .



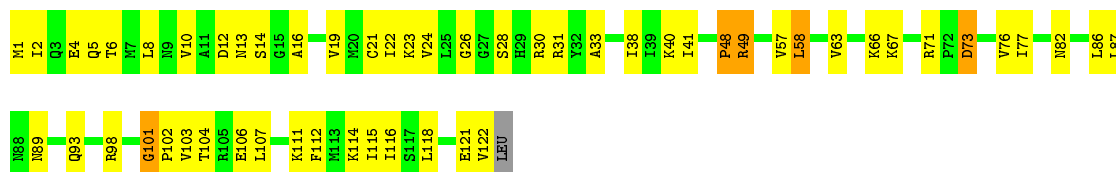
- Molecule 15: 50S ribosomal protein L13

Chain 12: 70% 30% .



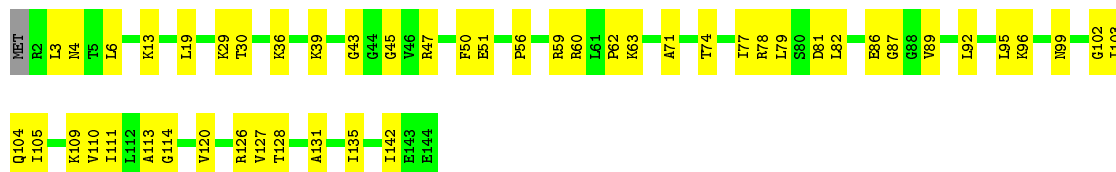
- Molecule 16: 50S ribosomal protein L14

Chain 13: 54% 41% . .



- Molecule 17: 50S ribosomal protein L15

Chain 14: 65% 34% .



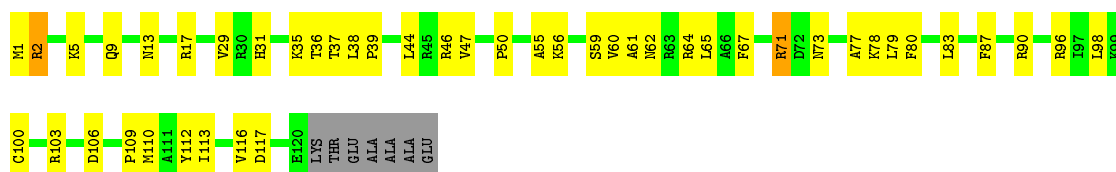
- Molecule 18: 50S ribosomal protein L16

Chain 15: 68% 30% .



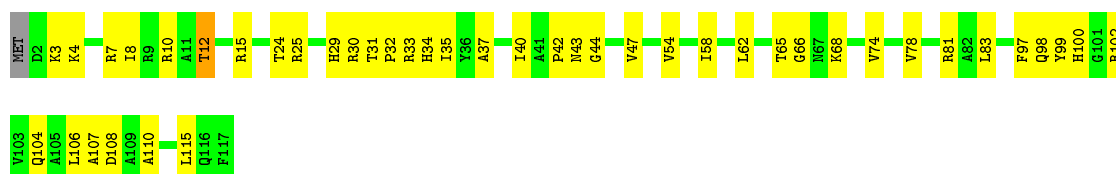
- Molecule 19: 50S ribosomal protein L17

Chain 16: 58% 35% 6%



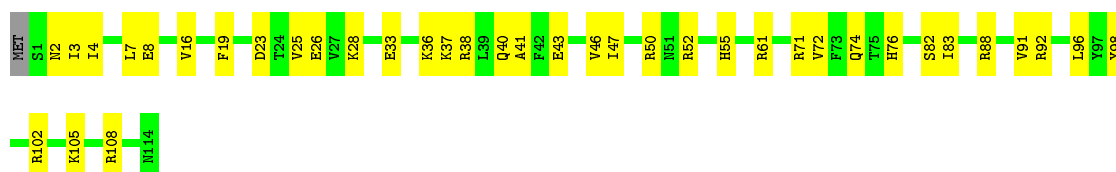
- Molecule 20: 50S ribosomal protein L18

Chain 17: 62% 36% 2%



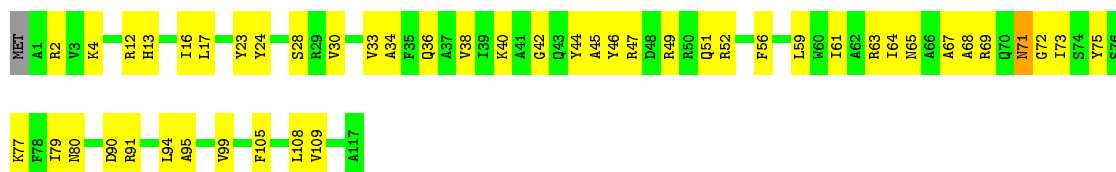
- Molecule 21: 50S ribosomal protein L19

Chain 18: 66% 33% 1%



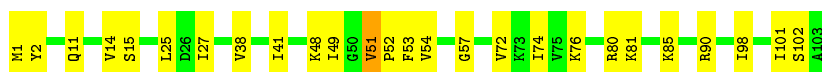
- Molecule 22: 50S ribosomal protein L20

Chain 19: 59% 39% 2%



- Molecule 23: 50S ribosomal protein L21

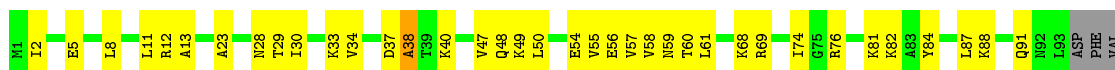
Chain 20: 75% 24% 1%



- Molecule 24: 50S ribosomal protein L22

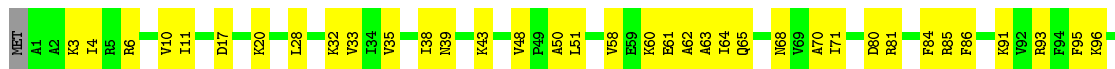


- Molecule 25: 50S ribosomal protein L23



GLY  
GLY  
ALA  
GLU

- Molecule 26: 50S ribosomal protein L24



E100  
I101  
I102  
LYS

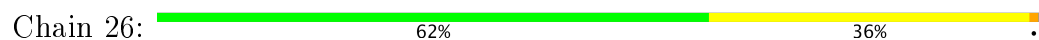
- Molecule 27: 50S ribosomal protein L25



- Molecule 28: 50S ribosomal protein L27



- Molecule 29: 50S ribosomal protein L28



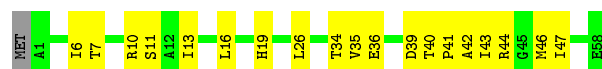
- Molecule 30: 50S ribosomal protein L29

Chain 27:  59% 38% .



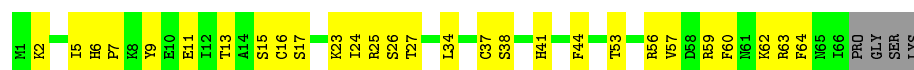
- Molecule 31: 50S ribosomal protein L30

Chain 28:  66% 32% .



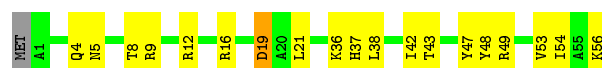
- Molecule 32: 50S ribosomal protein L31

Chain 29:  54% 40% 6%



- Molecule 33: 50S ribosomal protein L32

Chain 30:  65% 32% . .



- Molecule 34: 50S ribosomal protein L33

Chain 31:  71% 20% 9%




- Molecule 35: 50S ribosomal protein L34

Chain 32:  57% 43%



- Molecule 36: 50S ribosomal protein L35

Chain 33:  74% 22% . .



- Molecule 37: 50S ribosomal protein L36

Chain 34:  55% 42% .





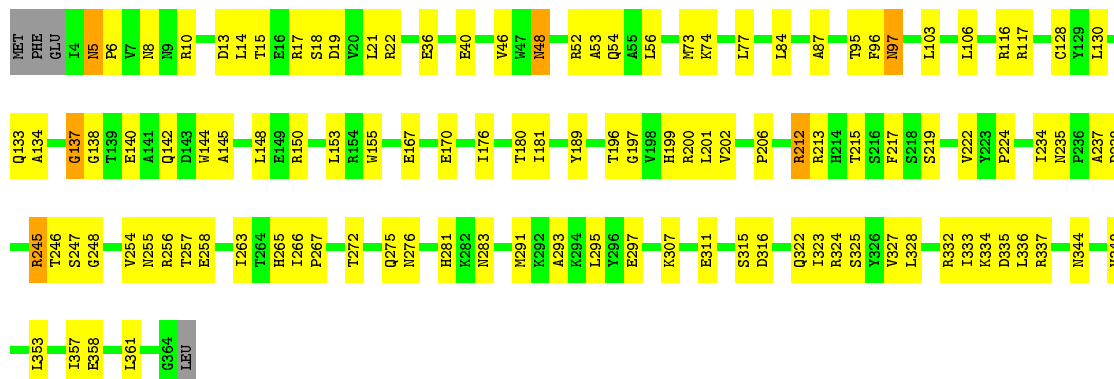
- Molecule 38: truncated mRNA

Chain V: 79% 21%



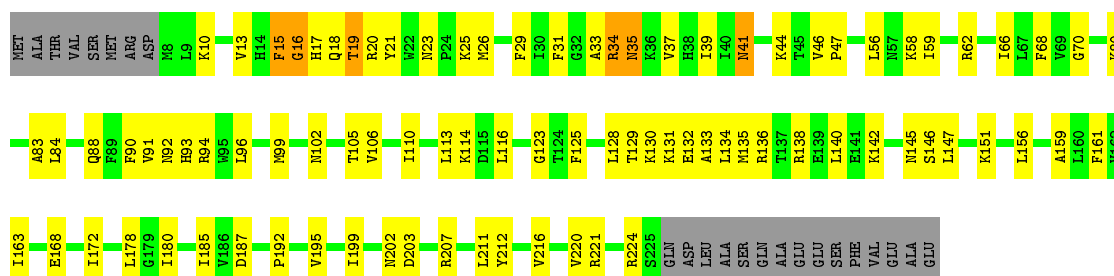
- Molecule 39: Peptide chain release factor RF2

Chain Z: 68% 30% ..



- Molecule 40: 30S ribosomal protein S2

Chain B: 54% 34% 10%

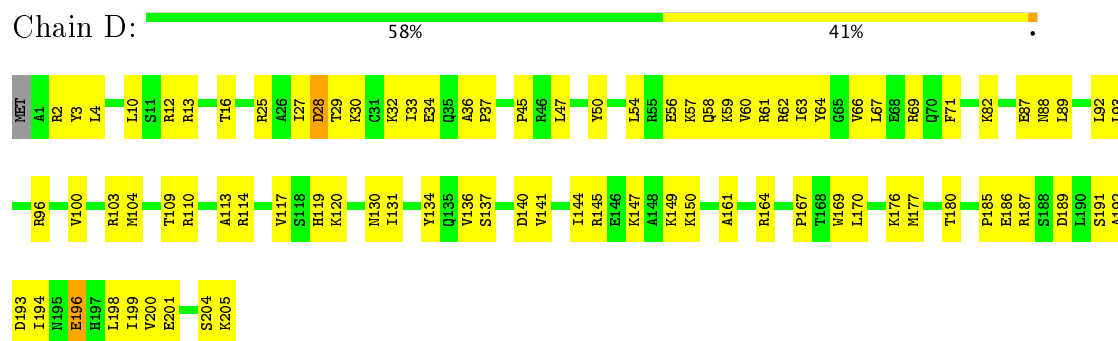


- Molecule 41: 30S ribosomal protein S3

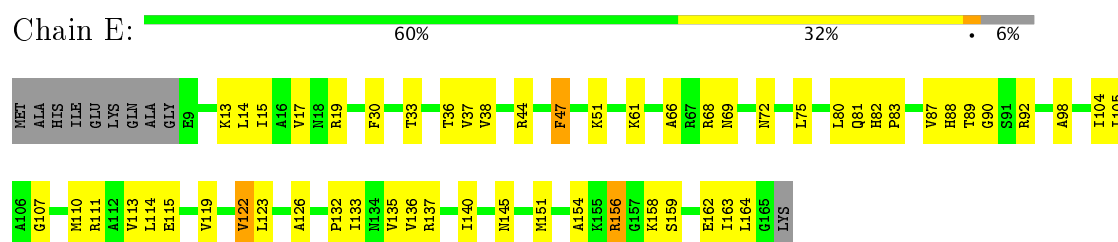
Chain C: 64% 25% 12%



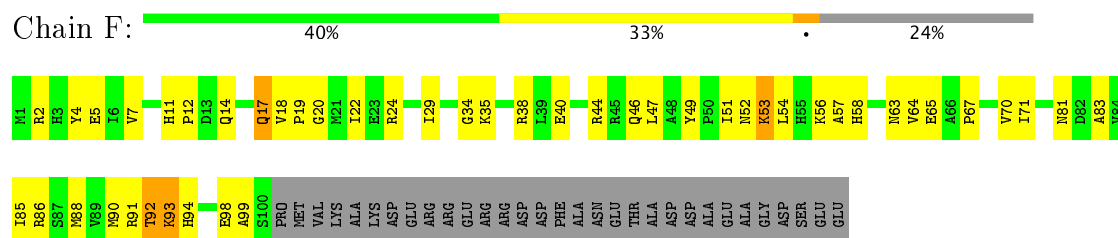
- Molecule 42: 30S ribosomal protein S4



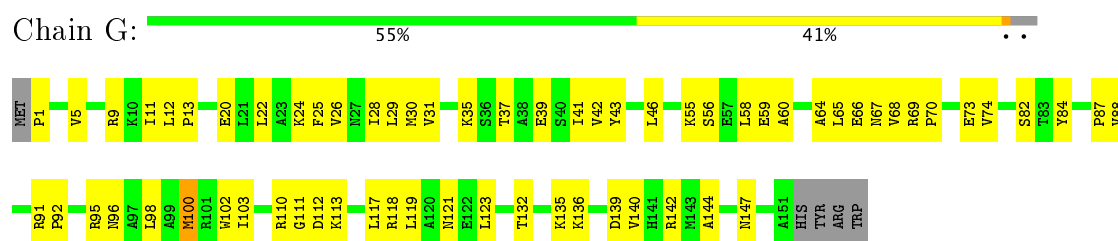
- Molecule 43: 30S ribosomal protein S5



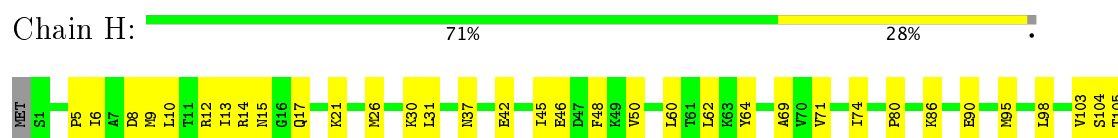
- Molecule 44: 30S ribosomal protein S6



- Molecule 45: 30S ribosomal protein S7



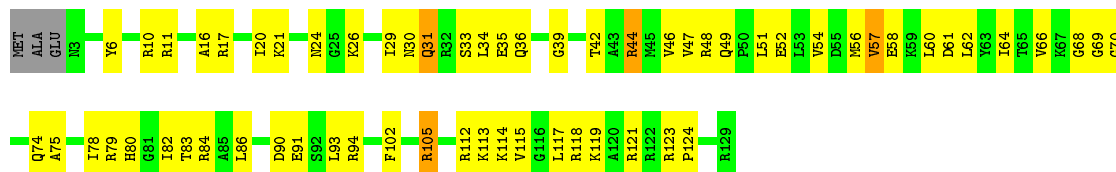
- Molecule 46: 30S ribosomal protein S8





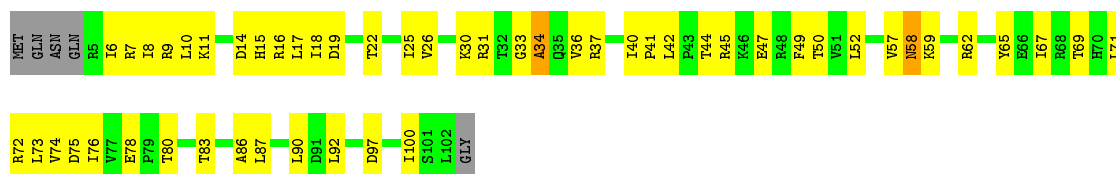
- Molecule 47: 30S ribosomal protein S9

Chain I: 



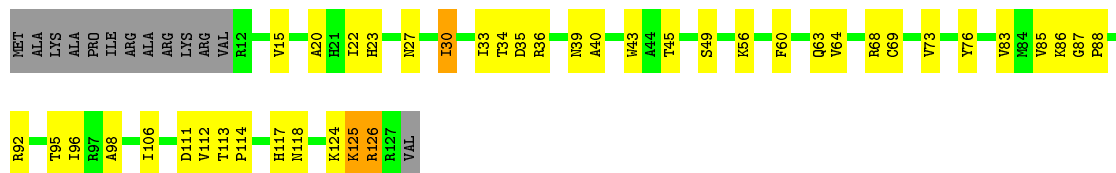
- Molecule 48: 30S ribosomal protein S10

Chain J: 



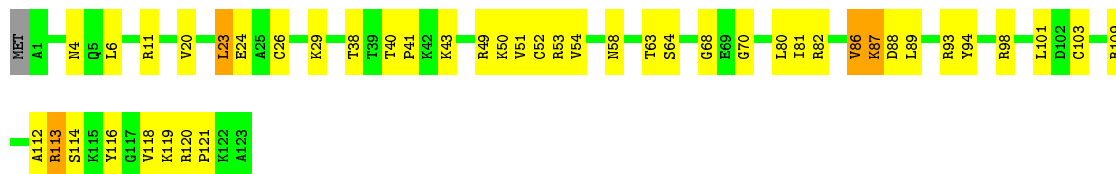
- Molecule 49: 30S ribosomal protein S11

Chain K: 



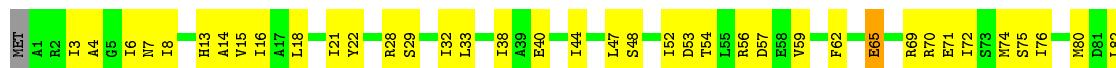
- Molecule 50: 30S ribosomal protein S12

Chain L: 



- Molecule 51: 30S ribosomal protein S13

Chain M: 





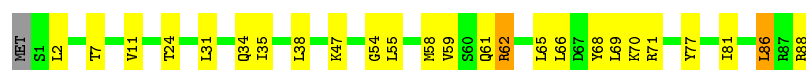
- Molecule 52: 30S ribosomal protein S14

Chain N: 47% 46% 6% ..



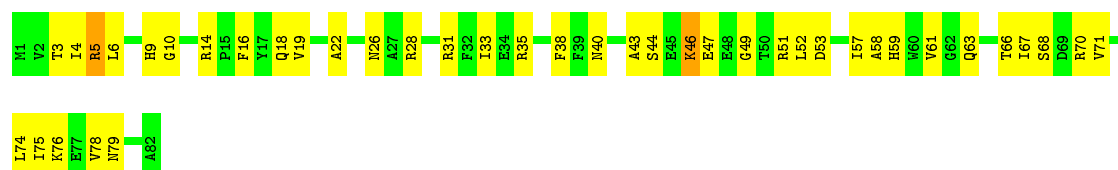
- Molecule 53: 30S ribosomal protein S15

Chain O: 71% 26% ..



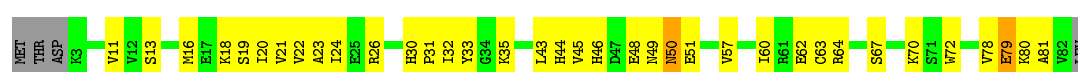
- Molecule 54: 30S ribosomal protein S16

Chain P: 50% 48% .



- Molecule 55: 30S ribosomal protein S17

Chain Q: 52% 40% . 5%



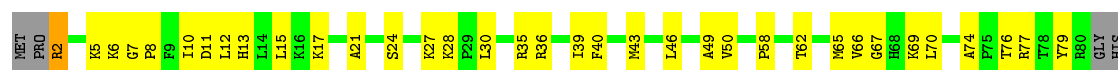
- Molecule 56: 30S ribosomal protein S18

Chain R: 57% 28% . 13%



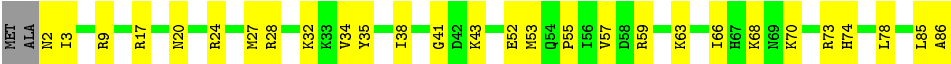
- Molecule 57: 30S ribosomal protein S19

Chain S: 48% 37% . 14%

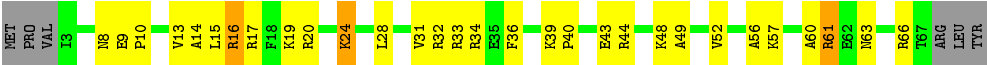


ALA  
ALA  
ASP  
LYS  
LYS  
ALA  
LYS  
LYS  
LYS

- Molecule 58: 30S ribosomal protein S20



- Molecule 59: 30S ribosomal protein S21



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	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	A	0.25	0/36963	0.65	0/57662
10	07	0.32	0/1434	0.56	0/1926
11	08	0.30	0/1343	0.60	0/1816
12	09	0.32	0/1122	0.64	0/1515
13	10	0.40	0/1001	0.93	3/1350 (0.2%)
14	11	0.32	0/1046	0.60	0/1410
15	12	0.31	0/1152	0.56	0/1551
16	13	0.32	0/947	0.63	1/1268 (0.1%)
17	14	0.31	0/1054	0.58	0/1403
18	15	0.33	0/1093	0.59	0/1460
19	16	0.32	0/973	0.57	0/1301
2	01	0.25	0/69797	0.65	1/108890 (0.0%)
20	17	0.29	0/902	0.54	0/1209
21	18	0.31	0/929	0.56	0/1242
22	19	0.30	0/960	0.47	0/1278
23	20	0.33	0/829	0.64	1/1107 (0.1%)
24	21	0.29	0/864	0.59	0/1156
25	22	0.31	0/744	0.59	0/994
26	23	0.33	0/787	0.59	0/1051
27	24	0.31	0/766	0.53	0/1025
28	25	0.34	0/582	0.59	0/769
29	26	0.31	0/635	0.54	0/848
3	02	0.26	0/2847	0.65	0/4440
30	27	0.28	0/510	0.49	0/677
31	28	0.29	0/453	0.55	0/605
32	29	0.34	0/531	0.56	0/709
33	30	0.30	0/450	0.57	0/599
34	31	0.33	0/416	0.54	0/554
35	32	0.32	0/380	0.57	0/498
36	33	0.30	0/513	0.58	0/676
37	34	0.23	0/303	0.40	0/397
38	V	0.20	0/345	0.60	0/538

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	Z	0.28	0/2884	0.49	0/3884
4	Y	0.30	0/383	0.51	0/504
40	B	0.32	0/1735	0.58	1/2338 (0.0%)
41	C	0.30	0/1651	0.54	0/2225
42	D	0.29	0/1665	0.58	0/2227
43	E	0.33	0/1169	0.66	0/1573
44	F	0.33	0/835	0.71	2/1128 (0.2%)
45	G	0.29	0/1195	0.53	0/1602
46	H	0.29	0/989	0.56	0/1326
47	I	0.31	0/1034	0.63	0/1375
48	J	0.29	0/796	0.60	0/1077
49	K	0.32	0/885	0.59	1/1195 (0.1%)
5	W	0.24	0/1832	0.64	0/2855
5	X	0.29	0/1811	0.66	0/2822
50	L	0.32	0/969	0.68	0/1300
51	M	0.28	0/892	0.59	0/1193
52	N	0.37	0/817	0.73	3/1088 (0.3%)
53	O	0.28	0/722	0.50	0/964
54	P	0.34	0/659	0.60	0/884
55	Q	0.33	0/657	0.59	0/881
56	R	0.29	0/544	0.51	0/731
57	S	0.32	0/652	0.58	0/877
58	T	0.30	0/671	0.48	0/888
59	U	0.36	0/550	0.71	0/728
6	03	0.29	0/1361	0.57	0/1796
7	04	0.30	0/2121	0.61	0/2852
8	05	0.33	0/1586	0.60	0/2134
9	06	0.31	0/1571	0.59	0/2113
All	All	0.27	0/165307	0.63	13/246484 (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
52	N	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	10	118	ILE	C-N-CD	-18.15	80.67	120.60
13	10	118	ILE	C-N-CA	7.52	153.59	122.00
52	N	55	SER	N-CA-C	6.88	129.58	111.00
49	K	125	LYS	N-CA-C	6.75	129.21	111.00
40	B	16	GLY	N-CA-C	6.51	129.38	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	N	86	ALA	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	33012	0	16618	477	0
2	01	62318	0	31345	788	0
3	02	2546	0	1292	50	0
4	Y	377	0	383	29	0
5	W	1640	0	837	11	0
5	X	1622	0	827	28	0
6	03	1353	0	1159	38	0
7	04	2082	0	2157	78	0
8	05	1565	0	1616	68	0
9	06	1552	0	1619	56	0
10	07	1410	0	1447	72	0
11	08	1323	0	1374	56	0
12	09	1111	0	1148	31	0
13	10	988	0	1025	47	0
14	11	1032	0	1088	56	0
15	12	1129	0	1162	44	0
16	13	938	0	1012	51	0
17	14	1045	0	1117	46	0
18	15	1074	0	1157	38	0
19	16	960	0	1000	47	0
20	17	892	0	923	39	0
21	18	917	0	965	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	19	947	0	1022	45	0
23	20	816	0	839	25	0
24	21	857	0	922	23	0
25	22	738	0	807	26	0
26	23	779	0	834	32	0
27	24	753	0	780	27	0
28	25	575	0	592	30	0
29	26	625	0	655	25	0
30	27	509	0	543	25	0
31	28	449	0	491	14	0
32	29	522	0	524	26	0
33	30	444	0	461	24	0
34	31	409	0	440	8	0
35	32	377	0	418	19	0
36	33	504	0	574	19	0
37	34	302	0	340	23	0
38	V	306	0	154	1	0
39	Z	2844	0	2739	113	0
40	B	1704	0	1732	77	0
41	C	1624	0	1699	50	0
42	D	1643	0	1710	82	0
43	E	1156	0	1199	55	0
44	F	817	0	808	36	0
45	G	1181	0	1240	45	0
46	H	979	0	1034	32	0
47	I	1022	0	1070	65	0
48	J	786	0	828	54	0
49	K	869	0	878	44	0
50	L	955	0	1019	42	0
51	M	883	0	944	52	0
52	N	805	0	847	63	0
53	O	714	0	737	19	0
54	P	649	0	666	39	0
55	Q	648	0	691	35	0
56	R	535	0	552	19	0
57	S	637	0	665	45	0
58	T	665	0	714	23	0
59	U	544	0	579	43	0
60	01	221	0	0	0	0
60	02	6	0	0	0	0
60	17	1	0	0	0	0
60	19	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	30	1	0	0	0	0
60	31	1	0	0	0	0
60	34	1	0	0	0	0
60	A	118	0	0	0	0
60	I	1	0	0	0	0
60	V	1	0	0	0	0
60	W	3	0	0	0	0
60	X	5	0	0	0	0
61	34	1	0	0	0	0
All	All	152819	0	104018	3184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 3184 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)
2:01:45:G:H5''	2:01:46:G:H5'	1.26	1.14
1:A:291:U:H2'	1:A:292:G:H5''	1.31	1.12
13:10:117:LEU:C	13:10:119:PRO:HD2	1.71	1.10
1:A:376:G:H2'	1:A:377:G:H5''	1.35	1.07
51:M:3:ILE:HG12	51:M:7:ASN:HB2	1.25	1.07

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	
4	Y	45/72 (62%)	40 (89%)	5 (11%)	0	100	100
6	03	218/234 (93%)	195 (89%)	23 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	04	269/273 (98%)	242 (90%)	25 (9%)	2 (1%)	25	68
8	05	207/209 (99%)	189 (91%)	17 (8%)	1 (0%)	32	74
9	06	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	18	61
10	07	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
11	08	174/177 (98%)	154 (88%)	17 (10%)	3 (2%)	11	48
12	09	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	9	44
13	10	129/165 (78%)	95 (74%)	28 (22%)	6 (5%)	3	20
14	11	139/142 (98%)	120 (86%)	18 (13%)	1 (1%)	25	68
15	12	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
16	13	120/123 (98%)	100 (83%)	18 (15%)	2 (2%)	11	48
17	14	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
18	15	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	12	51
19	16	118/127 (93%)	106 (90%)	11 (9%)	1 (1%)	22	65
20	17	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	20	64
21	18	112/115 (97%)	98 (88%)	14 (12%)	0	100	100
22	19	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
23	20	101/103 (98%)	84 (83%)	16 (16%)	1 (1%)	18	61
24	21	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
25	22	91/100 (91%)	77 (85%)	13 (14%)	1 (1%)	17	58
26	23	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
27	24	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
28	25	73/85 (86%)	60 (82%)	11 (15%)	2 (3%)	6	35
29	26	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
30	27	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
31	28	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
32	29	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
33	30	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
34	31	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
35	32	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	7	40
36	33	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	30
37	34	36/38 (95%)	31 (86%)	5 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Z	359/365 (98%)	332 (92%)	26 (7%)	1 (0%)	44	81
40	B	216/241 (90%)	188 (87%)	26 (12%)	2 (1%)	20	64
41	C	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
42	D	203/206 (98%)	177 (87%)	25 (12%)	1 (0%)	32	74
43	E	155/167 (93%)	125 (81%)	29 (19%)	1 (1%)	28	72
44	F	98/131 (75%)	77 (79%)	16 (16%)	5 (5%)	2	18
45	G	149/156 (96%)	134 (90%)	14 (9%)	1 (1%)	25	68
46	H	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
47	I	125/130 (96%)	101 (81%)	22 (18%)	2 (2%)	11	50
48	J	96/103 (93%)	85 (88%)	9 (9%)	2 (2%)	8	42
49	K	114/129 (88%)	102 (90%)	11 (10%)	1 (1%)	20	64
50	L	121/124 (98%)	92 (76%)	23 (19%)	6 (5%)	2	19
51	M	112/118 (95%)	94 (84%)	16 (14%)	2 (2%)	10	47
52	N	98/101 (97%)	79 (81%)	13 (13%)	6 (6%)	2	13
53	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
54	P	80/82 (98%)	65 (81%)	13 (16%)	2 (2%)	6	38
55	Q	78/84 (93%)	63 (81%)	14 (18%)	1 (1%)	14	55
56	R	63/75 (84%)	60 (95%)	3 (5%)	0	100	100
57	S	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	14	55
58	T	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
59	U	63/71 (89%)	44 (70%)	17 (27%)	2 (3%)	5	30
All	All	6468/6864 (94%)	5705 (88%)	696 (11%)	67 (1%)	23	61

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	06	83	VAL
11	08	12	ALA
12	09	9	VAL
13	10	55	VAL
13	10	119	PRO

### 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	
4	Y	38/59 (64%)	38 (100%)	0	100	100
6	03	106/181 (59%)	104 (98%)	2 (2%)	62	86
7	04	216/218 (99%)	213 (99%)	3 (1%)	71	90
8	05	164/164 (100%)	162 (99%)	2 (1%)	75	91
9	06	165/165 (100%)	164 (99%)	1 (1%)	89	96
10	07	148/150 (99%)	147 (99%)	1 (1%)	87	96
11	08	137/138 (99%)	136 (99%)	1 (1%)	87	96
12	09	114/114 (100%)	113 (99%)	1 (1%)	82	94
13	10	100/123 (81%)	98 (98%)	2 (2%)	60	86
14	11	109/110 (99%)	109 (100%)	0	100	100
15	12	116/116 (100%)	115 (99%)	1 (1%)	82	94
16	13	103/104 (99%)	99 (96%)	4 (4%)	37	74
17	14	102/103 (99%)	101 (99%)	1 (1%)	80	93
18	15	109/109 (100%)	107 (98%)	2 (2%)	64	87
19	16	100/104 (96%)	99 (99%)	1 (1%)	80	93
20	17	86/87 (99%)	84 (98%)	2 (2%)	56	84
21	18	99/100 (99%)	98 (99%)	1 (1%)	80	93
22	19	89/90 (99%)	88 (99%)	1 (1%)	78	92
23	20	84/84 (100%)	84 (100%)	0	100	100
24	21	93/93 (100%)	92 (99%)	1 (1%)	78	92
25	22	80/84 (95%)	80 (100%)	0	100	100
26	23	83/85 (98%)	83 (100%)	0	100	100
27	24	78/78 (100%)	77 (99%)	1 (1%)	73	91
28	25	57/63 (90%)	56 (98%)	1 (2%)	64	87
29	26	67/68 (98%)	66 (98%)	1 (2%)	70	90
30	27	55/55 (100%)	53 (96%)	2 (4%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	28	48/49 (98%)	48 (100%)	0	100	100
32	29	59/62 (95%)	59 (100%)	0	100	100
33	30	47/48 (98%)	46 (98%)	1 (2%)	59	85
34	31	45/49 (92%)	44 (98%)	1 (2%)	57	85
35	32	38/38 (100%)	38 (100%)	0	100	100
36	33	51/52 (98%)	51 (100%)	0	100	100
37	34	34/34 (100%)	33 (97%)	1 (3%)	48	80
39	Z	303/311 (97%)	298 (98%)	5 (2%)	66	88
40	B	180/199 (90%)	176 (98%)	4 (2%)	57	85
41	C	170/190 (90%)	170 (100%)	0	100	100
42	D	172/173 (99%)	169 (98%)	3 (2%)	66	88
43	E	119/126 (94%)	116 (98%)	3 (2%)	53	83
44	F	87/112 (78%)	85 (98%)	2 (2%)	56	84
45	G	124/129 (96%)	122 (98%)	2 (2%)	68	89
46	H	104/105 (99%)	103 (99%)	1 (1%)	80	93
47	I	105/107 (98%)	102 (97%)	3 (3%)	48	80
48	J	86/90 (96%)	85 (99%)	1 (1%)	75	91
49	K	89/99 (90%)	86 (97%)	3 (3%)	42	77
50	L	103/104 (99%)	102 (99%)	1 (1%)	80	93
51	M	92/96 (96%)	92 (100%)	0	100	100
52	N	83/84 (99%)	83 (100%)	0	100	100
53	O	76/77 (99%)	74 (97%)	2 (3%)	51	83
54	P	65/65 (100%)	63 (97%)	2 (3%)	45	79
55	Q	74/78 (95%)	73 (99%)	1 (1%)	71	90
56	R	56/65 (86%)	55 (98%)	1 (2%)	64	87
57	S	70/79 (89%)	69 (99%)	1 (1%)	71	90
58	T	65/66 (98%)	64 (98%)	1 (2%)	70	90
59	U	55/61 (90%)	53 (96%)	2 (4%)	40	76
All	All	5298/5593 (95%)	5225 (99%)	73 (1%)	74	90

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	31	25	ASN
40	B	15	PHE
55	Q	79	GLU
39	Z	97	ASN
40	B	35	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
29	26	15	ASN
39	Z	5	ASN
52	N	59	GLN
30	27	20	ASN
33	30	40	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1538/1539 (99%)	182 (11%)	1 (0%)
2	01	2902/2903 (99%)	320 (11%)	6 (0%)
3	02	118/119 (99%)	11 (9%)	1 (0%)
38	V	13/14 (92%)	1 (7%)	0
5	W	76/77 (98%)	8 (10%)	0
5	X	76/77 (98%)	19 (25%)	1 (1%)
All	All	4723/4729 (99%)	541 (11%)	9 (0%)

5 of 541 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	6	G
1	A	9	G
1	A	22	G
1	A	31	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	01	1130	U
5	X	17(A)	U
2	01	2326	C

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Mol	Chain	Res	Type
2	01	859	G
2	01	2296	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 361 ligands modelled in this entry, 361 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](#)

There are no chain breaks in this entry.