



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 7, 2016 – 08:35 PM EST

PDB ID : 5T5H
EMDB ID: : EMD-8361
Title : Structure and assembly model for the Trypanosoma cruzi 60S ribosomal subunit
Authors : Liu, Z.; Gutierrez-Vargas, C.; Wei, J.; Grassucci, R.A.; Ramesh, M.; Espina, N.; Sun, M.; Tutuncuoglu, B.; Madison-Antenucci, S.; Woolford Jr., J.L.; Tong, L.; Frank, J.
Deposited on : 2016-08-31
Resolution : 2.54 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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

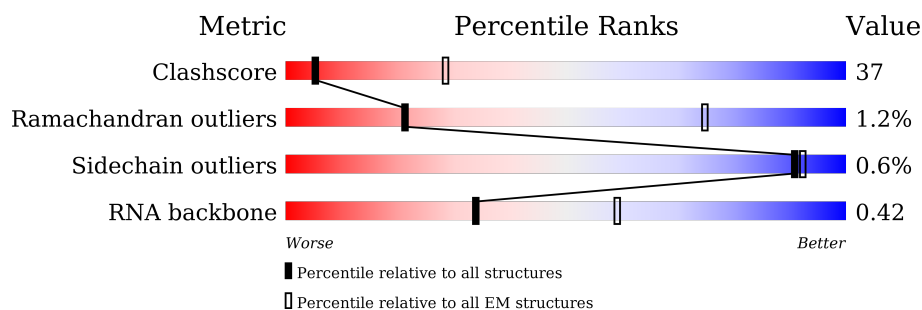
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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.



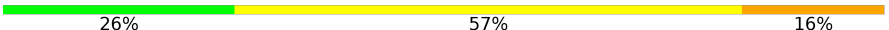



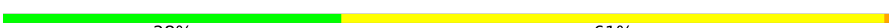
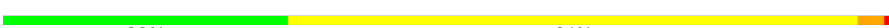







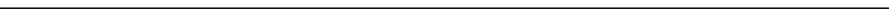




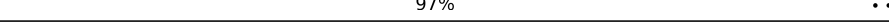
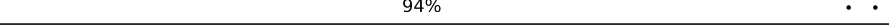
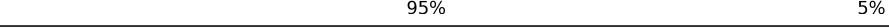
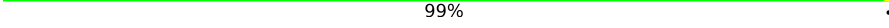
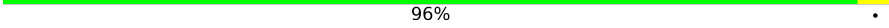
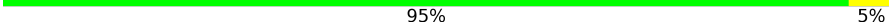

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	1278	24% 52% 23% .
2	B	941	23% 55% 22%
3	C	169	20% 48% 18% . 13%
4	D	118	20% 61% 15% .
5	E	146	21% 59% 18% .
6	F	46	26% 33% 41%
7	G	123	27% 51% 19% . .


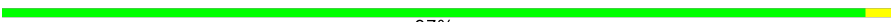







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	91	
9	I	192	
10	L	65	
11	N	205	
12	O	203	
13	P	149	
14	Q	203	
15	R	152	
16	S	177	
17	T	150	
18	U	146	
19	V	99	
20	W	127	
21	X	116	
22	Y	61	
23	Z	113	
24	a	132	
25	b	144	
26	c	125	
27	d	63	
28	e	245	
29	f	397	
30	g	66	
31	h	169	
32	i	113	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	j	104	 100%
34	k	120	 93% 6%
35	l	136	 97%
36	m	95	 97%
37	n	81	 99%
38	o	85	 96%
39	p	58	 88% 10%
40	q	50	 98%
41	r	337	 96%
42	t	93	 99%
43	u	254	 75% 24%
44	v	171	 76% 23%
45	w	215	 99%
46	x	223	 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	OMC	A	1053	-	-	X	-
1	OMC	A	919	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 105124 atoms, of which 12 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 RNA LARGE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1278	Total	C	H	N	O	P	0	0
			27453	12272	12	5035	8856	1278		

- Molecule 2 is a RNA chain called RNA LARGE SUBUNIT BETA, RNA LARGE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	941	Total	C	N	O	P	0	0
			20110	9007	3606	6556	941		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	147	Total	C	N	O	P	0	0
			3140	1408	557	1028	147		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	114	Total	C	N	O	P	0	0
			2432	1084	435	799	114		

- Molecule 5 is a RNA chain called srRNA1, srRNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	146	Total	C	N	O	P	0	0
			3110	1390	552	1022	146		

- Molecule 6 is a RNA chain called srRNA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	46	Total	C	N	O	P	0	0
			965	433	165	321	46		

- Molecule 7 is a RNA chain called srRNA2,srRNA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	121	Total	C	N	O	P	0	0
			2578	1150	455	852	121		

- Molecule 8 is a RNA chain called srRNA4,srRNA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	P	0	0
			1946	867	354	634	91		

- Molecule 9 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1515	951	308	250	6		

- Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	65	Total	C	N	O	S	0	0
			535	333	112	85	5		

- Molecule 11 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	172	Total	C	N	O	S	0	0
			1413	892	291	224	6		

- Molecule 12 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	203	Total	C	N	O	S	0	1
			1642	1046	322	269	5		

- Molecule 13 is a protein called 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	149	Total	C	N	O	S	0	0
			1186	746	235	203	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	72	LYS	ARG	conflict	UNP Q4DQ35

- Molecule 14 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	203	Total	C	N	O	S	1	0
			1710	1076	365	263	6		

- Molecule 15 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	152	Total	C	N	O	S	0	0
			1226	768	243	205	10		

- Molecule 16 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	177	Total	C	N	O	S	0	0
			1449	919	282	242	6		

- Molecule 17 is a protein called Ribosomal protein L19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	150	Total	C	N	O	S	0	0
			1273	789	273	205	6		

- Molecule 18 is a protein called Ribosomal protein L21E (60S).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	126	Total	C	N	O	S	0	0
			1016	642	207	163	4		

- Molecule 19 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	85	Total	C	N	O	S	0	0
			730	481	127	120	2		

- Molecule 20 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	127	Total	C	N	O	S	0	0
			960	611	180	166	3		

- Molecule 21 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	109	Total	C	N	O	S	0	0
			890	565	164	157	4		

- Molecule 22 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	61	Total	C	N	O	S	0	0
			519	340	98	77	4		

- Molecule 23 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	113	Total	C	N	O	S	0	0
			919	571	195	150	3		

- Molecule 24 is a protein called Ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	105	Total	C	N	O	S	0	0
			877	565	175	135	2		

- Molecule 25 is a protein called 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	144	Total	C	N	O	S	0	0
			1135	720	226	185	4		

- Molecule 26 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	120	Total	C	N	O	S	0	0
			935	583	187	161	4		

- Molecule 27 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	63	Total	C	N	O	S	0	0
			518	314	122	81	1		

- Molecule 28 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	245	Total	C	N	O	S	0	0
			1874	1170	379	314	11		

- Molecule 29 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	397	Total	C	N	O	S	0	0
			3189	2010	630	537	12		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	66	Total	C	N	O	S	0	0
			523	335	91	93	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	91	VAL	ALA	conflict	UNP Q4DIC9
g	92	LEU	GLY	conflict	UNP Q4DIC9
g	93	SER	ASN	conflict	UNP Q4DIC9
g	94	ILE	ASN	conflict	UNP Q4DIC9
g	95	THR	LEU	conflict	UNP Q4DIC9
g	97	VAL	LEU	conflict	UNP Q4DIC9

- Molecule 31 is a protein called 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	150	Total	C	N	O	S	0	0
			1064	671	208	183	2		

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	113	Total	C	N	O	S	0	0
			928	585	185	154	4		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	104	Total	C	N	O	S	0	0
			863	532	191	137	3		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	113	Total	C	N	O	S	0	0
			967	602	212	150	3		

- Molecule 35 is a protein called Ribosomal protein L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1057	662	217	174	4		

- Molecule 36 is a protein called Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	95	Total	C	N	O	S	0	0
			757	474	159	121	3		

- Molecule 37 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	81	Total	C	N	O	S	0	0
			679	413	154	106	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	64	MET	CYS	conflict	UNP Q4DXW6

- Molecule 38 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	85	Total	C	N	O	S	0	0
			669	413	141	108	7		

- Molecule 39 is a protein called Ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	52	Total	C	N	O	S	0	0
			432	277	82	71	2		

- Molecule 40 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	50	Total	C	N	O		0	0
			456	297	98	61			

- Molecule 41 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	325	Total	C	N	O	S	0	0
			2513	1575	489	434	15		

- Molecule 42 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	93	Total	C	N	O	S	0	0
			763	486	149	123	5		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	193	Total	C	N	O	S	0	0
			1541	982	292	262	5		

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	132	Total	C	N	O	S	0	0
			1037	661	194	179	3		

- Molecule 45 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	215	Total	C	N	O	S	0	0
			1749	1110	342	288	9		

- Molecule 46 is a protein called Ribosomal protein L7a-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	208	Total	C	N	O	S	0	0
			1690	1062	338	284	6		

- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	G	1	Total	Mg	0
			1	1	
47	D	1	Total	Mg	0
			1	1	
47	E	1	Total	Mg	0
			1	1	
47	H	1	Total	Mg	0
			1	1	
47	B	32	Total	Mg	0
			32	32	
47	C	2	Total	Mg	0
			2	2	
47	A	66	Total	Mg	0
			66	66	
47	F	1	Total	Mg	0
			1	1	

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	Zn	0
			1	1	
48	t	1	Total	Zn	0
			1	1	
48	n	1	Total	Zn	0
			1	1	

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	A	38	Total	O	0
			38	38	
49	B	26	Total	O	0
			26	26	
49	C	1	Total	O	0
			1	1	

Continued on next page...

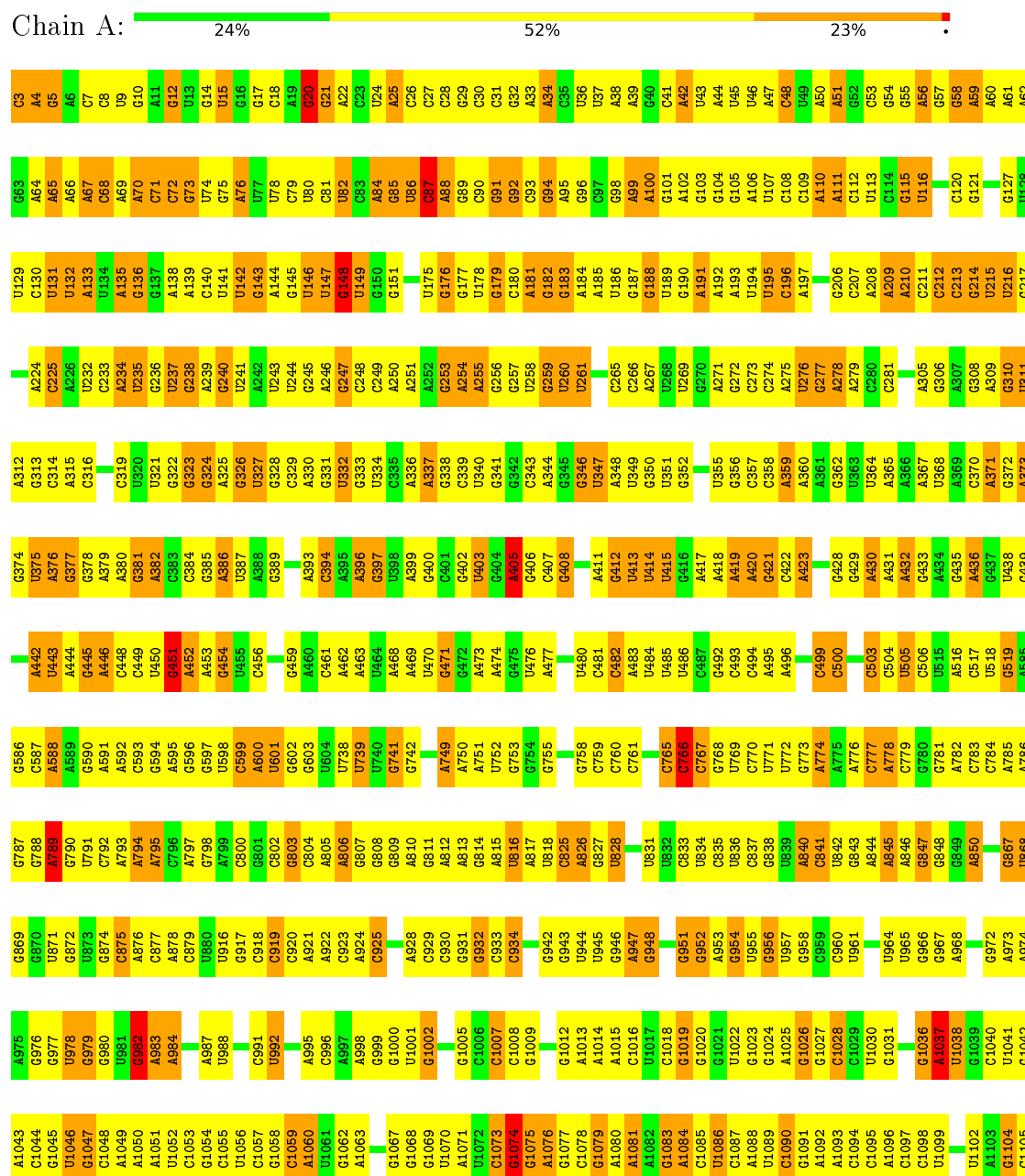
Continued from previous page...

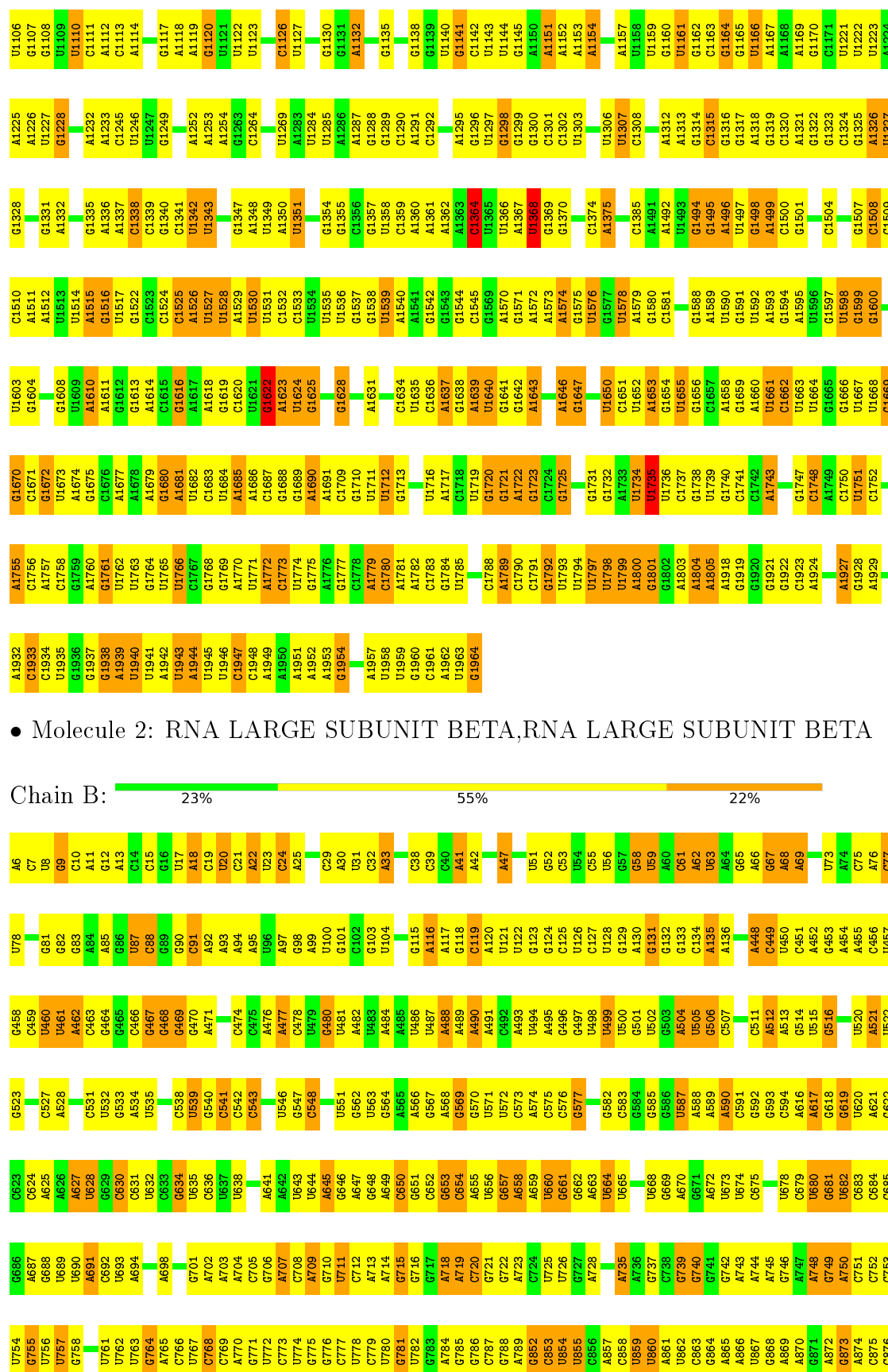
Mol	Chain	Residues	Atoms		AltConf
49	E	1	Total 1	O 1	0
49	G	3	Total 3	O 3	0
49	H	2	Total 2	O 2	0
49	I	1	Total 1	O 1	0
49	R	1	Total 1	O 1	0
49	a	1	Total 1	O 1	0
49	b	1	Total 1	O 1	0
49	e	2	Total 2	O 2	0
49	f	1	Total 1	O 1	0
49	j	1	Total 1	O 1	0
49	k	1	Total 1	O 1	0
49	n	1	Total 1	O 1	0
49	w	1	Total 1	O 1	0
49	x	1	Total 1	O 1	0

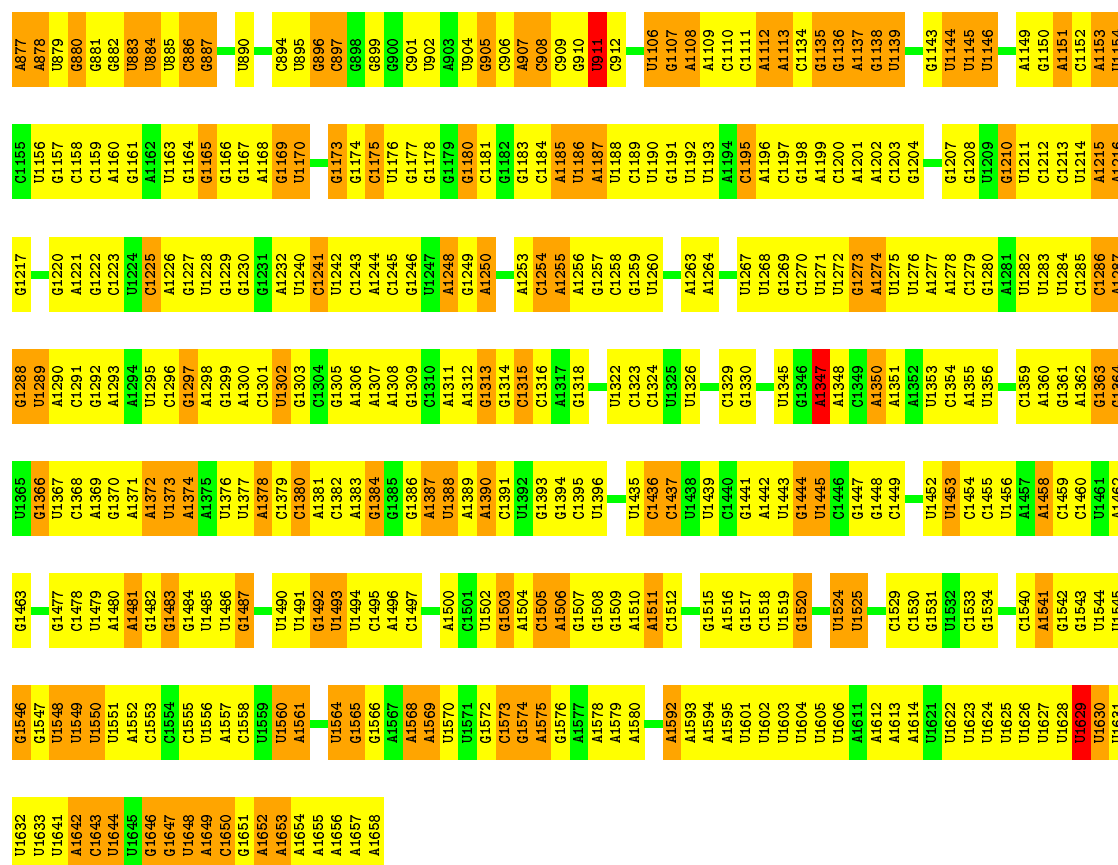
3 Residue-property plots

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

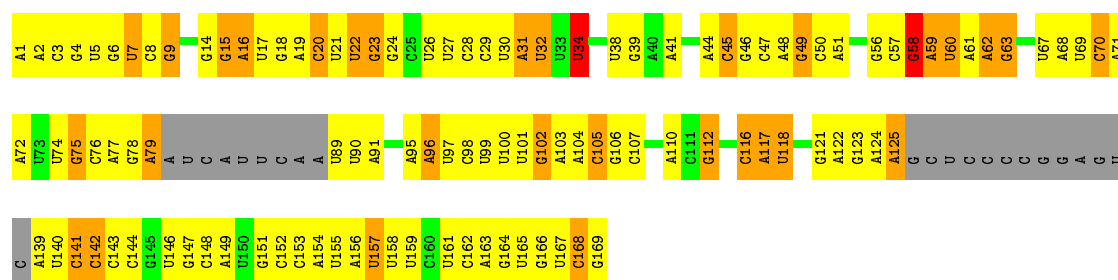
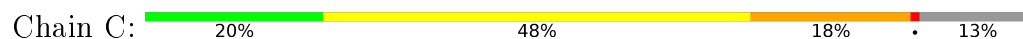
• Molecule 1: RNA LARGE SUBUNIT ALPHA



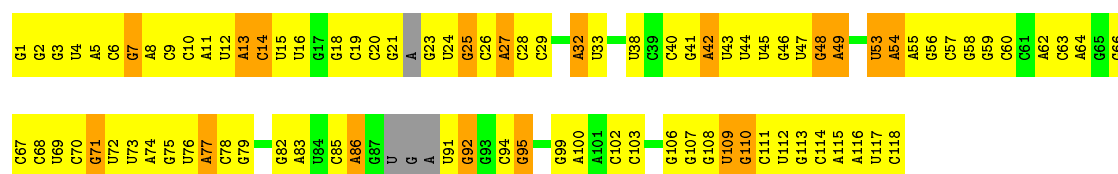




- Molecule 3: 5.8S rRNA

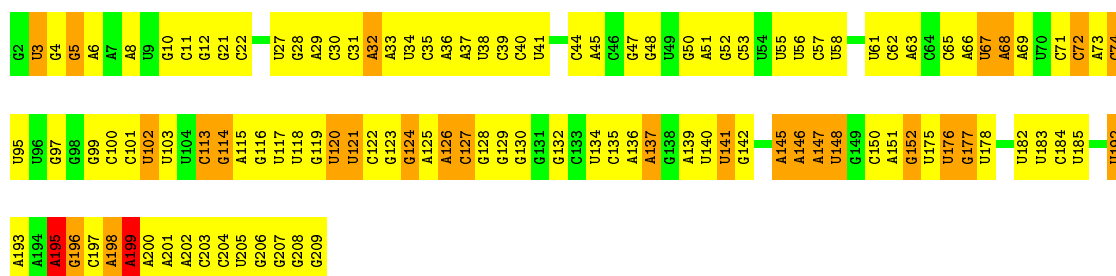


- Molecule 4: 5S rRNA

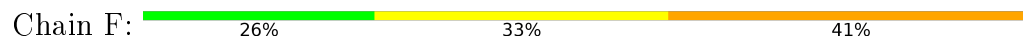


- Molecule 5: srRNA1,srRNA1

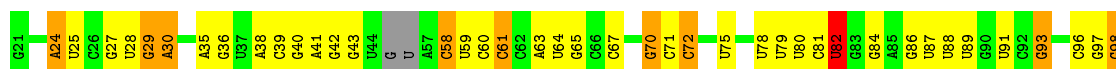




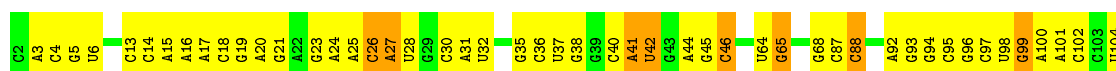
• Molecule 6: srRNA3



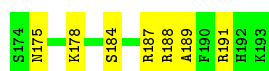
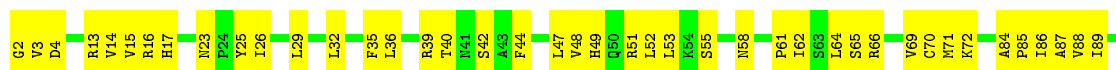
• Molecule 7: srRNA2,srRNA2



• Molecule 8: srRNA4,srRNA4

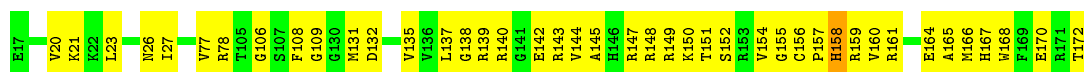


• Molecule 9: 60S ribosomal protein L18



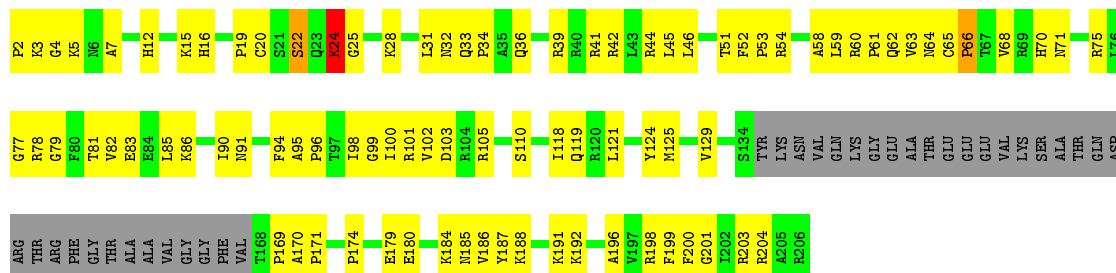
• Molecule 10: 60S ribosomal protein L11





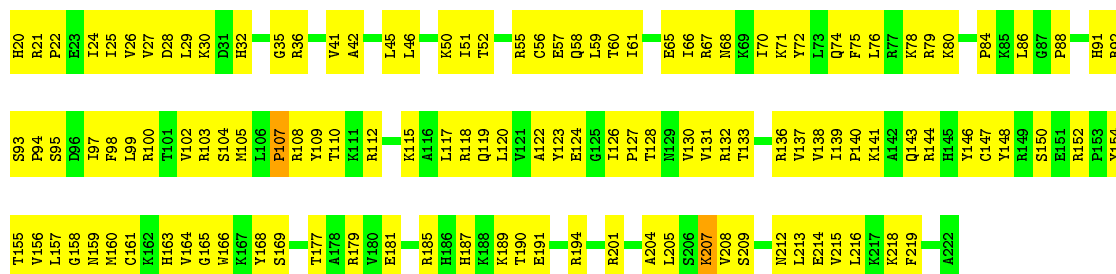
- Molecule 11: 60S ribosomal protein L13

Chain N: 40% 42% • 16%




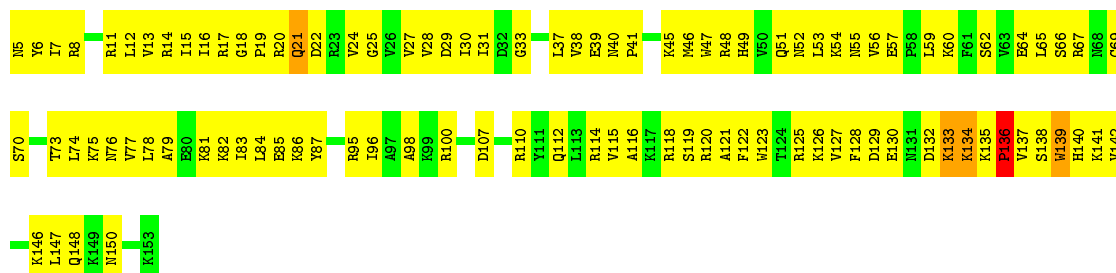
- Molecule 12: 60S ribosomal protein L13a

Chain O:  38% 61%



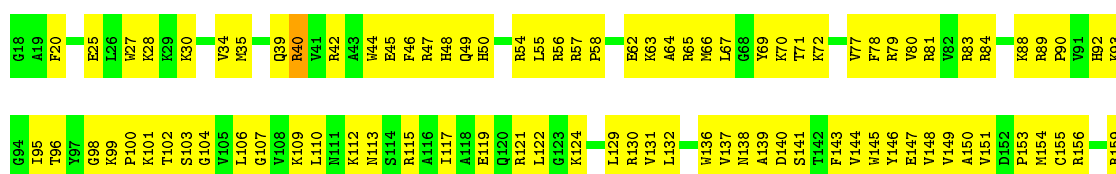
- Molecule 13: 40S ribosomal protein L14

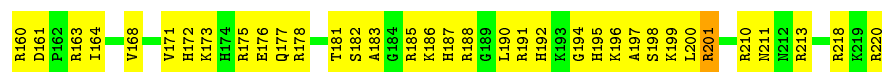
Chain P:  32% 64% .



- Molecule 14: Ribosomal protein L15

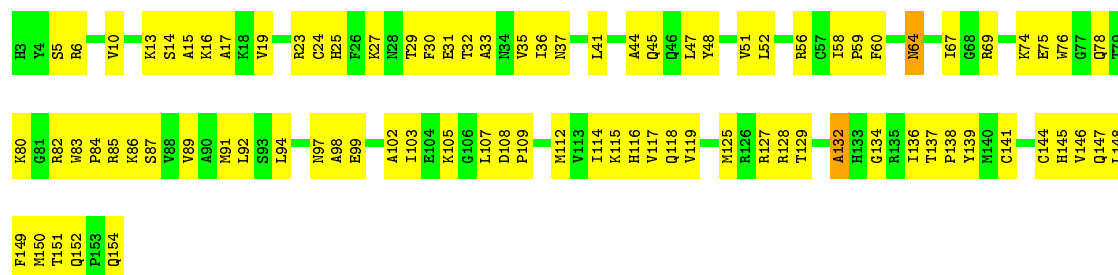
Chain Q: 39% 60%





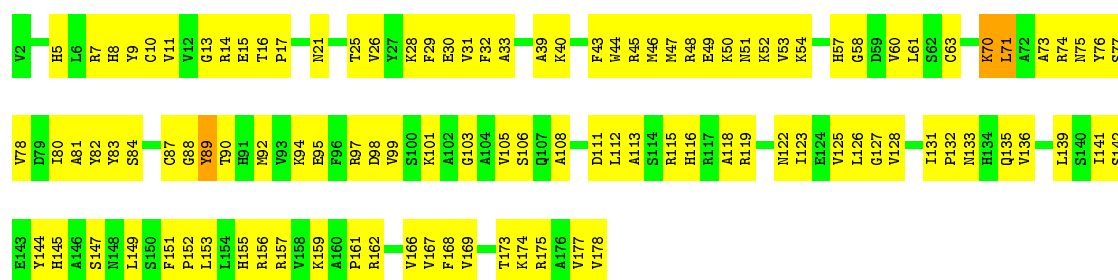
• Molecule 15: 60S ribosomal protein L17

Chain R: 43% 56%



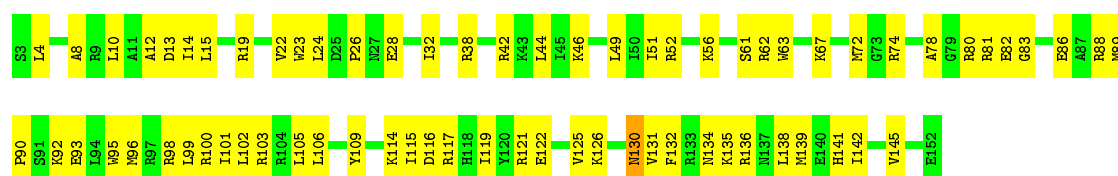
• Molecule 16: 60S ribosomal protein L18a

Chain S: 38% 60%



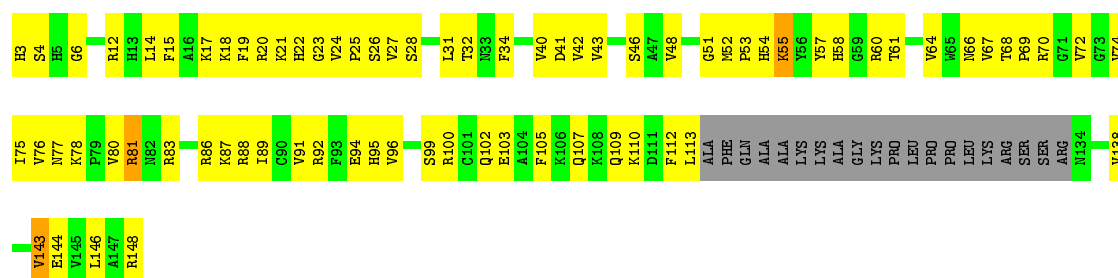
• Molecule 17: Ribosomal protein L19-like protein

Chain T: 53% 46%

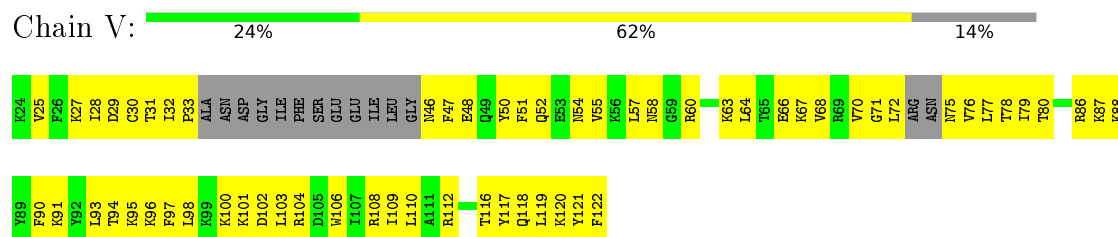


• Molecule 18: Ribosomal protein L21E (60S)

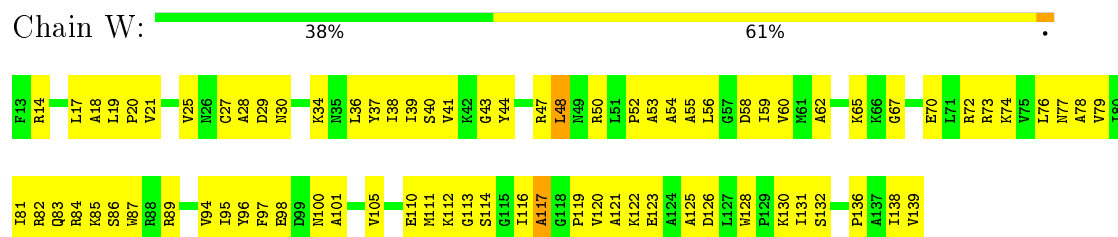
Chain U: 35% 49% 14%



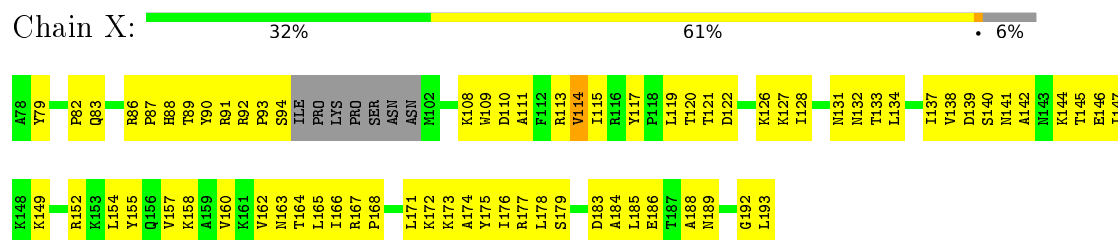
- Molecule 19: 60S ribosomal protein L22



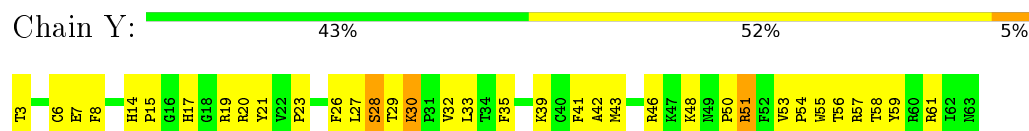
- Molecule 20: 60S ribosomal protein L23



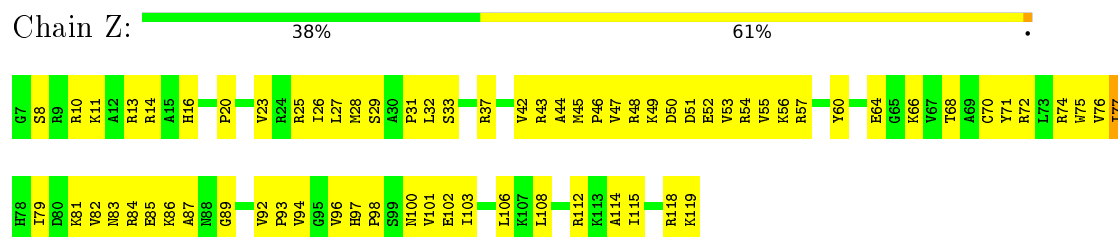
- Molecule 21: 60S ribosomal protein L23a



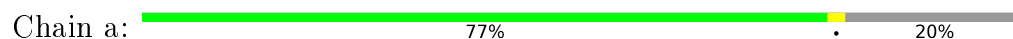
- Molecule 22: Ribosomal protein L24

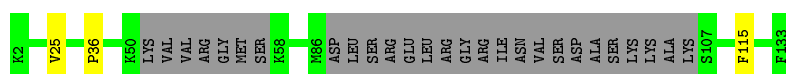


- Molecule 23: 60S ribosomal protein L26



- Molecule 24: Ribosomal protein L27





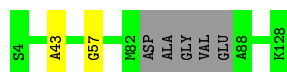
- Molecule 25: 60S ribosomal protein L27A/L29

Chain b: 97% ..



- Molecule 26: 60S ribosomal protein L28

Chain c: 94% . .



- Molecule 27: Ribosomal protein L29

Chain d: 95% 5%



- Molecule 28: 60S ribosomal protein L2

Chain e: 99% .



- Molecule 29: Ribosomal protein L13

Chain f: 96% .



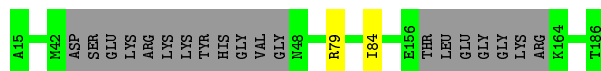
- Molecule 30: 60S ribosomal protein L30

Chain g: 95% 5%



- Molecule 31: 60S ribosomal subunit protein L31

Chain h: 88% . 11%



- Molecule 32: 60S ribosomal protein L32

Chain i:  99%



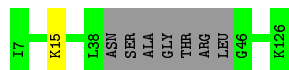
- Molecule 33: 60S ribosomal protein L34

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 60S ribosomal protein L35

Chain k:  93% • 6%



- Molecule 35: Ribosomal protein L35A

Chain l:  97%



- Molecule 36: Ribosomal protein L36

Chain m:  97%



- Molecule 37: Ribosomal protein L37

Chain n:  99%




- Molecule 38: 60S ribosomal protein L37a

Chain o:  96%



- Molecule 39: Ribosomal protein L38

Chain p:  88% • 10%



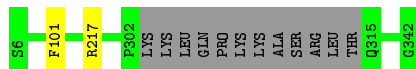
- Molecule 40: Ribosomal protein L39

Chain q: 98%



- Molecule 41: 60S ribosomal protein L4

Chain r: 96%



- Molecule 42: 60S ribosomal protein L44

Chain t: 99%



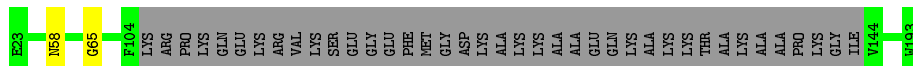
- Molecule 43: 60S ribosomal protein L5

Chain u: 75%



- Molecule 44: 60S ribosomal protein L6

Chain v: 76%



- Molecule 45: 60S ribosomal protein L7

Chain w: 99%



- Molecule 46: Ribosomal protein L7a-like protein

Chain x: 93%

R88	D169
VAL	
ALA	
THR	
GLU	
LYS	
LYS	
LYS	
ASN	
PRO	
GLU	
ALA	
SER	
LYS	
LYS	
A185	P216
	N310

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	235000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, ZN, OMG, OMU, MG, 5MC, 7MG, A2M

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	1.31	11/29897 (0.0%)	1.06	45/46554 (0.1%)
10	L	0.38	0/542	0.52	0/718
11	N	0.66	0/1442	0.65	1/1926 (0.1%)
12	O	0.67	0/1673	0.62	0/2244
13	P	0.51	0/1204	0.60	1/1618 (0.1%)
14	Q	0.82	0/1752	0.80	7/2341 (0.3%)
15	R	0.74	0/1251	0.67	0/1678
16	S	0.62	0/1484	0.60	0/1997
17	T	0.57	0/1292	0.58	0/1711
18	U	0.67	0/1037	0.62	0/1389
19	V	0.49	0/742	0.57	0/986
2	B	1.14	4/21699 (0.0%)	1.00	16/33776 (0.0%)
20	W	0.64	0/977	0.61	0/1318
21	X	0.65	0/905	0.65	0/1215
22	Y	0.69	0/539	0.66	0/728
23	Z	0.56	0/934	0.59	0/1249
24	a	0.45	0/895	0.55	0/1190
25	b	0.73	0/1164	0.69	2/1558 (0.1%)
26	c	0.55	0/946	0.58	0/1263
27	d	0.57	0/527	0.67	0/703
28	e	0.72	0/1915	0.66	0/2576
29	f	0.72	0/3257	0.69	3/4376 (0.1%)
3	C	1.23	0/3306	1.04	3/5144 (0.1%)
30	g	0.43	0/530	0.55	0/712
31	h	0.61	0/1076	0.60	0/1450
32	i	0.74	0/948	0.67	0/1265
33	j	0.62	0/879	0.62	0/1174
34	k	0.53	0/972	0.61	0/1283
35	l	0.77	0/1079	0.66	0/1451
36	m	0.53	0/767	0.62	0/1017
37	n	0.85	0/692	0.75	0/921
38	o	0.74	0/681	0.67	0/905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	p	0.45	0/437	0.56	0/579
4	D	0.83	0/2715	0.90	0/4226
40	q	0.66	0/470	0.65	0/626
41	r	0.70	0/2560	0.63	0/3444
42	t	0.62	0/777	0.65	0/1030
43	u	0.52	0/1568	0.56	0/2104
44	v	0.51	0/1055	0.57	0/1420
45	w	0.68	0/1780	0.62	0/2384
46	x	0.60	0/1715	0.64	0/2306
5	E	0.95	2/3472 (0.1%)	0.92	1/5396 (0.0%)
6	F	0.88	0/1074	0.98	3/1665 (0.2%)
7	G	1.25	1/2849 (0.0%)	1.06	5/4431 (0.1%)
8	H	1.16	0/2171	1.01	1/3374 (0.0%)
9	I	0.67	0/1540	0.67	0/2058
All	All	1.02	18/111187 (0.0%)	0.90	88/163479 (0.1%)

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
14	Q	0	1
24	a	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1610	A	N9-C4	-6.70	1.33	1.37
1	A	1079	G	N9-C4	-6.39	1.32	1.38
2	B	1347	A	N9-C4	-6.00	1.34	1.37
1	A	20	G	N9-C4	-5.97	1.33	1.38
1	A	405	A	N9-C4	-5.83	1.34	1.37

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1578	U	OP2-P-O3'	-10.15	82.87	105.20
1	A	1578	U	OP1-P-O3'	-9.94	83.34	105.20
14	Q	40[A]	ARG	CA-C-O	9.91	140.91	120.10
14	Q	40[B]	ARG	CA-C-O	9.91	140.91	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	G	N3-C4-C5	9.68	133.44	128.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Q	200	LEU	Peptide
24	a	115	PHE	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	27441	12	13883	1171	0
2	B	20110	0	10205	827	0
3	C	3140	0	1600	143	0
4	D	2432	0	1234	113	0
5	E	3110	0	1574	131	0
6	F	965	0	497	59	0
7	G	2578	0	1309	98	0
8	H	1946	0	991	76	0
9	I	1515	0	1619	116	0
10	L	535	0	547	51	0
11	N	1413	0	1518	98	0
12	O	1642	0	1763	155	0
13	P	1186	0	1212	140	0
14	Q	1710	0	1798	155	0
15	R	1226	0	1276	125	0
16	S	1449	0	1489	162	0
17	T	1273	0	1361	118	0
18	U	1016	0	1056	98	0
19	V	730	0	781	74	0
20	W	960	0	1017	102	0
21	X	890	0	932	78	0
22	Y	519	0	519	57	0
23	Z	919	0	981	96	0
24	a	877	0	933	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	1135	0	1175	0	0
26	c	935	0	1003	0	0
27	d	518	0	541	0	0
28	e	1874	0	1938	0	0
29	f	3189	0	3322	0	0
30	g	523	0	565	0	0
31	h	1064	0	1012	0	0
32	i	928	0	971	0	0
33	j	863	0	912	0	0
34	k	967	0	1092	0	0
35	l	1057	0	1072	0	0
36	m	757	0	834	0	0
37	n	679	0	694	0	0
38	o	669	0	690	0	0
39	p	432	0	473	0	0
40	q	456	0	495	0	0
41	r	2513	0	2582	0	0
42	t	763	0	821	0	0
43	u	1541	0	1596	0	0
44	v	1037	0	1106	0	0
45	w	1749	0	1845	0	0
46	x	1690	0	1805	0	0
47	A	66	0	0	0	0
47	B	32	0	0	0	0
47	C	2	0	0	0	0
47	D	1	0	0	0	0
47	E	1	0	0	0	0
47	F	1	0	0	0	0
47	G	1	0	0	0	0
47	H	1	0	0	0	0
48	n	1	0	0	0	0
48	o	1	0	0	0	0
48	t	1	0	0	0	0
49	A	38	0	0	1	0
49	B	26	0	0	1	0
49	C	1	0	0	0	0
49	E	1	0	0	0	0
49	G	3	0	0	0	0
49	H	2	0	0	0	0
49	I	1	0	0	0	0
49	R	1	0	0	0	0
49	a	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	b	1	0	0	0	0
49	e	2	0	0	0	0
49	f	1	0	0	0	0
49	j	1	0	0	0	0
49	k	1	0	0	0	0
49	n	1	0	0	0	0
49	w	1	0	0	0	0
49	x	1	0	0	0	0
All	All	105112	12	76639	3680	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 37.

The worst 5 of 3680 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:B:1516:A2M:H5'	2:B:1517:G:H5'	1.28	1.12
13:P:123:TRP:O	13:P:127:VAL:HG23	1.50	1.11
6:F:50:C:H5'	13:P:118:ARG:HH12	1.19	1.07
17:T:115:ILE:HB	17:T:119:ILE:HD11	1.13	1.07
2:B:62:A:H3'	2:B:63:U:H5'	1.30	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	
9	I	190/192 (99%)	177 (93%)	11 (6%)	2 (1%)	17	30
10	L	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	11	17
11	N	168/205 (82%)	154 (92%)	12 (7%)	2 (1%)	16	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	O	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	19	33
13	P	147/149 (99%)	133 (90%)	11 (8%)	3 (2%)	9	14
14	Q	202/203 (100%)	188 (93%)	14 (7%)	0	100	100
15	R	150/152 (99%)	138 (92%)	10 (7%)	2 (1%)	15	25
16	S	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	8	11
17	T	148/150 (99%)	144 (97%)	3 (2%)	1 (1%)	26	44
18	U	122/146 (84%)	111 (91%)	7 (6%)	4 (3%)	5	6
19	V	79/99 (80%)	70 (89%)	9 (11%)	0	100	100
20	W	125/127 (98%)	120 (96%)	3 (2%)	2 (2%)	12	20
21	X	105/116 (90%)	101 (96%)	3 (3%)	1 (1%)	19	33
22	Y	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
23	Z	111/113 (98%)	100 (90%)	10 (9%)	1 (1%)	21	36
24	a	99/132 (75%)	92 (93%)	5 (5%)	2 (2%)	9	14
25	b	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	26	44
26	c	116/125 (93%)	108 (93%)	6 (5%)	2 (2%)	11	18
27	d	61/63 (97%)	56 (92%)	2 (3%)	3 (5%)	3	2
28	e	243/245 (99%)	225 (93%)	16 (7%)	2 (1%)	24	40
29	f	395/397 (100%)	372 (94%)	19 (5%)	4 (1%)	19	33
30	g	62/66 (94%)	59 (95%)	2 (3%)	1 (2%)	12	20
31	h	140/169 (83%)	133 (95%)	7 (5%)	0	100	100
32	i	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	21	36
33	j	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
34	k	109/120 (91%)	105 (96%)	3 (3%)	1 (1%)	21	36
35	l	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	13	22
36	m	93/95 (98%)	87 (94%)	3 (3%)	3 (3%)	5	6
37	n	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15	25
38	o	83/85 (98%)	76 (92%)	4 (5%)	3 (4%)	4	5
39	p	48/58 (83%)	44 (92%)	3 (6%)	1 (2%)	9	13
40	q	48/50 (96%)	43 (90%)	4 (8%)	1 (2%)	9	13
41	r	321/337 (95%)	309 (96%)	10 (3%)	2 (1%)	30	48
42	t	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	17	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	u	187/254 (74%)	176 (94%)	9 (5%)	2 (1%)	17	30
44	v	128/171 (75%)	119 (93%)	7 (6%)	2 (2%)	12	20
45	w	213/215 (99%)	194 (91%)	16 (8%)	3 (1%)	14	23
46	x	204/223 (92%)	196 (96%)	7 (3%)	1 (0%)	34	54
All	All	5248/5634 (93%)	4903 (93%)	281 (5%)	64 (1%)	21	27

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	142	ASN
11	N	66	PRO
11	N	174	PRO
13	P	21	GLN
15	R	132	ALA

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	
9	I	160/160 (100%)	160 (100%)	0	100	100
10	L	57/57 (100%)	57 (100%)	0	100	100
11	N	153/178 (86%)	150 (98%)	3 (2%)	63	85
12	O	175/175 (100%)	175 (100%)	0	100	100
13	P	119/131 (91%)	115 (97%)	4 (3%)	44	70
14	Q	177/176 (101%)	177 (100%)	0	100	100
15	R	131/131 (100%)	131 (100%)	0	100	100
16	S	158/158 (100%)	158 (100%)	0	100	100
17	T	134/134 (100%)	134 (100%)	0	100	100
18	U	108/123 (88%)	108 (100%)	0	100	100
19	V	79/90 (88%)	79 (100%)	0	100	100
20	W	99/99 (100%)	99 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	X	96/103 (93%)	96 (100%)	0	100	100
22	Y	55/55 (100%)	52 (94%)	3 (6%)	27	46
23	Z	97/97 (100%)	97 (100%)	0	100	100
24	a	93/116 (80%)	93 (100%)	0	100	100
25	b	116/116 (100%)	114 (98%)	2 (2%)	68	88
26	c	99/102 (97%)	99 (100%)	0	100	100
27	d	52/52 (100%)	52 (100%)	0	100	100
28	e	194/194 (100%)	194 (100%)	0	100	100
29	f	339/339 (100%)	332 (98%)	7 (2%)	61	84
30	g	62/62 (100%)	60 (97%)	2 (3%)	46	72
31	h	91/144 (63%)	89 (98%)	2 (2%)	60	83
32	i	100/100 (100%)	100 (100%)	0	100	100
33	j	90/90 (100%)	90 (100%)	0	100	100
34	k	103/108 (95%)	103 (100%)	0	100	100
35	l	102/112 (91%)	100 (98%)	2 (2%)	63	85
36	m	77/77 (100%)	77 (100%)	0	100	100
37	n	69/69 (100%)	69 (100%)	0	100	100
38	o	68/68 (100%)	68 (100%)	0	100	100
39	p	48/53 (91%)	48 (100%)	0	100	100
40	q	46/46 (100%)	46 (100%)	0	100	100
41	r	262/273 (96%)	262 (100%)	0	100	100
42	t	82/82 (100%)	82 (100%)	0	100	100
43	u	155/207 (75%)	155 (100%)	0	100	100
44	v	112/141 (79%)	112 (100%)	0	100	100
45	w	180/180 (100%)	180 (100%)	0	100	100
46	x	182/194 (94%)	182 (100%)	0	100	100
All	All	4520/4792 (94%)	4495 (99%)	25 (1%)	91	97

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	b	45	PHE
29	f	66	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	l	25	LYS
29	f	65	SER
29	f	67	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
23	Z	97	HIS
27	d	30	HIS
43	u	201	HIS
23	Z	100	ASN
25	b	60	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1249/1278 (97%)	348 (27%)	33 (2%)
2	B	925/941 (98%)	275 (29%)	18 (1%)
3	C	144/169 (85%)	39 (27%)	2 (1%)
4	D	111/118 (94%)	23 (20%)	4 (3%)
5	E	141/146 (96%)	30 (21%)	4 (2%)
6	F	44/46 (95%)	21 (47%)	7 (15%)
7	G	117/123 (95%)	28 (23%)	2 (1%)
8	H	86/91 (94%)	20 (23%)	3 (3%)
All	All	2817/2912 (96%)	784 (27%)	73 (2%)

5 of 784 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	5	G
1	A	12	G
1	A	15	U
1	A	20	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	68	A
2	B	1112	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	67	A
2	B	854	U
2	B	1153	A

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

72 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	A2M	A	1043	1	18,25,26	4.39	7 (38%)	18,36,39	3.58	2 (11%)
1	7MG	A	1045	1	20,26,27	3.07	6 (30%)	23,39,42	1.81	6 (26%)
1	OMC	A	1053	1	15,22,23	1.95	6 (40%)	20,31,34	3.32	1 (5%)
1	A2M	A	1071	1	18,25,26	4.51	7 (38%)	18,36,39	3.26	4 (22%)
1	5MC	A	1073	1	14,22,23	1.98	5 (35%)	17,32,35	0.98	1 (5%)
1	OMG	A	1075	1	18,26,27	2.34	6 (33%)	21,38,41	6.88	5 (23%)
1	OMU	A	1127	1	13,22,23	2.41	4 (30%)	17,31,34	0.72	0
1	OMU	A	1227	1	14,22,23	2.81	5 (35%)	19,31,34	1.31	1 (5%)
1	OMG	A	1316	1	18,26,27	2.37	6 (33%)	21,38,41	5.61	6 (28%)
1	OMU	A	1497	1	14,22,23	2.75	5 (35%)	19,31,34	1.46	1 (5%)
1	5MC	A	1525	1	14,22,23	1.97	5 (35%)	17,32,35	0.85	0
1	OMG	A	1659	1	18,26,27	2.22	6 (33%)	21,38,41	5.55	6 (28%)
1	OMC	A	1662	1	15,22,23	2.25	5 (33%)	20,31,34	1.37	1 (5%)
1	A2M	A	1674	1,47,2	18,25,26	4.42	8 (44%)	18,36,39	3.17	3 (16%)
1	OMG	A	1675	1,2	18,26,27	2.17	6 (33%)	21,38,41	5.71	6 (28%)
1	OMG	A	1710	1	18,26,27	2.37	6 (33%)	21,38,41	6.30	5 (23%)
1	7MG	A	1725	1,2	20,26,27	2.97	7 (35%)	23,39,42	1.98	5 (21%)
1	A2M	A	1804	1	18,25,26	4.35	8 (44%)	18,36,39	3.48	5 (27%)
1	OMC	A	343	1	15,22,23	2.42	5 (33%)	20,31,34	2.09	2 (10%)
1	A2M	A	423	1	18,25,26	4.34	8 (44%)	18,36,39	3.30	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A	775	1,2	18,25,26	4.47	8 (44%)	18,36,39	3.04	3 (16%)
1	OMC	A	777	1	15,22,23	2.54	6 (40%)	20,31,34	1.61	1 (5%)
1	A2M	A	778	1	18,25,26	4.30	7 (38%)	18,36,39	2.87	3 (16%)
1	OMC	A	792	1	15,22,23	2.34	5 (33%)	20,31,34	1.26	1 (5%)
1	A2M	A	794	1	18,25,26	4.45	6 (33%)	18,36,39	3.87	7 (38%)
1	OMC	A	919	1	15,22,23	2.43	6 (40%)	20,31,34	1.72	2 (10%)
1	OMG	A	927	1	18,26,27	2.33	6 (33%)	21,38,41	5.88	6 (28%)
1	7MG	A	931	1	20,26,27	2.88	7 (35%)	23,39,42	2.09	7 (30%)
1	OMG	A	958	1	18,26,27	2.23	6 (33%)	21,38,41	5.60	6 (28%)
1	OMU	A	963	1	14,22,23	2.80	5 (35%)	19,31,34	1.37	1 (5%)
1	OMG	A	972	1	18,26,27	2.32	6 (33%)	21,38,41	5.07	7 (33%)
1	A2M	A	974	1	18,25,26	4.26	7 (38%)	18,36,39	3.50	6 (33%)
2	7MG	B	1107	2	20,26,27	3.17	7 (35%)	23,39,42	2.08	7 (30%)
2	7MG	B	1138	2	20,26,27	3.28	7 (35%)	23,39,42	2.03	8 (34%)
2	OMG	B	1169	2	18,26,27	2.24	6 (33%)	21,38,41	5.77	6 (28%)
2	OMG	B	1210	2	18,26,27	2.25	6 (33%)	21,38,41	5.32	8 (38%)
2	OMU	B	1345	2	14,22,23	2.77	5 (35%)	19,31,34	1.42	1 (5%)
2	OMG	B	1361	2	18,26,27	2.31	6 (33%)	21,38,41	5.76	5 (23%)
2	OMG	B	1363	2	18,26,27	2.43	6 (33%)	21,38,41	5.36	6 (28%)
2	OMC	B	1380	2	15,22,23	2.38	6 (40%)	20,31,34	1.78	1 (5%)
2	OMG	B	1385	2	18,26,27	2.29	6 (33%)	21,38,41	5.67	6 (28%)
2	OMC	B	1449	2	15,22,23	2.34	5 (33%)	20,31,34	1.92	1 (5%)
2	OMU	B	1491	2	14,22,23	2.68	5 (35%)	19,31,34	1.11	1 (5%)
2	OMG	B	1492	2	18,26,27	2.38	6 (33%)	21,38,41	6.37	5 (23%)
2	A2M	B	1516	47,2	18,25,26	4.48	8 (44%)	18,36,39	3.45	5 (27%)
2	OMC	B	1529	2	15,22,23	2.31	5 (33%)	20,31,34	1.66	1 (5%)
2	OMC	B	21	1,2	15,22,23	2.34	5 (33%)	20,31,34	1.93	2 (10%)
2	A2M	B	482	2	18,25,26	4.33	8 (44%)	18,36,39	3.31	2 (11%)
2	A2M	B	50	47,2	18,25,26	4.34	8 (44%)	18,36,39	2.97	2 (11%)
2	OMC	B	543	2	15,22,23	2.34	6 (40%)	20,31,34	1.71	1 (5%)
2	OMG	B	564	2	18,26,27	2.48	6 (33%)	21,38,41	6.05	5 (23%)
2	5MC	B	624	2	14,22,23	2.01	5 (35%)	17,32,35	0.79	1 (5%)
2	A2M	B	627	2	18,25,26	4.23	8 (44%)	18,36,39	3.21	6 (33%)
2	OMG	B	634	2	18,26,27	2.25	6 (33%)	21,38,41	6.15	6 (28%)
2	7MG	B	657	47,2	20,26,27	3.06	7 (35%)	23,39,42	1.98	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	B	683	2	15,22,23	2.30	5 (33%)	20,31,34	1.79	3 (15%)
2	A2M	B	691	2	18,25,26	4.47	8 (44%)	18,36,39	4.01	8 (44%)
2	OMG	B	71	2	18,26,27	2.44	6 (33%)	21,38,41	5.26	5 (23%)
2	A2M	B	728	2	18,25,26	4.35	7 (38%)	18,36,39	3.04	4 (22%)
2	OMU	B	73	2	14,22,23	2.77	5 (35%)	19,31,34	1.36	1 (5%)
2	OMG	B	755	2	18,26,27	2.30	6 (33%)	21,38,41	5.82	5 (23%)
2	OMU	B	767	2	14,22,23	2.65	5 (35%)	19,31,34	1.45	1 (5%)
2	OMC	B	77	2	15,22,23	2.50	6 (40%)	20,31,34	1.98	1 (5%)
3	OMC	C	105	47,3	15,22,23	2.40	6 (40%)	20,31,34	2.13	2 (10%)
3	OMU	C	118	3	14,22,23	2.67	5 (35%)	19,31,34	1.36	2 (10%)
3	A2M	C	163	1,3	18,25,26	4.35	8 (44%)	18,36,39	3.10	3 (16%)
3	OMG	C	166	1,3	18,26,27	2.25	6 (33%)	21,38,41	5.75	5 (23%)
3	7MG	C	42	3	20,26,27	2.94	7 (35%)	23,39,42	2.04	7 (30%)
3	A2M	C	43	3	18,25,26	4.41	7 (38%)	18,36,39	3.30	4 (22%)
3	OMU	C	7	1,3	14,22,23	2.94	5 (35%)	19,31,34	1.34	1 (5%)
3	OMG	C	75	3	18,26,27	2.35	6 (33%)	21,38,41	5.78	6 (28%)
7	OMG	G	70	7	18,26,27	2.20	6 (33%)	21,38,41	5.38	6 (28%)

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
1	A2M	A	1043	1	-	0/5/27/28	0/3/3/3
1	7MG	A	1045	1	-	0/7/37/38	0/3/3/3
1	OMC	A	1053	1	-	0/5/27/28	0/2/2/2
1	A2M	A	1071	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1073	1	-	0/3/25/26	0/2/2/2
1	OMG	A	1075	1	-	0/5/27/28	0/3/3/3
1	OMU	A	1127	1	-	0/5/27/28	0/2/2/2
1	OMU	A	1227	1	-	0/5/27/28	0/2/2/2
1	OMG	A	1316	1	-	0/5/27/28	0/3/3/3
1	OMU	A	1497	1	-	0/5/27/28	0/2/2/2
1	5MC	A	1525	1	-	0/3/25/26	0/2/2/2
1	OMG	A	1659	1	-	0/5/27/28	0/3/3/3
1	OMC	A	1662	1	-	0/5/27/28	0/2/2/2
1	A2M	A	1674	1,47,2	-	0/5/27/28	0/3/3/3
1	OMG	A	1675	1,2	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	1710	1	-	0/5/27/28	0/3/3/3
1	7MG	A	1725	1,2	-	0/7/37/38	0/3/3/3
1	A2M	A	1804	1	-	0/5/27/28	0/3/3/3
1	OMC	A	343	1	-	0/5/27/28	0/2/2/2
1	A2M	A	423	1	-	0/5/27/28	0/3/3/3
1	A2M	A	775	1,2	-	0/5/27/28	0/3/3/3
1	OMC	A	777	1	-	0/5/27/28	0/2/2/2
1	A2M	A	778	1	-	0/5/27/28	0/3/3/3
1	OMC	A	792	1	-	0/5/27/28	0/2/2/2
1	A2M	A	794	1	-	0/5/27/28	0/3/3/3
1	OMC	A	919	1	-	0/5/27/28	0/2/2/2
1	OMG	A	927	1	-	0/5/27/28	0/3/3/3
1	7MG	A	931	1	-	0/7/37/38	0/3/3/3
1	OMG	A	958	1	-	0/5/27/28	0/3/3/3
1	OMU	A	963	1	-	0/5/27/28	0/2/2/2
1	OMG	A	972	1	-	0/5/27/28	0/3/3/3
1	A2M	A	974	1	-	0/5/27/28	0/3/3/3
2	7MG	B	1107	2	-	0/7/37/38	0/3/3/3
2	7MG	B	1138	2	-	0/7/37/38	0/3/3/3
2	OMG	B	1169	2	-	0/5/27/28	0/3/3/3
2	OMG	B	1210	2	-	0/5/27/28	0/3/3/3
2	OMU	B	1345	2	-	0/5/27/28	0/2/2/2
2	OMG	B	1361	2	-	0/5/27/28	0/3/3/3
2	OMG	B	1363	2	-	0/5/27/28	0/3/3/3
2	OMC	B	1380	2	-	0/5/27/28	0/2/2/2
2	OMG	B	1385	2	-	0/5/27/28	0/3/3/3
2	OMC	B	1449	2	-	0/5/27/28	0/2/2/2
2	OMU	B	1491	2	-	0/5/27/28	0/2/2/2
2	OMG	B	1492	2	-	0/5/27/28	0/3/3/3
2	A2M	B	1516	47,2	-	0/5/27/28	0/3/3/3
2	OMC	B	1529	2	-	0/5/27/28	0/2/2/2
2	OMC	B	21	1,2	-	0/5/27/28	0/2/2/2
2	A2M	B	482	2	-	0/5/27/28	0/3/3/3
2	A2M	B	50	47,2	-	0/5/27/28	0/3/3/3
2	OMC	B	543	2	-	0/5/27/28	0/2/2/2
2	OMG	B	564	2	-	0/5/27/28	0/3/3/3
2	5MC	B	624	2	-	0/3/25/26	0/2/2/2
2	A2M	B	627	2	-	0/5/27/28	0/3/3/3
2	OMG	B	634	2	-	0/5/27/28	0/3/3/3
2	7MG	B	657	47,2	-	0/7/37/38	0/3/3/3
2	OMC	B	683	2	-	0/5/27/28	0/2/2/2
2	A2M	B	691	2	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	B	71	2	-	0/5/27/28	0/3/3/3
2	A2M	B	728	2	-	0/5/27/28	0/3/3/3
2	OMU	B	73	2	-	0/5/27/28	0/2/2/2
2	OMG	B	755	2	-	0/5/27/28	0/3/3/3
2	OMU	B	767	2	-	0/5/27/28	0/2/2/2
2	OMC	B	77	2	-	0/5/27/28	0/2/2/2
3	OMC	C	105	47,3	-	0/5/27/28	0/2/2/2
3	OMU	C	118	3	-	0/5/27/28	0/2/2/2
3	A2M	C	163	1,3	-	0/5/27/28	0/3/3/3
3	OMG	C	166	1,3	-	0/5/27/28	0/3/3/3
3	7MG	C	42	3	-	0/7/37/38	0/3/3/3
3	A2M	C	43	3	-	0/5/27/28	0/3/3/3
3	OMU	C	7	1,3	-	0/5/27/28	0/2/2/2
3	OMG	C	75	3	-	0/5/27/28	0/3/3/3
7	OMG	G	70	7	-	0/5/27/28	0/3/3/3

The worst 5 of 443 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	A2M	C2'-C1'	-9.46	1.27	1.53
3	C	43	A2M	C2'-C1'	-9.28	1.27	1.53
1	A	1043	A2M	C2'-C1'	-9.20	1.28	1.53
3	C	163	A2M	C2'-C1'	-9.19	1.28	1.53
2	B	1516	A2M	C2'-C1'	-9.17	1.28	1.53

The worst 5 of 271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	A2M	N3-C2-N1	-12.97	118.68	128.87
2	B	691	A2M	N3-C2-N1	-12.56	119.00	128.87
2	B	1516	A2M	N3-C2-N1	-12.34	119.18	128.87
1	A	1804	A2M	N3-C2-N1	-12.17	119.31	128.87
3	C	43	A2M	N3-C2-N1	-12.06	119.40	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

58 monomers are involved in 166 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1043	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1045	7MG	1	0
1	A	1053	OMC	7	0
1	A	1071	A2M	3	0
1	A	1073	5MC	2	0
1	A	1075	OMG	1	0
1	A	1127	OMU	1	0
1	A	1316	OMG	5	0
1	A	1525	5MC	2	0
1	A	1659	OMG	3	0
1	A	1662	OMC	1	0
1	A	1674	A2M	1	0
1	A	1710	OMG	3	0
1	A	1725	7MG	2	0
1	A	1804	A2M	7	0
1	A	343	OMC	4	0
1	A	423	A2M	1	0
1	A	777	OMC	4	0
1	A	778	A2M	3	0
1	A	792	OMC	2	0
1	A	794	A2M	4	0
1	A	919	OMC	7	0
1	A	931	7MG	4	0
1	A	958	OMG	3	0
1	A	972	OMG	2	0
1	A	974	A2M	1	0
2	B	1107	7MG	3	0
2	B	1138	7MG	2	0
2	B	1169	OMG	5	0
2	B	1210	OMG	1	0
2	B	1345	OMU	2	0
2	B	1361	OMG	3	0
2	B	1363	OMG	2	0
2	B	1380	OMC	4	0
2	B	1492	OMG	3	0
2	B	1516	A2M	6	0
2	B	1529	OMC	3	0
2	B	21	OMC	2	0
2	B	482	A2M	3	0
2	B	543	OMC	2	0
2	B	564	OMG	2	0
2	B	624	5MC	2	0
2	B	627	A2M	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	634	OMG	3	0
2	B	657	7MG	3	0
2	B	683	OMC	3	0
2	B	691	A2M	4	0
2	B	728	A2M	4	0
2	B	73	OMU	1	0
2	B	755	OMG	6	0
2	B	767	OMU	2	0
2	B	77	OMC	2	0
3	C	105	OMC	2	0
3	C	118	OMU	1	0
3	C	166	OMG	6	0
3	C	7	OMU	1	0
3	C	75	OMG	2	0
7	G	70	OMG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 108 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
1	A	30
2	B	16
5	E	5
8	H	4
10	L	3
7	G	2
31	h	2
30	g	1
6	F	1

The worst 5 of 64 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	282:U	O3'	304:A	P	49.48
1	A	1269:U	O3'	1283:A	P	36.80
1	B	913:U	O3'	1105:C	P	35.79
1	A	1233:A	O3'	1245:C	P	34.48
1	A	154:A	O3'	175:U	P	29.48