



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

Feb 21, 2017 – 04:13 PM EST

PDB ID : 5UMD  
EMDB ID: : EMD-8576  
Title : Structure of the Plasmodium falciparum 80S ribosome bound to the antimalarial drug mefloquine  
Authors : Wong, W.; Bai, X.-C.; Brown, A.; Scheres, S.; Baum, J.  
Deposited on : 2017-01-27  
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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

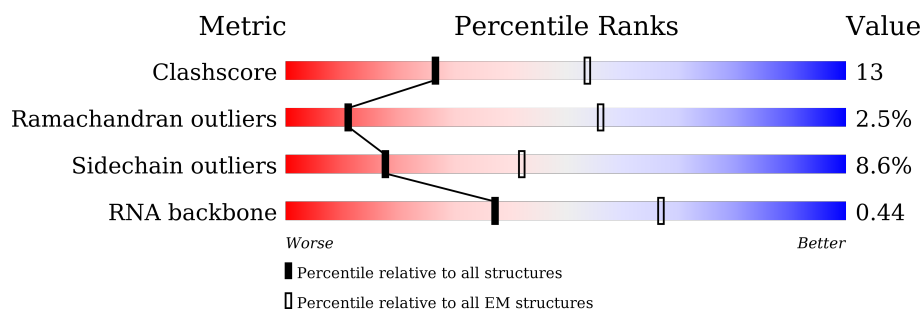
# 1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	3788	30% 41% 13% 16%
2	B	119	46% 46% 7% .
3	C	159	34% 44% 16% . 5%
4	D	260	61% 25% 8% 5%
5	E	386	69% 26% . .
6	F	411	72% 19% . 5%
7	G	173	45% 24% . 28%
8	H	190	68% 23% 5% . .



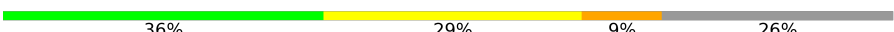









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Mol	Chain	Length	Quality of chain
9	I	221	
10	J	283	
11	K	202	
12	L	215	
13	M	139	
14	N	165	
15	O	148	
16	P	205	
17	Q	219	
18	R	294	
19	S	187	
20	T	182	
21	U	184	
22	V	161	
23	W	203	
24	X	139	
25	Y	190	
26	Z	126	
27	0	162	
28	1	146	
29	2	127	
30	3	124	
31	4	67	
32	5	257	
33	6	108	

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Mol	Chain	Length	Quality of chain
34	7	120	
35	8	131	
36	9	140	
37	a	150	
38	b	112	
39	c	92	
40	d	87	
41	e	51	
42	f	128	
43	g	39	
44	h	96	
45	i	104	

## 2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 124502 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3191	Total	C	N	O	P	0	0
			67935	30426	12044	22274	3191		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	821	C	U	conflict	GB 1013064538

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2525	1128	461	818	118		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	A	C	conflict	GB 1016052399
B	24	U	C	conflict	GB 1016052399
B	119	G	U	conflict	GB 1016052399

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	P	0	0
			3224	1444	589	1040	151		

- Molecule 4 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1866	1166	374	317	9		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total	C	N	O	S	0	0
			3061	1948	575	521	17		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	390	Total	C	N	O	S	0	0
			3094	1962	594	527	11		

- Molecule 7 is a protein called 60S ribosomal protein L11a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	124	Total	C	N	O	S	0	0
			1010	636	197	171	6		

- Molecule 8 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1460	938	261	255	6		

- Molecule 9 is a protein called 60S ribosomal protein L6-2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	207	Total	C	N	O	S	0	0
			1684	1096	298	285	5		

- Molecule 10 is a protein called 60S ribosomal protein L7-3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	222	Total	C	N	O	S	0	0
			1813	1174	323	309	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1659	1064	311	276	8		

- Molecule 12 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1756	1116	346	290	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	19	HIS	ARG	conflict	UNP Q8IAX6
L	20	ARG	HIS	conflict	UNP Q8IAX6
L	201	CYS	ARG	conflict	UNP Q8IAX6

- Molecule 13 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 14 is a protein called 60S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1197	779	210	202	6		

- Molecule 15 is a protein called 60S ribosomal protein L27a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 17 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1544	984	291	261	8		

- Molecule 18 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	252	Total	C	N	O	S	0	0
			2045	1298	384	357	6		

- Molecule 19 is a protein called 60S ribosomal protein L18-2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	186	Total	C	N	O	S	0	0
			1502	958	299	240	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	181	Total	C	N	O	S	0	0
			1505	949	308	244	4		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	180	Total	C	N	O	S	0	0
			1496	946	289	254	7		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	155	Total	C	N	O	S	0	0
			1275	814	241	214	6		

- Molecule 23 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	170	Total	C	N	O	S	0	0
			1318	824	266	221	7		

- Molecule 24 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			824	548	135	139	2		

- Molecule 25 is a protein called 60S ribosomal protein L23.



Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	101	Total	C	N	O	S	0	0
			796	502	144	144	6		

- Molecule 26 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	121	Total	C	N	O	S	0	0
			1000	626	206	165	3		

- Molecule 27 is a protein called 60S ribosomal protein L24, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	62	Total	C	N	O	S	0	0
			521	336	97	87	1		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	104	Total	C	N	O	S	0	0
			830	529	151	147	3		

- Molecule 30 is a protein called 60S ribosomal protein L35, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	119	Total	C	N	O	S	0	0
			994	635	194	163	2		

- Molecule 31 is a protein called 60S ribosomal protein L29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 32 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 33 is a protein called 60S ribosomal protein L30e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	98	Total	C	N	O	S	0	0
			740	462	132	139	7		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			793	508	151	129	5		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	125	Total	C	N	O	S	0	0
			1036	660	206	163	7		

- Molecule 36 is a protein called 60S ribosomal protein L35Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	103	Total	C	N	O	S	0	0
			844	543	163	135	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	106	Total	C	N	O	S	0	0
			858	530	184	138	6		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	95	Total	C	N	O	S	0	0
			756	477	150	129			

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	89	Total	C	N	O	S	0	0
			705	439	150	111	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	72	Total	C	N	O	S	0	0
			603	395	107	99	2		

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	51	Total	C	N	O	S	0	0
			413	255	87	66	5		

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	37	Total	C	N	O	S	0	0
			342	210	86	44	2		

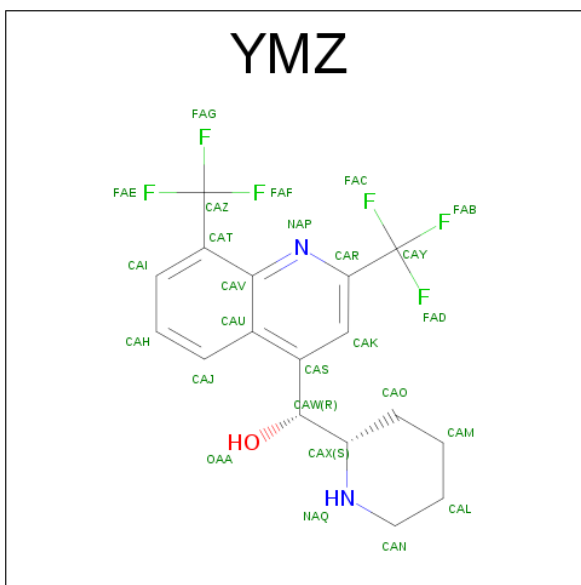
- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	85	Total	C	N	O	S	0	0
			658	417	127	107	7		

- Molecule 45 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	95	Total	C	N	O	S	0	0
			778	490	152	127	9		

- Molecule 46 is Mefloquine (three-letter code: YMZ) (formula: C<sub>17</sub>H<sub>16</sub>F<sub>6</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	F	N	O	0
			26	17	6	2	1	
46	K	1	Total	C	F	N	O	0
			26	17	6	2	1	

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

Mol	Chain	Residues	Atoms		AltConf
47	B	3	Total	Mg	0
			3	3	
47	A	155	Total	Mg	0
			155	155	
47	C	5	Total	Mg	0
			5	5	
47	M	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
48	h	1	Total	Zn	0
			1	1	
48	a	1	Total	Zn	0
			1	1	
48	c	1	Total	Zn	0
			1	1	

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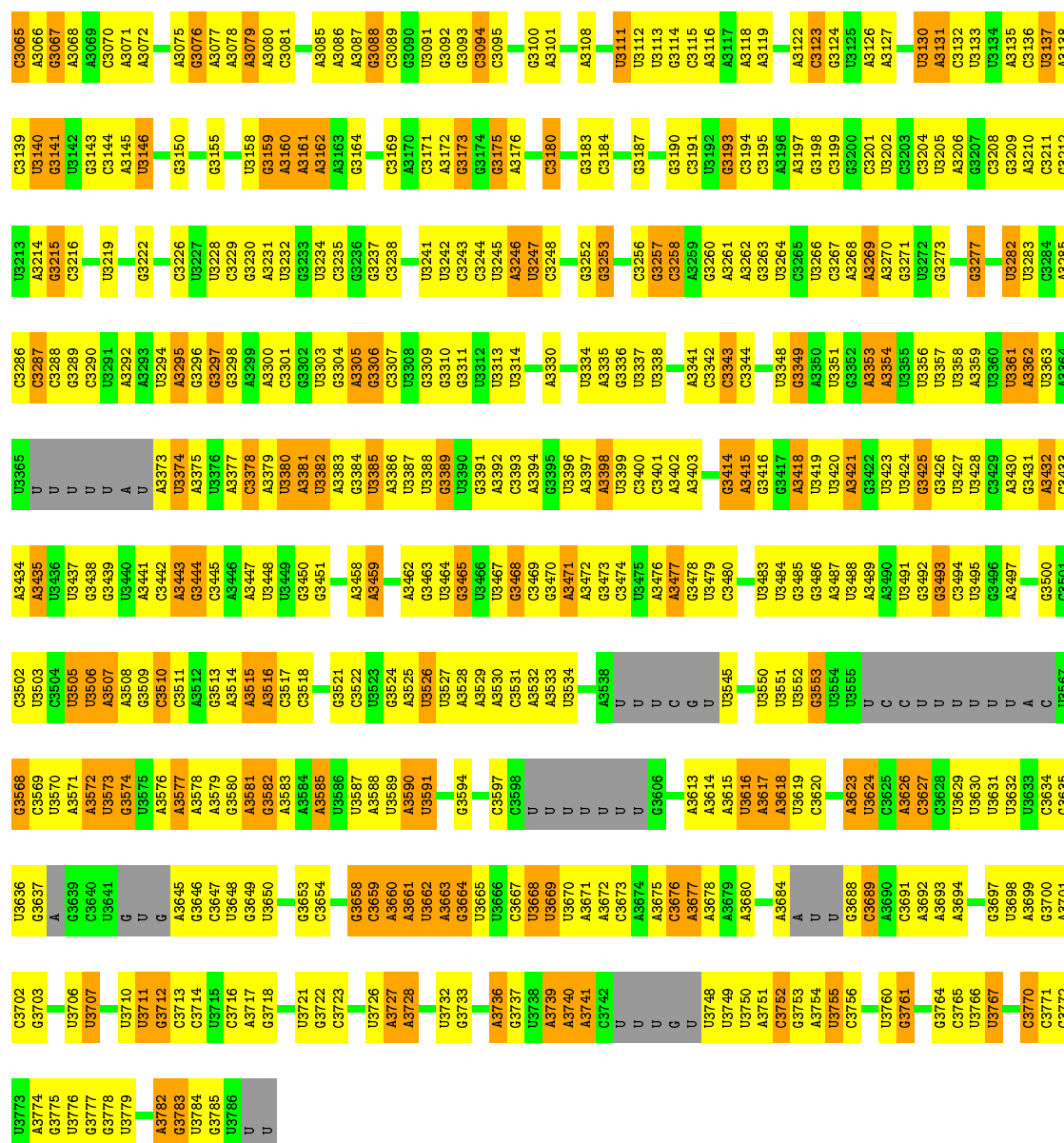
Mol	Chain	Residues	Atoms		AltConf
48	f	1	Total 1	Zn 1	0
48	i	1	Total 1	Zn 1	0



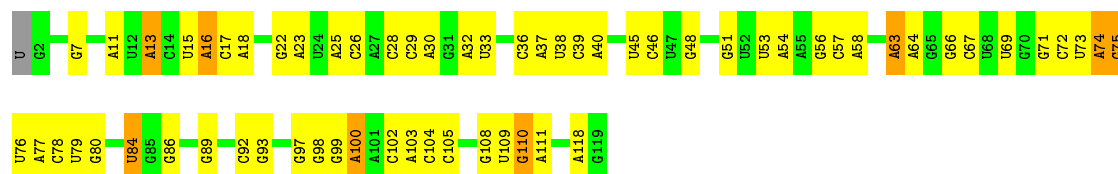
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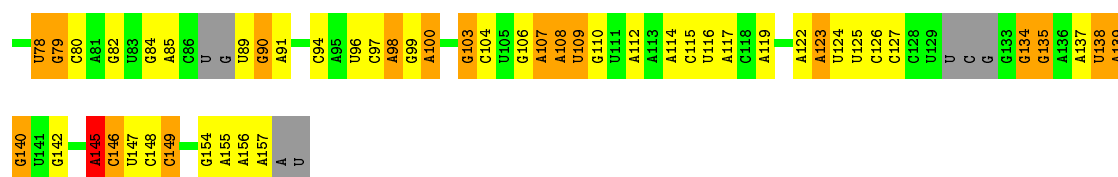




Chain B: 46% 46% 7%

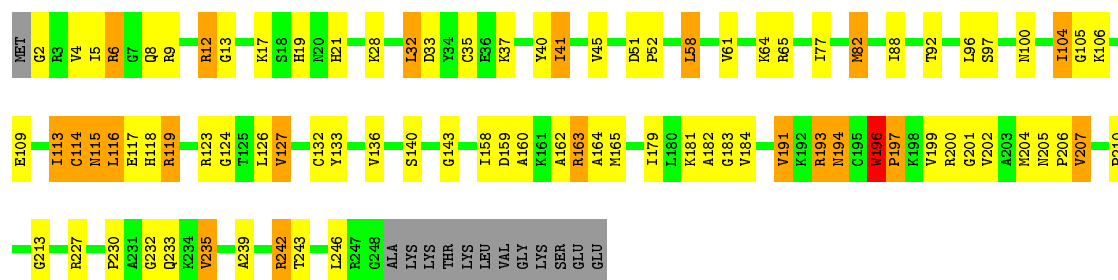


Chain C: 34% 44% 16% 5%



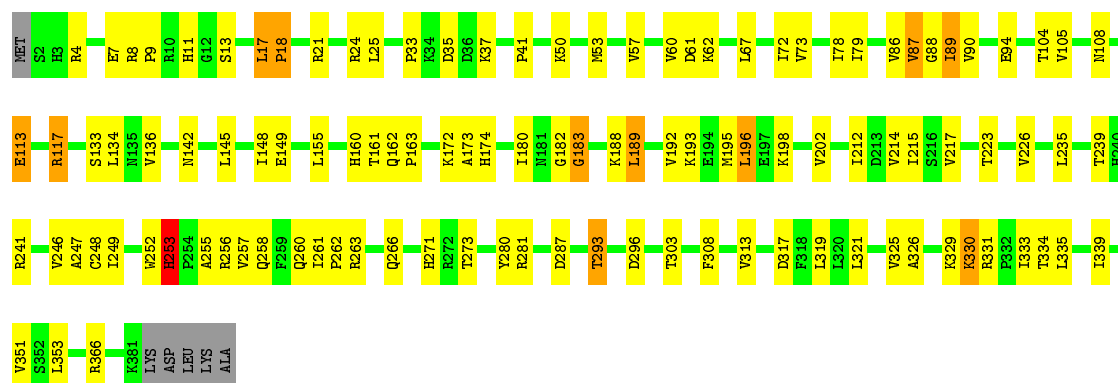
- Molecule 4: 60S ribosomal protein L2

Chain D:  61% 25% 8% 5%



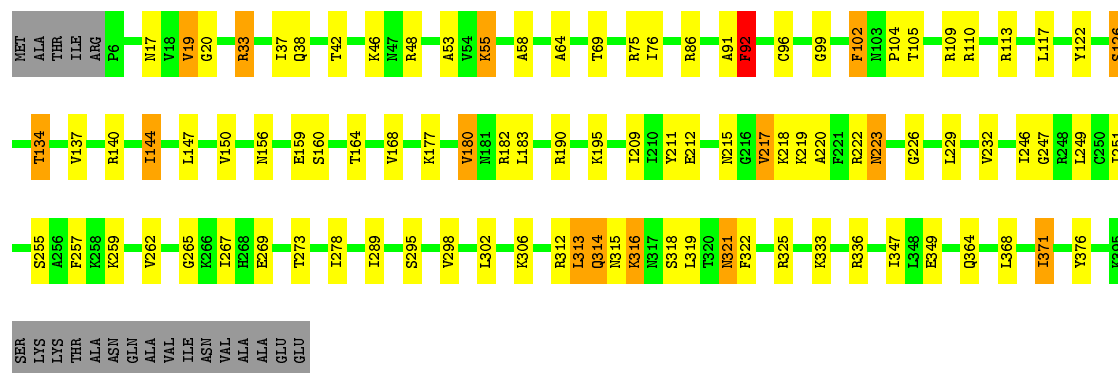
- Molecule 5: 60S ribosomal protein L3

Chain E:  69% 26% .



- Molecule 6: 60S ribosomal protein L4

Chain F:  72% 19% • 5%



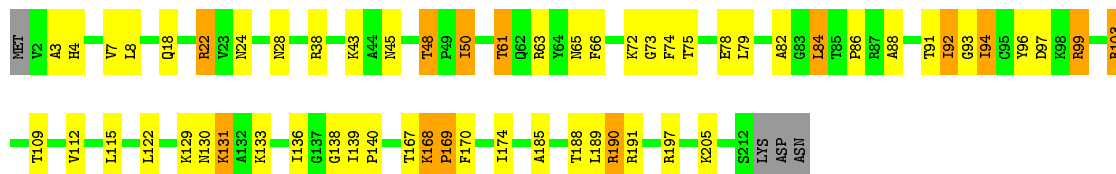
- Molecule 7: 60S ribosomal protein L11a, putative





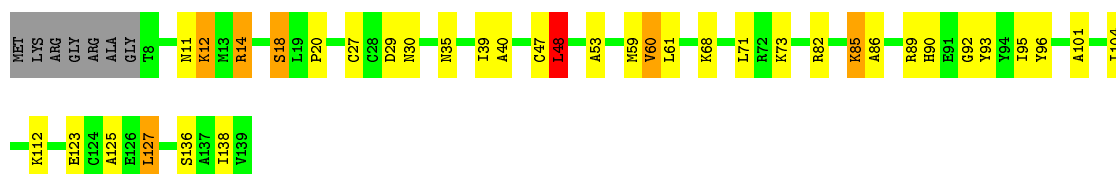
- Molecule 12: 60S ribosomal protein L13

Chain L: 71% 21% 6% .



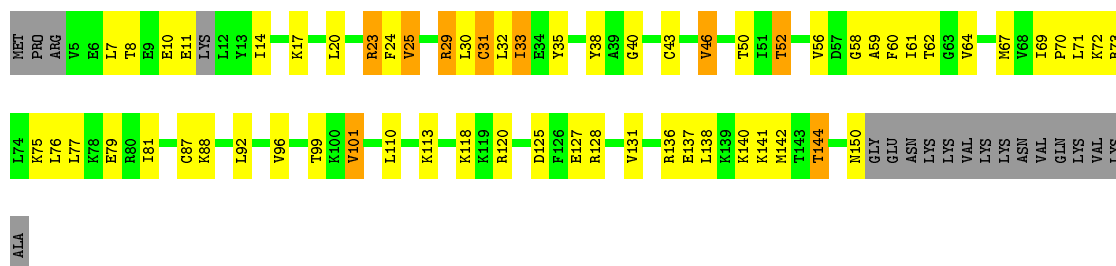
- Molecule 13: 60S ribosomal protein L23, putative

Chain M: 68% 22% . • 5%



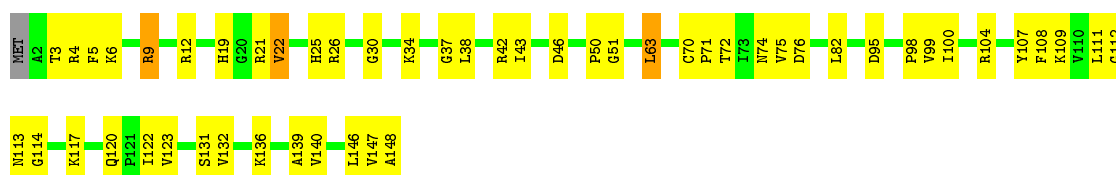
- Molecule 14: 60S ribosomal protein L14, putative

Chain N: 51% 32% 5% 12%



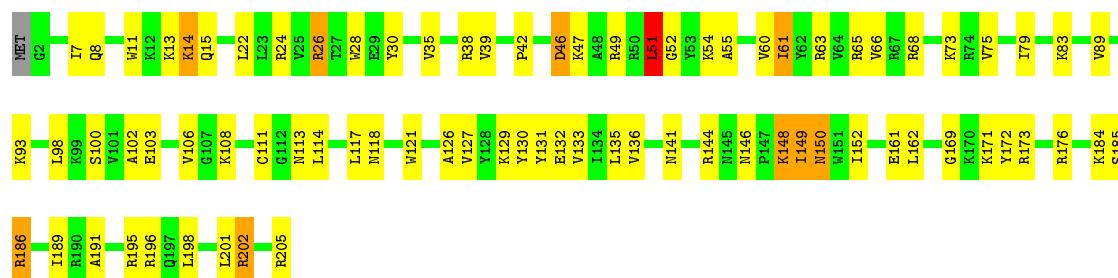
- Molecule 15: 60S ribosomal protein L27a, putative

Chain O: 64% 33% ..



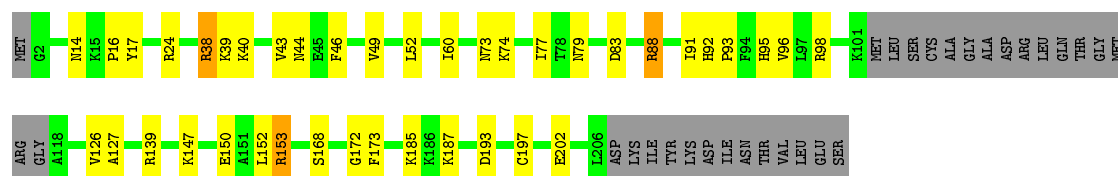
- Molecule 16: Ribosomal protein L15

Chain P: 60% 34% .



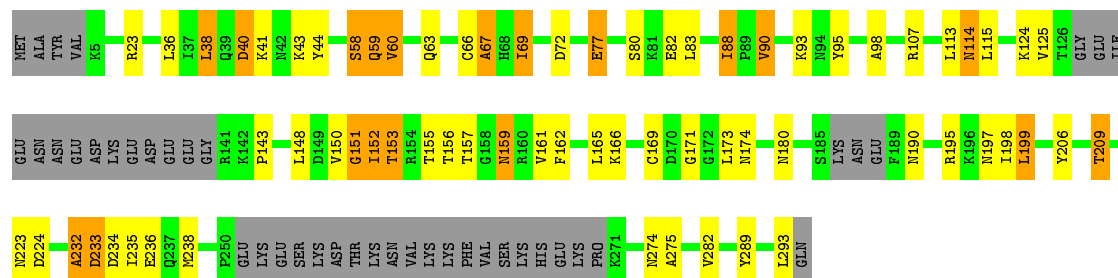
- Molecule 17: 60S ribosomal protein L10, putative

Chain Q: 68% 17% 14%



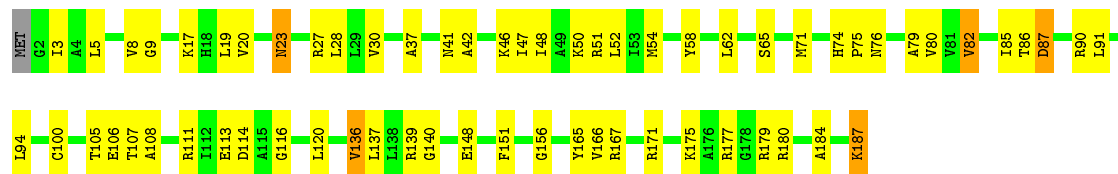
- Molecule 18: 60S ribosomal protein L5, putative

Chain R: 62% 17% 6% 14%



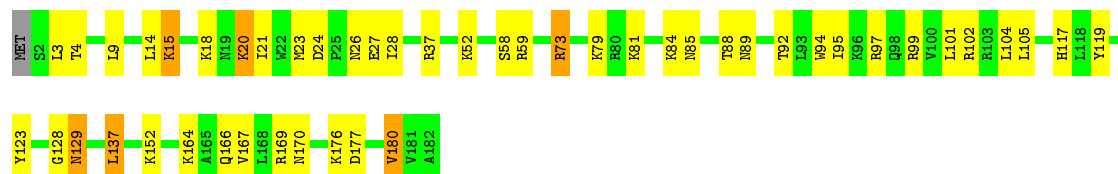
- Molecule 19: 60S ribosomal protein L18-2, putative

Chain S: 65% 32% 2%



- Molecule 20: 60S ribosomal protein L19

Chain T: 73% 23% 2%



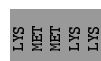
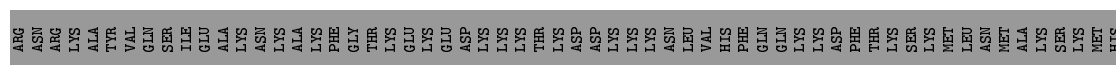
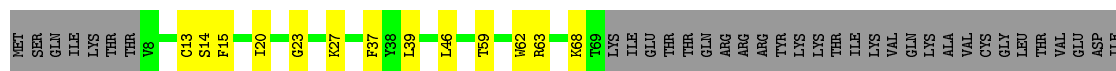
- [illegible]



- Molecule 26: 60S ribosomal protein L26, putative



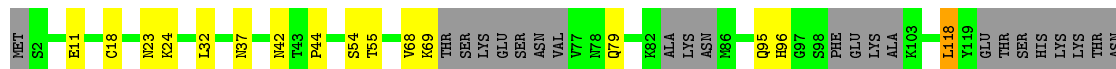
- Molecule 27: 60S ribosomal protein L24, putative



- Molecule 28: 60S ribosomal protein L27



- Molecule 29: 60S ribosomal protein L28

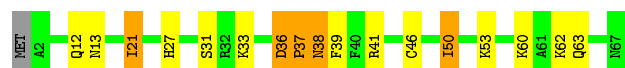


- Molecule 30: 60S ribosomal protein L35, putative



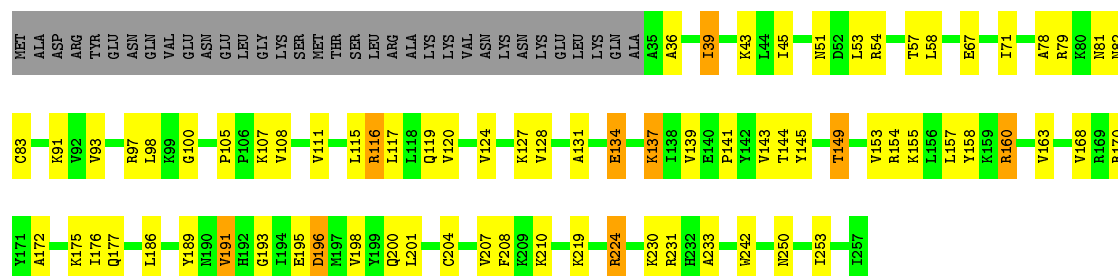
- Molecule 31: 60S ribosomal protein L29, putative

Chain 4: 



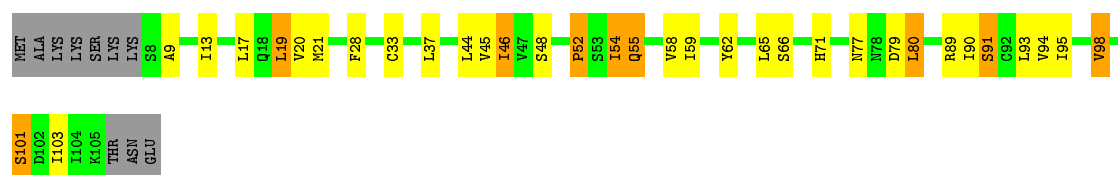
- Molecule 32: 60S ribosomal protein L7, putative

Chain 5: 



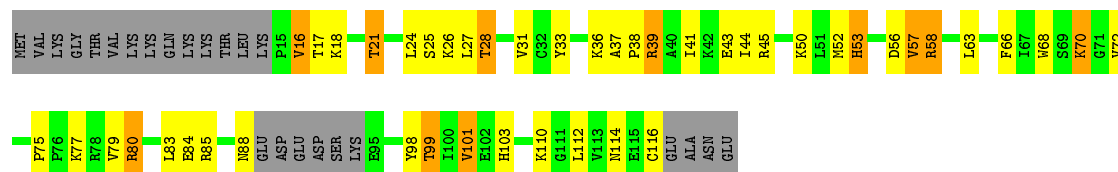
- Molecule 33: 60S ribosomal protein L30e, putative

Chain 6: 



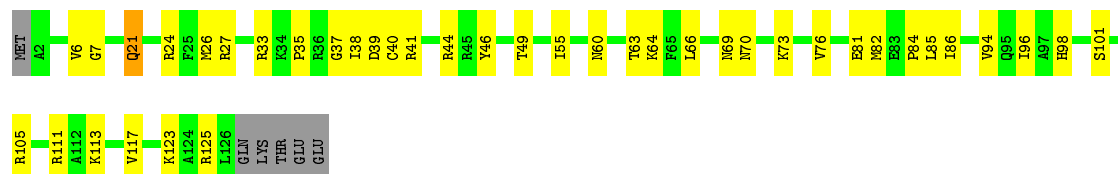
- Molecule 34: 60S ribosomal protein L31

Chain 7: 



- Molecule 35: 60S ribosomal protein L32

Chain 8: 

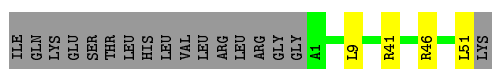


- Molecule 36: 60S ribosomal protein L35Ae, putative

Chain 9: 







- Molecule 43: 60S ribosomal protein L41

Chain g: 85% 10% 5%



- Molecule 44: 60S ribosomal protein L37a

Chain h: 83% 5% 11%



- Molecule 45: 60S ribosomal protein L44

Chain i: 84% 7% 9%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	43184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	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	104748	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: ZN, YMZ, 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	0.20	1/75982 (0.0%)	0.66	5/118263 (0.0%)
10	J	0.33	0/1840	0.63	0/2456
11	K	0.32	0/1689	0.64	0/2260
12	L	0.33	0/1788	0.62	0/2381
13	M	0.33	0/1012	0.60	0/1363
14	N	0.35	0/1213	0.64	0/1616
15	O	0.31	0/1199	0.58	0/1597
16	P	0.32	0/1735	0.60	0/2320
17	Q	0.31	0/1579	0.52	0/2113
18	R	0.33	0/2074	0.64	0/2772
19	S	0.32	0/1530	0.63	0/2040
2	B	0.18	0/2826	0.64	0/4404
20	T	0.35	0/1521	0.63	0/2012
21	U	0.33	0/1526	0.56	0/2043
22	V	0.27	0/1300	0.46	0/1732
23	W	0.30	0/1338	0.56	0/1793
24	X	0.35	0/841	0.59	0/1125
25	Y	0.34	0/805	0.61	0/1074
26	Z	0.28	0/1012	0.53	1/1339 (0.1%)
27	0	0.35	0/533	0.57	0/711
28	1	0.29	0/1151	0.53	0/1531
29	2	0.30	0/839	0.52	0/1114
3	C	0.19	0/3608	0.66	2/5615 (0.0%)
30	3	0.34	0/1004	0.64	0/1329
31	4	0.34	0/564	0.63	0/737
32	5	0.33	0/1917	0.62	0/2562
33	6	0.34	0/748	0.67	0/1001
34	7	0.34	0/805	0.64	0/1073
35	8	0.34	0/1053	0.60	0/1399
36	9	0.34	0/864	0.64	0/1160
37	a	0.28	0/871	0.53	0/1161
38	b	0.33	0/762	0.63	0/1008

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	c	0.33	0/718	0.60	0/946
4	D	0.37	0/1901	0.65	0/2544
40	d	0.34	0/611	0.64	0/812
41	e	0.35	0/396	0.59	0/521
42	f	0.36	0/418	0.63	0/556
43	g	0.35	0/347	0.60	0/448
44	h	0.29	0/667	0.52	0/887
45	i	0.32	0/788	0.57	0/1032
5	E	0.32	0/3129	0.57	0/4195
6	F	0.32	0/3144	0.62	0/4205
7	G	0.33	0/1020	0.61	0/1349
8	H	0.31	0/1485	0.59	2/2009 (0.1%)
9	I	0.30	0/1707	0.58	0/2274
All	All	0.25	1/133860 (0.0%)	0.64	10/196882 (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
33	6	0	1
36	9	0	1
4	D	0	1
5	E	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1475	G	O3'-P	-5.31	1.54	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1805	U	C2'-C3'-O3'	6.73	124.47	113.70
26	Z	105	LEU	CA-CB-CG	6.13	129.40	115.30
3	C	134	G	C2'-C3'-O3'	5.93	123.19	113.70
3	C	145	A	C2'-C3'-O3'	5.63	122.71	113.70
1	A	652	A	C2'-C3'-O3'	5.47	122.46	113.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	6	52	PRO	Peptide
36	9	136	TYR	Peptide
4	D	196	TRP	Peptide
5	E	17	LEU	Peptide
5	E	253	HIS	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	67935	0	34198	1791	0
2	B	2525	0	1274	38	0
3	C	3224	0	1630	93	0
4	D	1866	0	1964	66	0
5	E	3061	0	3205	87	0
6	F	3094	0	3333	72	0
7	G	1010	0	1073	29	0
8	H	1460	0	1532	31	0
9	I	1684	0	1849	25	0
10	J	1813	0	1985	34	0
11	K	1659	0	1782	26	0
12	L	1756	0	1888	37	0
13	M	996	0	1044	20	0
14	N	1197	0	1312	46	0
15	O	1172	0	1230	37	0
16	P	1697	0	1802	55	0
17	Q	1544	0	1582	23	0
18	R	2045	0	2134	36	0
19	S	1502	0	1636	51	0
20	T	1505	0	1671	30	0
21	U	1496	0	1556	45	0
22	V	1275	0	1355	20	0
23	W	1318	0	1319	24	0
24	X	824	0	882	14	0
25	Y	796	0	850	18	0
26	Z	1000	0	1099	22	0
27	0	521	0	539	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	1	1134	0	1245	18	0
29	2	830	0	887	9	0
30	3	994	0	1121	10	0
31	4	555	0	599	12	0
32	5	1879	0	2005	54	0
33	6	740	0	763	15	0
34	7	793	0	869	32	0
35	8	1036	0	1139	26	0
36	9	844	0	886	37	0
37	a	858	0	911	0	0
38	b	756	0	842	0	0
39	c	705	0	755	0	0
40	d	603	0	686	0	0
41	e	388	0	421	0	0
42	f	413	0	450	0	0
43	g	342	0	388	0	0
44	h	658	0	725	0	0
45	i	778	0	858	0	0
46	A	26	0	0	3	0
46	K	26	0	0	0	0
47	A	155	0	0	0	0
47	B	3	0	0	0	0
47	C	5	0	0	0	0
47	M	1	0	0	0	0
48	a	1	0	0	0	0
48	c	1	0	0	0	0
48	f	1	0	0	0	0
48	h	1	0	0	0	0
48	i	1	0	0	0	0
All	All	124502	0	91274	2716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2716 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)
1:A:1102:U:O4	1:A:1231:A:N1	1.59	1.34
1:A:3505:U:N3	1:A:3508:A:N6	1.77	1.33
1:A:2995:A:N6	1:A:3052:U:H3	1.26	1.32
1:A:1316:U:H3	1:A:1445:A:N6	1.28	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:U:H3	1:A:333:A:N6	1.28	1.26

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	
4	D	245/260 (94%)	224 (91%)	18 (7%)	3 (1%)	16	60
5	E	378/386 (98%)	340 (90%)	31 (8%)	7 (2%)	10	50
6	F	388/411 (94%)	363 (94%)	16 (4%)	9 (2%)	8	44
7	G	116/173 (67%)	101 (87%)	11 (10%)	4 (3%)	5	31
8	H	183/190 (96%)	158 (86%)	20 (11%)	5 (3%)	6	39
9	I	203/221 (92%)	174 (86%)	24 (12%)	5 (2%)	7	41
10	J	216/283 (76%)	198 (92%)	14 (6%)	4 (2%)	10	50
11	K	199/202 (98%)	181 (91%)	15 (8%)	3 (2%)	13	55
12	L	209/215 (97%)	183 (88%)	18 (9%)	8 (4%)	4	28
13	M	130/139 (94%)	117 (90%)	9 (7%)	4 (3%)	5	34
14	N	144/165 (87%)	137 (95%)	3 (2%)	4 (3%)	6	37
15	O	145/148 (98%)	131 (90%)	12 (8%)	2 (1%)	14	57
16	P	202/205 (98%)	184 (91%)	11 (5%)	7 (4%)	4	31
17	Q	185/219 (84%)	155 (84%)	27 (15%)	3 (2%)	12	54
18	R	244/294 (83%)	216 (88%)	18 (7%)	10 (4%)	3	27
19	S	184/187 (98%)	164 (89%)	14 (8%)	6 (3%)	5	32
20	T	179/182 (98%)	172 (96%)	4 (2%)	3 (2%)	11	52
21	U	178/184 (97%)	166 (93%)	8 (4%)	4 (2%)	8	45
22	V	153/161 (95%)	139 (91%)	10 (6%)	4 (3%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	166/203 (82%)	151 (91%)	11 (7%)	4 (2%)	7	43
24	X	95/139 (68%)	82 (86%)	9 (10%)	4 (4%)	3	26
25	Y	99/190 (52%)	91 (92%)	6 (6%)	2 (2%)	9	48
26	Z	119/126 (94%)	107 (90%)	10 (8%)	2 (2%)	11	52
27	0	60/162 (37%)	55 (92%)	4 (7%)	1 (2%)	11	52
28	1	136/146 (93%)	128 (94%)	3 (2%)	5 (4%)	4	29
29	2	96/127 (76%)	84 (88%)	11 (12%)	1 (1%)	19	65
30	3	117/124 (94%)	108 (92%)	4 (3%)	5 (4%)	3	25
31	4	64/67 (96%)	56 (88%)	5 (8%)	3 (5%)	3	22
32	5	221/257 (86%)	199 (90%)	17 (8%)	5 (2%)	8	44
33	6	96/108 (89%)	89 (93%)	4 (4%)	3 (3%)	5	34
34	7	92/120 (77%)	87 (95%)	5 (5%)	0	100	100
35	8	123/131 (94%)	110 (89%)	9 (7%)	4 (3%)	5	32
36	9	101/140 (72%)	87 (86%)	8 (8%)	6 (6%)	2	16
37	a	104/150 (69%)	96 (92%)	7 (7%)	1 (1%)	19	65
38	b	91/112 (81%)	84 (92%)	5 (6%)	2 (2%)	8	45
39	c	87/92 (95%)	72 (83%)	11 (13%)	4 (5%)	3	23
40	d	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
41	e	39/51 (76%)	38 (97%)	1 (3%)	0	100	100
42	f	49/128 (38%)	46 (94%)	3 (6%)	0	100	100
43	g	35/39 (90%)	31 (89%)	2 (6%)	2 (6%)	2	17
44	h	83/96 (86%)	72 (87%)	10 (12%)	1 (1%)	16	60
45	i	93/104 (89%)	83 (89%)	5 (5%)	5 (5%)	2	19
All	All	6115/7124 (86%)	5524 (90%)	436 (7%)	155 (2%)	11	41

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	PRO
5	E	18	PRO
5	E	196	LEU
6	F	102	PHE
6	F	265	GLY

### 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	D	191/202 (95%)	163 (85%)	28 (15%)	4	18
5	E	335/340 (98%)	319 (95%)	16 (5%)	31	72
6	F	336/352 (96%)	310 (92%)	26 (8%)	16	54
7	G	110/155 (71%)	97 (88%)	13 (12%)	6	29
8	H	164/173 (95%)	145 (88%)	19 (12%)	7	30
9	I	189/203 (93%)	169 (89%)	20 (11%)	8	34
10	J	204/260 (78%)	181 (89%)	23 (11%)	7	31
11	K	181/182 (100%)	171 (94%)	10 (6%)	27	68
12	L	190/194 (98%)	169 (89%)	21 (11%)	8	32
13	M	106/110 (96%)	94 (89%)	12 (11%)	7	31
14	N	134/152 (88%)	117 (87%)	17 (13%)	5	25
15	O	121/122 (99%)	110 (91%)	11 (9%)	12	42
16	P	179/180 (99%)	164 (92%)	15 (8%)	14	48
17	Q	165/190 (87%)	157 (95%)	8 (5%)	31	72
18	R	214/254 (84%)	189 (88%)	25 (12%)	7	30
19	S	158/159 (99%)	147 (93%)	11 (7%)	19	58
20	T	161/163 (99%)	146 (91%)	15 (9%)	11	41
21	U	162/166 (98%)	150 (93%)	12 (7%)	17	56
22	V	140/144 (97%)	135 (96%)	5 (4%)	42	79
23	W	128/178 (72%)	121 (94%)	7 (6%)	27	68
24	X	92/131 (70%)	87 (95%)	5 (5%)	27	68
25	Y	90/177 (51%)	84 (93%)	6 (7%)	20	60
26	Z	111/115 (96%)	103 (93%)	8 (7%)	18	57
27	0	53/146 (36%)	51 (96%)	2 (4%)	40	78
28	1	127/132 (96%)	118 (93%)	9 (7%)	18	57
29	2	97/118 (82%)	92 (95%)	5 (5%)	29	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	3	110/115 (96%)	101 (92%)	9 (8%)	14	50
31	4	60/61 (98%)	55 (92%)	5 (8%)	14	49
32	5	201/231 (87%)	187 (93%)	14 (7%)	19	58
33	6	83/92 (90%)	69 (83%)	14 (17%)	2	13
34	7	90/112 (80%)	72 (80%)	18 (20%)	1	8
35	8	114/120 (95%)	105 (92%)	9 (8%)	15	53
36	9	90/127 (71%)	78 (87%)	12 (13%)	5	23
37	a	89/128 (70%)	81 (91%)	8 (9%)	12	43
38	b	82/97 (84%)	81 (99%)	1 (1%)	78	93
39	c	73/77 (95%)	69 (94%)	4 (6%)	27	68
40	d	69/83 (83%)	61 (88%)	8 (12%)	7	30
41	e	40/48 (83%)	35 (88%)	5 (12%)	6	26
42	f	45/114 (40%)	41 (91%)	4 (9%)	12	44
43	g	34/35 (97%)	32 (94%)	2 (6%)	24	65
44	h	70/80 (88%)	66 (94%)	4 (6%)	25	67
45	i	87/93 (94%)	83 (95%)	4 (5%)	33	74
All	All	5475/6311 (87%)	5005 (91%)	470 (9%)	18	46

5 of 470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	95	ASP
18	R	274	ASN
37	a	59	PRO
16	P	26	ARG
17	Q	193	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	42	ASN
20	T	129	ASN
37	a	12	HIS
18	R	45	ASN
18	R	223	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3155/3788 (83%)	972 (30%)	177 (5%)
2	B	117/119 (98%)	24 (20%)	4 (3%)
3	C	148/159 (93%)	46 (31%)	9 (6%)
All	All	3420/4066 (84%)	1042 (30%)	190 (5%)

5 of 1042 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	13	G
1	A	14	U
1	A	16	A
1	A	18	G

5 of 190 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1574	C
1	A	2033	C
1	A	3711	U
1	A	1643	U
1	A	1873	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 171 ligands modelled in this entry, 169 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
46	YMZ	A	3801	-	28,28,28	3.63	9 (32%)	39,43,43	2.55	12 (30%)
46	YMZ	K	301	-	28,28,28	2.85	6 (21%)	39,43,43	2.44	12 (30%)

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
46	YMZ	A	3801	-	-	0/20/28/28	0/3/3/3
46	YMZ	K	301	-	-	0/20/28/28	1/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	3801	YMZ	CAZ-CAT	-11.11	1.38	1.50
46	A	3801	YMZ	CAS-CAW	-9.85	1.38	1.52
46	K	301	YMZ	CAZ-CAT	-8.80	1.40	1.50
46	A	3801	YMZ	CAY-CAR	-8.43	1.37	1.50
46	K	301	YMZ	CAS-CAW	-7.49	1.41	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	K	301	YMZ	CAK-CAR-NAP	-9.30	119.94	125.51
46	A	3801	YMZ	CAK-CAR-NAP	-9.09	120.06	125.51
46	A	3801	YMZ	FAG-CAZ-CAT	-5.43	106.59	112.40
46	A	3801	YMZ	OAA-CAW-CAS	-4.14	104.47	111.01
46	A	3801	YMZ	CAN-NAQ-CAX	-3.99	108.91	111.58

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	K	301	YMZ	CAL-CAM-CAN-CAO-CAX-NAQ

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	3801	YMZ	3	0

## 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	9

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3631:U	O3'	3632:U	P	5.96
1	A	3018:A	O3'	3019:A	P	4.60
1	A	1909:U	O3'	1910:C	P	4.15
1	A	3657:G	O3'	3658:G	P	3.84
1	A	181:C	O3'	182:U	P	3.44