wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:35 PM BST

PDB ID	:	4UER
EMDB ID:	:	EMD-2845
Title	:	40S-eIF1-eIF1A-eIF3-eIF3j translation initiation complex from Lachancea kluyveri
Authors	:	Aylett, C.H.S.; Boehringer, D.; Erzberger, J.P.; Schaefer, T.; Ban, N.
Deposited on	:	2014-12-18
Resolution	:	6.47 Å(reported)
Based on PDB ID	:	3U5B

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

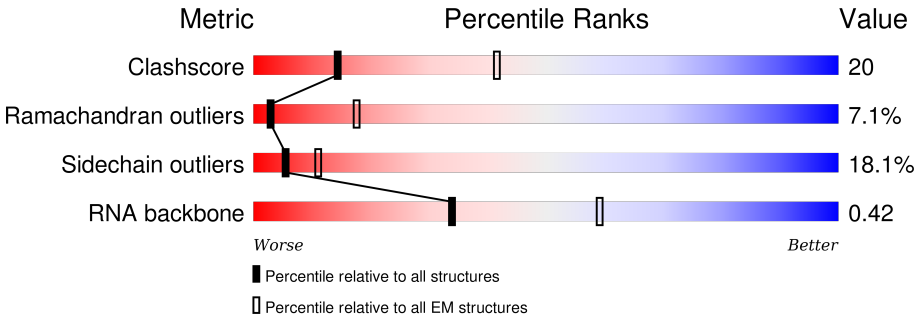
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.47 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 <=5%

Mol	Chain	Length	Quality of chain
1	0	100	42% 51% 6% •
2	1	63	27% 49% 24%
3	2	188	56% 31% 12% •
4	3	184	40% 38% 19% •
5	4	214	32% 40% 21% 7%
6	5	97	42% 39% 13% 5%
7	6	81	58% 35% 6% •
8	7	96	42% 39% 18% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	8	70	31% 39% 24% 6%
10	9	71	41% 41% 14% •
11	A	1781	33% 38% 23% 6%
12	B	206	36% 41% 19% •
13	C	223	53% 33% 13% •
14	D	185	51% 33% 15% •
15	E	217	52% 36% 11% •
16	F	83	46% 46% 7% •
17	G	206	50% 38% 10% •
18	H	129	47% 39% 12% •
19	I	141	43% 39% 16% •
20	J	107	42% 39% 19%
21	K	127	49% 36% 10% 5%
22	L	144	49% 38% 10% •
23	M	145	39% 43% 15% •
24	N	53	47% 42% 8% •
25	O	150	53% 33% 12% •
26	P	134	55% 30% 12% •
27	Q	155	52% 38% 8% •
28	R	318	58% 36% 6% •
29	S	124	50% 38% 9% •
30	T	143	39% 45% 15% •
31	U	124	31% 48% 16% 5%
32	V	120	49% 36% 11% •
33	W	260	46% 43% 10% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	X	60	48% 45% 7%
35	Y	226	52% 35% 12%
36	Z	87	49% 28% 21%
37	a	964	47% 53%
38	b	763	73% 25%
39	c	812	65% 33%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 89319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called EIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	100	805	495	148	157	5	0	0

- Molecule 2 is a protein called ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	63	497	306	99	91	1	0	0

- Molecule 3 is a protein called ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	188	1489	925	298	264	2	0	0

- Molecule 4 is a protein called ES7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	184	1481	951	265	265	0	0

- Molecule 5 is a protein called ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	214	1709	1084	310	311	4	0	0

- Molecule 6 is a protein called ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	97	769	475	160	129	5	0	0

- Molecule 7 is a protein called ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 8 is a protein called ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 9 is a protein called ES25.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 10 is a protein called ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

- Molecule 11 is a RNA chain called 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 12 is a protein called US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 13 is a protein called US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 14 is a protein called US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 15 is a protein called US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 16 is a protein called EIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	83	Total	C	N	O	S	0	0
			671	423	124	120	4		

- Molecule 17 is a protein called US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 18 is a protein called US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 19 is a protein called US9.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	I	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 21 is a protein called US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 22 is a protein called US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 23 is a protein called US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 24 is a protein called US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 25 is a protein called US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 26 is a protein called ES24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 27 is a protein called US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 28 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 29 is a protein called US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 30 is a protein called ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 31 is a protein called ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 32 is a protein called ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	V	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 33 is a protein called ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	W	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 34 is a protein called ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 35 is a protein called ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Y	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 36 is a protein called ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 37 is a protein called EIF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	449	Total	C	N	O	S	0	0
			3656	2350	616	683	7		

- Molecule 38 is a protein called EIF3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	572	Total	C	N	O	S	0	92
			3978	2578	667	720	13		

- Molecule 39 is a protein called EIF3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	544	Total	C	N	O	S	0	0
			4442	2845	736	849	12		

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

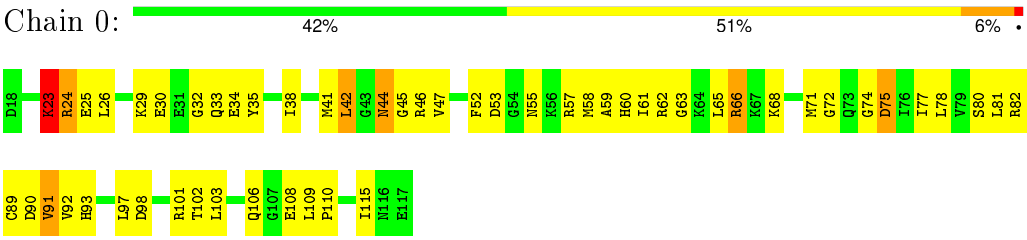
Mol	Chain	Residues	Atoms		AltConf
40	9	1	Total	Zn	0
			1	1	
40	N	1	Total	Zn	0
			1	1	
40	6	1	Total	Zn	0
			1	1	
40	5	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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.

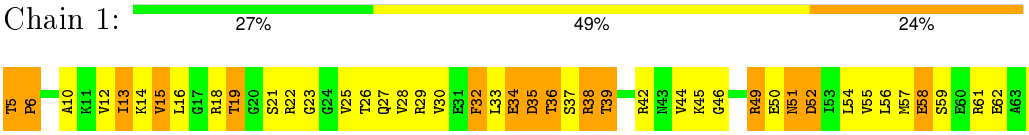
- Molecule 1: EIF1A

Chain 0:



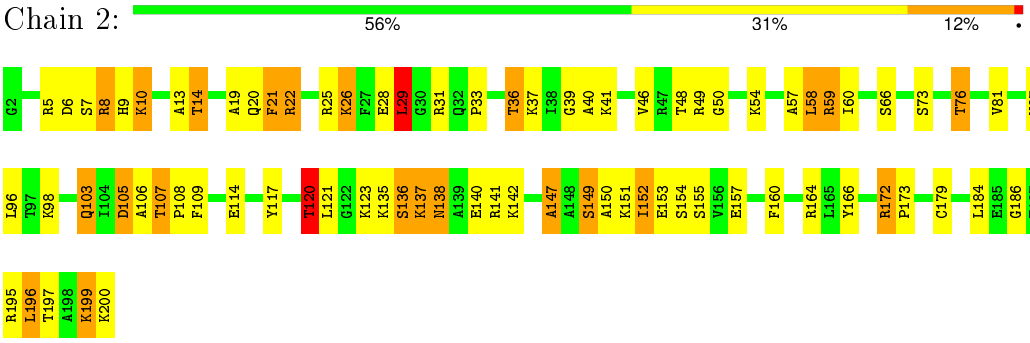
- Molecule 2: ES28

Chain 1:



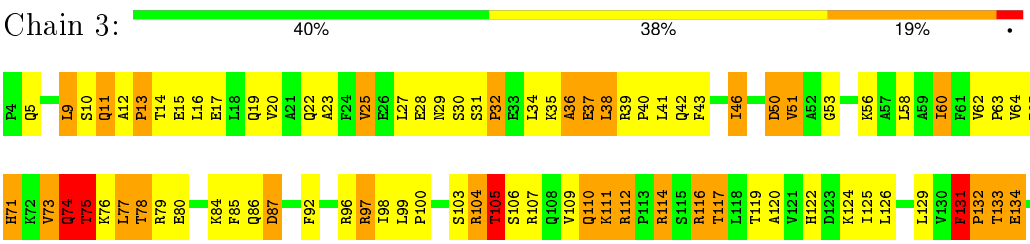
- Molecule 3: ES8

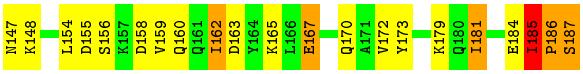
Chain 2:



- Molecule 4: ES7

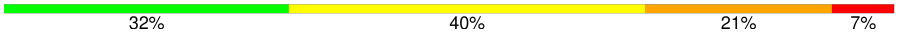
Chain 3:

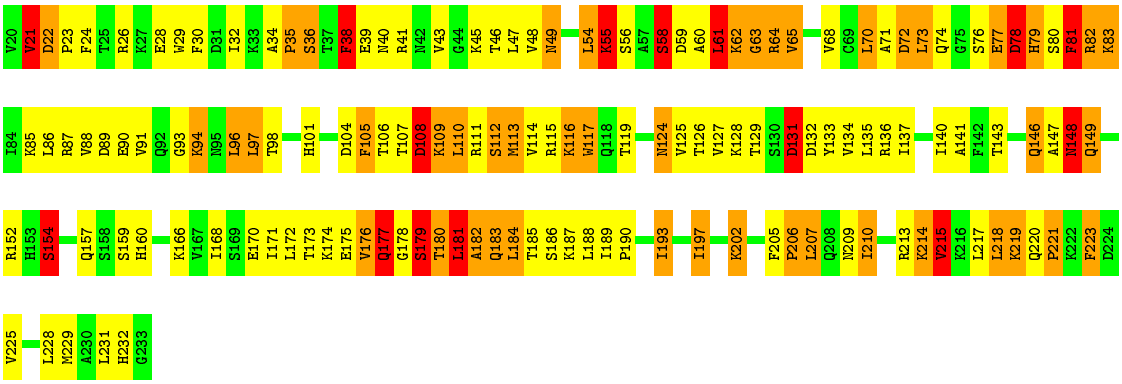




- Molecule 5: ES1

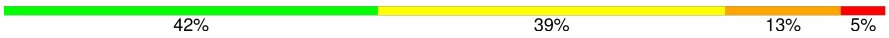
Chain 4:

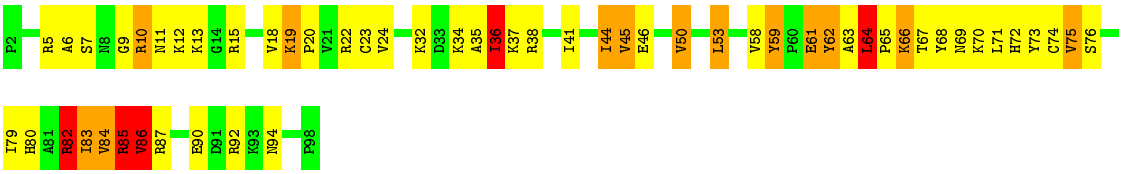




- Molecule 6: ES26

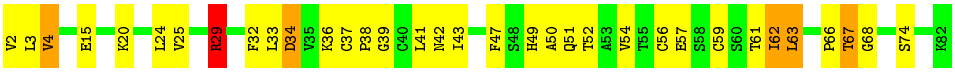
Chain 5:





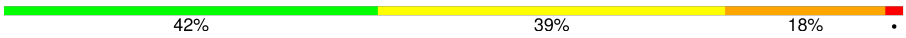
- Molecule 7: ES27

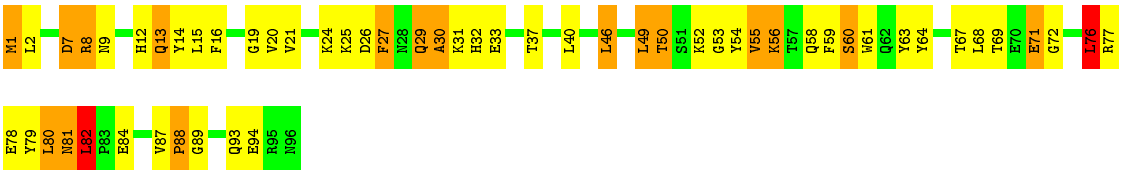
Chain 6:



- Molecule 8: ES10

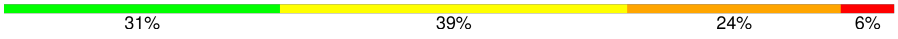
Chain 7:





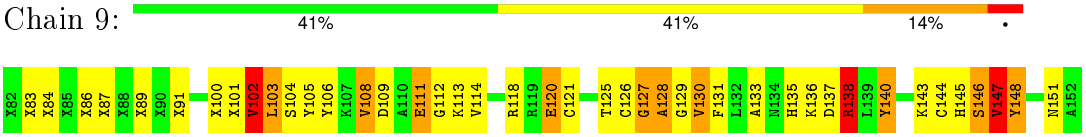
- Molecule 9: ES25

Chain 8:



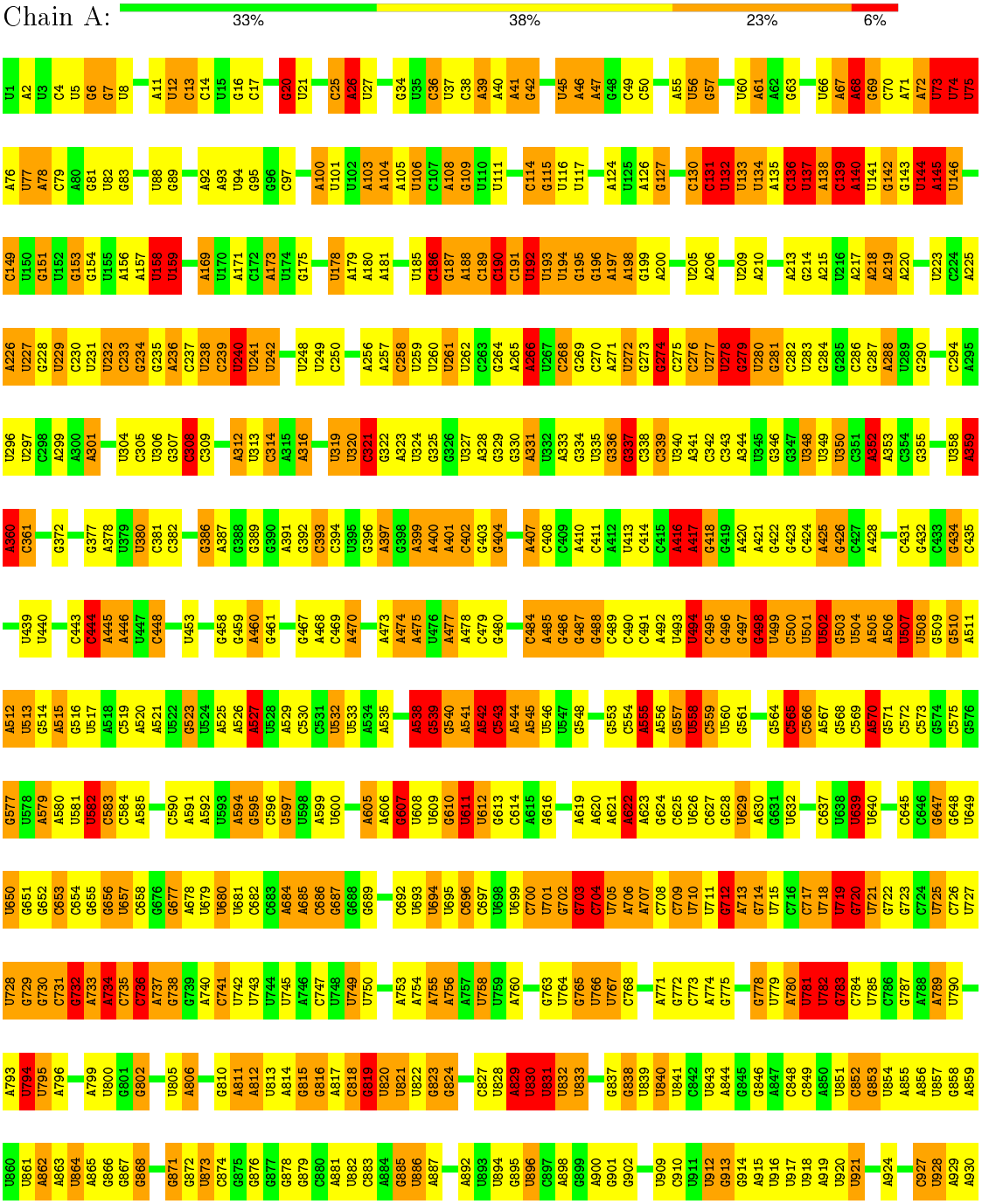
- Molecule 10: ES31

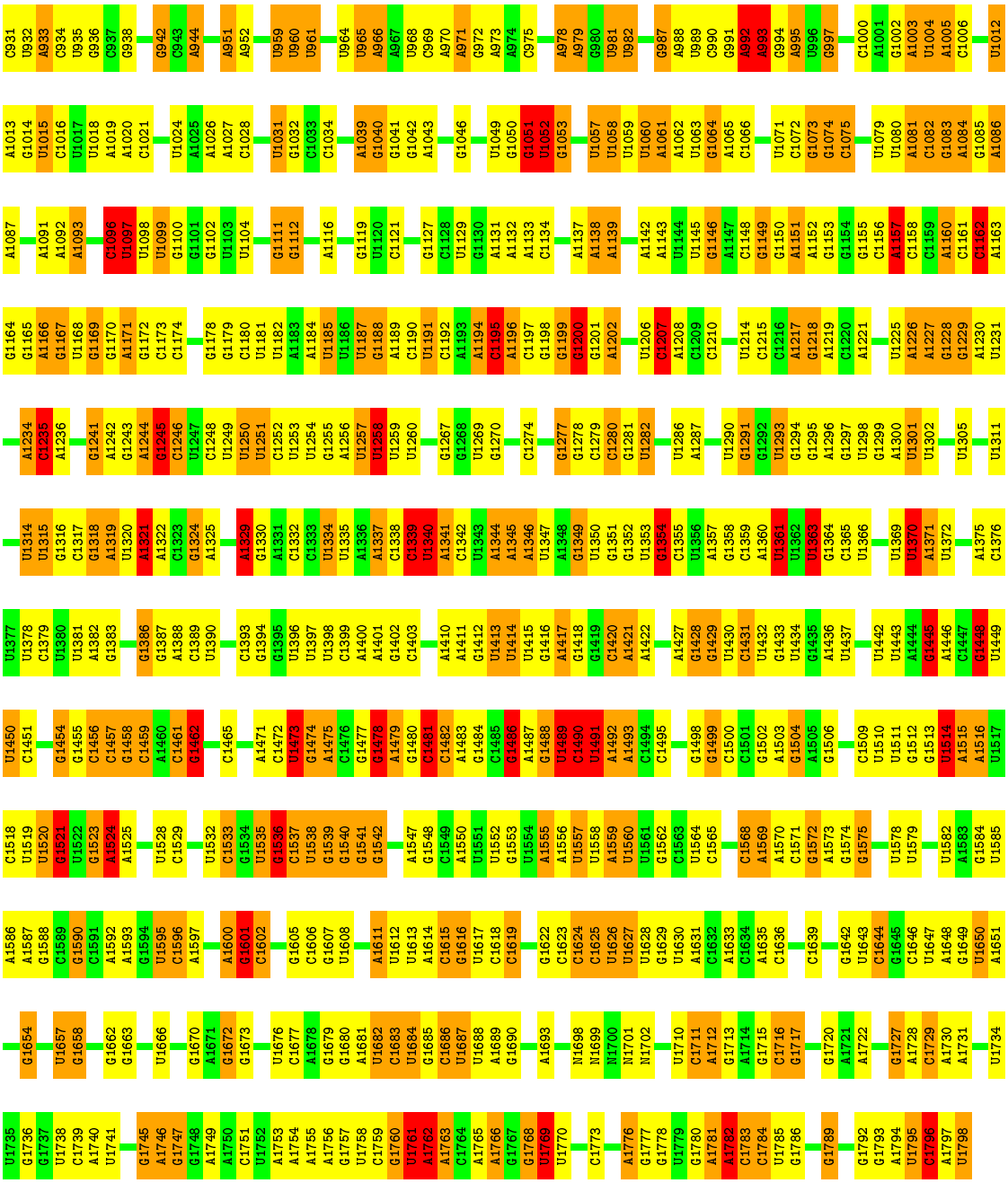
Chain 9:



- Molecule 11: 18S RRNA

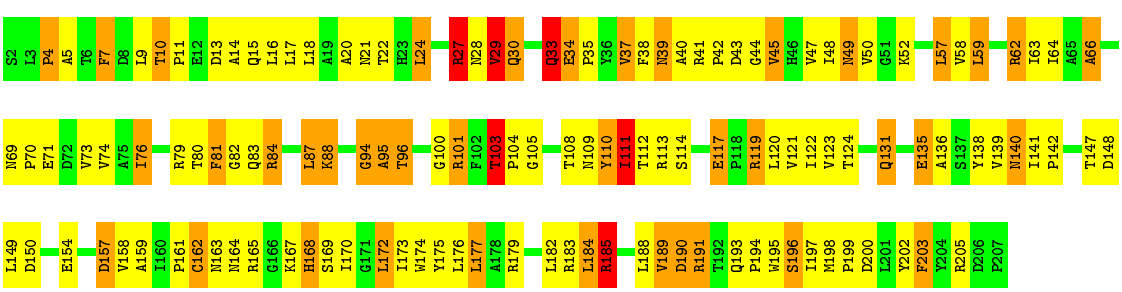
Chain A:





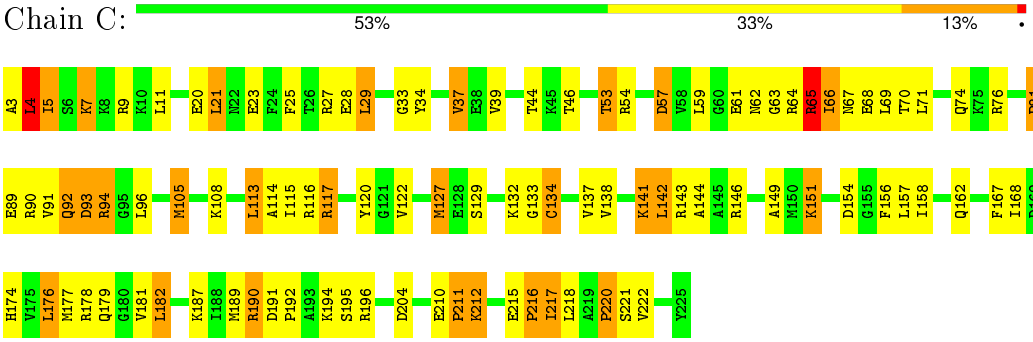
- Molecule 12: US2

Chain B:



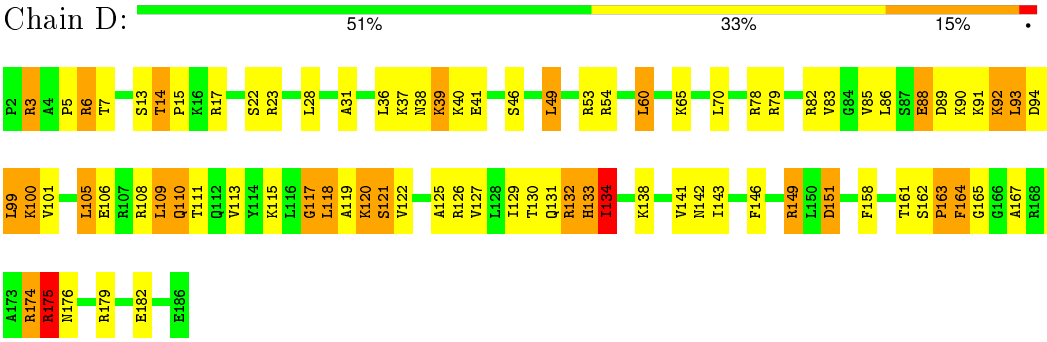
- Molecule 13: US3

Chain C:



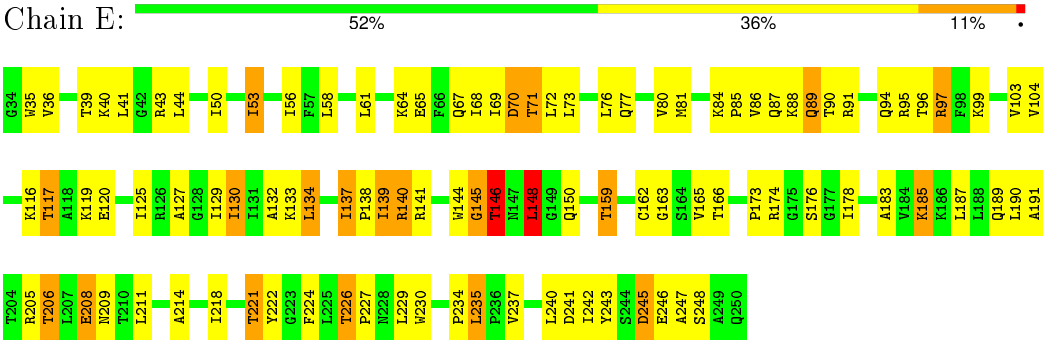
- Molecule 14: US4

Chain D:



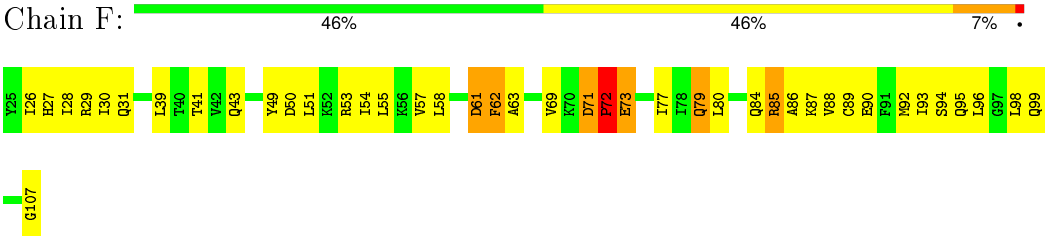
- Molecule 15: US5

Chain E:



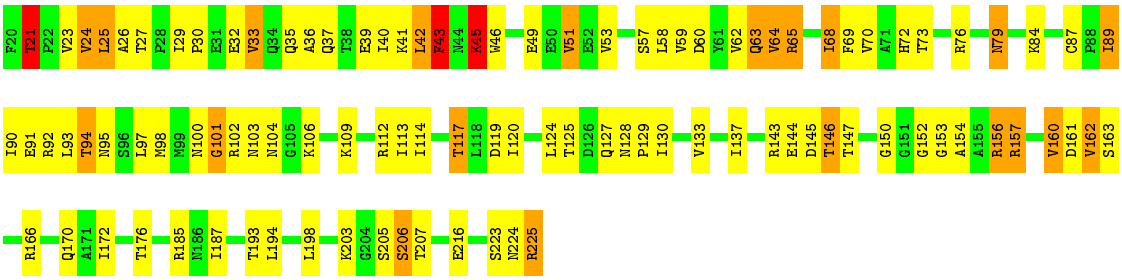
- Molecule 16: EIF1

Chain F:



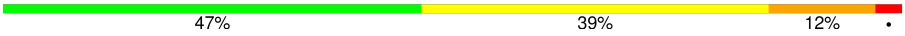
- Molecule 17: US7

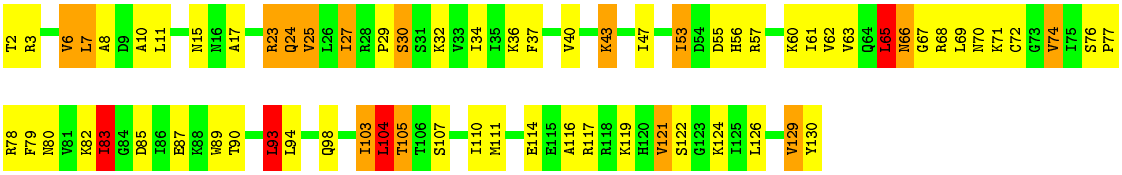
Chain G:



- Molecule 18: US8

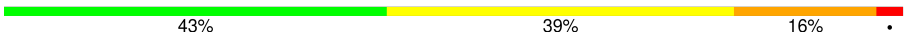
Chain H:

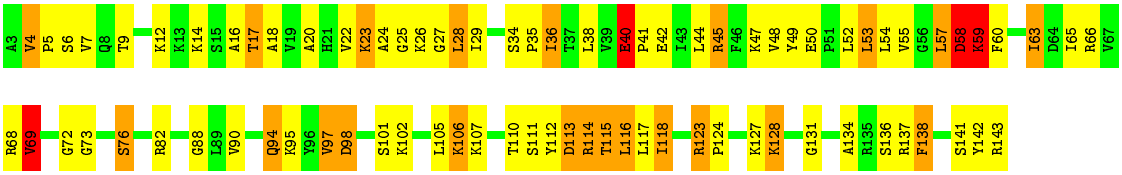




- Molecule 19: US9

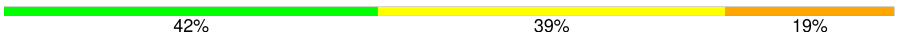
Chain I:

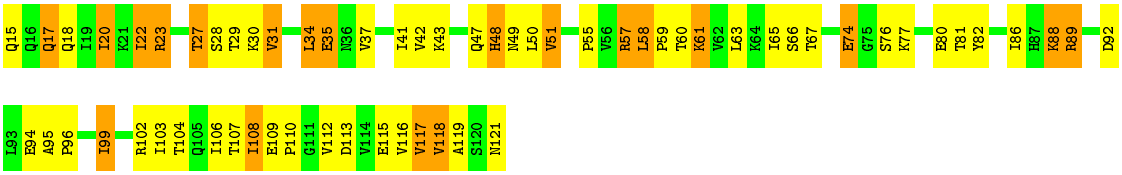




- Molecule 20: US10

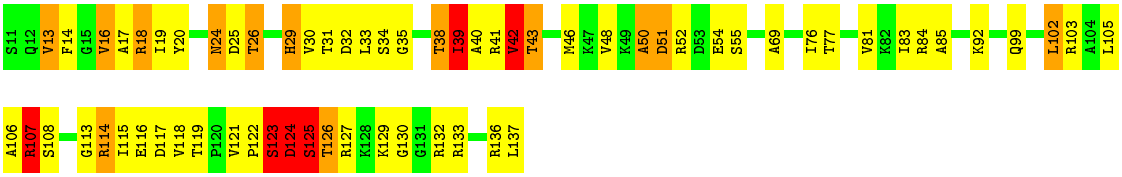
Chain J:





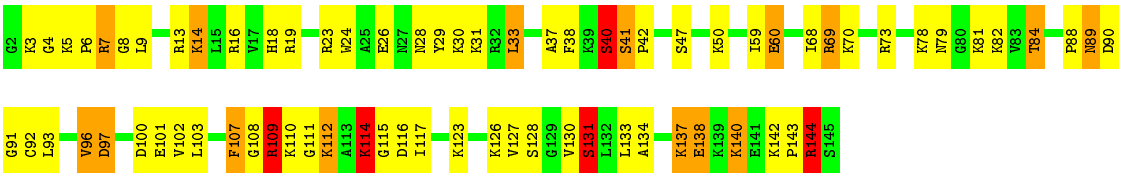
- Molecule 21: US11

Chain K:



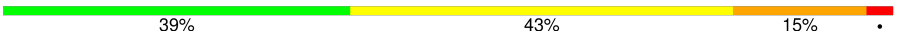
- Molecule 22: US12

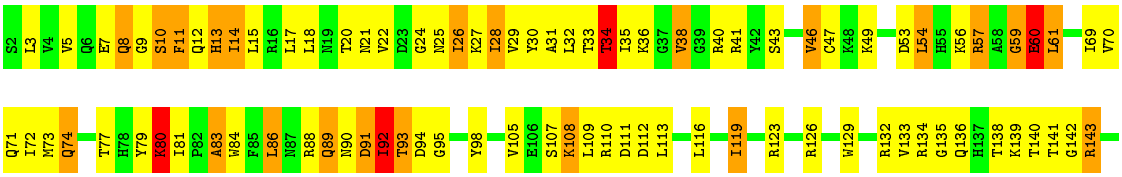
Chain L:



- Molecule 23: US13

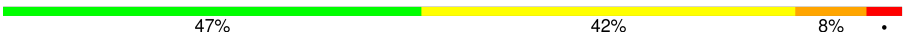
Chain M:





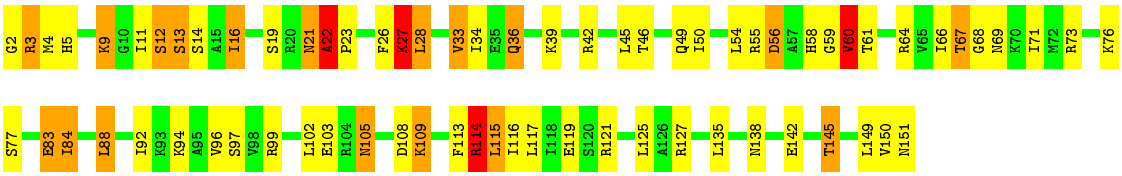
- Molecule 24: US14

Chain N:



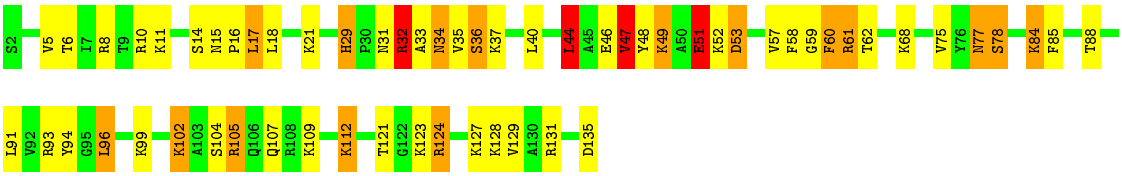
- Molecule 25: US15

Chain O:



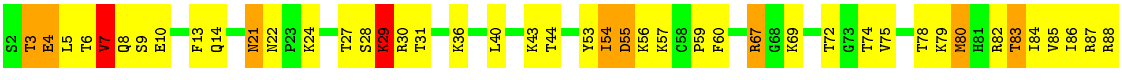
- Molecule 26: ES24

Chain P:



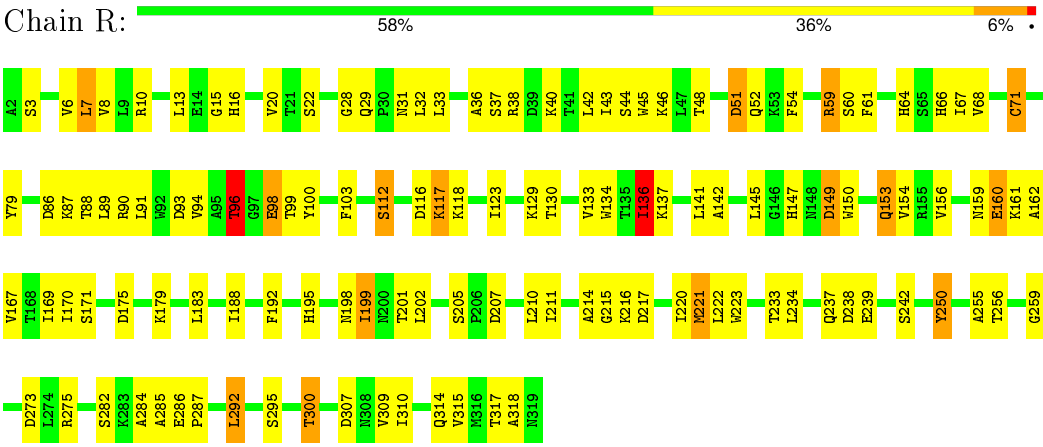
- Molecule 27: US17

Chain Q:



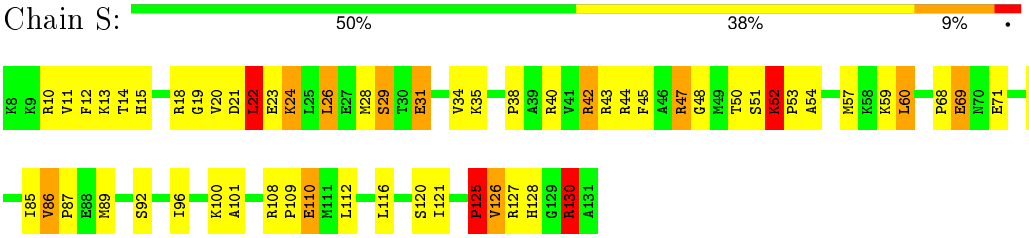
- Molecule 28: RACK1

Chain R:



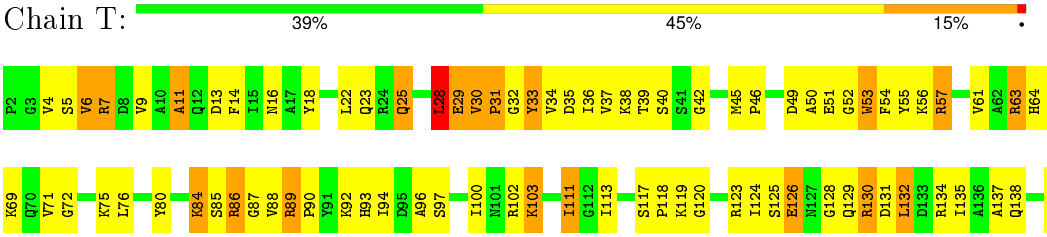
- Molecule 29: US19

Chain S:



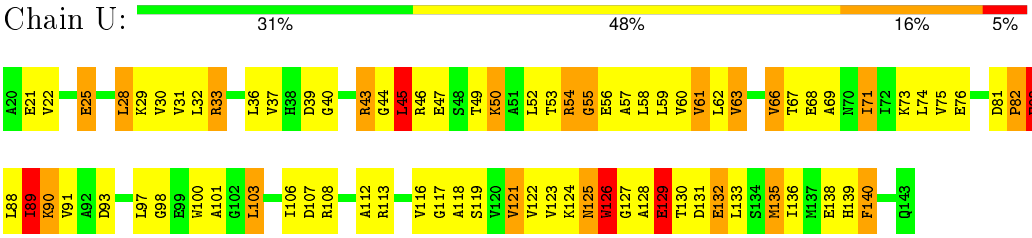
- Molecule 30: ES19

Chain T:



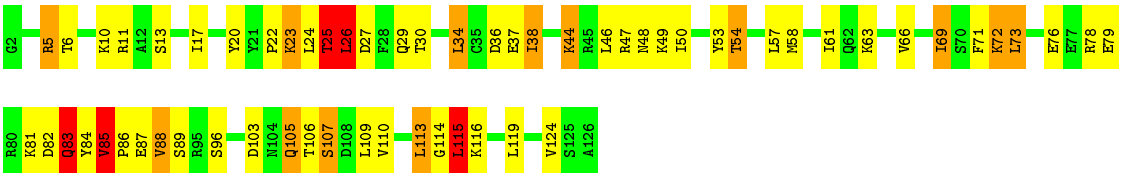
- Molecule 31: ES12

Chain U:



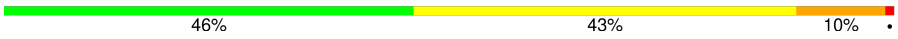
- Molecule 32: ES17

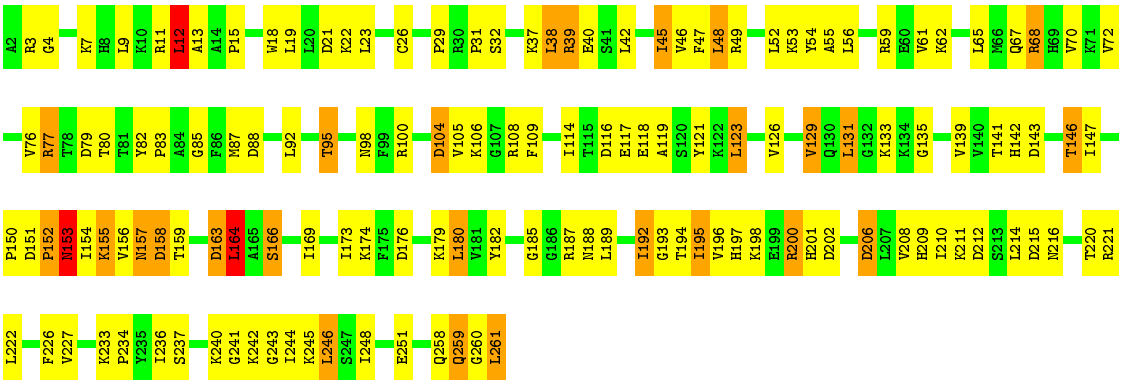
Chain V:



- Molecule 33: ES4

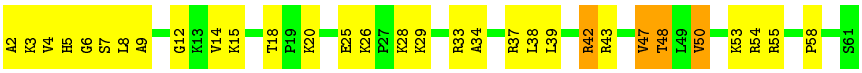
Chain W:





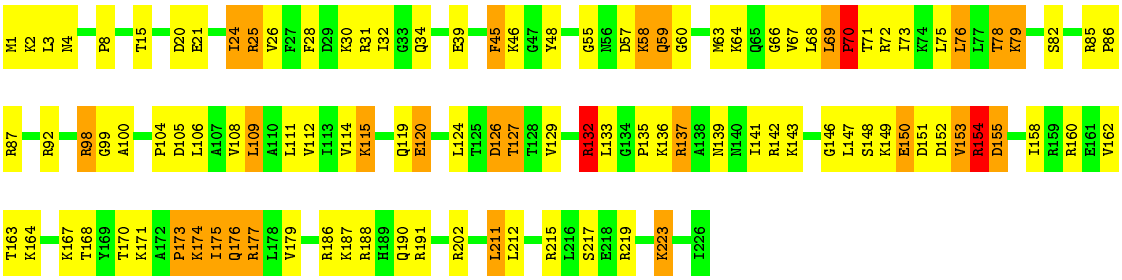
- Molecule 34: ES30

Chain X:



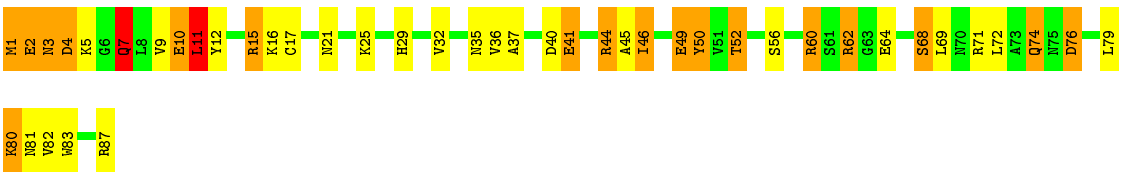
- Molecule 35: ES6

Chain Y:



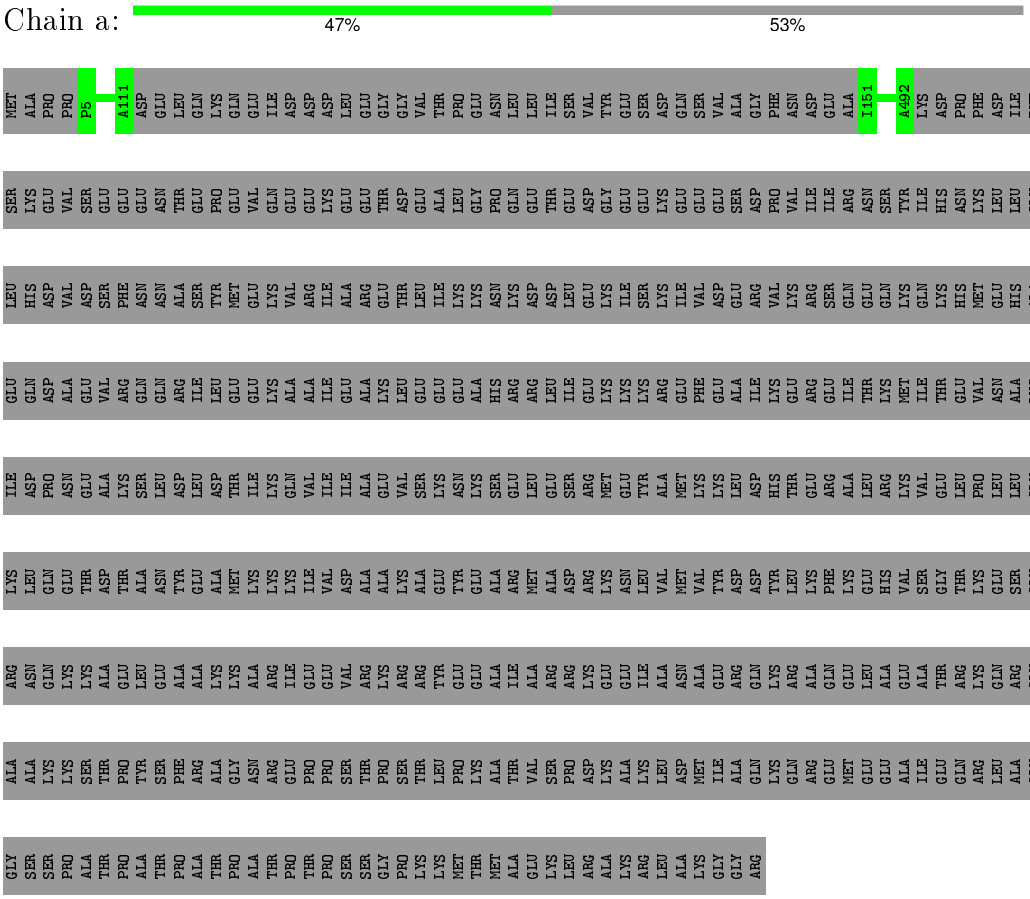
- Molecule 36: ES21

Chain Z:



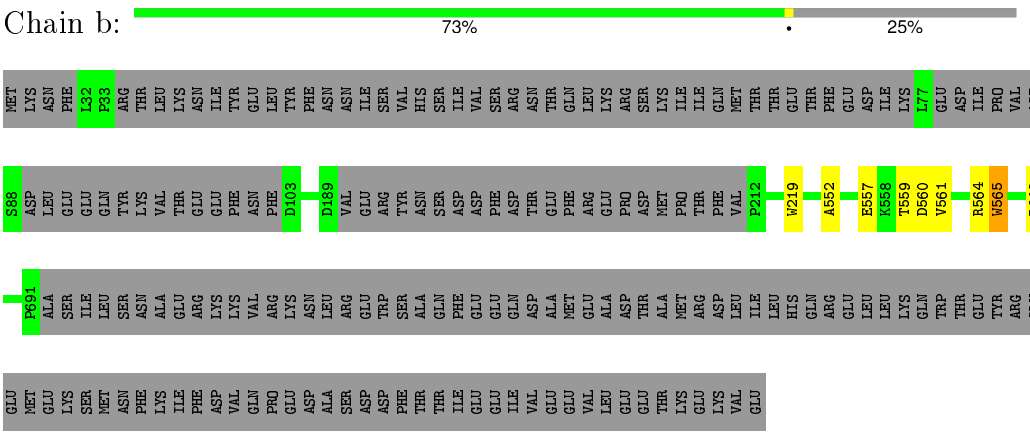
- Molecule 37: EIF3A

Chain a:



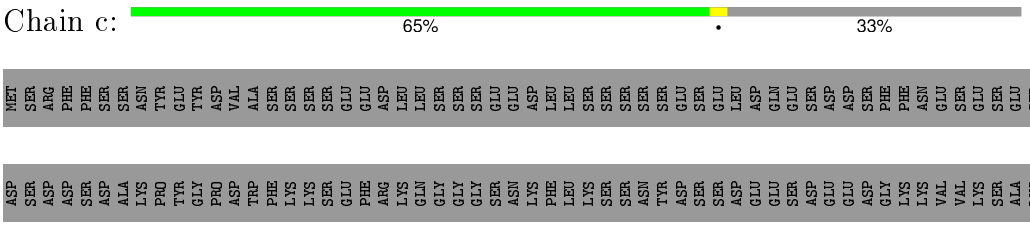
- Molecule 38: EIF3B

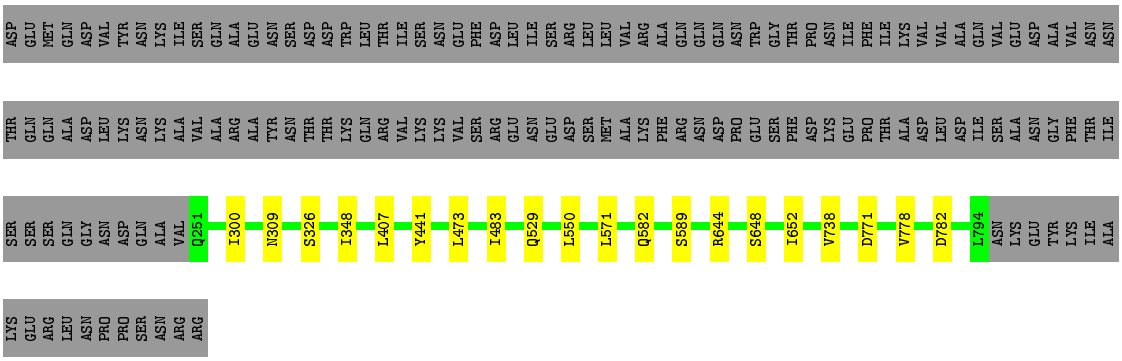
Chain b:



- Molecule 39: EIF3C

Chain c:




ASP GLU MET GLN ASP VAL TYR ASN LYS ILE SER GLN ALA GLU ASN SER ASP ASP TRP LEU THR ILE SER ASN GLU PHE ASP LEU ILE SER ARG LEU LEU VAL ARG ALA GLN GLN GLN ASN TRP GLY THR PRO ASN ILE PHE ILE LYS VAL VAL ALA GLN VAL GLU ASP ALA VAL ASN ASN
THR GLN GLN ALA ASP LEU LYS ASN LYS ALA VAL ALA ARG ALA TYR ASN THR THR LYS GLN ARG VAL LYS LYS VAL SER ARG GLU ASN GLU ASP SER MET ALA LYS PHE ARG ASN ASP PRO GLU SER PHE ASP LYS GLU PRO THR ALA ASP LEU ASP ILE SER ALA ASN GLY PHE THR ILE
SER SER SER GLN GLY ASN ASP GLN ALA VAL Q251 I300 N309 S326 I348 L407 Y441 L473 I483 Q529 L550 L571 Q582 S589 R644 S648 I652 V738 D771 V778 D782 L794 ASN LYS GLU TYR LYS ILE ALA
LYS GLU ARG LEU ASN PRO PRO SER ASN ARG ARG

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	BY IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0	0.64	0/815	1.14	3/1087 (0.3%)
10	9	0.53	0/404	0.99	1/542 (0.2%)
11	A	0.96	38/42127 (0.1%)	1.50	830/65638 (1.3%)
12	B	0.54	0/1617	0.80	0/2215
13	C	0.59	0/1759	0.74	0/2368
14	D	0.60	0/1519	0.82	1/2035 (0.0%)
15	E	0.60	0/1665	0.78	0/2263
16	F	0.64	0/678	1.18	6/903 (0.7%)
17	G	0.49	0/1629	0.72	0/2202
18	H	0.66	0/1038	0.86	3/1395 (0.2%)
19	I	0.57	0/1125	0.85	3/1510 (0.2%)
2	1	0.44	0/499	0.72	0/670
20	J	0.55	0/865	0.76	0/1169
21	K	0.49	0/901	0.82	1/1217 (0.1%)
22	L	0.72	0/1139	0.91	2/1518 (0.1%)
23	M	0.59	0/1211	0.80	0/1628
24	N	0.71	0/452	0.94	1/600 (0.2%)
25	O	0.61	0/1215	0.83	3/1638 (0.2%)
26	P	0.56	0/1087	0.77	1/1449 (0.1%)
27	Q	0.70	0/1239	0.81	0/1673
28	R	0.49	0/2490	0.70	0/3389
29	S	0.60	0/998	0.86	2/1341 (0.1%)
3	2	0.68	0/1514	0.88	2/2021 (0.1%)
30	T	0.57	0/1130	0.81	0/1517
31	U	0.49	0/898	0.76	0/1220
32	V	0.54	0/935	0.81	0/1254
33	W	0.58	0/2109	0.86	1/2839 (0.0%)
34	X	0.50	0/483	0.72	0/643
35	Y	0.55	0/1823	0.75	0/2439
36	Z	0.53	0/693	0.75	0/935
37	a	0.32	0/3729	0.51	0/5041
38	b	0.42	1/3999 (0.0%)	0.57	2/5440 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	c	0.33	0/4525	0.53	0/6120
4	3	0.52	0/1506	0.77	0/2028
5	4	0.45	0/1735	0.81	0/2335
6	5	0.54	0/782	0.77	0/1047
7	6	0.53	0/620	0.82	1/838 (0.1%)
8	7	0.56	0/789	0.83	3/1067 (0.3%)
9	8	0.50	0/571	0.86	1/768 (0.1%)
All	All	0.75	39/94313 (0.0%)	1.18	867/136002 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
10	9	0	2
16	F	0	1
21	K	0	1
27	Q	0	1
32	V	0	2
39	c	0	1
4	3	0	1
5	4	0	1
7	6	0	1
9	8	0	3
All	All	0	15

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1626	U	O3'-P	48.27	2.19	1.61
11	A	553	G	C6-N1	8.08	1.45	1.39
11	A	377	G	N9-C4	-7.20	1.32	1.38
11	A	1456	C	N3-C4	-7.04	1.29	1.33
11	A	1455	G	C6-O6	6.88	1.30	1.24

The worst 5 of 867 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1626	U	O3'-P-O5'	27.80	156.82	104.00
11	A	1626	U	OP1-P-O3'	-21.44	58.04	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1626	U	P-O3'-C3'	-19.41	96.41	119.70
11	A	553	G	N1-C6-O6	18.48	130.99	119.90
11	A	1200	G	N1-C6-O6	17.91	130.65	119.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	23	LYS	Peptide
4	3	131	PHE	Peptide
5	4	131	ASP	Peptide
7	6	42	ASN	Peptide
9	8	54	VAL	Peptide

5.2 Too-close contacts (i)

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	0	805	0	790	147	0
2	1	497	0	535	36	0
3	2	1489	0	1525	59	0
4	3	1481	0	1572	80	0
5	4	1709	0	1784	125	0
6	5	769	0	814	51	0
7	6	610	0	630	24	0
8	7	772	0	727	42	0
9	8	563	0	603	45	0
10	9	516	0	517	42	0
11	A	37835	0	19056	1168	0
12	B	1577	0	1566	221	0
13	C	1734	0	1817	80	0
14	D	1494	0	1573	81	0
15	E	1635	0	1715	88	0
16	F	671	0	707	80	0
17	G	1609	0	1675	70	0
18	H	1021	0	1060	54	0
19	I	1105	0	1166	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	855	0	917	41	0
21	K	891	0	883	63	0
22	L	1121	0	1196	61	0
23	M	1192	0	1222	63	0
24	N	442	0	428	24	0
25	O	1192	0	1255	45	0
26	P	1073	0	1132	41	0
27	Q	1213	0	1257	50	0
28	R	2437	0	2386	77	0
29	S	977	0	1002	41	0
30	T	1112	0	1124	69	0
31	U	890	0	887	43	0
32	V	926	0	930	76	0
33	W	2068	0	2154	71	0
34	X	475	0	523	86	0
35	Y	1799	0	1879	88	0
36	Z	684	0	672	39	0
37	a	3656	0	3708	0	0
38	b	3978	0	3768	0	0
39	c	4442	0	4474	0	0
40	5	1	0	0	0	0
40	6	1	0	0	0	0
40	9	1	0	0	0	0
40	N	1	0	0	0	0
All	All	89319	0	71629	2907	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 20.

The worst 5 of 2907 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)
11:A:1151:A:C2'	11:A:1152:A:H5'	1.10	1.57
11:A:1151:A:C6	11:A:1152:A:C8	1.93	1.57
11:A:1293:U:H1'	12:B:111:ILE:CB	1.21	1.57
11:A:1293:U:H1'	12:B:111:ILE:CG1	1.27	1.56
1:0:46:ARG:CD	34:X:3:LYS:HE3	1.39	1.53

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	98/100 (98%)	89 (91%)	6 (6%)	3 (3%)	5 42
2	1	61/63 (97%)	47 (77%)	9 (15%)	5 (8%)	1 18
3	2	184/188 (98%)	155 (84%)	14 (8%)	15 (8%)	1 18
4	3	182/184 (99%)	128 (70%)	27 (15%)	27 (15%)	0 5
5	4	212/214 (99%)	132 (62%)	42 (20%)	38 (18%)	0 4
6	5	95/97 (98%)	58 (61%)	20 (21%)	17 (18%)	0 4
7	6	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	2 30
8	7	94/96 (98%)	66 (70%)	18 (19%)	10 (11%)	0 11
9	8	68/70 (97%)	46 (68%)	11 (16%)	11 (16%)	0 5
10	9	50/71 (70%)	30 (60%)	9 (18%)	11 (22%)	0 2
12	B	204/206 (99%)	143 (70%)	35 (17%)	26 (13%)	0 8
13	C	221/223 (99%)	180 (81%)	28 (13%)	13 (6%)	2 26
14	D	183/185 (99%)	153 (84%)	18 (10%)	12 (7%)	1 24
15	E	215/217 (99%)	187 (87%)	16 (7%)	12 (6%)	2 28
16	F	81/83 (98%)	75 (93%)	5 (6%)	1 (1%)	16 61
17	G	204/206 (99%)	154 (76%)	31 (15%)	19 (9%)	1 16
18	H	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	7 47
19	I	139/141 (99%)	114 (82%)	14 (10%)	11 (8%)	1 19
20	J	105/107 (98%)	87 (83%)	13 (12%)	5 (5%)	3 31
21	K	125/127 (98%)	94 (75%)	16 (13%)	15 (12%)	0 8
22	L	142/144 (99%)	111 (78%)	13 (9%)	18 (13%)	0 8
23	M	143/145 (99%)	110 (77%)	19 (13%)	14 (10%)	1 14
24	N	51/53 (96%)	42 (82%)	7 (14%)	2 (4%)	4 36
25	O	148/150 (99%)	125 (84%)	15 (10%)	8 (5%)	2 29
26	P	132/134 (98%)	106 (80%)	13 (10%)	13 (10%)	1 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	Q	153/155 (99%)	125 (82%)	19 (12%)	9 (6%)	2 26
28	R	316/318 (99%)	273 (86%)	30 (10%)	13 (4%)	3 35
29	S	122/124 (98%)	92 (75%)	15 (12%)	15 (12%)	0 8
30	T	141/143 (99%)	111 (79%)	18 (13%)	12 (8%)	1 18
31	U	122/124 (98%)	66 (54%)	23 (19%)	33 (27%)	0 1
32	V	116/120 (97%)	87 (75%)	17 (15%)	12 (10%)	1 12
33	W	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1 20
34	X	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	5 40
35	Y	224/226 (99%)	190 (85%)	22 (10%)	12 (5%)	2 29
36	Z	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0 9
37	a	445/964 (46%)	438 (98%)	7 (2%)	0	100 100
38	b	478/763 (63%)	452 (95%)	24 (5%)	2 (0%)	39 80
39	c	542/812 (67%)	507 (94%)	35 (6%)	0	100 100
All	All	6403/7570 (85%)	5264 (82%)	686 (11%)	453 (7%)	3 22

5 of 453 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	24	ARG
2	1	36	THR
2	1	51	ASN
3	2	13	ALA
3	2	22	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	86/86 (100%)	84 (98%)	2 (2%)	58 82
2	1	56/56 (100%)	38 (68%)	18 (32%)	0 2
3	2	150/150 (100%)	118 (79%)	32 (21%)	1 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	3	165/165 (100%)	124 (75%)	41 (25%)	1 6
5	4	191/191 (100%)	137 (72%)	54 (28%)	0 3
6	5	83/83 (100%)	65 (78%)	18 (22%)	1 9
7	6	70/70 (100%)	62 (89%)	8 (11%)	7 32
8	7	77/89 (86%)	58 (75%)	19 (25%)	1 6
9	8	61/61 (100%)	43 (70%)	18 (30%)	0 3
10	9	43/43 (100%)	32 (74%)	11 (26%)	0 6
12	B	164/173 (95%)	122 (74%)	42 (26%)	0 6
13	C	182/182 (100%)	137 (75%)	45 (25%)	1 6
14	D	158/158 (100%)	117 (74%)	41 (26%)	0 5
15	E	176/176 (100%)	130 (74%)	46 (26%)	0 5
16	F	74/74 (100%)	73 (99%)	1 (1%)	74 89
17	G	173/173 (100%)	137 (79%)	36 (21%)	1 10
18	H	110/110 (100%)	84 (76%)	26 (24%)	1 7
19	I	117/117 (100%)	84 (72%)	33 (28%)	0 3
20	J	100/100 (100%)	71 (71%)	29 (29%)	0 3
21	K	81/96 (84%)	57 (70%)	24 (30%)	0 3
22	L	119/119 (100%)	96 (81%)	23 (19%)	2 13
23	M	128/128 (100%)	87 (68%)	41 (32%)	0 2
24	N	47/47 (100%)	38 (81%)	9 (19%)	2 13
25	O	127/127 (100%)	91 (72%)	36 (28%)	0 3
26	P	112/112 (100%)	84 (75%)	28 (25%)	1 6
27	Q	129/136 (95%)	105 (81%)	24 (19%)	2 14
28	R	259/261 (99%)	222 (86%)	37 (14%)	4 25
29	S	101/104 (97%)	82 (81%)	19 (19%)	2 13
30	T	115/115 (100%)	84 (73%)	31 (27%)	0 5
31	U	88/100 (88%)	55 (62%)	33 (38%)	0 1
32	V	94/109 (86%)	70 (74%)	24 (26%)	1 6
33	W	221/221 (100%)	166 (75%)	55 (25%)	1 6
34	X	51/51 (100%)	43 (84%)	8 (16%)	3 21
35	Y	188/193 (97%)	149 (79%)	39 (21%)	1 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	Z	74/74 (100%)	56 (76%)	18 (24%)	1 6
37	a	404/846 (48%)	404 (100%)	0	100 100
38	b	430/693 (62%)	421 (98%)	9 (2%)	61 84
39	c	506/749 (68%)	487 (96%)	19 (4%)	40 73
All	All	5510/6538 (84%)	4513 (82%)	997 (18%)	5 15

5 of 997 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	H	98	GLN
22	L	110	LYS
35	Y	78	THR
19	I	36	ILE
20	J	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
17	G	104	ASN
19	I	62	ASN
39	c	529	GLN
17	G	170	GLN
19	I	74	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1763/1781 (98%)	544 (30%)	86 (4%)

5 of 544 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	2	A
11	A	4	C
11	A	8	U
11	A	16	G
11	A	20	G

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	542	A
11	A	755	A
11	A	1568	C
11	A	555	A
11	A	685	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.