wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:43 PM BST

PDB ID	:	4V91
EMDB ID:	:	EMD-2599
Title	:	Kluyveromyces lactis 80S ribosome in complex with CrPV-IRES
Authors	:	Fernandez, I.S.; Bai, X.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-03-21
Resolution	:	3.70 Å(reported)
Based on PDB ID	:	3B31

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

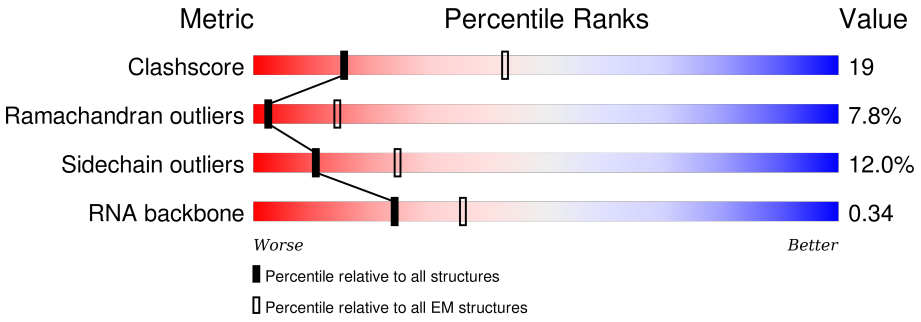
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.70 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	1	3397	27% 38% 23% 7% 6%
2	3	121	39% 39% 17% 5%
3	4	158	29% 39% 27% 6%
4	A	254	44% 47% 6% • •
5	B	387	46% 40% 11% •
6	C	362	46% 44% 7% •
7	D	297	53% 41% 5% •
8	E	176	54% 28% 5% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	244	45% 40% 6% 9%
10	G	256	45% 38% 7% 9%
11	H	191	51% 41% 8%
12	I	221	49% 38% 7% 5%
13	J	174	50% 36% 8%
14	L	199	42% 43% 10%
15	M	138	51% 40% 7%
16	N	204	42% 48% 9%
17	O	398	21% 19% 6% 51%
18	P	184	46% 46% 6%
19	Q	186	51% 39% 9%
20	R	189	49% 40% 7%
21	S	172	41% 49% 9%
22	T	160	45% 49%
23	U	121	62% 18% 17%
24	V	137	50% 40% 8%
25	W	155	19% 19% 61%
26	X	142	48% 28% 8% 15%
27	Y	127	43% 49% 7%
28	Z	136	41% 50% 7%
29	a	149	85% 11%
30	b	59	83% 10%
31	c	105	73% 17% 8%
32	d	113	81% 13%
33	e	130	81% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	107	
35	g	121	
36	h	120	
37	i	100	
38	j	88	
39	k	78	
40	l	51	
41	m	128	
42	n	25	
43	o	106	
44	p	92	
45	t	217	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 125665 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 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3203	68514	30602	12358	22351	3203	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1152	461	845	121	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called UL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	252	1914	1191	388	334	1	0	0

- Molecule 5 is a protein called UL3.

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

- Molecule 6 is a protein called UL4.

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

- Molecule 7 is a protein called UL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called EL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called UL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called EL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called UL6.

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

- Molecule 12 is a protein called UL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called UL5.

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

- Molecule 14 is a protein called EL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	193	Total 1543	C 962	N 315	O 266	0	0

- Molecule 15 is a protein called EL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	136	Total 1053	C 675	N 199	O 177	S 2	0	0

- Molecule 16 is a protein called EL15.

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

- Molecule 17 is a protein called UL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	197	Total 1555	C 1003	N 289	O 262	S 1	0	0

- Molecule 18 is a protein called UL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	183	Total 1420	C 882	N 281	O 257	0	0

- Molecule 19 is a protein called EL18.

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

- Molecule 20 is a protein called EL19.

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

- Molecule 21 is a protein called EL20.

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

- Molecule 22 is a protein called EL21.

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

- Molecule 23 is a protein called EL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 24 is a protein called UL14.

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

- Molecule 25 is a protein called EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	60	Total	C	N	O	S	0	0
			500	322	98	79	1		

- Molecule 26 is a protein called UL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called UL24.

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

- Molecule 28 is a protein called EL27.

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

- Molecule 29 is a protein called UL15.

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

- Molecule 30 is a protein called EL29.

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

- Molecule 31 is a protein called EL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 32 is a protein called EL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called EL32.

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

- Molecule 34 is a protein called EL33.

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

- Molecule 35 is a protein called EL34.

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

- Molecule 36 is a protein called UL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 37 is a protein called EL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called EL37.

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

- Molecule 39 is a protein called EL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 40 is a protein called EL39.

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

- Molecule 41 is a protein called EL40.

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

- Molecule 42 is a protein called EL41.

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

- Molecule 43 is a protein called EL42.

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

- Molecule 44 is a protein called EL43.

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

- Molecule 45 is a protein called UL1.

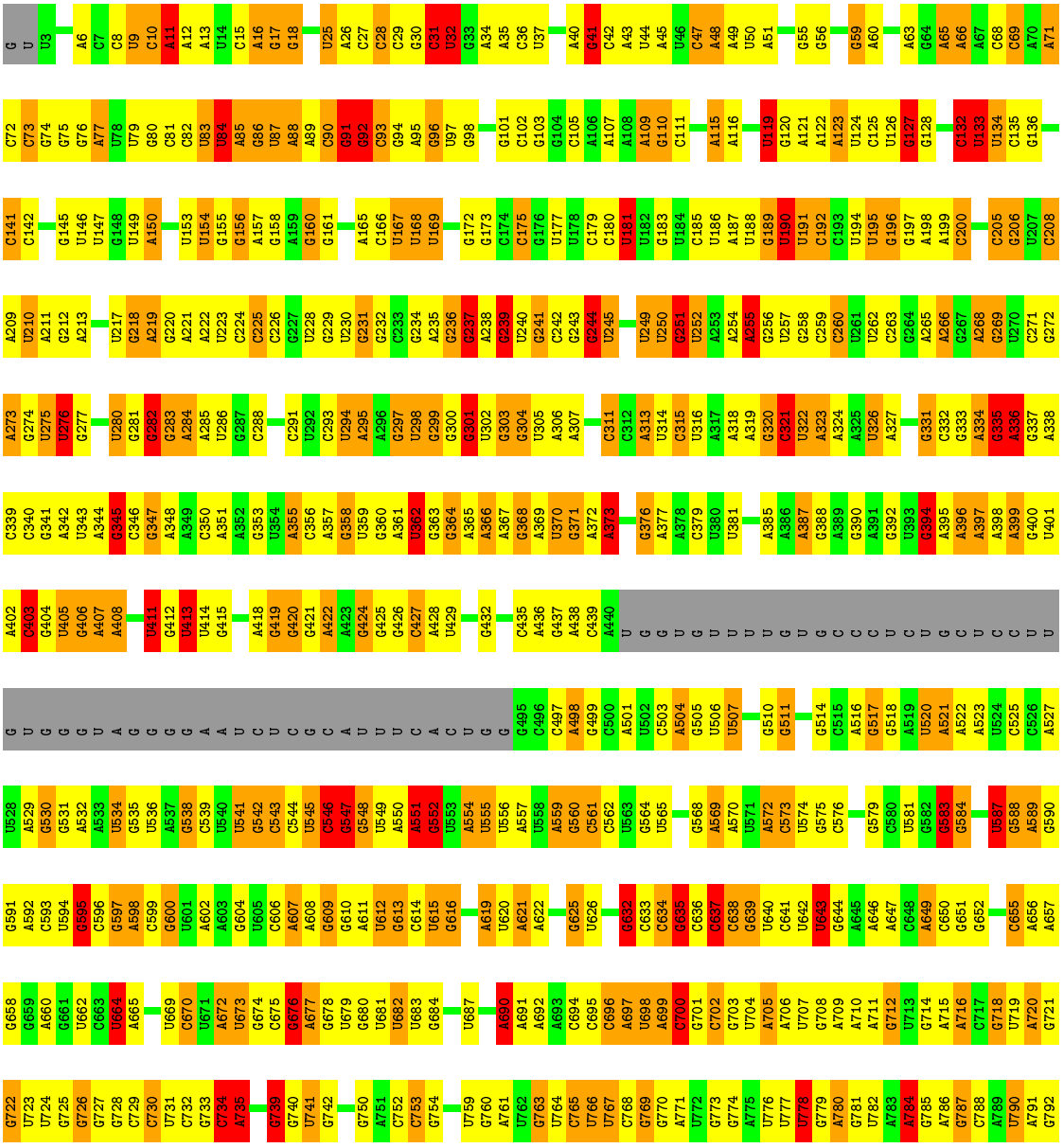
Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

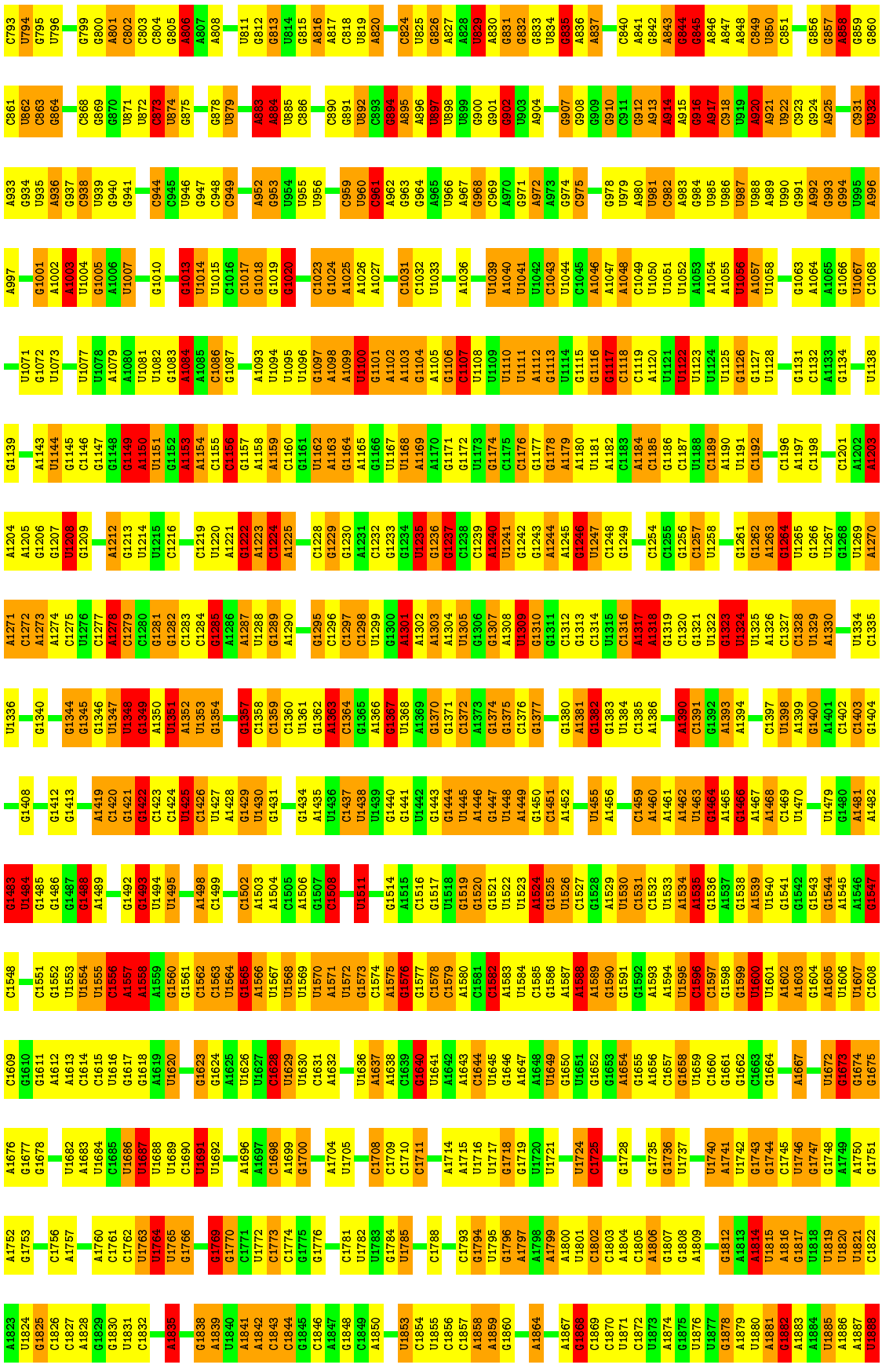
3 Residue-property plots (i)

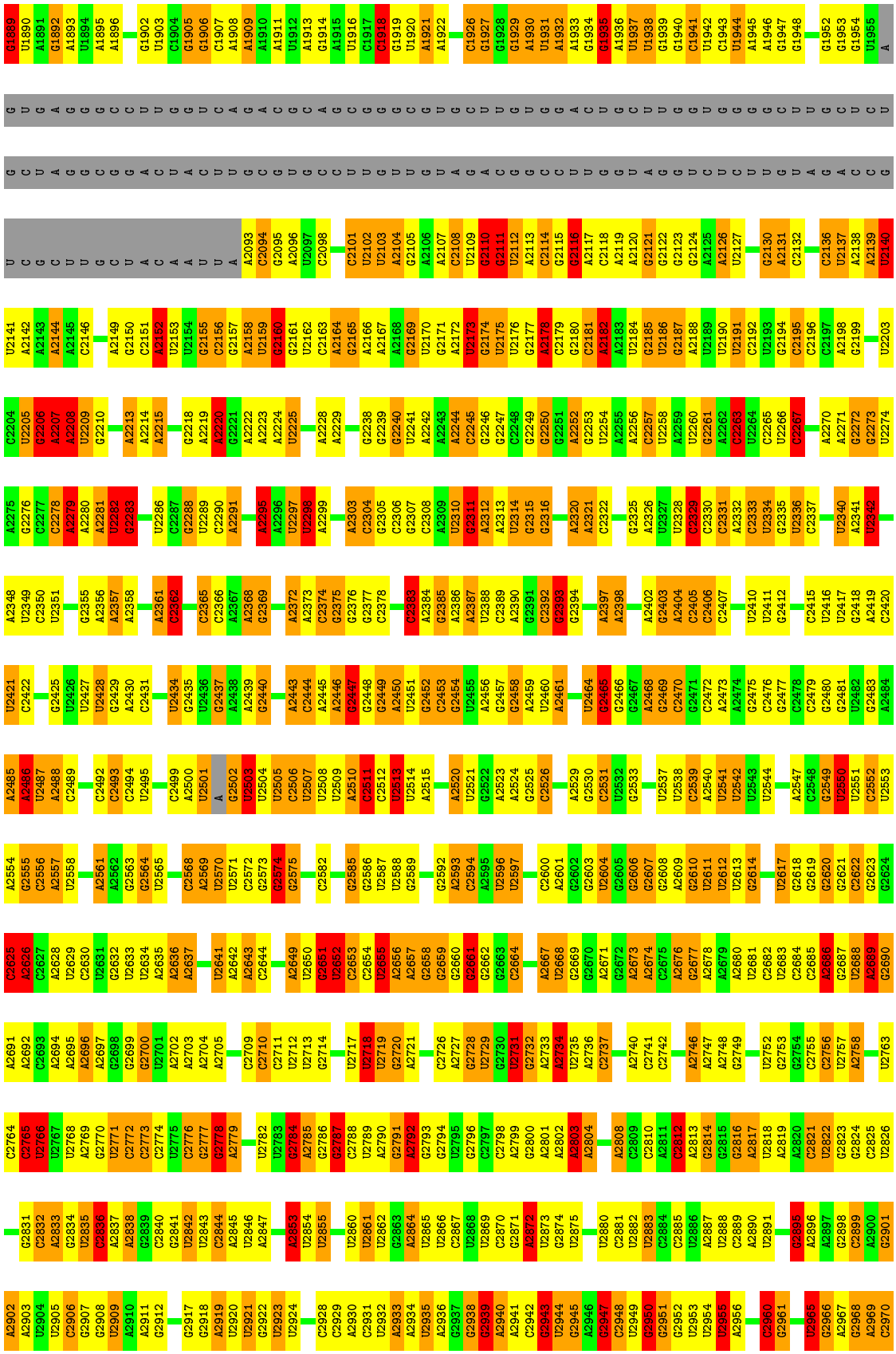
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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.

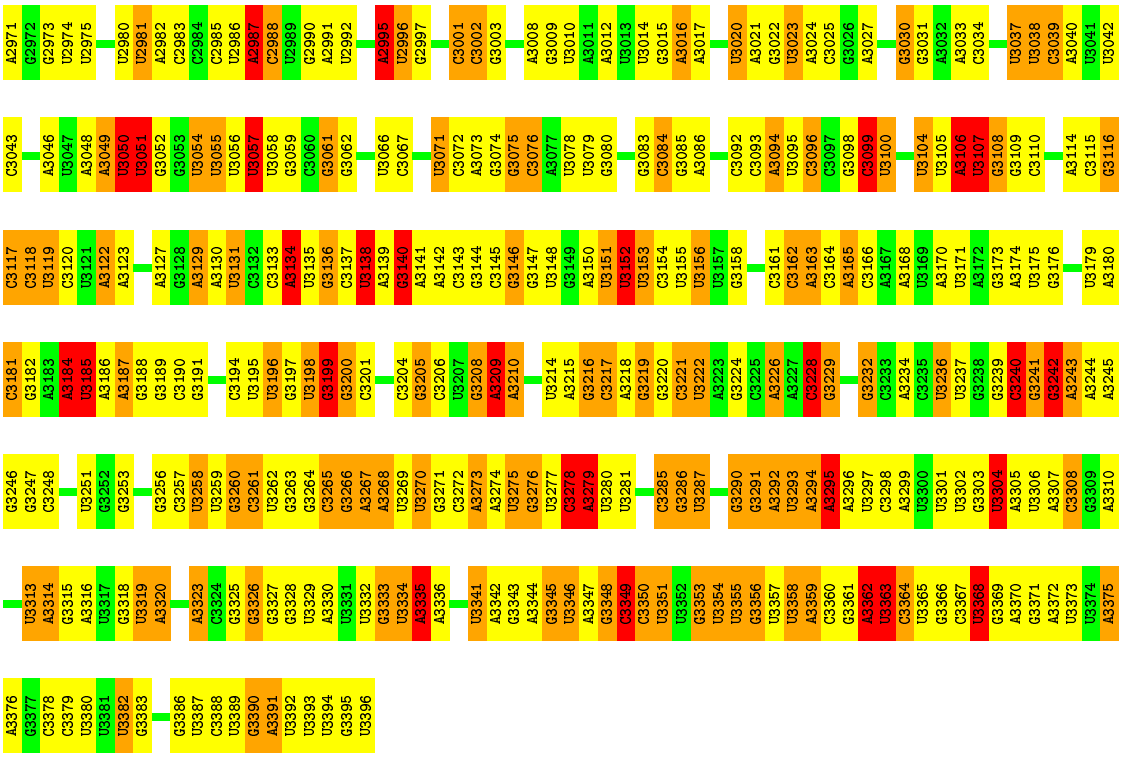
- Molecule 1: 25S RRNA

Chain 1: 27% 38% 23% 7% 6%



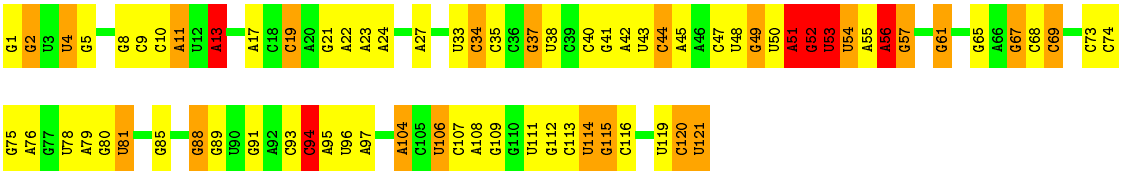



G1889 U1890 A1891 G1892 A1893 U1894 A1895 A1896 G1902 U1903 C1904 G1905 G1906 C1907 A1908 A1909 A1910 A1911 U1912 A1913 G1914 A1915 U1916 C1917 C1918 G1919 U1920 A1921 A1922 C1926 G1927 G1928 G1929 A1930 U1931 A1932 A1933 G1934 G1935 A1936 U1937 U1938 G1939 G1940 C1941 U1942 C1943 U1944 A1945 A1946 G1947 G1948 G1952 G1953 G1954 U1955 A
G C U A G G C C U G C A G G C C U G C A G G C C U G C



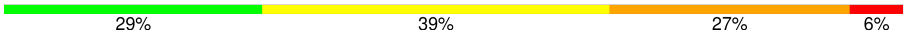
- Molecule 2: 5S RRNA

Chain 3:



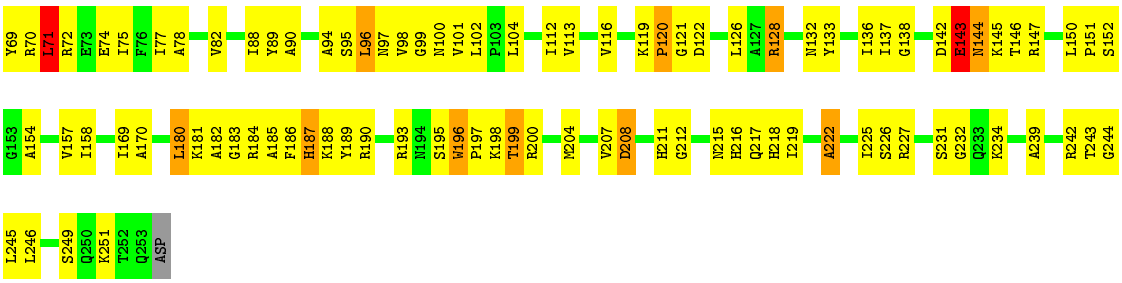
- Molecule 3: 5.8S RRNA

Chain 4:



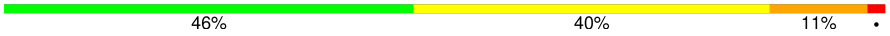
- Molecule 4: UL2

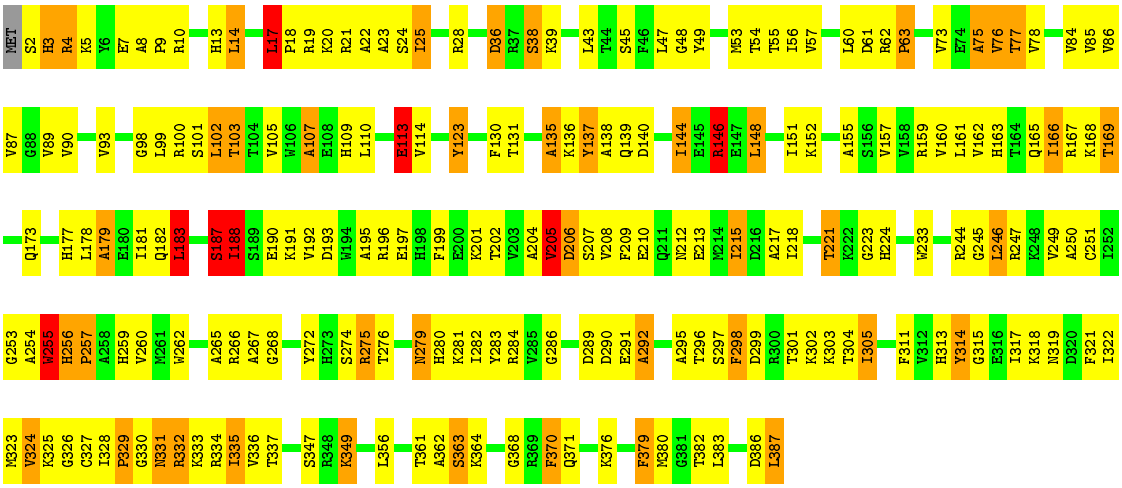
Chain A:



• Molecule 5: UL3

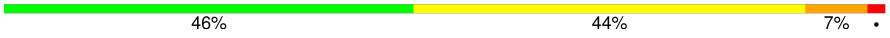
Chain B:

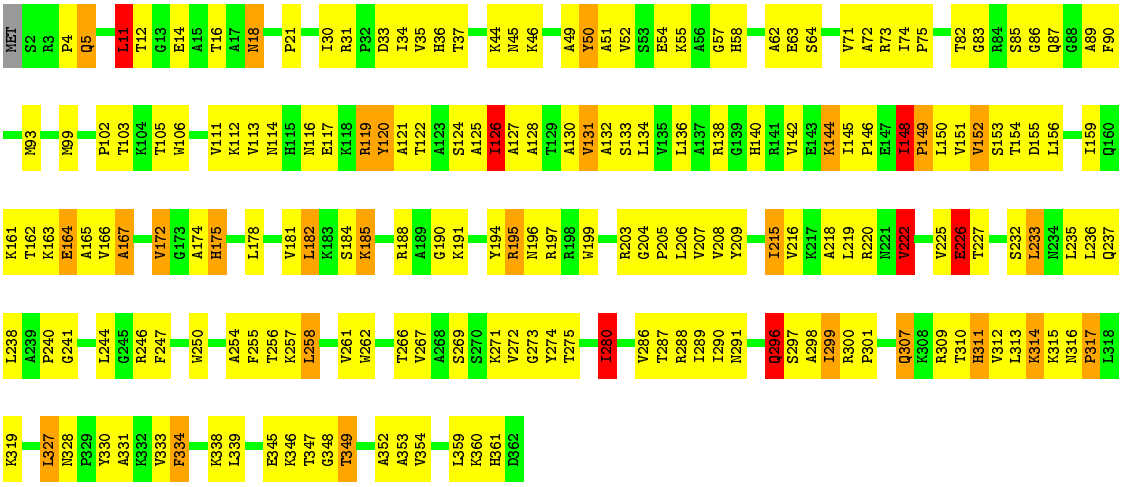




• Molecule 6: UL4

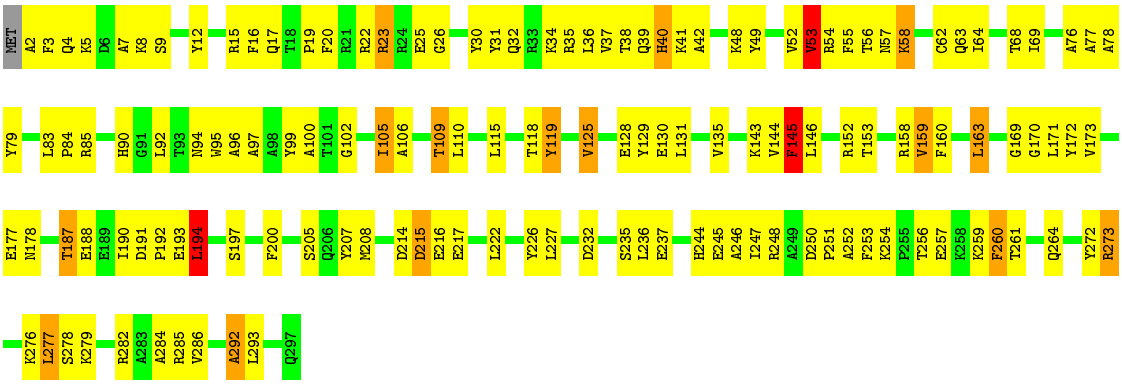
Chain C:





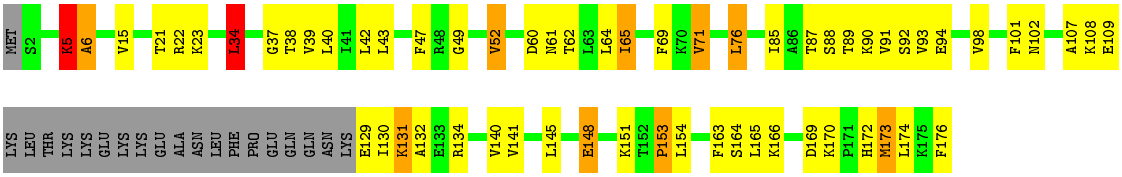
• Molecule 7: UL18

Chain D:



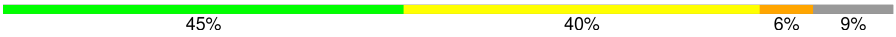
- Molecule 8: EL6

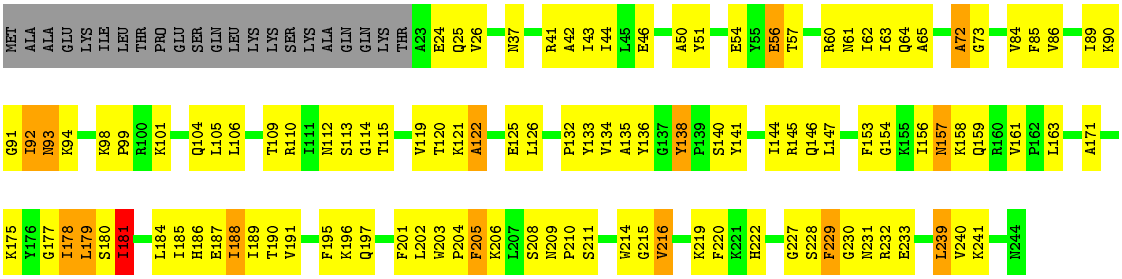
Chain E:



- Molecule 9: UL30

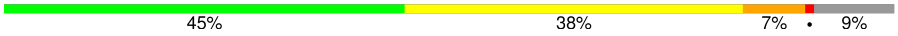
Chain F:

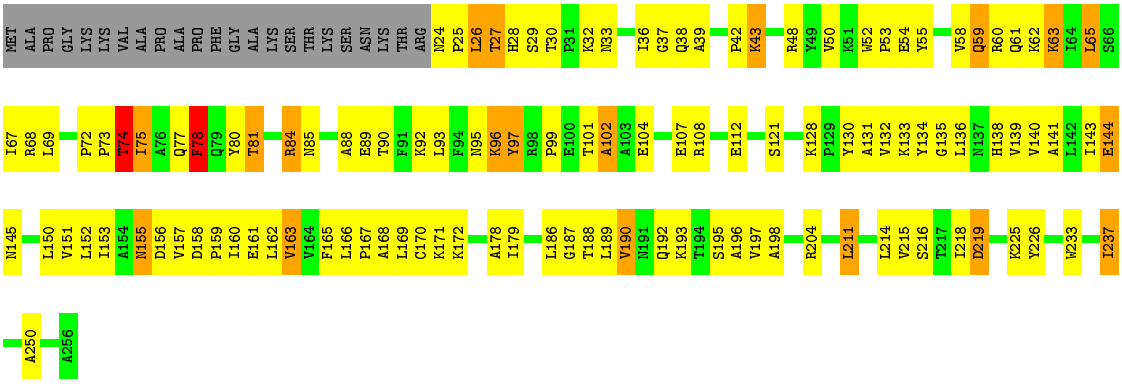




- Molecule 10: EL8

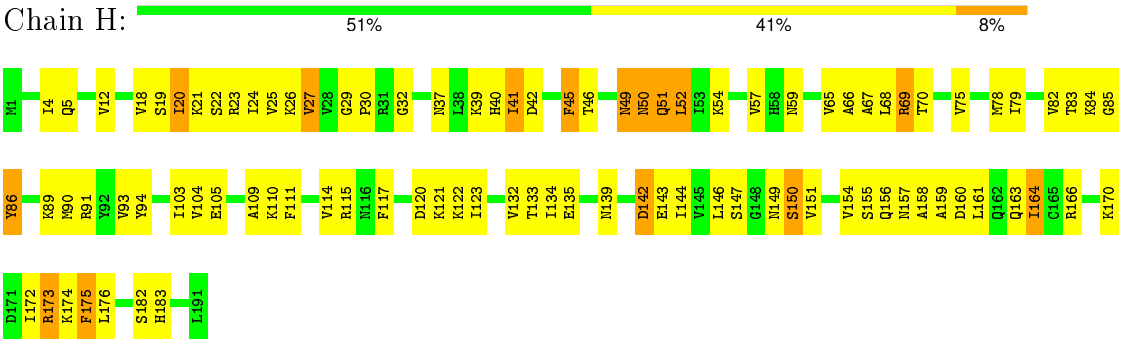
Chain G:





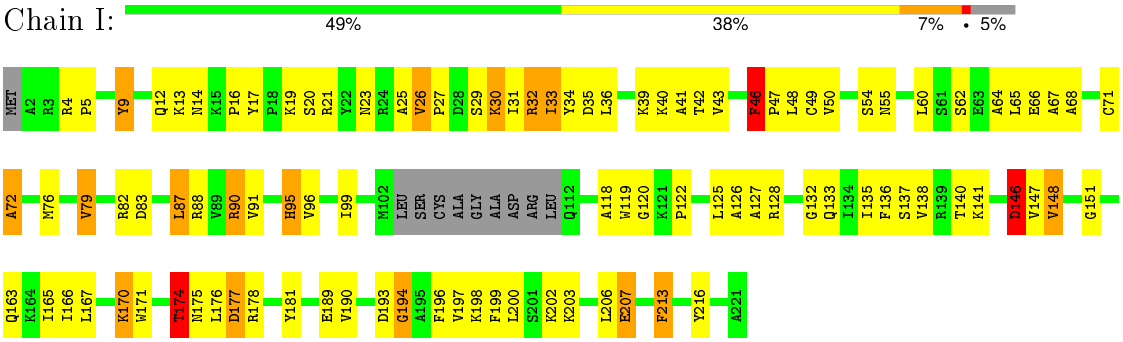
- Molecule 11: UL6

Chain H:



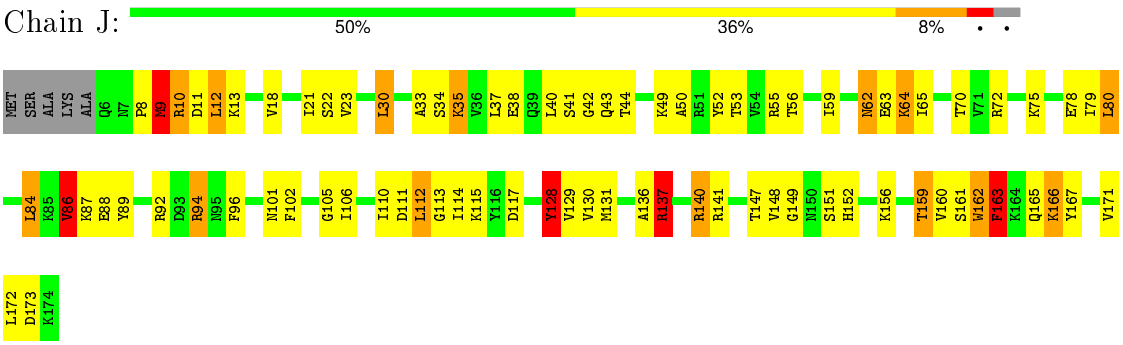
- Molecule 12: UL16

Chain I:



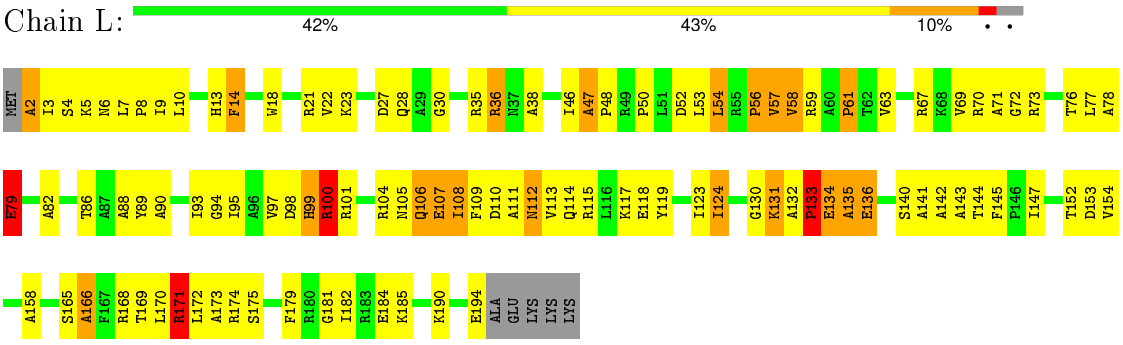
- Molecule 13: UL5

Chain J:



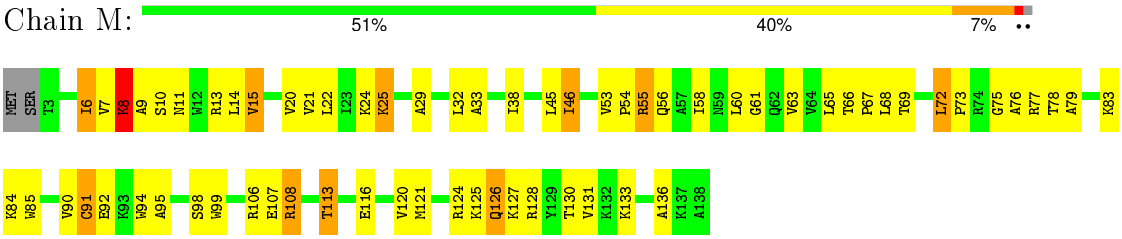
- Molecule 14: EL13

Chain L:



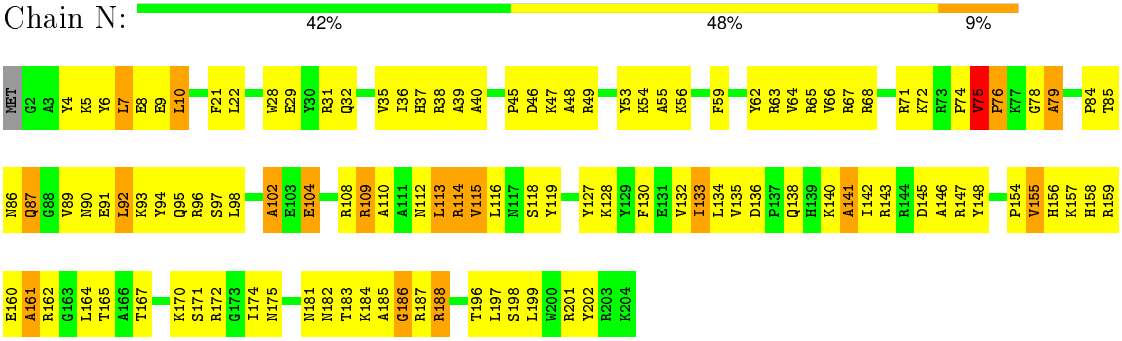
- Molecule 15: EL14

Chain M:



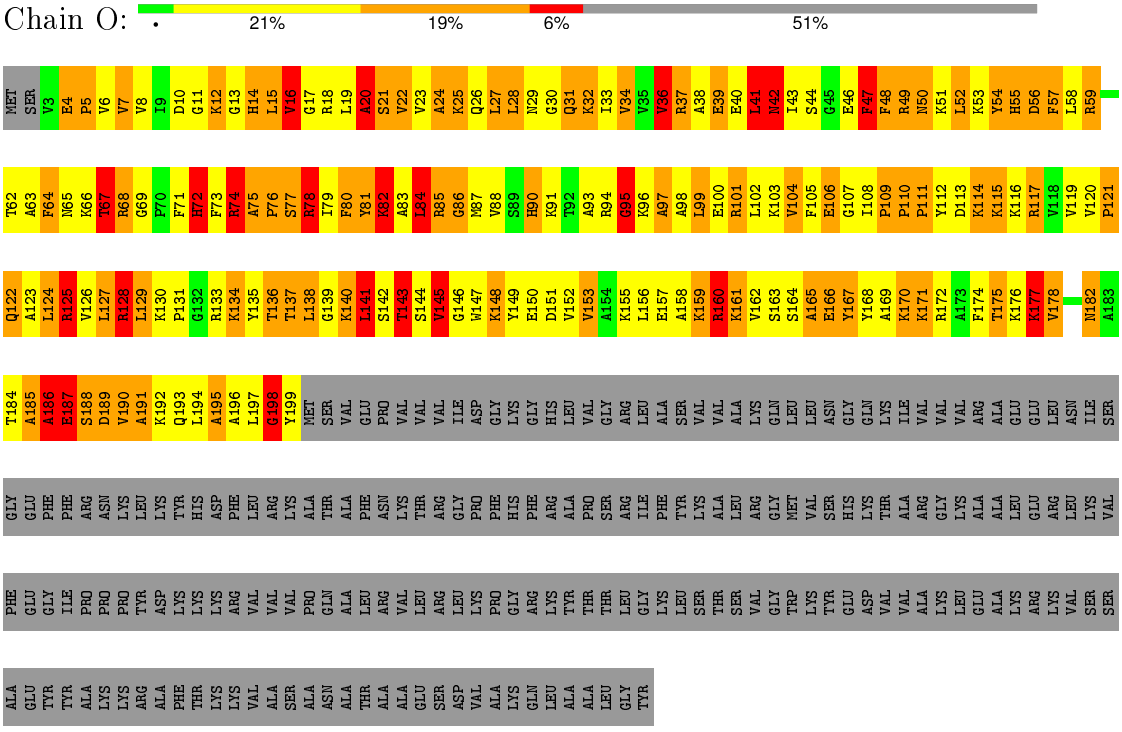
- Molecule 16: EL15

Chain N:



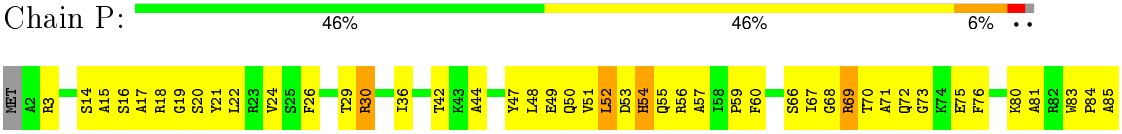
- Molecule 17: UL13

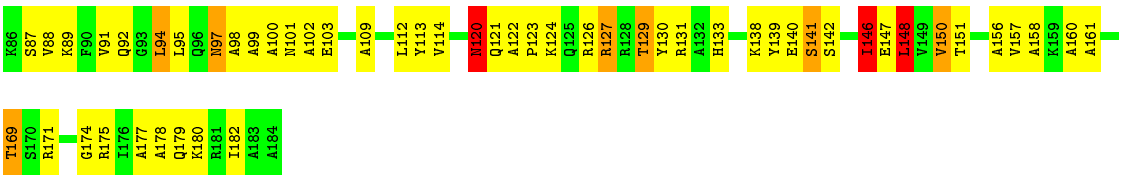
Chain O:



- Molecule 18: UL22

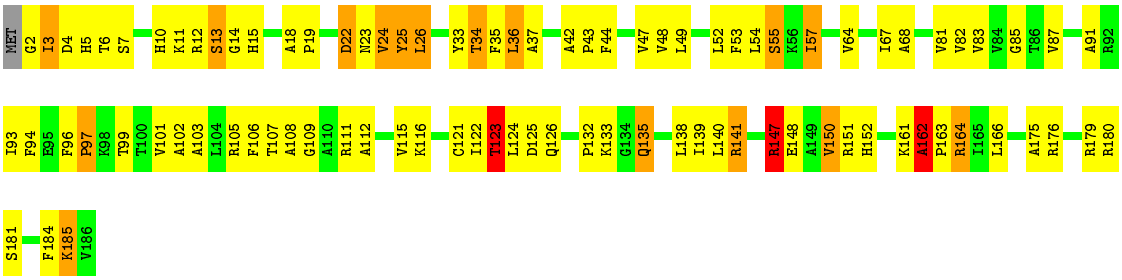
Chain P:





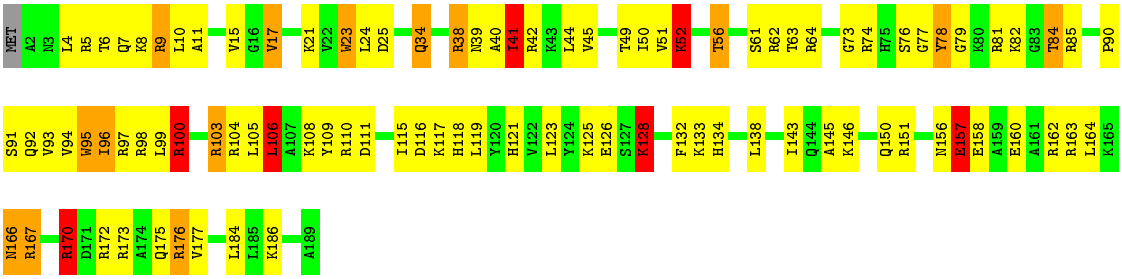
- Molecule 19: EL18

Chain Q:



- Molecule 20: EL19

Chain R:

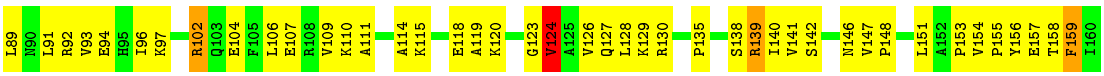


- Molecule 21: EL20

Chain S:

- Molecule 22: EL21

Chain T:

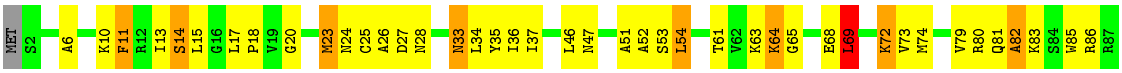


- Molecule 23: EL22

Chain U:

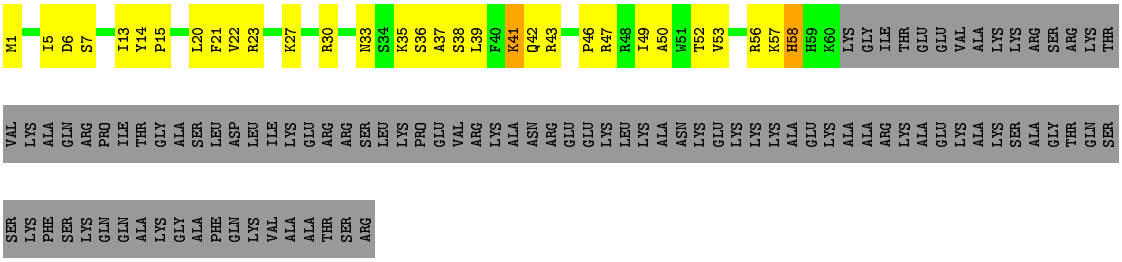
- Molecule 24: UL14

Chain V:



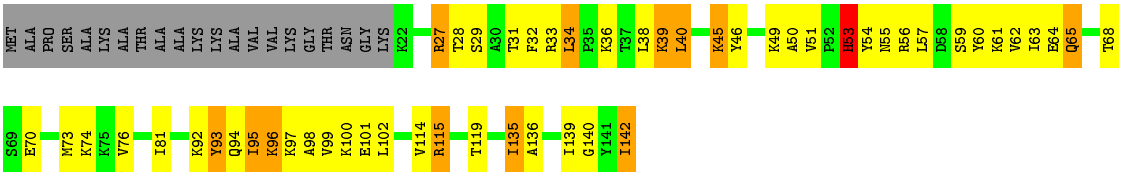
- Molecule 25: EL24

Chain W:



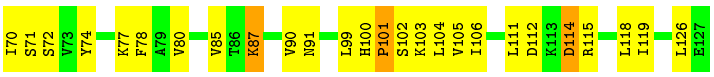
- Molecule 26: UL23

Chain X:



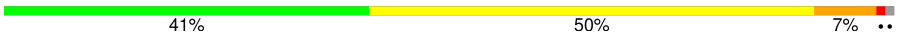
- Molecule 27: UL24

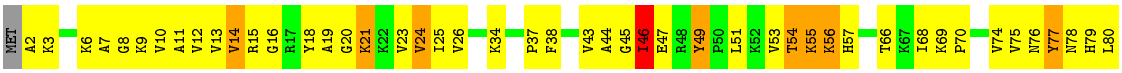
Chain Y:



- Molecule 28: EL27

Chain Z:



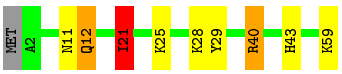


- Molecule 29: UL15

Chain a:

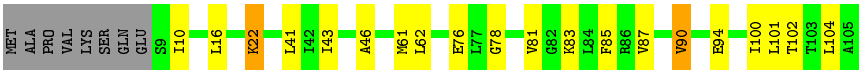
- Molecule 30: EL29

Chain b:



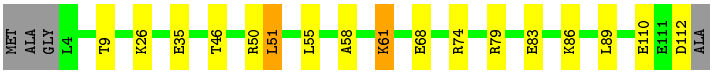
- Molecule 31: EL30

Chain c:



- Molecule 32: EL31

Chain d:



- Molecule 33: EL32

Chain e:

- Molecule 34: EL33

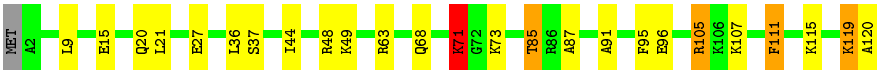
Chain f:

- Molecule 35: EL34

Chain g:

- Molecule 36: UL29

Chain h:

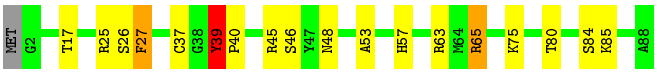


- Molecule 37: EL36

Chain i:

- Molecule 38: EL37

Chain j:

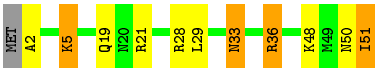


- Molecule 39: EL38

Chain k:

- Molecule 40: EL39

Chain l:

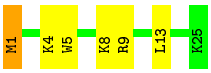


- Molecule 41: EL40

Chain m:

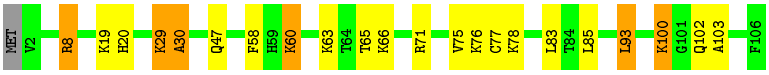
- Molecule 42: EL41

Chain n:



- Molecule 43: EL42

Chain o:

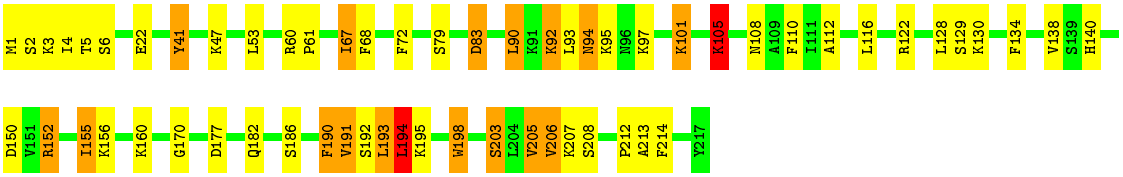


- Molecule 44: EL43

Chain p:

- Molecule 45: UL1

Chain t:



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	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1.8	Depositor
Maximum defocus (nm)	3	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4KX4K)	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.86	28/76106 (0.0%)	1.13	1805/117228 (1.5%)
10	G	0.35	0/1771	0.89	16/2286 (0.7%)
11	H	0.36	0/1493	0.89	12/1935 (0.6%)
12	I	0.75	1/1690 (0.1%)	0.88	12/2182 (0.5%)
13	J	0.35	0/1339	0.92	10/1737 (0.6%)
14	L	0.82	1/1518 (0.1%)	0.98	16/1956 (0.8%)
15	M	0.32	0/1040	0.77	4/1354 (0.3%)
16	N	0.35	0/1706	0.87	12/2201 (0.5%)
17	O	2.16	23/1577 (1.5%)	4.80	87/2104 (4.1%)
18	P	0.35	0/1400	0.91	13/1815 (0.7%)
19	Q	0.33	0/1417	0.96	12/1821 (0.7%)
2	3	0.27	0/2857	1.10	75/4387 (1.7%)
20	R	0.58	1/1492 (0.1%)	1.10	22/1912 (1.2%)
21	S	0.32	0/1435	0.88	10/1852 (0.5%)
22	T	0.33	0/1266	0.82	4/1641 (0.2%)
23	U	0.38	0/788	0.81	3/1027 (0.3%)
24	V	0.36	0/984	0.86	5/1267 (0.4%)
25	W	0.31	0/496	0.73	2/632 (0.3%)
26	X	0.30	0/957	0.76	5/1255 (0.4%)
27	Y	0.32	0/974	0.95	11/1251 (0.9%)
28	Z	0.38	0/1080	0.97	7/1383 (0.5%)
29	a	0.32	0/1163	0.82	8/1489 (0.5%)
3	4	1.27	3/3723 (0.1%)	1.19	101/5740 (1.8%)
30	b	0.31	0/456	0.94	4/578 (0.7%)
31	c	0.38	0/727	0.96	7/936 (0.7%)
32	d	0.32	0/867	0.81	4/1127 (0.4%)
33	e	0.32	0/1015	0.91	5/1316 (0.4%)
34	f	0.36	0/837	0.95	8/1075 (0.7%)
35	g	0.39	0/863	1.12	13/1108 (1.2%)
36	h	0.31	0/948	0.85	9/1211 (0.7%)
37	i	0.33	0/748	0.92	7/944 (0.7%)
38	j	0.37	0/674	0.97	8/857 (0.9%)
39	k	1.22	1/599 (0.2%)	0.93	6/769 (0.8%)
4	A	0.34	0/1881	0.90	15/2416 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
40	l	0.39	0/431	1.01	6/552 (1.1%)
41	m	0.30	0/409	0.64	0/520
42	n	0.66	0/228	1.00	1/282 (0.4%)
43	o	0.37	0/843	0.99	10/1085 (0.9%)
44	p	0.36	0/684	0.86	5/883 (0.6%)
45	t	0.48	0/1692	1.11	24/2183 (1.1%)
5	B	0.38	0/3064	0.97	35/3982 (0.9%)
6	C	0.36	0/2721	0.90	19/3553 (0.5%)
7	D	0.38	0/2353	0.91	18/3055 (0.6%)
8	E	0.35	0/1233	0.88	9/1613 (0.6%)
9	F	0.35	0/1773	0.90	14/2307 (0.6%)
All	All	0.77	58/133318 (0.0%)	1.17	2479/192807 (1.3%)

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	1	103	0
10	G	6	0
11	H	5	0
12	I	4	0
13	J	3	0
14	L	6	1
15	M	2	0
16	N	2	0
17	O	3	16
18	P	5	0
19	Q	4	0
2	3	1	0
20	R	13	0
21	S	5	0
22	T	6	0
24	V	3	0
25	W	2	0
26	X	2	0
27	Y	4	0
28	Z	2	0
29	a	3	0
3	4	4	0
30	b	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
31	c	3	0
32	d	3	0
33	e	2	0
34	f	4	2
35	g	4	0
36	h	4	0
37	i	2	0
38	j	3	1
4	A	7	0
40	l	3	0
43	o	7	0
44	p	1	0
45	t	8	5
5	B	11	3
6	C	11	3
7	D	6	0
8	E	3	0
9	F	5	0
All	All	277	31

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	41	G	O3'-P	49.28	2.20	1.61
1	1	1708	C	O3'-P	49.19	2.20	1.61
1	1	2361	A	O3'-P	49.04	2.19	1.61
1	1	554	A	O3'-P	48.77	2.19	1.61
1	1	968	G	O3'-P	48.44	2.19	1.61

The worst 5 of 2479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	72	HIS	O-C-N	-63.40	21.26	122.70
17	O	186	ALA	O-C-N	-61.98	23.52	122.70
17	O	64	PHE	O-C-N	-60.21	26.36	122.70
17	O	129	LEU	O-C-N	-56.56	32.21	122.70
17	O	153	VAL	O-C-N	-52.15	39.27	122.70

5 of 277 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	69	C	C2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	1	92	G	C2'
1	1	95	A	C2'
1	1	109	A	C3'
1	1	167	U	C3'

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	17	LEU	Peptide
5	B	256	HIS	Peptide
5	B	36	ASP	Peptide
6	C	148	ILE	Peptide
6	C	226	GLU	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	1	68514	0	35042	1249	0
2	3	2579	0	1330	31	0
3	4	3353	0	1721	62	0
4	A	1914	0	1914	145	0
5	B	3075	0	3060	180	0
6	C	2748	0	2780	160	0
7	D	2375	0	2253	92	0
8	E	1239	0	1299	33	0
9	F	1784	0	1814	84	0
10	G	1804	0	1812	91	0
11	H	1518	0	1541	64	0
12	I	1705	0	1684	73	0
13	J	1353	0	1348	49	0
14	L	1543	0	1557	86	0
15	M	1053	0	1121	42	0
16	N	1720	0	1728	110	0
17	O	1555	0	1635	457	0
18	P	1420	0	1394	75	0
19	Q	1441	0	1495	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	1521	0	1571	73	0
21	S	1445	0	1441	74	0
22	T	1276	0	1289	52	0
23	U	796	0	788	13	0
24	V	1003	0	1014	58	0
25	W	500	0	508	21	0
26	X	964	0	1003	29	0
27	Y	993	0	1051	49	0
28	Z	1092	0	1117	51	0
29	a	1173	0	1174	0	0
30	b	462	0	474	0	0
31	c	743	0	773	0	0
32	d	876	0	889	0	0
33	e	1020	0	1064	0	0
34	f	850	0	849	0	0
35	g	880	0	918	0	0
36	h	969	0	1048	0	0
37	i	771	0	819	0	0
38	j	681	0	665	0	0
39	k	612	0	662	0	0
40	l	436	0	463	0	0
41	m	417	0	445	0	0
42	n	233	0	278	0	0
43	o	847	0	901	0	0
44	p	694	0	721	0	0
45	t	1718	0	1758	0	0
All	All	125665	0	90211	3435	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 19.

The worst 5 of 3435 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:128:ARG:C	17:O:129:LEU:CA	1.80	1.50
17:O:190:VAL:C	17:O:191:ALA:N	1.67	1.46
17:O:128:ARG:C	17:O:129:LEU:N	1.71	1.44
17:O:63:ALA:O	17:O:64:PHE:CA	1.65	1.41
17:O:48:PHE:HB3	17:O:49:ARG:N	1.26	1.40

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	A	135/254 (53%)	107 (79%)	21 (16%)	7 (5%)	2 30
5	B	240/387 (62%)	198 (82%)	25 (10%)	17 (7%)	1 22
6	C	215/362 (59%)	168 (78%)	26 (12%)	21 (10%)	1 13
7	D	164/297 (55%)	128 (78%)	25 (15%)	11 (7%)	1 24
8	E	103/176 (58%)	91 (88%)	7 (7%)	5 (5%)	3 32
9	F	136/244 (56%)	121 (89%)	10 (7%)	5 (4%)	4 40
10	G	122/256 (48%)	100 (82%)	13 (11%)	9 (7%)	1 21
11	H	106/191 (56%)	84 (79%)	18 (17%)	4 (4%)	4 39
12	I	119/221 (54%)	102 (86%)	12 (10%)	5 (4%)	3 36
13	J	103/174 (59%)	85 (82%)	10 (10%)	8 (8%)	1 19
14	L	103/199 (52%)	79 (77%)	14 (14%)	10 (10%)	1 13
15	M	84/138 (61%)	68 (81%)	10 (12%)	6 (7%)	1 22
16	N	114/204 (56%)	94 (82%)	11 (10%)	9 (8%)	1 18
17	O	181/398 (46%)	69 (38%)	53 (29%)	59 (33%)	0 0
18	P	106/184 (58%)	96 (91%)	7 (7%)	3 (3%)	6 47
19	Q	100/186 (54%)	81 (81%)	13 (13%)	6 (6%)	2 26
20	R	105/189 (56%)	74 (70%)	26 (25%)	5 (5%)	3 32
21	S	87/172 (51%)	63 (72%)	17 (20%)	7 (8%)	1 18
22	T	93/160 (58%)	69 (74%)	19 (20%)	5 (5%)	2 29
23	U	58/121 (48%)	50 (86%)	5 (9%)	3 (5%)	2 30
24	V	73/137 (53%)	65 (89%)	6 (8%)	2 (3%)	6 48
25	W	33/155 (21%)	29 (88%)	4 (12%)	0	100 100
26	X	76/142 (54%)	63 (83%)	8 (10%)	5 (7%)	1 24
27	Y	71/127 (56%)	50 (70%)	17 (24%)	4 (6%)	2 28
28	Z	66/136 (48%)	48 (73%)	13 (20%)	5 (8%)	1 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	a	75/149 (50%)	56 (75%)	13 (17%)	6 (8%)	1 18
30	b	27/59 (46%)	19 (70%)	5 (18%)	3 (11%)	0 10
31	c	56/105 (53%)	44 (79%)	8 (14%)	4 (7%)	1 22
32	d	68/113 (60%)	59 (87%)	6 (9%)	3 (4%)	3 35
33	e	82/130 (63%)	68 (83%)	8 (10%)	6 (7%)	1 21
34	f	52/107 (49%)	42 (81%)	7 (14%)	3 (6%)	2 27
35	g	65/121 (54%)	57 (88%)	6 (9%)	2 (3%)	5 45
36	h	66/120 (55%)	52 (79%)	8 (12%)	6 (9%)	1 15
37	i	47/100 (47%)	33 (70%)	10 (21%)	4 (8%)	1 16
38	j	48/88 (54%)	35 (73%)	7 (15%)	6 (12%)	0 8
39	k	43/78 (55%)	32 (74%)	9 (21%)	2 (5%)	3 33
40	l	27/51 (53%)	20 (74%)	5 (18%)	2 (7%)	1 21
41	m	26/128 (20%)	22 (85%)	3 (12%)	1 (4%)	4 39
42	n	14/25 (56%)	9 (64%)	4 (29%)	1 (7%)	1 22
43	o	71/106 (67%)	58 (82%)	10 (14%)	3 (4%)	3 36
44	p	59/92 (64%)	53 (90%)	4 (7%)	2 (3%)	5 43
45	t	121/217 (56%)	82 (68%)	24 (20%)	15 (12%)	0 8
All	All	3740/6999 (53%)	2923 (78%)	527 (14%)	290 (8%)	2 19

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	33	ASP
4	A	120	PRO
5	B	61	ASP
5	B	113	GLU
5	B	146	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
4	A	193/196 (98%)	172 (89%)	21 (11%)	8 40
5	B	321/323 (99%)	278 (87%)	43 (13%)	5 31
6	C	288/289 (100%)	261 (91%)	27 (9%)	11 48
7	D	244/245 (100%)	215 (88%)	29 (12%)	6 35
8	E	134/153 (88%)	123 (92%)	11 (8%)	14 53
9	F	186/205 (91%)	172 (92%)	14 (8%)	17 57
10	G	187/208 (90%)	170 (91%)	17 (9%)	12 49
11	H	171/171 (100%)	154 (90%)	17 (10%)	10 45
12	I	177/187 (95%)	156 (88%)	21 (12%)	6 35
13	J	147/150 (98%)	123 (84%)	24 (16%)	3 21
14	L	154/159 (97%)	140 (91%)	14 (9%)	12 49
15	M	107/109 (98%)	92 (86%)	15 (14%)	4 29
16	N	175/176 (99%)	162 (93%)	13 (7%)	17 58
17	O	160/324 (49%)	134 (84%)	26 (16%)	3 21
18	P	140/146 (96%)	120 (86%)	20 (14%)	4 28
19	Q	150/151 (99%)	133 (89%)	17 (11%)	7 38
20	R	153/154 (99%)	132 (86%)	21 (14%)	4 30
21	S	156/156 (100%)	143 (92%)	13 (8%)	14 53
22	T	136/137 (99%)	117 (86%)	19 (14%)	4 29
23	U	87/107 (81%)	81 (93%)	6 (7%)	19 61
24	V	104/105 (99%)	93 (89%)	11 (11%)	8 42
25	W	53/129 (41%)	48 (91%)	5 (9%)	11 48
26	X	104/118 (88%)	88 (85%)	16 (15%)	3 24
27	Y	109/110 (99%)	99 (91%)	10 (9%)	11 49
28	Z	115/116 (99%)	101 (88%)	14 (12%)	6 34
29	a	118/119 (99%)	107 (91%)	11 (9%)	11 49
30	b	46/47 (98%)	40 (87%)	6 (13%)	5 32
31	c	81/88 (92%)	70 (86%)	11 (14%)	5 30
32	d	92/97 (95%)	80 (87%)	12 (13%)	5 32
33	e	109/111 (98%)	96 (88%)	13 (12%)	6 35
34	f	90/91 (99%)	83 (92%)	7 (8%)	16 56
35	g	95/103 (92%)	84 (88%)	11 (12%)	7 37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	h	104/105 (99%)	88 (85%)	16 (15%)	3 24
37	i	81/82 (99%)	71 (88%)	10 (12%)	6 34
38	j	70/71 (99%)	62 (89%)	8 (11%)	7 38
39	k	68/69 (99%)	50 (74%)	18 (26%)	0 5
40	l	45/46 (98%)	38 (84%)	7 (16%)	3 24
41	m	47/116 (40%)	44 (94%)	3 (6%)	22 64
42	n	23/23 (100%)	18 (78%)	5 (22%)	1 9
43	o	90/91 (99%)	75 (83%)	15 (17%)	3 19
44	p	71/72 (99%)	61 (86%)	10 (14%)	4 29
45	t	198/198 (100%)	161 (81%)	37 (19%)	2 14
All	All	5379/5853 (92%)	4735 (88%)	644 (12%)	11 35

5 of 644 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	O	187	GLU
21	S	155	ARG
43	o	93	LEU
18	P	94	LEU
19	Q	164	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	87	GLN
18	P	55	GLN
44	p	25	GLN
16	N	139	HIS
17	O	31	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2683/3397 (78%)	1145 (42%)	379 (14%)
2	3	97/121 (80%)	31 (31%)	10 (10%)
3	4	135/158 (85%)	52 (38%)	14 (10%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2915/3676 (79%)	1228 (42%)	403 (13%)

5 of 1228 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	9	U
1	1	10	C
1	1	11	A
1	1	15	C

5 of 403 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1605	A
1	1	2156	C
1	1	3323	A
1	1	1691	U
1	1	1839	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)

There are no ligands in this entry.

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	1	613
5	B	82
6	C	79
7	D	72
4	A	67
10	G	65
45	t	53
12	I	52
16	N	51
14	L	51
19	Q	48
9	F	48
21	S	46
20	R	46
11	H	46
18	P	43
29	a	41
28	Z	38
13	J	35
24	V	34
22	T	34
34	f	31
36	h	30
37	i	30
27	Y	30
15	M	28
35	g	27
8	E	27
33	e	26
3	4	26
2	3	26
31	c	24
23	U	24
32	d	23
26	X	22
38	j	22
39	k	20
17	O	18
43	o	17
44	p	17
30	b	17
25	W	16
41	m	14

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
40	l	12
42	n	6

The worst 5 of 2177 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	171:ASP	C	172:ARG	N	8.98
1	t	52:SER	C	53:LEU	N	8.07
1	1	2511:C	O3'	2512:C	P	7.92
1	R	170:ARG	C	171:ASP	N	7.88
1	1	2468:A	O3'	2469:G	P	6.79