wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:30 PM BST

PDB ID	:	3J7Y
EMDB ID:	:	EMD-2762
Title	:	Structure of the large ribosomal subunit from human mitochondria
Authors	:	Brown, A.; Amunts, A.; Bai, X.C.; Sugimoto, Y.; Edwards, P.C.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-08-26
Resolution	:	3.40 Å(reported)

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

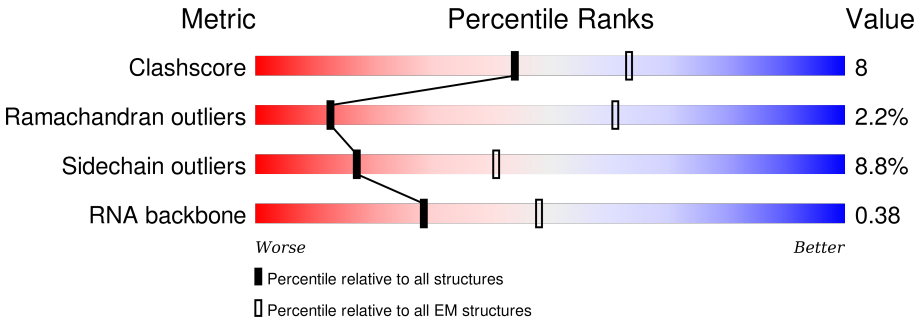
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.40 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	A	1559	36% 43% 14% • 6%
2	B	73	38% 29% 11% 22%
3	D	305	65% 11% • 23%
4	E	348	67% 18% • 14%
5	F	311	61% 19% • 20%
6	H	267	28% 7% 64%
7	I	261	44% 13% • 39%
8	J	192	56% 14% • 27%

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Mol	Chain	Length	Quality of chain
9	K	178	78% 19%
10	L	145	64% 15% 21%
11	M	296	77% 17%
12	N	251	69% 11% 18%
13	O	175	59% 22% 5% 13%
14	P	179	52% 20% 26%
15	Q	292	52% 15% 30%
16	R	149	77% 17% 6%
17	S	205	62% 12% 24%
18	T	212	59% 17% 22%
19	U	153	54% 18% 27%
20	V	216	73% 14% 13%
21	W	148	51% 19% 28%
22	X	256	76% 15% 5%
23	Y	250	54% 15% 30%
24	Z	161	59% 16% 25%
25	0	188	35% 15% 48%
26	1	65	60% 17% 20%
27	2	92	38% 8% 53%
28	3	188	42% 7% 49%
29	4	103	23% 10% 65%
30	5	423	65% 21% 11%
31	6	380	67% 16% 14%
32	7	338	67% 12% 21%
33	8	206	25% 72%

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Mol	Chain	Length	Quality of chain
34	9	137	64% 15% 20%
35	a	142	25% 73%
36	b	155	85% 10% 5%
37	c	332	76% 7% 17%
38	d	306	50% 47%
39	e	279	41% 6% 52%
40	f	211	41% 55%
41	g	166	69% 8% 22%
42	h	158	54% 9% 37%
43	i	128	64% 10% 25%
44	j	123	63% 6% 31%
45	k	112	64% 10% 25%
46	o	102	80% 11% 8%
47	p	206	35% 5% 60%
48	q	222	55% 42%
49	r	196	66% 9% 26%
50	s	439	76% 8% 16%
51	t	127	97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	ZN	0	200	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 94121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1472	31261	14025	5642	10122	1472	0	0

- Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	57	1211	543	217	394	57	0	0

- Molecule 3 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	236	1842	1145	373	315	9	0	0

- Molecule 4 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	300	2365	1523	410	422	10	0	0

- Molecule 5 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	250	2013	1294	365	348	6	0	0

- Molecule 6 is a protein called bL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	95	784	498	152	134	0	0

- Molecule 7 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 15 is a protein called bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	204	Total	C	N	O	S	0	0
			1704	1094	303	299	8		

- Molecule 16 is a protein called bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 20 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 21 is a protein called bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	107	Total	C	N	O	S	0	0
			842	542	158	139	3		

- Molecule 22 is a protein called bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

- Molecule 23 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	98	Total	C	N	O	S	0	0
			803	501	159	137	6		

- Molecule 26 is a protein called bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 28 is a protein called bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 30 is a protein called mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 31 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 32 is a protein called mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 33 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	57	Total	C	N	O	S	0	0
			482	302	86	92	2		

- Molecule 34 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	39	Total	C	N	O	S	0	0
			343	217	68	55	3		

- Molecule 36 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	134	Total	C	N	O	S	0	0
			1082	690	193	196	3		

- Molecule 40 is a protein called mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	95	Total	C	N	O	S	0	0
			703	448	119	133	3		

- Molecule 41 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	96	Total	C	N	O	S	0	0
			816	526	161	125	4		

- Molecule 44 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 47 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	83	Total	C	N	O	S	0	0
			674	421	125	125	3		

- Molecule 48 is a protein called CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 49 is a protein called bS18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

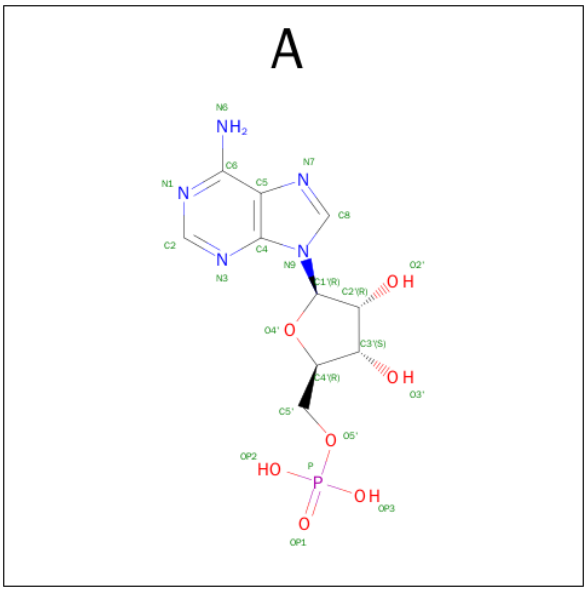
- Molecule 50 is a protein called mS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 51 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	t	123	Total	C	N	O	0	0
			615	369	123	123		

- Molecule 52 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	65	Total	Mg	0
			65	65	

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Mol	Chain	Residues	Atoms	AltConf
53	E	1	Total Mg 1 1	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

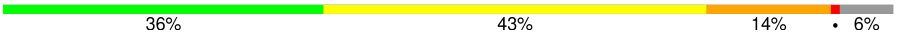
Mol	Chain	Residues	Atoms	AltConf
54	0	1	Total Zn 1 1	0
54	r	1	Total Zn 1 1	0
54	4	1	Total Zn 1 1	0

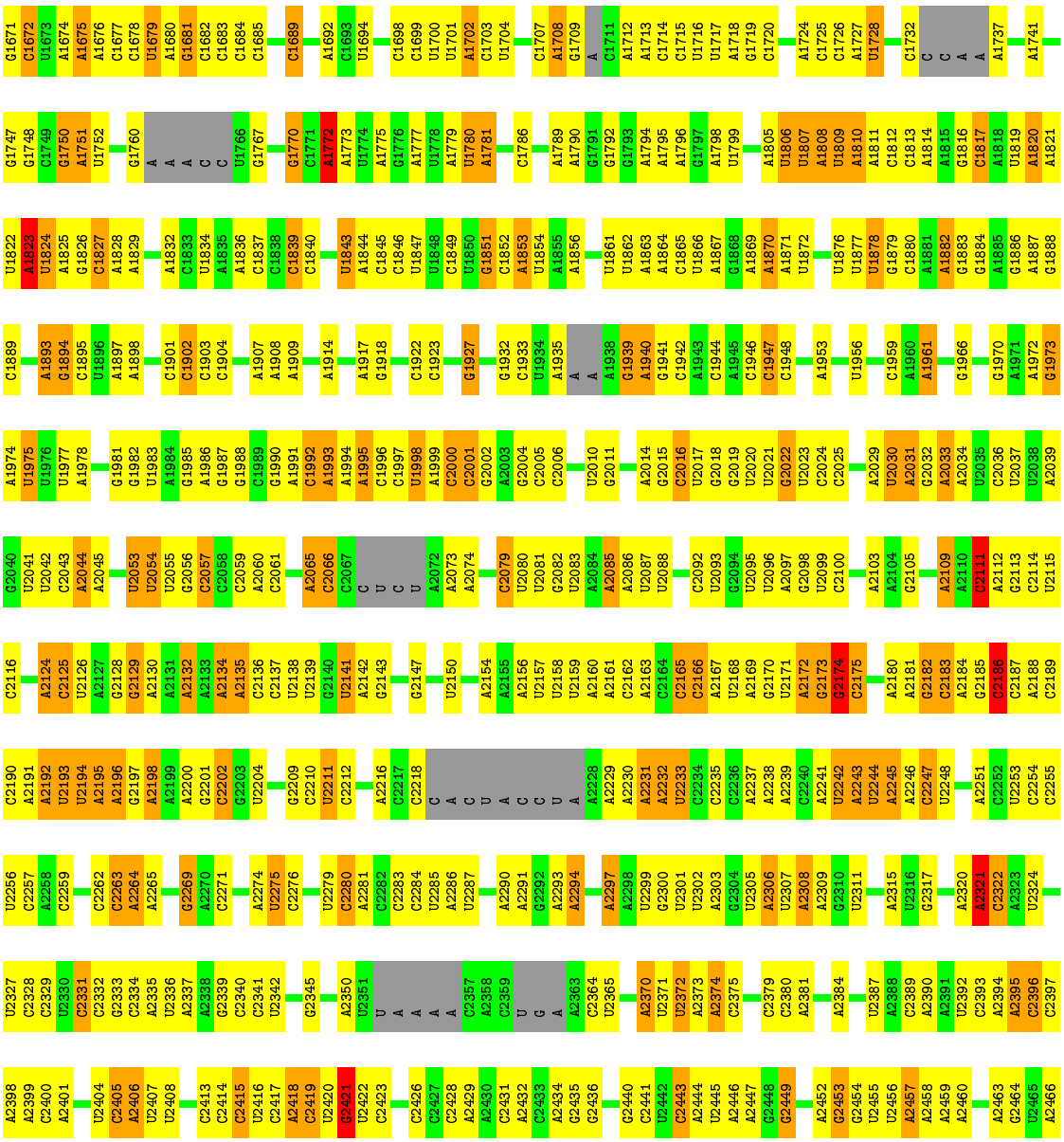
3 Residue-property plots (i)

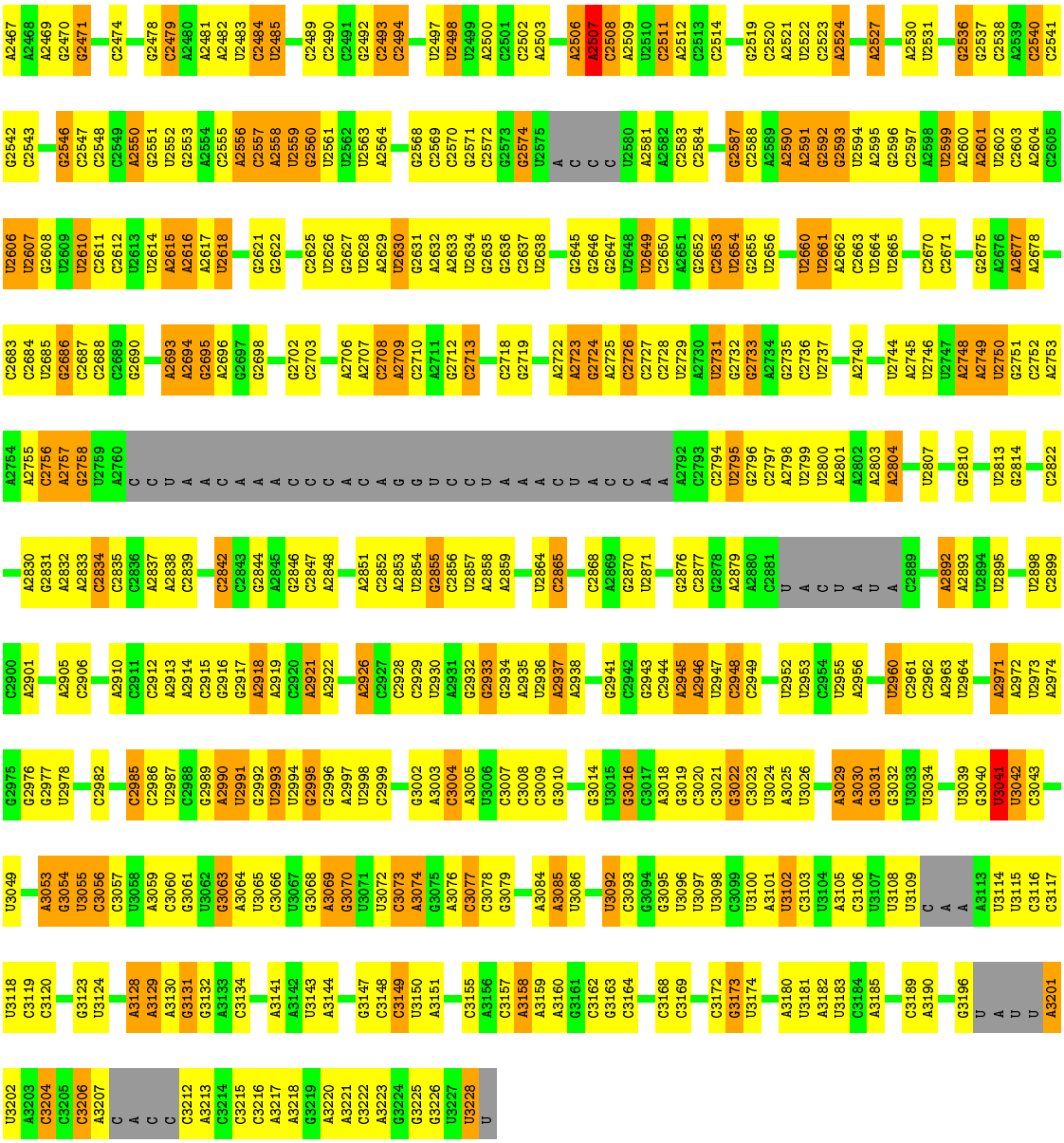
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 16S rRNA

Chain A:

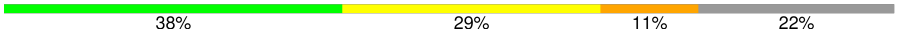


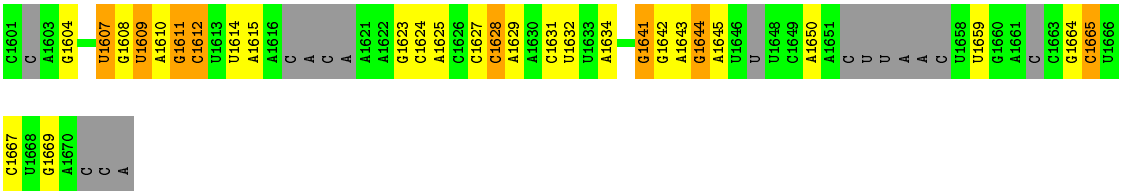




- Molecule 2: mt-tRNAVal

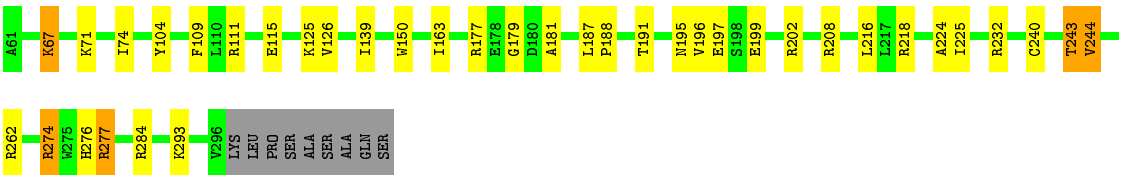
Chain B:





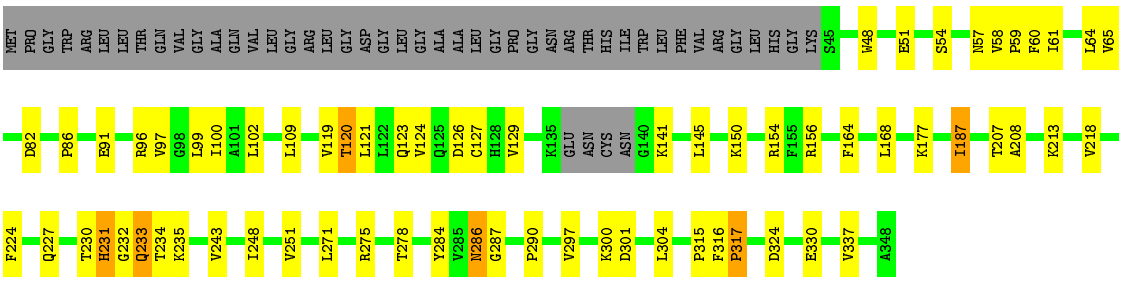
- Molecule 3: uL2

Chain D:



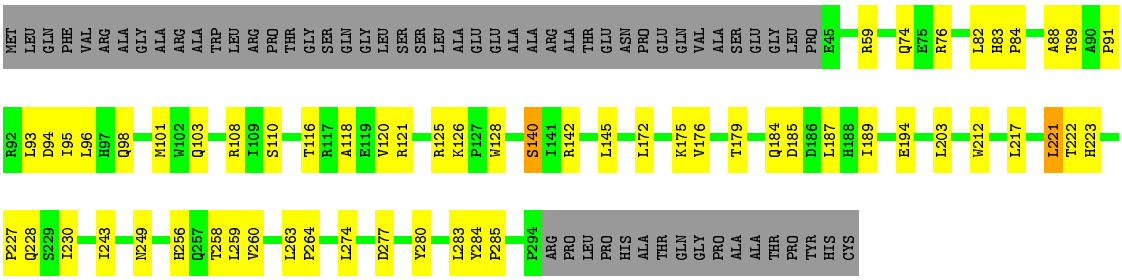
- Molecule 4: uL3

Chain E:



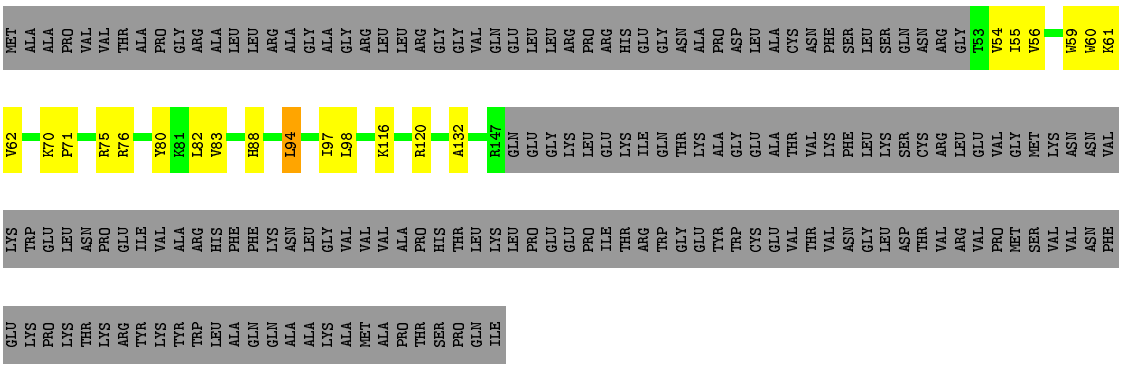
- Molecule 5: uL4

Chain F:



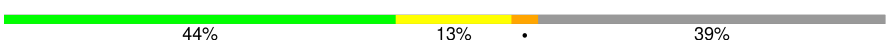
- Molecule 6: bL9

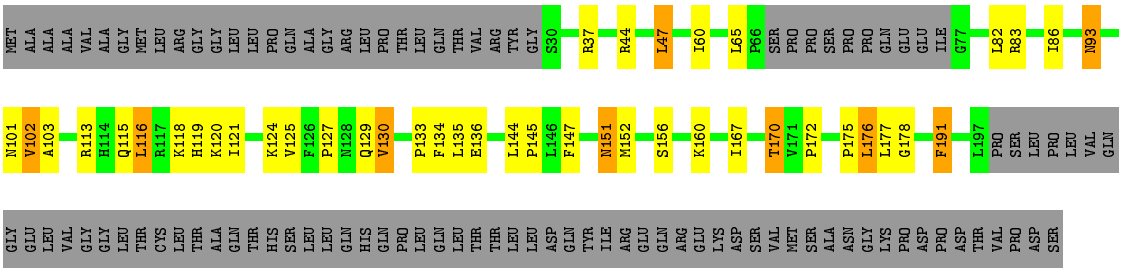
Chain H:



- Molecule 7: uL10

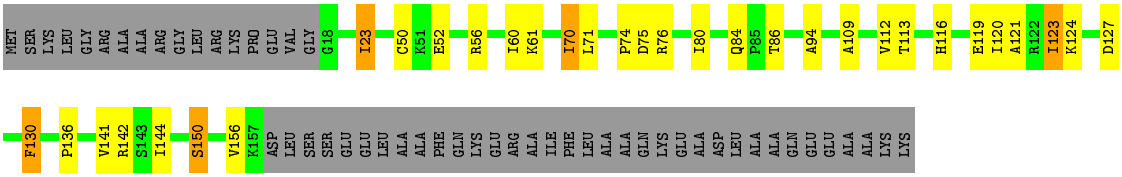
Chain I:





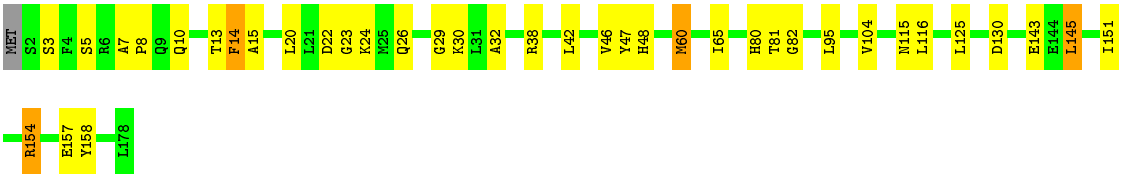
- Molecule 8: uL11

Chain J:



- Molecule 9: uL13

Chain K:

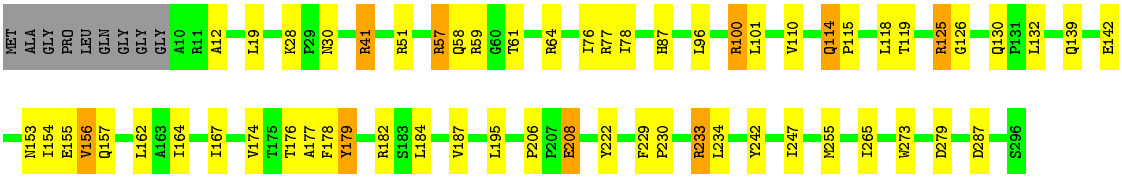


- Molecule 10: uL14

Chain L:

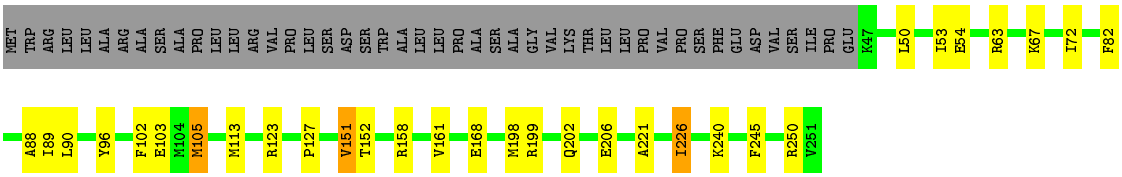
- Molecule 11: uL15

Chain M:



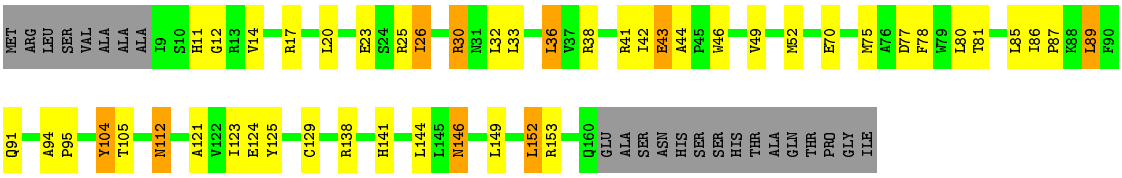
- Molecule 12: uL16

Chain N:



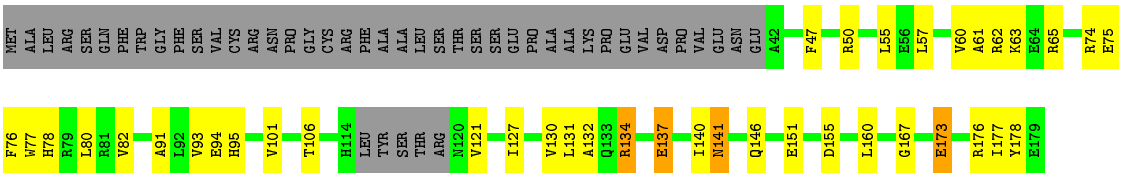
- Molecule 13: bL17

Chain O:



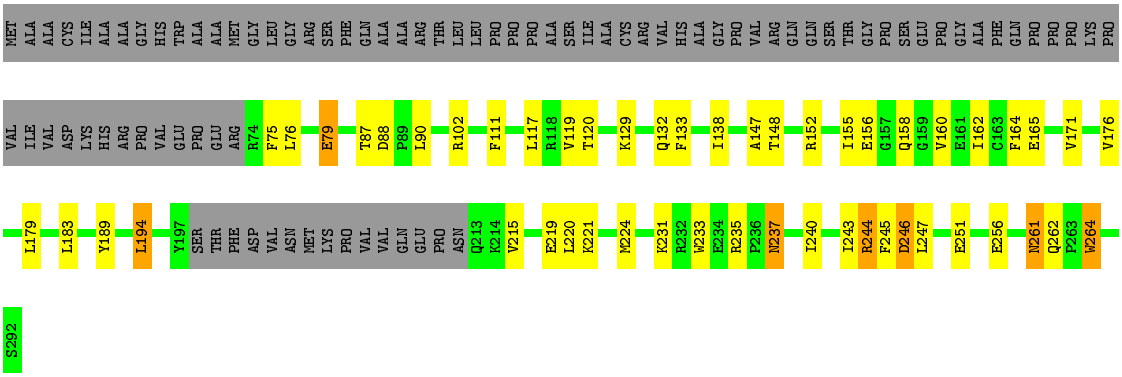
- Molecule 14: uL18

Chain P:



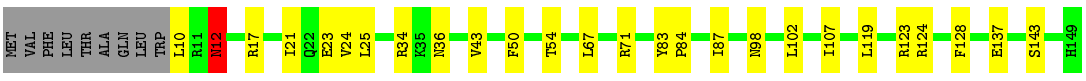
- Molecule 15: bL19

Chain Q:



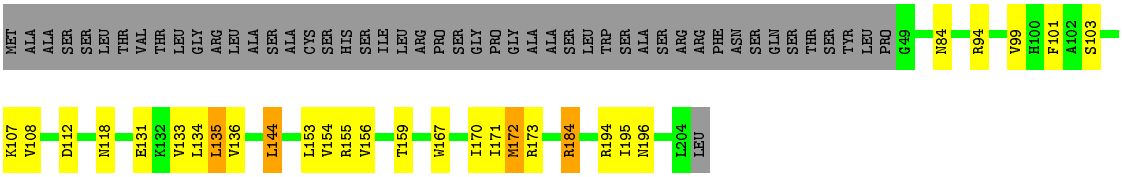
- Molecule 16: bL20

Chain R:



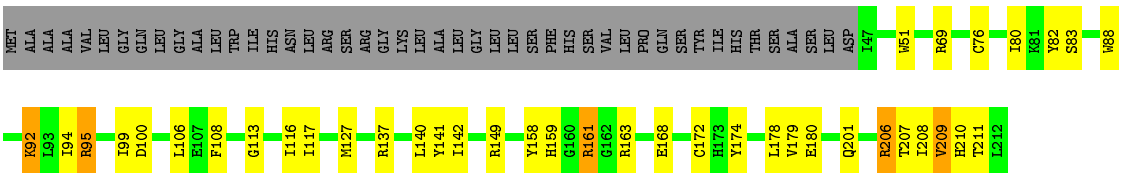
- Molecule 17: bL21

Chain S:



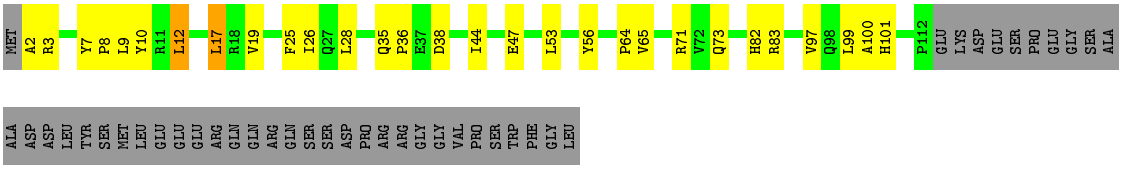
- Molecule 18: uL22

Chain T:



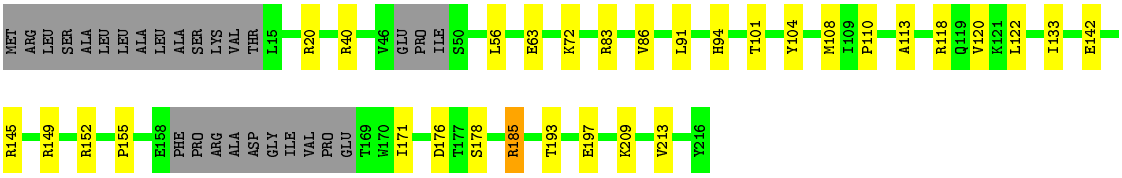
- Molecule 19: uL23

Chain U:



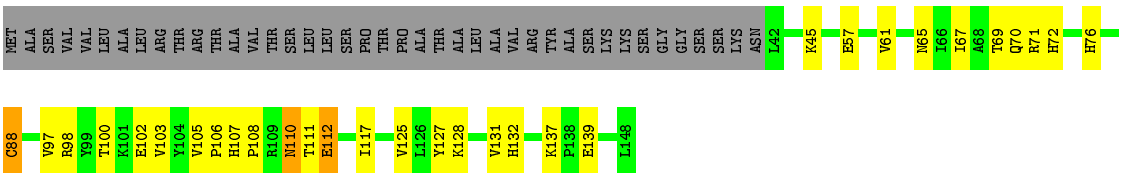
- Molecule 20: uL24

Chain V:



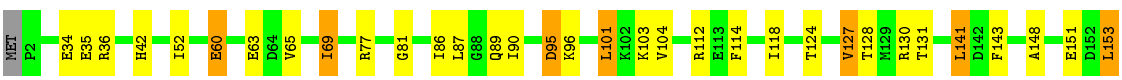
- Molecule 21: bL27

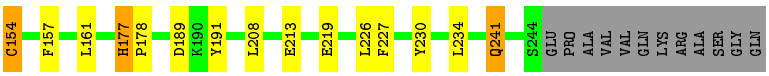
Chain W:



- Molecule 22: bL28

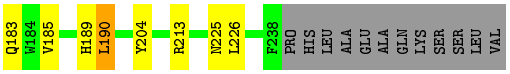
Chain X:





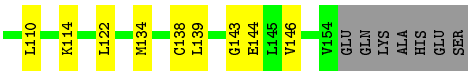
- Molecule 23: uL29

Chain Y:



- Molecule 24: uL30

Chain Z:



- Molecule 25: bL32

Chain 0:

- Molecule 26: bL33

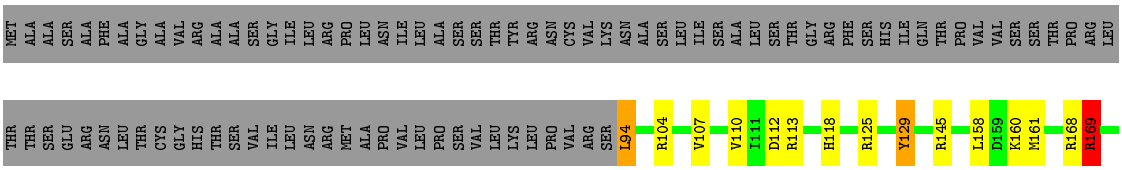
Chain 1:

- Molecule 27: bL34

Chain 2:

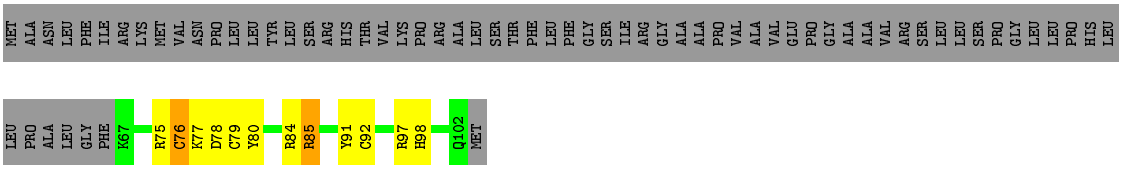
- Molecule 28: bL35

Chain 3:



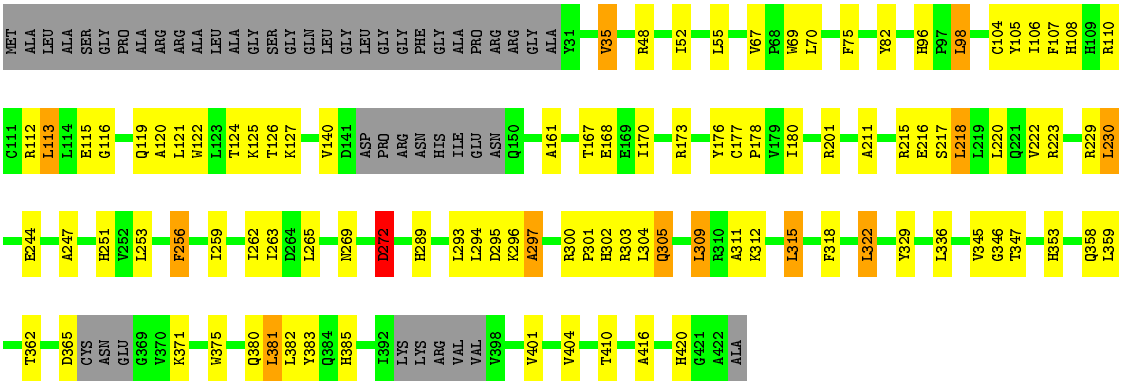
- Molecule 29: bL36

Chain 4:



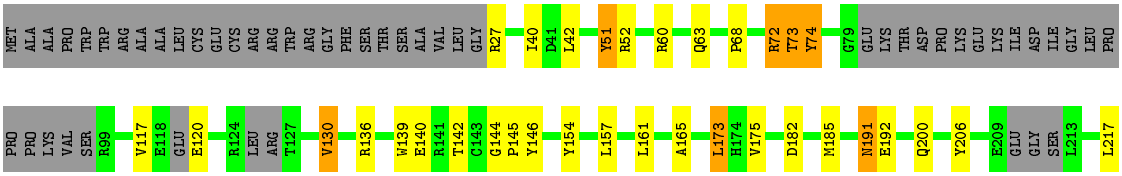
- Molecule 30: mL37

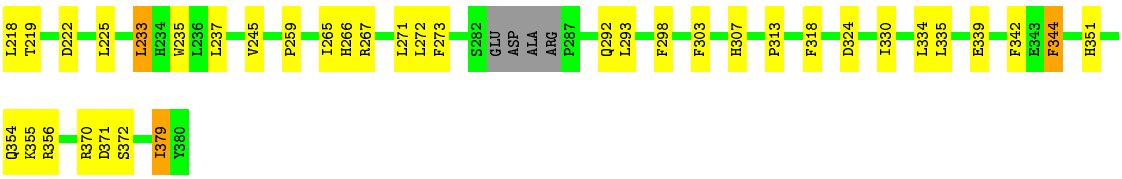
Chain 5:



- Molecule 31: mL38

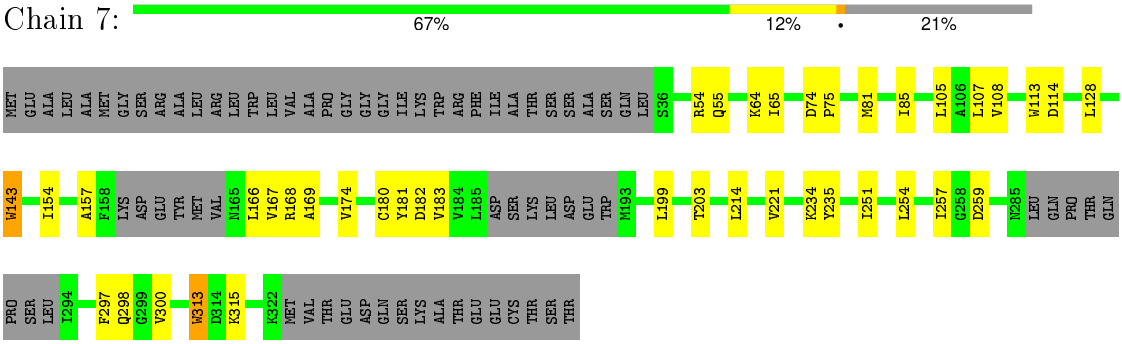
Chain 6:





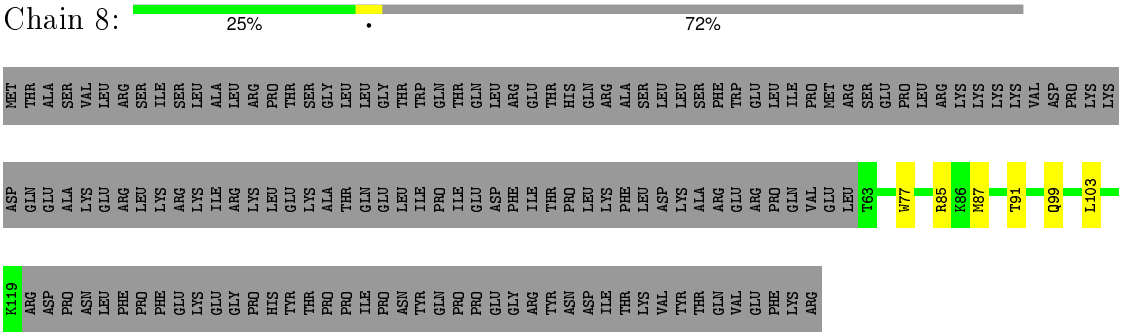
- Molecule 32: mL39

Chain 7:



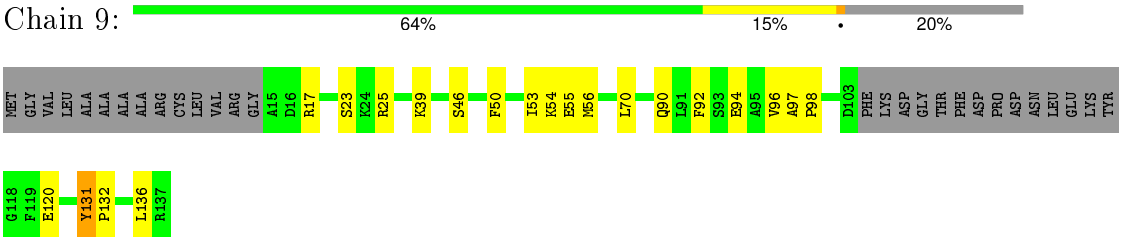
- Molecule 33: mL40

Chain 8:



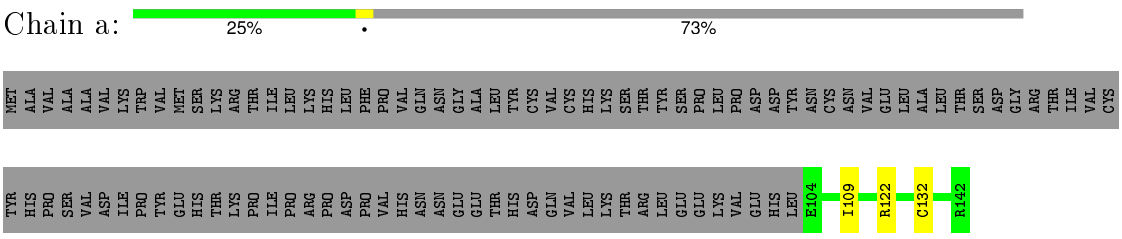
- Molecule 34: mL41

Chain 9:



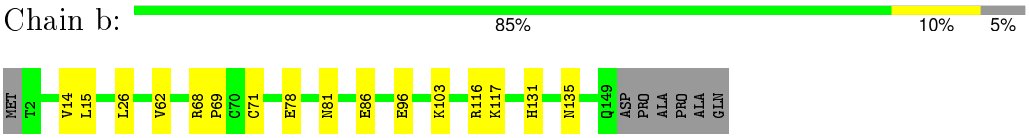
- Molecule 35: mL42

Chain a:



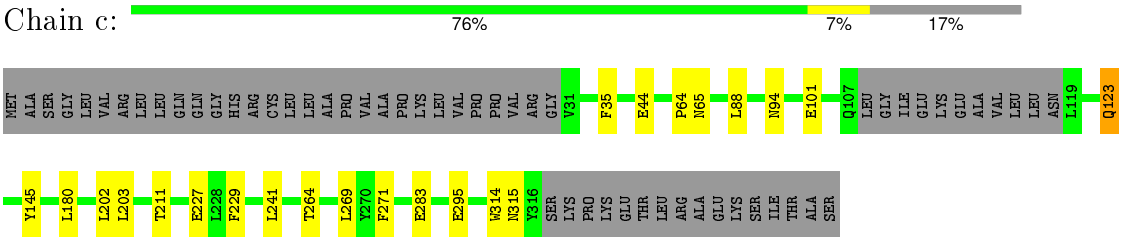
- Molecule 36: mL43

Chain b:



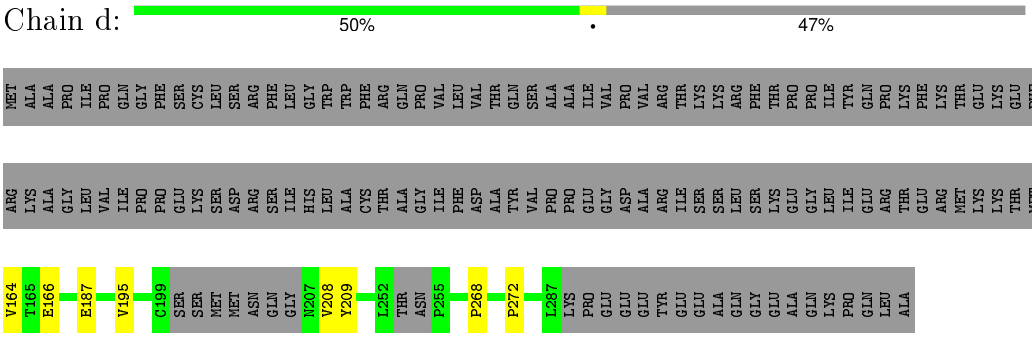
- Molecule 37: mL44

Chain c:



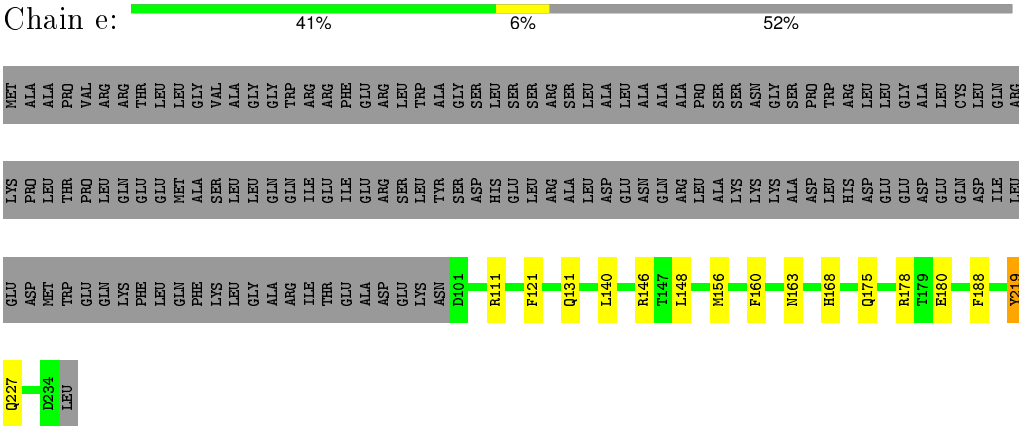
- Molecule 38: mL45

Chain d:



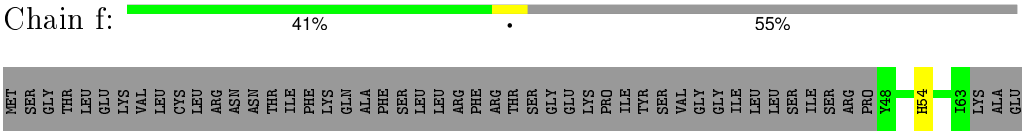
- Molecule 39: mL46

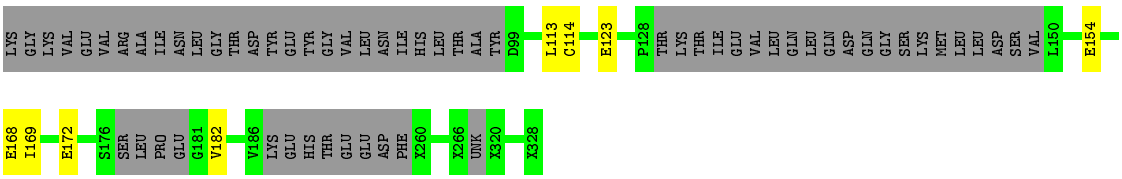
Chain e:



- Molecule 40: mL48

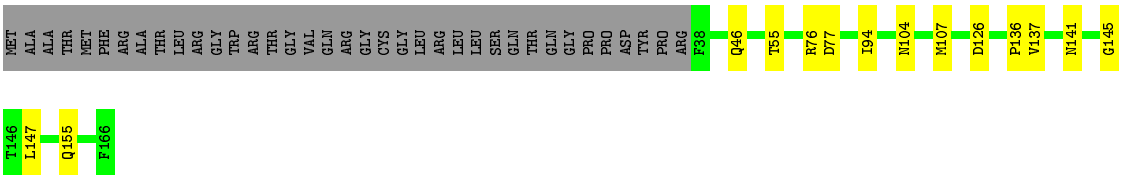
Chain f:





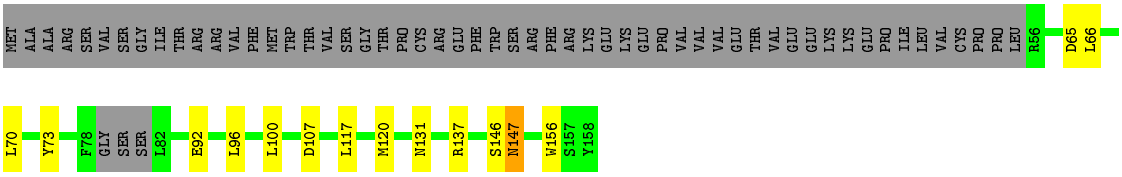
- Molecule 41: mL49

Chain g:



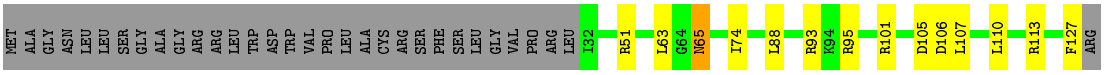
- Molecule 42: mL50

Chain h:



- Molecule 43: mL51

Chain i:



- Molecule 44: mL52

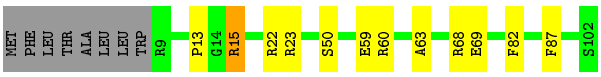
Chain j:

- Molecule 45: mL53

Chain k:

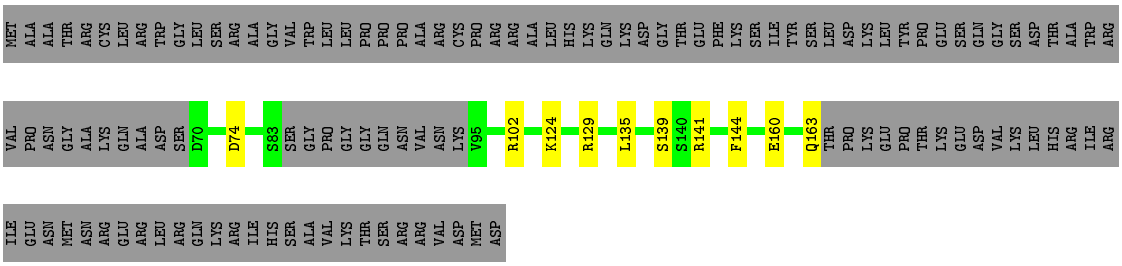
- Molecule 46: mL63

Chain o:



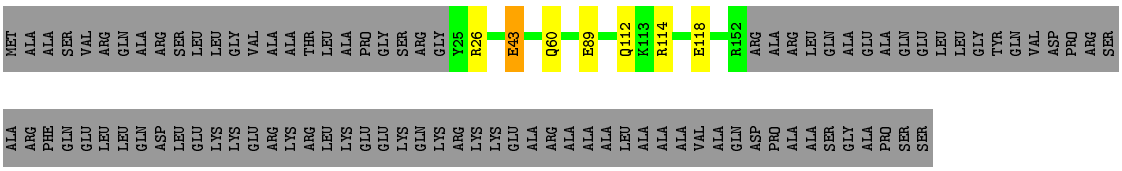
• Molecule 47: ICT1

Chain p:



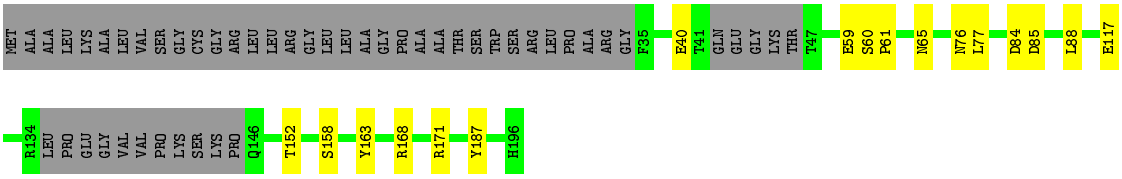
• Molecule 48: CRIF1

Chain q:



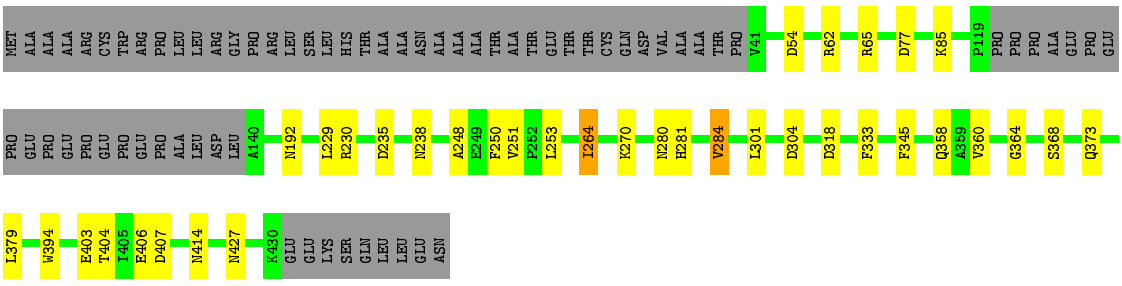
• Molecule 49: bS18a

Chain r:



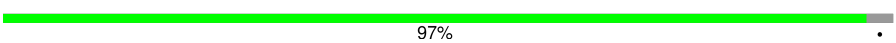
• Molecule 50: mS30

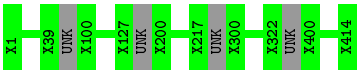
Chain s:



• Molecule 51: unknown protein

Chain t:




X1
X39
UNK
X100
X127
UNK
X200
X217
UNK
X300
X322
UNK
X400
X414

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	107679	Depositor
Resolution determination method	FSC 0.143 gold-standard	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	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, 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	0.29	0/34967	0.76	15/54407 (0.0%)
10	L	0.39	0/904	0.71	0/1218
11	M	0.44	2/2359 (0.1%)	0.79	0/3185
12	N	0.45	1/1697 (0.1%)	0.76	1/2281 (0.0%)
13	O	0.58	3/1269 (0.2%)	0.85	0/1708
14	P	0.80	2/1103 (0.2%)	0.73	0/1491
15	Q	0.55	3/1741 (0.2%)	0.73	1/2340 (0.0%)
16	R	0.77	2/1174 (0.2%)	0.85	0/1572
17	S	0.37	0/1276	0.72	0/1729
18	T	0.47	0/1402	0.78	0/1886
19	U	0.63	2/946 (0.2%)	0.77	0/1283
2	B	0.23	0/1349	0.71	2/2086 (0.1%)
20	V	0.44	1/1590 (0.1%)	0.71	0/2151
21	W	0.47	0/864	0.76	0/1166
22	X	0.48	2/2081 (0.1%)	0.72	0/2812
23	Y	0.50	1/1552 (0.1%)	0.83	1/2079 (0.0%)
24	Z	0.50	1/1003 (0.1%)	0.64	0/1354
25	0	0.57	2/816 (0.2%)	0.80	1/1093 (0.1%)
26	1	0.53	1/438 (0.2%)	0.81	0/583
27	2	0.46	0/357	0.92	0/475
28	3	0.42	0/852	0.81	1/1136 (0.1%)
29	4	0.33	0/329	0.68	0/435
3	D	0.47	1/1879 (0.1%)	0.76	1/2527 (0.0%)
30	5	0.44	0/3154	0.75	1/4295 (0.0%)
31	6	0.51	3/2722 (0.1%)	0.74	0/3709
32	7	0.49	1/2207 (0.0%)	0.71	0/2978
33	8	0.52	0/487	0.83	0/649
34	9	0.75	6/896 (0.7%)	0.72	0/1205
35	a	0.46	0/355	0.76	0/475
36	b	0.80	4/1202 (0.3%)	0.73	0/1626
37	c	0.54	3/2264 (0.1%)	0.78	2/3059 (0.1%)
38	d	0.43	0/1385	0.67	0/1877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	e	0.67	1/1107 (0.1%)	0.72	0/1494
4	E	0.42	1/2433 (0.0%)	0.72	0/3299
40	f	0.97	3/632 (0.5%)	0.70	0/850
41	g	0.42	0/1102	0.72	1/1503 (0.1%)
42	h	0.45	0/847	0.73	0/1150
43	i	0.46	0/838	0.85	0/1121
44	j	0.61	3/698 (0.4%)	0.79	0/940
45	k	0.61	0/665	0.77	0/897
46	o	0.56	1/818 (0.1%)	0.97	1/1097 (0.1%)
47	p	0.48	1/682 (0.1%)	0.75	0/917
48	q	0.55	2/1107 (0.2%)	0.78	0/1498
49	r	0.39	0/1238	0.67	0/1676
5	F	0.41	0/2071	0.73	0/2817
50	s	0.55	4/3114 (0.1%)	0.77	2/4225 (0.0%)
6	H	0.46	0/798	0.78	1/1073 (0.1%)
7	I	0.45	0/1308	0.79	0/1761
8	J	0.46	0/1077	0.77	0/1452
9	K	0.48	1/1495 (0.1%)	0.76	1/2029 (0.0%)
All	All	0.45	58/98650 (0.1%)	0.76	32/140669 (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
31	6	0	1
45	k	0	1
46	o	0	1
5	F	0	1
9	K	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	23	GLU	CD-OE2	18.73	1.46	1.25
14	P	151	GLU	CD-OE2	18.14	1.45	1.25
39	e	180	GLU	CD-OE2	15.19	1.42	1.25
36	b	78	GLU	CD-OE2	14.77	1.41	1.25
40	f	123	GLU	CD-OE1	14.32	1.41	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	o	15	ARG	NE-CZ-NH2	-7.78	116.41	120.30
25	0	108	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	1772	A	C2'-C3'-O3'	7.47	125.93	109.50
28	3	169	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	2174	G	C2'-C3'-O3'	7.26	125.47	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	6	191	ASN	Sidechain
5	F	140	SER	Peptide
9	K	82	GLY	Peptide
45	k	61	GLU	Peptide
46	o	63	ALA	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	A	31261	0	15879	642	0
2	B	1211	0	619	12	0
3	D	1842	0	1896	18	0
4	E	2365	0	2378	38	0
5	F	2013	0	2044	24	0
6	H	784	0	832	16	0
7	I	1283	0	1370	33	0
8	J	1061	0	1141	13	0
9	K	1451	0	1448	20	0
10	L	889	0	941	12	0
11	M	2305	0	2378	27	0
12	N	1654	0	1681	13	0
13	O	1245	0	1283	29	0
14	P	1080	0	1081	27	0
15	Q	1704	0	1744	35	0
16	R	1153	0	1214	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	1251	0	1322	11	0
18	T	1368	0	1410	26	0
19	U	922	0	935	17	0
20	V	1551	0	1558	5	0
21	W	842	0	869	25	0
22	X	2027	0	2040	35	0
23	Y	1517	0	1561	24	0
24	Z	978	0	1030	11	0
25	0	803	0	837	16	0
26	1	433	0	475	2	0
27	2	351	0	375	3	0
28	3	831	0	883	11	0
29	4	322	0	344	12	0
30	5	3064	0	3059	67	0
31	6	2636	0	2450	23	0
32	7	2158	0	2173	22	0
33	8	482	0	494	2	0
34	9	873	0	878	10	0
35	a	343	0	334	0	0
36	b	1178	0	1180	0	0
37	c	2217	0	2220	0	0
38	d	1347	0	1343	0	0
39	e	1082	0	1071	0	0
40	f	703	0	654	0	0
41	g	1067	0	1056	0	0
42	h	827	0	806	0	0
43	i	816	0	844	0	0
44	j	684	0	673	0	0
45	k	655	0	656	0	0
46	o	797	0	804	0	0
47	p	674	0	690	0	0
48	q	1076	0	1049	0	0
49	r	1203	0	1221	0	0
50	s	3036	0	3022	0	0
51	t	615	0	143	0	0
52	A	22	0	12	0	0
53	A	65	0	0	0	0
53	E	1	0	0	0	0
54	0	1	0	0	3	0
54	4	1	0	0	1	0
54	r	1	0	0	0	0
All	All	94121	0	78400	1181	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 8.

The worst 5 of 1181 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)
15:Q:244:ARG:HH11	15:Q:247:LEU:CD1	1.40	1.34
1:A:2556:A:C2	1:A:2559:U:O2	1.86	1.27
1:A:2556:A:H2	1:A:2559:U:O2	1.15	1.26
30:5:127:LYS:CD	30:5:251:HIS:CE1	2.20	1.25
1:A:2194:U:H2'	1:A:2195:A:C8	1.80	1.16

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	
3	D	234/305 (77%)	222 (95%)	11 (5%)	1 (0%)	39	79
4	E	296/348 (85%)	268 (90%)	21 (7%)	7 (2%)	7	44
5	F	248/311 (80%)	228 (92%)	17 (7%)	3 (1%)	16	59
6	H	93/267 (35%)	81 (87%)	10 (11%)	2 (2%)	8	46
7	I	154/261 (59%)	143 (93%)	6 (4%)	5 (3%)	5	38
8	J	138/192 (72%)	115 (83%)	16 (12%)	7 (5%)	2	24
9	K	175/178 (98%)	157 (90%)	10 (6%)	8 (5%)	3	26
10	L	113/145 (78%)	100 (88%)	10 (9%)	3 (3%)	6	41
11	M	285/296 (96%)	256 (90%)	23 (8%)	6 (2%)	9	47
12	N	203/251 (81%)	186 (92%)	15 (7%)	2 (1%)	19	63
13	O	150/175 (86%)	133 (89%)	15 (10%)	2 (1%)	15	57
14	P	129/179 (72%)	115 (89%)	12 (9%)	2 (2%)	12	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	Q	200/292 (68%)	179 (90%)	17 (8%)	4 (2%)	9 48
16	R	138/149 (93%)	128 (93%)	7 (5%)	3 (2%)	8 46
17	S	154/205 (75%)	144 (94%)	9 (6%)	1 (1%)	30 72
18	T	164/212 (77%)	152 (93%)	9 (6%)	3 (2%)	11 50
19	U	109/153 (71%)	96 (88%)	12 (11%)	1 (1%)	21 65
20	V	183/216 (85%)	161 (88%)	15 (8%)	7 (4%)	4 32
21	W	105/148 (71%)	102 (97%)	2 (2%)	1 (1%)	19 63
22	X	241/256 (94%)	220 (91%)	16 (7%)	5 (2%)	9 47
23	Y	174/250 (70%)	157 (90%)	17 (10%)	0	100 100
24	Z	118/161 (73%)	107 (91%)	9 (8%)	2 (2%)	11 51
25	0	94/188 (50%)	81 (86%)	7 (7%)	6 (6%)	2 17
26	1	50/65 (77%)	46 (92%)	2 (4%)	2 (4%)	4 31
27	2	41/92 (45%)	40 (98%)	0	1 (2%)	7 44
28	3	93/188 (50%)	88 (95%)	5 (5%)	0	100 100
29	4	34/103 (33%)	34 (100%)	0	0	100 100
30	5	368/423 (87%)	329 (89%)	26 (7%)	13 (4%)	4 35
31	6	313/380 (82%)	274 (88%)	30 (10%)	9 (3%)	6 40
32	7	258/338 (76%)	236 (92%)	21 (8%)	1 (0%)	39 79
33	8	55/206 (27%)	53 (96%)	2 (4%)	0	100 100
34	9	105/137 (77%)	93 (89%)	9 (9%)	3 (3%)	6 40
35	a	37/142 (26%)	35 (95%)	2 (5%)	0	100 100
36	b	146/155 (94%)	125 (86%)	17 (12%)	4 (3%)	6 41
37	c	271/332 (82%)	238 (88%)	27 (10%)	6 (2%)	8 46
38	d	156/306 (51%)	139 (89%)	11 (7%)	6 (4%)	4 32
39	e	132/279 (47%)	103 (78%)	25 (19%)	4 (3%)	5 39
40	f	71/211 (34%)	63 (89%)	7 (10%)	1 (1%)	14 55
41	g	127/166 (76%)	116 (91%)	8 (6%)	3 (2%)	7 44
42	h	96/158 (61%)	82 (85%)	10 (10%)	4 (4%)	3 29
43	i	94/128 (73%)	80 (85%)	13 (14%)	1 (1%)	17 61
44	j	83/123 (68%)	79 (95%)	3 (4%)	1 (1%)	16 59
45	k	82/112 (73%)	64 (78%)	13 (16%)	5 (6%)	2 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	o	92/102 (90%)	80 (87%)	9 (10%)	3 (3%)	5 37
47	p	79/206 (38%)	73 (92%)	5 (6%)	1 (1%)	15 57
48	q	126/222 (57%)	120 (95%)	5 (4%)	1 (1%)	24 67
49	r	140/196 (71%)	125 (89%)	12 (9%)	3 (2%)	9 47
50	s	366/439 (83%)	326 (89%)	32 (9%)	8 (2%)	8 46
All	All	7313/10347 (71%)	6572 (90%)	580 (8%)	161 (2%)	13 46

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	102	VAL
8	J	70	ILE
12	N	67	LYS
16	R	12	ASN
22	X	69	ILE

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
3	D	190/245 (78%)	175 (92%)	15 (8%)	15 52
4	E	255/290 (88%)	234 (92%)	21 (8%)	14 50
5	F	217/262 (83%)	193 (89%)	24 (11%)	8 33
6	H	86/228 (38%)	81 (94%)	5 (6%)	25 65
7	I	145/232 (62%)	135 (93%)	10 (7%)	19 59
8	J	113/150 (75%)	101 (89%)	12 (11%)	8 36
9	K	155/156 (99%)	144 (93%)	11 (7%)	18 58
10	L	98/124 (79%)	93 (95%)	5 (5%)	29 69
11	M	245/249 (98%)	218 (89%)	27 (11%)	8 34
12	N	172/211 (82%)	158 (92%)	14 (8%)	15 51
13	O	133/150 (89%)	113 (85%)	20 (15%)	3 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	P	115/154 (75%)	108 (94%)	7 (6%)	23 63
15	Q	186/256 (73%)	171 (92%)	15 (8%)	15 51
16	R	118/126 (94%)	108 (92%)	10 (8%)	13 48
17	S	141/180 (78%)	125 (89%)	16 (11%)	7 32
18	T	146/182 (80%)	131 (90%)	15 (10%)	9 37
19	U	99/135 (73%)	91 (92%)	8 (8%)	15 51
20	V	169/191 (88%)	154 (91%)	15 (9%)	12 45
21	W	87/119 (73%)	78 (90%)	9 (10%)	9 37
22	X	217/227 (96%)	198 (91%)	19 (9%)	12 46
23	Y	159/223 (71%)	144 (91%)	15 (9%)	11 42
24	Z	111/147 (76%)	105 (95%)	6 (5%)	27 67
25	0	88/164 (54%)	74 (84%)	14 (16%)	3 17
26	1	49/60 (82%)	41 (84%)	8 (16%)	3 16
27	2	38/72 (53%)	34 (90%)	4 (10%)	8 36
28	3	88/166 (53%)	83 (94%)	5 (6%)	25 65
29	4	35/89 (39%)	33 (94%)	2 (6%)	25 65
30	5	337/368 (92%)	306 (91%)	31 (9%)	11 43
31	6	266/332 (80%)	230 (86%)	36 (14%)	5 24
32	7	242/303 (80%)	231 (96%)	11 (4%)	34 73
33	8	51/190 (27%)	49 (96%)	2 (4%)	39 76
34	9	91/112 (81%)	87 (96%)	4 (4%)	35 73
35	a	37/133 (28%)	34 (92%)	3 (8%)	15 51
36	b	130/135 (96%)	120 (92%)	10 (8%)	16 53
37	c	241/288 (84%)	227 (94%)	14 (6%)	25 65
38	d	151/274 (55%)	148 (98%)	3 (2%)	63 87
39	e	114/236 (48%)	99 (87%)	15 (13%)	5 25
40	f	70/173 (40%)	64 (91%)	6 (9%)	13 48
41	g	119/148 (80%)	109 (92%)	10 (8%)	14 49
42	h	95/148 (64%)	83 (87%)	12 (13%)	5 27
43	i	85/110 (77%)	71 (84%)	14 (16%)	3 15
44	j	68/97 (70%)	63 (93%)	5 (7%)	17 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	k	74/90 (82%)	67 (90%)	7 (10%)	11 41
46	o	80/87 (92%)	72 (90%)	8 (10%)	9 38
47	p	75/181 (41%)	67 (89%)	8 (11%)	8 35
48	q	110/178 (62%)	104 (94%)	6 (6%)	27 66
49	r	133/169 (79%)	119 (90%)	14 (10%)	8 36
50	s	326/381 (86%)	300 (92%)	26 (8%)	15 51
All	All	6550/8921 (73%)	5973 (91%)	577 (9%)	17 46

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	X	69	ILE
27	2	72	THR
48	q	60	GLN
22	X	143	PHE
24	Z	77	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
29	4	98	HIS
30	5	380	GLN
48	q	137	GLN
30	5	102	GLN
30	5	251	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1458/1559 (93%)	550 (37%)	118 (8%)
2	B	51/73 (69%)	21 (41%)	3 (5%)
All	All	1509/1632 (92%)	571 (37%)	121 (8%)

5 of 571 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1672	C
1	A	1674	A

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Mol	Chain	Res	Type
1	A	1675	A
1	A	1676	A
1	A	1677	C

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2274	A
1	A	2444	A
1	A	3092	U
1	A	2321	A
1	A	2380	C

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 70 ligands modelled in this entry, 69 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
52	A	A	3301	-	17,24,25	0.53	0	16,35,38	0.48	0

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
52	A	A	3301	-	-	0/3/25/26	0/3/3/3

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.