wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:16 PM BST

PDB ID	:	4CE4
EMDB ID:	:	EMD-2490
Title	:	39S large subunit of the porcine mitochondrial ribosome
Authors	:	Greber, B.J.; Boehringer, D.; Leitner, A.; Bieri, P.; Voigts-Hoffmann, F.; Erzberger, J.P.; Leibundgut, M.; Aebersold, R.; Ban, N.
Deposited on	:	2013-11-08
Resolution	:	4.90 Å(reported)
Based on PDB ID	:	3V2D 1R73 2QYQ 1QF6 1O0W 2CW9 2XZN 1J26 1S3A

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

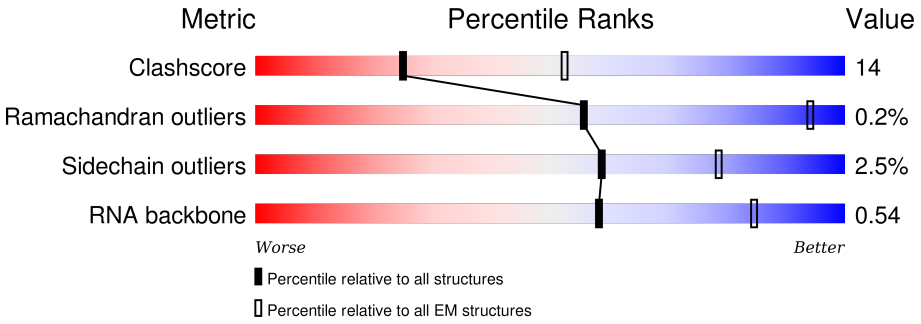
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 4.90 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	148	42% 9% • 49%
2	1	256	17% 5% 77%
3	2	252	24% 6% 70%
4	3	161	25% 11% 63%
5	5	146	25% 21% 53%
6	6	65	52% 22% 26%
7	7	95	31% 15% 55%
8	8	188	20% 12% 68%

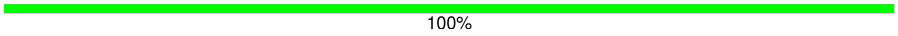
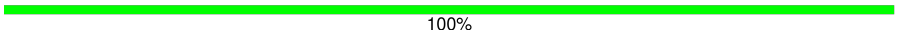
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	9	100	29% 7% 64%
10	A	1570	50% 32% 10% 8%
11	B	29	93% 7%
12	D	306	52% 14% 35%
13	E	399	36% 16% 48%
14	F	224	72% 28%
15	I	268	15% 6% 79%
16	N	178	63% 20% 17%
17	O	145	59% 19% 21%
18	P	288	40% 18% 41%
19	Q	208	53% 21% 26%
20	R	169	56% 14% 29%
21	S	180	43% 9% 48%
22	T	292	27% 13% 59%
23	U	132	69% 23% 7%
24	V	207	38% 14% 47%
25	W	134	64% 35%
26	X	87	64% 34%
27	Y	216	40% 7% 52%
28	b	380	48% 49%
29	c	301	93%
30	h	298	90% 9%
31	i	312	50% 48%
32	l	166	42% 54%
33	o	56	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	u	205	
35	v	91	
35	w	91	
36	x	85	
37	z	426	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 65473 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 MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	76	607	392	114	99	2	0	0

- Molecule 2 is a protein called MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	58	489	312	90	85	2	0	0

- Molecule 3 is a protein called MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	76	633	394	116	119	4	0	0

- Molecule 4 is a protein called MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	59	491	321	95	74	1	0	0

- Molecule 5 is a protein called MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	68	508	317	103	83	5	0	0

- Molecule 6 is a protein called MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	48	391	253	70	66	2	0	0

- Molecule 7 is a protein called MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			362	224	82	55	1		

- Molecule 8 is a protein called MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	60	Total	C	N	O	S	0	0
			520	338	106	74	2		

- Molecule 9 is a protein called MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	36	Total	C	N	O	S	0	0
			316	200	68	45	3		

- Molecule 10 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1444	Total	C	N	O	P	0	0
			30656	13760	5548	9904	1444		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	INSERTION	GB AJ002189

- Molecule 11 is a RNA chain called UNASSIGNED RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	B	29	Total	C	O	P	0	0
			348	145	174	29		

- Molecule 12 is a protein called MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	200	Total	C	N	O	S	0	0
			1531	944	309	269	9		

- Molecule 13 is a protein called MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	208	Total	C	N	O	S	0	0
			1621	1040	300	274	7		

- Molecule 14 is a protein called MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	224	Total	C	N	O	S	0	0
			1713	1101	310	298	4		

- Molecule 15 is a protein called MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	57	Total	C	N	O	0	0
			447	282	79	86		

- Molecule 16 is a protein called MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	147	Total	C	N	O	S	0	0
			1178	756	210	204	8		

- Molecule 17 is a protein called MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	114	Total	C	N	O	S	0	0
			891	559	175	153	4		

- Molecule 18 is a protein called MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	169	Total	C	N	O	S	0	0
			1309	816	258	233	2		

- Molecule 19 is a protein called MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	154	Total	C	N	O	S	0	0
			1179	758	218	195	8		

- Molecule 20 is a protein called MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	120	Total	C	N	O	S	0	0
			982	619	187	172	4		

- Molecule 21 is a protein called MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	94	Total	C	N	O	S	0	0
			748	467	146	131	4		

- Molecule 22 is a protein called MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	119	Total	C	N	O	S	0	0
			962	615	166	177	4		

- Molecule 23 is a protein called MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	123	Total	C	N	O	S	0	0
			1018	647	212	156	3		

- Molecule 24 is a protein called MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	109	Total	C	N	O	S	0	0
			877	565	156	154	2		

- Molecule 25 is a protein called MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	134	Total	C	N	O	S	0	0
			1058	679	191	182	6		

- Molecule 26 is a protein called MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	87	Total	C	N	O	S	0	0
			689	436	133	118	2		

- Molecule 27 is a protein called MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	103	Total	C	N	O	S	0	0
			835	526	156	151	2		

- Molecule 28 is a protein called MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	192	Total	C	N	O	S	0	0
			1562	1006	266	284	6		

- Molecule 29 is a protein called MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	292	Total	C	N	O	S	0	0
			2310	1489	391	415	15		

- Molecule 30 is a protein called MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	272	Total	C	N	O	S	0	0
			2075	1333	344	391	7		

- Molecule 31 is a protein called MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	161	Total	C	N	O	S	0	0
			1335	845	243	239	8		

- Molecule 32 is a protein called MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	76	Total	C	N	O	S	0	0
			619	398	108	111	2		

- Molecule 33 is a protein called MRPL52.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	o	56	Total	C	N	O	0	0
			336	224	56	56		

- Molecule 34 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	90	Total	C	N	O	S	0	0
			717	444	137	132	4		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	v	91	Total	C	N	O	0	0
			546	364	91	91		
35	w	91	Total	C	N	O	0	0
			546	364	91	91		

- Molecule 36 is a protein called THIOREDOXIN FOLD.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	x	85	Total	C	N	O	0	0
			510	340	85	85		

- Molecule 37 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	z	426	Total	C	N	O	0	0
			2556	1704	426	426		

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

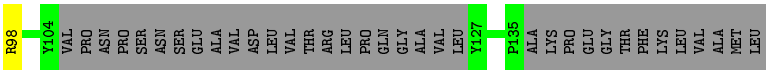
Mol	Chain	Residues	Atoms		AltConf
38	9	1	Total	Zn	0
			1	1	
38	5	1	Total	Zn	0
			1	1	

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: MRPL27

Chain 0:

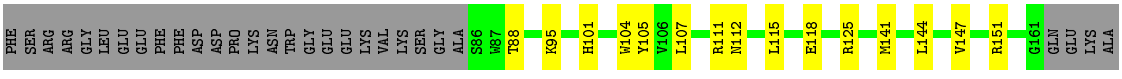


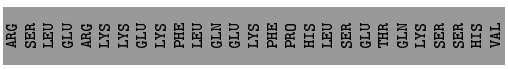
- Molecule 2: MRPL28

Chain 1:

- Molecule 3: MRPL47

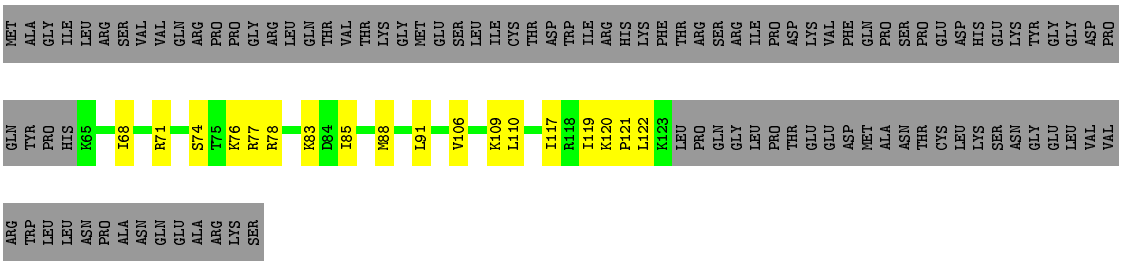
Chain 2:





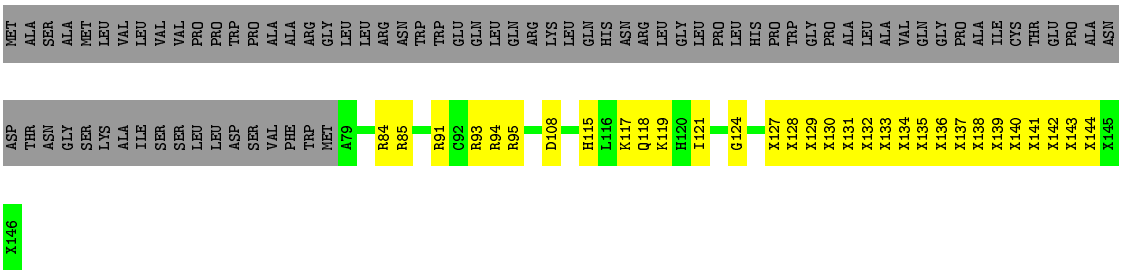
- Molecule 4: MRPL30

Chain 3:



- Molecule 5: MRPL32

Chain 5:

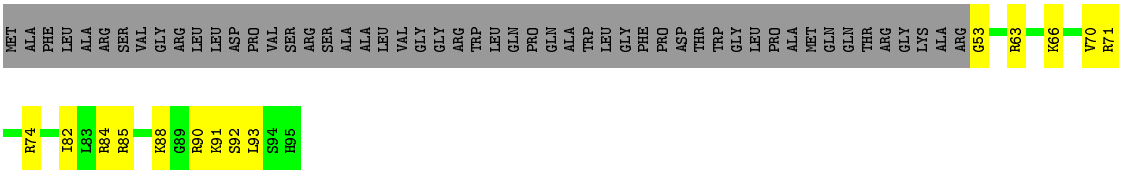


- Molecule 6: MRPL33

Chain 6:

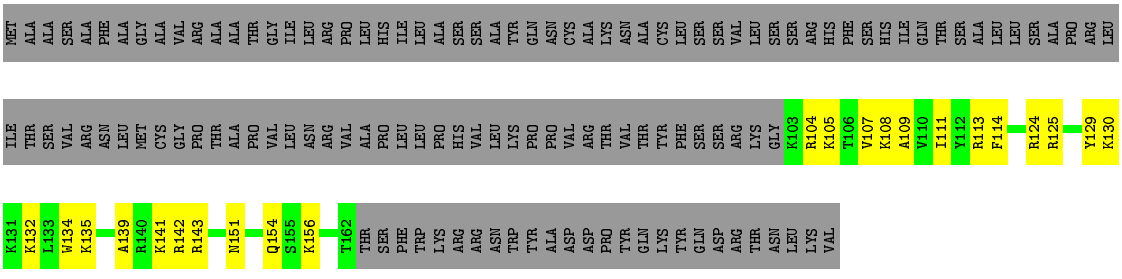
- Molecule 7: MRPL34

Chain 7:



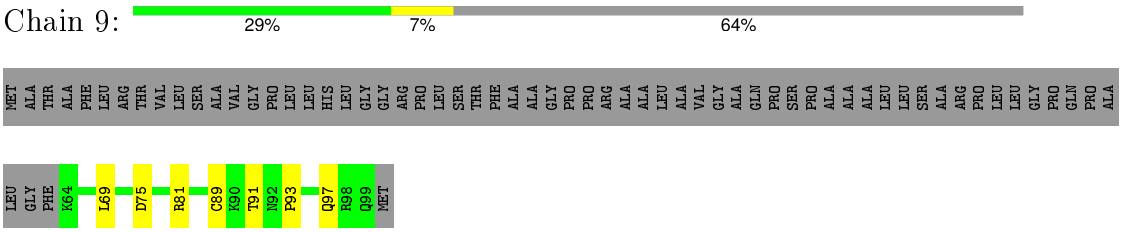
- Molecule 8: MRPL35

Chain 8:



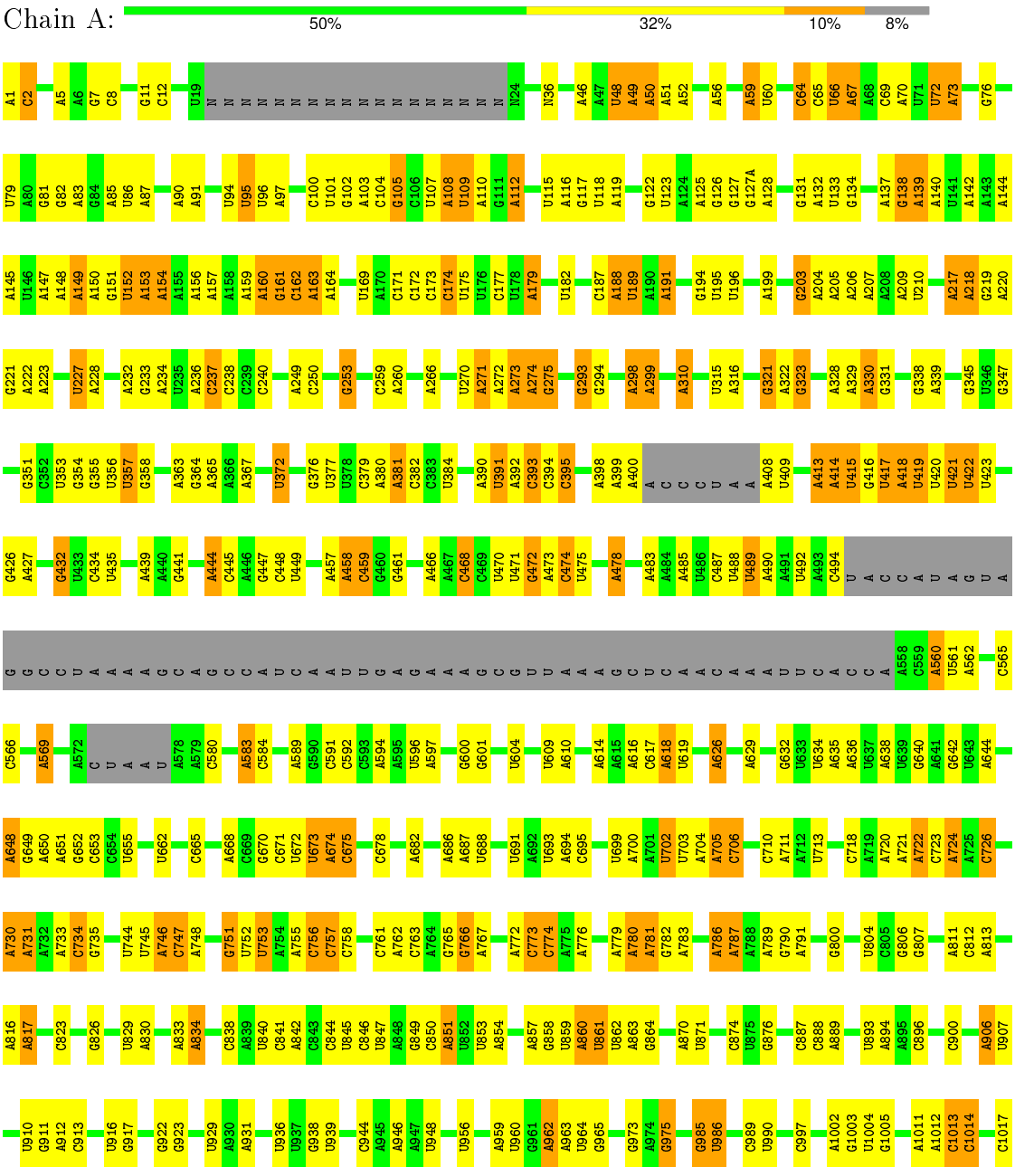
- Molecule 9: MRPL36

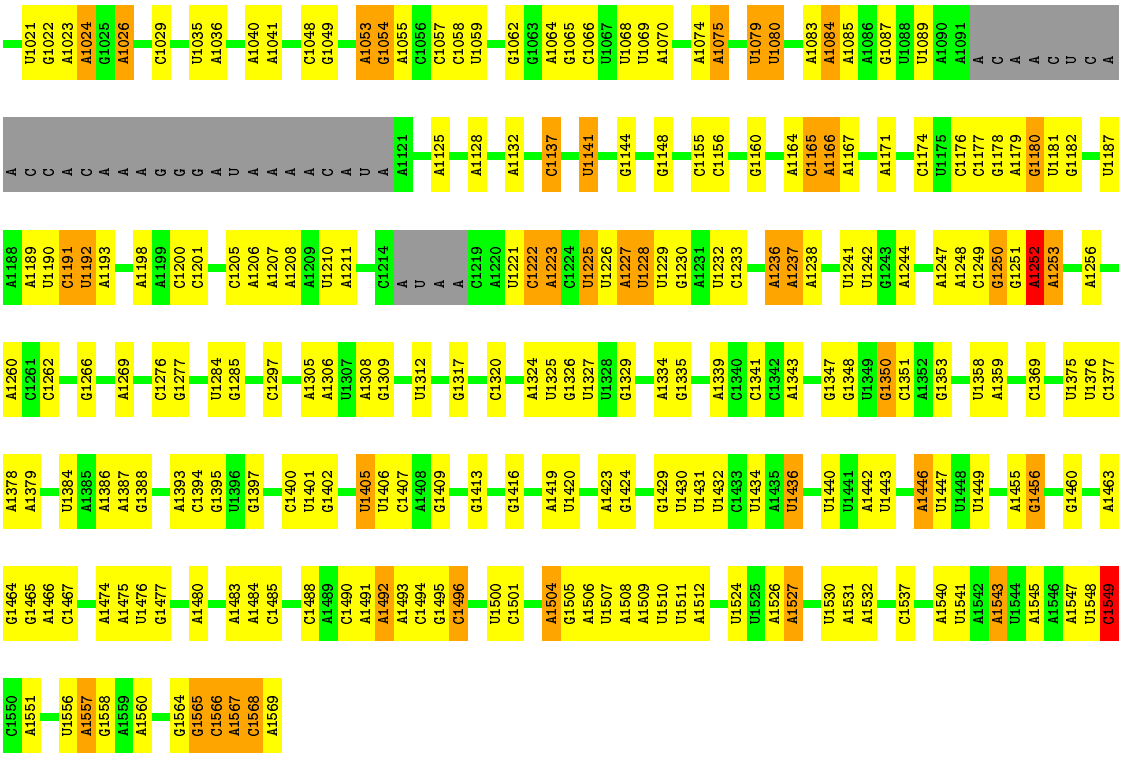
Chain 9:



- Molecule 10: 16S RRNA

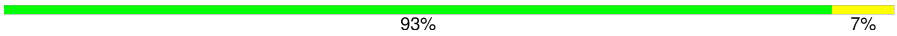
Chain A:





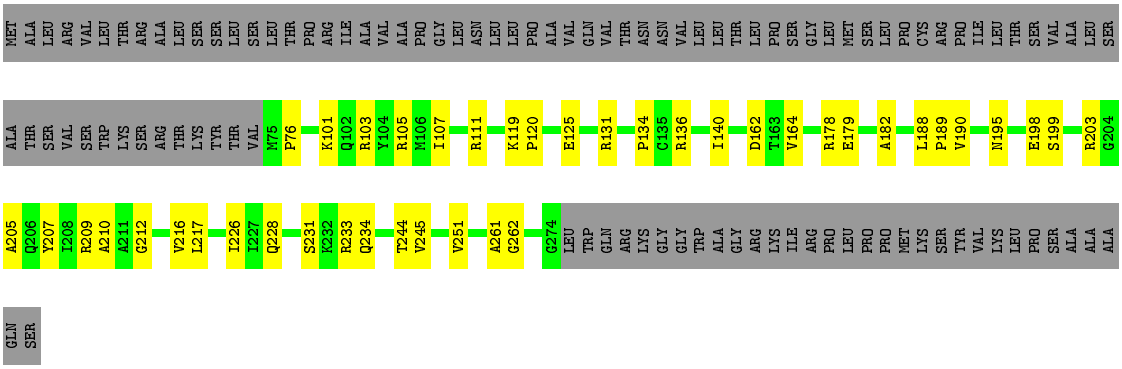
- Molecule 11: UNASSIGNED RNA

Chain B:



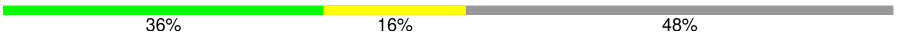
- Molecule 12: MRPL2

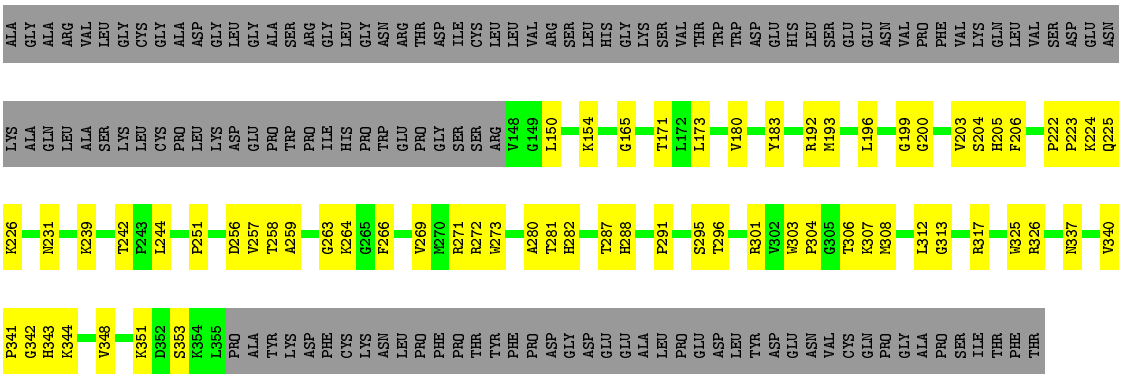
Chain D:



- Molecule 13: MRPL3

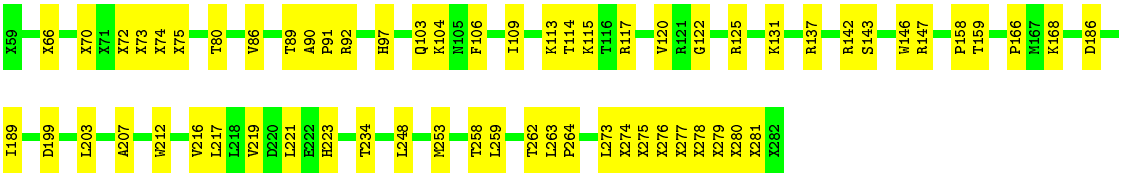
Chain E:





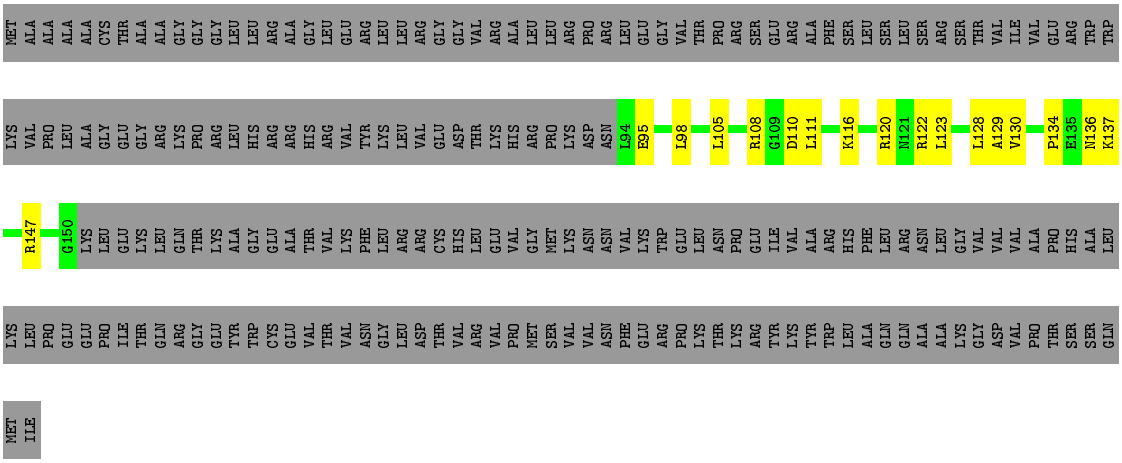
- Molecule 14: MRPL4

Chain F:



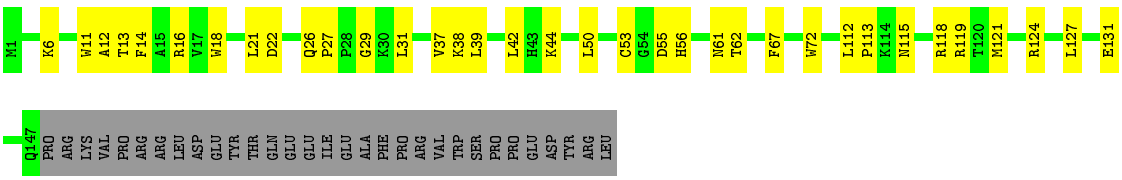
- Molecule 15: MRPL9

Chain I:



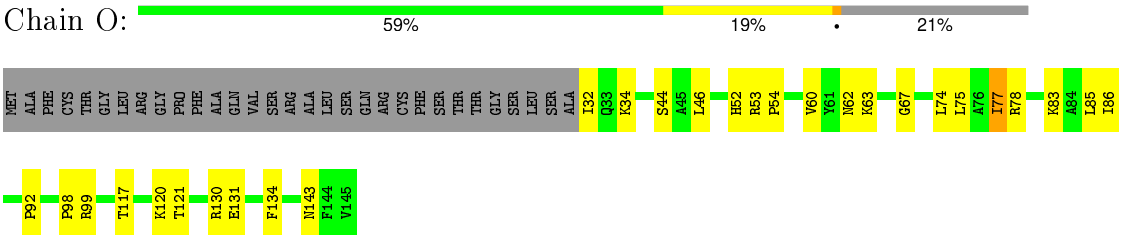
- Molecule 16: MRPL13

Chain N:



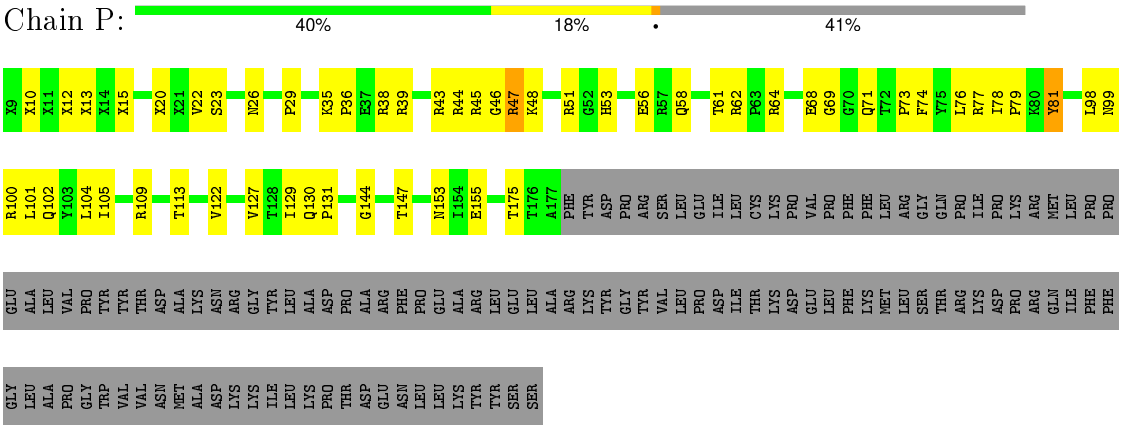
- Molecule 17: MRPL14

Chain O:



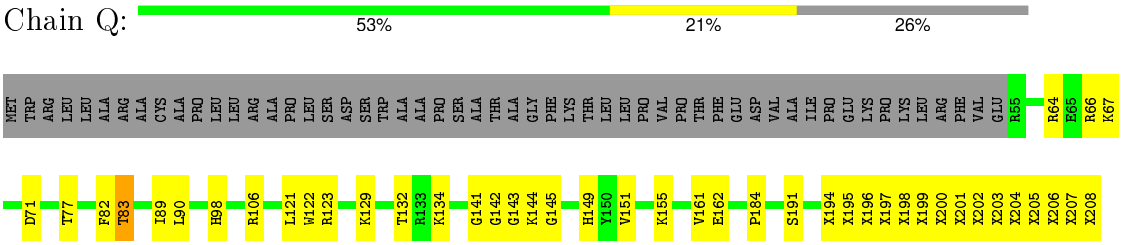
- Molecule 18: MRPL15

Chain P:



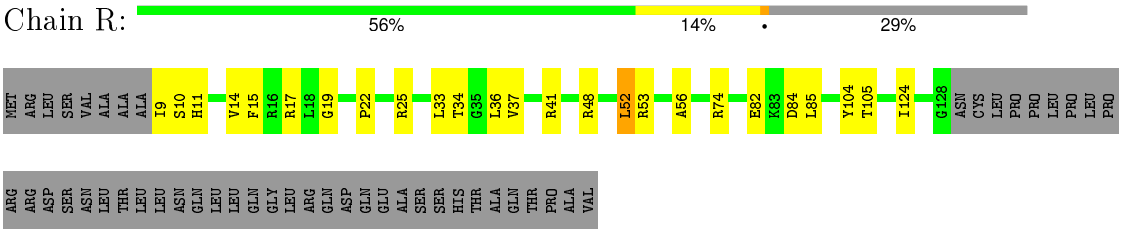
- Molecule 19: MRPL16

Chain Q:



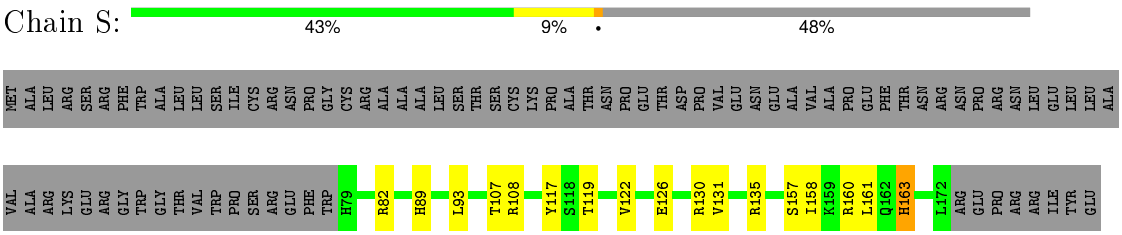
- Molecule 20: MRPL17

Chain R:



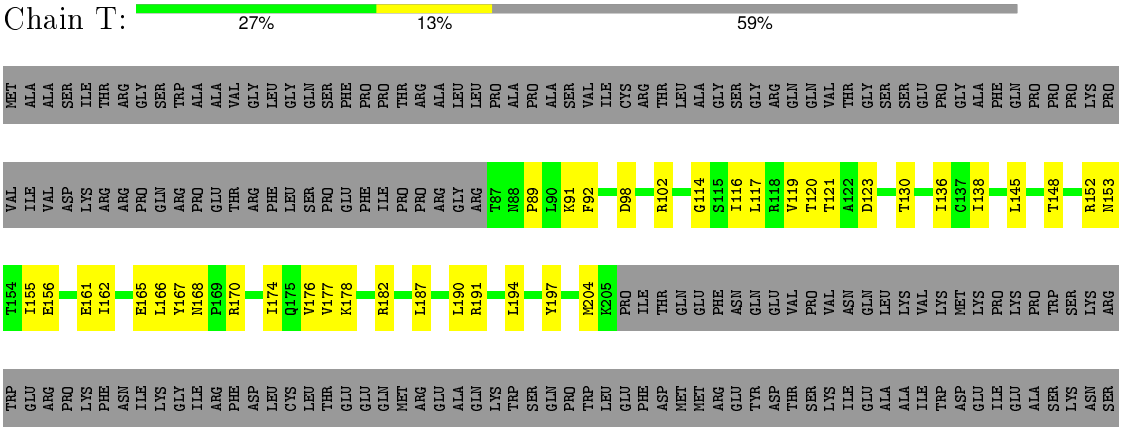
- Molecule 21: MRPL18

Chain S:



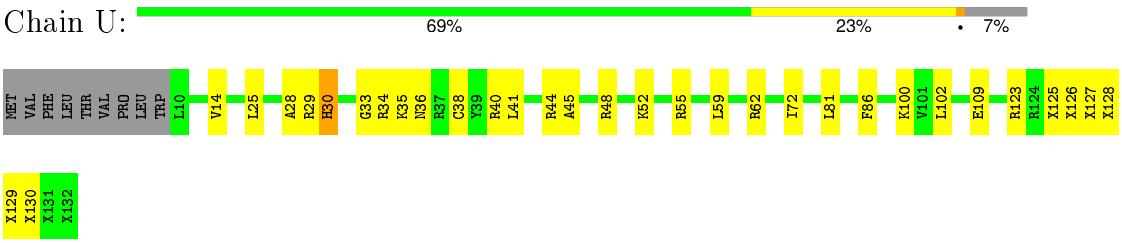
- Molecule 22: MRPL19

Chain T:



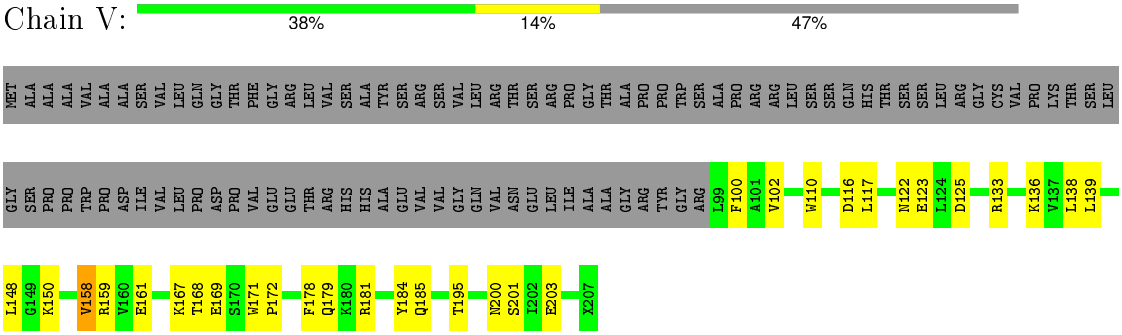
- Molecule 23: MRPL20

Chain U:



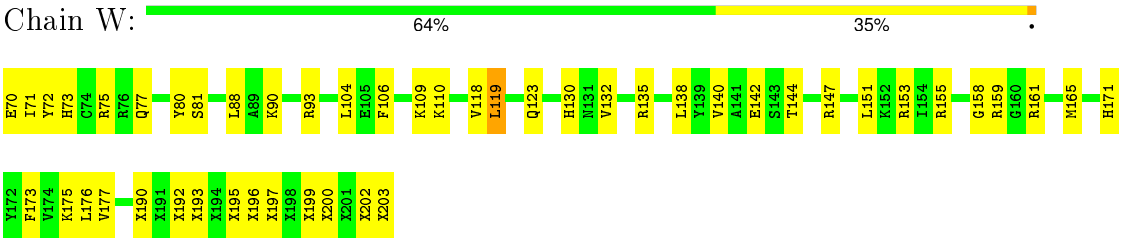
- Molecule 24: MRPL21

Chain V:



- Molecule 25: MRPL22

Chain W:

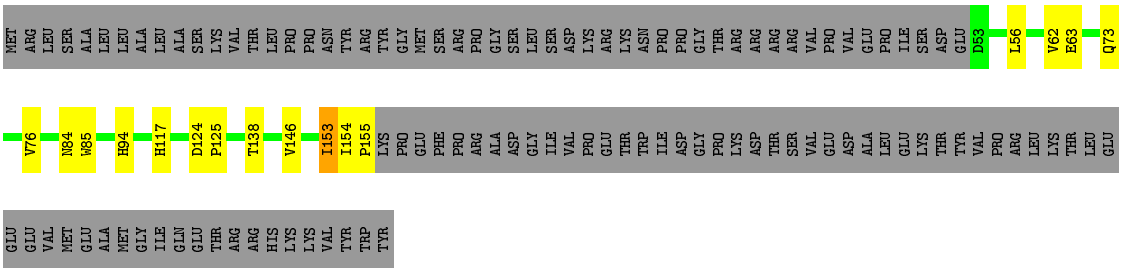


- Molecule 26: MRPL23

Chain X:

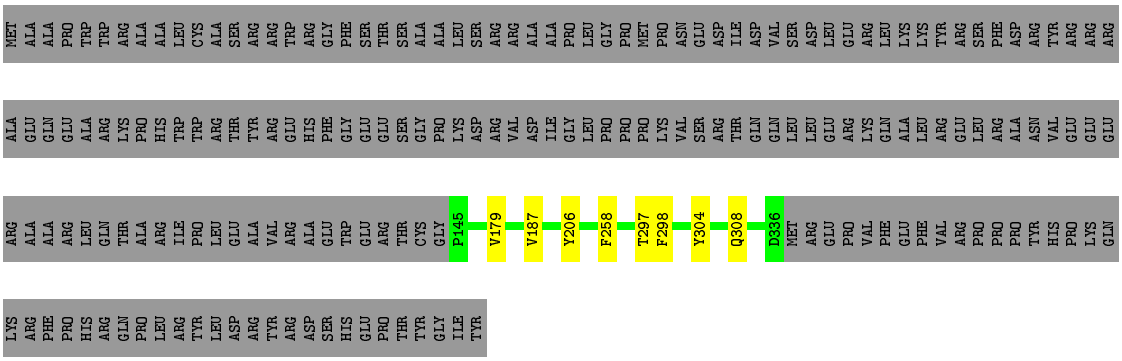
- Molecule 27: MRPL24

Chain Y:



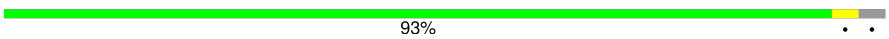
- Molecule 28: MRPL38

Chain b:



- Molecule 29: MRPL39

Chain c:

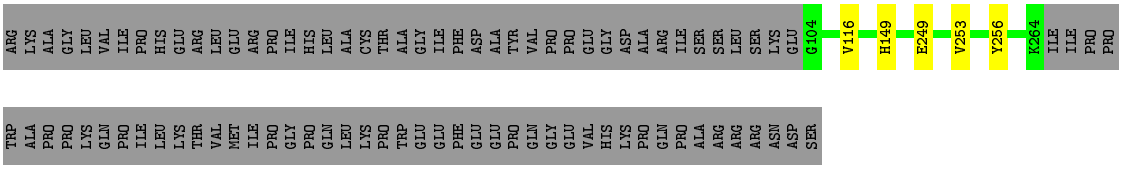


- Molecule 30: MRPL44

Chain h:

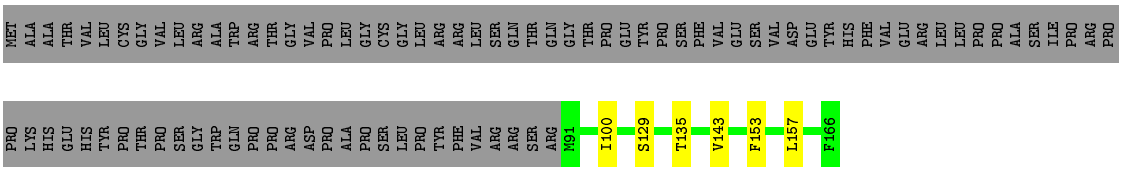
- Molecule 31: MRPL45

Chain i:



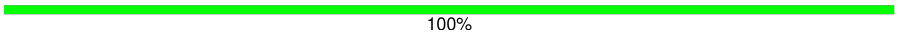
- Molecule 32: MRPL49

Chain l:



- Molecule 33: MRPL52

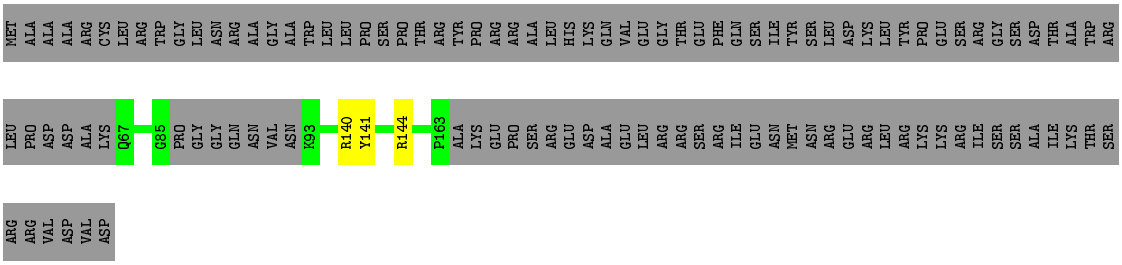
Chain o:



There are no outlier residues recorded for this chain.

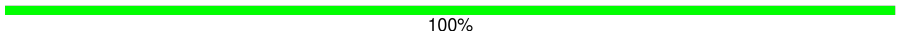
- Molecule 34: ICT1

Chain u:



- Molecule 35: UNASSIGNED HELICES

Chain v:



There are no outlier residues recorded for this chain.

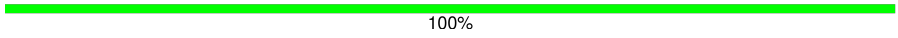
- Molecule 35: UNASSIGNED HELICES

Chain w:

There are no outlier residues recorded for this chain.

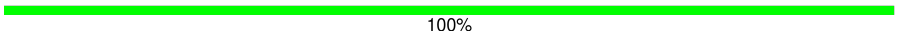
- Molecule 36: THIOREDOXIN FOLD

Chain x:



There are no outlier residues recorded for this chain.

- Molecule 37: UNASSIGNED HELICES

Chain z: 

There are no outlier residues recorded for this chain.

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	PER DETECTOR FRAME	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON I AND FEI FALCON II	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	0.20	0/624	0.34	0/836
10	A	0.16	0/34230	0.72	8/53284 (0.0%)
12	D	0.19	0/1557	0.36	0/2093
13	E	0.21	0/1662	0.37	0/2246
14	F	0.20	0/1582	0.38	0/2148
15	I	0.20	0/450	0.37	0/603
16	N	0.21	0/1211	0.40	0/1639
17	O	0.21	0/907	0.40	0/1224
18	P	0.21	0/1254	0.40	0/1686
19	Q	0.21	0/1104	0.36	0/1483
2	1	0.20	0/498	0.41	0/670
20	R	0.21	0/1000	0.38	0/1342
21	S	0.18	0/763	0.36	0/1033
22	T	0.22	0/978	0.39	0/1318
23	U	0.21	0/986	0.36	0/1319
24	V	0.21	0/866	0.41	0/1168
25	W	0.20	0/931	0.33	0/1241
26	X	0.20	0/585	0.37	0/788
27	Y	0.20	0/853	0.40	0/1155
28	b	0.21	0/1616	0.39	0/2205
29	c	0.29	1/2171 (0.0%)	0.43	1/2937 (0.0%)
3	2	0.19	0/641	0.32	0/862
30	h	0.23	0/1918	0.38	0/2597
31	i	0.21	0/1366	0.41	0/1844
32	l	0.22	0/632	0.42	0/855
34	u	0.20	0/726	0.38	0/975
4	3	0.19	0/501	0.40	0/671
5	5	0.19	0/393	0.37	0/524
6	6	0.21	0/396	0.36	0/526
7	7	0.19	0/370	0.35	0/492
8	8	0.21	0/529	0.33	0/698
9	9	0.20	0/322	0.32	0/424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>2$	RMSZ	$\#\|Z\|>2$
All	All	0.19	1/63622 (0.0%)	0.60	9/92886 (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
29	c	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	141	ARG	C-N	6.05	1.48	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	753	U	C2-N1-C1'	7.69	126.93	117.70
10	A	1549	C	N3-C2-O2	-7.49	116.66	121.90
10	A	753	U	N1-C2-O2	7.31	127.92	122.80
10	A	753	U	N3-C2-O2	-6.98	117.31	122.20
10	A	1549	C	C6-N1-C2	-6.66	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	c	70	THR	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	607	0	611	9	0
2	1	489	0	501	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	633	0	649	13	0
4	3	491	0	559	16	0
5	5	508	0	527	33	0
6	6	391	0	429	8	0
7	7	362	0	382	15	0
8	8	520	0	585	31	0
9	9	316	0	341	5	0
10	A	30656	0	15523	415	0
11	B	348	0	234	2	0
12	D	1531	0	1569	29	0
13	E	1621	0	1680	48	0
14	F	1713	0	1762	49	0
15	I	447	0	472	10	0
16	N	1178	0	1185	31	0
17	O	891	0	941	19	0
18	P	1309	0	1335	51	0
19	Q	1179	0	1211	34	0
20	R	982	0	995	15	0
21	S	748	0	752	12	0
22	T	962	0	987	29	0
23	U	1018	0	1099	29	0
24	V	877	0	925	25	0
25	W	1058	0	1069	38	0
26	X	689	0	708	22	0
27	Y	835	0	838	8	0
28	b	1562	0	1469	0	0
29	c	2310	0	2310	0	0
30	h	2075	0	2091	0	0
31	i	1335	0	1323	0	0
32	l	619	0	628	0	0
33	o	336	0	338	0	0
34	u	717	0	730	0	0
35	v	546	0	556	0	0
35	w	546	0	556	0	0
36	x	510	0	514	0	0
37	z	2556	0	2598	0	0
38	5	1	0	0	0	0
38	9	1	0	0	0	0
All	All	65473	0	50982	814	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 14.

The worst 5 of 814 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)
13:E:258:THR:OG1	13:E:351:LYS:NZ	2.02	0.92
10:A:1543:A:OP1	13:E:351:LYS:NZ	2.05	0.89
10:A:444:A:OP2	19:Q:67:LYS:NZ	2.03	0.89
8:8:108:LYS:NZ	10:A:79:U:O4	2.06	0.89
10:A:83:A:OP2	10:A:1233:C:O2'	1.94	0.86

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	72/148 (49%)	69 (96%)	3 (4%)	0	100	100
2	1	56/256 (22%)	51 (91%)	5 (9%)	0	100	100
3	2	74/252 (29%)	73 (99%)	1 (1%)	0	100	100
4	3	57/161 (35%)	56 (98%)	1 (2%)	0	100	100
5	5	47/146 (32%)	44 (94%)	3 (6%)	0	100	100
6	6	46/65 (71%)	43 (94%)	3 (6%)	0	100	100
7	7	41/95 (43%)	41 (100%)	0	0	100	100
8	8	58/188 (31%)	58 (100%)	0	0	100	100
9	9	34/100 (34%)	34 (100%)	0	0	100	100
12	D	198/306 (65%)	188 (95%)	10 (5%)	0	100	100
13	E	206/399 (52%)	194 (94%)	12 (6%)	0	100	100
14	F	196/224 (88%)	188 (96%)	8 (4%)	0	100	100
15	I	55/268 (20%)	47 (86%)	8 (14%)	0	100	100
16	N	145/178 (82%)	132 (91%)	13 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	112/145 (77%)	109 (97%)	3 (3%)	0	100	100
18	P	155/288 (54%)	144 (93%)	10 (6%)	1 (1%)	30	74
19	Q	136/208 (65%)	131 (96%)	5 (4%)	0	100	100
20	R	118/169 (70%)	107 (91%)	11 (9%)	0	100	100
21	S	92/180 (51%)	87 (95%)	5 (5%)	0	100	100
22	T	117/292 (40%)	113 (97%)	4 (3%)	0	100	100
23	U	114/132 (86%)	110 (96%)	3 (3%)	1 (1%)	21	67
24	V	104/207 (50%)	97 (93%)	7 (7%)	0	100	100
25	W	109/134 (81%)	106 (97%)	3 (3%)	0	100	100
26	X	68/87 (78%)	68 (100%)	0	0	100	100
27	Y	101/216 (47%)	95 (94%)	6 (6%)	0	100	100
28	b	190/380 (50%)	179 (94%)	10 (5%)	1 (0%)	34	77
29	c	259/301 (86%)	246 (95%)	12 (5%)	1 (0%)	39	80
30	h	239/298 (80%)	220 (92%)	18 (8%)	1 (0%)	39	80
31	i	159/312 (51%)	148 (93%)	11 (7%)	0	100	100
32	l	74/166 (45%)	70 (95%)	3 (4%)	1 (1%)	14	58
34	u	86/205 (42%)	77 (90%)	9 (10%)	0	100	100
All	All	3518/6506 (54%)	3325 (94%)	187 (5%)	6 (0%)	56	86

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	l	143	VAL
23	U	14	VAL
28	b	187	VAL
18	P	47	ARG
30	h	223	MET

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	62/115 (54%)	60 (97%)	2 (3%)	46	77
2	1	54/229 (24%)	51 (94%)	3 (6%)	26	65
3	2	72/228 (32%)	72 (100%)	0	100	100
4	3	56/147 (38%)	56 (100%)	0	100	100
5	5	44/108 (41%)	43 (98%)	1 (2%)	58	83
6	6	45/60 (75%)	45 (100%)	0	100	100
7	7	39/78 (50%)	39 (100%)	0	100	100
8	8	54/162 (33%)	52 (96%)	2 (4%)	41	74
9	9	34/77 (44%)	34 (100%)	0	100	100
12	D	158/248 (64%)	158 (100%)	0	100	100
13	E	173/320 (54%)	171 (99%)	2 (1%)	78	90
14	F	166/166 (100%)	161 (97%)	5 (3%)	48	78
15	I	50/228 (22%)	48 (96%)	2 (4%)	38	72
16	N	127/157 (81%)	126 (99%)	1 (1%)	86	93
17	O	99/123 (80%)	97 (98%)	2 (2%)	63	86
18	P	129/235 (55%)	125 (97%)	4 (3%)	47	78
19	Q	111/155 (72%)	106 (96%)	5 (4%)	34	70
20	R	101/143 (71%)	96 (95%)	5 (5%)	30	67
21	S	80/153 (52%)	78 (98%)	2 (2%)	55	82
22	T	107/258 (42%)	105 (98%)	2 (2%)	65	86
23	U	100/109 (92%)	98 (98%)	2 (2%)	63	86
24	V	94/173 (54%)	92 (98%)	2 (2%)	61	85
25	W	95/95 (100%)	94 (99%)	1 (1%)	80	91
26	X	62/62 (100%)	61 (98%)	1 (2%)	70	88
27	Y	91/192 (47%)	88 (97%)	3 (3%)	45	77
28	b	165/328 (50%)	158 (96%)	7 (4%)	36	71
29	c	236/244 (97%)	228 (97%)	8 (3%)	44	76
30	h	206/230 (90%)	203 (98%)	3 (2%)	72	89
31	i	148/281 (53%)	143 (97%)	5 (3%)	44	76
32	l	68/147 (46%)	63 (93%)	5 (7%)	17	56
34	u	79/177 (45%)	76 (96%)	3 (4%)	40	74
All	All	3105/5428 (57%)	3027 (98%)	78 (2%)	59	82

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	S	163	HIS
26	X	56	TYR
32	l	135	THR
22	T	166	LEU
23	U	81	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	36	ASN
25	W	73	HIS
34	u	103	HIS
23	U	79	HIS
23	U	89	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1431/1570 (91%)	368 (25%)	25 (1%)
11	B	0/29	-	-
All	All	1431/1599 (89%)	368 (25%)	25 (1%)

5 of 368 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	2	C
10	A	5	A
10	A	7	G
10	A	8	C
10	A	46	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	746	A
10	A	756	C
10	A	1566	C
10	A	751	G
10	A	786	A

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.