wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 03:18 PM JST

PDB ID	:	8IA0
EMDB ID	:	EMD-35290
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - State Puf6
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	2.70 Å(reported)
Based on initial model	:	.

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

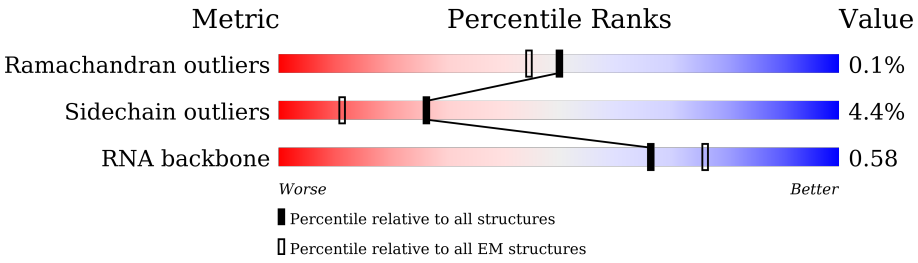
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.70 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	C1	3341	70% 17% 12%
2	C2	319	63% 18% 20%
3	CA	316	78% · 21%
4	CB	391	63% · 34%
5	CC	801	79% · 18%
6	CD	495	89% · 7%
7	CE	598	75% · 23%
8	CF	270	88% · 9%
9	CG	184	94% · ·

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Mol	Chain	Length	Quality of chain
10	CH	661	78% 18%
11	CI	414	34% 65%
12	CJ	679	69% 27%
13	CK	261	83% 5% 12%
14	CL	558	70% 29%
15	CM	249	86% 10%
15	LF	249	98%
16	CN	246	97%
17	CO	120	50% 48%
18	CP	751	46% 53%
19	CQ	225	75% 20%
20	CR	237	68% 30%
21	CS	834	72% 25%
22	CT	688	68% 29%
23	CU	451	38% 61%
24	CV	147	91% 5%
25	CW	679	75% 20%
26	CX	203	43% 57%
27	CY	788	50% 47%
28	CZ	697	79% 17%
29	Ca	227	48% 48%
30	Cz	123	54% 43%
31	LA	254	62% 35%
32	LB	392	89% 9%
33	LC	365	96%

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Mol	Chain	Length	Quality of chain
34	LE	200	88% 10%
35	LG	262	77% 22%
36	LH	192	97%
37	LK	165	85% 12%
38	LL	213	54% 45%
39	LM	142	94%
40	LN	203	87% 10%
41	LO	204	98%
42	LP	187	89% 10%
43	LQ	213	59% 39%
44	LR	2898	5% 95%
45	LS	174	97%
46	LT	160	77% 21%
47	LU	127	82% 17%
48	LV	139	95%
49	LX	156	86% 12%
50	LY	138	92% 5%
51	LZ	135	95% 5%
52	Lc	108	87% 9%
53	Ld	120	89% 9%
54	Le	131	94%
55	Lf	109	96%
56	Lg	119	96%
57	Lh	935	13% 87%
58	Li	110	78% 20%

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Mol	Chain	Length	Quality of chain
59	Lj	95	
60	Lk	81	
61	Lp	92	
62	Ll	51	
63	Lq	217	

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 177631 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	2928	62650	27959	11356	20407	2928	0	0

- Molecule 2 is a RNA chain called RNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	256	5456	2435	974	1791	256	0	0

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	251	2069	1324	381	357	7	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	260	2063	1322	367	371	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	CC	658	5297	3368	931	983	2	13	0	0

- Molecule 6 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CD	460	3468	2173	610	679	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	88	ASP	GLU	conflict	UNP G0SFB5

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CE	463	Total	C	N	O	S	0	0
			3673	2352	643	667	11		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 8 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CF	245	Total	C	N	O	S	0	0
			1945	1222	352	362	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CG	177	Total	C	N	O	S	0	0
			1396	884	247	253	12		

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CH	542	Total	C	N	O	S	0	0
			4388	2784	770	818	16		

- Molecule 11 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CJ	494	Total	C	N	O	S	0	0
			4040	2575	719	734	12		

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CK	229	Total	C	N	O	S	0	0
			1835	1149	362	320	4		

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CL	397	Total	C	N	O	0	0
			2239	1350	459	430		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CM	223	Total	C	N	O	S	0	0
			1820	1169	340	308	3		
15	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 17 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	356	Total	C	N	O	S	0	0
			2798	1777	495	510	16		

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	179	Total	C	N	O	S	0	0
			1485	926	304	245	10		

- Molecule 20 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CS	629	Total	C	N	O	S	0	0
			5082	3220	925	918	19		

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CT	488	Total	C	N	O	S	0	0
			3911	2486	690	719	16		

- Molecule 23 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

- Molecule 24 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	CV	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 25 is a protein called ATP-dependent RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CW	540	Total	C	N	O	S	0	0
			4310	2748	765	783	14		

- Molecule 26 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CX	88	Total	C	N	O	S	0	0
			701	435	128	135	3		

- Molecule 27 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CY	420	Total	C	N	O	S	0	0
			3413	2191	619	591	12		

- Molecule 28 is a protein called PUM-HD domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CZ	576	Total	C	N	O	S	0	0
			3975	2502	708	753	12		

- Molecule 29 is a protein called Nucleolar protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ca	117	Total	C	N	O	S	0	0
			982	609	199	173	1		

- Molecule 30 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Cz	70	Total	C	N	O	S	0	0
			592	368	120	101	3		

- Molecule 31 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LA	166	Total	C	N	O	S	0	0
			1259	798	233	226	2		

- Molecule 32 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LB	356	Total	C	N	O	S	0	0
			2829	1798	518	501	12		

- Molecule 33 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 34 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LE	179	Total	C	N	O	S	0	0
			1403	898	255	247	3		

- Molecule 35 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LG	205	Total	C	N	O	S	0	0
			1651	1065	298	283	5		

- Molecule 36 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 37 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LK	146	Total	C	N	O	S	0	0
			1112	701	203	206	2		

- Molecule 38 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 39 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 40 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 41 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 42 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LP	169	Total	C	N	O	S	0	0
			1345	835	273	234	3		

- Molecule 43 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 44 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LR	148	Total	C	N	O	S	0	0
			1219	756	253	205	5		

- Molecule 45 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 46 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 47 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LU	105	Total	C	N	O	S	0	0
			850	551	147	151	1		

- Molecule 48 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 49 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	LX	137	Total	C	N	O	0	0
			1062	678	194	190		

- Molecule 50 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 51 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 52 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lc	98	Total	C	N	O	S	0	0
			731	463	126	137	5		

- Molecule 53 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ld	109	Total	C	N	O	S	0	0
			890	563	171	155	1		

- Molecule 54 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Le	127	Total	C	N	O	S	0	0
			1025	645	209	164	7		

- Molecule 55 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 56 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lg	117	Total	C	N	O	S	0	0
			930	578	189	159	4		

- Molecule 57 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Lh	121	Total	C	N	O	0	0
			995	633	196	166		

- Molecule 58 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 59 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Lk	75	Total	C	N	O	S	0	0
			620	394	117	107	2		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	SER	deletion	UNP G0SG89
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89

- Molecule 61 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lp	58	Total	C	N	O	S	0	0
			436	266	85	79	6		

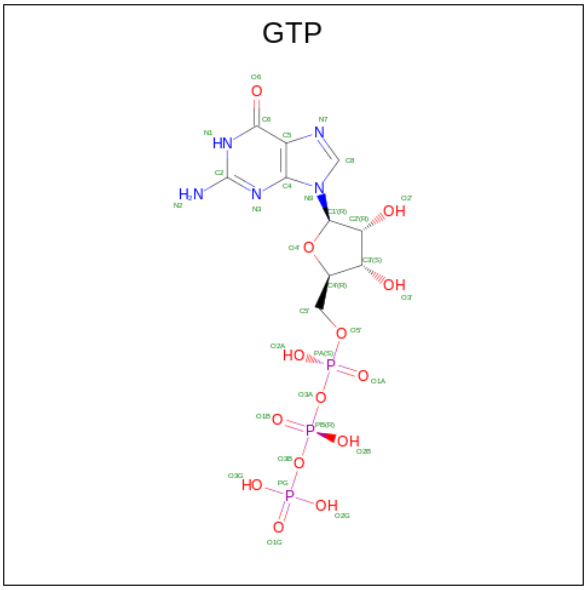
- Molecule 62 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	Ll	38	Total	C	N	O	0	0
			322	204	68	50		

- Molecule 63 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lq	207	Total	C	N	O	S	0	0
			1600	1016	285	291	8		

- Molecule 64 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

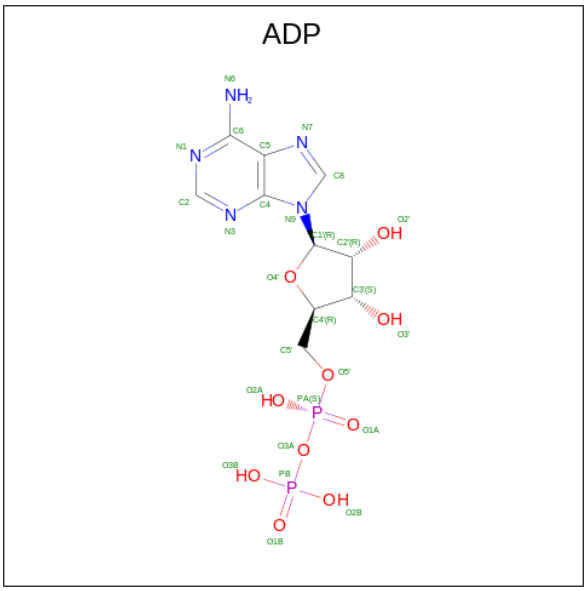


Mol	Chain	Residues	Atoms					AltConf
64	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
65	CQ	1	Total	Zn	0
			1	1	
65	Lj	1	Total	Zn	0
			1	1	
65	Lp	1	Total	Zn	0
			1	1	

- Molecule 66 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
66	CW	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

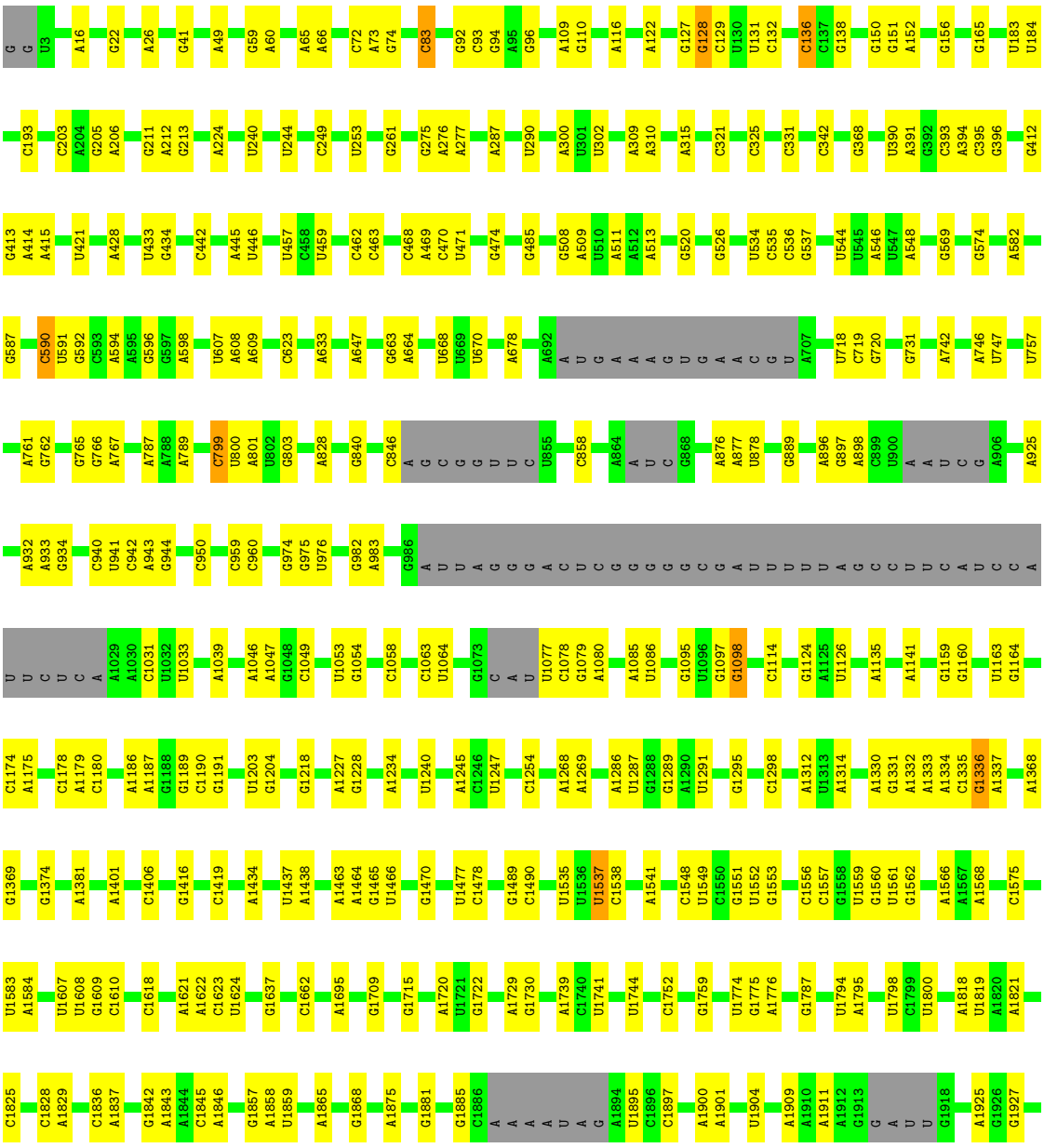
Mol	Chain	Residues	Atoms		AltConf
67	CW	1	Total	Mg	0
			1	1	

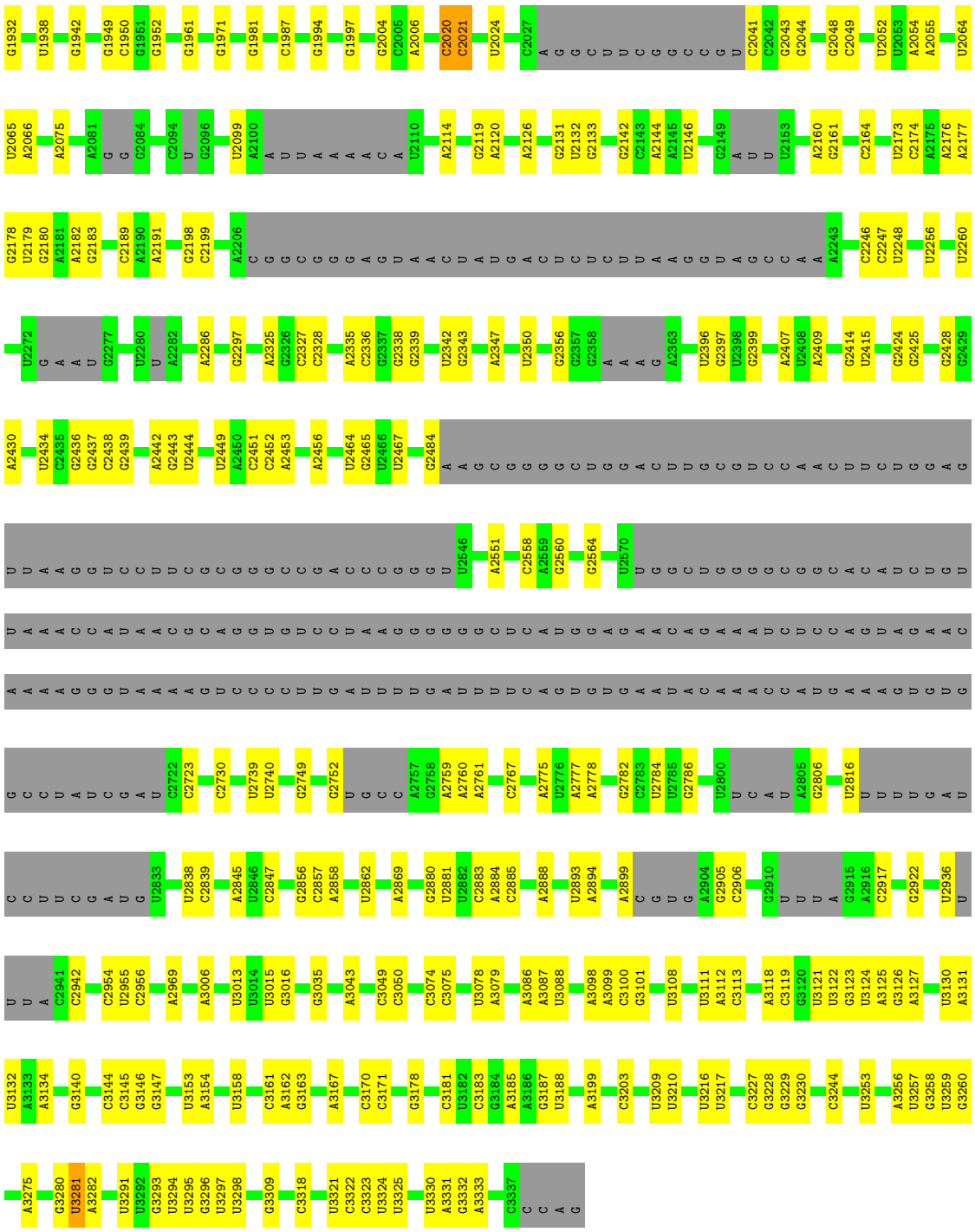
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: RNA (3341-MER)

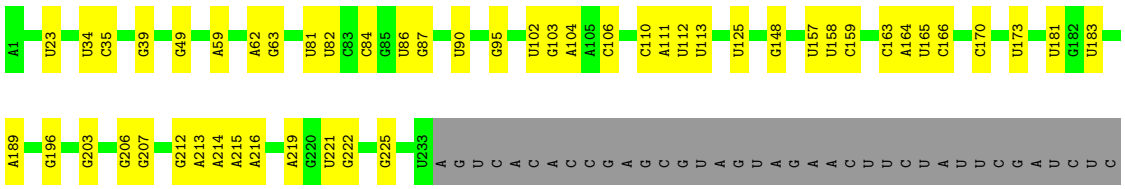
Chain C1:





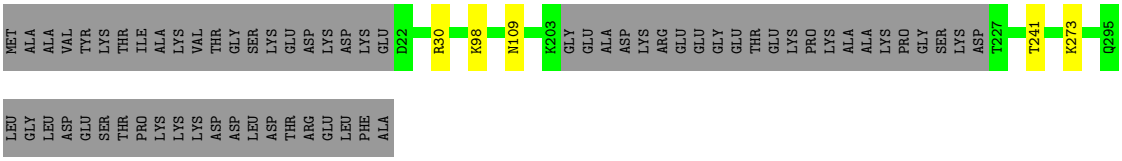
• Molecule 2: RNA (319-MER)

Chain C2:



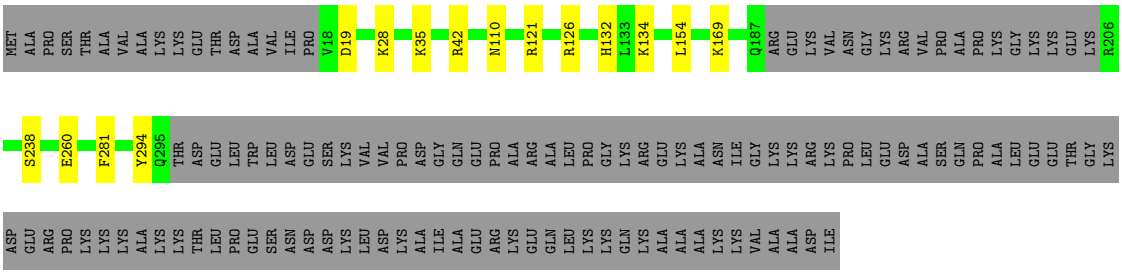
• Molecule 3: Brix domain-containing protein

Chain CA:



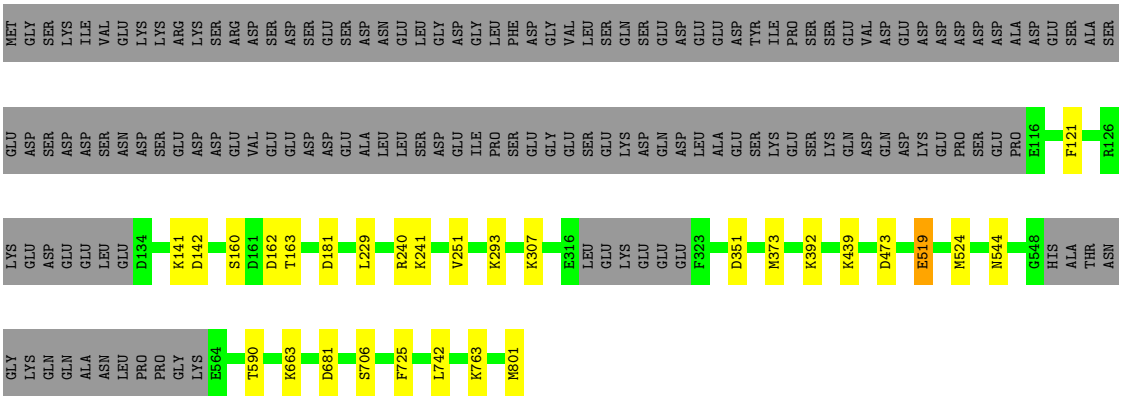
• Molecule 4: Ribosome biogenesis protein C8F11.04

Chain CB:



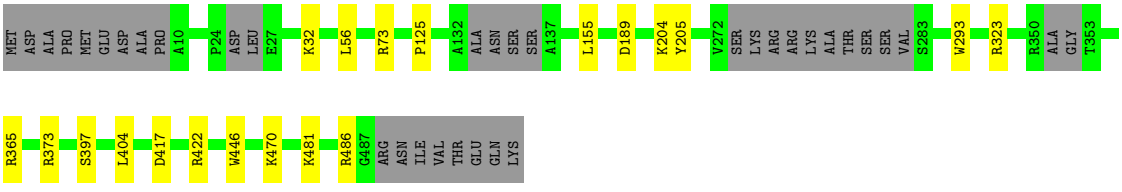
• Molecule 5: Ribosome biogenesis protein ERB1

Chain CC:



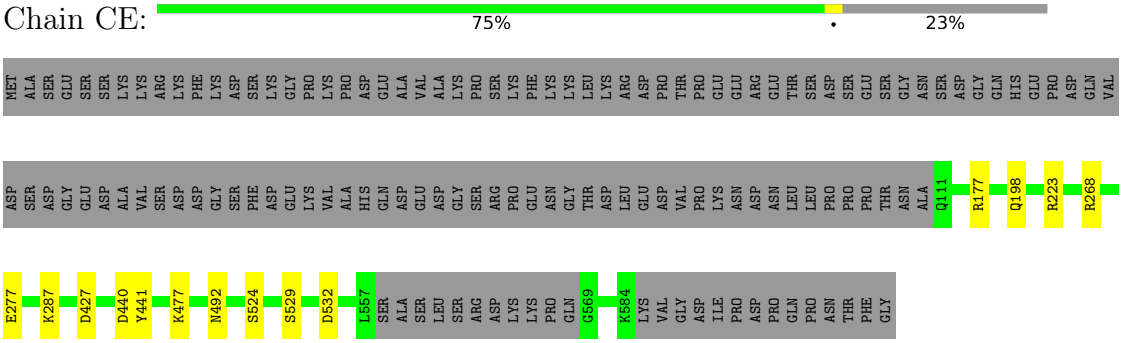
• Molecule 6: Ribosome biogenesis protein YTM1

Chain CD:



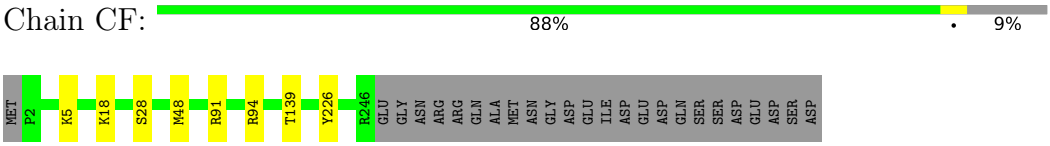
• Molecule 7: RNA helicase

Chain CE:



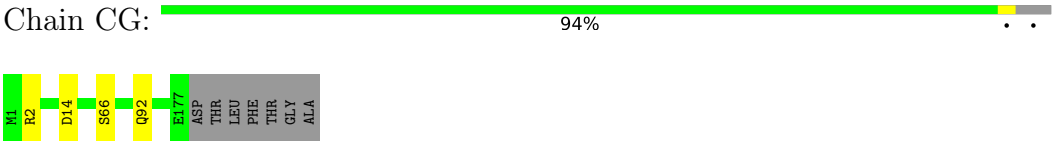
• Molecule 8: Ribosome assembly factor mrt4

Chain CF:



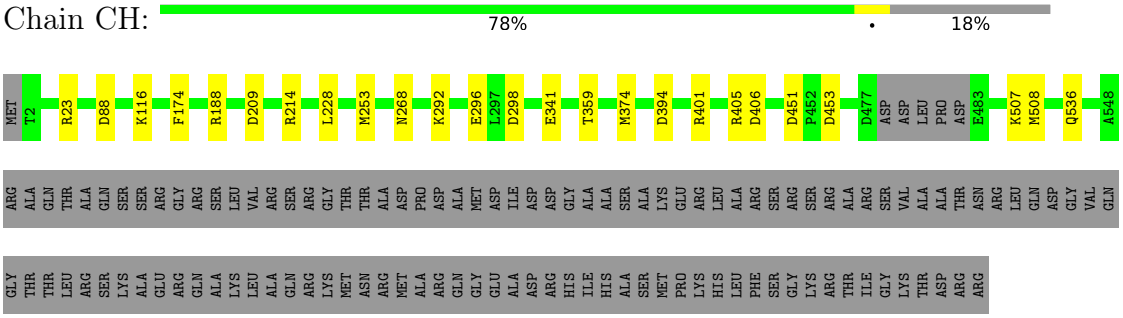
• Molecule 9: 60S ribosome subunit biogenesis protein NIP7

Chain CG:



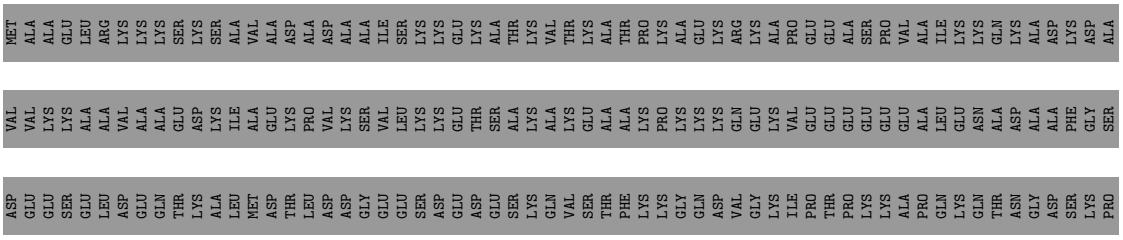
• Molecule 10: Nucleolar GTP-binding protein 1

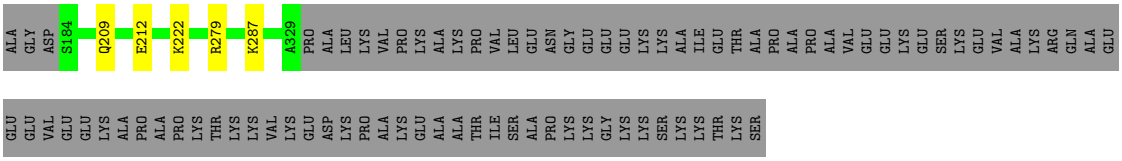
Chain CH:



• Molecule 11: Putative RNA-binding protein

Chain CI:



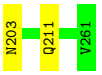


• Molecule 12: Pescadillo homolog

Chain CJ:

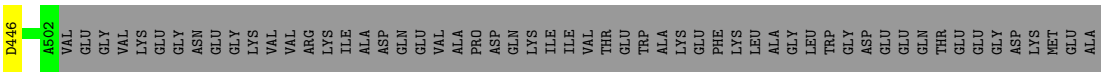
• Molecule 13: Ribosome biogenesis protein NSA2 homolog

Chain CK:



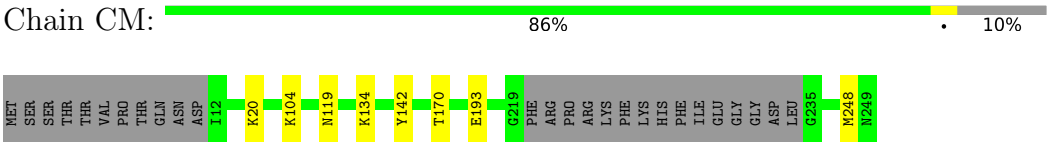
• Molecule 14: Putative GTP binding protein

Chain CL:



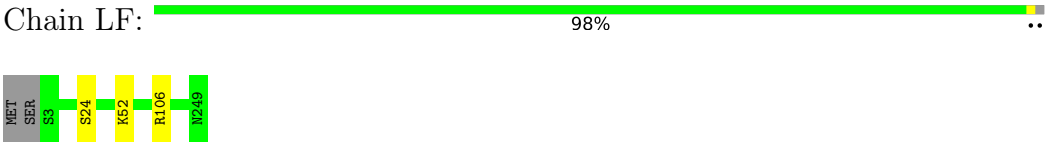
• Molecule 15: 60S ribosomal protein l7-like protein

Chain CM:



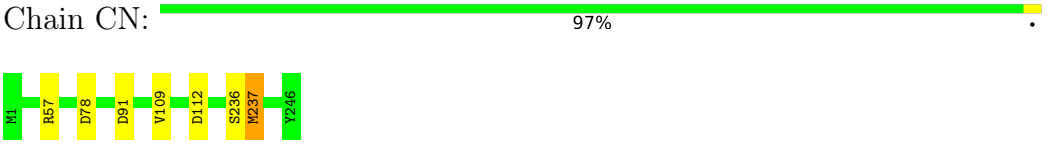
• Molecule 15: 60S ribosomal protein l7-like protein

Chain LF:



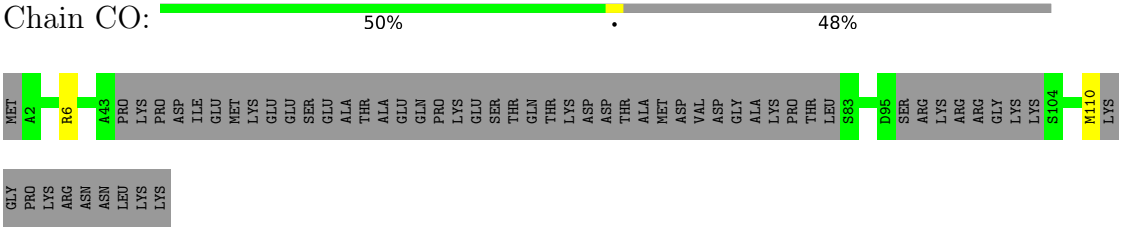
• Molecule 16: Eukaryotic translation initiation factor 6

Chain CN:



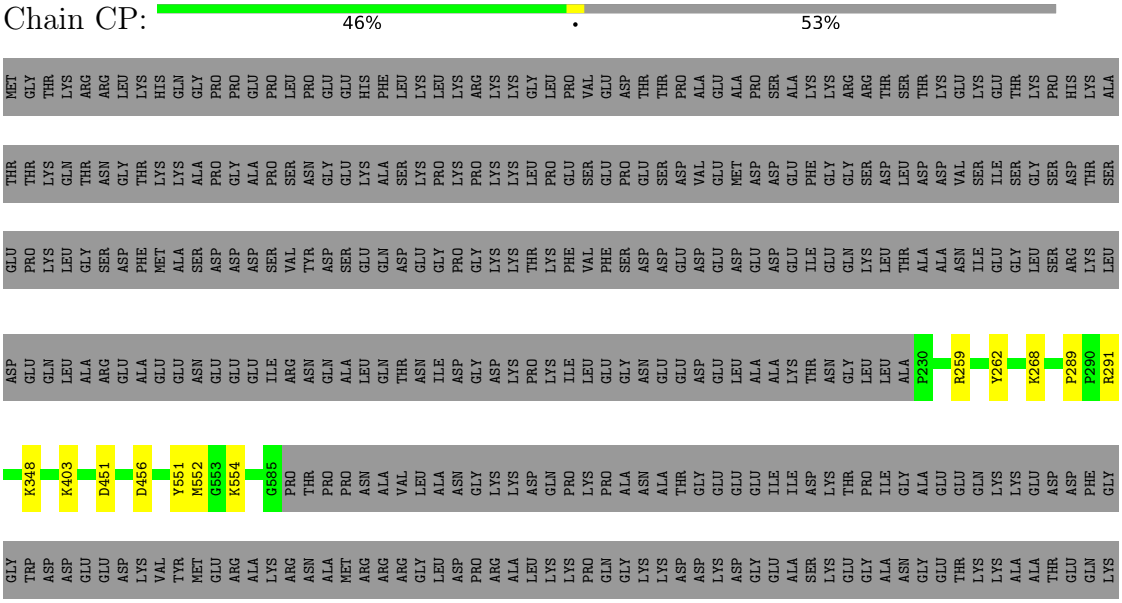
• Molecule 17: DUF2423 domain-containing protein

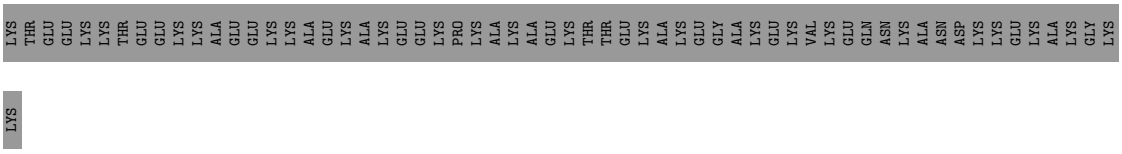
Chain CO:



• Molecule 18: RNA methyltransferase nop2-like protein

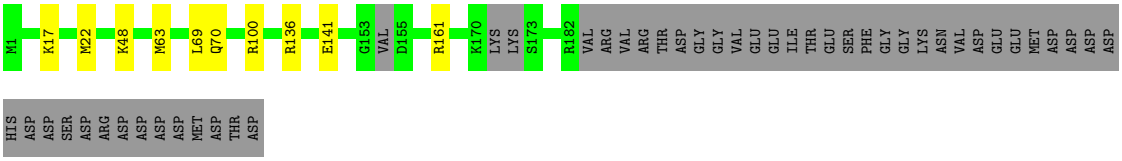
Chain CP:





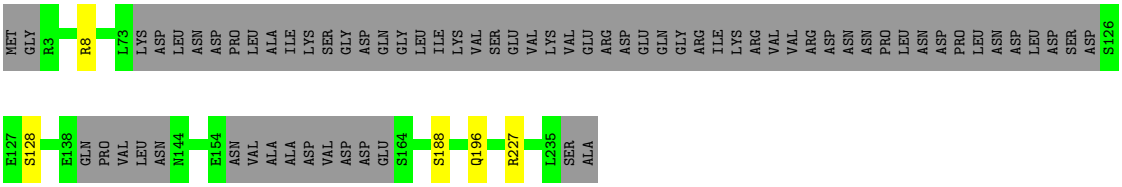
• Molecule 19: Ribosome biogenesis protein RLP24

Chain CQ:



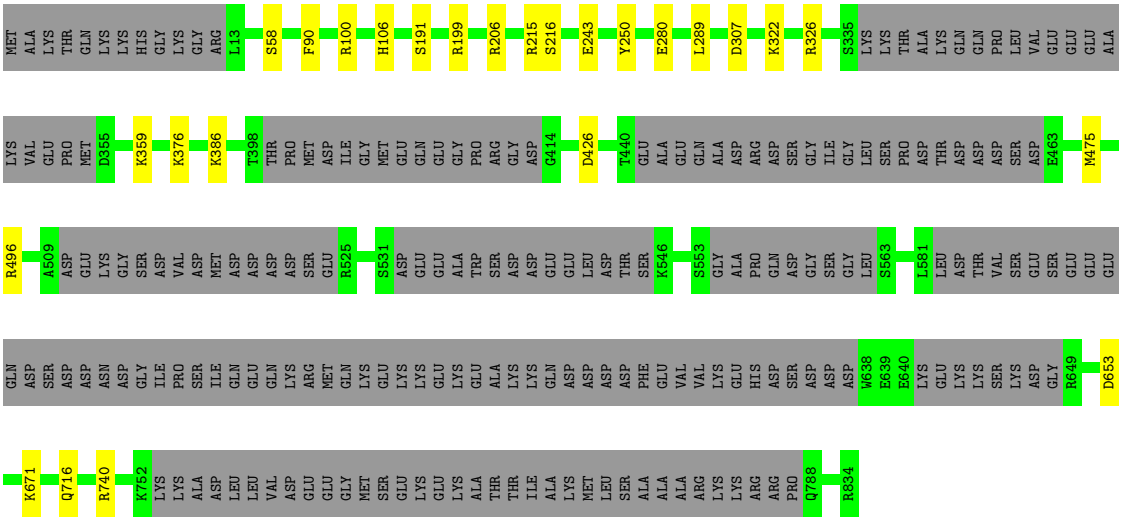
• Molecule 20: Nucleolar protein 16

Chain CR:



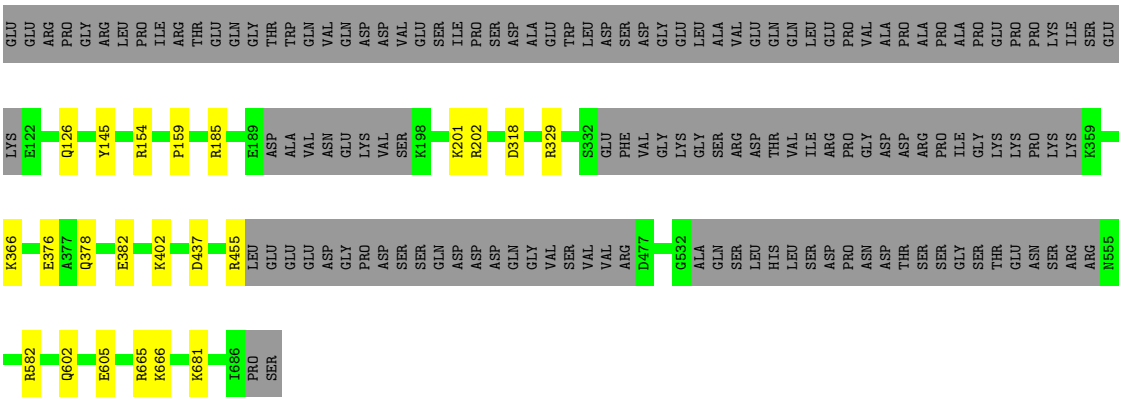
• Molecule 21: AdoMet-dependent rRNA methyltransferase SPB1

Chain CS:



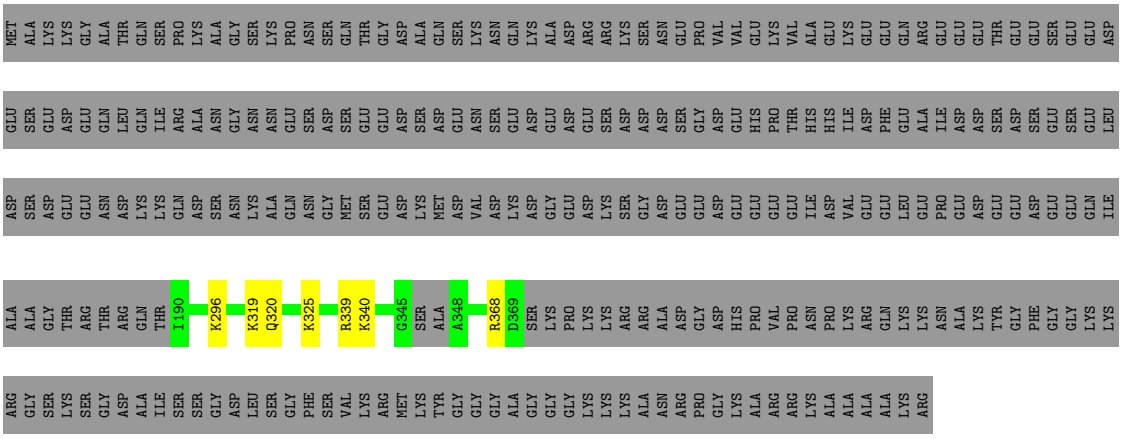
• Molecule 22: Nucleolar complex-associated protein 3

Chain CT:



• Molecule 23: rRNA-processing protein EBP2

Chain CU:

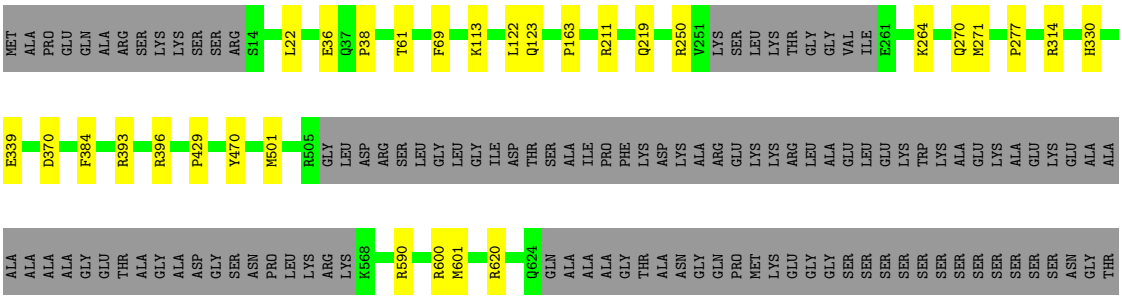


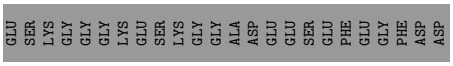
• Molecule 24: Putative 60S ribosomal protein

Chain CV:

• Molecule 25: ATP-dependent RNA helicase

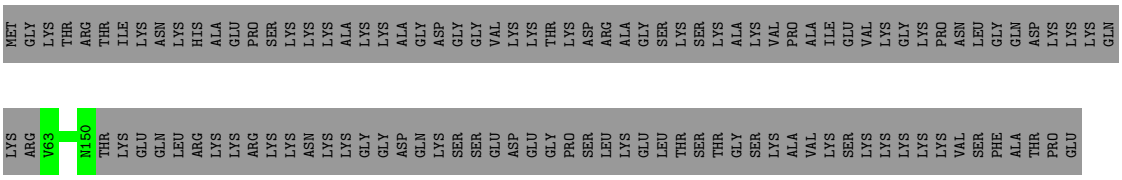
Chain CW:





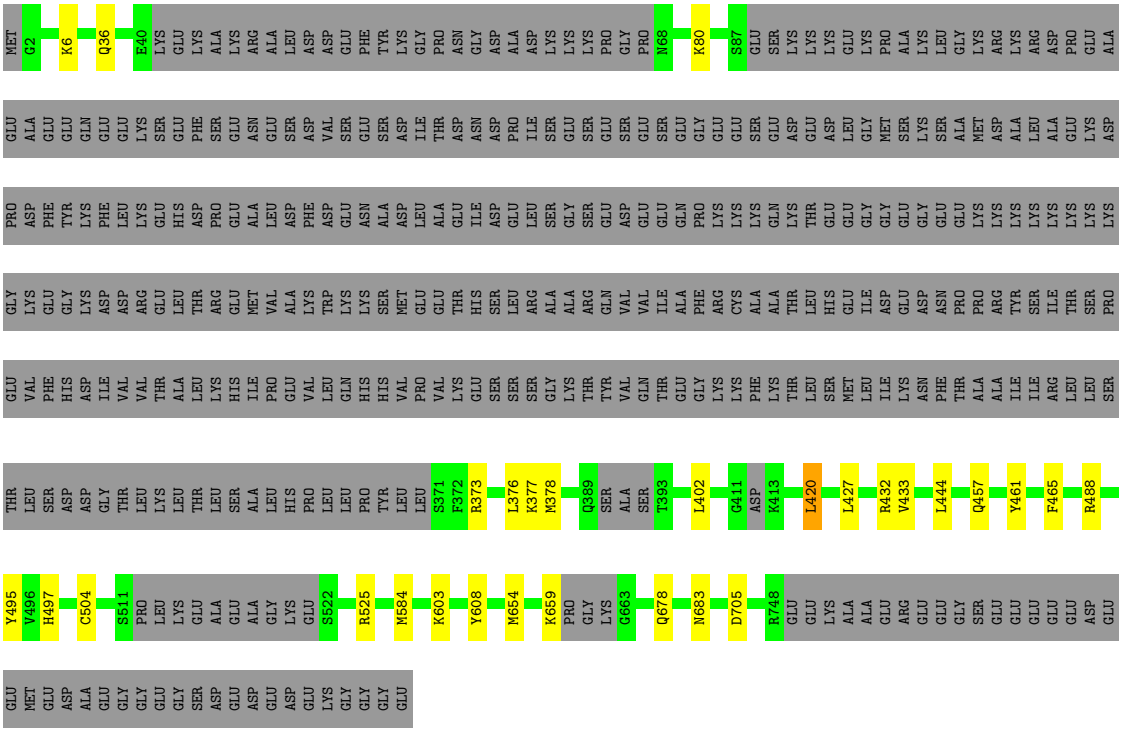
• Molecule 26: 60S ribosomal subunit-like protein

Chain CX:



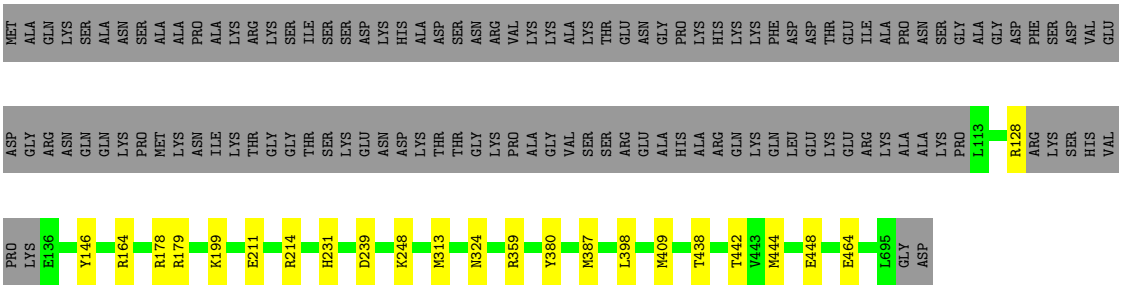
• Molecule 27: Putative NOC2 family protein

Chain CY:



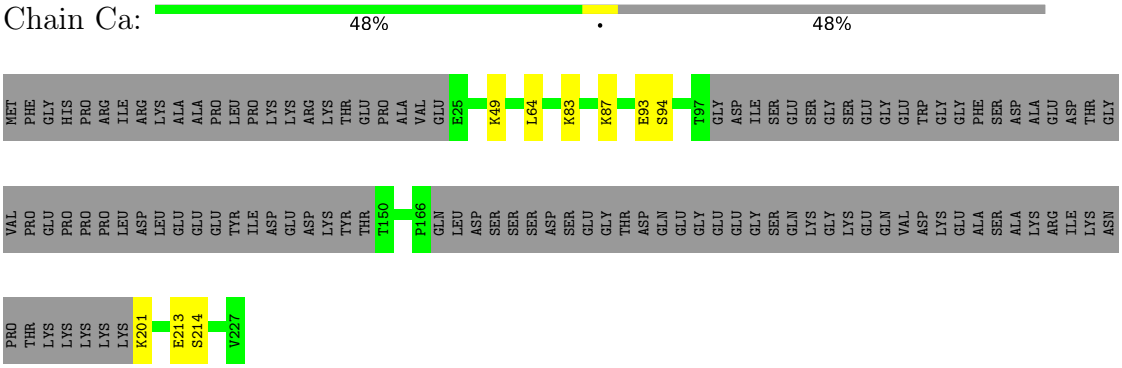
• Molecule 28: PUM-HD domain-containing protein

Chain CZ:



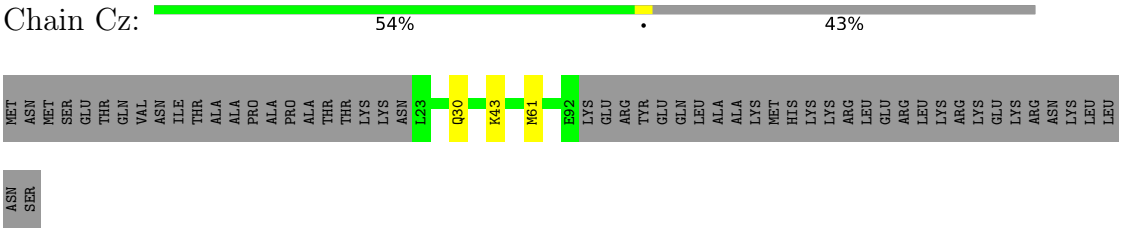
• Molecule 29: Nucleolar protein 12

Chain Ca:



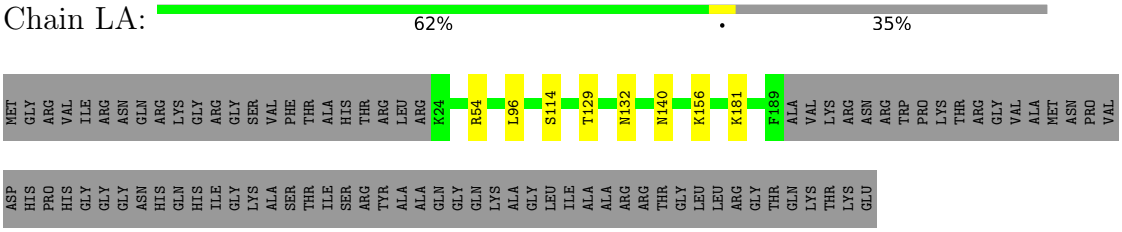
• Molecule 30: rRNA-processing protein

Chain Cz:



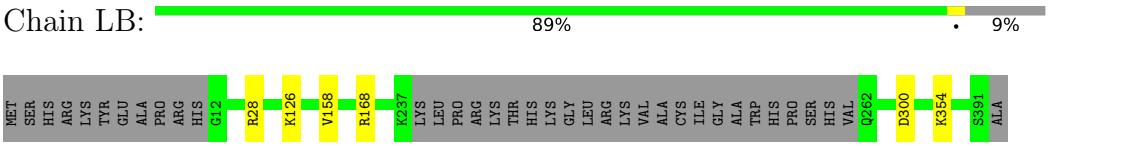
• Molecule 31: 60S ribosomal protein L2-like protein

Chain LA:



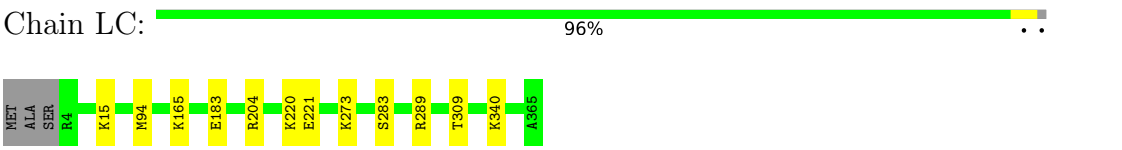
• Molecule 32: 60S ribosomal protein L3-like protein

Chain LB:



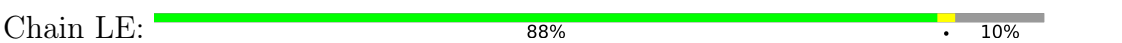
• Molecule 33: 60S ribosomal protein L4-like protein

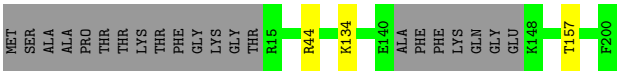
Chain LC:



• Molecule 34: 60S ribosomal protein L6

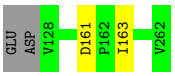
Chain LE:





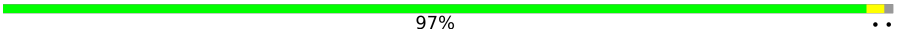
• Molecule 35: 60S ribosomal protein L8

Chain LG:



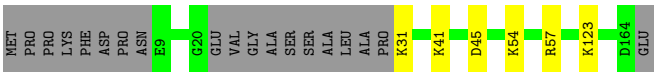
• Molecule 36: 60S ribosomal protein l9-like protein

Chain LH:



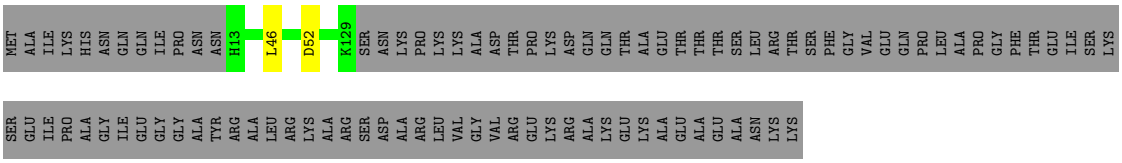
• Molecule 37: 60S ribosomal protein L12-like protein

Chain LK:



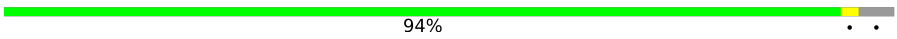
• Molecule 38: 60S ribosomal protein L13

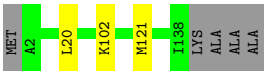
Chain LL:



• Molecule 39: 60S ribosomal protein L14-like protein

Chain LM:



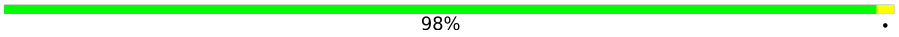


• Molecule 40: Ribosomal protein L15

Chain LN:

• Molecule 41: 60S ribosomal protein L16-like protein

Chain LO:

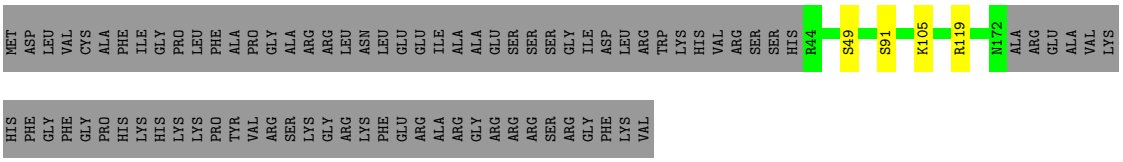


• Molecule 42: 60S ribosomal protein l17-like protein

Chain LP:

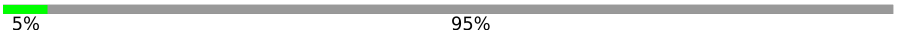
• Molecule 43: Ribosomal protein L18-like protein

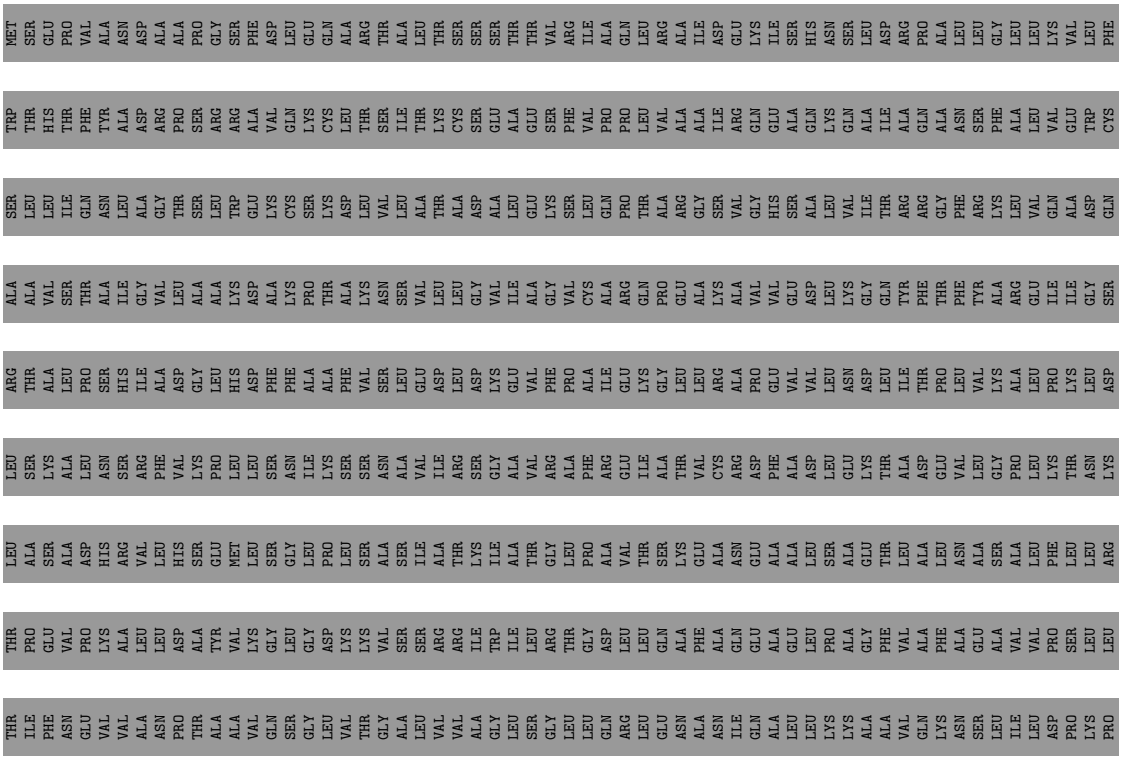
Chain LQ:

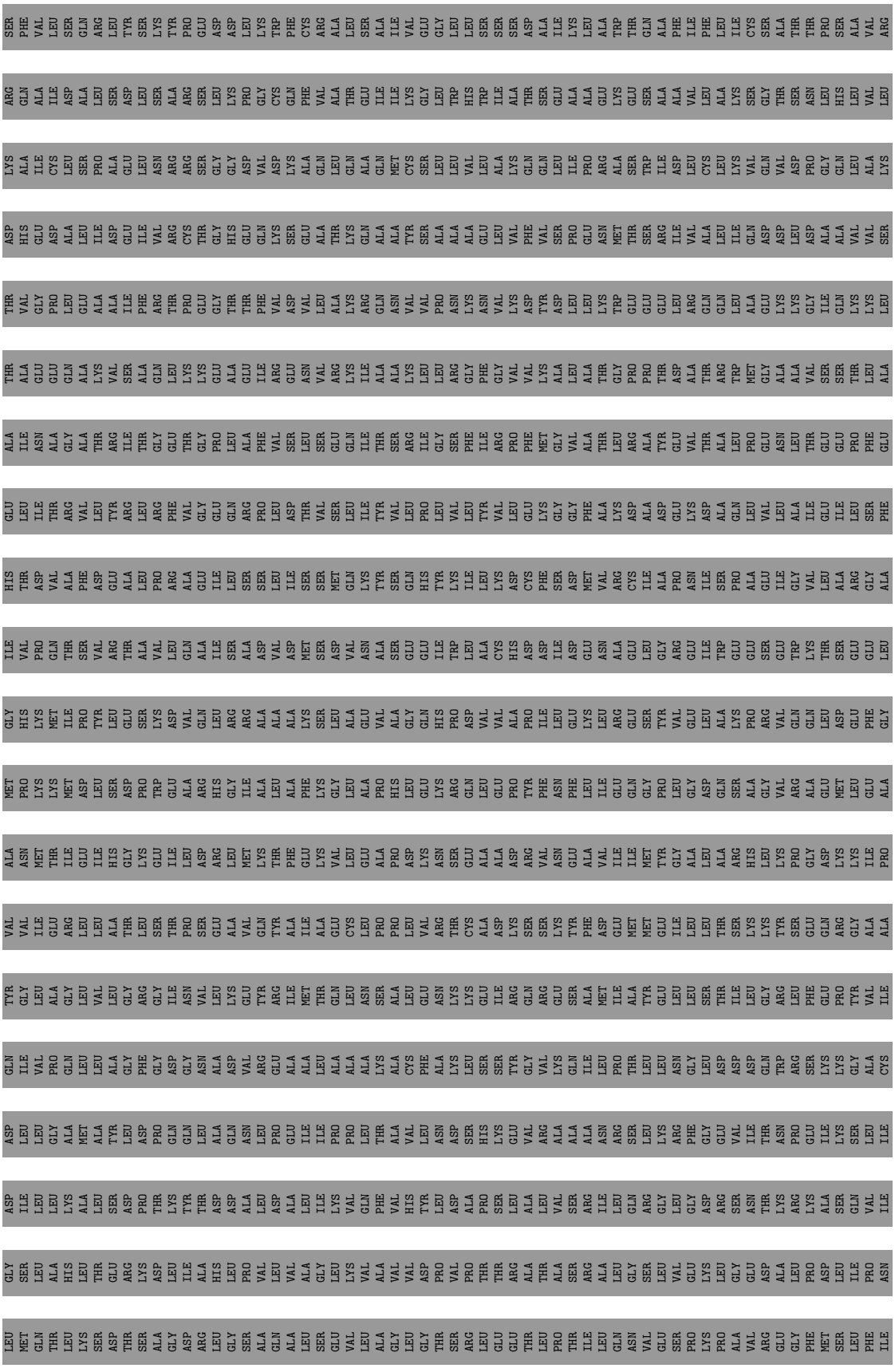


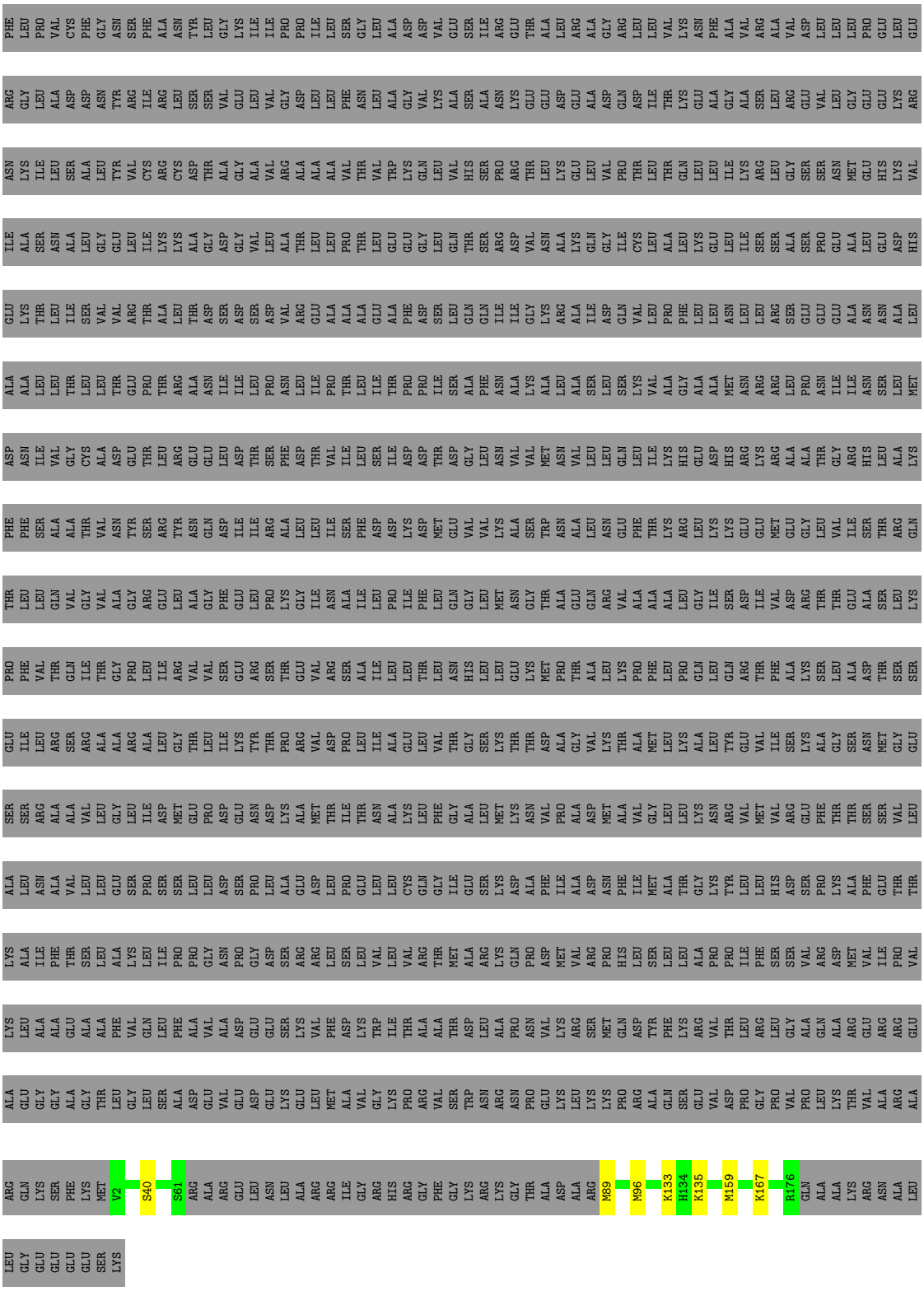
• Molecule 44: Ribosomal protein L19

Chain LR:



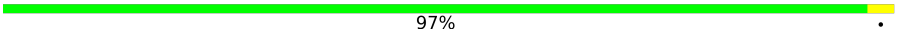


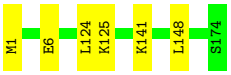




• Molecule 45: 60S ribosomal protein L20

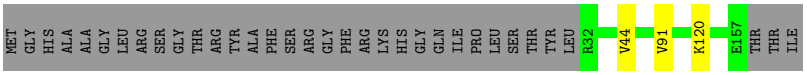
Chain LS:





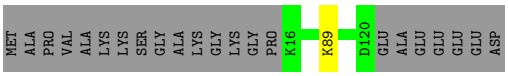
• Molecule 46: 60S ribosomal protein l21-like protein

Chain LT:



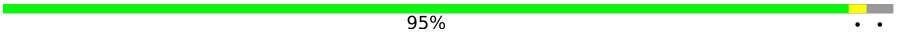
• Molecule 47: 60S ribosomal protein L22-like protein

Chain LU:



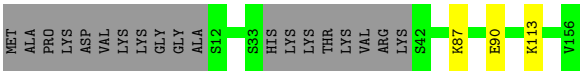
• Molecule 48: 60S ribosomal protein l23-like protein

Chain LV:



• Molecule 49: 60S ribosomal protein L25-like protein

Chain LX:

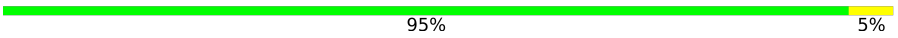


• Molecule 50: 60S ribosomal protein L26-like protein

Chain LY:

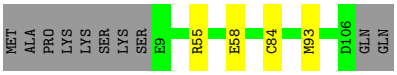
• Molecule 51: 60S ribosomal protein L27

Chain LZ:



• Molecule 52: 60S ribosomal protein l30-like protein

Chain Lc:

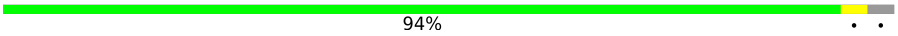


• Molecule 53: Putative 60S ribosomal protein

Chain Ld:

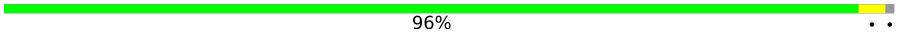
• Molecule 54: 60S ribosomal protein L32-like protein

Chain Le:



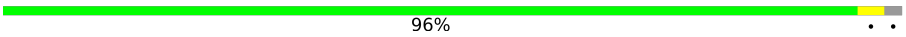
• Molecule 55: 60S ribosomal protein l33-like protein

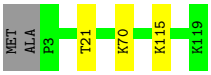
Chain Lf:



• Molecule 56: Ribosomal protein l34-like protein

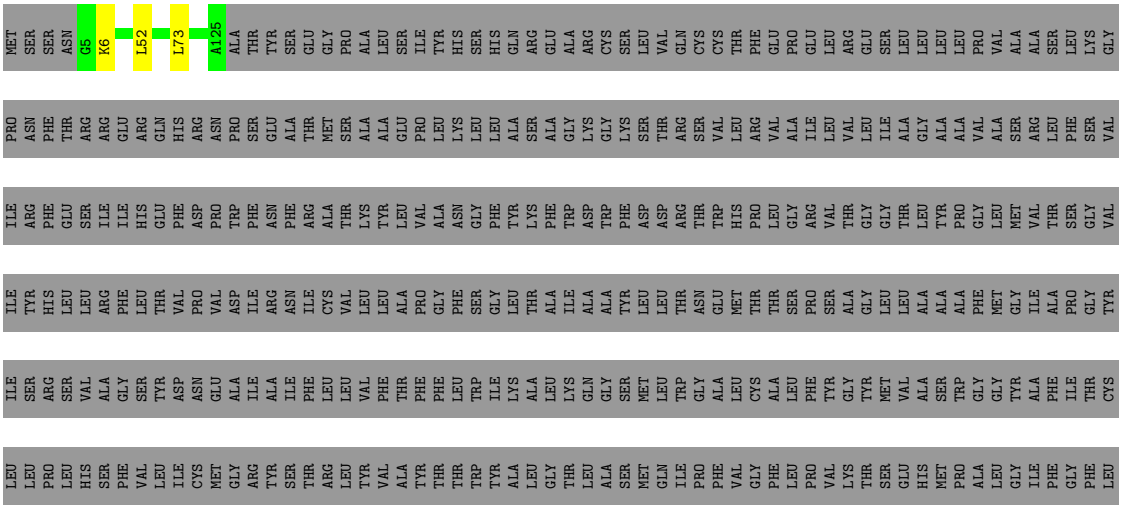
Chain Lg:

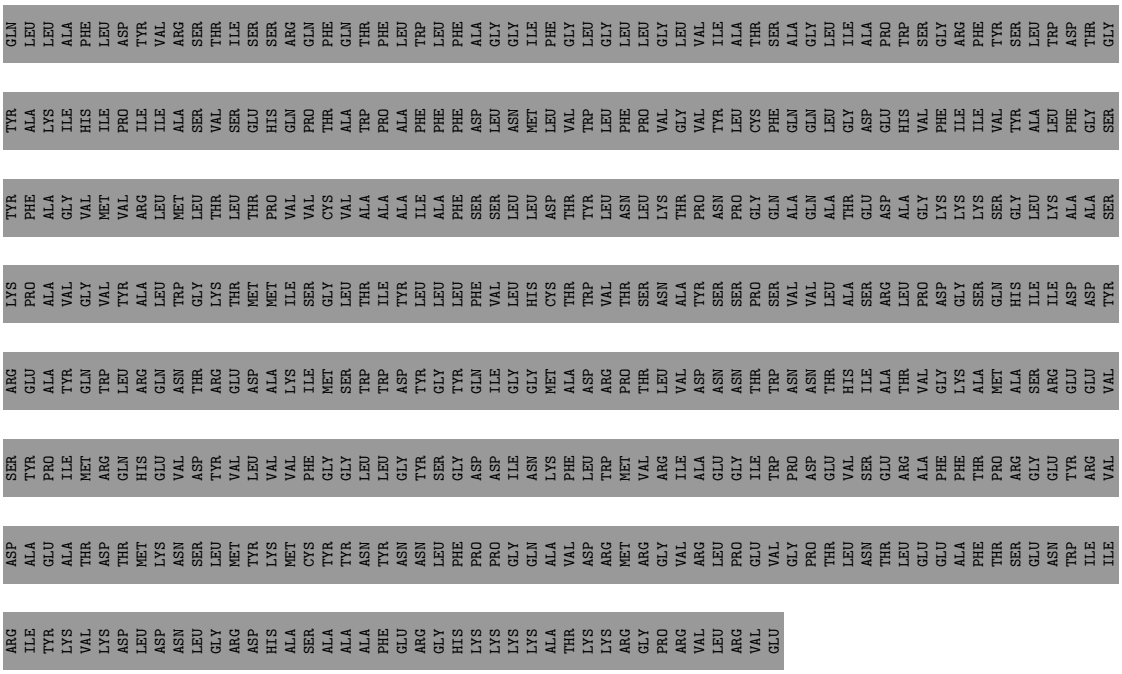




• Molecule 57: dolichyl-diphosphooligosaccharide--protein glycotransferase

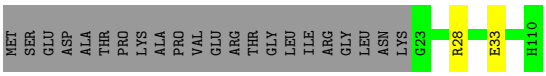
Chain Lh:





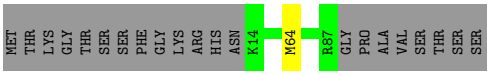
• Molecule 58: 60S ribosomal protein L36

Chain Li:



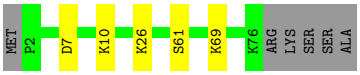
• Molecule 59: Ribosomal protein L37

Chain Lj:



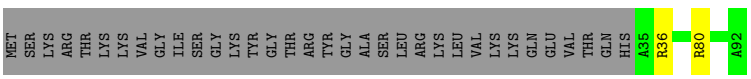
• Molecule 60: 60S ribosomal protein L38-like protein

Chain Lk:



• Molecule 61: 60S ribosomal protein L43-like protein

Chain Lp:

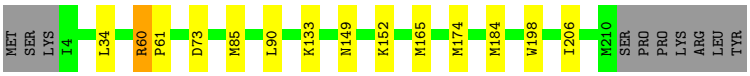


• Molecule 62: 60S ribosomal protein L39

Chain Ll:

• Molecule 63: Ribosomal protein

Chain Lq:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GTP, ADP, TPO, SEP

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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C1	0.28	0/70087	0.82	60/109235 (0.1%)
2	C2	0.25	0/6097	0.77	1/9499 (0.0%)
3	CA	0.26	0/2115	0.51	0/2840
4	CB	0.27	0/2109	0.56	0/2866
5	CC	0.27	0/5423	0.51	0/7380
6	CD	0.26	0/3543	0.60	2/4824 (0.0%)
7	CE	0.27	0/3743	0.53	1/5045 (0.0%)
8	CF	0.26	0/1982	0.54	0/2671
9	CG	0.26	0/1422	0.50	0/1920
10	CH	0.27	0/4468	0.50	1/6029 (0.0%)
11	CI	0.27	0/1225	0.54	0/1645
12	CJ	0.28	0/4125	0.52	0/5548
13	CK	0.26	0/1863	0.51	0/2494
14	CL	0.26	0/2247	0.49	0/3076
15	CM	0.27	0/1851	0.51	0/2481
15	LF	0.26	0/2055	0.49	0/2758
16	CN	0.26	0/1881	0.55	2/2560 (0.1%)
17	CO	0.25	0/470	0.50	0/619
18	CP	0.29	0/2859	0.59	1/3870 (0.0%)
19	CQ	0.28	0/1507	0.59	0/1996
20	CR	0.25	0/1369	0.54	0/1828
21	CS	0.27	0/5162	0.54	0/6904
22	CT	0.27	0/3974	0.52	2/5357 (0.0%)
23	CU	0.26	0/1428	0.51	0/1910
24	CV	0.26	0/1091	0.51	0/1468
25	CW	0.32	0/4397	0.65	3/5951 (0.1%)
26	CX	0.24	0/705	0.48	0/938
27	CY	0.28	0/3470	0.61	2/4659 (0.0%)
28	CZ	0.27	0/4025	0.52	1/5467 (0.0%)
29	Ca	0.27	0/988	0.56	0/1302
30	Cz	0.25	0/598	0.52	0/785
31	LA	0.28	0/1286	0.57	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LB	0.27	0/2885	0.53	0/3872
33	LC	0.26	0/2809	0.50	0/3787
34	LE	0.26	0/1428	0.49	0/1921
35	LG	0.26	0/1674	0.47	0/2240
36	LH	0.27	0/1516	0.51	0/2038
37	LK	0.25	0/1124	0.55	0/1507
38	LL	0.25	0/983	0.58	0/1318
39	LM	0.25	0/1120	0.52	0/1507
40	LN	0.26	0/1595	0.56	0/2132
41	LO	0.27	0/1652	0.52	0/2215
42	LP	0.24	0/1367	0.53	0/1838
43	LQ	0.25	0/1033	0.55	0/1391
44	LR	0.25	0/1235	0.53	0/1644
45	LS	0.27	0/1468	0.51	0/1975
46	LT	0.26	0/1033	0.56	0/1389
47	LU	0.26	0/863	0.46	0/1155
48	LV	0.28	0/1013	0.49	0/1361
49	LX	0.24	0/1078	0.47	0/1451
50	LY	0.24	0/1079	0.53	0/1443
51	LZ	0.27	0/1135	0.53	0/1519
52	Lc	0.25	0/740	0.47	0/995
53	Ld	0.26	0/904	0.53	0/1209
54	Le	0.25	0/1043	0.53	0/1389
55	Lf	0.28	0/883	0.57	0/1187
56	Lg	0.25	0/943	0.56	0/1258
57	Lh	0.24	0/1006	0.50	0/1338
58	Li	0.25	0/738	0.56	0/971
59	Lj	0.26	0/606	0.59	0/803
60	Lk	0.26	0/628	0.54	0/835
61	Lp	0.24	0/441	0.60	0/590
62	Ll	0.23	0/329	0.51	0/440
63	Lq	0.27	0/1621	0.62	0/2180
All	All	0.27	0/187537	0.67	76/268557 (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
5	CC	0	1
63	Lq	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	CP	289	PRO	CA-N-CD	-12.12	94.54	111.50
22	CT	159	PRO	CA-N-CD	-11.33	95.64	111.50
1	C1	136	C	N3-C2-O2	-9.16	115.49	121.90
1	C1	2452	C	N3-C2-O2	-9.16	115.49	121.90
1	C1	2021	C	N3-C2-O2	-9.01	115.59	121.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	CC	519	GLU	Peptide
63	Lq	60	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	CA	247/316 (78%)	232 (94%)	15 (6%)	0	100	100
4	CB	256/391 (66%)	239 (93%)	17 (7%)	0	100	100
5	CC	648/801 (81%)	623 (96%)	24 (4%)	1 (0%)	44	68
6	CD	450/495 (91%)	425 (94%)	25 (6%)	0	100	100
7	CE	459/598 (77%)	449 (98%)	10 (2%)	0	100	100
8	CF	243/270 (90%)	234 (96%)	9 (4%)	0	100	100
9	CG	175/184 (95%)	165 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CH	538/661 (81%)	522 (97%)	16 (3%)	0	100	100
11	CI	144/414 (35%)	140 (97%)	4 (3%)	0	100	100
12	CJ	484/679 (71%)	473 (98%)	11 (2%)	0	100	100
13	CK	223/261 (85%)	214 (96%)	9 (4%)	0	100	100
14	CL	393/558 (70%)	368 (94%)	23 (6%)	2 (0%)	25	49
15	CM	219/249 (88%)	212 (97%)	7 (3%)	0	100	100
15	LF	245/249 (98%)	237 (97%)	8 (3%)	0	100	100
16	CN	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	354/751 (47%)	336 (95%)	18 (5%)	0	100	100
19	CQ	173/225 (77%)	167 (96%)	6 (4%)	0	100	100
20	CR	159/237 (67%)	158 (99%)	1 (1%)	0	100	100
21	CS	609/834 (73%)	584 (96%)	25 (4%)	0	100	100
22	CT	478/688 (70%)	461 (96%)	17 (4%)	0	100	100
23	CU	174/451 (39%)	170 (98%)	4 (2%)	0	100	100
24	CV	137/147 (93%)	135 (98%)	2 (2%)	0	100	100
25	CW	534/679 (79%)	479 (90%)	54 (10%)	1 (0%)	44	68
26	CX	86/203 (42%)	85 (99%)	1 (1%)	0	100	100
27	CY	406/788 (52%)	380 (94%)	25 (6%)	1 (0%)	44	68
28	CZ	572/697 (82%)	552 (96%)	20 (4%)	0	100	100
29	Ca	111/227 (49%)	109 (98%)	2 (2%)	0	100	100
30	Cz	68/123 (55%)	66 (97%)	2 (3%)	0	100	100
31	LA	164/254 (65%)	155 (94%)	9 (6%)	0	100	100
32	LB	352/392 (90%)	335 (95%)	17 (5%)	0	100	100
33	LC	360/365 (99%)	346 (96%)	14 (4%)	0	100	100
34	LE	175/200 (88%)	169 (97%)	6 (3%)	0	100	100
35	LG	201/262 (77%)	197 (98%)	4 (2%)	0	100	100
36	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
37	LK	142/165 (86%)	136 (96%)	6 (4%)	0	100	100
38	LL	115/213 (54%)	112 (97%)	3 (3%)	0	100	100
39	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	LN	179/203 (88%)	170 (95%)	9 (5%)	0	100	100
41	LO	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
42	LP	165/187 (88%)	160 (97%)	5 (3%)	0	100	100
43	LQ	127/213 (60%)	121 (95%)	6 (5%)	0	100	100
44	LR	144/2898 (5%)	143 (99%)	1 (1%)	0	100	100
45	LS	172/174 (99%)	165 (96%)	7 (4%)	0	100	100
46	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	16	38
47	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
48	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
49	LX	133/156 (85%)	131 (98%)	2 (2%)	0	100	100
50	LY	132/138 (96%)	127 (96%)	5 (4%)	0	100	100
51	LZ	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
52	Lc	96/108 (89%)	96 (100%)	0	0	100	100
53	Ld	107/120 (89%)	105 (98%)	2 (2%)	0	100	100
54	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100
55	Lf	106/109 (97%)	104 (98%)	2 (2%)	0	100	100
56	Lg	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
57	Lh	119/935 (13%)	116 (98%)	3 (2%)	0	100	100
58	Li	86/110 (78%)	86 (100%)	0	0	100	100
59	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
60	Lk	73/81 (90%)	68 (93%)	5 (7%)	0	100	100
61	Lp	56/92 (61%)	52 (93%)	4 (7%)	0	100	100
62	Ll	36/51 (71%)	35 (97%)	1 (3%)	0	100	100
63	Lq	205/217 (94%)	183 (89%)	21 (10%)	1 (0%)	25	49
All	All	13660/21629 (63%)	13103 (96%)	550 (4%)	7 (0%)	50	73

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	CW	393	ARG
27	CY	457	GLN
14	CL	439	ASP
14	CL	446	ASP
46	LT	44	VAL

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	CA	223/276 (81%)	218 (98%)	5 (2%)	47 76
4	CB	222/329 (68%)	207 (93%)	15 (7%)	13 32
5	CC	578/708 (82%)	552 (96%)	26 (4%)	23 50
6	CD	381/410 (93%)	363 (95%)	18 (5%)	22 49
7	CE	398/517 (77%)	385 (97%)	13 (3%)	33 62
8	CF	214/236 (91%)	206 (96%)	8 (4%)	29 58
9	CG	150/155 (97%)	146 (97%)	4 (3%)	40 69
10	CH	481/575 (84%)	457 (95%)	24 (5%)	20 46
11	CI	121/336 (36%)	116 (96%)	5 (4%)	26 54
12	CJ	428/579 (74%)	401 (94%)	27 (6%)	15 35
13	CK	195/225 (87%)	183 (94%)	12 (6%)	15 36
14	CL	72/458 (16%)	68 (94%)	4 (6%)	17 41
15	CM	191/215 (89%)	183 (96%)	8 (4%)	25 53
15	LF	213/215 (99%)	210 (99%)	3 (1%)	62 84
16	CN	206/206 (100%)	199 (97%)	7 (3%)	32 61
17	CO	48/99 (48%)	46 (96%)	2 (4%)	25 53
18	CP	302/632 (48%)	291 (96%)	11 (4%)	30 59
19	CQ	150/192 (78%)	140 (93%)	10 (7%)	13 33
20	CR	144/206 (70%)	139 (96%)	5 (4%)	31 60
21	CS	532/716 (74%)	506 (95%)	26 (5%)	21 47
22	CT	427/600 (71%)	407 (95%)	20 (5%)	22 49
23	CU	149/376 (40%)	142 (95%)	7 (5%)	22 49
24	CV	109/112 (97%)	104 (95%)	5 (5%)	23 49
25	CW	476/577 (82%)	450 (94%)	26 (6%)	18 41
26	CX	76/172 (44%)	76 (100%)	0	100 100
27	CY	369/686 (54%)	342 (93%)	27 (7%)	11 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	CZ	310/581 (53%)	288 (93%)	22 (7%)	12	30
29	Ca	101/195 (52%)	92 (91%)	9 (9%)	8	20
30	Cz	60/107 (56%)	57 (95%)	3 (5%)	20	46
31	LA	131/198 (66%)	123 (94%)	8 (6%)	15	36
32	LB	301/331 (91%)	295 (98%)	6 (2%)	50	78
33	LC	283/285 (99%)	271 (96%)	12 (4%)	25	53
34	LE	151/166 (91%)	148 (98%)	3 (2%)	50	78
35	LG	176/222 (79%)	172 (98%)	4 (2%)	45	74
36	LH	167/169 (99%)	163 (98%)	4 (2%)	44	73
37	LK	121/136 (89%)	115 (95%)	6 (5%)	20	46
38	LL	99/176 (56%)	97 (98%)	2 (2%)	50	78
39	LM	115/117 (98%)	112 (97%)	3 (3%)	41	70
40	LN	164/180 (91%)	157 (96%)	7 (4%)	25	52
41	LO	163/163 (100%)	158 (97%)	5 (3%)	35	64
42	LP	137/152 (90%)	134 (98%)	3 (2%)	47	76
43	LQ	110/178 (62%)	106 (96%)	4 (4%)	30	59
44	LR	128/2396 (5%)	121 (94%)	7 (6%)	18	41
45	LS	154/154 (100%)	148 (96%)	6 (4%)	27	56
46	LT	109/135 (81%)	107 (98%)	2 (2%)	54	80
47	LU	93/108 (86%)	92 (99%)	1 (1%)	70	87
48	LV	99/102 (97%)	96 (97%)	3 (3%)	36	65
49	LX	114/129 (88%)	111 (97%)	3 (3%)	41	70
50	LY	117/119 (98%)	110 (94%)	7 (6%)	16	38
51	LZ	121/121 (100%)	114 (94%)	7 (6%)	17	39
52	Lc	79/88 (90%)	75 (95%)	4 (5%)	20	45
53	Ld	95/105 (90%)	93 (98%)	2 (2%)	48	76
54	Le	110/114 (96%)	106 (96%)	4 (4%)	30	59
55	Lf	89/90 (99%)	86 (97%)	3 (3%)	32	61
56	Lg	101/102 (99%)	98 (97%)	3 (3%)	36	65
57	Lh	108/781 (14%)	105 (97%)	3 (3%)	38	68
58	Li	75/93 (81%)	73 (97%)	2 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
59	Lj	61/78 (78%)	60 (98%)	1 (2%)	58 82
60	Lk	71/76 (93%)	66 (93%)	5 (7%)	12 31
61	Lp	45/74 (61%)	43 (96%)	2 (4%)	24 51
62	Ll	34/46 (74%)	33 (97%)	1 (3%)	37 67
63	Lq	179/189 (95%)	166 (93%)	13 (7%)	11 29
All	All	11426/18264 (63%)	10928 (96%)	498 (4%)	26 51

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	CT	145	TYR
50	LY	10	SER
25	CW	601	MET
49	LX	87	LYS
57	Lh	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
25	CW	287	GLN
27	CY	494	GLN
28	CZ	394	HIS
28	CZ	139	GLN
5	CC	707	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2903/3341 (86%)	554 (19%)	22 (0%)
2	C2	254/319 (79%)	54 (21%)	1 (0%)
All	All	3157/3660 (86%)	608 (19%)	23 (0%)

5 of 608 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	16	A
1	C1	22	G
1	C1	26	A

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Mol	Chain	Res	Type
1	C1	41	G
1	C1	49	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	3162	A
1	C1	3229	G
1	C1	3216	U
1	C1	3257	U
1	C1	1077	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
5	TPO	CC	163	5	8,10,11	1.65	1 (12%)	10,14,16	1.12	1 (10%)
5	SEP	CC	160	5	8,9,10	1.52	1 (12%)	8,12,14	1.51	2 (25%)

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
5	TPO	CC	163	5	-	7/9/11/13	-
5	SEP	CC	160	5	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	CC	163	TPO	P-O1P	3.40	1.61	1.50
5	CC	160	SEP	P-O1P	3.32	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	CC	160	SEP	P-OG-CB	-2.88	110.36	118.30
5	CC	160	SEP	OG-CB-CA	2.53	110.61	108.14
5	CC	163	TPO	P-OG1-CB	-2.45	115.79	123.21

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	N-CA-CB-CG2
5	CC	163	TPO	N-CA-CB-OG1
5	CC	163	TPO	C-CA-CB-CG2
5	CC	163	TPO	O-C-CA-CB
5	CC	163	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
66	ADP	CW	1001	67	24,29,29	0.68	0	29,45,45	0.82	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
64	GTP	CH	1001	-	26,34,34	1.14	2 (7%)	32,54,54	1.49	7 (21%)

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
66	ADP	CW	1001	67	-	5/12/32/32	0/3/3/3
64	GTP	CH	1001	-	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	CH	1001	GTP	C5-C6	-4.03	1.39	1.47
64	CH	1001	GTP	C2-N3	2.03	1.38	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	CH	1001	GTP	C5-C6-N1	3.26	119.70	113.95
64	CH	1001	GTP	C8-N7-C5	3.04	108.78	102.99
64	CH	1001	GTP	C2-N1-C6	-2.83	119.88	125.10
64	CH	1001	GTP	PA-O3A-PB	-2.71	123.53	132.83
64	CH	1001	GTP	PB-O3B-PG	-2.69	123.60	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	CW	1001	ADP	C4'-C5'-O5'-PA
66	CW	1001	ADP	O4'-C4'-C5'-O5'
66	CW	1001	ADP	C3'-C4'-C5'-O5'
64	CH	1001	GTP	PB-O3A-PA-O1A
64	CH	1001	GTP	C3'-C4'-C5'-O5'

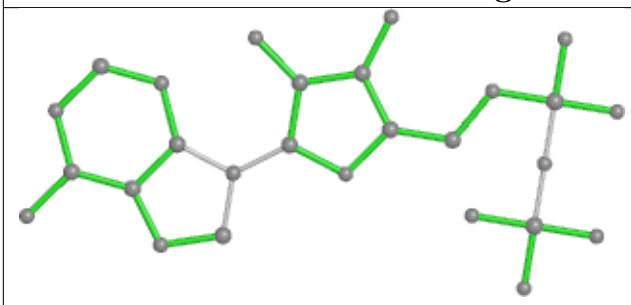
There are no ring outliers.

No monomer is involved in short contacts.

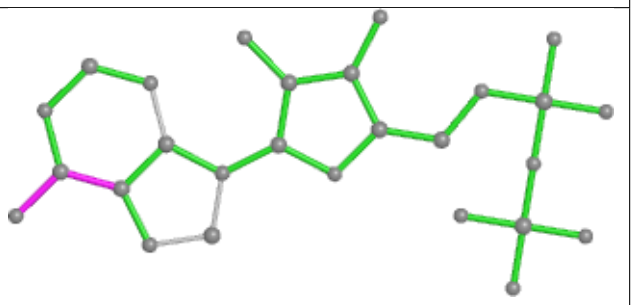
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

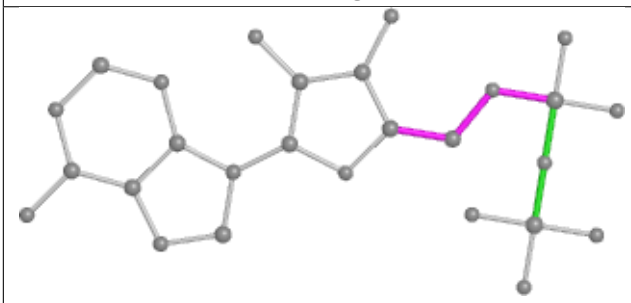
Ligand ADP CW 1001



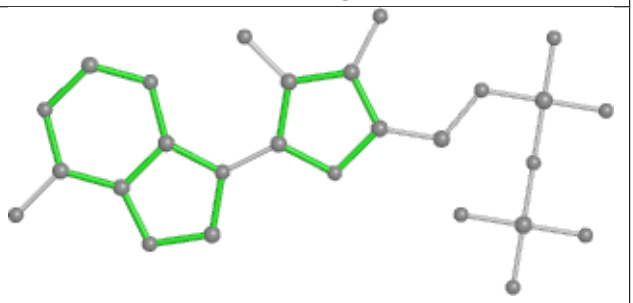
Bond lengths



Bond angles

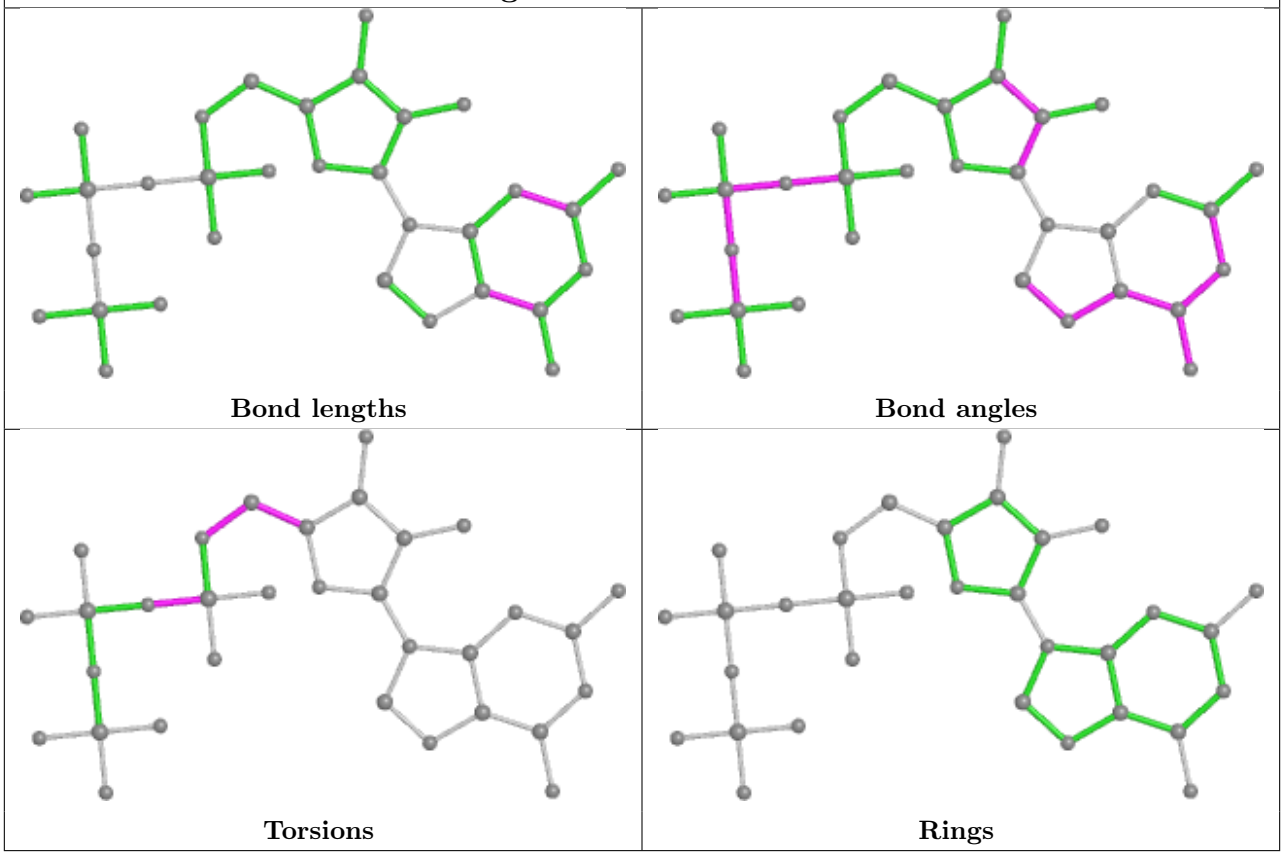


Torsions



Rings

Ligand GTP CH 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.