wwPDB EM Validation Summary Report

Nov 5, 2024 – 10:50 AM JST

PDB ID	:	8I9Y
EMDB ID	:	EMD-35288
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - Ytm1-2
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	3.10 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

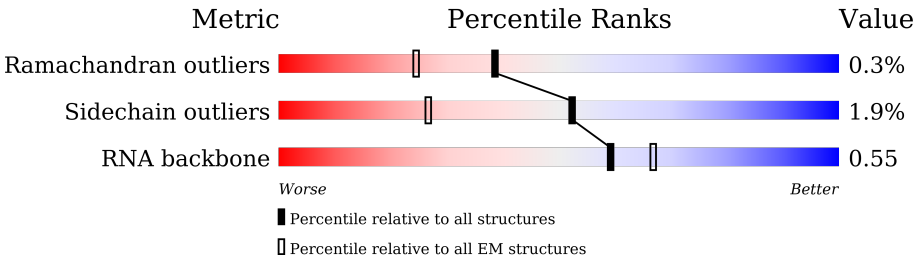
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	60% 18% 22%
2	C2	319	65% 16% 20%
3	CA	316	76% · 21%
4	CB	391	63% · 34%
5	CC	801	80% · 18%
6	CD	495	93% 7%
7	CE	598	74% · 23%
8	CF	270	89% · 9%
9	CG	184	94% · ·

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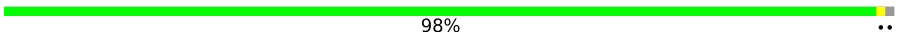
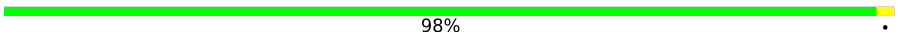
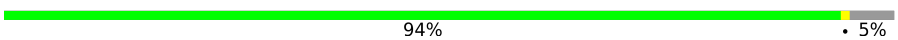
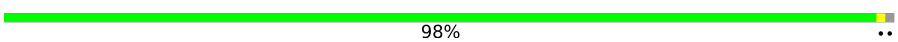
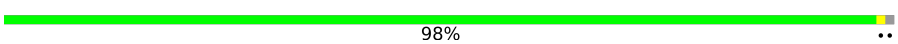
Mol	Chain	Length	Quality of chain
10	CH	661	
11	CI	414	
12	CJ	679	
13	CK	261	
14	CL	558	
15	CM	249	
15	LF	249	
16	CN	246	
17	CO	120	
18	CP	751	
19	CQ	225	
20	CR	237	
21	CS	834	
22	CT	688	
23	CU	451	
24	CV	147	
25	CX	203	
26	CY	788	
27	Cz	123	
28	LB	392	
29	LC	365	
30	LE	200	
31	LG	262	
32	LH	192	
33	LK	165	

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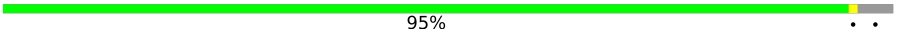
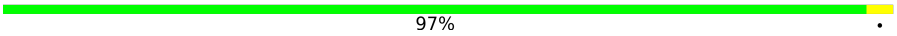
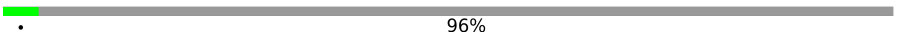
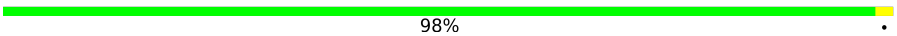
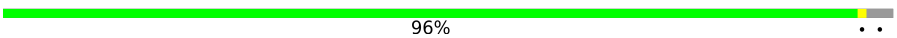
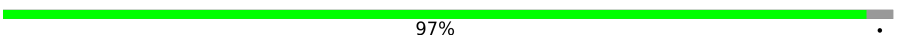
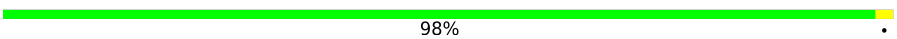
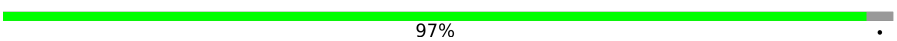
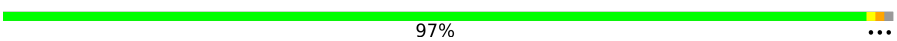
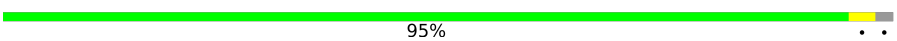
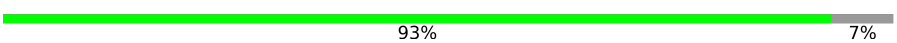
Mol	Chain	Length	Quality of chain
34	LL	213	
35	LM	142	
36	LN	203	
37	LO	204	
38	LP	187	
39	LQ	213	
40	LR	2898	
41	LS	174	
42	LT	160	
43	LU	127	
44	LV	139	
45	LX	156	
46	LY	138	
47	LZ	135	
48	Lc	108	
49	Ld	120	
50	Le	131	
51	Lf	109	
52	Lg	119	
53	Lh	935	
54	Li	110	
55	Lj	95	
56	Lk	81	
57	Ll	51	
58	Lq	217	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 156553 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	2609	55815	24911	10105	18190	2609	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	462	Total	C	N	O	S	0	0
			3669	2350	642	666	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	262	Total	C	N	O	S	0	0
			2105	1322	399	377	7		

- 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 60S ribosomal subunit-like protein.

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

- Molecule 26 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CY	420	Total	C	N	O	S	0	0
			3399	2181	616	590	12		

- Molecule 27 is a protein called rRNA-processing protein.

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

- Molecule 28 is a protein called 60S ribosomal protein L3-like protein.

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

- Molecule 29 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 30 is a protein called 60S ribosomal protein L6.

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

- Molecule 31 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	204	Total	C	N	O	S	0	0
			1644	1060	297	282	5		

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 33 is a protein called 60S ribosomal protein L12-like protein.

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

- Molecule 34 is a protein called 60S ribosomal protein L13.

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

- Molecule 35 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 36 is a protein called Ribosomal protein L15.

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

- Molecule 37 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 38 is a protein called 60S ribosomal protein l17-like protein.

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

- Molecule 39 is a protein called Ribosomal protein L18-like protein.

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

- Molecule 40 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LR	119	Total	C	N	O	S	0	0
			969	610	196	159	4		

- Molecule 41 is a protein called 60S ribosomal protein L20.

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

- Molecule 42 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 43 is a protein called 60S ribosomal protein L22-like protein.

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

- Molecule 44 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 45 is a protein called 60S ribosomal protein L25-like protein.

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

- Molecule 46 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 47 is a protein called 60S ribosomal protein L27.

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

- Molecule 48 is a protein called 60S ribosomal protein l30-like protein.

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

- Molecule 49 is a protein called Putative 60S ribosomal protein.

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

- Molecule 50 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 51 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 52 is a protein called Ribosomal protein l34-like protein.

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

- Molecule 53 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 54 is a protein called 60S ribosomal protein L36.

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

- Molecule 55 is a protein called Ribosomal protein L37.

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

- Molecule 56 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	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

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Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	THR	deletion	UNP G0SG89

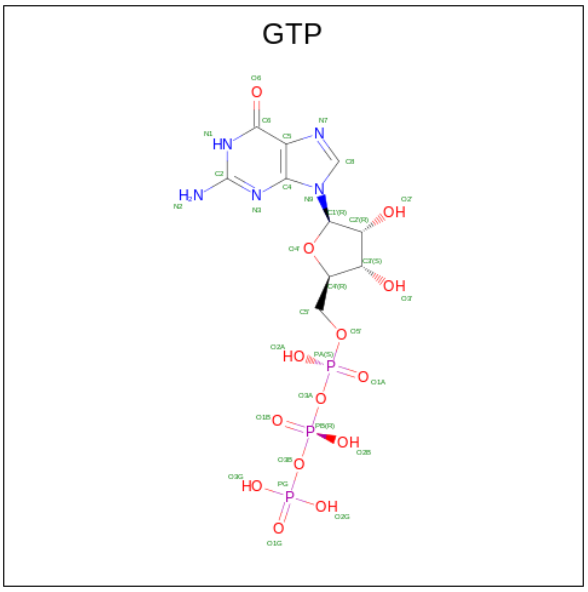
- Molecule 57 is a protein called 60S ribosomal protein L39.

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

- Molecule 58 is a protein called Ribosomal protein.

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

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	CQ	1	Total	Zn	0
			1	1	

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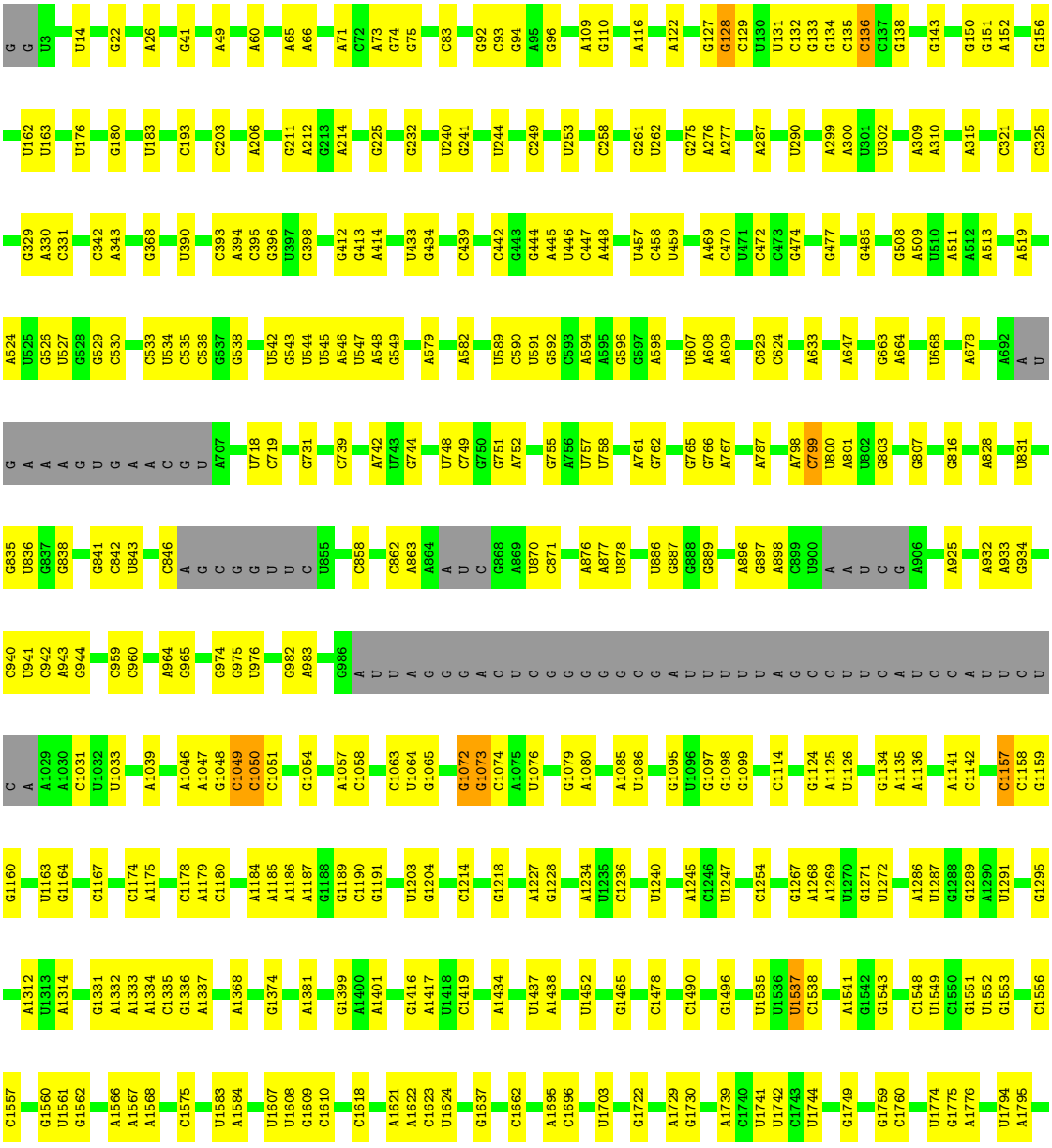
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	Lj	1	1	1	0

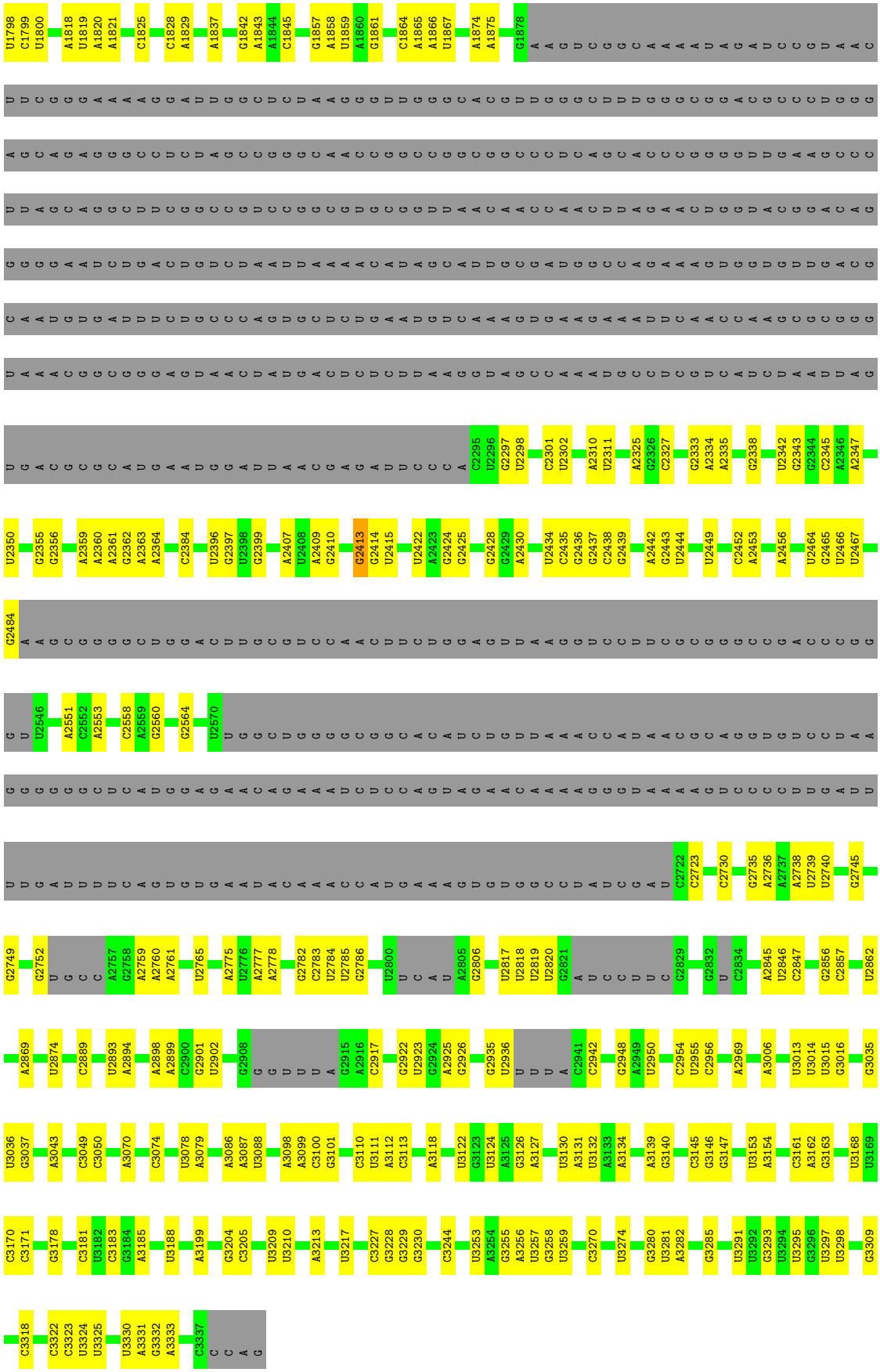
3 Residue-property plots (i)

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)

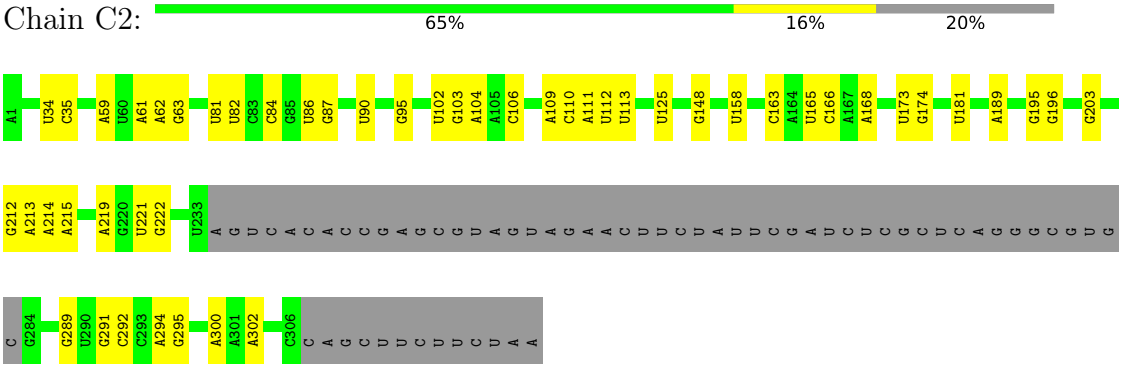
Chain C1:





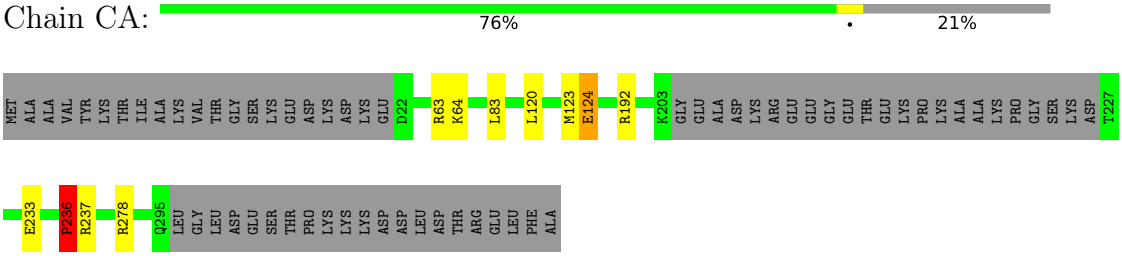
• Molecule 2: RNA (319-MER)

Chain C2:



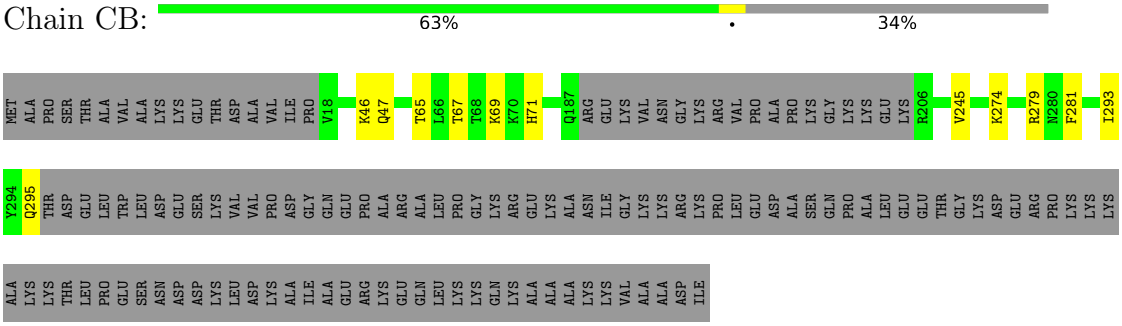
• Molecule 3: Brix domain-containing protein

Chain CA:



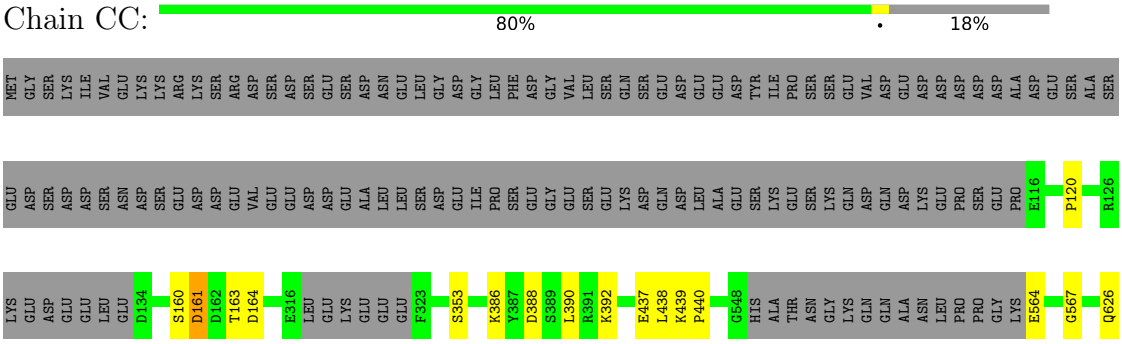
• Molecule 4: Ribosome biogenesis protein C8F11.04

Chain CB:



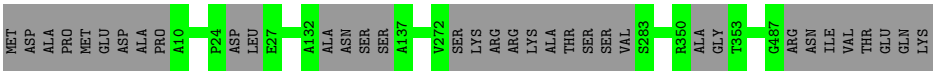
• Molecule 5: Ribosome biogenesis protein ERB1

Chain CC:



• Molecule 6: Ribosome biogenesis protein YTM1

Chain CD:



• Molecule 7: RNA helicase

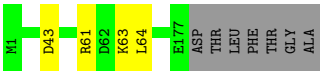
Chain CE:

• Molecule 8: Ribosome assembly factor mrt4

Chain CF:

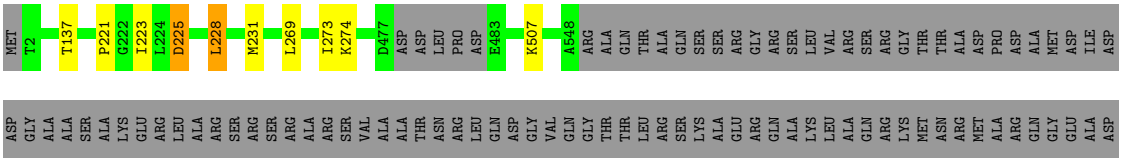
• Molecule 9: 60S ribosome subunit biogenesis protein NIP7

Chain CG:



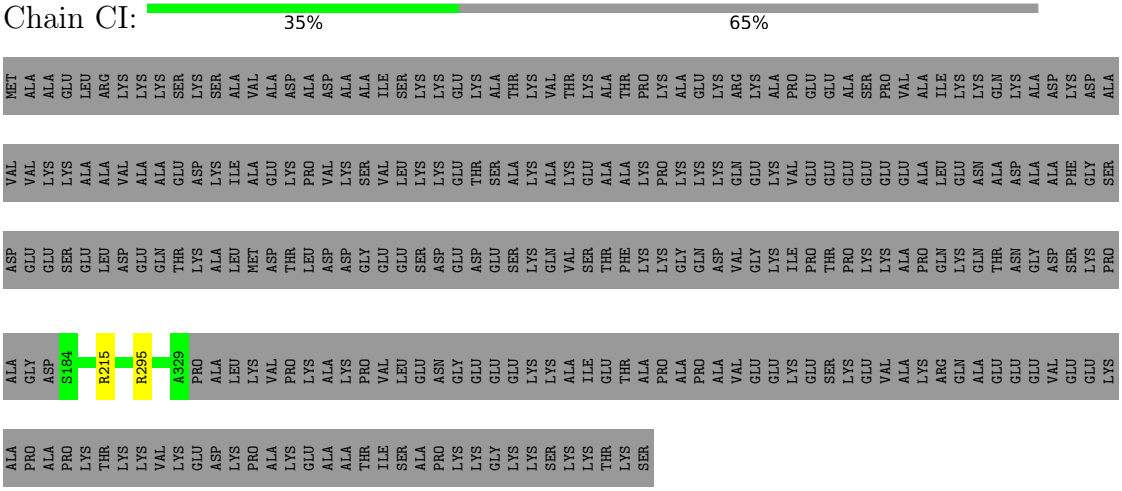
• Molecule 10: Nucleolar GTP-binding protein 1

Chain CH:



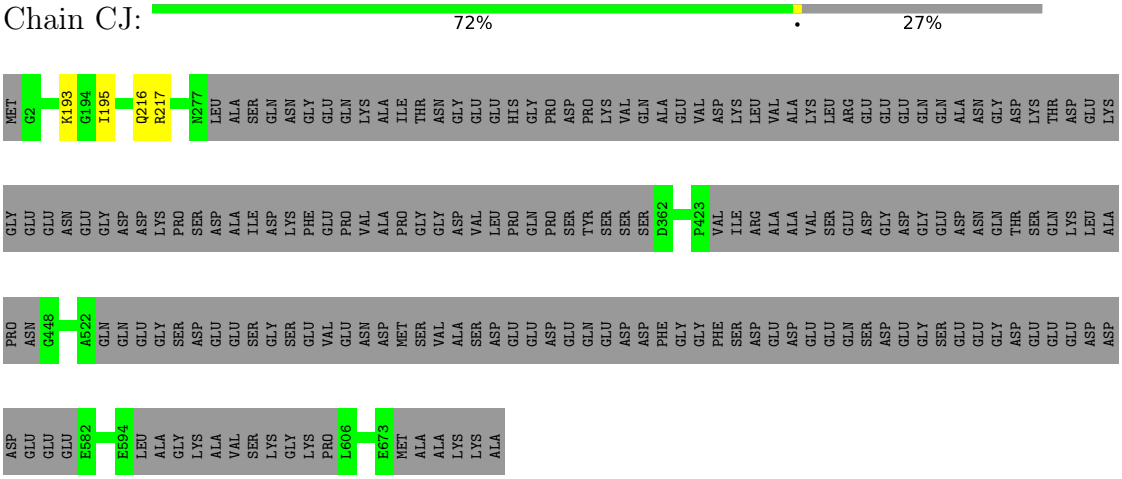
• Molecule 11: Putative RNA-binding protein

Chain CI:



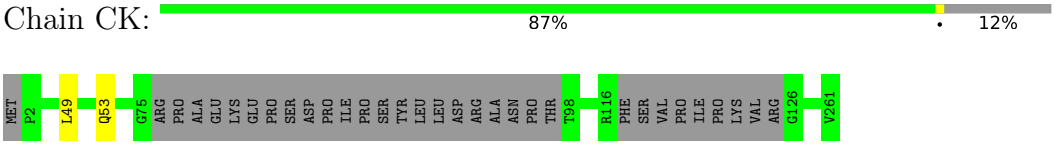
• Molecule 12: Pescadillo homolog

Chain CJ:



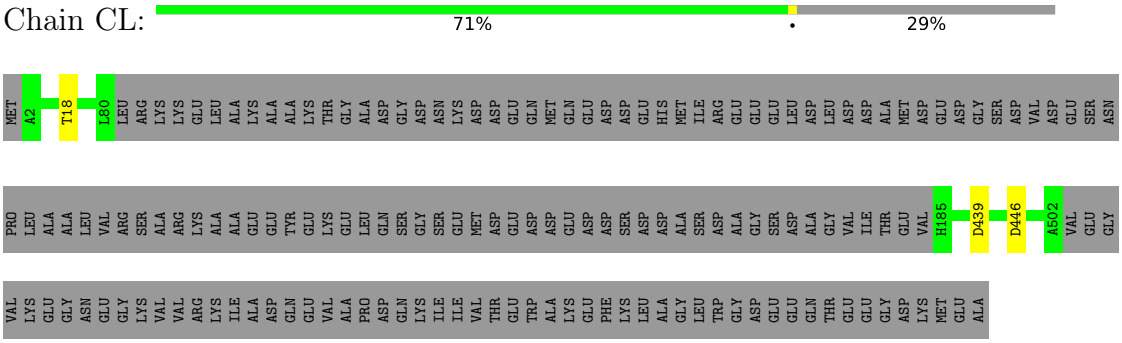
• Molecule 13: Ribosome biogenesis protein NSA2 homolog

Chain CK:



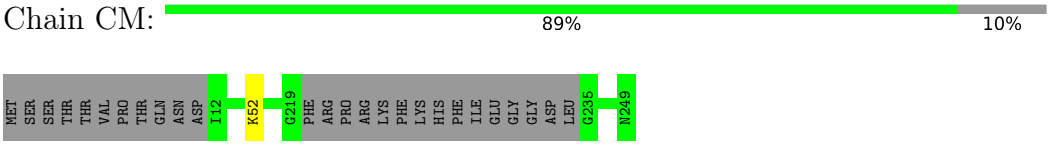
• Molecule 14: Putative GTP binding protein

Chain CL:



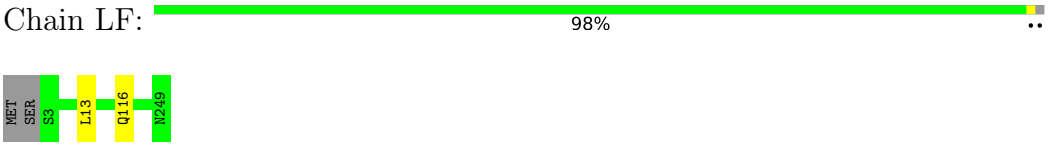
• Molecule 15: 60S ribosomal protein l7-like protein

Chain CM:



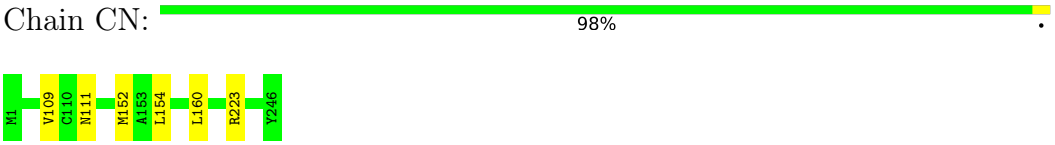
• Molecule 15: 60S ribosomal protein l7-like protein

Chain LF:



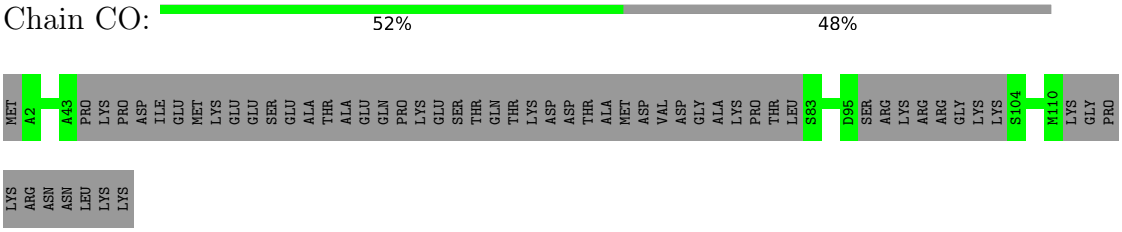
• Molecule 16: Eukaryotic translation initiation factor 6

Chain CN:



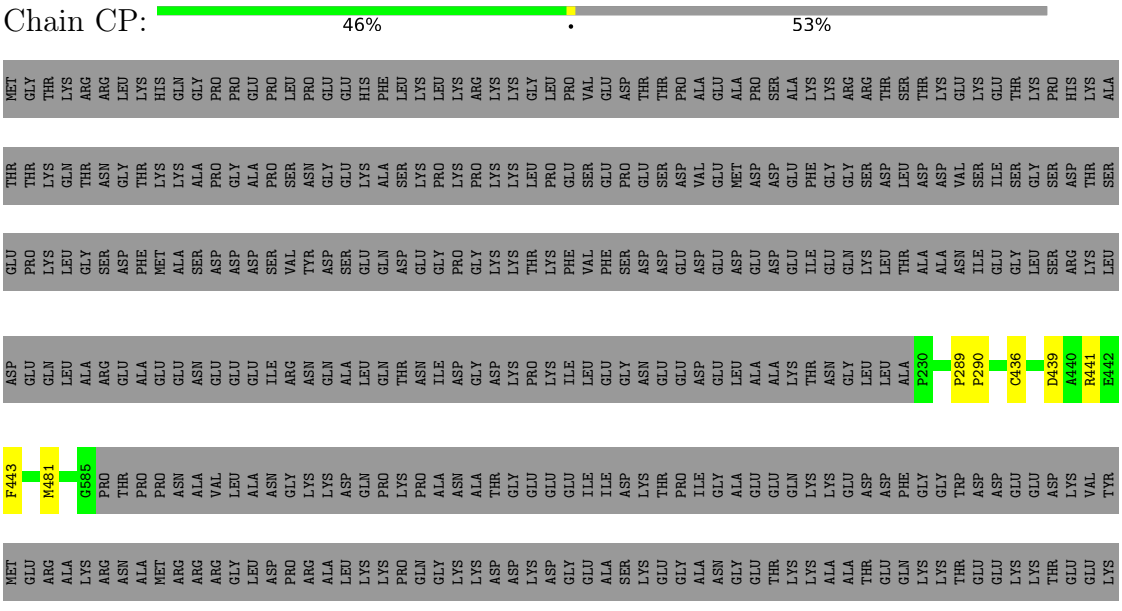
• Molecule 17: DUF2423 domain-containing protein

Chain CO:



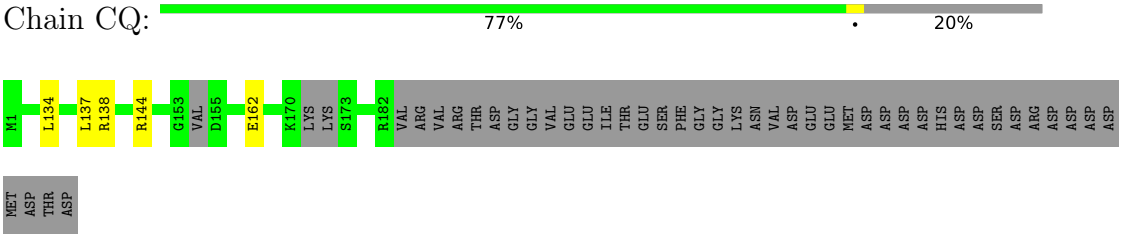
• Molecule 18: RNA methyltransferase nop2-like protein

Chain CP:



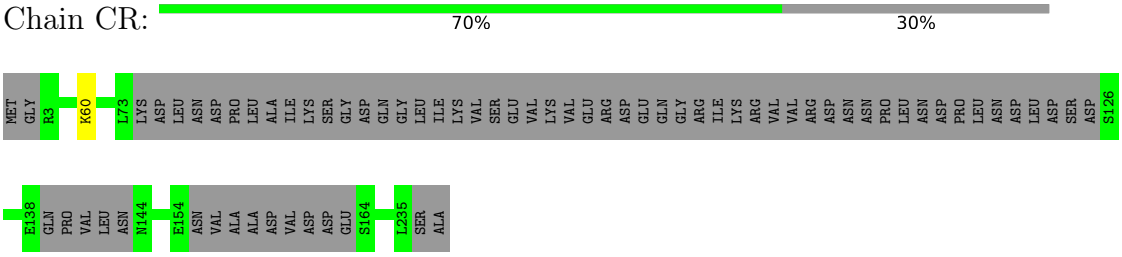
• Molecule 19: Ribosome biogenesis protein RLP24

Chain CQ:



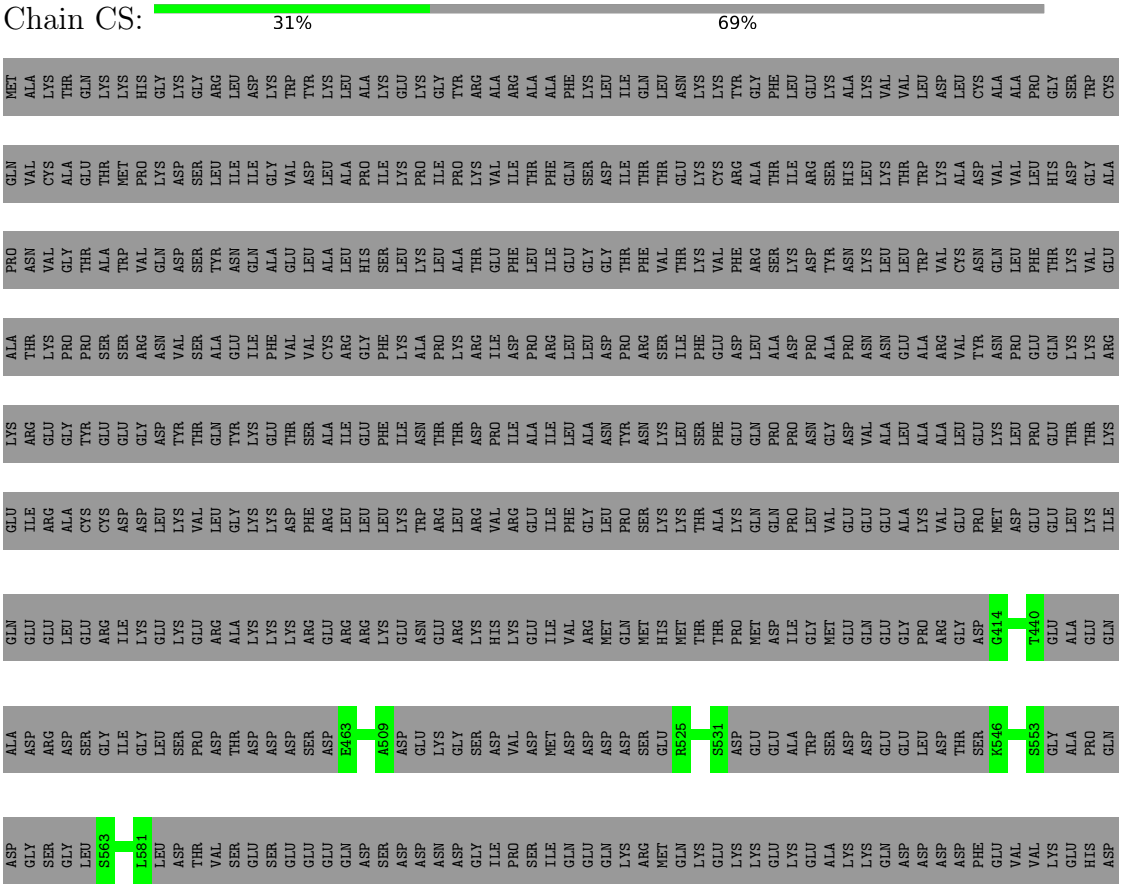
• Molecule 20: Nucleolar protein 16

Chain CR:



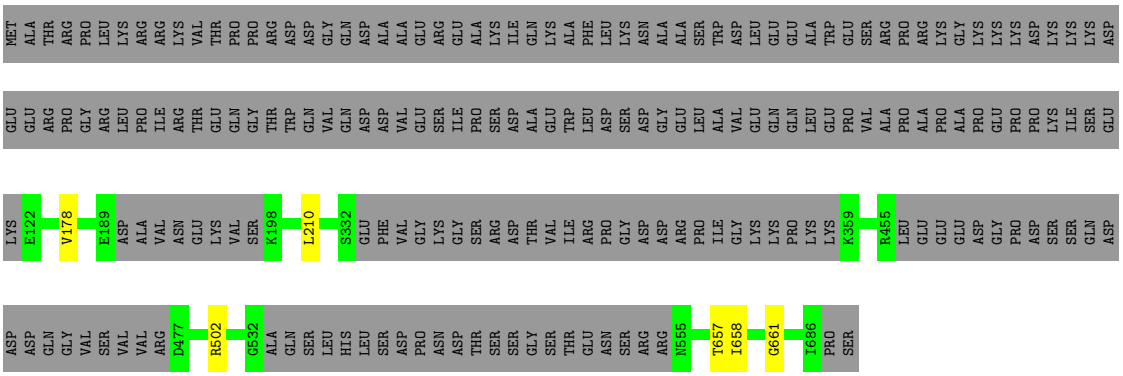
• Molecule 21: AdoMet-dependent rRNA methyltransferase SPB1

Chain CS:



• Molecule 22: Nucleolar complex-associated protein 3

Chain CT:

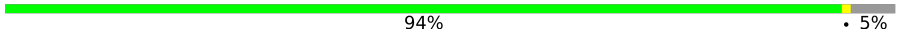


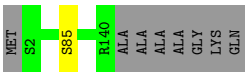
• Molecule 23: rRNA-processing protein EBP2

Chain CU:

• Molecule 24: Putative 60S ribosomal protein

Chain CV:



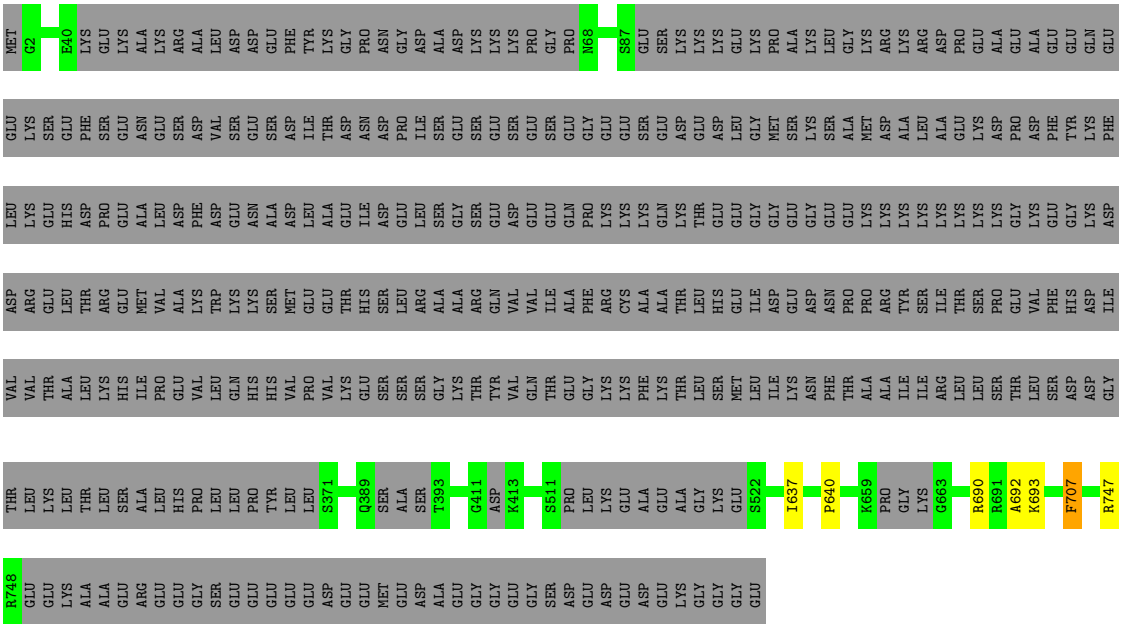


• Molecule 25: 60S ribosomal subunit-like protein

Chain CX:

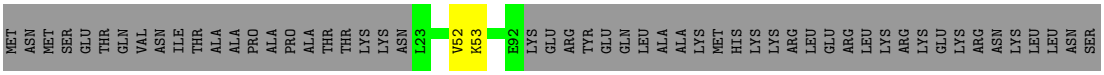
• Molecule 26: Putative NOC2 family protein

Chain CY:



• Molecule 27: rRNA-processing protein

Chain Cz:

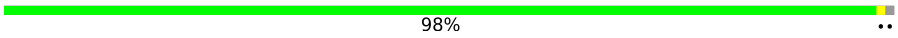


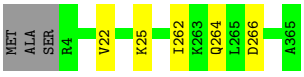
• Molecule 28: 60S ribosomal protein L3-like protein

Chain LB:

• Molecule 29: 60S ribosomal protein L4-like protein

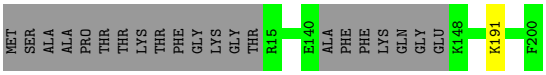
Chain LC:





• Molecule 30: 60S ribosomal protein L6

Chain LE:

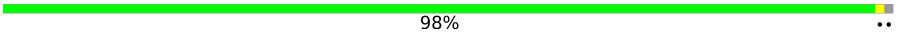


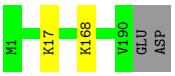
• Molecule 31: 60S ribosomal protein L8

Chain LG:

• Molecule 32: 60S ribosomal protein l9-like protein

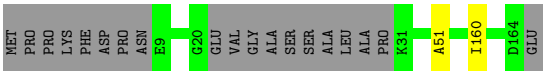
Chain LH:





• Molecule 33: 60S ribosomal protein L12-like protein

Chain LK:

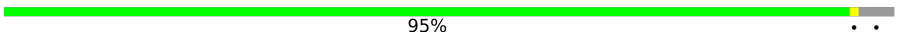


• Molecule 34: 60S ribosomal protein L13

Chain LL:

• Molecule 35: 60S ribosomal protein L14-like protein

Chain LM:

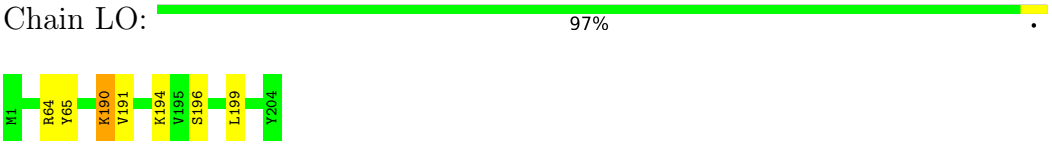


• Molecule 36: Ribosomal protein L15

Chain LN:

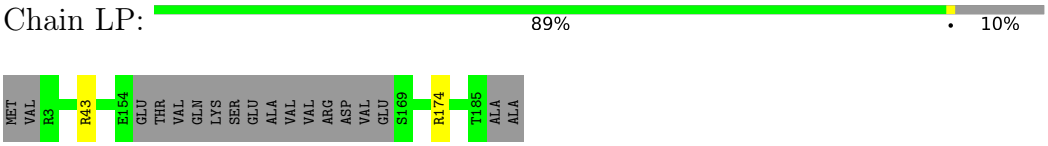
• Molecule 37: 60S ribosomal protein L16-like protein

Chain LO:



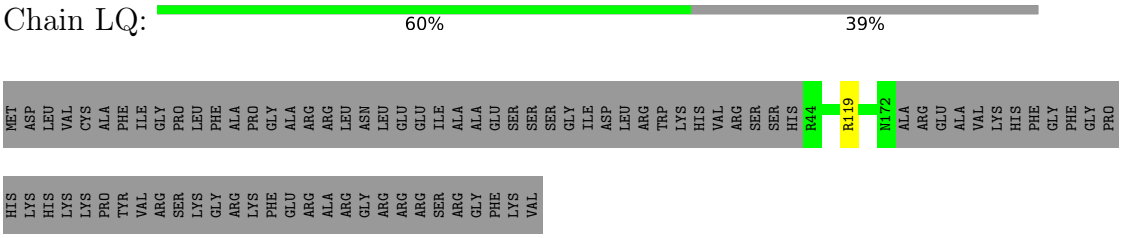
• Molecule 38: 60S ribosomal protein l17-like protein

Chain LP:



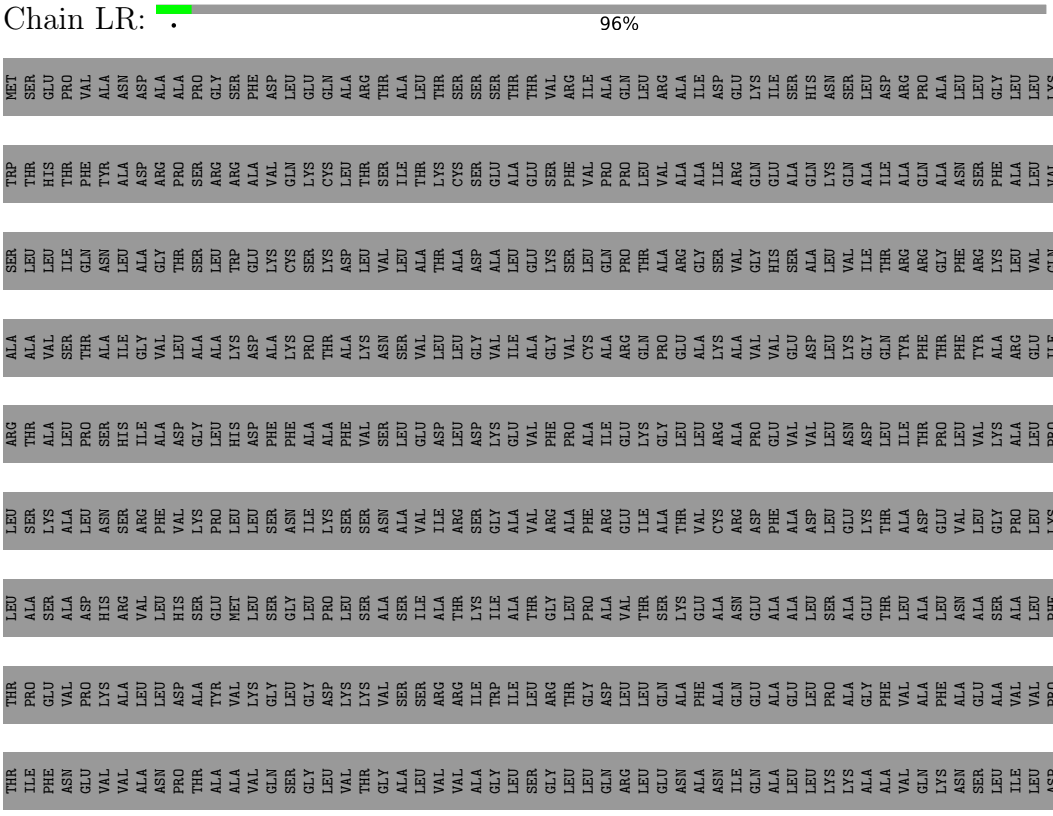
• Molecule 39: Ribosomal protein L18-like protein

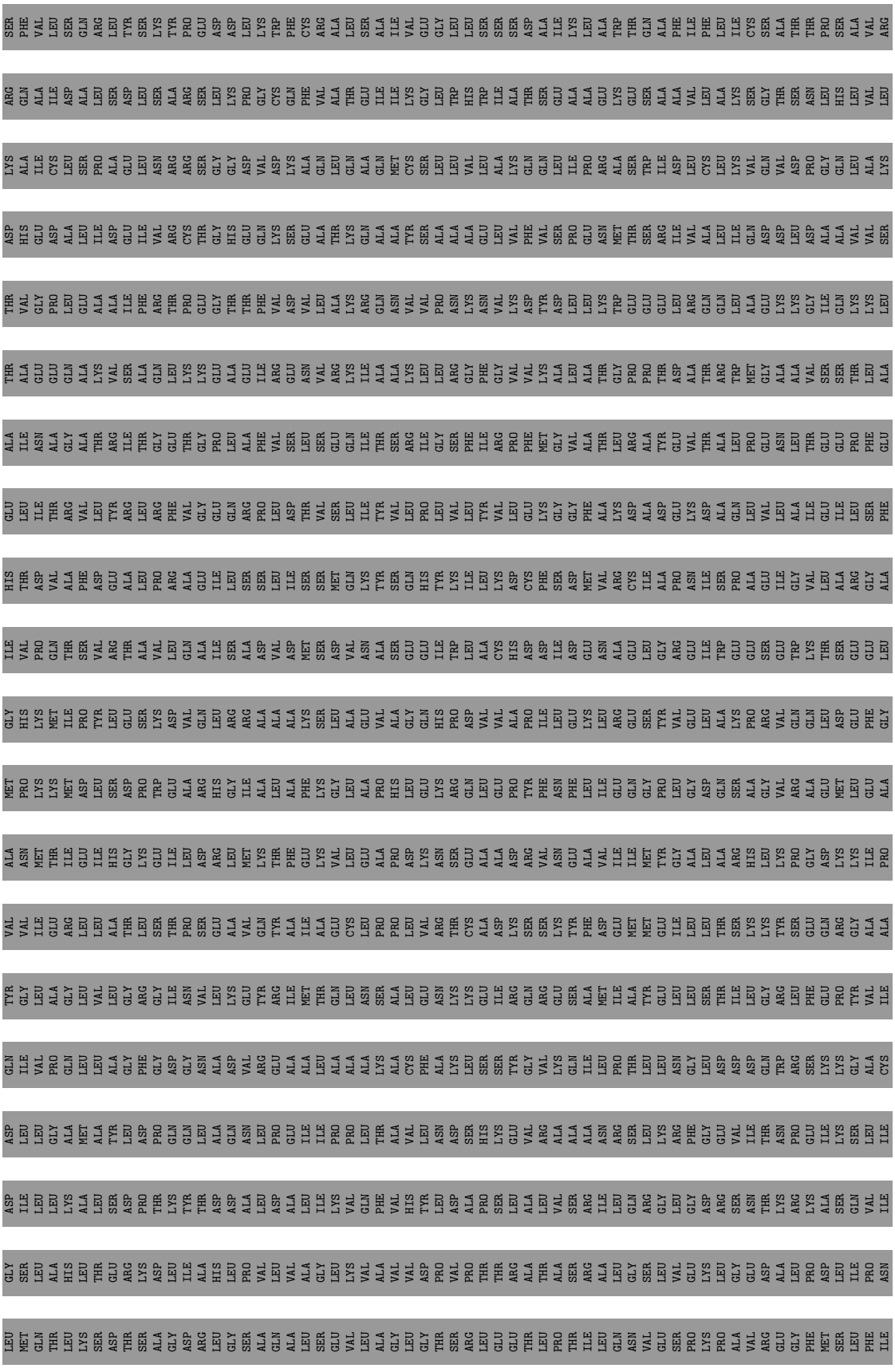
Chain LQ:

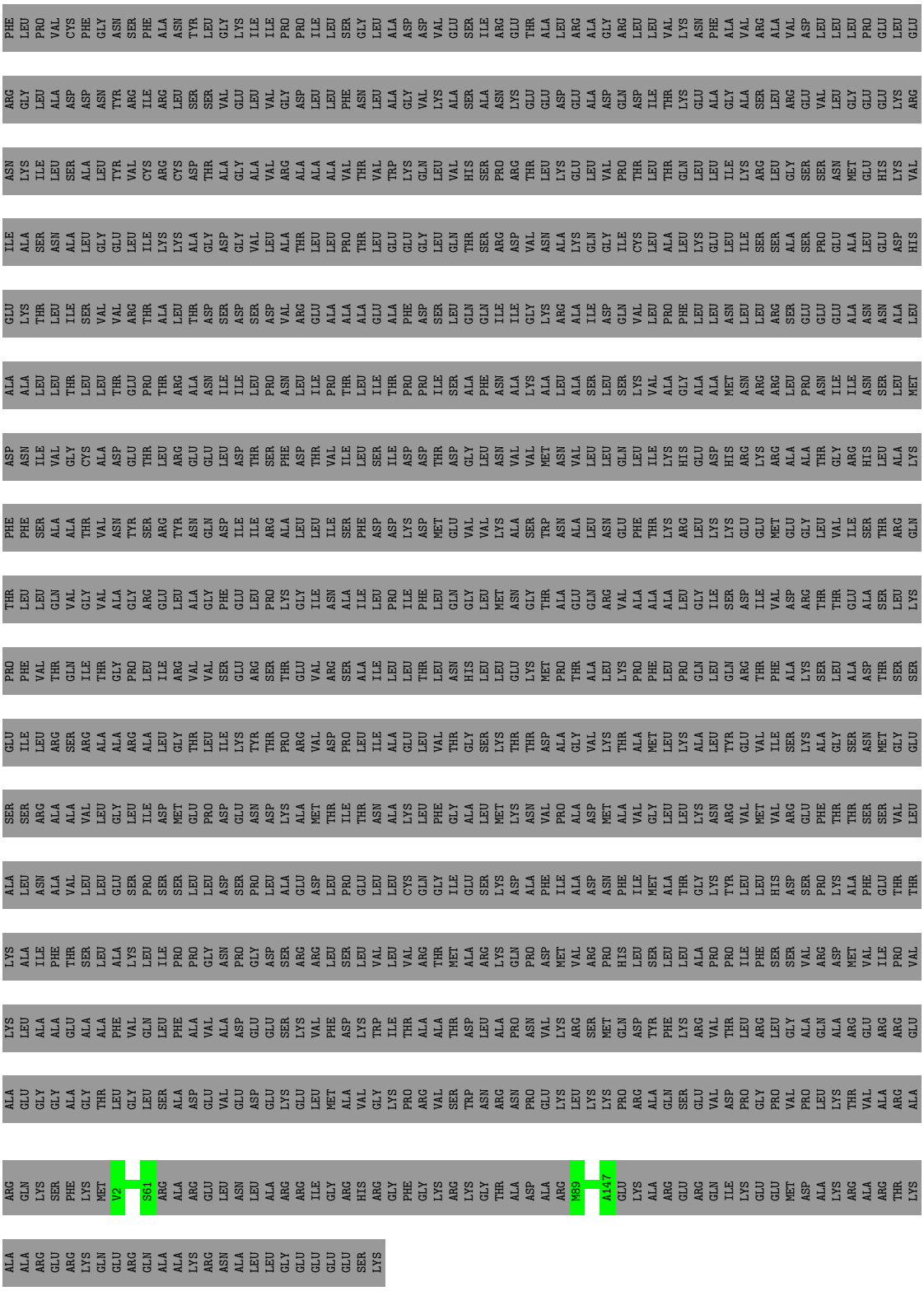


• Molecule 40: Ribosomal protein L19

Chain LR:

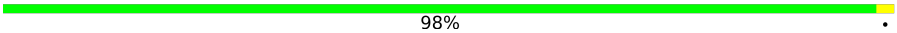


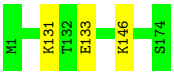




• Molecule 41: 60S ribosomal protein L20

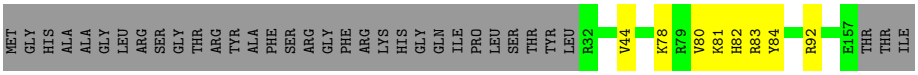
Chain LS:





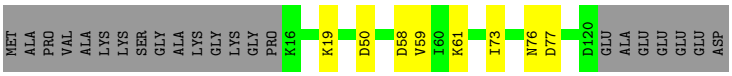
• Molecule 42: 60S ribosomal protein l21-like protein

Chain LT:



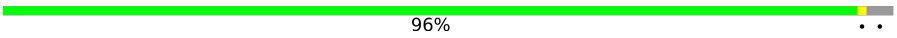
• Molecule 43: 60S ribosomal protein L22-like protein

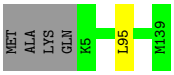
Chain LU:



• Molecule 44: 60S ribosomal protein l23-like protein

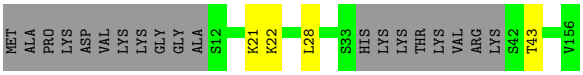
Chain LV:





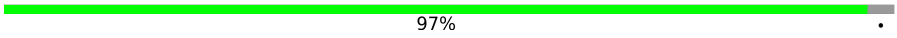
• Molecule 45: 60S ribosomal protein L25-like protein

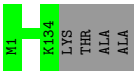
Chain LX:



• Molecule 46: 60S ribosomal protein L26-like protein

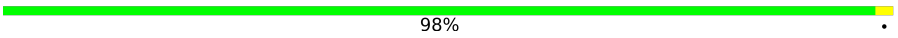
Chain LY:





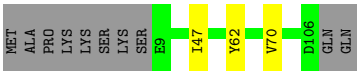
• Molecule 47: 60S ribosomal protein L27

Chain LZ:



• Molecule 48: 60S ribosomal protein l30-like protein

Chain Lc:

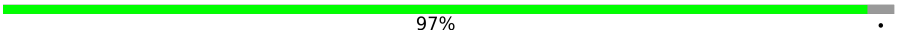


• Molecule 49: Putative 60S ribosomal protein

Chain Ld:

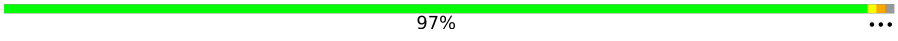
• Molecule 50: 60S ribosomal protein L32-like protein

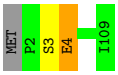
Chain Le:



• Molecule 51: 60S ribosomal protein l33-like protein

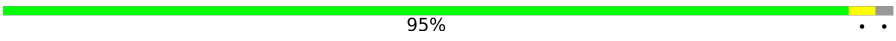
Chain Lf:

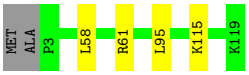




• Molecule 52: Ribosomal protein l34-like protein

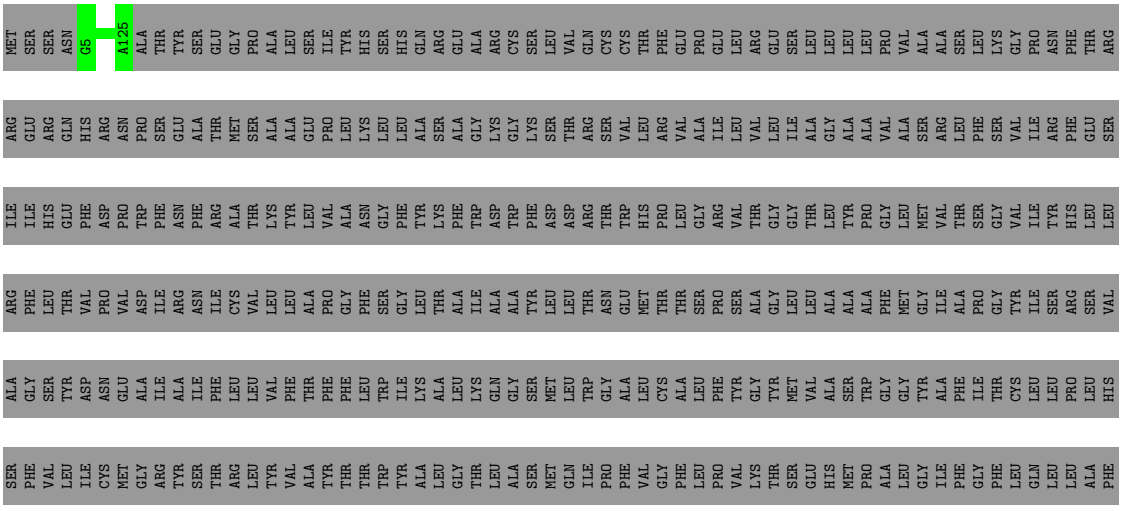
Chain Lg:

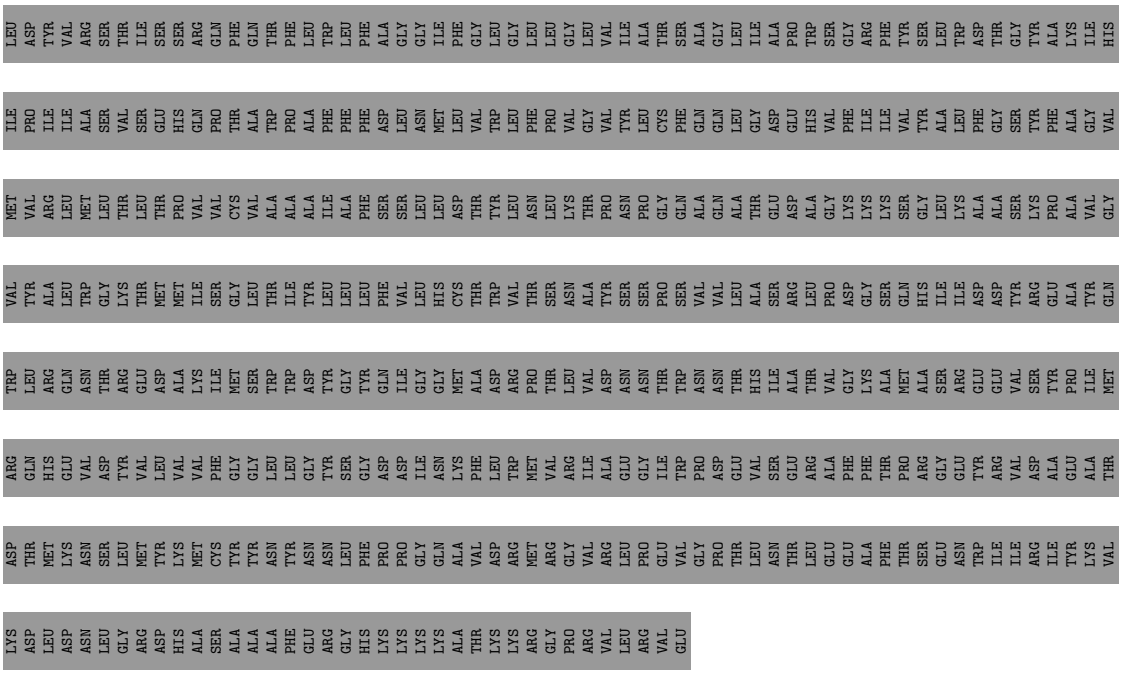




• Molecule 53: dolichyl-diphosphooligosaccharide--protein glycotransferase

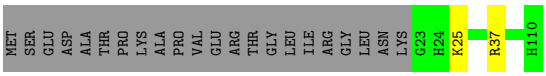
Chain Lh:





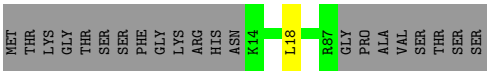
• Molecule 54: 60S ribosomal protein L36

Chain Li:



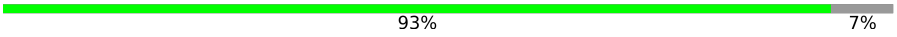
• Molecule 55: Ribosomal protein L37

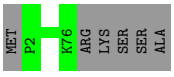
Chain Lj:



• Molecule 56: 60S ribosomal protein L38-like protein

Chain Lk:





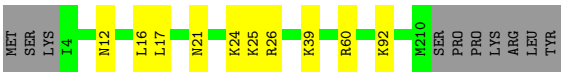
• Molecule 57: 60S ribosomal protein L39

Chain Ll:

• Molecule 58: Ribosomal protein

Chain Lq:


91%
5%
5%


MET
SER
LYS
I4
N12
L16
L17
N21
K24
K25
R26
K39
R60
K92
M210
SER
PRO
PRO
LYS
ARG
LEU
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70516	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, GTP, TPO, 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C1	0.34	0/62448	0.82	37/97346 (0.0%)
2	C2	0.30	0/6097	0.77	0/9499
3	CA	0.35	0/2115	0.63	1/2840 (0.0%)
4	CB	0.36	0/2109	0.65	0/2866
5	CC	0.31	0/5423	0.59	0/7380
6	CD	0.26	0/3543	0.58	0/4824
7	CE	0.33	0/3739	0.58	0/5040
8	CF	0.30	0/1982	0.58	0/2671
9	CG	0.31	0/1422	0.57	0/1920
10	CH	0.32	0/4468	0.57	0/6029
11	CI	0.32	0/1225	0.63	0/1645
12	CJ	0.31	0/4125	0.58	0/5548
13	CK	0.27	0/1863	0.55	0/2494
14	CL	0.29	0/2247	0.51	0/3076
15	CM	0.31	0/1851	0.58	0/2481
15	LF	0.31	0/2055	0.59	1/2758 (0.0%)
16	CN	0.31	0/1881	0.62	0/2560
17	CO	0.26	0/470	0.52	0/619
18	CP	0.32	0/2859	0.59	0/3870
19	CQ	0.32	0/1507	0.64	0/1996
20	CR	0.27	0/1369	0.59	0/1828
21	CS	0.26	0/2127	0.53	0/2817
22	CT	0.29	0/3974	0.57	0/5357
23	CU	0.31	0/1428	0.59	0/1910
24	CV	0.26	0/1091	0.54	0/1468
25	CX	0.29	0/705	0.55	0/938
26	CY	0.31	0/3454	0.63	0/4637
27	Cz	0.30	0/598	0.62	0/785
28	LB	0.32	0/2885	0.61	0/3872
29	LC	0.30	0/2809	0.55	0/3787
30	LE	0.28	0/1428	0.53	0/1921
31	LG	0.32	0/1667	0.55	0/2230

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LH	0.28	0/1516	0.56	0/2038
33	LK	0.25	0/1124	0.54	0/1507
34	LL	0.30	0/983	0.63	0/1318
35	LM	0.32	0/1120	0.59	0/1507
36	LN	0.30	0/1595	0.62	1/2132 (0.0%)
37	LO	0.33	0/1652	0.58	0/2215
38	LP	0.26	0/1367	0.59	0/1838
39	LQ	0.28	0/1033	0.58	0/1391
40	LR	0.26	0/985	0.55	0/1318
41	LS	0.30	0/1468	0.58	0/1975
42	LT	0.29	0/1033	0.53	0/1389
43	LU	0.34	0/863	0.57	0/1155
44	LV	0.29	0/1013	0.54	0/1361
45	LX	0.30	0/1078	0.52	0/1451
46	LY	0.26	0/1079	0.56	0/1443
47	LZ	0.30	0/1135	0.61	0/1519
48	Lc	0.35	0/740	0.59	0/995
49	Ld	0.33	0/904	0.59	0/1209
50	Le	0.25	0/1043	0.54	0/1389
51	Lf	0.33	0/883	0.62	0/1187
52	Lg	0.34	0/943	0.61	0/1258
53	Lh	0.25	0/1006	0.54	0/1338
54	Li	0.28	0/738	0.62	0/971
55	Lj	0.34	0/606	0.68	0/803
56	Lk	0.26	0/628	0.57	0/835
57	Ll	0.24	0/329	0.54	0/440
58	Lq	0.29	0/1621	0.63	0/2180
All	All	0.32	0/165449	0.70	40/237174 (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
58	Lq	0	1

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1050	C	N3-C2-O2	-12.25	113.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1050	C	N1-C2-O2	10.69	125.31	118.90
1	C1	1583	U	C2-N1-C1'	8.47	127.87	117.70
1	C1	136	C	N3-C2-O2	-8.14	116.20	121.90
1	C1	2723	C	N3-C2-O2	-7.78	116.46	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	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%)	228 (92%)	16 (6%)	3 (1%)	11 38
4	CB	256/391 (66%)	228 (89%)	28 (11%)	0	100 100
5	CC	648/801 (81%)	606 (94%)	38 (6%)	4 (1%)	22 53
6	CD	450/495 (91%)	416 (92%)	34 (8%)	0	100 100
7	CE	458/598 (77%)	428 (93%)	30 (7%)	0	100 100
8	CF	243/270 (90%)	227 (93%)	14 (6%)	2 (1%)	16 48
9	CG	175/184 (95%)	163 (93%)	11 (6%)	1 (1%)	22 53
10	CH	538/661 (81%)	511 (95%)	25 (5%)	2 (0%)	30 63
11	CI	144/414 (35%)	135 (94%)	9 (6%)	0	100 100
12	CJ	484/679 (71%)	462 (96%)	21 (4%)	1 (0%)	44 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CK	223/261 (85%)	212 (95%)	11 (5%)	0	100	100
14	CL	393/558 (70%)	366 (93%)	25 (6%)	2 (0%)	25	58
15	CM	219/249 (88%)	210 (96%)	9 (4%)	0	100	100
15	LF	245/249 (98%)	238 (97%)	7 (3%)	0	100	100
16	CN	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	354/751 (47%)	330 (93%)	24 (7%)	0	100	100
19	CQ	173/225 (77%)	165 (95%)	8 (5%)	0	100	100
20	CR	159/237 (67%)	157 (99%)	2 (1%)	0	100	100
21	CS	246/834 (30%)	238 (97%)	8 (3%)	0	100	100
22	CT	478/688 (70%)	452 (95%)	24 (5%)	2 (0%)	30	63
23	CU	174/451 (39%)	170 (98%)	3 (2%)	1 (1%)	22	53
24	CV	137/147 (93%)	135 (98%)	1 (1%)	1 (1%)	19	51
25	CX	86/203 (42%)	84 (98%)	2 (2%)	0	100	100
26	CY	406/788 (52%)	371 (91%)	33 (8%)	2 (0%)	25	58
27	Cz	68/123 (55%)	64 (94%)	4 (6%)	0	100	100
28	LB	352/392 (90%)	333 (95%)	19 (5%)	0	100	100
29	LC	360/365 (99%)	344 (96%)	16 (4%)	0	100	100
30	LE	175/200 (88%)	163 (93%)	11 (6%)	1 (1%)	22	53
31	LG	200/262 (76%)	189 (94%)	11 (6%)	0	100	100
32	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
33	LK	142/165 (86%)	129 (91%)	11 (8%)	2 (1%)	9	34
34	LL	115/213 (54%)	107 (93%)	7 (6%)	1 (1%)	14	45
35	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
36	LN	179/203 (88%)	170 (95%)	9 (5%)	0	100	100
37	LO	202/204 (99%)	190 (94%)	9 (4%)	3 (2%)	8	33
38	LP	165/187 (88%)	160 (97%)	5 (3%)	0	100	100
39	LQ	127/213 (60%)	121 (95%)	6 (5%)	0	100	100
40	LR	115/2898 (4%)	115 (100%)	0	0	100	100
41	LS	172/174 (99%)	160 (93%)	12 (7%)	0	100	100
42	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	LU	103/127 (81%)	96 (93%)	7 (7%)	0	100	100
44	LV	133/139 (96%)	128 (96%)	5 (4%)	0	100	100
45	LX	133/156 (85%)	129 (97%)	4 (3%)	0	100	100
46	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
47	LZ	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
48	Lc	96/108 (89%)	93 (97%)	3 (3%)	0	100	100
49	Ld	107/120 (89%)	101 (94%)	6 (6%)	0	100	100
50	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100
51	Lf	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	6	27
52	Lg	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
53	Lh	119/935 (13%)	113 (95%)	6 (5%)	0	100	100
54	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
55	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
56	Lk	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
57	Ll	36/51 (71%)	33 (92%)	3 (8%)	0	100	100
58	Lq	205/217 (94%)	179 (87%)	25 (12%)	1 (0%)	25	58
All	All	11829/19680 (60%)	11173 (94%)	624 (5%)	32 (0%)	38	68

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	CA	236	PRO
5	CC	161	ASP
22	CT	502	ARG
26	CY	692	ALA
26	CY	707	PHE

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%)	213 (96%)	10 (4%)	23 53
4	CB	222/329 (68%)	210 (95%)	12 (5%)	18 47
5	CC	578/708 (82%)	566 (98%)	12 (2%)	48 72
6	CD	381/410 (93%)	381 (100%)	0	100 100
7	CE	398/517 (77%)	381 (96%)	17 (4%)	25 55
8	CF	214/236 (91%)	211 (99%)	3 (1%)	62 81
9	CG	150/155 (97%)	147 (98%)	3 (2%)	50 74
10	CH	481/575 (84%)	471 (98%)	10 (2%)	48 72
11	CI	121/336 (36%)	119 (98%)	2 (2%)	56 78
12	CJ	428/579 (74%)	425 (99%)	3 (1%)	81 90
13	CK	195/225 (87%)	193 (99%)	2 (1%)	73 86
14	CL	72/458 (16%)	71 (99%)	1 (1%)	62 81
15	CM	191/215 (89%)	190 (100%)	1 (0%)	86 92
15	LF	213/215 (99%)	212 (100%)	1 (0%)	86 92
16	CN	206/206 (100%)	200 (97%)	6 (3%)	37 65
17	CO	48/99 (48%)	48 (100%)	0	100 100
18	CP	302/632 (48%)	295 (98%)	7 (2%)	45 70
19	CQ	150/192 (78%)	145 (97%)	5 (3%)	33 62
20	CR	144/206 (70%)	143 (99%)	1 (1%)	81 90
21	CS	209/716 (29%)	207 (99%)	2 (1%)	73 86
22	CT	427/600 (71%)	423 (99%)	4 (1%)	75 88
23	CU	149/376 (40%)	147 (99%)	2 (1%)	65 82
24	CV	109/112 (97%)	109 (100%)	0	100 100
25	CX	76/172 (44%)	76 (100%)	0	100 100
26	CY	364/686 (53%)	358 (98%)	6 (2%)	58 79
27	Cz	60/107 (56%)	58 (97%)	2 (3%)	33 62
28	LB	301/331 (91%)	293 (97%)	8 (3%)	40 67
29	LC	283/285 (99%)	278 (98%)	5 (2%)	54 76
30	LE	151/166 (91%)	151 (100%)	0	100 100
31	LG	175/222 (79%)	173 (99%)	2 (1%)	70 84
32	LH	167/169 (99%)	165 (99%)	2 (1%)	67 83
33	LK	121/136 (89%)	121 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	LL	99/176 (56%)	99 (100%)	0	100 100
35	LM	115/117 (98%)	113 (98%)	2 (2%)	56 78
36	LN	164/180 (91%)	163 (99%)	1 (1%)	84 91
37	LO	163/163 (100%)	158 (97%)	5 (3%)	35 63
38	LP	137/152 (90%)	135 (98%)	2 (2%)	60 80
39	LQ	110/178 (62%)	109 (99%)	1 (1%)	75 88
40	LR	104/2396 (4%)	104 (100%)	0	100 100
41	LS	154/154 (100%)	151 (98%)	3 (2%)	52 75
42	LT	109/135 (81%)	102 (94%)	7 (6%)	14 42
43	LU	93/108 (86%)	85 (91%)	8 (9%)	8 31
44	LV	99/102 (97%)	98 (99%)	1 (1%)	73 86
45	LX	114/129 (88%)	110 (96%)	4 (4%)	31 61
46	LY	117/119 (98%)	117 (100%)	0	100 100
47	LZ	121/121 (100%)	118 (98%)	3 (2%)	42 69
48	Lc	79/88 (90%)	76 (96%)	3 (4%)	28 59
49	Ld	95/105 (90%)	94 (99%)	1 (1%)	70 84
50	Le	110/114 (96%)	110 (100%)	0	100 100
51	Lf	89/90 (99%)	88 (99%)	1 (1%)	70 84
52	Lg	101/102 (99%)	97 (96%)	4 (4%)	27 58
53	Lh	108/781 (14%)	108 (100%)	0	100 100
54	Li	75/93 (81%)	73 (97%)	2 (3%)	40 67
55	Lj	61/78 (78%)	60 (98%)	1 (2%)	58 79
56	Lk	71/76 (93%)	71 (100%)	0	100 100
57	Ll	34/46 (74%)	34 (100%)	0	100 100
58	Lq	179/189 (95%)	171 (96%)	8 (4%)	23 53
All	All	10010/16639 (60%)	9824 (98%)	186 (2%)	52 75

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	LB	349	ARG
42	LT	78	LYS
29	LC	22	VAL

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Mol	Chain	Res	Type
35	LM	122	ARG
43	LU	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
22	CT	323	ASN
31	LG	212	ASN
22	CT	436	GLN
26	CY	636	ASN
35	LM	98	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2594/3341 (77%)	571 (22%)	40 (1%)
2	C2	254/319 (79%)	49 (19%)	1 (0%)
All	All	2848/3660 (77%)	620 (21%)	41 (1%)

5 of 620 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	22	G
1	C1	26	A
1	C1	41	G
1	C1	49	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	3013	U
1	C1	3229	G
1	C1	3014	U
1	C1	3162	A
1	C1	3257	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	0.76	0	10,14,16	1.32	2 (20%)
5	SEP	CC	160	5	8,9,10	1.54	1 (12%)	8,12,14	1.50	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	-	6/9/11/13	-
5	SEP	CC	160	5	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	CC	160	SEP	P-O1P	3.39	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	CC	160	SEP	P-OG-CB	-2.81	110.56	118.30
5	CC	163	TPO	O-C-CA	-2.80	117.44	124.78
5	CC	160	SEP	OG-CB-CA	2.61	110.68	108.14
5	CC	163	TPO	P-OG1-CB	2.23	129.94	123.21

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	C-CA-CB-CG2
5	CC	163	TPO	O-C-CA-CB
5	CC	163	TPO	CG2-CB-OG1-P
5	CC	163	TPO	CB-OG1-P-O1P

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	GTP	CH	1001	-	26,34,34	1.12	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
59	GTP	CH	1001	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CH	1001	GTP	C5-C6	-3.96	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CH	1001	GTP	C2-N3	2.12	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	CH	1001	GTP	C5-C6-N1	3.22	119.63	113.95
59	CH	1001	GTP	C8-N7-C5	3.08	108.85	102.99
59	CH	1001	GTP	PB-O3B-PG	-3.01	122.51	132.83
59	CH	1001	GTP	PA-O3A-PB	-2.92	122.79	132.83
59	CH	1001	GTP	C2-N1-C6	-2.85	119.85	125.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

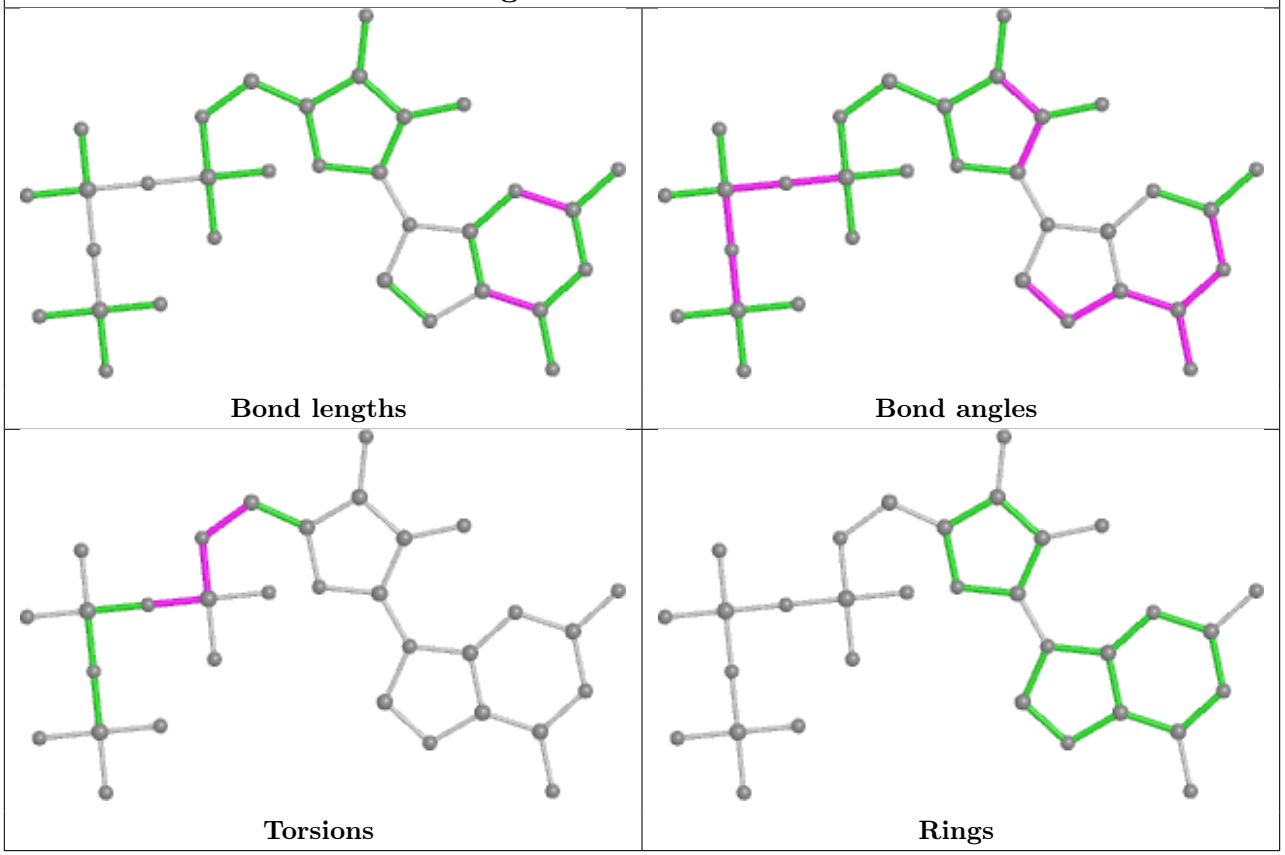
Mol	Chain	Res	Type	Atoms
59	CH	1001	GTP	C5'-O5'-PA-O3A
59	CH	1001	GTP	PB-O3A-PA-O2A
59	CH	1001	GTP	C4'-C5'-O5'-PA
59	CH	1001	GTP	C5'-O5'-PA-O2A

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 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.