Full wwPDB EM Validation Report ⓘ

May 21, 2024 – 10:27 AM JST

PDB ID	:	8I9V
EMDB ID	:	EMD-35285
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - State Dbp10-2
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation 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:

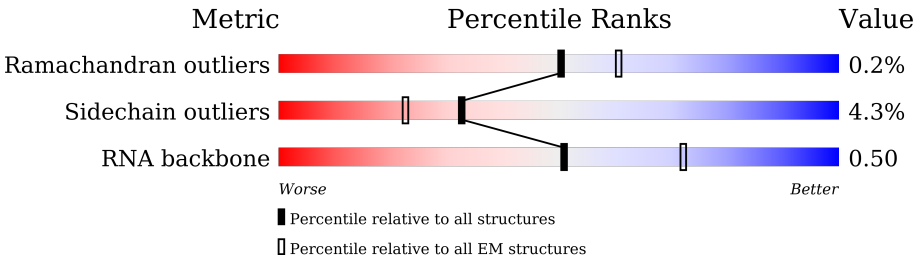
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	48% 15% • 36%
2	C2	256	49% 12% 38%
3	C3	161	37% 23% • 39%
4	CA	316	78% 5% 18%
5	CB	391	61% 5% • 34%
6	CC	801	34% • 64%
7	CE	598	73% 5% 23%
8	CF	270	86% • 9%
9	CG	184	91% 5% •

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Mol	Chain	Length	Quality of chain
10	CH	661	68% 28%
11	CI	414	34% 65%
12	CJ	679	55% 44%
13	CK	261	84% 5% 11%
14	CL	558	68% 30%
15	CM	249	71% 25%
15	LF	249	94%
16	CN	246	97%
17	CO	120	51% 48%
18	CP	751	40% 57%
19	CQ	225	46% 50%
20	CR	237	67% 30%
21	CS	834	35% 64%
22	CT	688	66% 33%
23	CU	451	39% 61%
24	CX	203	42% 57%
25	CY	788	41% 59%
26	Cz	123	56% 43%
27	Cb	924	67% 31%
28	LB	392	84% 13%
29	LC	365	97%
30	LE	200	83% 15%
31	LG	262	73% 25%
32	LH	192	92% 7%
33	LK	165	84% 12%

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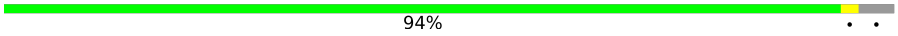
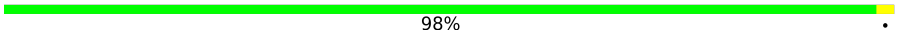
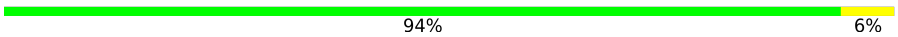
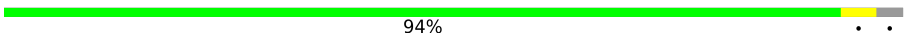
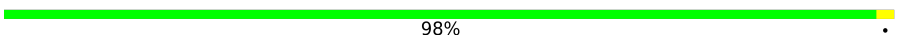
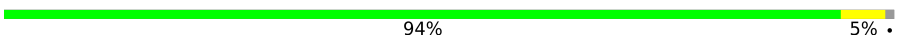
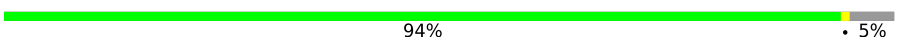
Mol	Chain	Length	Quality of chain
34	LL	213	
35	LM	142	
36	LN	203	
37	LO	204	
38	LP	187	
39	LQ	213	
40	LS	174	
41	LT	160	
42	LV	139	
43	LX	156	
44	LY	138	
45	Ld	120	
46	Le	131	
47	Lf	109	
48	Lh	935	
49	Li	110	
50	Lj	95	
51	Lq	217	
52	Cc	282	
53	Cd	436	
54	Ce	336	
55	Cf	570	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 138001 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	2152	46025	20547	8331	14995	2152	0	0

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	158	3359	1502	593	1106	158	0	0

- Molecule 3 is a RNA chain called RNA (161-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C3	98	2097	933	381	685	98	0	0

- Molecule 4 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CA	260	2144	1371	393	373	7	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein C8F11.04.

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

- Molecule 6 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CC	289	2388	1520	399	462	7	0	0

- 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	476	Total	C	N	O	S	0	0
			3851	2451	669	716	15		

- 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	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CK	232	Total	C	N	O	S	0	0
			1855	1165	363	323	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CL	390	Total	C	N	O	0	0
			2173	1307	446	420		

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	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
15	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	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	324	Total	C	N	O	S	0	0
			2535	1618	445	457	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	112	Total	C	N	O	S	0	0
			960	607	195	148	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	298	Total	C	N	O	S	0	0
			1750	1072	330	347	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
22	CT	458	Total	C	N	O	0	0
			2269	1353	458	458		

- 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 60S ribosomal subunit-like protein.

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

- Molecule 25 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	CY	324	Total 1608	C 960	N 324	O 324	0	0

- Molecule 26 is a protein called rRNA-processing protein.

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

- Molecule 27 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Cb	642	Total 5058	C 3216	N 918	O 911	S 13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LB	341	Total 2708	C 1721	N 493	O 482	S 12	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LE	170	Total 1338	C 861	N 241	O 233	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	196	Total 1583	C 1021	N 287	O 270	S 5	0	0

- 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
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	154	Total	C	N	O	S	0	0
			1212	758	233	218	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 60S ribosomal protein L20.

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

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LX	22	Total	C	N	O	0	0
			148	91	31	26		

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

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

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

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

- Molecule 46 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Le	131	Total	C	N	O	S	0	0
			1055	663	213	172	7		

- Molecule 47 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 48 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 49 is a protein called 60S ribosomal protein L36.

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

- Molecule 50 is a protein called Ribosomal protein L37.

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

- Molecule 51 is a protein called Ribosomal protein.

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

- Molecule 52 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Cc	236	Total	C	N	O	S	0	0
			1898	1208	337	343	10		

- Molecule 53 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Cd	342	Total	C	N	O	S	0	0
			2763	1743	533	483	4		

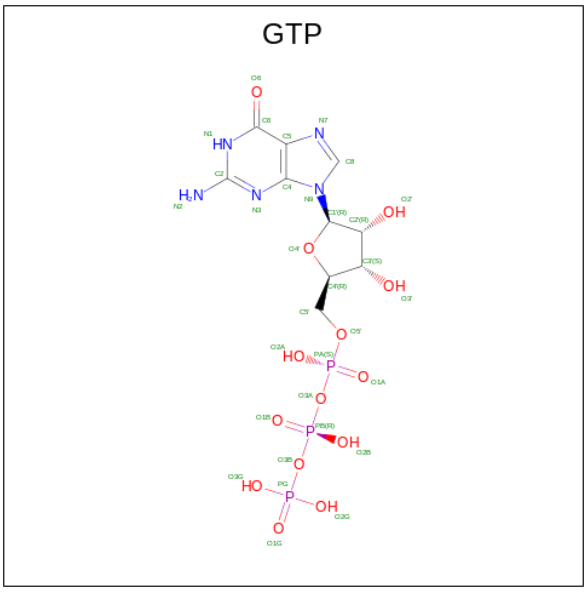
- Molecule 54 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ce	194	Total	C	N	O	S	0	0
			1609	1020	304	276	9		

- Molecule 55 is a protein called 60S ribosome biogenesis protein Rrp14.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Cf	59	Total	C	N	O	0	0
			513	310	111	92		

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

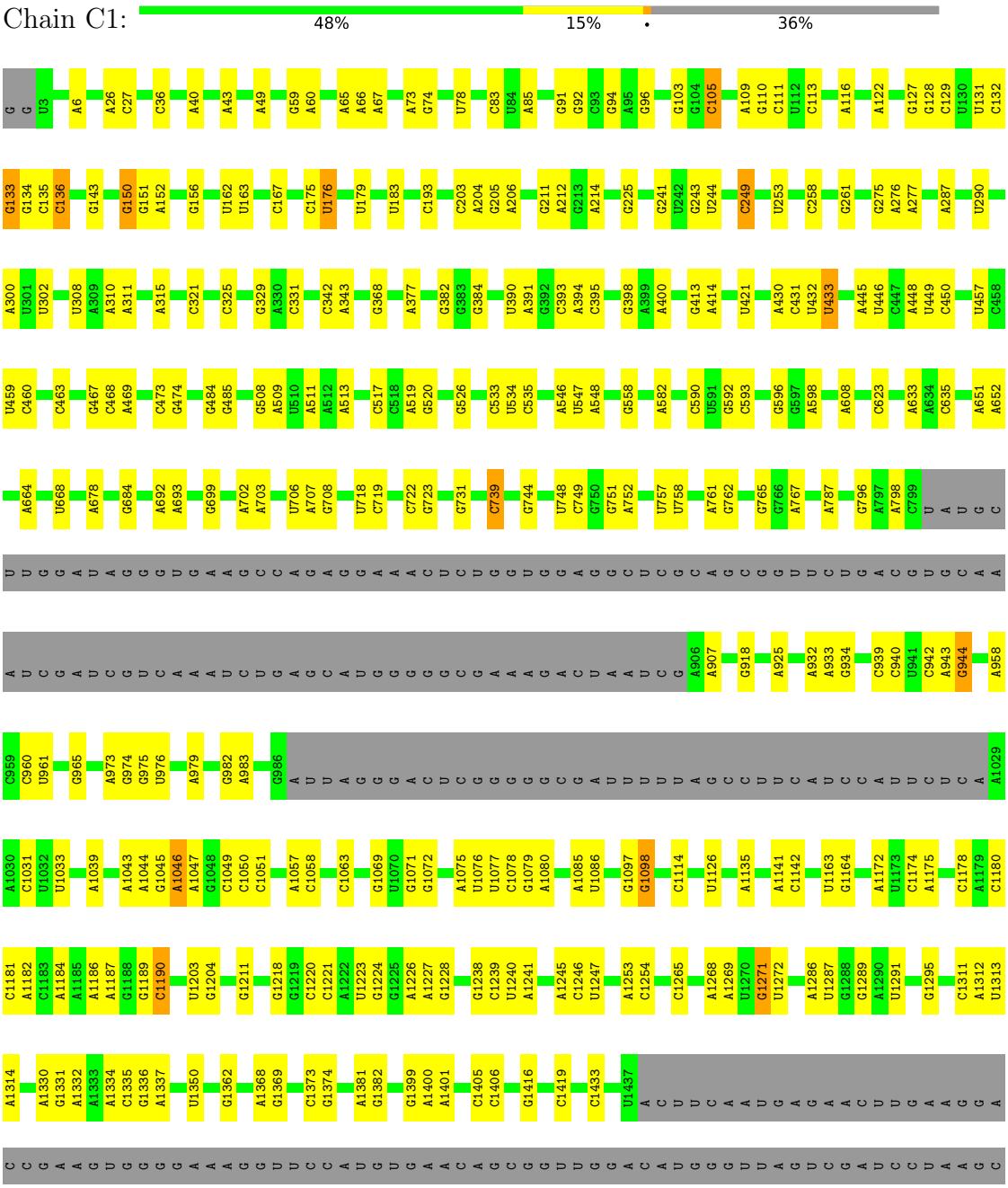
Mol	Chain	Residues	Atoms		AltConf
57	CQ	1	Total	Zn	0
			1	1	
57	Lj	1	Total	Zn	0
			1	1	
57	Ce	1	Total	Zn	0
			1	1	

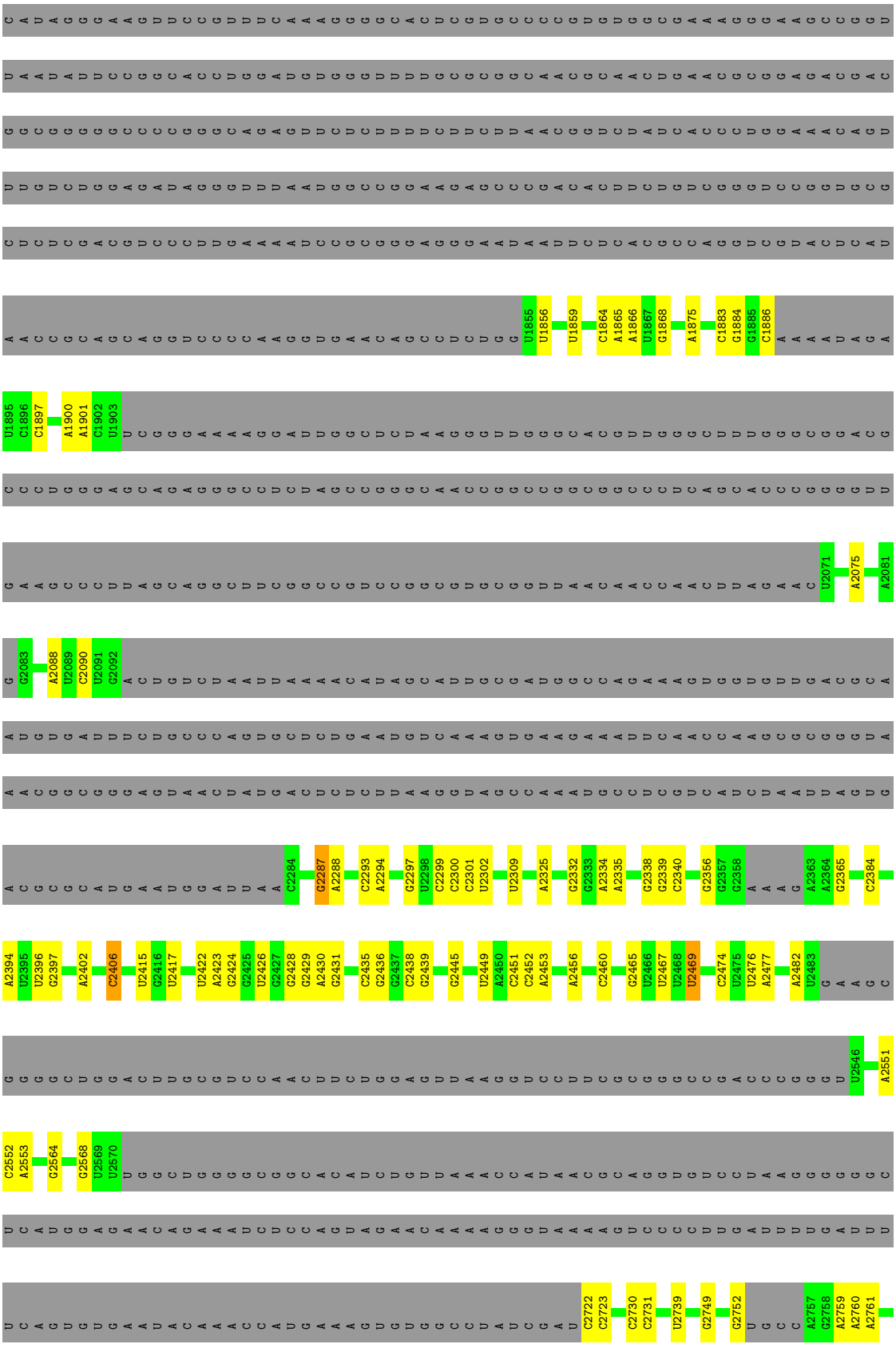
3 Residue-property plots (i)

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:




U1855
U1856
U1859
C1864
A1865
A1866
U1867
G1868
A1875
C1883
G1884
G1885
C1886
U1895
C1896
C1897
A1900
A1901
C1902
U1903
U2071
A2075
A2081
G2083
A2088
U2089
C2090
U2091
G2092
C2284
G2287
A2288
C2293
A2294
G2297
U2298
C2299
C2300
C2301
U2302
U2309
A2325
G2332
G2333
A2334
A2335
G2338
G2339
C2340
G2356
G2357
G2358
A2363
A2364
G2365
C2384
A2394
U2395
U2396
G2397
A2402
C2406
U2415
G2416
U2417
U2422
A2423
G2424
G2425
U2426
G2427
G2428
G2429
A2430
G2431
C2435
G2436
G2437
C2438
G2439
G2445
U2449
A2450
C2451
C2452
A2453
A2456
C2460
G2465
U2466
U2467
U2468
U2469
C2474
U2475
U2476
A2477
A2482
U2483
U2546
A2551
C2552
A2553
G2564
G2568
U2569
U2570
C2722
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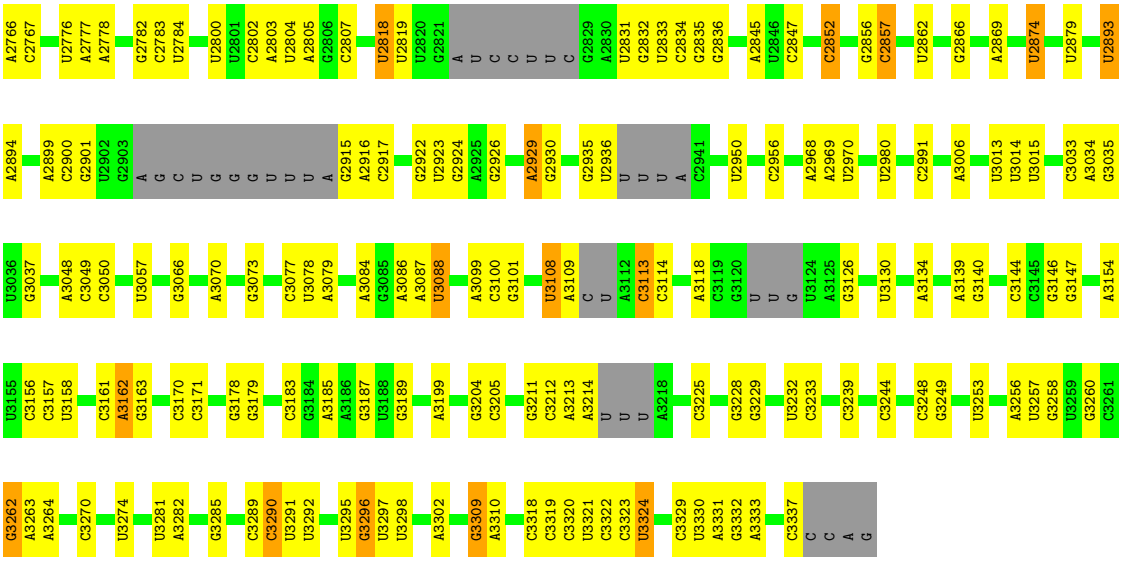
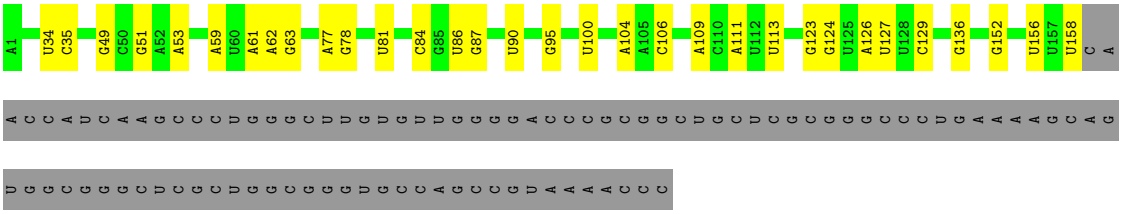
A2757
G2758
A2759
A2760
A2761



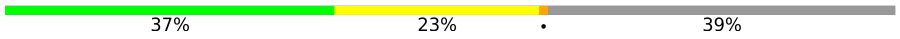
• Molecule 2: RNA (256-MER)

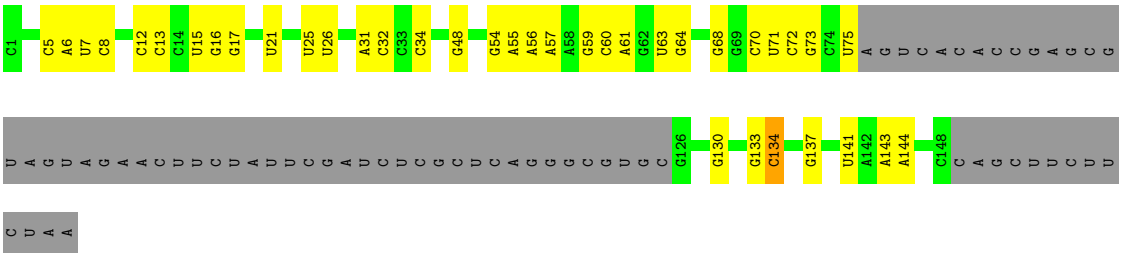
Chain C2:



• Molecule 3: RNA (161-MER)

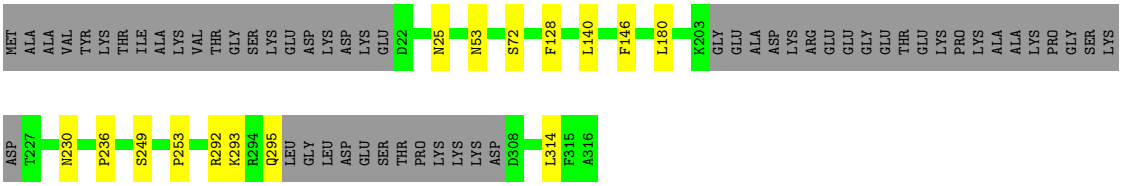
Chain C3:





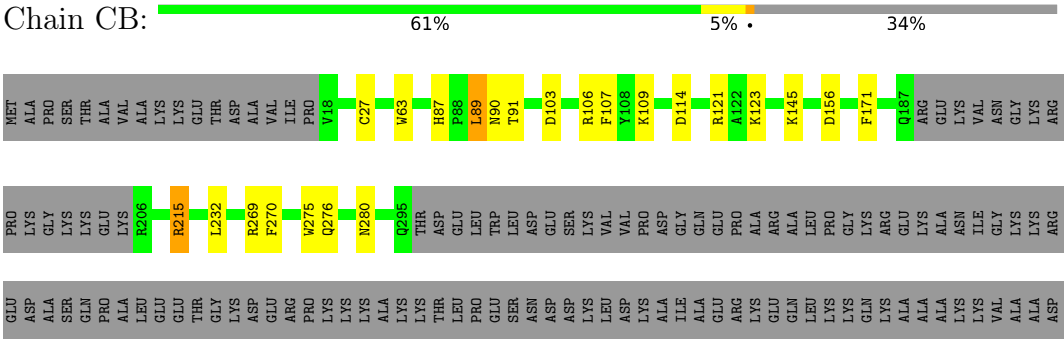
• Molecule 4: Brix domain-containing protein

Chain CA:



• Molecule 5: Ribosome biogenesis protein C8F11.04

Chain CB:

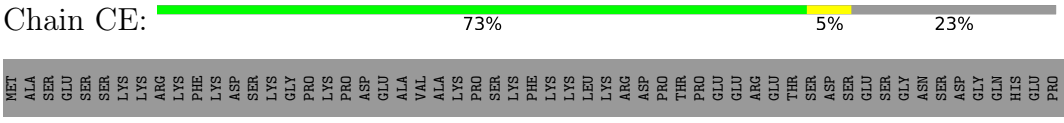


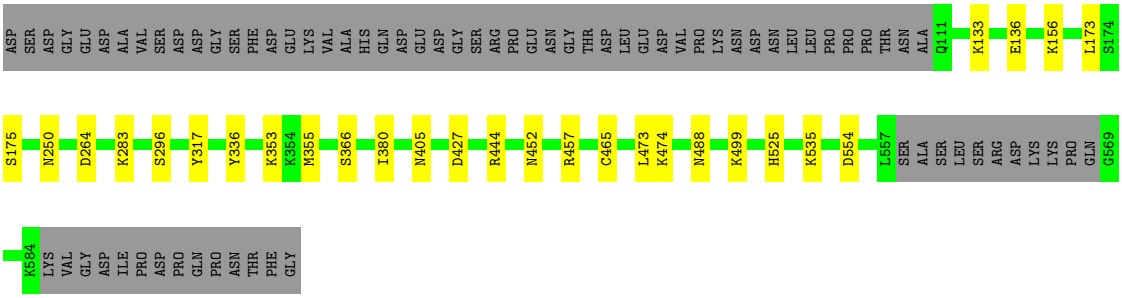
• Molecule 6: Ribosome biogenesis protein ERB1

Chain CC:

• Molecule 7: RNA helicase

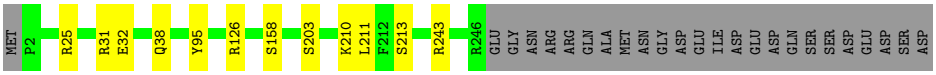
Chain CE:





• Molecule 8: Ribosome assembly factor mrt4

Chain CF:

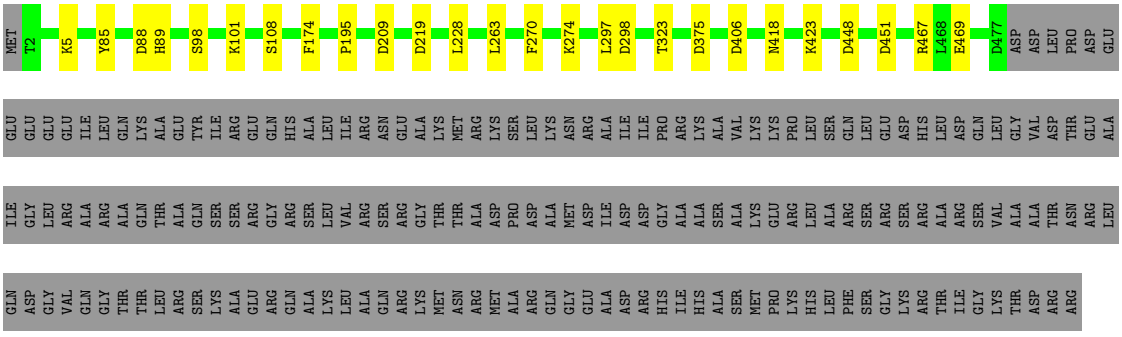


• Molecule 9: 60S ribosome subunit biogenesis protein NIP7

Chain CG:

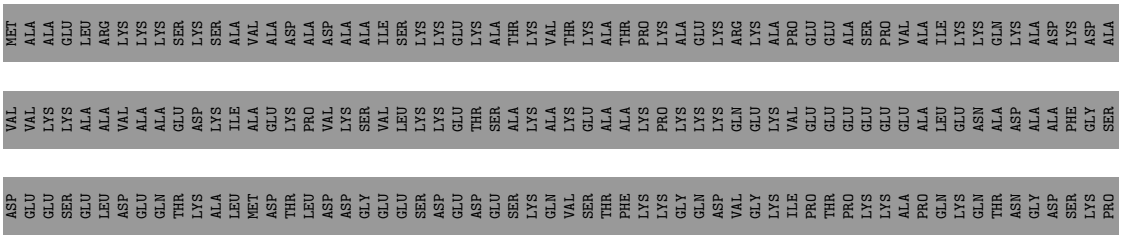
• Molecule 10: Nucleolar GTP-binding protein 1

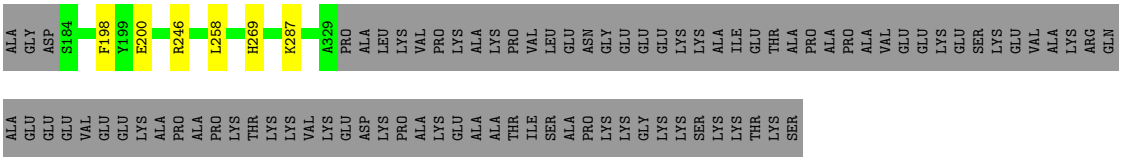
Chain CH:



• Molecule 11: Putative RNA-binding protein

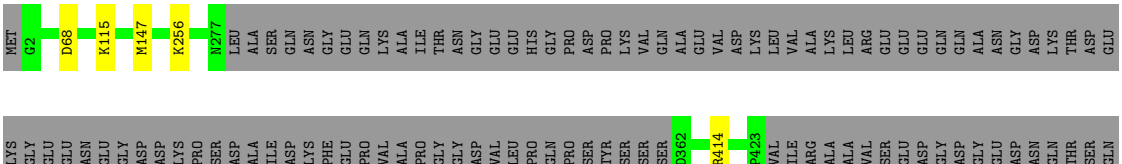
Chain CI:





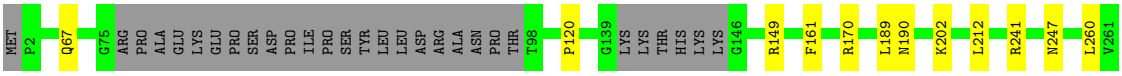
• Molecule 12: Pescadillo homolog

Chain CJ:



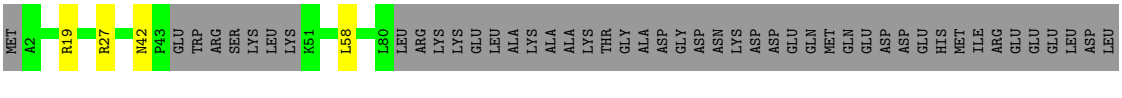
• Molecule 13: Ribosome biogenesis protein NSA2 homolog

Chain CK:



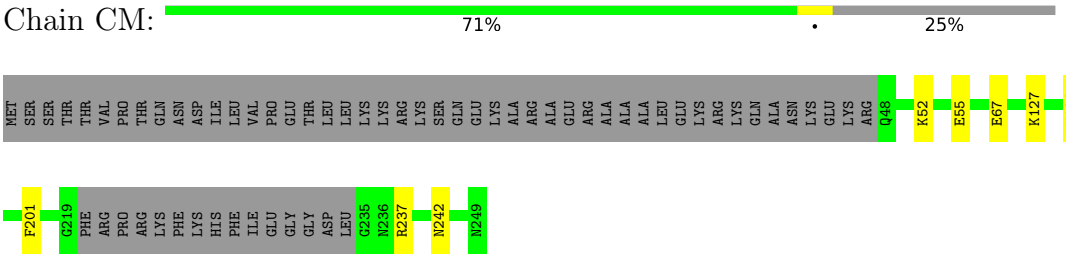
• Molecule 14: Putative GTP binding protein

Chain CL:



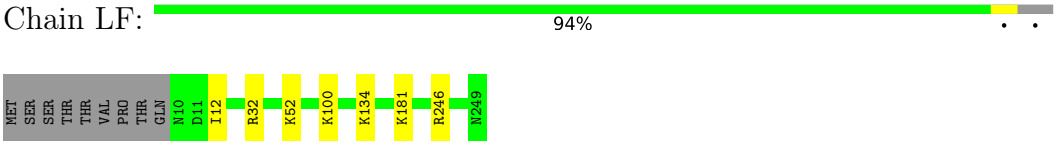
• Molecule 15: 60S ribosomal protein l7-like protein

Chain CM:



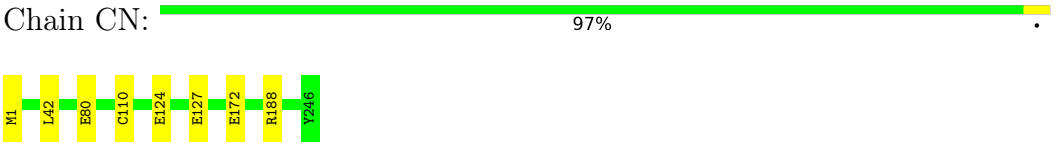
• Molecule 15: 60S ribosomal protein l7-like protein

Chain LF:



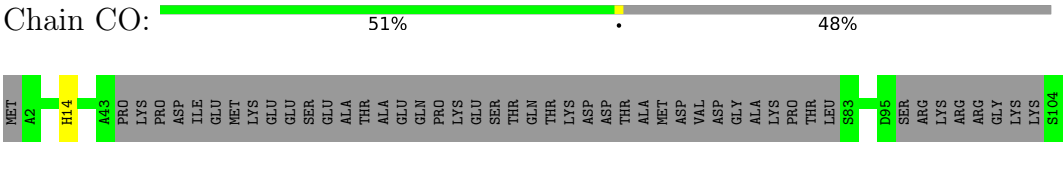
• Molecule 16: Eukaryotic translation initiation factor 6

Chain CN:



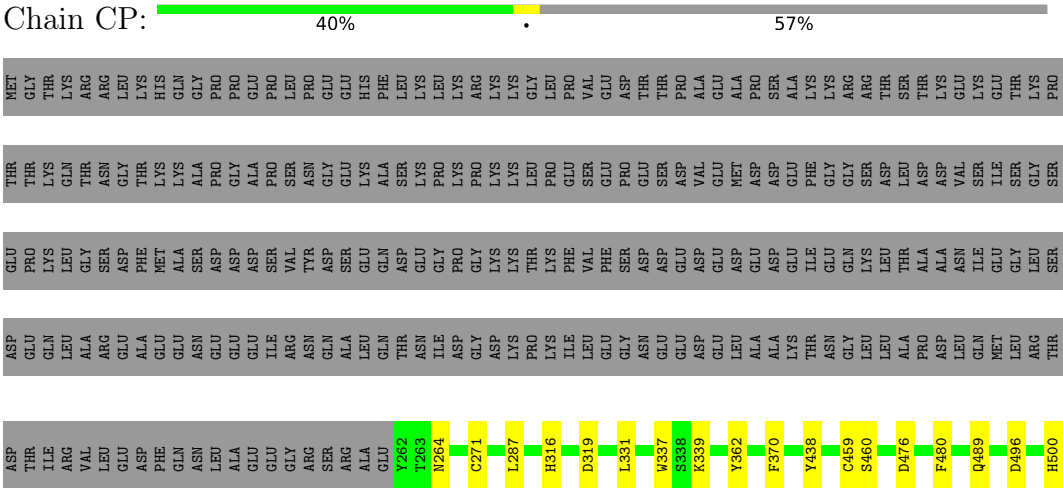
• Molecule 17: DUF2423 domain-containing protein

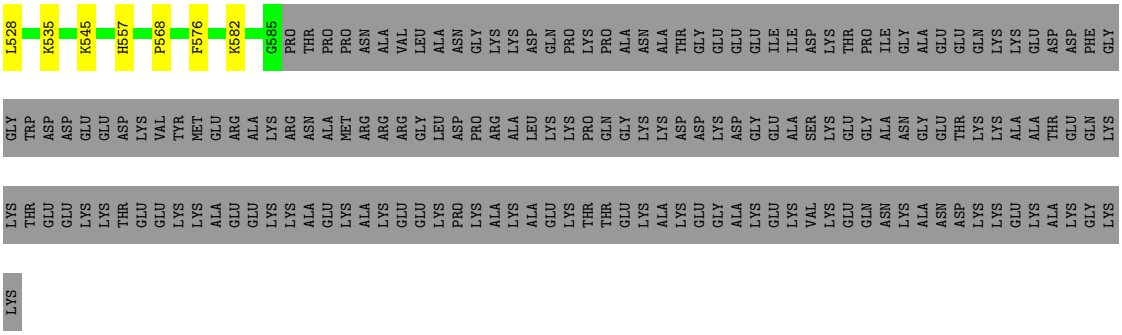
Chain CO:



• Molecule 18: RNA methyltransferase nop2-like protein

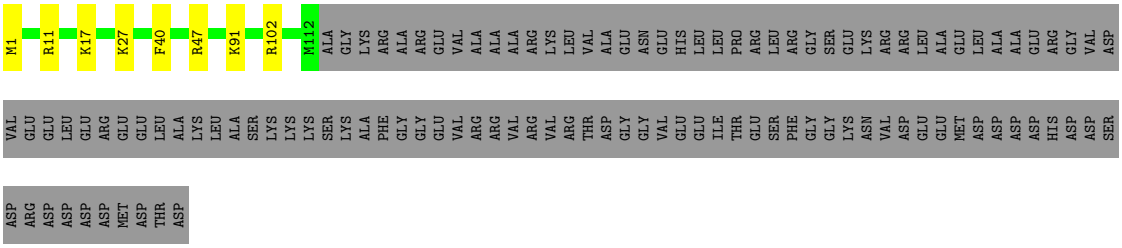
Chain CP:





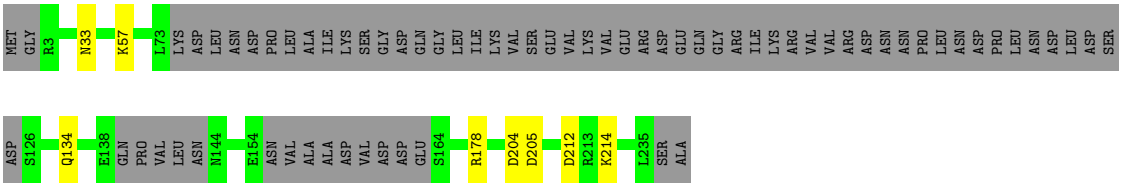
• Molecule 19: Ribosome biogenesis protein RLP24

Chain CQ:



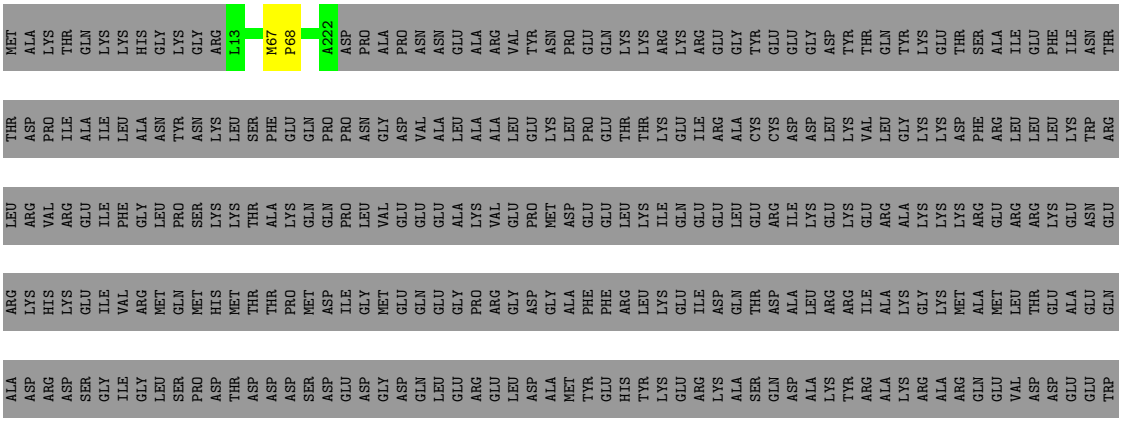
• Molecule 20: Nucleolar protein 16

Chain CR:



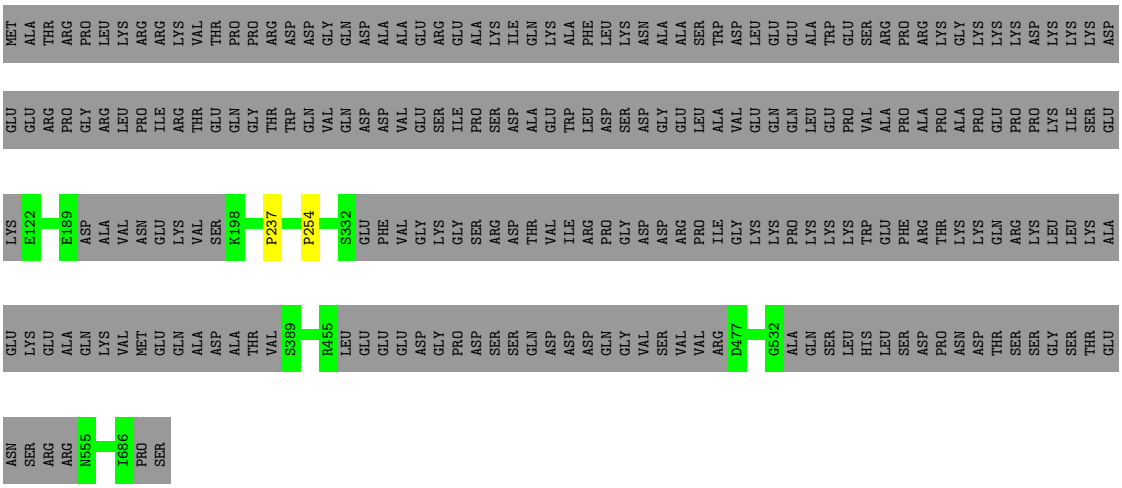
• Molecule 21: AdoMet-dependent rRNA methyltransferase SPB1

Chain CS:



• Molecule 22: Nucleolar complex-associated protein 3

Chain CT:

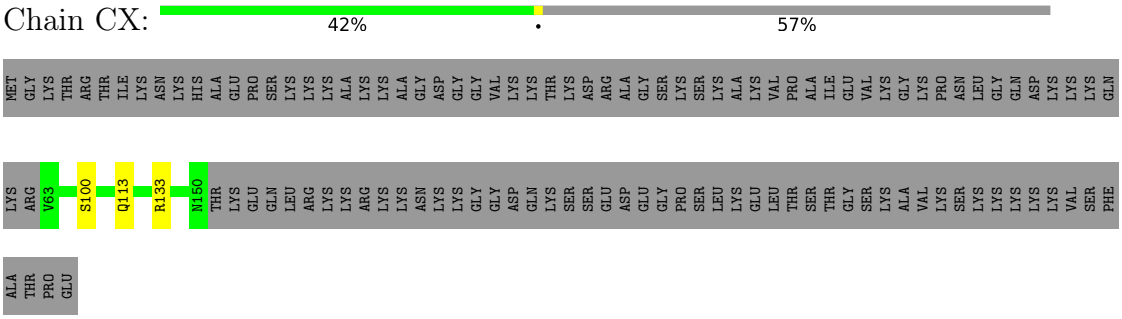


• Molecule 23: rRNA-processing protein EBP2

Chain CU:

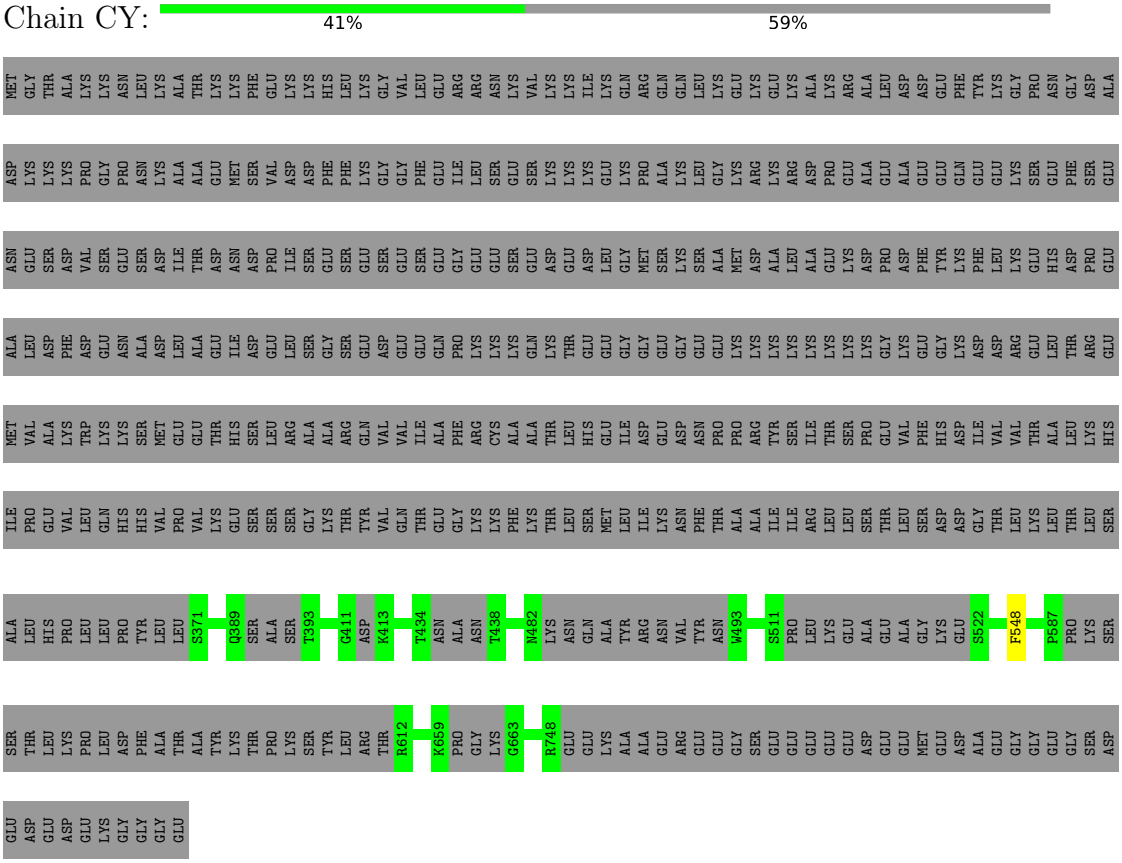
• Molecule 24: 60S ribosomal subunit-like protein

Chain CX:



• Molecule 25: Putative NOC2 family protein

Chain CY:

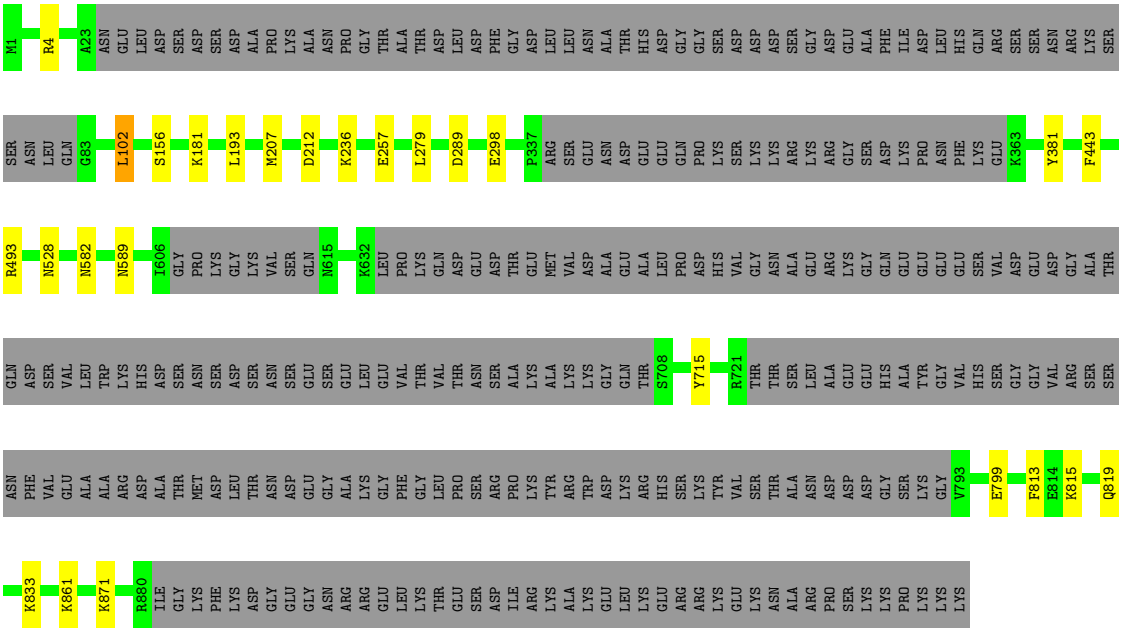


• Molecule 26: rRNA-processing protein

Chain Cz:

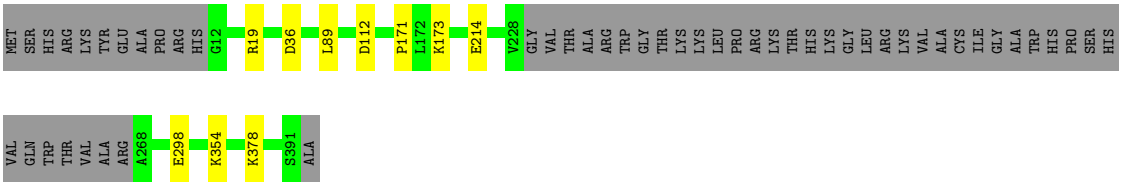
• Molecule 27: ATP-dependent RNA helicase DBP10

Chain Cb:



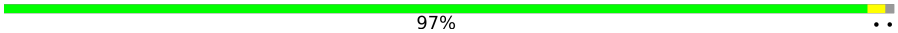
• Molecule 28: 60S ribosomal protein L3-like protein

Chain LB:



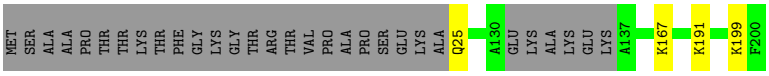
• Molecule 29: 60S ribosomal protein L4-like protein

Chain LC:



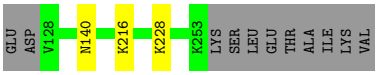
• Molecule 30: 60S ribosomal protein L6

Chain LE:



• Molecule 31: 60S ribosomal protein L8

Chain LG:

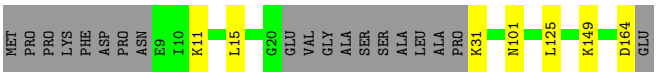


• Molecule 32: 60S ribosomal protein l9-like protein

Chain LH:

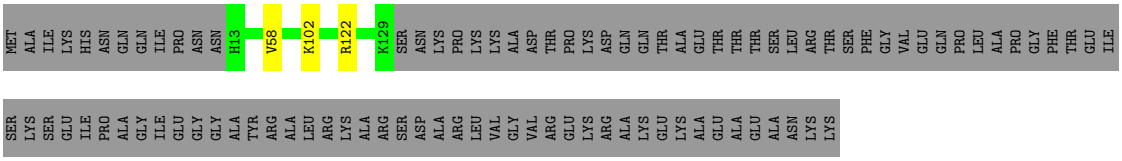
• Molecule 33: 60S ribosomal protein L12-like protein

Chain LK:



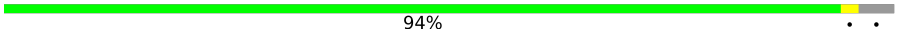
• Molecule 34: 60S ribosomal protein L13

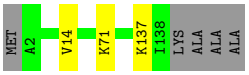
Chain LL:



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

Chain LM:



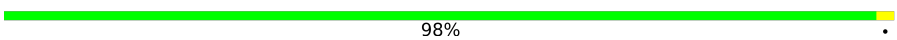


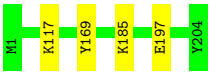
• Molecule 36: Ribosomal protein L15

Chain LN:

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

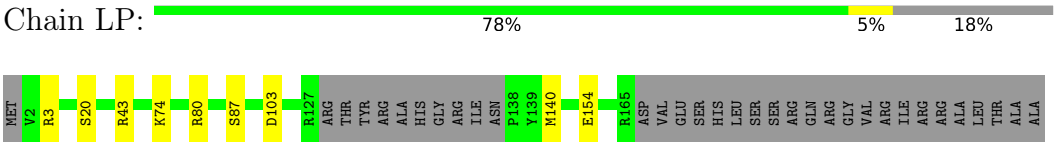
Chain LO:





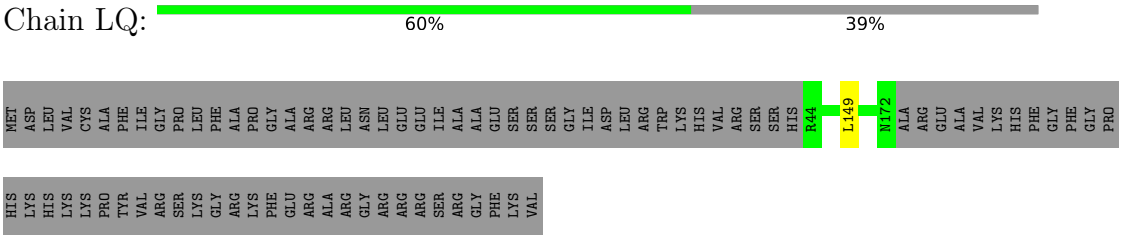
• Molecule 38: 60S ribosomal protein l17-like protein

Chain LP:



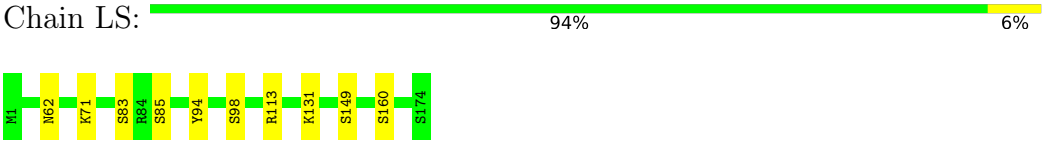
• Molecule 39: Ribosomal protein L18-like protein

Chain LQ:



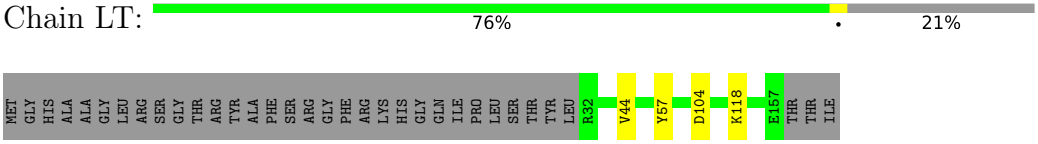
• Molecule 40: 60S ribosomal protein L20

Chain LS:



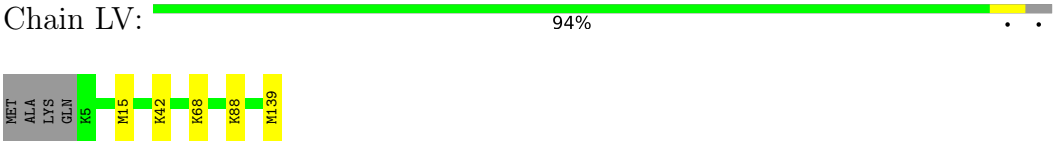
• Molecule 41: 60S ribosomal protein l21-like protein

Chain LT:



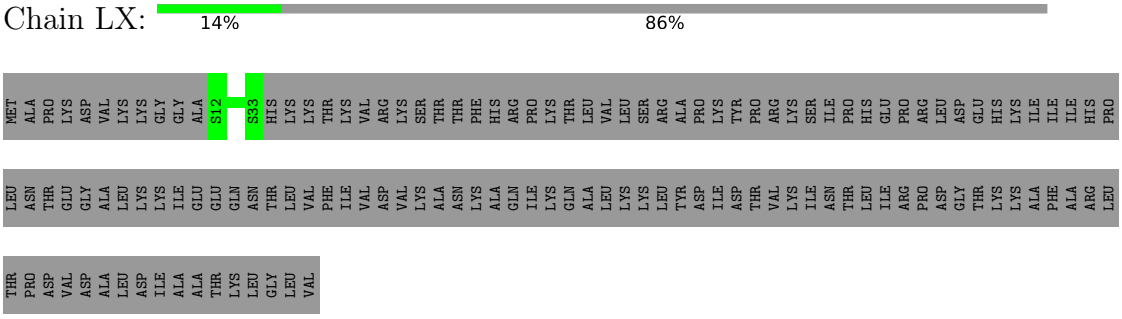
• Molecule 42: 60S ribosomal protein l23-like protein

Chain LV:



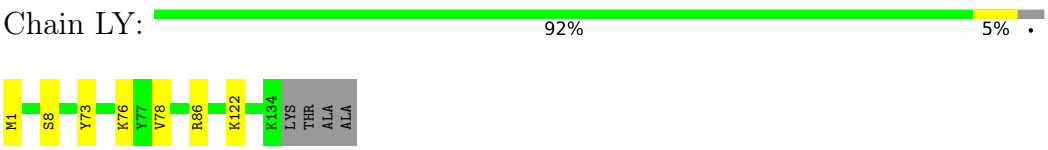
• Molecule 43: 60S ribosomal protein L25-like protein

Chain LX:



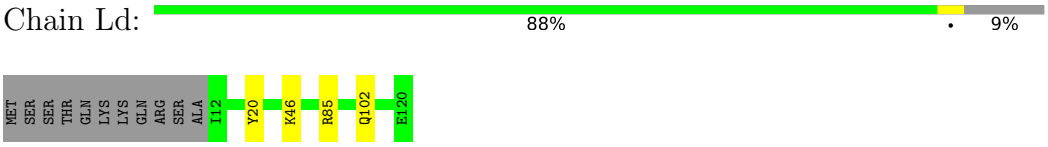
• Molecule 44: 60S ribosomal protein L26-like protein

Chain LY:



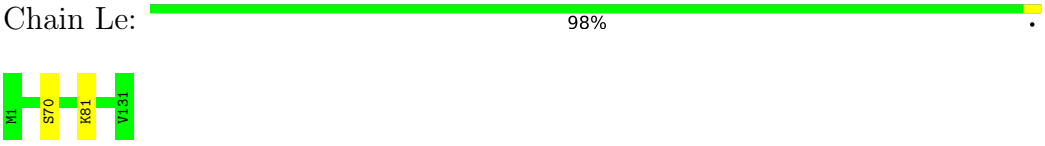
• Molecule 45: Putative 60S ribosomal protein

Chain Ld:



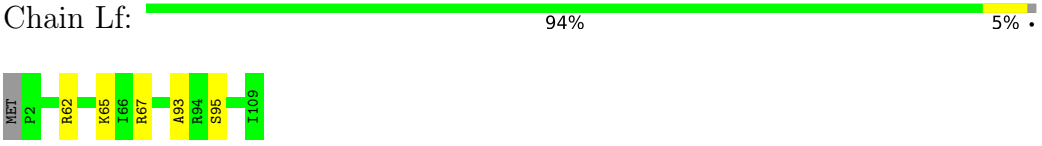
• Molecule 46: 60S ribosomal protein L32-like protein

Chain Le:



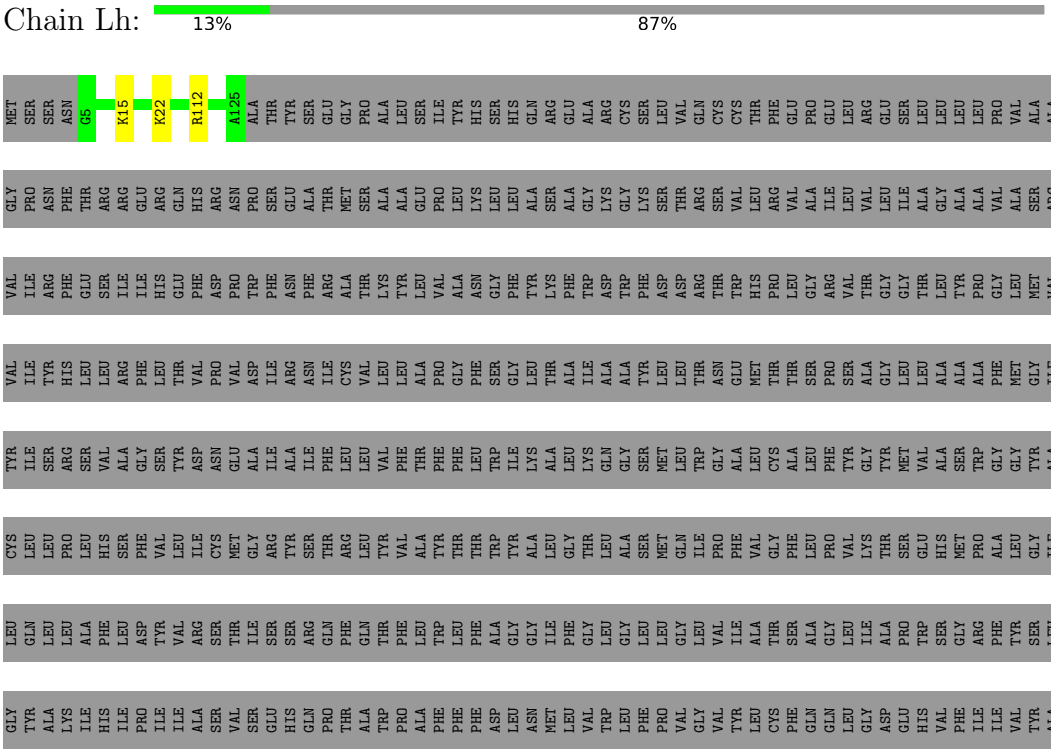
• Molecule 47: 60S ribosomal protein l33-like protein

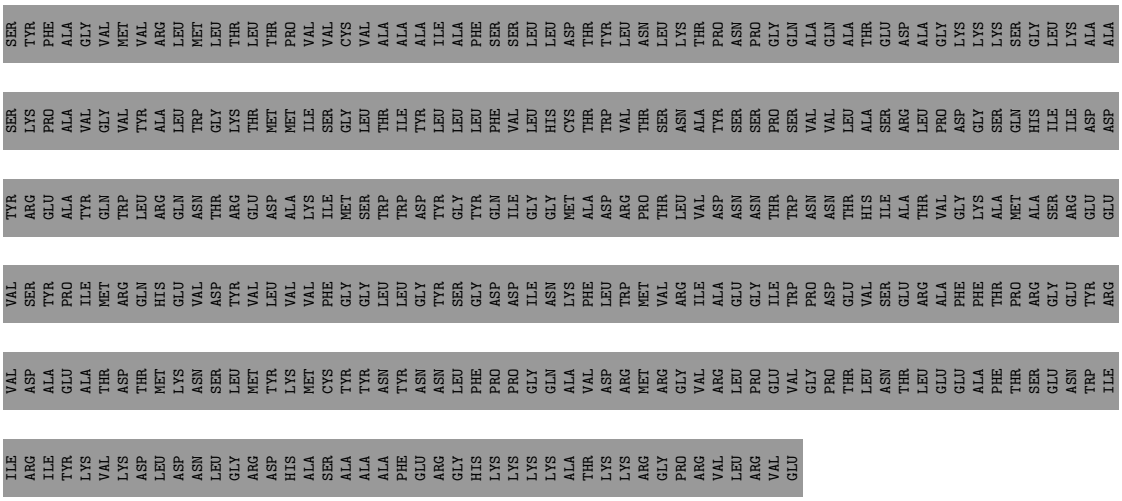
Chain Lf:



• Molecule 48: dolichyl-diphosphooligosaccharide--protein glycotransferase

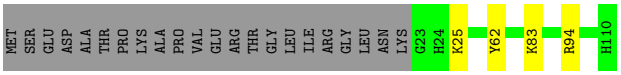
Chain Lh:





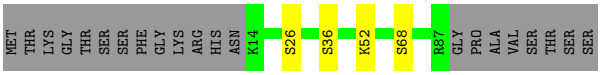
• Molecule 49: 60S ribosomal protein L36

Chain Li:



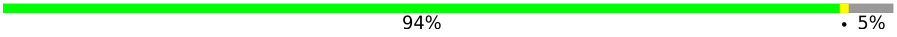
• Molecule 50: Ribosomal protein L37

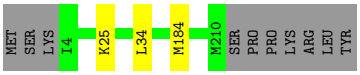
Chain Lj:



• Molecule 51: Ribosomal protein

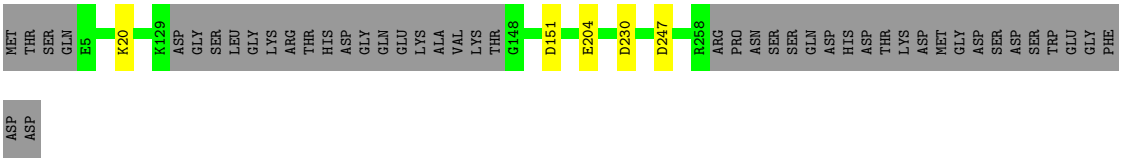
Chain Lq:





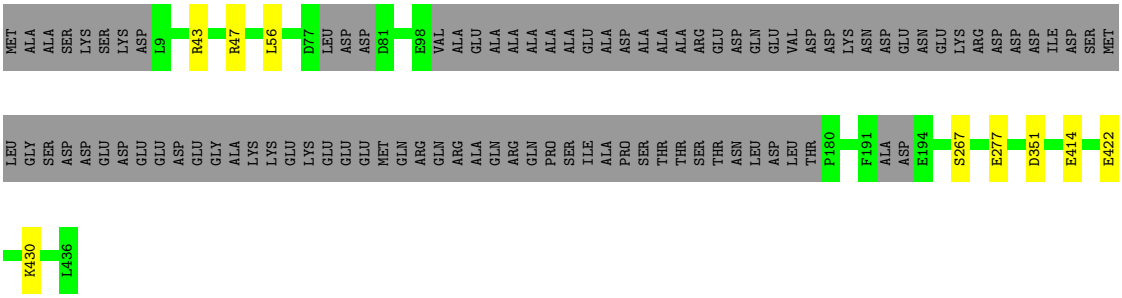
• Molecule 52: Ribosomal RNA-processing protein 1

Chain Cc:



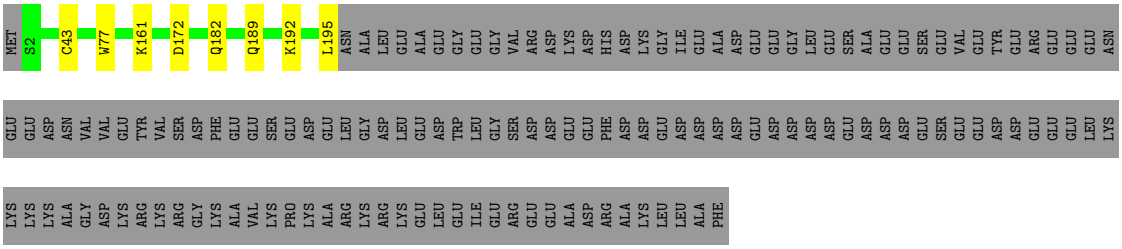
• Molecule 53: Brix domain-containing protein

Chain Cd:



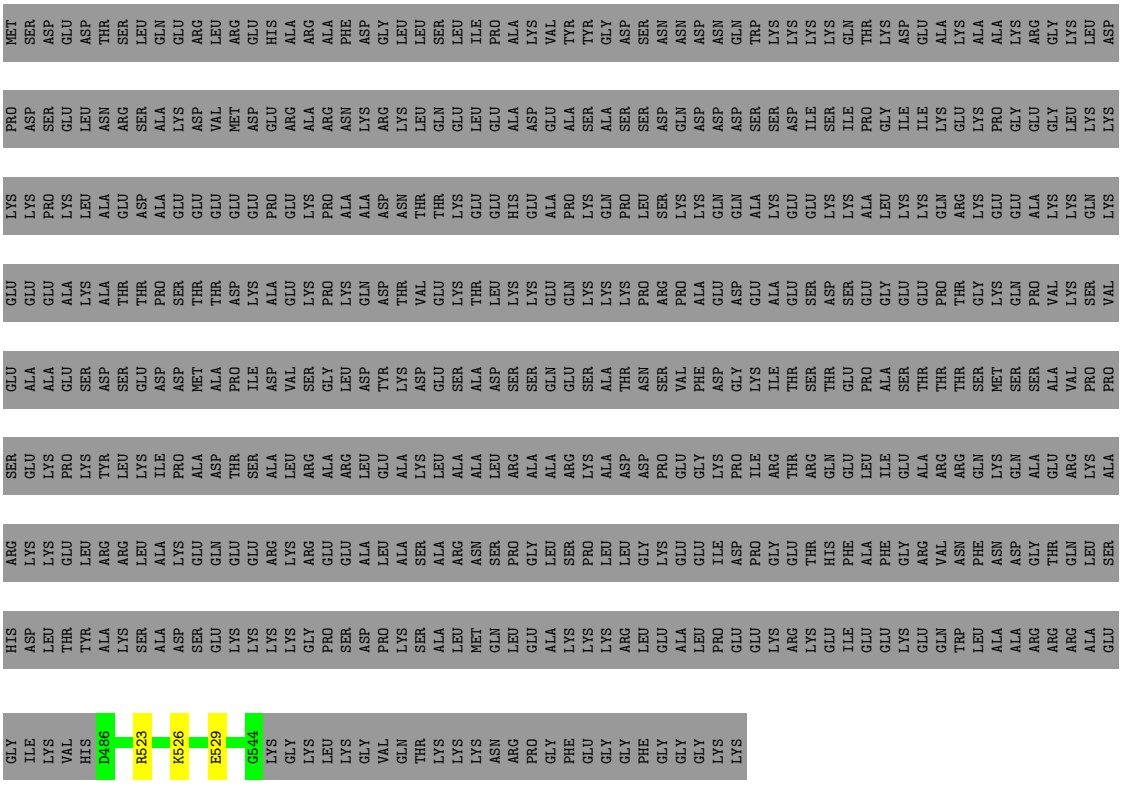
• Molecule 54: Protein MAK16

Chain Ce:



• Molecule 55: 60S ribosome biogenesis protein Rrp14

Chain Cf:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16465	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: GTP, 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	0.43	0/51490	1.00	169/80245 (0.2%)
2	C2	0.39	0/3754	0.90	1/5846 (0.0%)
3	C3	0.39	0/2342	1.07	11/3649 (0.3%)
4	CA	0.30	0/2190	0.61	1/2940 (0.0%)
5	CB	0.36	0/2109	0.72	3/2866 (0.1%)
6	CC	0.29	0/2459	0.56	0/3350
7	CE	0.31	0/3743	0.64	5/5045 (0.1%)
8	CF	0.30	0/1982	0.65	0/2671
9	CG	0.32	0/1422	0.70	2/1920 (0.1%)
10	CH	0.35	0/3927	0.70	7/5307 (0.1%)
11	CI	0.33	0/1225	0.68	1/1645 (0.1%)
12	CJ	0.27	0/3189	0.53	0/4309
13	CK	0.30	0/1885	0.64	2/2529 (0.1%)
14	CL	0.26	0/2178	0.48	0/2983
15	CM	0.32	0/1555	0.67	2/2091 (0.1%)
15	LF	0.29	0/2004	0.56	0/2686
16	CN	0.29	0/1881	0.64	1/2560 (0.0%)
17	CO	0.29	0/470	0.55	0/619
18	CP	0.33	0/2594	0.68	4/3514 (0.1%)
19	CQ	0.32	0/981	0.70	1/1301 (0.1%)
20	CR	0.29	0/1369	0.64	1/1828 (0.1%)
21	CS	0.26	0/1762	0.45	0/2417
22	CT	0.28	0/2264	0.47	0/3149
23	CU	0.33	0/1428	0.66	1/1910 (0.1%)
24	CX	0.27	0/705	0.57	0/938
25	CY	0.31	0/1600	0.47	0/2220
26	Cz	0.29	0/598	0.56	0/785
27	Cb	0.32	0/5150	0.68	4/6936 (0.1%)
28	LB	0.33	0/2760	0.65	2/3701 (0.1%)
29	LC	0.32	0/2809	0.57	0/3787
30	LE	0.30	0/1363	0.55	0/1833
31	LG	0.32	0/1606	0.57	0/2149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LH	0.29	0/1516	0.58	1/2038 (0.0%)
33	LK	0.30	0/1124	0.70	2/1507 (0.1%)
34	LL	0.34	0/983	0.65	0/1318
35	LM	0.29	0/1120	0.57	0/1507
36	LN	0.30	0/1595	0.62	0/2132
37	LO	0.31	0/1652	0.56	0/2215
38	LP	0.31	0/1231	0.61	0/1658
39	LQ	0.30	0/1033	0.63	0/1391
40	LS	0.31	0/1468	0.61	0/1975
41	LT	0.28	0/1033	0.68	1/1389 (0.1%)
42	LV	0.32	0/1013	0.57	0/1361
43	LX	0.24	0/148	0.35	0/194
44	LY	0.29	0/1079	0.61	0/1443
45	Ld	0.26	0/904	0.61	0/1209
46	Le	0.29	0/1073	0.56	0/1431
47	Lf	0.33	0/883	0.63	0/1187
48	Lh	0.28	0/1006	0.59	0/1338
49	Li	0.30	0/738	0.64	0/971
50	Lj	0.32	0/606	0.65	0/803
51	Lq	0.25	0/1621	0.55	0/2180
52	Cc	0.31	0/1934	0.57	0/2614
53	Cd	0.31	0/2818	0.61	0/3786
54	Ce	0.30	0/1638	0.56	0/2196
55	Cf	0.27	0/514	0.57	0/669
All	All	0.36	0/145524	0.80	222/208241 (0.1%)

There are no bond length outliers.

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1050	C	N3-C2-O2	-11.53	113.83	121.90
1	C1	136	C	N3-C2-O2	-10.12	114.82	121.90
1	C1	2852	C	N3-C2-O2	-10.01	114.89	121.90
1	C1	939	C	N3-C2-O2	-9.73	115.09	121.90
28	LB	171	PRO	CA-N-CD	-9.15	98.69	111.50
1	C1	1190	C	N1-C2-O2	8.92	124.25	118.90
1	C1	2723	C	N3-C2-O2	-8.72	115.79	121.90
10	CH	451	ASP	CB-CG-OD2	8.60	126.03	118.30
1	C1	3320	C	C6-N1-C2	-8.46	116.92	120.30
1	C1	1050	C	N1-C2-O2	8.45	123.97	118.90
1	C1	2300	C	N3-C2-O2	-8.42	116.01	121.90
28	LB	36	ASP	CB-CG-OD1	8.34	125.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3290	C	N3-C2-O2	-8.19	116.17	121.90
1	C1	2438	C	C6-N1-C2	-8.18	117.03	120.30
1	C1	36	C	N1-C2-O2	8.07	123.74	118.90
1	C1	136	C	N1-C2-O2	7.98	123.69	118.90
18	CP	476	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C1	3114	C	N3-C2-O2	-7.84	116.41	121.90
1	C1	1050	C	C6-N1-C2	-7.84	117.17	120.30
1	C1	1190	C	N3-C2-O2	-7.78	116.45	121.90
3	C3	70	C	C5-C6-N1	7.72	124.86	121.00
1	C1	2406	C	C5-C6-N1	7.71	124.85	121.00
10	CH	195	PRO	CA-N-CD	-7.70	100.72	111.50
10	CH	375	ASP	CB-CG-OD1	7.70	125.23	118.30
10	CH	228	LEU	CA-CB-CG	7.67	132.95	115.30
1	C1	2406	C	C2-N1-C1'	7.61	127.17	118.80
1	C1	249	C	N1-C2-O2	7.60	123.46	118.90
1	C1	1051	C	N3-C2-O2	-7.59	116.59	121.90
1	C1	249	C	N3-C2-O2	-7.56	116.61	121.90
18	CP	568	PRO	CA-N-CD	-7.46	101.06	111.50
1	C1	2852	C	C6-N1-C2	-7.44	117.32	120.30
1	C1	2417	U	C2-N1-C1'	7.43	126.61	117.70
1	C1	635	C	N1-C2-O2	7.35	123.31	118.90
1	C1	3320	C	N3-C2-O2	-7.27	116.81	121.90
1	C1	2300	C	C6-N1-C2	-7.26	117.40	120.30
1	C1	739	C	C2-N1-C1'	7.17	126.69	118.80
1	C1	3088	U	C2-N1-C1'	7.15	126.28	117.70
1	C1	1190	C	C2-N1-C1'	7.14	126.66	118.80
1	C1	1406	C	N3-C2-O2	-7.05	116.96	121.90
1	C1	2866	G	N3-C2-N2	-6.95	115.03	119.90
10	CH	219	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C1	2406	C	C6-N1-C2	-6.83	117.57	120.30
3	C3	34	C	N3-C2-O2	-6.80	117.14	121.90
7	CE	264	ASP	CB-CG-OD1	6.73	124.36	118.30
1	C1	3113	C	N1-C2-O2	6.72	122.93	118.90
1	C1	433	U	C2-N1-C1'	6.71	125.75	117.70
1	C1	2406	C	N1-C2-O2	6.71	122.92	118.90
1	C1	127	G	N3-C4-N9	6.64	129.98	126.00
1	C1	1049	C	N1-C2-O2	6.62	122.87	118.90
27	Cb	102	LEU	CA-CB-CG	6.54	130.35	115.30
1	C1	2818	U	N1-C2-O2	6.46	127.32	122.80
1	C1	1098	G	C4-N9-C1'	6.45	134.88	126.50
1	C1	1049	C	N3-C2-O2	-6.44	117.39	121.90
1	C1	136	C	C6-N1-C2	-6.43	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3319	C	N1-C2-O2	6.42	122.75	118.90
1	C1	1406	C	C6-N1-C2	-6.40	117.74	120.30
3	C3	70	C	C6-N1-C2	-6.37	117.75	120.30
1	C1	2929	A	P-O3'-C3'	6.37	127.34	119.70
9	CG	107	PRO	CA-N-CD	-6.36	102.59	111.50
1	C1	2818	U	N3-C2-O2	-6.36	117.75	122.20
1	C1	3290	C	N1-C2-O2	6.35	122.71	118.90
1	C1	722	C	C2-N1-C1'	6.34	125.77	118.80
1	C1	3113	C	C2-N1-C1'	6.33	125.76	118.80
1	C1	2731	C	N1-C2-O2	6.30	122.68	118.90
1	C1	113	C	C2-N1-C1'	6.29	125.72	118.80
1	C1	463	C	C2-N1-C1'	6.29	125.72	118.80
1	C1	473	C	C2-N1-C1'	6.25	125.68	118.80
32	LH	37	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C1	1051	C	C6-N1-C2	-6.23	117.81	120.30
5	CB	232	LEU	CA-CB-CG	6.22	129.61	115.30
27	Cb	289	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C1	2991	C	N1-C2-O2	6.15	122.59	118.90
1	C1	2866	G	N9-C4-C5	6.11	107.84	105.40
1	C1	2417	U	N1-C2-O2	6.11	127.07	122.80
1	C1	2417	U	N3-C2-O2	-6.09	117.94	122.20
1	C1	635	C	C2-N1-C1'	6.07	125.48	118.80
16	CN	42	LEU	CA-CB-CG	6.07	129.25	115.30
1	C1	167	C	C2-N1-C1'	6.04	125.45	118.80
23	CU	275	MET	CB-CG-SD	6.03	130.50	112.40
10	CH	298	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C1	398	G	O4'-C1'-N9	6.02	113.01	108.20
3	C3	12	C	C2-N1-C1'	5.99	125.39	118.80
1	C1	83	C	C6-N1-C1'	5.97	127.97	120.80
1	C1	1271	G	O4'-C1'-N9	5.97	112.97	108.20
1	C1	83	C	N3-C2-O2	-5.94	117.75	121.90
1	C1	1265	C	N1-C2-O2	5.94	122.46	118.90
18	CP	287	LEU	CA-CB-CG	5.94	128.95	115.30
1	C1	939	C	C6-N1-C2	-5.85	117.96	120.30
1	C1	433	U	N1-C2-O2	5.84	126.89	122.80
1	C1	83	C	C2-N1-C1'	-5.83	112.38	118.80
1	C1	1265	C	N3-C2-O2	-5.83	117.82	121.90
1	C1	2438	C	N3-C2-O2	-5.82	117.83	121.90
3	C3	70	C	C2-N1-C1'	5.82	125.20	118.80
1	C1	2857	C	C2-N1-C1'	5.81	125.19	118.80
1	C1	635	C	N3-C2-O2	-5.80	117.84	121.90
1	C1	36	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	2287	G	C4-C5-N7	5.80	113.12	110.80
1	C1	3229	G	N3-C4-N9	5.77	129.46	126.00
1	C1	243	G	C4-N9-C1'	5.75	133.98	126.50
1	C1	2287	G	N9-C4-C5	-5.75	103.10	105.40
7	CE	427	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C1	1071	G	N1-C2-N2	-5.75	111.02	116.20
1	C1	1072	G	N1-C2-N2	-5.75	111.03	116.20
1	C1	1072	G	N1-C6-O6	-5.75	116.45	119.90
5	CB	156	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C1	2287	G	C6-C5-N7	-5.72	126.97	130.40
1	C1	3108	U	N1-C2-O2	5.71	126.80	122.80
27	Cb	207	MET	CB-CG-SD	5.70	129.50	112.40
10	CH	263	LEU	CA-CB-CG	5.68	128.37	115.30
1	C1	1350	U	N1-C2-O2	5.67	126.77	122.80
1	C1	939	C	N1-C2-N3	5.67	123.17	119.20
1	C1	1071	G	N3-C2-N2	5.63	123.84	119.90
1	C1	2287	G	C8-N9-C1'	-5.61	119.71	127.00
1	C1	3108	U	N3-C2-O2	-5.61	118.27	122.20
1	C1	1098	G	C8-N9-C1'	-5.59	119.73	127.00
3	C3	70	C	N1-C2-O2	5.59	122.25	118.90
1	C1	3319	C	C2-N1-C1'	5.58	124.94	118.80
1	C1	83	C	N3-C4-N4	-5.58	114.09	118.00
3	C3	13	C	N3-C2-O2	-5.57	118.00	121.90
1	C1	1239	C	C6-N1-C2	-5.56	118.08	120.30
1	C1	243	G	N3-C4-N9	5.54	129.32	126.00
1	C1	2287	G	C4-N9-C1'	5.54	133.70	126.50
1	C1	2340	C	C2-N1-C1'	5.54	124.89	118.80
1	C1	2866	G	N3-C4-N9	-5.53	122.68	126.00
7	CE	380	ILE	CG1-CB-CG2	-5.53	99.23	111.40
1	C1	944	G	N1-C6-O6	-5.53	116.58	119.90
1	C1	2731	C	C2-N1-C1'	5.51	124.87	118.80
1	C1	1405	C	N1-C2-O2	5.51	122.21	118.90
1	C1	150	G	P-O3'-C3'	5.51	126.31	119.70
1	C1	3309	G	N3-C4-C5	-5.49	125.86	128.60
20	CR	205	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C1	127	G	N9-C4-C5	-5.46	103.22	105.40
1	C1	2474	C	N3-C2-O2	-5.46	118.08	121.90
1	C1	3320	C	N1-C2-N3	5.46	123.02	119.20
1	C1	127	G	C8-N9-C1'	-5.45	119.92	127.00
1	C1	83	C	C5-C4-N4	5.43	124.00	120.20
2	C2	156	U	C2-N1-C1'	5.43	124.21	117.70
3	C3	134	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3324	U	C2-N1-C1'	5.39	124.17	117.70
3	C3	34	C	C6-N1-C1'	5.39	127.27	120.80
1	C1	2893	U	N3-C2-O2	-5.39	118.43	122.20
1	C1	3296	G	N1-C2-N2	-5.38	111.36	116.20
1	C1	27	C	N3-C2-O2	-5.38	118.14	121.90
13	CK	120	PRO	CA-N-CD	-5.37	103.99	111.50
1	C1	105	C	C2-N1-C1'	5.36	124.70	118.80
1	C1	133	G	N3-C4-C5	-5.36	125.92	128.60
5	CB	215	ARG	CA-CB-CG	5.36	125.19	113.40
1	C1	3233	C	N1-C2-O2	5.35	122.11	118.90
1	C1	2299	C	N1-C2-O2	5.34	122.10	118.90
1	C1	3162	A	P-O3'-C3'	5.33	126.09	119.70
27	Cb	279	LEU	CA-CB-CG	5.33	127.55	115.30
1	C1	2723	C	C6-N1-C2	-5.32	118.17	120.30
1	C1	2460	C	C2-N1-C1'	5.32	124.65	118.80
1	C1	27	C	N1-C2-O2	5.32	122.09	118.90
15	CM	132	MET	CG-SD-CE	5.32	108.71	100.20
3	C3	134	C	N1-C2-O2	5.31	122.09	118.90
1	C1	2991	C	N3-C2-O2	-5.31	118.19	121.90
1	C1	3114	C	C6-N1-C2	-5.31	118.18	120.30
1	C1	176	U	N1-C2-O2	5.30	126.51	122.80
1	C1	2915	G	C4-N9-C1'	5.30	133.39	126.50
1	C1	1190	C	C6-N1-C2	-5.29	118.18	120.30
19	CQ	102	ARG	CG-CD-NE	5.29	122.92	111.80
1	C1	2752	G	C5-C6-O6	5.29	131.78	128.60
1	C1	3289	C	N1-C2-O2	5.28	122.06	118.90
1	C1	162	U	N3-C2-O2	-5.27	118.51	122.20
1	C1	2922	G	C4-N9-C1'	5.27	133.36	126.50
1	C1	243	G	N3-C4-C5	-5.27	125.96	128.60
1	C1	175	C	C2-N1-C1'	5.26	124.59	118.80
1	C1	3156	C	C2-N1-C1'	5.26	124.59	118.80
1	C1	3158	U	C2-N1-C1'	5.26	124.02	117.70
1	C1	2866	G	C5-C6-O6	5.25	131.75	128.60
1	C1	1406	C	N1-C2-N3	5.25	122.88	119.20
1	C1	2915	G	N3-C4-C5	-5.24	125.98	128.60
4	CA	314	LEU	CA-CB-CG	5.24	127.36	115.30
1	C1	2893	U	N1-C2-O2	5.24	126.47	122.80
1	C1	3088	U	N1-C2-O2	5.24	126.47	122.80
1	C1	2287	G	N3-C4-N9	5.23	129.14	126.00
9	CG	20	MET	CB-CG-SD	5.21	128.04	112.40
1	C1	3296	G	P-O3'-C3'	5.21	125.95	119.70
1	C1	2874	U	C5-C6-N1	5.20	125.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	CE	173	LEU	CA-CB-CG	5.19	127.24	115.30
1	C1	1172	A	C4-N9-C1'	5.19	135.63	126.30
1	C1	3309	G	N3-C4-N9	5.19	129.11	126.00
1	C1	78	U	N3-C2-O2	-5.18	118.57	122.20
1	C1	135	C	N1-C2-O2	5.18	122.01	118.90
1	C1	3239	C	C2-N1-C1'	5.17	124.49	118.80
1	C1	1046	A	P-O3'-C3'	5.17	125.90	119.70
1	C1	2866	G	N1-C6-O6	-5.16	116.80	119.90
1	C1	421	U	C2-N1-C1'	5.16	123.89	117.70
1	C1	2722	C	N1-C2-O2	5.16	121.99	118.90
1	C1	2731	C	C6-N1-C2	-5.14	118.24	120.30
1	C1	1051	C	N1-C2-O2	5.14	121.98	118.90
33	LK	15	LEU	CA-CB-CG	5.13	127.09	115.30
1	C1	103	G	C5-C6-O6	5.11	131.67	128.60
1	C1	1239	C	C5-C6-N1	5.11	123.56	121.00
1	C1	127	G	C4-N9-C1'	5.11	133.14	126.50
13	CK	260	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C1	2469	U	C2-N1-C1'	5.09	123.81	117.70
3	C3	13	C	N1-C2-O2	5.09	121.95	118.90
1	C1	2731	C	N3-C2-O2	-5.08	118.34	121.90
1	C1	2417	U	O4'-C1'-N1	5.08	112.27	108.20
1	C1	1311	C	O4'-C1'-N1	5.08	112.27	108.20
11	CI	200	GLU	CA-CB-CG	5.08	124.58	113.40
18	CP	528	LEU	CA-CB-CG	5.08	126.98	115.30
1	C1	2090	C	C5-C6-N1	5.07	123.54	121.00
41	LT	104	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C1	3229	G	C8-N9-C1'	-5.07	120.41	127.00
1	C1	421	U	N3-C2-O2	-5.06	118.66	122.20
7	CE	133	LYS	CA-CB-CG	5.06	124.54	113.40
1	C1	133	G	C2-N3-C4	5.05	114.43	111.90
1	C1	1058	C	N1-C2-O2	5.05	121.93	118.90
1	C1	3113	C	C5-C6-N1	5.05	123.52	121.00
1	C1	3262	G	O4'-C1'-N9	5.04	112.23	108.20
1	C1	3229	G	C4-N9-C1'	5.04	133.05	126.50
33	LK	125	LEU	CA-CB-CG	5.04	126.89	115.30
1	C1	3073	G	N1-C6-O6	-5.03	116.88	119.90
1	C1	2406	C	C2-N3-C4	5.03	122.41	119.90
15	CM	132	MET	CA-CB-CG	5.01	121.82	113.30
1	C1	2818	U	C2-N1-C1'	5.01	123.71	117.70
1	C1	517	C	C2-N1-C1'	5.00	124.30	118.80
1	C1	2451	C	C2-N1-C1'	5.00	124.31	118.80
1	C1	179	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CA	254/316 (80%)	234 (92%)	19 (8%)	1 (0%)	34	69
5	CB	256/391 (66%)	244 (95%)	10 (4%)	2 (1%)	19	54
6	CC	283/801 (35%)	272 (96%)	11 (4%)	0	100	100
7	CE	459/598 (77%)	445 (97%)	13 (3%)	1 (0%)	47	79
8	CF	243/270 (90%)	234 (96%)	9 (4%)	0	100	100
9	CG	175/184 (95%)	167 (95%)	8 (5%)	0	100	100
10	CH	474/661 (72%)	456 (96%)	18 (4%)	0	100	100
11	CI	144/414 (35%)	136 (94%)	8 (6%)	0	100	100
12	CJ	374/679 (55%)	365 (98%)	9 (2%)	0	100	100
13	CK	226/261 (87%)	216 (96%)	10 (4%)	0	100	100
14	CL	384/558 (69%)	357 (93%)	22 (6%)	5 (1%)	12	42
15	CM	183/249 (74%)	175 (96%)	8 (4%)	0	100	100
15	LF	238/249 (96%)	228 (96%)	9 (4%)	1 (0%)	34	69
16	CN	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	322/751 (43%)	307 (95%)	15 (5%)	0	100	100
19	CQ	110/225 (49%)	106 (96%)	4 (4%)	0	100	100
20	CR	159/237 (67%)	155 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	CS	294/834 (35%)	286 (97%)	6 (2%)	2 (1%)	22 57
22	CT	448/688 (65%)	425 (95%)	21 (5%)	2 (0%)	34 69
23	CU	174/451 (39%)	166 (95%)	8 (5%)	0	100 100
24	CX	86/203 (42%)	82 (95%)	4 (5%)	0	100 100
25	CY	308/788 (39%)	292 (95%)	15 (5%)	1 (0%)	41 73
26	Cz	68/123 (55%)	67 (98%)	1 (2%)	0	100 100
27	Cb	630/924 (68%)	597 (95%)	33 (5%)	0	100 100
28	LB	337/392 (86%)	320 (95%)	17 (5%)	0	100 100
29	LC	360/365 (99%)	348 (97%)	12 (3%)	0	100 100
30	LE	166/200 (83%)	160 (96%)	6 (4%)	0	100 100
31	LG	192/262 (73%)	188 (98%)	4 (2%)	0	100 100
32	LH	188/192 (98%)	178 (95%)	10 (5%)	0	100 100
33	LK	142/165 (86%)	132 (93%)	10 (7%)	0	100 100
34	LL	115/213 (54%)	109 (95%)	6 (5%)	0	100 100
35	LM	135/142 (95%)	131 (97%)	4 (3%)	0	100 100
36	LN	179/203 (88%)	174 (97%)	5 (3%)	0	100 100
37	LO	202/204 (99%)	198 (98%)	4 (2%)	0	100 100
38	LP	150/187 (80%)	149 (99%)	1 (1%)	0	100 100
39	LQ	127/213 (60%)	123 (97%)	4 (3%)	0	100 100
40	LS	172/174 (99%)	166 (96%)	6 (4%)	0	100 100
41	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	19 54
42	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100 100
43	LX	20/156 (13%)	20 (100%)	0	0	100 100
44	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100 100
45	Ld	107/120 (89%)	102 (95%)	5 (5%)	0	100 100
46	Le	129/131 (98%)	126 (98%)	3 (2%)	0	100 100
47	Lf	106/109 (97%)	102 (96%)	3 (3%)	1 (1%)	17 52
48	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100 100
49	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100 100
50	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100 100
51	Lq	205/217 (94%)	186 (91%)	19 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Cc	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
53	Cd	334/436 (77%)	323 (97%)	11 (3%)	0	100	100
54	Ce	192/336 (57%)	185 (96%)	7 (4%)	0	100	100
55	Cf	57/570 (10%)	57 (100%)	0	0	100	100
All	All	11105/18067 (62%)	10656 (96%)	432 (4%)	17 (0%)	50	79

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CA	236	PRO
5	CB	103	ASP
14	CL	414	VAL
21	CS	67	MET
22	CT	254	PRO
25	CY	548	PHE
14	CL	446	ASP
15	LF	12	ILE
47	Lf	93	ALA
14	CL	42	ASN
14	CL	278	ASN
14	CL	439	ASP
5	CB	89	LEU
7	CE	452	ASN
41	LT	44	VAL
21	CS	68	PRO
22	CT	237	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CA	231/276 (84%)	218 (94%)	13 (6%)	21	52
5	CB	222/329 (68%)	202 (91%)	20 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	CC	266/710 (38%)	252 (95%)	14 (5%)	22 54
7	CE	398/517 (77%)	376 (94%)	22 (6%)	21 53
8	CF	214/236 (91%)	202 (94%)	12 (6%)	21 52
9	CG	150/155 (97%)	143 (95%)	7 (5%)	26 59
10	CH	424/575 (74%)	405 (96%)	19 (4%)	27 60
11	CI	121/336 (36%)	116 (96%)	5 (4%)	30 64
12	CJ	332/579 (57%)	324 (98%)	8 (2%)	49 76
13	CK	198/225 (88%)	188 (95%)	10 (5%)	24 56
14	CL	65/458 (14%)	62 (95%)	3 (5%)	27 59
15	CM	161/215 (75%)	153 (95%)	8 (5%)	24 57
15	LF	206/215 (96%)	200 (97%)	6 (3%)	42 72
16	CN	206/206 (100%)	199 (97%)	7 (3%)	37 69
17	CO	48/99 (48%)	47 (98%)	1 (2%)	53 79
18	CP	273/632 (43%)	251 (92%)	22 (8%)	11 39
19	CQ	100/192 (52%)	93 (93%)	7 (7%)	15 45
20	CR	144/206 (70%)	137 (95%)	7 (5%)	25 57
21	CS	73/716 (10%)	72 (99%)	1 (1%)	67 86
23	CU	149/376 (40%)	146 (98%)	3 (2%)	55 80
24	CX	76/172 (44%)	73 (96%)	3 (4%)	32 65
26	Cz	60/107 (56%)	59 (98%)	1 (2%)	60 83
27	Cb	540/779 (69%)	517 (96%)	23 (4%)	29 62
28	LB	290/331 (88%)	282 (97%)	8 (3%)	43 73
29	LC	283/285 (99%)	275 (97%)	8 (3%)	43 73
30	LE	143/166 (86%)	139 (97%)	4 (3%)	43 73
31	LG	168/222 (76%)	163 (97%)	5 (3%)	41 71
32	LH	167/169 (99%)	155 (93%)	12 (7%)	14 44
33	LK	121/136 (89%)	116 (96%)	5 (4%)	30 64
34	LL	99/176 (56%)	96 (97%)	3 (3%)	41 71
35	LM	115/117 (98%)	112 (97%)	3 (3%)	46 74
36	LN	164/180 (91%)	157 (96%)	7 (4%)	29 62
37	LO	163/163 (100%)	159 (98%)	4 (2%)	47 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	LP	125/152 (82%)	116 (93%)	9 (7%)	14 44
39	LQ	110/178 (62%)	109 (99%)	1 (1%)	78 91
40	LS	154/154 (100%)	144 (94%)	10 (6%)	17 47
41	LT	109/135 (81%)	107 (98%)	2 (2%)	59 82
42	LV	99/102 (97%)	94 (95%)	5 (5%)	24 56
43	LX	12/129 (9%)	12 (100%)	0	100 100
44	LY	117/119 (98%)	110 (94%)	7 (6%)	19 49
45	Ld	95/105 (90%)	91 (96%)	4 (4%)	30 62
46	Le	114/114 (100%)	112 (98%)	2 (2%)	59 82
47	Lf	89/90 (99%)	85 (96%)	4 (4%)	27 60
48	Lh	108/781 (14%)	105 (97%)	3 (3%)	43 73
49	Li	75/93 (81%)	71 (95%)	4 (5%)	22 54
50	Lj	61/78 (78%)	57 (93%)	4 (7%)	16 47
51	Lq	179/189 (95%)	176 (98%)	3 (2%)	60 83
52	Cc	204/244 (84%)	199 (98%)	5 (2%)	47 75
53	Cd	291/367 (79%)	282 (97%)	9 (3%)	40 70
54	Ce	173/297 (58%)	165 (95%)	8 (5%)	27 59
55	Cf	53/482 (11%)	50 (94%)	3 (6%)	20 52
All	All	8538/14065 (61%)	8174 (96%)	364 (4%)	33 62

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CA	25	ASN
4	CA	53	ASN
4	CA	72	SER
4	CA	128	PHE
4	CA	140	LEU
4	CA	146	PHE
4	CA	180	LEU
4	CA	230	ASN
4	CA	249	SER
4	CA	253	PRO
4	CA	292	ARG
4	CA	293	LYS
4	CA	295	GLN

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Mol	Chain	Res	Type
5	CB	27	CYS
5	CB	63	TRP
5	CB	87	HIS
5	CB	89	LEU
5	CB	90	ASN
5	CB	91	THR
5	CB	106	ARG
5	CB	107	PHE
5	CB	109	LYS
5	CB	114	ASP
5	CB	121	ARG
5	CB	123	LYS
5	CB	145	LYS
5	CB	171	PHE
5	CB	215	ARG
5	CB	269	ARG
5	CB	270	PHE
5	CB	275	TRP
5	CB	276	GLN
5	CB	280	ASN
6	CC	125	PRO
6	CC	137	TYR
6	CC	189	ASP
6	CC	193	LYS
6	CC	196	MET
6	CC	255	TYR
6	CC	302	ARG
6	CC	306	TYR
6	CC	338	MET
6	CC	351	ASP
6	CC	373	MET
6	CC	378	ARG
6	CC	382	TYR
6	CC	408	MET
7	CE	136	GLU
7	CE	156	LYS
7	CE	175	SER
7	CE	250	ASN
7	CE	283	LYS
7	CE	296	SER
7	CE	317	TYR
7	CE	336	TYR

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Mol	Chain	Res	Type
7	CE	353	LYS
7	CE	355	MET
7	CE	366	SER
7	CE	405	ASN
7	CE	444	ARG
7	CE	457	ARG
7	CE	465	CYS
7	CE	473	LEU
7	CE	474	LYS
7	CE	488	ASN
7	CE	499	LYS
7	CE	525	HIS
7	CE	535	LYS
7	CE	554	ASP
8	CF	25	ARG
8	CF	31	ARG
8	CF	32	GLU
8	CF	38	GLN
8	CF	95	TYR
8	CF	126	ARG
8	CF	158	SER
8	CF	203	SER
8	CF	210	LYS
8	CF	211	LEU
8	CF	213	SER
8	CF	243	ARG
9	CG	1	MET
9	CG	15	LYS
9	CG	58	CYS
9	CG	71	LEU
9	CG	158	ASP
9	CG	164	CYS
9	CG	169	ASP
10	CH	5	LYS
10	CH	85	TYR
10	CH	88	ASP
10	CH	89	HIS
10	CH	98	SER
10	CH	101	LYS
10	CH	108	SER
10	CH	174	PHE
10	CH	209	ASP

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Mol	Chain	Res	Type
10	CH	270	PHE
10	CH	274	LYS
10	CH	297	LEU
10	CH	323	THR
10	CH	406	ASP
10	CH	418	ASN
10	CH	423	LYS
10	CH	448	ASP
10	CH	467	ARG
10	CH	469	GLU
11	CI	198	PHE
11	CI	246	ARG
11	CI	258	LEU
11	CI	269	HIS
11	CI	287	LYS
12	CJ	68	ASP
12	CJ	115	LYS
12	CJ	147	MET
12	CJ	256	LYS
12	CJ	414	ARG
12	CJ	453	ARG
12	CJ	462	TRP
12	CJ	475	LEU
13	CK	67	GLN
13	CK	149	ARG
13	CK	161	PHE
13	CK	170	ARG
13	CK	189	LEU
13	CK	190	ASN
13	CK	202	LYS
13	CK	212	LEU
13	CK	241	ARG
13	CK	247	ASN
14	CL	19	ARG
14	CL	27	ARG
14	CL	58	LEU
15	CM	52	LYS
15	CM	55	GLU
15	CM	67	GLU
15	CM	127	LYS
15	CM	155	TYR
15	CM	201	PHE

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Mol	Chain	Res	Type
15	CM	237	ARG
15	CM	242	ASN
16	CN	1	MET
16	CN	80	GLU
16	CN	110	CYS
16	CN	124	GLU
16	CN	127	GLU
16	CN	172	GLU
16	CN	188	ARG
17	CO	14	HIS
18	CP	264	ASN
18	CP	271	CYS
18	CP	316	HIS
18	CP	319	ASP
18	CP	331	LEU
18	CP	337	TRP
18	CP	339	LYS
18	CP	362	TYR
18	CP	370	PHE
18	CP	438	TYR
18	CP	459	CYS
18	CP	460	SER
18	CP	480	PHE
18	CP	489	GLN
18	CP	496	ASP
18	CP	500	HIS
18	CP	520	ASN
18	CP	535	LYS
18	CP	545	LYS
18	CP	557	HIS
18	CP	576	PHE
18	CP	582	LYS
19	CQ	1	MET
19	CQ	11	ARG
19	CQ	17	LYS
19	CQ	27	LYS
19	CQ	40	PHE
19	CQ	47	ARG
19	CQ	91	LYS
20	CR	33	ASN
20	CR	57	LYS
20	CR	134	GLN

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Mol	Chain	Res	Type
20	CR	178	ARG
20	CR	204	ASP
20	CR	212	ASP
20	CR	214	LYS
21	CS	660	MET
23	CU	318	GLN
23	CU	327	LYS
23	CU	329	GLU
24	CX	100	SER
24	CX	113	GLN
24	CX	133	ARG
26	Cz	37	LYS
27	Cb	4	ARG
27	Cb	102	LEU
27	Cb	156	SER
27	Cb	181	LYS
27	Cb	193	LEU
27	Cb	212	ASP
27	Cb	236	LYS
27	Cb	257	GLU
27	Cb	298	GLU
27	Cb	381	TYR
27	Cb	443	PHE
27	Cb	493	ARG
27	Cb	528	ASN
27	Cb	582	ASN
27	Cb	589	ASN
27	Cb	715	TYR
27	Cb	799	GLU
27	Cb	813	PHE
27	Cb	815	LYS
27	Cb	819	GLN
27	Cb	833	LYS
27	Cb	861	LYS
27	Cb	871	LYS
28	LB	19	ARG
28	LB	89	LEU
28	LB	112	ASP
28	LB	173	LYS
28	LB	214	GLU
28	LB	298	GLU
28	LB	354	LYS

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Mol	Chain	Res	Type
28	LB	378	LYS
29	LC	62	SER
29	LC	64	GLU
29	LC	70	ARG
29	LC	121	PHE
29	LC	271	SER
29	LC	321	ARG
29	LC	359	LYS
29	LC	360	GLU
30	LE	25	GLN
30	LE	167	LYS
30	LE	191	LYS
30	LE	199	LYS
15	LF	32	ARG
15	LF	52	LYS
15	LF	100	LYS
15	LF	134	LYS
15	LF	181	LYS
15	LF	246	ARG
31	LG	52	MET
31	LG	107	GLU
31	LG	140	ASN
31	LG	216	LYS
31	LG	228	LYS
32	LH	17	LYS
32	LH	19	SER
32	LH	23	ARG
32	LH	33	LYS
32	LH	36	LYS
32	LH	55	LEU
32	LH	63	LYS
32	LH	98	PRO
32	LH	108	GLU
32	LH	149	SER
32	LH	151	ASN
32	LH	157	SER
33	LK	11	LYS
33	LK	31	LYS
33	LK	101	ASN
33	LK	149	LYS
33	LK	164	ASP
34	LL	58	VAL

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Mol	Chain	Res	Type
34	LL	102	LYS
34	LL	122	ARG
35	LM	14	VAL
35	LM	71	LYS
35	LM	137	LYS
36	LN	23	LEU
36	LN	96	ARG
36	LN	108	ARG
36	LN	118	SER
36	LN	140	LYS
36	LN	187	ARG
36	LN	198	SER
37	LO	117	LYS
37	LO	169	TYR
37	LO	185	LYS
37	LO	197	GLU
38	LP	3	ARG
38	LP	20	SER
38	LP	43	ARG
38	LP	74	LYS
38	LP	80	ARG
38	LP	87	SER
38	LP	103	ASP
38	LP	140	MET
38	LP	154	GLU
39	LQ	149	LEU
40	LS	62	ASN
40	LS	71	LYS
40	LS	83	SER
40	LS	85	SER
40	LS	94	TYR
40	LS	98	SER
40	LS	113	ARG
40	LS	131	LYS
40	LS	149	SER
40	LS	160	SER
41	LT	57	TYR
41	LT	118	LYS
42	LV	15	MET
42	LV	42	LYS
42	LV	68	LYS
42	LV	88	LYS

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Mol	Chain	Res	Type
42	LV	139	MET
44	LY	1	MET
44	LY	8	SER
44	LY	73	TYR
44	LY	76	LYS
44	LY	78	VAL
44	LY	86	ARG
44	LY	122	LYS
45	Ld	20	TYR
45	Ld	46	LYS
45	Ld	85	ARG
45	Ld	102	GLN
46	Le	70	SER
46	Le	81	LYS
47	Lf	62	ARG
47	Lf	65	LYS
47	Lf	67	ARG
47	Lf	95	SER
48	Lh	15	LYS
48	Lh	22	LYS
48	Lh	112	ARG
49	Li	25	LYS
49	Li	62	TYR
49	Li	83	LYS
49	Li	94	ARG
50	Lj	26	SER
50	Lj	36	SER
50	Lj	52	LYS
50	Lj	68	SER
51	Lq	25	LYS
51	Lq	34	LEU
51	Lq	184	MET
52	Cc	20	LYS
52	Cc	151	ASP
52	Cc	204	GLU
52	Cc	230	ASP
52	Cc	247	ASP
53	Cd	43	ARG
53	Cd	47	ARG
53	Cd	56	LEU
53	Cd	267	SER
53	Cd	277	GLU

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Mol	Chain	Res	Type
53	Cd	351	ASP
53	Cd	414	GLU
53	Cd	422	GLU
53	Cd	430	LYS
54	Ce	43	CYS
54	Ce	77	TRP
54	Ce	161	LYS
54	Ce	172	ASP
54	Ce	182	GLN
54	Ce	189	GLN
54	Ce	192	LYS
54	Ce	195	LEU
55	Cf	523	ARG
55	Cf	526	LYS
55	Cf	529	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
7	CE	334	GLN
10	CH	258	GLN
12	CJ	485	HIS
13	CK	203	ASN
15	CM	119	ASN
16	CN	79	GLN
16	CN	156	ASN
19	CQ	58	ASN
20	CR	133	GLN
20	CR	148	GLN
31	LG	140	ASN
40	LS	21	ASN
41	LT	146	ASN
42	LV	76	HIS
48	Lh	37	GLN
49	Li	42	GLN
54	Ce	185	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2134/3341 (63%)	479 (22%)	15 (0%)
2	C2	157/256 (61%)	30 (19%)	1 (0%)
3	C3	96/161 (59%)	34 (35%)	0
All	All	2387/3758 (63%)	543 (22%)	16 (0%)

All (543) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	A
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	67	A
1	C1	73	A
1	C1	74	G
1	C1	85	A
1	C1	91	G
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	136	C
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G

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Mol	Chain	Res	Type
1	C1	163	U
1	C1	176	U
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	204	A
1	C1	205	G
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	214	A
1	C1	225	G
1	C1	241	G
1	C1	244	U
1	C1	249	C
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	300	A
1	C1	302	U
1	C1	308	U
1	C1	310	A
1	C1	311	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	377	A
1	C1	382	G
1	C1	384	G
1	C1	390	U
1	C1	391	A
1	C1	393	C

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Mol	Chain	Res	Type
1	C1	394	A
1	C1	395	C
1	C1	400	A
1	C1	413	G
1	C1	414	A
1	C1	430	A
1	C1	431	C
1	C1	432	U
1	C1	433	U
1	C1	445	A
1	C1	446	U
1	C1	448	A
1	C1	449	U
1	C1	450	C
1	C1	457	U
1	C1	459	U
1	C1	460	C
1	C1	467	G
1	C1	468	C
1	C1	469	A
1	C1	474	G
1	C1	484	G
1	C1	485	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	558	G
1	C1	582	A
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G
1	C1	598	A

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Mol	Chain	Res	Type
1	C1	608	A
1	C1	623	C
1	C1	633	A
1	C1	651	A
1	C1	652	A
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	684	G
1	C1	692	A
1	C1	693	A
1	C1	699	G
1	C1	702	A
1	C1	703	A
1	C1	706	U
1	C1	707	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	731	G
1	C1	739	C
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	767	A
1	C1	787	A
1	C1	796	G
1	C1	798	A
1	C1	907	A
1	C1	918	G
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G

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Mol	Chain	Res	Type
1	C1	940	C
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	958	A
1	C1	960	C
1	C1	961	U
1	C1	965	G
1	C1	973	A
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	979	A
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1043	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1063	C
1	C1	1069	G
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1097	G
1	C1	1098	G
1	C1	1114	C
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1163	U
1	C1	1164	G

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Mol	Chain	Res	Type
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1180	C
1	C1	1181	C
1	C1	1182	A
1	C1	1184	A
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1203	U
1	C1	1204	G
1	C1	1211	G
1	C1	1218	G
1	C1	1221	C
1	C1	1223	U
1	C1	1224	G
1	C1	1226	A
1	C1	1227	A
1	C1	1228	G
1	C1	1238	G
1	C1	1240	U
1	C1	1241	A
1	C1	1245	A
1	C1	1246	C
1	C1	1247	U
1	C1	1253	A
1	C1	1254	C
1	C1	1268	A
1	C1	1269	A
1	C1	1271	G
1	C1	1272	U
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A

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Mol	Chain	Res	Type
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1362	G
1	C1	1368	A
1	C1	1369	G
1	C1	1373	C
1	C1	1374	G
1	C1	1381	A
1	C1	1382	G
1	C1	1399	G
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1433	C
1	C1	1856	U
1	C1	1859	U
1	C1	1864	C
1	C1	1865	A
1	C1	1866	A
1	C1	1868	G
1	C1	1875	A
1	C1	1883	C
1	C1	1884	G
1	C1	1886	C
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	2075	A
1	C1	2088	A
1	C1	2287	G
1	C1	2288	A
1	C1	2293	C
1	C1	2294	A
1	C1	2297	G
1	C1	2302	U
1	C1	2309	U
1	C1	2325	A

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Mol	Chain	Res	Type
1	C1	2332	G
1	C1	2334	A
1	C1	2335	A
1	C1	2338	G
1	C1	2339	G
1	C1	2356	G
1	C1	2365	G
1	C1	2384	C
1	C1	2394	A
1	C1	2396	U
1	C1	2397	G
1	C1	2402	A
1	C1	2406	C
1	C1	2415	U
1	C1	2422	U
1	C1	2423	A
1	C1	2424	G
1	C1	2426	U
1	C1	2428	G
1	C1	2429	G
1	C1	2430	A
1	C1	2431	G
1	C1	2435	C
1	C1	2436	G
1	C1	2439	G
1	C1	2445	G
1	C1	2449	U
1	C1	2452	C
1	C1	2453	A
1	C1	2456	A
1	C1	2465	G
1	C1	2467	U
1	C1	2469	U
1	C1	2476	U
1	C1	2477	A
1	C1	2482	A
1	C1	2551	A
1	C1	2552	C
1	C1	2553	A
1	C1	2564	G
1	C1	2568	G
1	C1	2730	C

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Mol	Chain	Res	Type
1	C1	2739	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2766	A
1	C1	2767	C
1	C1	2776	U
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2800	U
1	C1	2802	C
1	C1	2803	A
1	C1	2804	U
1	C1	2805	A
1	C1	2807	C
1	C1	2818	U
1	C1	2819	U
1	C1	2831	U
1	C1	2832	G
1	C1	2833	U
1	C1	2834	C
1	C1	2835	G
1	C1	2836	G
1	C1	2845	A
1	C1	2847	C
1	C1	2852	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2879	U
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2900	C
1	C1	2901	G
1	C1	2916	A

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Mol	Chain	Res	Type
1	C1	2917	C
1	C1	2923	U
1	C1	2924	G
1	C1	2926	G
1	C1	2929	A
1	C1	2930	G
1	C1	2935	G
1	C1	2936	U
1	C1	2950	U
1	C1	2956	C
1	C1	2968	A
1	C1	2969	A
1	C1	2970	U
1	C1	2980	U
1	C1	3006	A
1	C1	3013	U
1	C1	3014	U
1	C1	3015	U
1	C1	3033	C
1	C1	3034	A
1	C1	3035	G
1	C1	3037	G
1	C1	3048	A
1	C1	3049	C
1	C1	3050	C
1	C1	3057	U
1	C1	3066	G
1	C1	3070	A
1	C1	3077	C
1	C1	3079	A
1	C1	3084	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3108	U
1	C1	3109	A
1	C1	3113	C
1	C1	3118	A
1	C1	3126	G

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Mol	Chain	Res	Type
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3144	C
1	C1	3146	G
1	C1	3147	G
1	C1	3154	A
1	C1	3157	C
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3179	G
1	C1	3183	C
1	C1	3185	A
1	C1	3187	G
1	C1	3189	G
1	C1	3199	A
1	C1	3205	C
1	C1	3211	G
1	C1	3212	C
1	C1	3213	A
1	C1	3214	A
1	C1	3225	C
1	C1	3228	G
1	C1	3232	U
1	C1	3244	C
1	C1	3248	C
1	C1	3249	G
1	C1	3253	U
1	C1	3256	A
1	C1	3257	U
1	C1	3258	G
1	C1	3260	G
1	C1	3262	G
1	C1	3263	A
1	C1	3264	A
1	C1	3270	C
1	C1	3274	U

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Mol	Chain	Res	Type
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3290	C
1	C1	3291	U
1	C1	3292	U
1	C1	3295	U
1	C1	3296	G
1	C1	3297	U
1	C1	3298	U
1	C1	3302	A
1	C1	3309	G
1	C1	3310	A
1	C1	3318	C
1	C1	3321	U
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3329	C
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	34	U
2	C2	35	C
2	C2	49	G
2	C2	51	G
2	C2	53	A
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	77	A
2	C2	78	G
2	C2	81	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	100	U

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Mol	Chain	Res	Type
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	111	A
2	C2	113	U
2	C2	124	G
2	C2	126	A
2	C2	127	U
2	C2	129	C
2	C2	136	G
2	C2	152	G
2	C2	158	U
3	C3	5	C
3	C3	6	A
3	C3	7	U
3	C3	8	C
3	C3	15	U
3	C3	16	G
3	C3	17	G
3	C3	21	U
3	C3	25	U
3	C3	26	U
3	C3	31	A
3	C3	32	C
3	C3	48	G
3	C3	54	G
3	C3	55	A
3	C3	56	A
3	C3	57	A
3	C3	59	G
3	C3	60	C
3	C3	61	A
3	C3	63	U
3	C3	64	G
3	C3	68	G
3	C3	71	U
3	C3	72	C
3	C3	73	G
3	C3	75	U
3	C3	130	G
3	C3	133	G
3	C3	134	C

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Mol	Chain	Res	Type
3	C3	137	G
3	C3	141	U
3	C3	143	A
3	C3	144	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	308	U
1	C1	519	A
1	C1	1044	A
1	C1	1046	A
1	C1	1220	C
1	C1	2301	C
1	C1	2929	A
1	C1	3078	U
1	C1	3162	A
1	C1	3204	G
1	C1	3257	U
1	C1	3263	A
1	C1	3296	G
1	C1	3297	U
2	C2	123	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
56	GTP	CH	701	-	26,34,34	1.16	2 (7%)	32,54,54	1.60	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
56	GTP	CH	701	-	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CH	701	GTP	C5-C6	-4.17	1.38	1.47
56	CH	701	GTP	C2-N3	2.11	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	CH	701	GTP	PB-O3B-PG	-3.73	120.02	132.83
56	CH	701	GTP	PA-O3A-PB	-3.20	121.86	132.83
56	CH	701	GTP	C5-C6-N1	3.15	119.51	113.95
56	CH	701	GTP	C3'-C2'-C1'	2.97	105.46	100.98
56	CH	701	GTP	C8-N7-C5	2.92	108.55	102.99
56	CH	701	GTP	C2-N1-C6	-2.87	119.81	125.10
56	CH	701	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

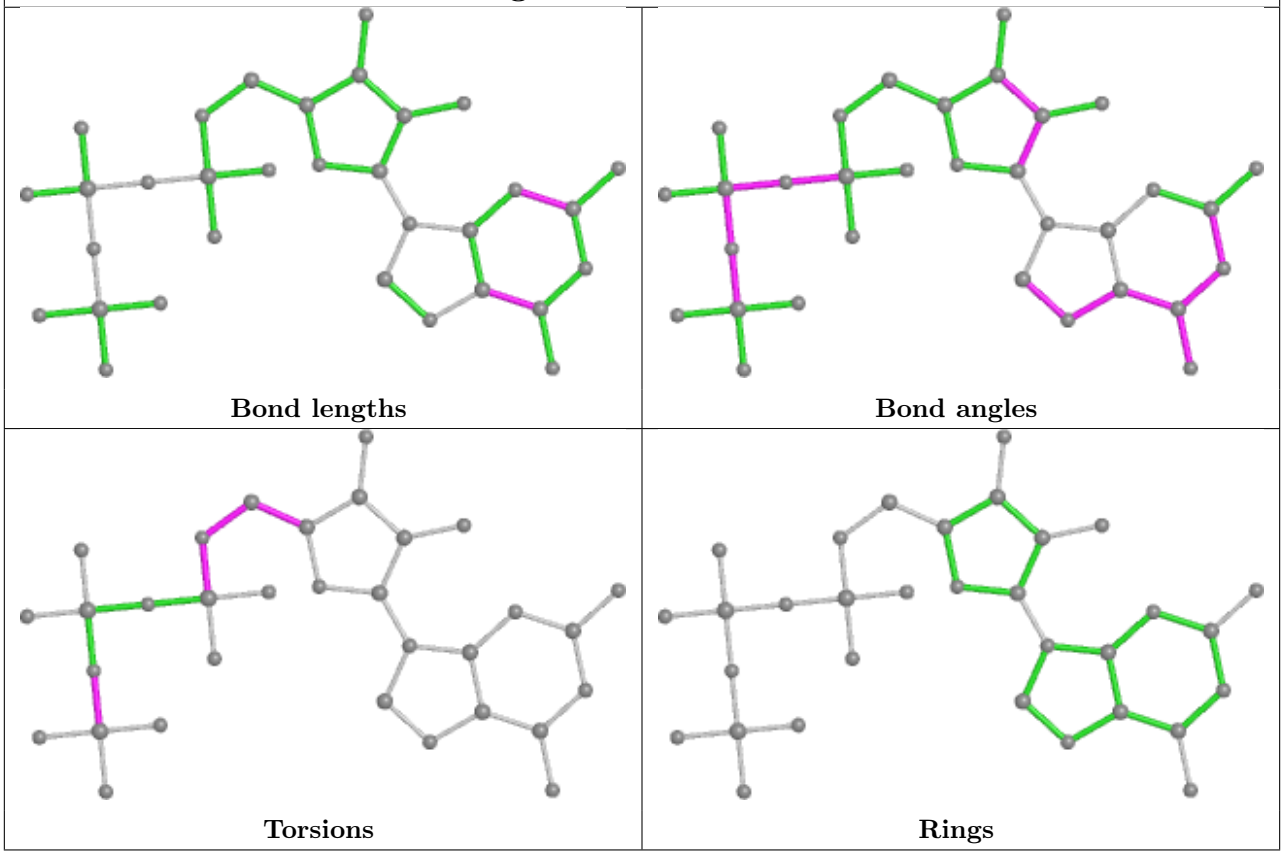
Mol	Chain	Res	Type	Atoms
56	CH	701	GTP	PB-O3B-PG-O2G
56	CH	701	GTP	PB-O3B-PG-O3G
56	CH	701	GTP	C5'-O5'-PA-O3A
56	CH	701	GTP	C4'-C5'-O5'-PA
56	CH	701	GTP	C5'-O5'-PA-O2A
56	CH	701	GTP	C3'-C4'-C5'-O5'

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 GTP CH 701



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.