



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:52 PM JST

PDB ID : 8I9Z  
EMDB ID : EMD-35289  
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit  
- State Spb4  
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.  
Deposited on : 2023-02-07  
Resolution : 2.70 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](mailto: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>.

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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

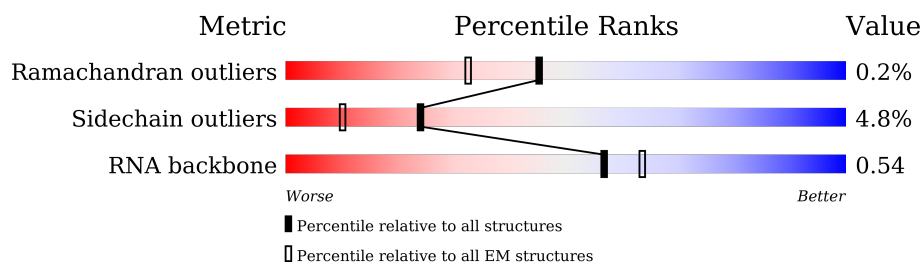
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









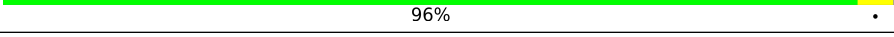
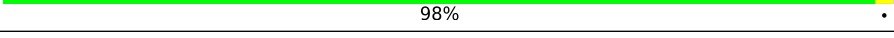


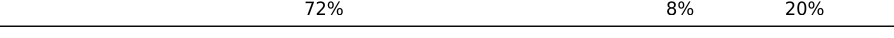
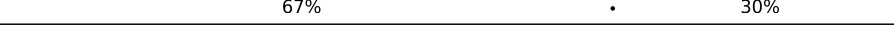

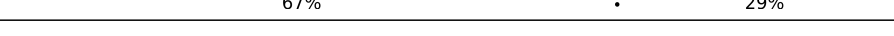

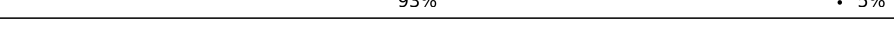
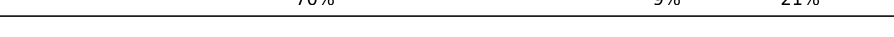

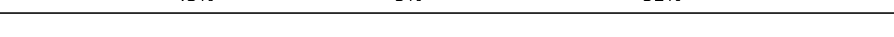






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	C1	3341	65% 17% . 17%
2	C2	319	62% 18% 20%
3	CA	316	77% . 21%
4	CB	391	62% . 34%
5	CC	801	79% . 18%
6	CD	495	87% 6% 7%
7	CE	598	74% . 22%
8	CF	270	88% . 9%
9	CG	184	93% . .



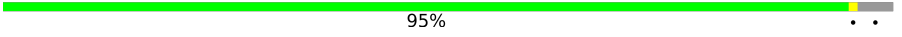

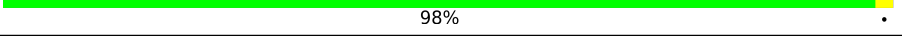


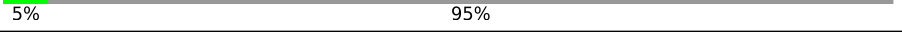
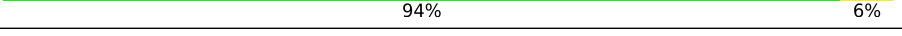

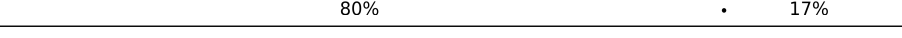
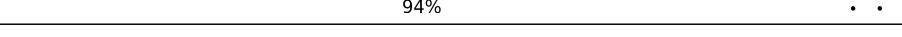

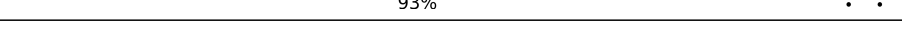
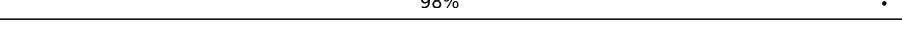

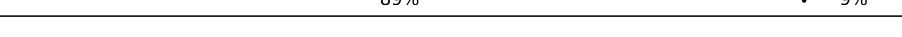
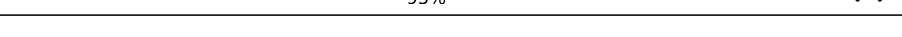
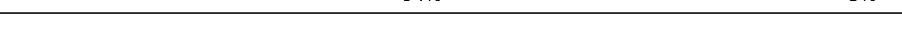






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Mol	Chain	Length	Quality of chain
10	CH	661	
11	CI	414	
12	CJ	679	
13	CK	261	
14	CL	558	
15	CM	249	
15	LF	249	
16	CN	246	
17	CO	120	
18	CP	751	
19	CQ	225	
20	CR	237	
21	CS	834	
22	CT	688	
23	CU	451	
24	CV	147	
25	CW	679	
26	CX	203	
27	CY	788	
28	Cz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


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Mol	Chain	Length	Quality of chain
34	LK	165	
35	LL	213	
36	LM	142	
37	LN	203	
38	LO	204	
39	LP	187	
40	LQ	213	
41	LR	2898	
42	LS	174	
43	LT	160	
44	LU	127	
45	LV	139	
46	LX	156	
47	LY	138	
48	LZ	135	
49	Lc	108	
50	Ld	120	
51	Le	131	
52	Lf	109	
53	Lg	119	
54	Lh	935	
55	Li	110	
56	Lj	95	
57	Lk	81	
58	Ll	51	

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Mol	Chain	Length	Quality of chain
59	Lq	217	 91% • 5%

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 167255 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
1	C1	2787	Total	C	N	O	P	0	0
			59633	26611	10807	19428	2787		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CC	658	Total	C	N	O	S	0	0
			5289	3368	931	977	13		

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

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

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	465	Total	C	N	O	S	0	0
			3689	2362	646	670	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	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	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	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	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	625	Total	C	N	O	S	0	0
			5036	3190	917	910	19		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CW	537	Total	C	N	O	S	0	0
			4284	2733	760	777	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CY	382	Total	C	N	O	S	0	0
			3035	1943	558	523	11		

- Molecule 28 is a protein called rRNA-processing protein.

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

- Molecule 29 is a protein called 60S ribosomal protein L3-like protein.

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

- Molecule 30 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 31 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LE	189	Total	C	N	O	S	0	0
			1475	944	267	261	3		

- Molecule 32 is a protein called 60S ribosomal protein L8.

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

- Molecule 33 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	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

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

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

- Molecule 35 is a protein called 60S ribosomal protein L13.

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

- Molecule 36 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 37 is a protein called Ribosomal protein L15.

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

- Molecule 38 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 39 is a protein called 60S ribosomal protein l17-like protein.

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

- Molecule 40 is a protein called Ribosomal protein L18-like protein.

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

- Molecule 41 is a protein called Ribosomal protein L19.

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

- Molecule 42 is a protein called 60S ribosomal protein L20.

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

- Molecule 43 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 44 is a protein called 60S ribosomal protein L22-like protein.

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

- Molecule 45 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 46 is a protein called 60S ribosomal protein L25-like protein.

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

- Molecule 47 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 48 is a protein called 60S ribosomal protein L27.

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

- Molecule 49 is a protein called 60S ribosomal protein l30-like protein.

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

- Molecule 50 is a protein called Putative 60S ribosomal protein.

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

- Molecule 51 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 52 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 53 is a protein called Ribosomal protein l34-like protein.

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

- Molecule 54 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 55 is a protein called 60S ribosomal protein L36.

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

- Molecule 56 is a protein called Ribosomal protein L37.

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

- Molecule 57 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	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

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

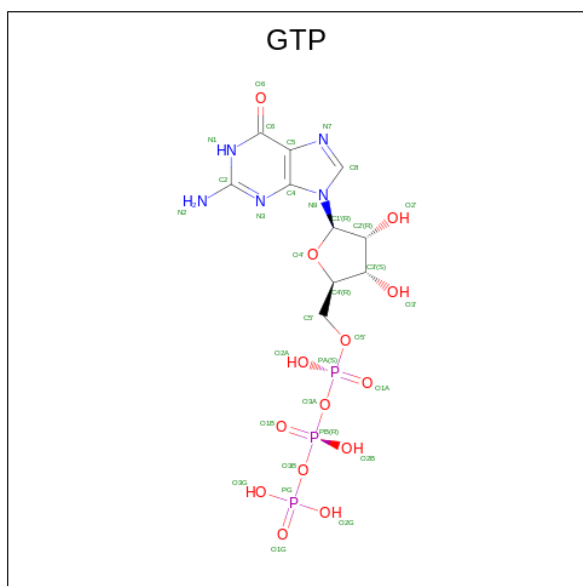
- Molecule 58 is a protein called 60S ribosomal protein L39.

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

- Molecule 59 is a protein called Ribosomal protein.

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

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

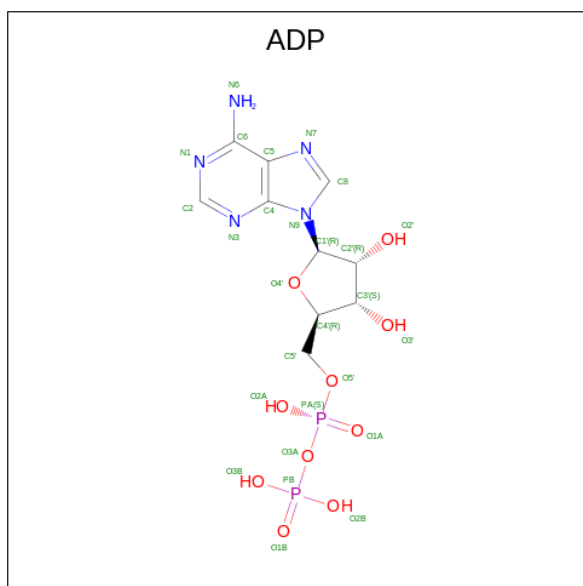


Mol	Chain	Residues	Atoms					AltConf
60	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total	Zn	0
			1	1	
61	Lj	1	Total	Zn	0
			1	1	

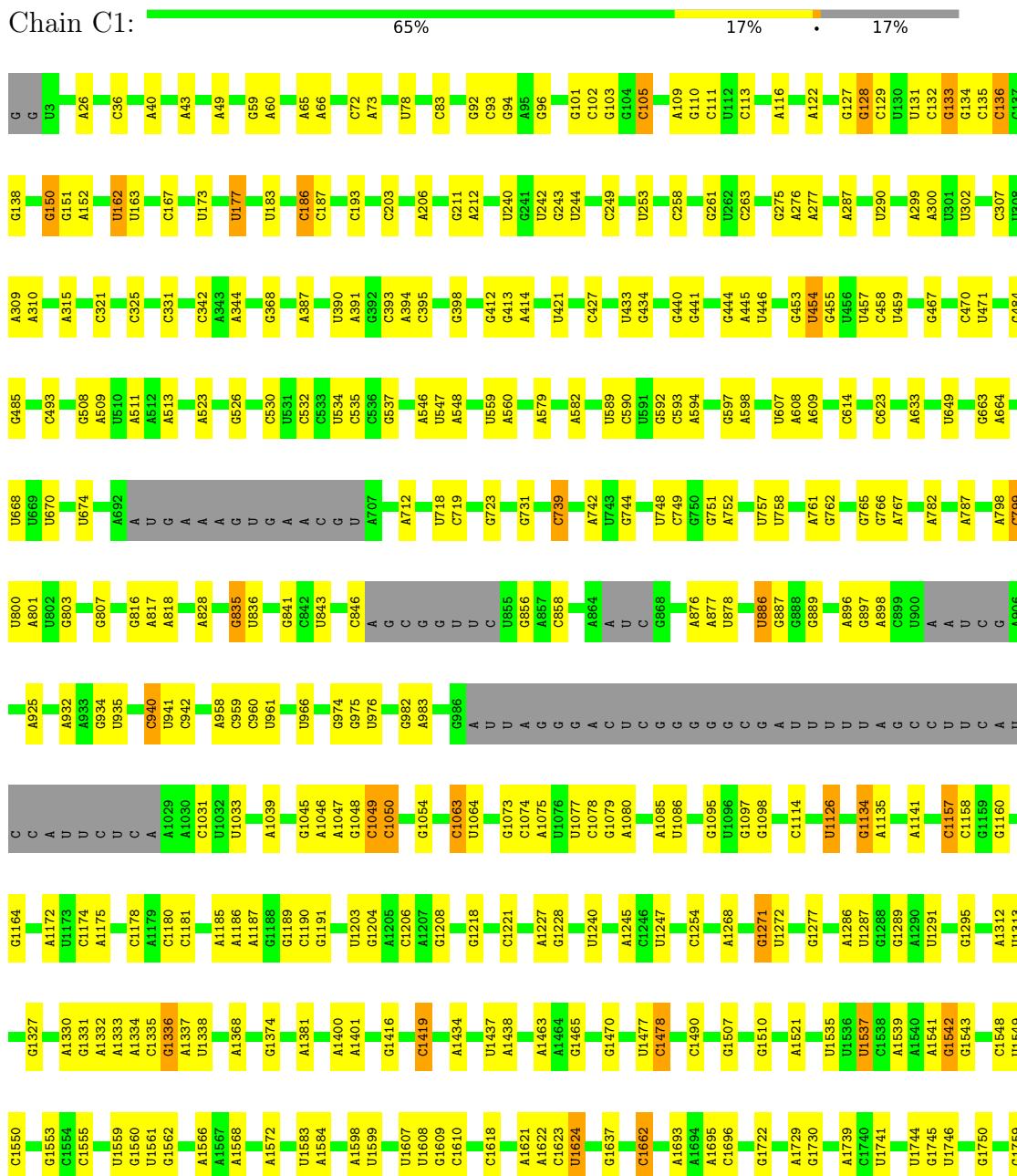
- Molecule 62 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



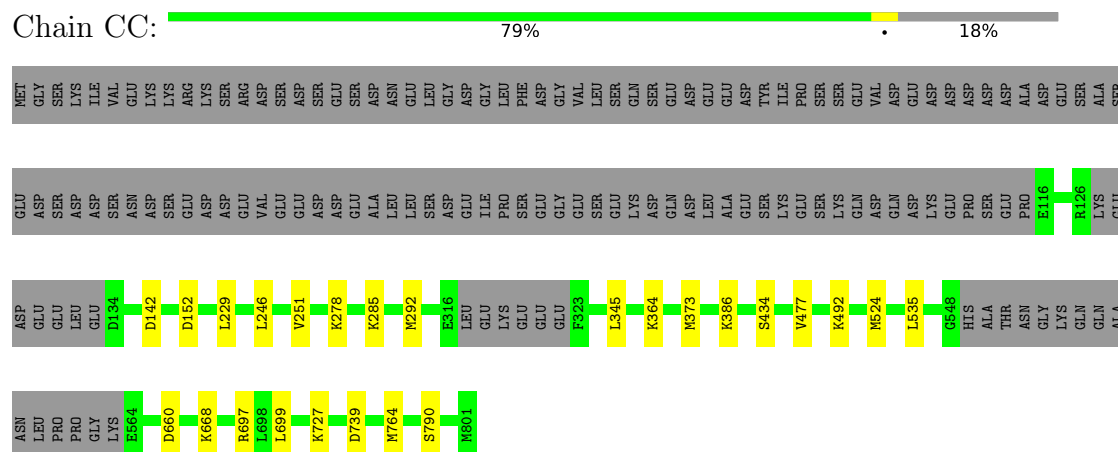
### 3 Residue-property plots

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.

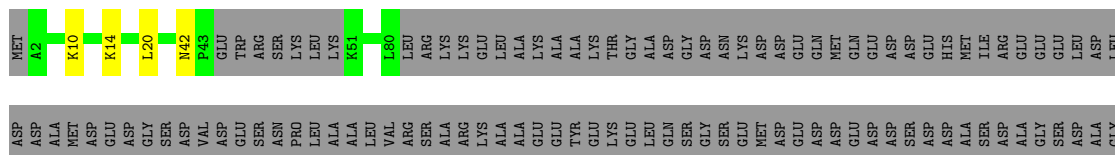
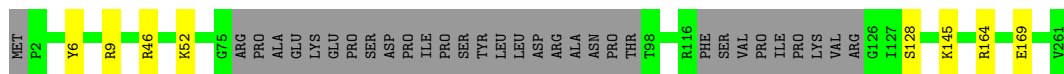
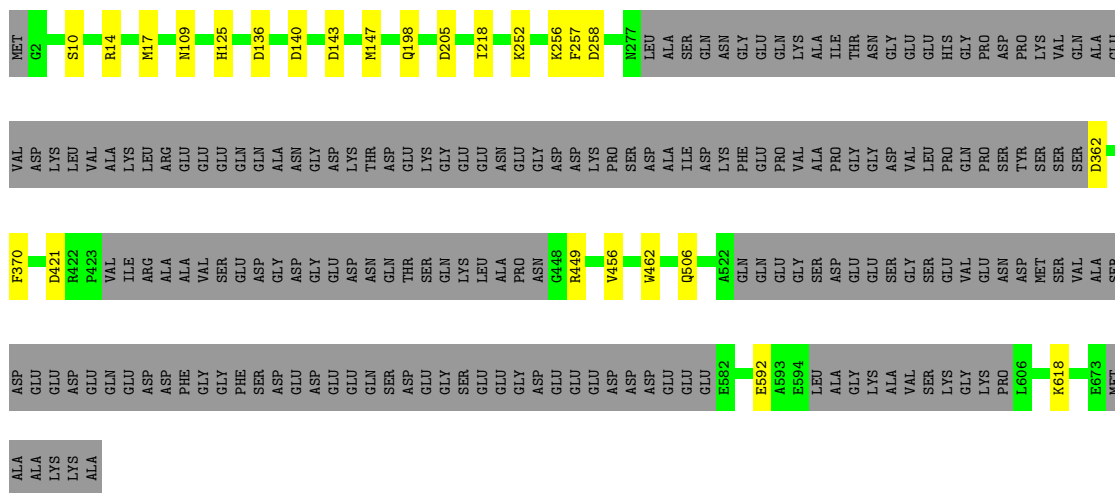
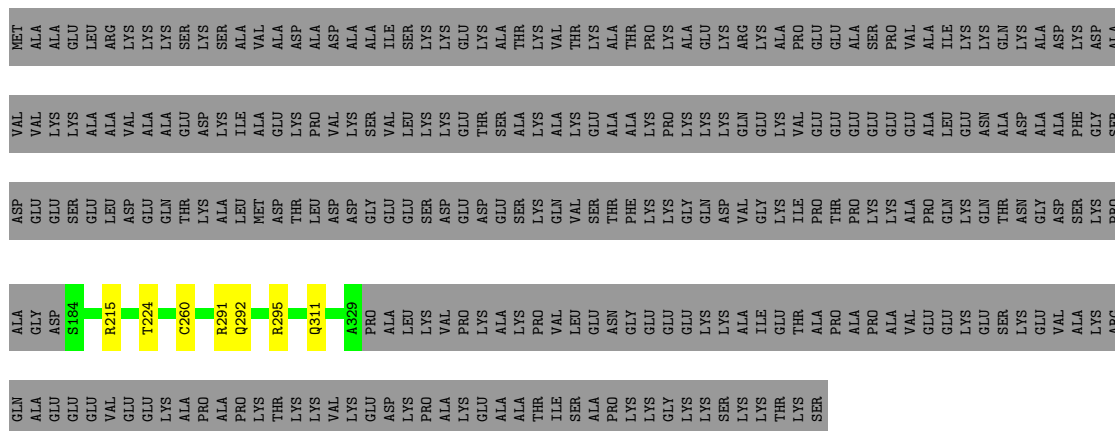
#### • Molecule 1: RNA (3341-MER)

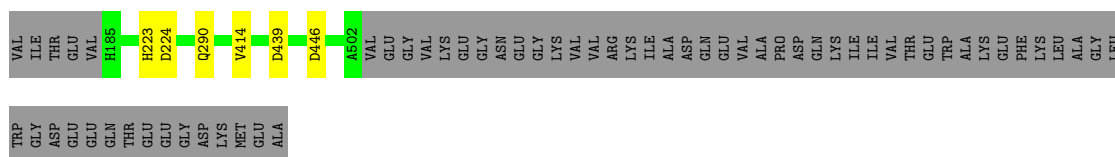




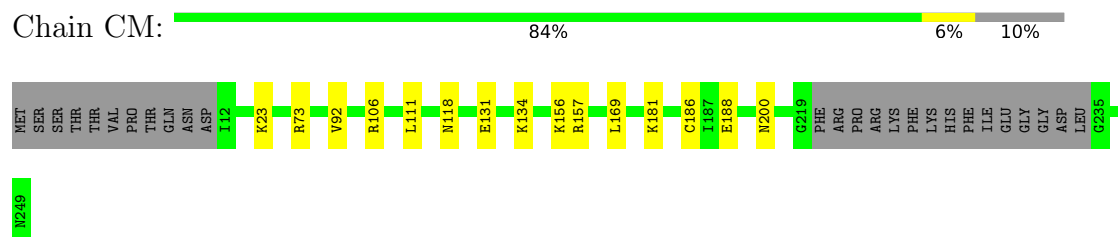




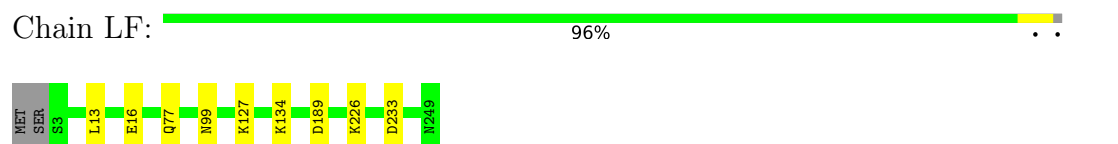




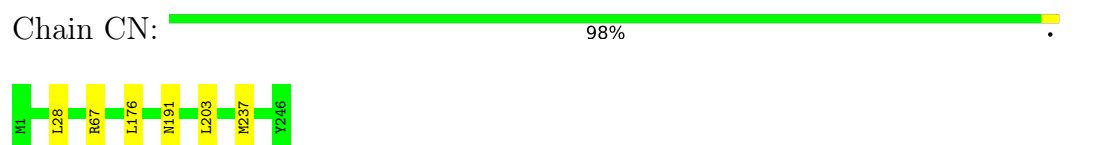
- Molecule 15: 60S ribosomal protein l7-like protein



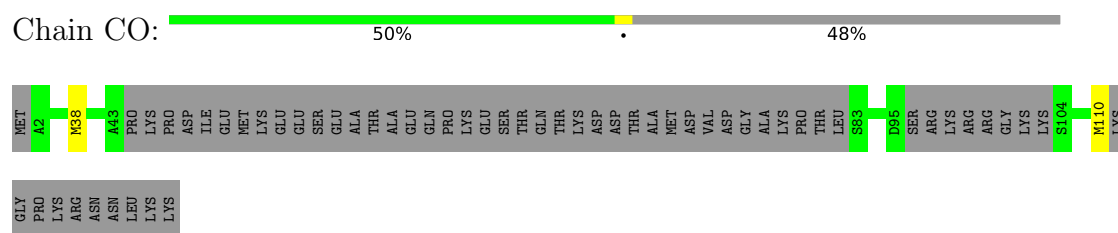
- Molecule 15: 60S ribosomal protein l7-like protein



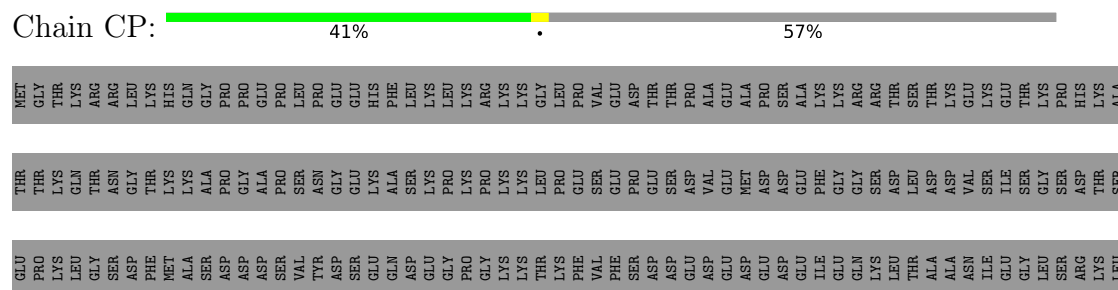
- Molecule 16: Eukaryotic translation initiation factor 6



- Molecule 17: DUF2423 domain-containing protein



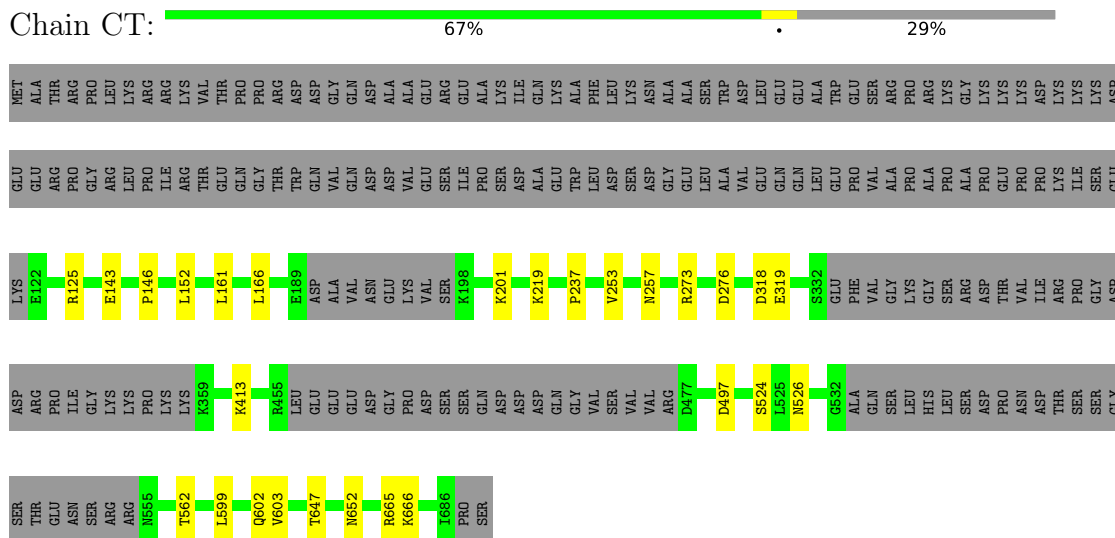
- Molecule 18: RNA methyltransferase nop2-like protein



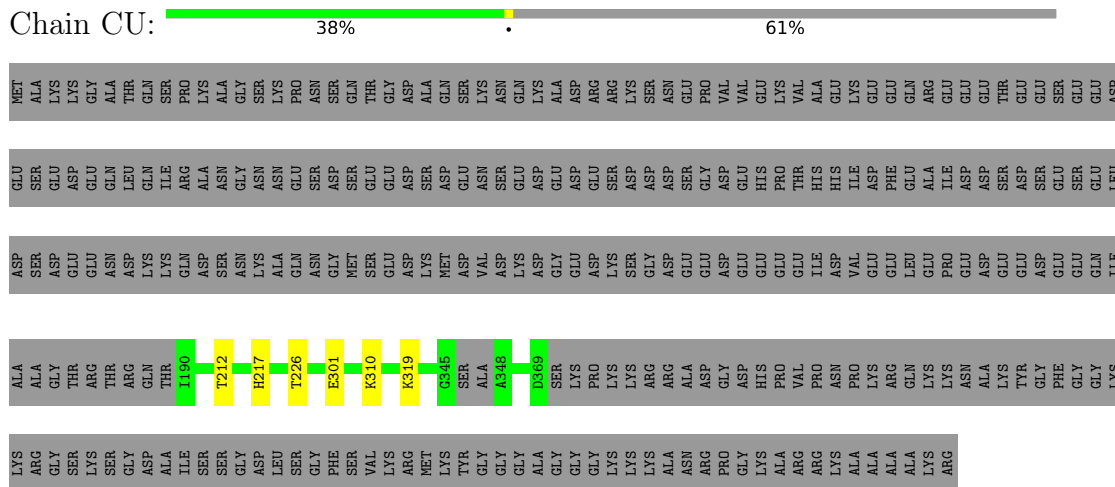




- Molecule 22: Nucleolar complex-associated protein 3



- Molecule 23: rRNA-processing protein EBP2



- Molecule 24: Putative 60S ribosomal protein



- Molecule 25: ATP-dependent RNA helicase









Opinion	Percentage
Doing a good job	60%
Doing a bad job	39%

HIS  
LYS  
LYS  
PRO  
TYR  
VAL  
ARG  
SER  
LYS  
GLY  
ARG  
LYS  
PHE  
GLU  
ARG  
ALA  
ARG  
GLY  
ARG  
ARG  
ARG  
SER  
ARG  
GLY  
PHE  
LYS  
VAL

- Molecule 41: Ribosomal protein L19

[illegible]

WORLDWIDE  
PDB  
PROTEIN DATA BANK




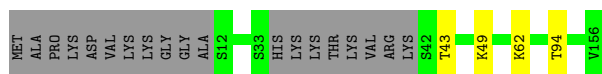


Chain LV:  94% . .



- Molecule 46: 60S ribosomal protein L25-like protein

Chain LX:  85% . 12%



- Molecule 47: 60S ribosomal protein L26-like protein

Chain LY:  93% . .




- Molecule 48: 60S ribosomal protein L27

Chain LZ:  98% .



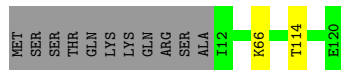
- Molecule 49: 60S ribosomal protein l30-like protein

Chain Lc:  86% 5% 9%



- Molecule 50: Putative 60S ribosomal protein

Chain Ld:  89% . 9%



- Molecule 51: 60S ribosomal protein L32-like protein

Chain Le:  95% . .



- Molecule 52: 60S ribosomal protein l33-like protein

Chain Lf:  94% 5% •



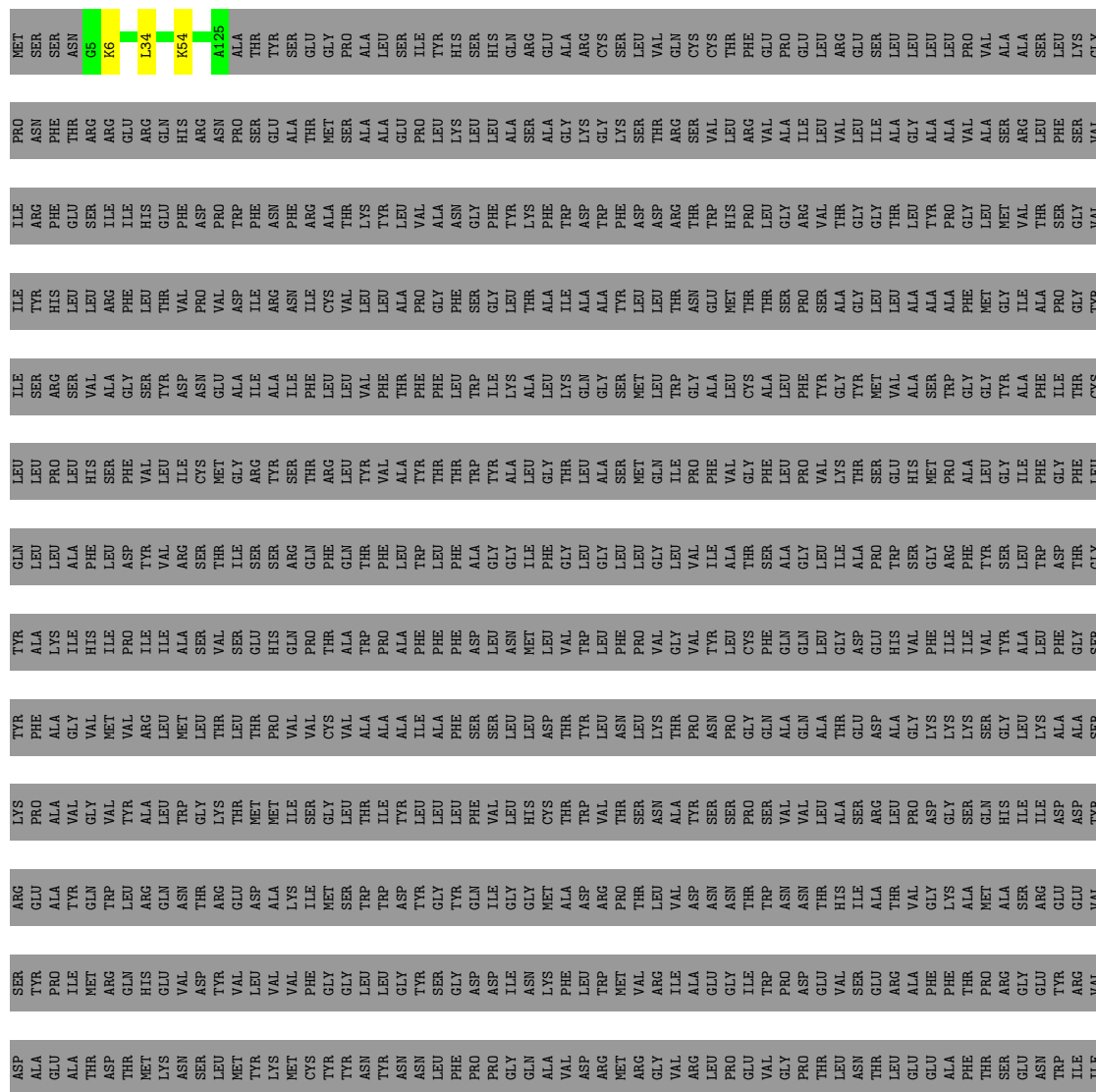
- Molecule 53: Ribosomal protein l34-like protein

Chain Lg:  97% ••




- Molecule 54: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:  13% 87%




ARG  
ILE  
TYR  
LYS  
VAL  
LYS  
ASP  
LEU  
ASP  
ASN  
LEU  
GLY  
ARG  
ASP  
HIS  
ALA  
SER  
ALA  
ALA  
ALA  
PHE  
GLU  
ARG  
GLY  
HIS  
LYS  
LYS  
LYS  
LYS  
ALA  
THR  
LYS  
LYS  
ARG  
GLY  
PRO  
ARG  
VAL  
LEU  
VAL  
GLU

- Molecule 55: 60S ribosomal protein L36

Chain Li:  78% 20%

MET  
SER  
GLU  
ASP  
ALA  
THR  
PRO  
LYS  
ALA  
PRO  
VAL  
GLU  
ARG  
THR  
GLY  
LEU  
ILE  
ARG  
GLY  
LEU  
ASN  
LYS  
G23  
K33  
R107  
H110

- Molecule 56: Ribosomal protein L37

Chain Lj:  74% 22%

MET  
THR  
GLY  
THR  
SER  
SER  
PHE  
GLY  
ARG  
LYS  
ASN  
K4  
R45  
R63  
K34  
R87  
GLY  
PRO  
ALA  
VAL  
SER  
THR  
SER  
SER

- Molecule 57: 60S ribosomal protein L38-like protein

Chain Lk:  89% 7%

MET  
F2  
K10  
R24  
K27  
K76  
ARG  
LYS  
SER  
SER  
ALA

- Molecule 58: 60S ribosomal protein L39

Chain Ll:  71% 25%

MET  
F2  
Q19  
Q25  
K39  
LYS  
ARG  
ARG  
HIS  
TRP  
ARG  
LYS  
THR  
ARG  
LEU  
GLY  
LEU

- Molecule 59: Ribosomal protein

Chain Lq:  91% 5%

MET  
SER  
LYS  
I4  
F49  
R60  
K92  
K98  
S113  
L116  
K133  
Y189  
I206  
K210  
SER  
PRO  
PRO  
LYS  
ARG  
LEU  
TYR

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173028	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 ( $e^-/\text{\AA}^2$ )	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: ZN, ADP, MG, GTP

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	0.46	0/66718	0.97	166/104004 (0.2%)
2	C2	0.42	0/6097	0.91	3/9499 (0.0%)
3	CA	0.32	0/2115	0.56	1/2840 (0.0%)
4	CB	0.32	0/2109	0.66	3/2866 (0.1%)
5	CC	0.32	0/5438	0.62	6/7404 (0.1%)
6	CD	0.31	0/3543	0.73	7/4824 (0.1%)
7	CE	0.30	0/3760	0.61	1/5068 (0.0%)
8	CF	0.33	0/1982	0.63	1/2671 (0.0%)
9	CG	0.33	0/1422	0.60	1/1920 (0.1%)
10	CH	0.34	0/4468	0.64	5/6029 (0.1%)
11	CI	0.30	0/1225	0.58	0/1645
12	CJ	0.33	0/4125	0.64	5/5548 (0.1%)
13	CK	0.31	0/1863	0.56	0/2494
14	CL	0.28	0/2178	0.54	0/2983
15	CM	0.30	0/1851	0.60	1/2481 (0.0%)
15	LF	0.32	0/2055	0.57	2/2758 (0.1%)
16	CN	0.33	0/1881	0.65	2/2560 (0.1%)
17	CO	0.28	0/470	0.61	1/619 (0.2%)
18	CP	0.32	0/2594	0.58	0/3514
19	CQ	0.40	0/1507	0.68	0/1996
20	CR	0.28	0/1369	0.59	1/1828 (0.1%)
21	CS	0.29	0/5115	0.59	3/6841 (0.0%)
22	CT	0.33	0/3974	0.61	4/5357 (0.1%)
23	CU	0.28	0/1428	0.57	0/1910
24	CV	0.30	0/1091	0.59	0/1468
25	CW	0.37	0/4371	0.80	12/5917 (0.2%)
26	CX	0.28	0/705	0.60	0/938
27	CY	0.33	0/3079	0.77	11/4136 (0.3%)
28	Cz	0.27	0/598	0.51	0/785
29	LB	0.33	0/2885	0.60	1/3872 (0.0%)
30	LC	0.32	0/2809	0.56	0/3787
31	LE	0.30	0/1502	0.56	0/2020

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LG	0.36	0/1667	0.58	0/2230
33	LH	0.32	0/1516	0.55	0/2038
34	LK	0.28	0/1124	0.64	2/1507 (0.1%)
35	LL	0.30	0/983	0.64	0/1318
36	LM	0.30	0/1120	0.58	1/1507 (0.1%)
37	LN	0.33	0/1595	0.61	0/2132
38	LO	0.33	0/1652	0.57	0/2215
39	LP	0.27	0/1367	0.56	1/1838 (0.1%)
40	LQ	0.30	0/1033	0.61	0/1391
41	LR	0.29	0/1235	0.62	1/1644 (0.1%)
42	LS	0.32	0/1468	0.59	0/1975
43	LT	0.27	0/1033	0.59	0/1389
44	LU	0.29	0/863	0.48	0/1155
45	LV	0.30	0/1013	0.53	0/1361
46	LX	0.26	0/1078	0.48	0/1451
47	LY	0.28	0/1079	0.60	0/1443
48	LZ	0.32	0/1135	0.55	0/1519
49	Lc	0.31	0/740	0.59	0/995
50	Ld	0.29	0/904	0.57	0/1209
51	Le	0.29	0/1043	0.56	0/1389
52	Lf	0.35	0/883	0.61	0/1187
53	Lg	0.31	0/943	0.62	0/1258
54	Lh	0.27	0/1006	0.54	1/1338 (0.1%)
55	Li	0.32	0/738	0.64	0/971
56	Lj	0.33	0/606	0.65	0/803
57	Lk	0.33	0/628	0.59	0/835
58	Ll	0.28	0/329	0.62	0/440
59	Lq	0.27	0/1621	0.64	1/2180 (0.0%)
All	All	0.38	0/176729	0.79	244/253300 (0.1%)

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
14	CL	0	1
22	CT	0	1
59	Lq	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2021	C	N3-C2-O2	-11.80	113.64	121.90
1	C1	1583	U	C2-N1-C1'	10.78	130.64	117.70
25	CW	277	PRO	CA-N-CD	-10.77	96.43	111.50
10	CH	72	ASP	CB-CG-OD1	10.72	127.95	118.30
1	C1	2022	C	N3-C2-O2	-10.09	114.84	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	CL	223	HIS	Peptide
22	CT	253	VAL	Peptide
59	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%)	235 (95%)	12 (5%)	0	100	100
4	CB	256/391 (66%)	242 (94%)	12 (5%)	2 (1%)	16	38
5	CC	650/801 (81%)	625 (96%)	24 (4%)	1 (0%)	44	68
6	CD	450/495 (91%)	429 (95%)	21 (5%)	0	100	100
7	CE	461/598 (77%)	440 (95%)	20 (4%)	1 (0%)	44	68
8	CF	243/270 (90%)	232 (96%)	10 (4%)	1 (0%)	30	55
9	CG	175/184 (95%)	169 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CH	538/661 (81%)	517 (96%)	21 (4%)	0	100	100
11	CI	144/414 (35%)	139 (96%)	5 (4%)	0	100	100
12	CJ	484/679 (71%)	468 (97%)	16 (3%)	0	100	100
13	CK	223/261 (85%)	216 (97%)	7 (3%)	0	100	100
14	CL	384/558 (69%)	353 (92%)	25 (6%)	6 (2%)	8	21
15	CM	219/249 (88%)	208 (95%)	11 (5%)	0	100	100
15	LF	245/249 (98%)	236 (96%)	9 (4%)	0	100	100
16	CN	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
17	CO	56/120 (47%)	55 (98%)	1 (2%)	0	100	100
18	CP	322/751 (43%)	309 (96%)	13 (4%)	0	100	100
19	CQ	173/225 (77%)	169 (98%)	4 (2%)	0	100	100
20	CR	159/237 (67%)	154 (97%)	5 (3%)	0	100	100
21	CS	607/834 (73%)	577 (95%)	29 (5%)	1 (0%)	44	68
22	CT	478/688 (70%)	454 (95%)	23 (5%)	1 (0%)	44	68
23	CU	174/451 (39%)	169 (97%)	4 (2%)	1 (1%)	22	45
24	CV	137/147 (93%)	131 (96%)	5 (4%)	1 (1%)	19	42
25	CW	531/679 (78%)	495 (93%)	34 (6%)	2 (0%)	30	55
26	CX	86/203 (42%)	85 (99%)	1 (1%)	0	100	100
27	CY	366/788 (46%)	346 (94%)	19 (5%)	1 (0%)	37	61
28	Cz	68/123 (55%)	65 (96%)	3 (4%)	0	100	100
29	LB	352/392 (90%)	338 (96%)	14 (4%)	0	100	100
30	LC	360/365 (99%)	345 (96%)	15 (4%)	0	100	100
31	LE	185/200 (92%)	172 (93%)	13 (7%)	0	100	100
32	LG	200/262 (76%)	189 (94%)	11 (6%)	0	100	100
33	LH	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
34	LK	142/165 (86%)	132 (93%)	8 (6%)	2 (1%)	9	24
35	LL	115/213 (54%)	109 (95%)	6 (5%)	0	100	100
36	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
37	LN	179/203 (88%)	173 (97%)	6 (3%)	0	100	100
38	LO	202/204 (99%)	200 (99%)	2 (1%)	0	100	100
39	LP	165/187 (88%)	162 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	LQ	127/213 (60%)	122 (96%)	5 (4%)	0	100	100
41	LR	144/2898 (5%)	143 (99%)	1 (1%)	0	100	100
42	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
43	LT	124/160 (78%)	118 (95%)	5 (4%)	1 (1%)	16	38
44	LU	103/127 (81%)	101 (98%)	2 (2%)	0	100	100
45	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
46	LX	133/156 (85%)	130 (98%)	3 (2%)	0	100	100
47	LY	132/138 (96%)	126 (96%)	6 (4%)	0	100	100
48	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
49	Lc	96/108 (89%)	95 (99%)	1 (1%)	0	100	100
50	Ld	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
51	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100
52	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
53	Lg	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
54	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
55	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
56	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
57	Lk	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
58	Ll	36/51 (71%)	36 (100%)	0	0	100	100
59	Lq	205/217 (94%)	184 (90%)	21 (10%)	0	100	100
All	All	12684/20359 (62%)	12128 (96%)	535 (4%)	21 (0%)	45	68

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	103	ASP
4	CB	104	PRO
7	CE	313	PRO
14	CL	224	ASP
14	CL	414	VAL

### 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	
3	CA	223/276 (81%)	217 (97%)	6 (3%)	40	69
4	CB	222/329 (68%)	208 (94%)	14 (6%)	15	35
5	CC	580/710 (82%)	562 (97%)	18 (3%)	35	64
6	CD	381/410 (93%)	355 (93%)	26 (7%)	13	32
7	CE	400/517 (77%)	382 (96%)	18 (4%)	23	50
8	CF	214/236 (91%)	209 (98%)	5 (2%)	45	74
9	CG	150/155 (97%)	145 (97%)	5 (3%)	33	62
10	CH	481/575 (84%)	465 (97%)	16 (3%)	33	62
11	CI	121/336 (36%)	114 (94%)	7 (6%)	17	39
12	CJ	428/579 (74%)	408 (95%)	20 (5%)	22	49
13	CK	195/225 (87%)	187 (96%)	8 (4%)	26	54
14	CL	65/458 (14%)	62 (95%)	3 (5%)	23	49
15	CM	191/215 (89%)	177 (93%)	14 (7%)	11	29
15	LF	213/215 (99%)	206 (97%)	7 (3%)	33	62
16	CN	206/206 (100%)	202 (98%)	4 (2%)	52	79
17	CO	48/99 (48%)	47 (98%)	1 (2%)	48	76
18	CP	273/632 (43%)	255 (93%)	18 (7%)	14	33
19	CQ	150/192 (78%)	133 (89%)	17 (11%)	4	11
20	CR	144/206 (70%)	137 (95%)	7 (5%)	21	47
21	CS	527/716 (74%)	504 (96%)	23 (4%)	24	51
22	CT	427/600 (71%)	405 (95%)	22 (5%)	19	44
23	CU	149/376 (40%)	144 (97%)	5 (3%)	32	61
24	CV	109/112 (97%)	107 (98%)	2 (2%)	54	80
25	CW	473/577 (82%)	422 (89%)	51 (11%)	5	13
26	CX	76/172 (44%)	71 (93%)	5 (7%)	14	33
27	CY	315/686 (46%)	283 (90%)	32 (10%)	6	15
28	Cz	60/107 (56%)	58 (97%)	2 (3%)	33	62
29	LB	301/331 (91%)	290 (96%)	11 (4%)	29	58
30	LC	283/285 (99%)	272 (96%)	11 (4%)	27	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LE	159/166 (96%)	149 (94%)	10 (6%)	15	35
32	LG	175/222 (79%)	165 (94%)	10 (6%)	17	40
33	LH	167/169 (99%)	159 (95%)	8 (5%)	21	48
34	LK	121/136 (89%)	114 (94%)	7 (6%)	17	39
35	LL	99/176 (56%)	97 (98%)	2 (2%)	50	78
36	LM	115/117 (98%)	114 (99%)	1 (1%)	75	90
37	LN	164/180 (91%)	157 (96%)	7 (4%)	25	52
38	LO	163/163 (100%)	159 (98%)	4 (2%)	42	72
39	LP	137/152 (90%)	130 (95%)	7 (5%)	20	45
40	LQ	110/178 (62%)	109 (99%)	1 (1%)	75	90
41	LR	128/2396 (5%)	120 (94%)	8 (6%)	15	35
42	LS	154/154 (100%)	144 (94%)	10 (6%)	14	34
43	LT	109/135 (81%)	101 (93%)	8 (7%)	11	29
44	LU	93/108 (86%)	90 (97%)	3 (3%)	34	63
45	LV	99/102 (97%)	95 (96%)	4 (4%)	27	55
46	LX	114/129 (88%)	110 (96%)	4 (4%)	31	60
47	LY	117/119 (98%)	112 (96%)	5 (4%)	25	52
48	LZ	121/121 (100%)	118 (98%)	3 (2%)	42	72
49	Lc	79/88 (90%)	74 (94%)	5 (6%)	15	35
50	Ld	95/105 (90%)	93 (98%)	2 (2%)	48	76
51	Le	110/114 (96%)	107 (97%)	3 (3%)	40	69
52	Lf	89/90 (99%)	84 (94%)	5 (6%)	17	41
53	Lg	101/102 (99%)	99 (98%)	2 (2%)	50	78
54	Lh	108/781 (14%)	106 (98%)	2 (2%)	52	79
55	Li	75/93 (81%)	73 (97%)	2 (3%)	40	69
56	Lj	61/78 (78%)	57 (93%)	4 (7%)	14	33
57	Lk	71/76 (93%)	68 (96%)	3 (4%)	25	53
58	Ll	34/46 (74%)	32 (94%)	2 (6%)	16	38
59	Lq	179/189 (95%)	172 (96%)	7 (4%)	27	56
All	All	10752/17218 (62%)	10235 (95%)	517 (5%)	24	48

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	LU	113	LYS
47	LY	76	LYS
44	LU	95	GLN
19	CQ	156	VAL
19	CQ	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
33	LH	118	ASN
35	LL	66	ASN
43	LT	146	ASN
41	LR	91	GLN
16	CN	106	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2770/3341 (82%)	564 (20%)	21 (0%)
2	C2	254/319 (79%)	54 (21%)	1 (0%)
All	All	3024/3660 (82%)	618 (20%)	22 (0%)

5 of 618 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	3078	U
1	C1	3204	G
1	C1	3162	A
1	C1	3209	U
1	C1	1046	A

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
62	ADP	CW	1001	63	24,29,29	0.69	0	29,45,45	0.78	1 (3%)
60	GTP	CH	701	-	26,34,34	1.18	1 (3%)	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
62	ADP	CW	1001	63	-	3/12/32/32	0/3/3/3
60	GTP	CH	701	-	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CH	701	GTP	C5-C6	-4.16	1.39	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CH	701	GTP	PB-O3B-PG	-3.63	120.38	132.83
60	CH	701	GTP	C5-C6-N1	3.20	119.61	113.95
60	CH	701	GTP	C3'-C2'-C1'	3.00	105.49	100.98
60	CH	701	GTP	C8-N7-C5	2.98	108.66	102.99
60	CH	701	GTP	C2-N1-C6	-2.85	119.85	125.10

There are no chirality outliers.

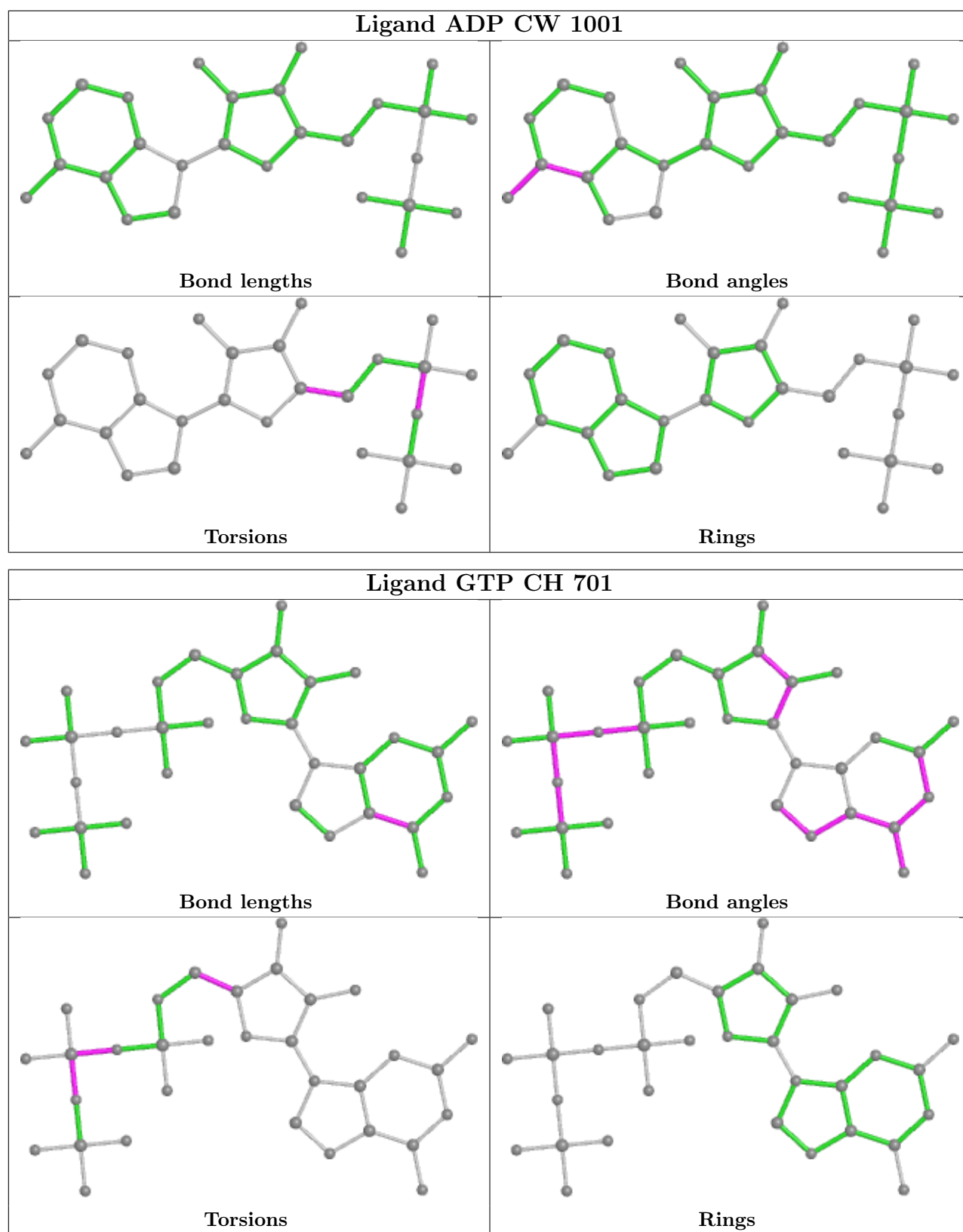
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	CW	1001	ADP	C3'-C4'-C5'-O5'
62	CW	1001	ADP	O4'-C4'-C5'-O5'
60	CH	701	GTP	PG-O3B-PB-O2B
62	CW	1001	ADP	PB-O3A-PA-O1A
60	CH	701	GTP	PA-O3A-PB-O3B

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 than 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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.