



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:18 PM JST

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

This is a Full wwPDB EM Validation 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

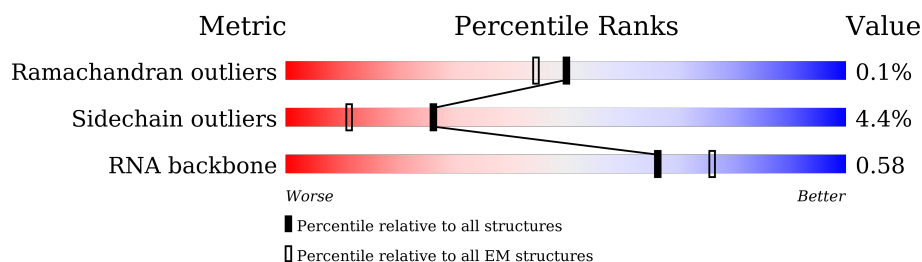
# 1 Overall quality at a glance

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.









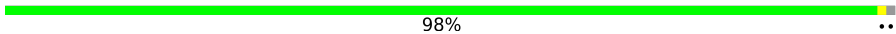
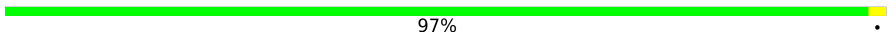
















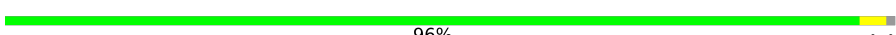
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	C2	319	
3	CA	316	
4	CB	391	
5	CC	801	
6	CD	495	
7	CE	598	
8	CF	270	
9	CG	184	

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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	697	
29	Ca	227	
30	Cz	123	
31	LA	254	
32	LB	392	
33	LC	365	






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Mol	Chain	Length	Quality of chain
34	LE	200	
35	LG	262	
36	LH	192	
37	LK	165	
38	LL	213	
39	LM	142	
40	LN	203	
41	LO	204	
42	LP	187	
43	LQ	213	
44	LR	2898	
45	LS	174	
46	LT	160	
47	LU	127	
48	LV	139	
49	LX	156	
50	LY	138	
51	LZ	135	
52	Lc	108	
53	Ld	120	
54	Le	131	
55	Lf	109	
56	Lg	119	
57	Lh	935	
58	Li	110	

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Mol	Chain	Length	Quality of chain
59	Lj	95	 77% 22%
60	Lk	81	 86% 6% 7%
61	Lp	92	 61% 37%
62	Ll	51	 73% 25%
63	Lq	217	 89% 6% 5%

## 2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 177631 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA (3341-MER).

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

- 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	P	S	0	0
			5297	3368	931	983	2	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	463	Total	C	N	O	S	0	0
			3673	2352	643	667	11		

There are 42 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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



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

- Molecule 12 is a protein called Pescadillo homolog.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Nucleolar protein 16.

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

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

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

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

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

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

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

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

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

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

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

- 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		
			701	435	128	135	3	0	0

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

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

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

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

- Molecule 29 is a protein called Nucleolar protein 12.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 37 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

- Molecule 40 is a protein called Ribosomal protein L15.

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

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

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

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

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

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

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

- Molecule 44 is a protein called Ribosomal protein L19.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is a protein called Ribosomal protein L37.



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

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

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

There are 13 discrepancies between the modelled and reference sequences:

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

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

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

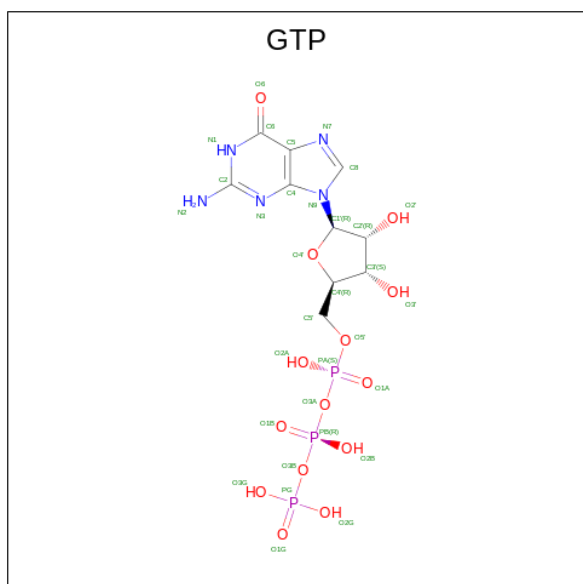
- Molecule 62 is a protein called 60S ribosomal protein L39.

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

- Molecule 63 is a protein called Ribosomal protein.

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

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

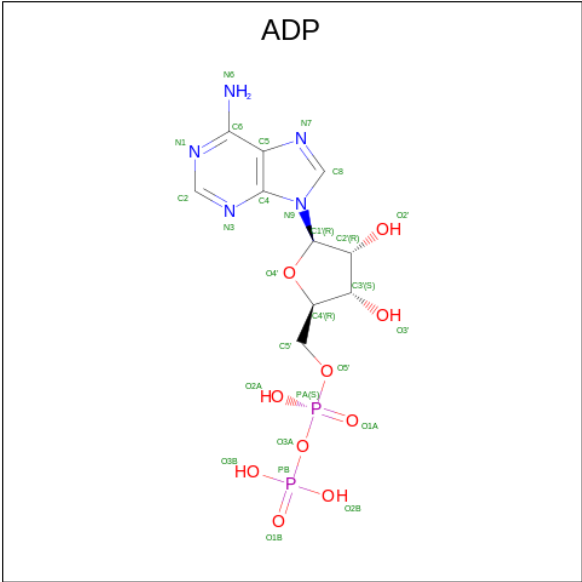


Mol	Chain	Residues	Atoms					AltConf
64	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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



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

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

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



U3132	A3275	U3133	A3134	G3140	C3144	C3145	U3291	G3292	U3293	U3294	U3295	G3296	U3297	U3298	G3309	C3318	U3321	C3322	C3323	U3324	U3325	U3330	A3331	G3332	A3333	C3337	C	C	A	G	A3199	C3203	U3209	U3210	U3216	U3217	C3227	G3228	G3229	G3230	C3244	U3253	A3256	U3257	G3258	U3259	G3260
U3132	A3275	U3133	A3134	G3140	C3144	C3145	U3291	G3292	U3293	U3294	U3295	G3296	U3297	U3298	G3309	C3318	U3321	C3322	C3323	U3324	U3325	U3330	A3331	G3332	A3333	C3337	C	C	A	G	A3199	C3203	U3209	U3210	U3216	U3217	C3227	G3228	G3229	G3230	C3244	U3253	A3256	U3257	G3258	U3259	G3260
C	U	C	U	C2941	C2942	C2954	U2955	C2956	A2969	A3006	U3013	U3014	U3015	G3016	G3035	A3043	C3049	C3050	C3074	C3075	U3078	A3079	A3086	A3087	U3088	A3098	A3099	C3100	G3101	U3108	U3111	A3112	C3113	A3118	C3119	G3120	U3121	U3122	G3123	U3124	A3125	G3126	A3127	U3130	A3131		
C	U	C	U	C2941	C2942	C2954	U2955	C2956	A2969	A3006	U3013	U3014	U3015	G3016	G3035	A3043	C3049	C3050	C3074	C3075	U3078	A3079	A3086	A3087	U3088	A3098	A3099	C3100	G3101	U3108	U3111	A3112	C3113	A3118	C3119	G3120	U3121	U3122	G3123	U3124	A3125	G3126	A3127	U3130	A3131		
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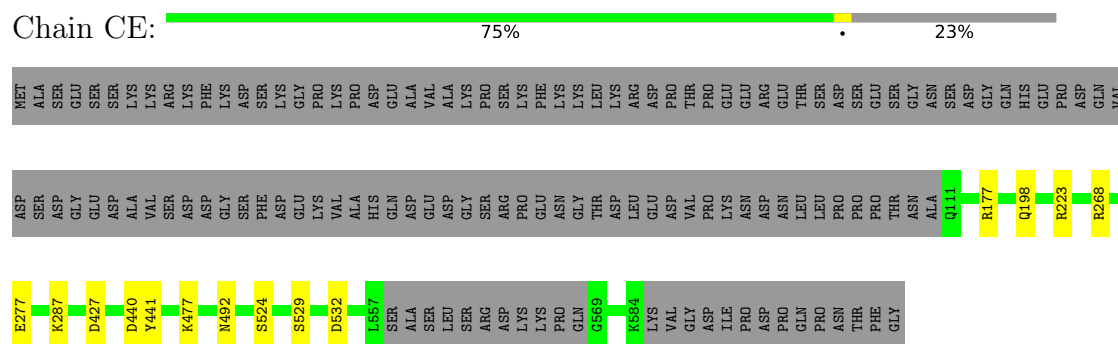
• Molecule 2: RNA (319-MER)

Chain C2:  63% 18% 20%

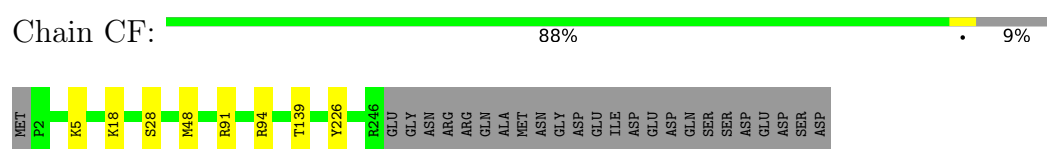
A1	U23	U34	C35	G39	G49	A59	A62	G63	U81	U82	C83	C84	U86	G87	U90	G95	U102	G103	A104	A105	C106	C110	A111	U112	U113	U125	G148	U157	U158	C159	C163	A164	U165	C166	C170	U173	U181	G182	U183
A189	G196	G203	G206	G207	G212	A213	A214	A215	A216	A219	G220	U221	G222	G225	U233	A	G	U	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	C



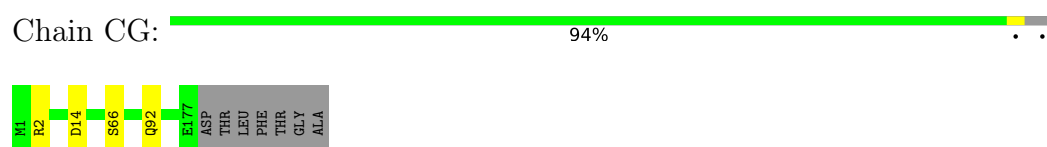
- Molecule 7: RNA helicase



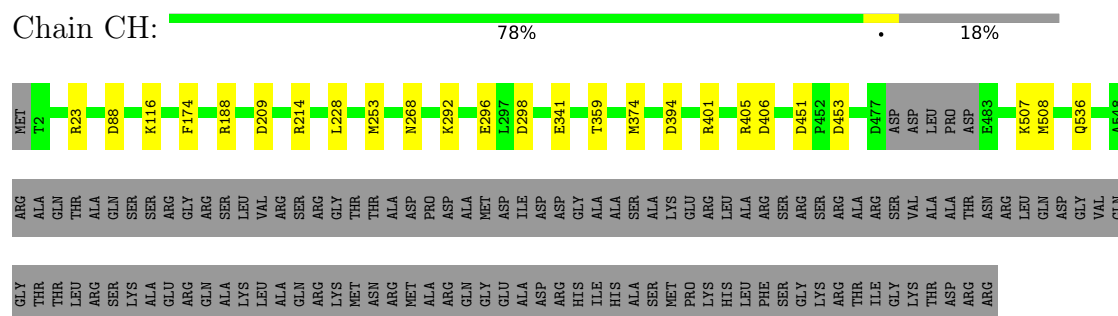
- Molecule 8: Ribosome assembly factor mrt4



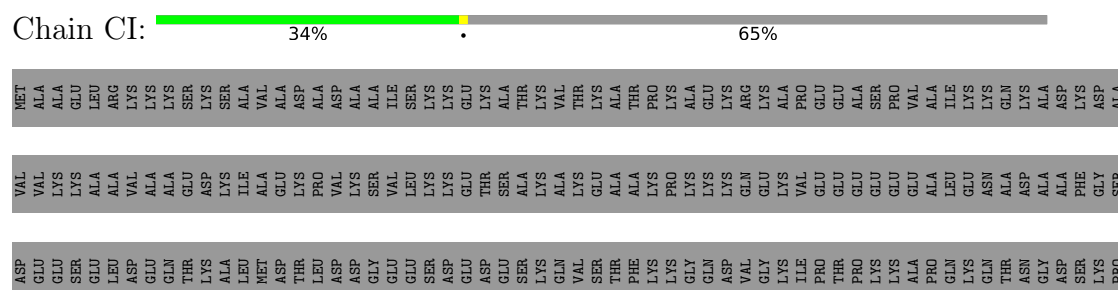
- Molecule 9: 60S ribosome subunit biogenesis protein NIP7

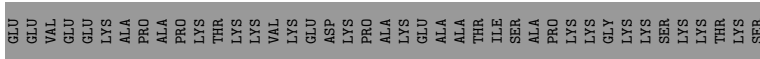


- Molecule 10: Nucleolar GTP-binding protein 1

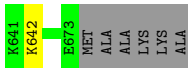
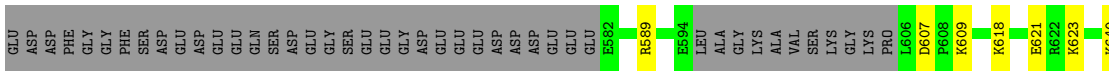


- Molecule 11: Putative RNA-binding protein

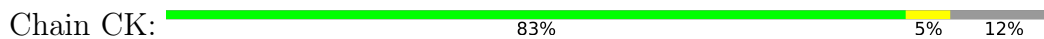




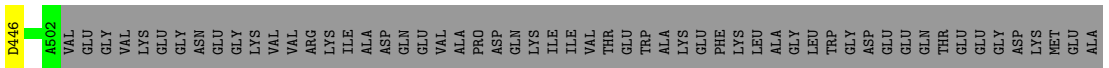
- Molecule 12: Pescadillo homolog



- Molecule 13: Ribosome biogenesis protein NSA2 homolog



- Molecule 14: Putative GTP binding protein



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



MET	SER	SER	THR	THR	THR	VAL	PRO	THR	GLN	ASN	ASP	ASP	GLY	GLY	GLY	ASP	LEU	G235	M248	N249
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- Chain LF:  98%

- Chain CN:  97%

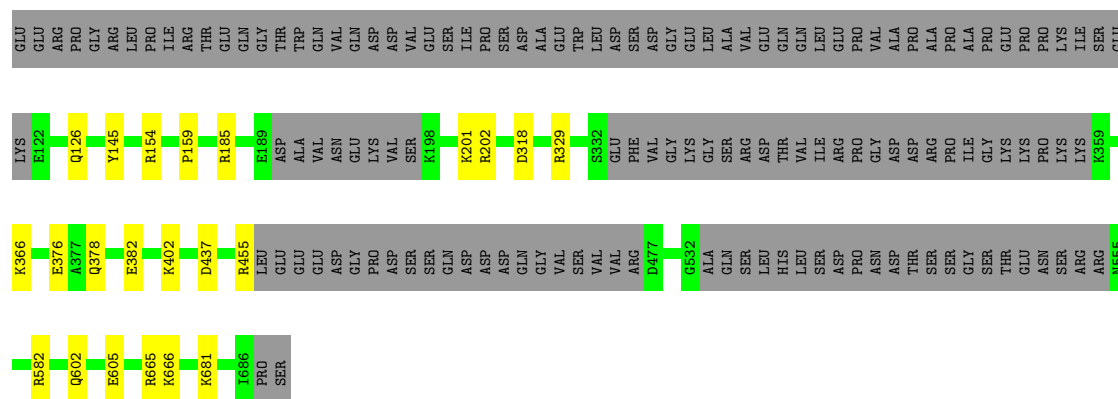
- Chain CO:  50% 48%

GLY	MET
PRO	A2
LYS	R6
ARG	A43
ASN	PRO
ASN	LYS
LEU	PRO
LYS	ASP
LYS	TLE
	GLU
	MET
	LYS
	GLU
	GLU
	SER
	GLU
	THR
	ALA
	GLU
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	PRO
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	SF3
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	ARG
	ARG
	GLY
	LYS
	LYS
	S104
	M110

- Chain CP: 

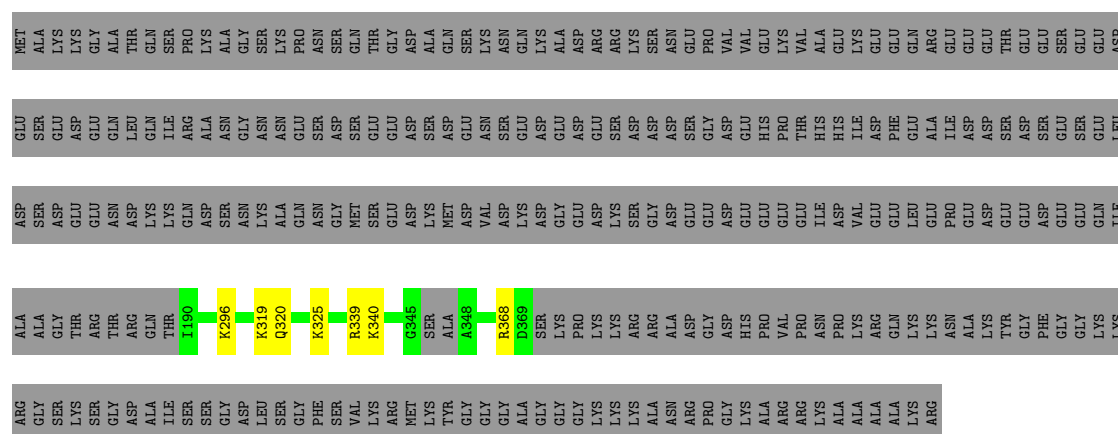
[illegible]





• Molecule 23: rRNA-processing protein EBP2

Chain CU: 38% 61%



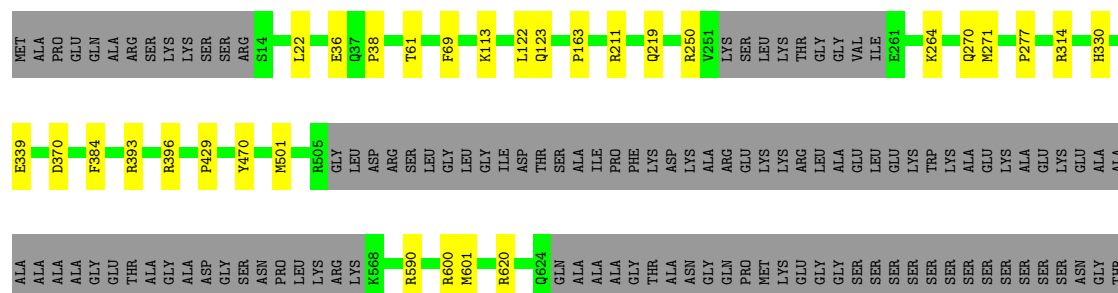
• Molecule 24: Putative 60S ribosomal protein

Chain CV: 91% 5%



• Molecule 25: ATP-dependent RNA helicase

Chain CW: 75% 20%



- Molecule 26: 60S ribosomal subunit-like protein

Chain CX:  43% 57%

MET	GLY	THR	ARG	THR	ILE	LYS	ASN	LYS	LYS	HIS	ALA	GLU	PRO	PRO	SER	LYS	LYS	LYS	LYS	LYS	ALA	GLY	ASP	GLY	GLY	VAL	LYS	LYS	THR	LYS	ASP	ARG	ARG	GLY	ALA	LYS	SER	LYS	LYS	VAL	LYS	VAL	PRO	PRO	ALA	ALA	ILE	GLU	VAL	LYS	LYS	GLY	LYS	LYS	PRO	ASN	LEU	GLY	GLN	ASP	LYS	LYS	LYS	LYS
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LYS	ARG	V63	N150	THR	LYS	GLU	GLN	LEU	ARG	LYS	LYS	ARG	LYS	LYS	ASN	LYS	LYS	GLY	GLY	ASP	GLN	LYS	SER	SER	GLU	ASP	GLU	GLY	GLY	PRO	SER	LEU	LEU	LYS	GLU	GLY	LEU	THR	SER	THR	GLY	SER	LYS	ALA	VAL	LYS	SER	LYS	LYS	LYS	LYS	VAL	SER	PHE	ALA	THR	PRO
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- Molecule 27: Putative NOC2 family protein

Chain CY:  50% 1% 47%

MET	G2		K6		Q36		E40	LYS	GLU	LYS	ALA	LYS	ARG	ALA	LEU	ASP	ASP	PHE	GLU	TYR	LYS	GLY	PRO	ASN	GLY	ASP	ALA	ASP	LYS	LYS	LYS	PRO	PRO	GLY	PRO	N68		K80		S87	GLU	SER	LYS	LYS	LYS	GLU	LYS	PRO	ALA	LYS	LEU	GLY	LYS	ARG	LYS	ARG	ASP	PRO	GLU
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GLU  
SER  
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ILE  
THR  
ASP  
ASN  
ASP  
PRO  
PRO  
LEU  
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GLY  
GLU  
GLU  
GLU  
GLU  
ASP  
ASP  
LEU  
GLY  
MET  
SER  
LYS  
ALA  
ALA  
LEU  
ALA  
GLU  
LYS

PRO ASP PHE TYR LYS PHE LEU LYS HIS ASP ASP PHE ASP ASP ASN ALA ALA LEU ALA LEU SER GLY SER ASP ASP GLU GLU GLN PRO LYS LYS LYS LYS LYS THR GLU GLU GLY GLY GLY GLY GLU GLU LYS LYS LYS LYS LYS LYS

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

THR	LEU	ASP	GLY	THR	LEU	LYS	THR	LEU	SER	ALA	HIS	PRO	LEU	PRO	TYR	LEU	S71	R373	L376	K377	M378	Q389	SER	ALA	SER	T393	L402	G411	ASP	K413	L420	L427	V432	F433	L444	Q457	Y461	F465	R488
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	------	------	------	-----	------	------	------	------	------	------	------	------	------	------

Y495	Y496	H497	C504	S511	PRO	LEU	LYS	ALA	ALA	ALA	GLY	LYS	GLU	S522	R526	M584	K603	Y608	M654	K659	PRO	LYS	GLY	G663	Q678	M683	D705	R748	GLU	GLU	LYS	ALA	ALA	GLU	ARG	GLU	GLU	GLY	SER	GLU	GLU	GLU	GLU	GLU	ASP
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GLU  
MET  
GLU  
ASP  
ALA  
GLU  
GLY  
GLY  
GLU  
GLY  
SER  
ASP  
GLU  
ASP  
GLU  
ASP  
GLU  
LYS  
GLY  
GLY  
GLY  
GLU

- Molecule 28: PUM-HD domain-containing protein

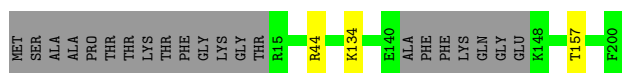
Chain CZ:  79% • 17%

MET	ALA	GLN	LYS	SER	ALA	ASN	SER	ALA	ALA	PRO	ALA	LYS	ARG	LYS	SER	SER	SER	ASN	ASP	HIS	ALA	ASP	SER	ASN	ARG	VAL	LYS	LYS	ALA	LYS	THR	GLU	GLN	GLY	PRO	LYS	HIS	LYS	LYS	PHE	ASP	ASP	THR	GLU	ILE	ALA	PRO	ASN	GLY	ALA	GLY	ASP	PHE	SER	ASP	VAL
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ASP	GLY	ARG	ASN	GLN	GLN	LYS	PRO	MET	LYS	ASN	ILE	LYS	THR	GLY	THR	SER	LYS	GLU	ASN	ASP	LYS	THR	THR	GLY	LYS	PRO	ALA	ALA	VAL	SER	SER	ARG	GLU	ALA	HIS	ALA	ALA	ARG	GLN	LYS	LYS	GLN	LEU	GLU	LYS	GLU	GLU	ARG	LYS	ALA	ALA	LYS	PRO	L113	R128	ARG	LYS	SER	HIS
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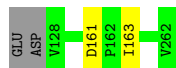
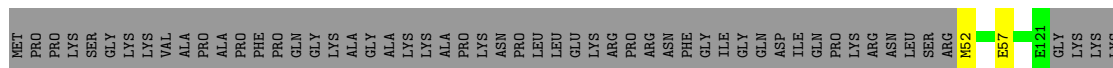
PRO	LYS	E136	Y146	R164	R178	R179	K199	E211	R214	H231	D239	K248	M313	M324	R359	Y380	M387	L398	M409	T438	T442	V443	M444	E448	E464	L695	GLY
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- Molecule 35: 60S ribosomal protein L8

Chain LG: 77% 22%



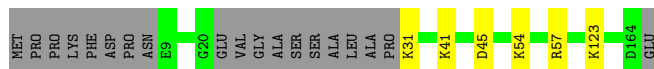
- Molecule 36: 60S ribosomal protein I9-like protein

Chain LH: 97% ..



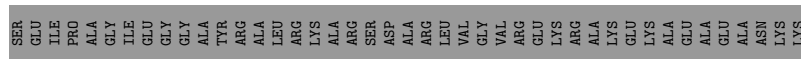
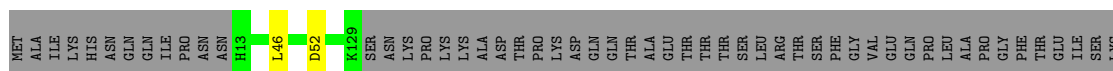
- Molecule 37: 60S ribosomal protein L12-like protein

Chain LK: 85% 12%



- Molecule 38: 60S ribosomal protein L13

Chain LL: 54% 45%



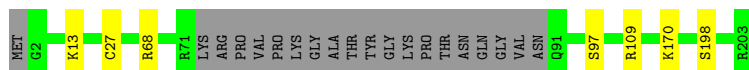
- Molecule 39: 60S ribosomal protein L14-like protein

Chain LM: 94% ..



- Molecule 40: Ribosomal protein L15

Chain LN: 87% 10%

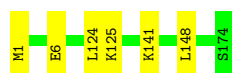






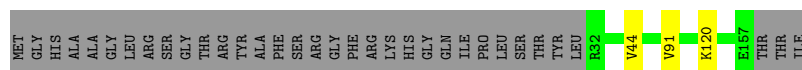






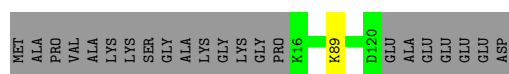
- Molecule 46: 60S ribosomal protein l21-like protein

Chain LT: 77% 21%



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

Chain LU: 82% 17%



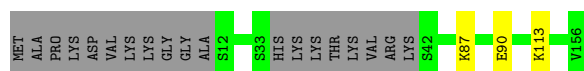
- Molecule 48: 60S ribosomal protein l23-like protein

Chain LV: 95% 2%



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

Chain LX: 86% 12%



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

Chain LY: 92% 5%



- Molecule 51: 60S ribosomal protein L27

Chain LZ: 95% 5%



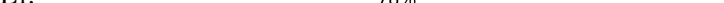
- Molecule 52: 60S ribosomal protein l30-like protein

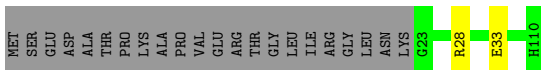
Chain Lc: 87% 9%



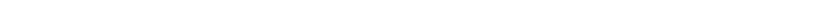
[illegible]

- Molecule 58: 60S ribosomal protein L36

Chain Li:  78% 20%



- Molecule 59: Ribosomal protein L37

Chain Lj:  77% . 22%



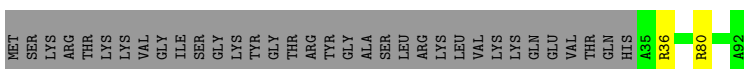
- Molecule 60: 60S ribosomal protein L38-like protein

Chain Lk:  86% 6% 7%



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

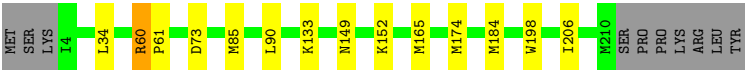
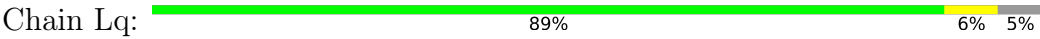
Chain Lp:  61% 1% 37%



- Molecule 62: 60S ribosomal protein L39



● Molecule 63: Ribosomal protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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: MG, ZN, GTP, ADP, TPO, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
32	LB	0.27	0/2885	0.53	0/3872
33	LC	0.26	0/2809	0.50	0/3787
34	LE	0.26	0/1428	0.49	0/1921
35	LG	0.26	0/1674	0.47	0/2240
36	LH	0.27	0/1516	0.51	0/2038
37	LK	0.25	0/1124	0.55	0/1507
38	LL	0.25	0/983	0.58	0/1318
39	LM	0.25	0/1120	0.52	0/1507
40	LN	0.26	0/1595	0.56	0/2132
41	LO	0.27	0/1652	0.52	0/2215
42	LP	0.24	0/1367	0.53	0/1838
43	LQ	0.25	0/1033	0.55	0/1391
44	LR	0.25	0/1235	0.53	0/1644
45	LS	0.27	0/1468	0.51	0/1975
46	LT	0.26	0/1033	0.56	0/1389
47	LU	0.26	0/863	0.46	0/1155
48	LV	0.28	0/1013	0.49	0/1361
49	LX	0.24	0/1078	0.47	0/1451
50	LY	0.24	0/1079	0.53	0/1443
51	LZ	0.27	0/1135	0.53	0/1519
52	Lc	0.25	0/740	0.47	0/995
53	Ld	0.26	0/904	0.53	0/1209
54	Le	0.25	0/1043	0.53	0/1389
55	Lf	0.28	0/883	0.57	0/1187
56	Lg	0.25	0/943	0.56	0/1258
57	Lh	0.24	0/1006	0.50	0/1338
58	Li	0.25	0/738	0.56	0/971
59	Lj	0.26	0/606	0.59	0/803
60	Lk	0.26	0/628	0.54	0/835
61	Lp	0.24	0/441	0.60	0/590
62	Ll	0.23	0/329	0.51	0/440
63	Lq	0.27	0/1621	0.62	0/2180
All	All	0.27	0/187537	0.67	76/268557 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CC	0	1
63	Lq	0	1
All	All	0	2



There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	CP	289	PRO	CA-N-CD	-12.12	94.54	111.50
22	CT	159	PRO	CA-N-CD	-11.33	95.64	111.50
1	C1	136	C	N3-C2-O2	-9.16	115.49	121.90
1	C1	2452	C	N3-C2-O2	-9.16	115.49	121.90
1	C1	2021	C	N3-C2-O2	-9.01	115.59	121.90
1	C1	1583	U	C2-N1-C1'	8.40	127.78	117.70
1	C1	2723	C	N3-C2-O2	-7.70	116.51	121.90
1	C1	1406	C	N3-C2-O2	-7.59	116.59	121.90
1	C1	1583	U	N1-C2-O2	7.31	127.92	122.80
1	C1	1836	C	N3-C2-O2	-7.18	116.88	121.90
1	C1	2041	C	N3-C2-O2	-7.10	116.93	121.90
1	C1	1098	G	C4-N9-C1'	6.88	135.45	126.50
1	C1	1477	U	C2-N1-C1'	6.86	125.93	117.70
1	C1	799	C	N3-C2-O2	-6.82	117.12	121.90
25	CW	429	PRO	CA-N-CD	-6.78	102.00	111.50
1	C1	127	G	N3-C4-N9	6.75	130.05	126.00
1	C1	1583	U	N3-C2-O2	-6.71	117.51	122.20
1	C1	2020	C	N1-C2-O2	6.67	122.90	118.90
1	C1	590	C	N1-C2-O2	6.67	122.90	118.90
1	C1	1537	U	C2-N1-C1'	6.47	125.46	117.70
1	C1	72	C	C2-N3-C4	-6.42	116.69	119.90
1	C1	249	C	N3-C2-O2	-6.30	117.49	121.90
1	C1	136	C	N1-C2-O2	6.26	122.66	118.90
1	C1	2452	C	N1-C2-O2	6.19	122.61	118.90
1	C1	2020	C	C2-N1-C1'	6.11	125.52	118.80
1	C1	1098	G	C8-N9-C1'	-6.08	119.10	127.00
1	C1	2451	C	N1-C2-O2	6.06	122.53	118.90
1	C1	1537	U	N3-C2-O2	-6.04	117.97	122.20
1	C1	128	G	C5-C6-O6	6.00	132.20	128.60
1	C1	1537	U	N1-C2-O2	5.96	126.97	122.80
6	CD	417	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C1	2021	C	C6-N1-C2	-5.92	117.93	120.30
1	C1	590	C	N3-C2-O2	-5.88	117.79	121.90
16	CN	237	MET	CA-CB-CG	5.80	123.16	113.30
1	C1	1836	C	N1-C2-N3	5.76	123.23	119.20
1	C1	3015	U	C2-N1-C1'	5.60	124.42	117.70
1	C1	83	C	C6-N1-C1'	5.57	127.49	120.80
10	CH	453	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C1	1406	C	N1-C2-N3	5.54	123.08	119.20
1	C1	1583	U	C6-N1-C1'	-5.54	113.45	121.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2297	G	O4'-C1'-N9	-5.54	103.77	108.20
1	C1	2246	C	N1-C2-O2	5.50	122.20	118.90
1	C1	2452	C	C6-N1-C2	-5.48	118.11	120.30
1	C1	799	C	N1-C2-O2	5.47	122.18	118.90
6	CD	56	LEU	CA-CB-CG	5.46	127.86	115.30
1	C1	2428	G	N1-C2-N2	-5.46	111.29	116.20
1	C1	950	C	N3-C2-O2	-5.42	118.10	121.90
28	CZ	398	LEU	CA-CB-CG	5.42	127.77	115.30
1	C1	3281	U	O4'-C1'-N1	-5.42	103.86	108.20
1	C1	1477	U	N1-C2-O2	5.37	126.56	122.80
1	C1	249	C	N1-C2-O2	5.37	122.12	118.90
1	C1	2752	G	C5-C6-O6	5.37	131.82	128.60
27	CY	420	LEU	CA-CB-CG	5.31	127.52	115.30
1	C1	1406	C	C6-N1-C2	-5.29	118.18	120.30
1	C1	127	G	C8-N9-C1'	-5.28	120.13	127.00
1	C1	1836	C	C6-N1-C2	-5.28	118.19	120.30
1	C1	1098	G	N3-C4-N9	5.24	129.15	126.00
1	C1	1336	G	C4-N9-C1'	5.24	133.31	126.50
1	C1	2428	G	N1-C6-O6	-5.20	116.78	119.90
1	C1	2752	G	N1-C6-O6	-5.20	116.78	119.90
1	C1	442	C	C2-N1-C1'	5.20	124.52	118.80
2	C2	207	G	N1-C6-O6	-5.19	116.79	119.90
16	CN	237	MET	CB-CG-SD	5.14	127.84	112.40
7	CE	440	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C1	127	G	C4-N9-C1'	5.10	133.13	126.50
1	C1	3158	U	C2-N1-C1'	5.10	123.82	117.70
1	C1	1477	U	N3-C2-O2	-5.09	118.64	122.20
1	C1	940	C	C2-N1-C1'	5.08	124.39	118.80
1	C1	128	G	N1-C6-O6	-5.07	116.86	119.90
22	CT	318	ASP	CB-CG-OD1	5.07	122.86	118.30
25	CW	163	PRO	CA-N-CD	-5.04	104.44	111.50
25	CW	277	PRO	CA-N-CD	-5.04	104.45	111.50
1	C1	2246	C	N3-C2-O2	-5.01	118.39	121.90
1	C1	1406	C	C5-C4-N4	5.01	123.70	120.20
27	CY	376	LEU	CA-CB-CG	5.01	126.82	115.30
1	C1	83	C	C5-C4-N4	5.00	123.70	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	CC	519	GLU	Peptide

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Mol	Chain	Res	Type	Group
63	Lq	60	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CA	247/316 (78%)	232 (94%)	15 (6%)	0	100	100
4	CB	256/391 (66%)	239 (93%)	17 (7%)	0	100	100
5	CC	648/801 (81%)	623 (96%)	24 (4%)	1 (0%)	44	68
6	CD	450/495 (91%)	425 (94%)	25 (6%)	0	100	100
7	CE	459/598 (77%)	449 (98%)	10 (2%)	0	100	100
8	CF	243/270 (90%)	234 (96%)	9 (4%)	0	100	100
9	CG	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
10	CH	538/661 (81%)	522 (97%)	16 (3%)	0	100	100
11	CI	144/414 (35%)	140 (97%)	4 (3%)	0	100	100
12	CJ	484/679 (71%)	473 (98%)	11 (2%)	0	100	100
13	CK	223/261 (85%)	214 (96%)	9 (4%)	0	100	100
14	CL	393/558 (70%)	368 (94%)	23 (6%)	2 (0%)	25	49
15	CM	219/249 (88%)	212 (97%)	7 (3%)	0	100	100
15	LF	245/249 (98%)	237 (97%)	8 (3%)	0	100	100
16	CN	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	354/751 (47%)	336 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CQ	173/225 (77%)	167 (96%)	6 (4%)	0	100	100
20	CR	159/237 (67%)	158 (99%)	1 (1%)	0	100	100
21	CS	609/834 (73%)	584 (96%)	25 (4%)	0	100	100
22	CT	478/688 (70%)	461 (96%)	17 (4%)	0	100	100
23	CU	174/451 (39%)	170 (98%)	4 (2%)	0	100	100
24	CV	137/147 (93%)	135 (98%)	2 (2%)	0	100	100
25	CW	534/679 (79%)	479 (90%)	54 (10%)	1 (0%)	44	68
26	CX	86/203 (42%)	85 (99%)	1 (1%)	0	100	100
27	CY	406/788 (52%)	380 (94%)	25 (6%)	1 (0%)	44	68
28	CZ	572/697 (82%)	552 (96%)	20 (4%)	0	100	100
29	Ca	111/227 (49%)	109 (98%)	2 (2%)	0	100	100
30	Cz	68/123 (55%)	66 (97%)	2 (3%)	0	100	100
31	LA	164/254 (65%)	155 (94%)	9 (6%)	0	100	100
32	LB	352/392 (90%)	335 (95%)	17 (5%)	0	100	100
33	LC	360/365 (99%)	346 (96%)	14 (4%)	0	100	100
34	LE	175/200 (88%)	169 (97%)	6 (3%)	0	100	100
35	LG	201/262 (77%)	197 (98%)	4 (2%)	0	100	100
36	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
37	LK	142/165 (86%)	136 (96%)	6 (4%)	0	100	100
38	LL	115/213 (54%)	112 (97%)	3 (3%)	0	100	100
39	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
40	LN	179/203 (88%)	170 (95%)	9 (5%)	0	100	100
41	LO	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
42	LP	165/187 (88%)	160 (97%)	5 (3%)	0	100	100
43	LQ	127/213 (60%)	121 (95%)	6 (5%)	0	100	100
44	LR	144/2898 (5%)	143 (99%)	1 (1%)	0	100	100
45	LS	172/174 (99%)	165 (96%)	7 (4%)	0	100	100
46	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	16	38
47	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
48	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
49	LX	133/156 (85%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	LY	132/138 (96%)	127 (96%)	5 (4%)	0	100	100
51	LZ	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
52	Lc	96/108 (89%)	96 (100%)	0	0	100	100
53	Ld	107/120 (89%)	105 (98%)	2 (2%)	0	100	100
54	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100
55	Lf	106/109 (97%)	104 (98%)	2 (2%)	0	100	100
56	Lg	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
57	Lh	119/935 (13%)	116 (98%)	3 (2%)	0	100	100
58	Li	86/110 (78%)	86 (100%)	0	0	100	100
59	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
60	Lk	73/81 (90%)	68 (93%)	5 (7%)	0	100	100
61	Lp	56/92 (61%)	52 (93%)	4 (7%)	0	100	100
62	Ll	36/51 (71%)	35 (97%)	1 (3%)	0	100	100
63	Lq	205/217 (94%)	183 (89%)	21 (10%)	1 (0%)	25	49
All	All	13660/21629 (63%)	13103 (96%)	550 (4%)	7 (0%)	50	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	CW	393	ARG
27	CY	457	GLN
14	CL	439	ASP
14	CL	446	ASP
46	LT	44	VAL
5	CC	251	VAL
63	Lq	61	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	
3	CA	223/276 (81%)	218 (98%)	5 (2%)	47	76
4	CB	222/329 (68%)	207 (93%)	15 (7%)	13	32
5	CC	578/708 (82%)	552 (96%)	26 (4%)	23	50
6	CD	381/410 (93%)	363 (95%)	18 (5%)	22	49
7	CE	398/517 (77%)	385 (97%)	13 (3%)	33	62
8	CF	214/236 (91%)	206 (96%)	8 (4%)	29	58
9	CG	150/155 (97%)	146 (97%)	4 (3%)	40	69
10	CH	481/575 (84%)	457 (95%)	24 (5%)	20	46
11	CI	121/336 (36%)	116 (96%)	5 (4%)	26	54
12	CJ	428/579 (74%)	401 (94%)	27 (6%)	15	35
13	CK	195/225 (87%)	183 (94%)	12 (6%)	15	36
14	CL	72/458 (16%)	68 (94%)	4 (6%)	17	41
15	CM	191/215 (89%)	183 (96%)	8 (4%)	25	53
15	LF	213/215 (99%)	210 (99%)	3 (1%)	62	84
16	CN	206/206 (100%)	199 (97%)	7 (3%)	32	61
17	CO	48/99 (48%)	46 (96%)	2 (4%)	25	53
18	CP	302/632 (48%)	291 (96%)	11 (4%)	30	59
19	CQ	150/192 (78%)	140 (93%)	10 (7%)	13	33
20	CR	144/206 (70%)	139 (96%)	5 (4%)	31	60
21	CS	532/716 (74%)	506 (95%)	26 (5%)	21	47
22	CT	427/600 (71%)	407 (95%)	20 (5%)	22	49
23	CU	149/376 (40%)	142 (95%)	7 (5%)	22	49
24	CV	109/112 (97%)	104 (95%)	5 (5%)	23	49
25	CW	476/577 (82%)	450 (94%)	26 (6%)	18	41
26	CX	76/172 (44%)	76 (100%)	0	100	100
27	CY	369/686 (54%)	342 (93%)	27 (7%)	11	29
28	CZ	310/581 (53%)	288 (93%)	22 (7%)	12	30
29	Ca	101/195 (52%)	92 (91%)	9 (9%)	8	20
30	Cz	60/107 (56%)	57 (95%)	3 (5%)	20	46
31	LA	131/198 (66%)	123 (94%)	8 (6%)	15	36
32	LB	301/331 (91%)	295 (98%)	6 (2%)	50	78
33	LC	283/285 (99%)	271 (96%)	12 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	LE	151/166 (91%)	148 (98%)	3 (2%)	50	78
35	LG	176/222 (79%)	172 (98%)	4 (2%)	45	74
36	LH	167/169 (99%)	163 (98%)	4 (2%)	44	73
37	LK	121/136 (89%)	115 (95%)	6 (5%)	20	46
38	LL	99/176 (56%)	97 (98%)	2 (2%)	50	78
39	LM	115/117 (98%)	112 (97%)	3 (3%)	41	70
40	LN	164/180 (91%)	157 (96%)	7 (4%)	25	52
41	LO	163/163 (100%)	158 (97%)	5 (3%)	35	64
42	LP	137/152 (90%)	134 (98%)	3 (2%)	47	76
43	LQ	110/178 (62%)	106 (96%)	4 (4%)	30	59
44	LR	128/2396 (5%)	121 (94%)	7 (6%)	18	41
45	LS	154/154 (100%)	148 (96%)	6 (4%)	27	56
46	LT	109/135 (81%)	107 (98%)	2 (2%)	54	80
47	LU	93/108 (86%)	92 (99%)	1 (1%)	70	87
48	LV	99/102 (97%)	96 (97%)	3 (3%)	36	65
49	LX	114/129 (88%)	111 (97%)	3 (3%)	41	70
50	LY	117/119 (98%)	110 (94%)	7 (6%)	16	38
51	LZ	121/121 (100%)	114 (94%)	7 (6%)	17	39
52	Lc	79/88 (90%)	75 (95%)	4 (5%)	20	45
53	Ld	95/105 (90%)	93 (98%)	2 (2%)	48	76
54	Le	110/114 (96%)	106 (96%)	4 (4%)	30	59
55	Lf	89/90 (99%)	86 (97%)	3 (3%)	32	61
56	Lg	101/102 (99%)	98 (97%)	3 (3%)	36	65
57	Lh	108/781 (14%)	105 (97%)	3 (3%)	38	68
58	Li	75/93 (81%)	73 (97%)	2 (3%)	40	69
59	Lj	61/78 (78%)	60 (98%)	1 (2%)	58	82
60	Lk	71/76 (93%)	66 (93%)	5 (7%)	12	31
61	Lp	45/74 (61%)	43 (96%)	2 (4%)	24	51
62	Ll	34/46 (74%)	33 (97%)	1 (3%)	37	67
63	Lq	179/189 (95%)	166 (93%)	13 (7%)	11	29
All	All	11426/18264 (63%)	10928 (96%)	498 (4%)	26	51

All (498) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	30	ARG
3	CA	98	LYS
3	CA	109	ASN
3	CA	241	THR
3	CA	273	LYS
4	CB	19	ASP
4	CB	28	LYS
4	CB	35	LYS
4	CB	42	ARG
4	CB	110	ASN
4	CB	121	ARG
4	CB	126	ARG
4	CB	132	HIS
4	CB	134	LYS
4	CB	154	LEU
4	CB	169	LYS
4	CB	238	SER
4	CB	260	GLU
4	CB	281	PHE
4	CB	294	TYR
5	CC	121	PHE
5	CC	141	LYS
5	CC	142	ASP
5	CC	162	ASP
5	CC	181	ASP
5	CC	229	LEU
5	CC	240	ARG
5	CC	241	LYS
5	CC	293	LYS
5	CC	307	LYS
5	CC	351	ASP
5	CC	373	MET
5	CC	392	LYS
5	CC	439	LYS
5	CC	473	ASP
5	CC	519	GLU
5	CC	524	MET
5	CC	544	ASN
5	CC	590	THR
5	CC	663	LYS
5	CC	681	ASP
5	CC	706	SER

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Mol	Chain	Res	Type
5	CC	725	PHE
5	CC	742	LEU
5	CC	763	LYS
5	CC	801	MET
6	CD	32	LYS
6	CD	73	ARG
6	CD	125	PRO
6	CD	155	LEU
6	CD	189	ASP
6	CD	204	LYS
6	CD	205	TYR
6	CD	293	TRP
6	CD	323	ARG
6	CD	365	ARG
6	CD	373	ARG
6	CD	397	SER
6	CD	404	LEU
6	CD	422	ARG
6	CD	446	TRP
6	CD	470	LYS
6	CD	481	LYS
6	CD	486	ARG
7	CE	177	ARG
7	CE	198	GLN
7	CE	223	ARG
7	CE	268	ARG
7	CE	277	GLU
7	CE	287	LYS
7	CE	427	ASP
7	CE	441	TYR
7	CE	477	LYS
7	CE	492	ASN
7	CE	524	SER
7	CE	529	SER
7	CE	532	ASP
8	CF	5	LYS
8	CF	18	LYS
8	CF	28	SER
8	CF	48	MET
8	CF	91	ARG
8	CF	94	ARG
8	CF	139	THR

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Mol	Chain	Res	Type
8	CF	226	TYR
9	CG	2	ARG
9	CG	14	ASP
9	CG	66	SER
9	CG	92	GLN
10	CH	23	ARG
10	CH	88	ASP
10	CH	116	LYS
10	CH	174	PHE
10	CH	188	ARG
10	CH	209	ASP
10	CH	214	ARG
10	CH	228	LEU
10	CH	253	MET
10	CH	268	ASN
10	CH	292	LYS
10	CH	296	GLU
10	CH	298	ASP
10	CH	341	GLU
10	CH	359	THR
10	CH	374	MET
10	CH	394	ASP
10	CH	401	ARG
10	CH	405	ARG
10	CH	406	ASP
10	CH	451	ASP
10	CH	507	LYS
10	CH	508	MET
10	CH	536	GLN
11	CI	209	GLN
11	CI	212	GLU
11	CI	222	LYS
11	CI	279	ARG
11	CI	287	LYS
12	CJ	136	ASP
12	CJ	143	ASP
12	CJ	151	PHE
12	CJ	164	MET
12	CJ	170	ARG
12	CJ	248	SER
12	CJ	256	LYS
12	CJ	370	PHE

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Mol	Chain	Res	Type
12	CJ	380	ARG
12	CJ	388	ARG
12	CJ	422	ARG
12	CJ	462	TRP
12	CJ	464	SER
12	CJ	471	LYS
12	CJ	474	GLU
12	CJ	481	GLN
12	CJ	504	GLU
12	CJ	505	GLU
12	CJ	506	GLN
12	CJ	589	ARG
12	CJ	607	ASP
12	CJ	609	LYS
12	CJ	618	LYS
12	CJ	621	GLU
12	CJ	623	LYS
12	CJ	640	LYS
12	CJ	642	LYS
13	CK	17	ARG
13	CK	43	ARG
13	CK	61	MET
13	CK	112	GLU
13	CK	132	MET
13	CK	137	LYS
13	CK	153	LYS
13	CK	170	ARG
13	CK	180	LYS
13	CK	192	THR
13	CK	203	ASN
13	CK	211	GLN
14	CL	7	LYS
14	CL	14	LYS
14	CL	33	ARG
14	CL	75	ARG
15	CM	20	LYS
15	CM	104	LYS
15	CM	119	ASN
15	CM	134	LYS
15	CM	142	TYR
15	CM	170	THR
15	CM	193	GLU

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Mol	Chain	Res	Type
15	CM	248	MET
16	CN	57	ARG
16	CN	78	ASP
16	CN	91	ASP
16	CN	109	VAL
16	CN	112	ASP
16	CN	236	SER
16	CN	237	MET
17	CO	6	ARG
17	CO	110	MET
18	CP	259	ARG
18	CP	262	TYR
18	CP	268	LYS
18	CP	291	ARG
18	CP	348	LYS
18	CP	403	LYS
18	CP	451	ASP
18	CP	456	ASP
18	CP	551	TYR
18	CP	552	MET
18	CP	554	LYS
19	CQ	17	LYS
19	CQ	22	MET
19	CQ	48	LYS
19	CQ	63	MET
19	CQ	69	LEU
19	CQ	70	GLN
19	CQ	100	ARG
19	CQ	136	ARG
19	CQ	141	GLU
19	CQ	161	ARG
20	CR	8	ARG
20	CR	128	SER
20	CR	188	SER
20	CR	196	GLN
20	CR	227	ARG
21	CS	58	SER
21	CS	90	PHE
21	CS	100	ARG
21	CS	106	HIS
21	CS	191	SER
21	CS	199	ARG

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Mol	Chain	Res	Type
21	CS	206	ARG
21	CS	215	ARG
21	CS	216	SER
21	CS	243	GLU
21	CS	250	TYR
21	CS	280	GLU
21	CS	289	LEU
21	CS	307	ASP
21	CS	322	LYS
21	CS	326	ARG
21	CS	359	LYS
21	CS	376	LYS
21	CS	386	LYS
21	CS	426	ASP
21	CS	475	MET
21	CS	496	ARG
21	CS	653	ASP
21	CS	671	LYS
21	CS	716	GLN
21	CS	740	ARG
22	CT	126	GLN
22	CT	145	TYR
22	CT	154	ARG
22	CT	185	ARG
22	CT	201	LYS
22	CT	202	ARG
22	CT	329	ARG
22	CT	366	LYS
22	CT	376	GLU
22	CT	378	GLN
22	CT	382	GLU
22	CT	402	LYS
22	CT	437	ASP
22	CT	455	ARG
22	CT	582	ARG
22	CT	602	GLN
22	CT	605	GLU
22	CT	665	ARG
22	CT	666	LYS
22	CT	681	LYS
23	CU	296	LYS
23	CU	319	LYS

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Mol	Chain	Res	Type
23	CU	320	GLN
23	CU	325	LYS
23	CU	339	ARG
23	CU	340	LYS
23	CU	368	ARG
24	CV	22	LYS
24	CV	34	ASN
24	CV	62	LYS
24	CV	69	LYS
24	CV	96	SER
25	CW	22	LEU
25	CW	36	GLU
25	CW	38	PRO
25	CW	61	THR
25	CW	69	PHE
25	CW	113	LYS
25	CW	122	LEU
25	CW	123	GLN
25	CW	211	ARG
25	CW	219	GLN
25	CW	250	ARG
25	CW	264	LYS
25	CW	270	GLN
25	CW	271	MET
25	CW	314	ARG
25	CW	330	HIS
25	CW	339	GLU
25	CW	370	ASP
25	CW	384	PHE
25	CW	396	ARG
25	CW	470	TYR
25	CW	501	MET
25	CW	590	ARG
25	CW	600	ARG
25	CW	601	MET
25	CW	620	ARG
27	CY	6	LYS
27	CY	36	GLN
27	CY	80	LYS
27	CY	373	ARG
27	CY	377	LYS
27	CY	378	MET

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Mol	Chain	Res	Type
27	CY	402	LEU
27	CY	420	LEU
27	CY	427	LEU
27	CY	432	ARG
27	CY	433	VAL
27	CY	444	LEU
27	CY	461	TYR
27	CY	465	PHE
27	CY	488	ARG
27	CY	495	TYR
27	CY	497	HIS
27	CY	504	CYS
27	CY	525	ARG
27	CY	584	MET
27	CY	603	LYS
27	CY	608	TYR
27	CY	654	MET
27	CY	659	LYS
27	CY	678	GLN
27	CY	683	ASN
27	CY	705	ASP
28	CZ	128	ARG
28	CZ	146	TYR
28	CZ	164	ARG
28	CZ	178	ARG
28	CZ	179	ARG
28	CZ	199	LYS
28	CZ	211	GLU
28	CZ	214	ARG
28	CZ	231	HIS
28	CZ	239	ASP
28	CZ	248	LYS
28	CZ	313	MET
28	CZ	324	ASN
28	CZ	359	ARG
28	CZ	380	TYR
28	CZ	387	MET
28	CZ	409	MET
28	CZ	438	THR
28	CZ	442	THR
28	CZ	444	MET
28	CZ	448	GLU

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Mol	Chain	Res	Type
28	CZ	464	GLU
29	Ca	49	LYS
29	Ca	64	LEU
29	Ca	83	LYS
29	Ca	87	LYS
29	Ca	93	GLU
29	Ca	94	SER
29	Ca	201	LYS
29	Ca	213	GLU
29	Ca	214	SER
30	Cz	30	GLN
30	Cz	43	LYS
30	Cz	61	MET
31	LA	54	ARG
31	LA	96	LEU
31	LA	114	SER
31	LA	129	THR
31	LA	132	ASN
31	LA	140	ASN
31	LA	156	LYS
31	LA	181	LYS
32	LB	28	ARG
32	LB	126	LYS
32	LB	158	VAL
32	LB	168	ARG
32	LB	300	ASP
32	LB	354	LYS
33	LC	15	LYS
33	LC	94	MET
33	LC	165	LYS
33	LC	183	GLU
33	LC	204	ARG
33	LC	220	LYS
33	LC	221	GLU
33	LC	273	LYS
33	LC	283	SER
33	LC	289	ARG
33	LC	309	THR
33	LC	340	LYS
34	LE	44	ARG
34	LE	134	LYS
34	LE	157	THR

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Mol	Chain	Res	Type
15	LF	24	SER
15	LF	52	LYS
15	LF	106	ARG
35	LG	52	MET
35	LG	57	GLU
35	LG	161	ASP
35	LG	163	ILE
36	LH	52	VAL
36	LH	148	LEU
36	LH	168	LYS
36	LH	173	ASP
37	LK	31	LYS
37	LK	41	LYS
37	LK	45	ASP
37	LK	54	LYS
37	LK	57	ARG
37	LK	123	LYS
38	LL	46	LEU
38	LL	52	ASP
39	LM	20	LEU
39	LM	102	LYS
39	LM	121	MET
40	LN	13	LYS
40	LN	27	CYS
40	LN	68	ARG
40	LN	97	SER
40	LN	109	ARG
40	LN	170	LYS
40	LN	198	SER
41	LO	1	MET
41	LO	17	LEU
41	LO	69	ARG
41	LO	87	ARG
41	LO	194	LYS
42	LP	54	LYS
42	LP	103	ASP
42	LP	174	ARG
43	LQ	49	SER
43	LQ	91	SER
43	LQ	105	LYS
43	LQ	119	ARG
44	LR	40	SER

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Mol	Chain	Res	Type
44	LR	89	MET
44	LR	96	MET
44	LR	133	LYS
44	LR	135	LYS
44	LR	159	MET
44	LR	167	LYS
45	LS	1	MET
45	LS	6	GLU
45	LS	124	LEU
45	LS	125	LYS
45	LS	141	LYS
45	LS	148	LEU
46	LT	91	VAL
46	LT	120	LYS
47	LU	89	LYS
48	LV	66	LYS
48	LV	98	GLU
48	LV	112	LYS
49	LX	87	LYS
49	LX	90	GLU
49	LX	113	LYS
50	LY	1	MET
50	LY	2	LYS
50	LY	10	SER
50	LY	23	SER
50	LY	68	LYS
50	LY	73	TYR
50	LY	76	LYS
51	LZ	11	LEU
51	LZ	16	ARG
51	LZ	29	ASP
51	LZ	72	LYS
51	LZ	107	GLU
51	LZ	123	SER
51	LZ	125	LYS
52	Lc	55	ARG
52	Lc	58	GLU
52	Lc	84	CYS
52	Lc	93	MET
53	Ld	65	LYS
53	Ld	104	VAL
54	Le	1	MET

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Mol	Chain	Res	Type
54	Le	45	ARG
54	Le	81	LYS
54	Le	104	ARG
55	Lf	23	ARG
55	Lf	50	ARG
55	Lf	80	SER
56	Lg	21	THR
56	Lg	70	LYS
56	Lg	115	LYS
57	Lh	6	LYS
57	Lh	52	LEU
57	Lh	73	LEU
58	Li	28	ARG
58	Li	33	GLU
59	Lj	64	MET
60	Lk	7	ASP
60	Lk	10	LYS
60	Lk	26	LYS
60	Lk	61	SER
60	Lk	69	LYS
61	Lp	36	ARG
61	Lp	80	ARG
62	Ll	21	ARG
63	Lq	34	LEU
63	Lq	60	ARG
63	Lq	73	ASP
63	Lq	85	MET
63	Lq	90	LEU
63	Lq	133	LYS
63	Lq	149	ASN
63	Lq	152	LYS
63	Lq	165	MET
63	Lq	174	MET
63	Lq	184	MET
63	Lq	198	TRP
63	Lq	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	193	ASN
4	CB	150	HIS

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Mol	Chain	Res	Type
5	CC	446	GLN
5	CC	494	ASN
5	CC	528	HIS
5	CC	544	ASN
5	CC	707	ASN
7	CE	391	GLN
7	CE	425	GLN
18	CP	365	GLN
20	CR	148	GLN
22	CT	208	GLN
24	CV	34	ASN
25	CW	90	GLN
25	CW	287	GLN
25	CW	623	ASN
27	CY	477	ASN
27	CY	494	GLN
28	CZ	139	GLN
28	CZ	394	HIS

### 5.3.3 RNA ⓘ

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

All (608) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	16	A
1	C1	22	G
1	C1	26	A
1	C1	41	G
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	73	A
1	C1	74	G
1	C1	83	C

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Mol	Chain	Res	Type
1	C1	92	G
1	C1	93	C
1	C1	94	G
1	C1	96	G
1	C1	109	A
1	C1	110	G
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	136	C
1	C1	138	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	165	G
1	C1	183	U
1	C1	184	U
1	C1	193	C
1	C1	203	C
1	C1	205	G
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	213	G
1	C1	224	A
1	C1	240	U
1	C1	244	U
1	C1	253	U
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	309	A
1	C1	310	A

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Mol	Chain	Res	Type
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	331	C
1	C1	342	C
1	C1	368	G
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	396	G
1	C1	412	G
1	C1	413	G
1	C1	414	A
1	C1	415	A
1	C1	421	U
1	C1	428	A
1	C1	433	U
1	C1	434	G
1	C1	446	U
1	C1	457	U
1	C1	459	U
1	C1	462	C
1	C1	463	C
1	C1	468	C
1	C1	469	A
1	C1	470	C
1	C1	471	U
1	C1	474	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	534	U
1	C1	535	C
1	C1	536	C
1	C1	537	G
1	C1	544	U

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Mol	Chain	Res	Type
1	C1	546	A
1	C1	548	A
1	C1	569	G
1	C1	574	G
1	C1	582	A
1	C1	587	G
1	C1	590	C
1	C1	591	U
1	C1	592	G
1	C1	594	A
1	C1	596	G
1	C1	598	A
1	C1	607	U
1	C1	608	A
1	C1	609	A
1	C1	623	C
1	C1	633	A
1	C1	647	A
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	670	U
1	C1	678	A
1	C1	718	U
1	C1	719	C
1	C1	720	G
1	C1	731	G
1	C1	742	A
1	C1	746	A
1	C1	747	U
1	C1	757	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	766	G
1	C1	767	A
1	C1	787	A
1	C1	789	A
1	C1	800	U
1	C1	801	A
1	C1	803	G
1	C1	828	A

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Mol	Chain	Res	Type
1	C1	840	G
1	C1	846	C
1	C1	858	C
1	C1	876	A
1	C1	877	A
1	C1	878	U
1	C1	889	G
1	C1	896	A
1	C1	898	A
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	941	U
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	959	C
1	C1	960	C
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1046	A
1	C1	1047	A
1	C1	1049	C
1	C1	1053	U
1	C1	1054	G
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1095	G
1	C1	1097	G

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Mol	Chain	Res	Type
1	C1	1098	G
1	C1	1114	C
1	C1	1124	G
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1159	G
1	C1	1160	G
1	C1	1163	U
1	C1	1164	G
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1179	A
1	C1	1180	C
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1191	G
1	C1	1203	U
1	C1	1204	G
1	C1	1218	G
1	C1	1227	A
1	C1	1228	G
1	C1	1234	A
1	C1	1240	U
1	C1	1245	A
1	C1	1247	U
1	C1	1254	C
1	C1	1268	A
1	C1	1269	A
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1298	C
1	C1	1312	A
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G

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Mol	Chain	Res	Type
1	C1	1332	A
1	C1	1333	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1368	A
1	C1	1369	G
1	C1	1374	G
1	C1	1381	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1434	A
1	C1	1437	U
1	C1	1438	A
1	C1	1463	A
1	C1	1464	A
1	C1	1465	G
1	C1	1466	U
1	C1	1470	G
1	C1	1478	C
1	C1	1489	G
1	C1	1490	C
1	C1	1535	U
1	C1	1537	U
1	C1	1538	C
1	C1	1541	A
1	C1	1548	C
1	C1	1549	U
1	C1	1551	G
1	C1	1552	U
1	C1	1553	G
1	C1	1556	C
1	C1	1557	C
1	C1	1559	U
1	C1	1560	G
1	C1	1561	U
1	C1	1562	G
1	C1	1566	A
1	C1	1568	A
1	C1	1575	C

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Mol	Chain	Res	Type
1	C1	1584	A
1	C1	1607	U
1	C1	1608	U
1	C1	1609	G
1	C1	1610	C
1	C1	1618	C
1	C1	1621	A
1	C1	1622	A
1	C1	1623	C
1	C1	1624	U
1	C1	1637	G
1	C1	1662	C
1	C1	1695	A
1	C1	1709	G
1	C1	1715	G
1	C1	1720	A
1	C1	1722	G
1	C1	1729	A
1	C1	1730	G
1	C1	1739	A
1	C1	1741	U
1	C1	1744	U
1	C1	1752	C
1	C1	1759	G
1	C1	1774	U
1	C1	1775	G
1	C1	1776	A
1	C1	1787	G
1	C1	1794	U
1	C1	1795	A
1	C1	1798	U
1	C1	1800	U
1	C1	1818	A
1	C1	1819	U
1	C1	1821	A
1	C1	1825	C
1	C1	1828	C
1	C1	1829	A
1	C1	1837	A
1	C1	1842	G
1	C1	1843	A
1	C1	1845	C

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Mol	Chain	Res	Type
1	C1	1846	A
1	C1	1857	G
1	C1	1858	A
1	C1	1859	U
1	C1	1865	A
1	C1	1868	G
1	C1	1875	A
1	C1	1881	G
1	C1	1885	G
1	C1	1895	U
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	1904	U
1	C1	1909	A
1	C1	1911	A
1	C1	1925	A
1	C1	1927	G
1	C1	1932	G
1	C1	1938	U
1	C1	1942	G
1	C1	1950	C
1	C1	1952	G
1	C1	1961	G
1	C1	1971	G
1	C1	1981	G
1	C1	1987	C
1	C1	1994	G
1	C1	1997	G
1	C1	2004	G
1	C1	2006	A
1	C1	2020	C
1	C1	2021	C
1	C1	2024	U
1	C1	2043	G
1	C1	2044	G
1	C1	2048	G
1	C1	2049	C
1	C1	2052	U
1	C1	2054	A
1	C1	2055	A
1	C1	2064	U

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Mol	Chain	Res	Type
1	C1	2065	U
1	C1	2066	A
1	C1	2075	A
1	C1	2099	U
1	C1	2114	A
1	C1	2119	G
1	C1	2120	A
1	C1	2126	A
1	C1	2131	G
1	C1	2132	U
1	C1	2133	G
1	C1	2142	G
1	C1	2144	A
1	C1	2146	U
1	C1	2160	A
1	C1	2161	G
1	C1	2164	C
1	C1	2174	C
1	C1	2177	A
1	C1	2178	G
1	C1	2179	U
1	C1	2180	G
1	C1	2182	A
1	C1	2183	G
1	C1	2189	C
1	C1	2191	A
1	C1	2198	G
1	C1	2199	C
1	C1	2247	C
1	C1	2248	U
1	C1	2256	U
1	C1	2260	U
1	C1	2286	A
1	C1	2325	A
1	C1	2327	C
1	C1	2328	C
1	C1	2335	A
1	C1	2336	C
1	C1	2338	G
1	C1	2339	G
1	C1	2342	U
1	C1	2343	G

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Mol	Chain	Res	Type
1	C1	2347	A
1	C1	2350	U
1	C1	2356	G
1	C1	2396	U
1	C1	2397	G
1	C1	2399	G
1	C1	2407	A
1	C1	2409	A
1	C1	2414	G
1	C1	2415	U
1	C1	2424	G
1	C1	2425	G
1	C1	2430	A
1	C1	2434	U
1	C1	2436	G
1	C1	2437	G
1	C1	2438	C
1	C1	2439	G
1	C1	2442	A
1	C1	2443	G
1	C1	2444	U
1	C1	2449	U
1	C1	2453	A
1	C1	2456	A
1	C1	2464	U
1	C1	2465	G
1	C1	2467	U
1	C1	2484	G
1	C1	2551	A
1	C1	2558	C
1	C1	2560	G
1	C1	2564	G
1	C1	2730	C
1	C1	2739	U
1	C1	2740	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2767	C
1	C1	2775	A
1	C1	2777	A

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Mol	Chain	Res	Type
1	C1	2778	A
1	C1	2782	G
1	C1	2784	U
1	C1	2786	G
1	C1	2806	G
1	C1	2816	U
1	C1	2838	U
1	C1	2839	C
1	C1	2845	A
1	C1	2847	C
1	C1	2856	G
1	C1	2857	C
1	C1	2858	A
1	C1	2862	U
1	C1	2869	A
1	C1	2880	G
1	C1	2881	U
1	C1	2883	C
1	C1	2884	A
1	C1	2885	C
1	C1	2888	A
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2905	G
1	C1	2906	C
1	C1	2917	C
1	C1	2922	G
1	C1	2936	U
1	C1	2942	C
1	C1	2954	C
1	C1	2955	U
1	C1	2956	C
1	C1	2969	A
1	C1	3006	A
1	C1	3013	U
1	C1	3016	G
1	C1	3035	G
1	C1	3043	A
1	C1	3049	C
1	C1	3050	C
1	C1	3074	C

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Mol	Chain	Res	Type
1	C1	3075	C
1	C1	3079	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3098	A
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3108	U
1	C1	3111	U
1	C1	3112	A
1	C1	3113	C
1	C1	3118	A
1	C1	3119	C
1	C1	3121	U
1	C1	3122	U
1	C1	3123	G
1	C1	3124	U
1	C1	3125	A
1	C1	3126	G
1	C1	3127	A
1	C1	3130	U
1	C1	3131	A
1	C1	3132	U
1	C1	3134	A
1	C1	3140	G
1	C1	3144	C
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3153	U
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3167	A
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3181	C
1	C1	3183	C

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Mol	Chain	Res	Type
1	C1	3185	A
1	C1	3187	G
1	C1	3188	U
1	C1	3199	A
1	C1	3203	C
1	C1	3210	U
1	C1	3217	U
1	C1	3227	C
1	C1	3228	G
1	C1	3229	G
1	C1	3230	G
1	C1	3244	C
1	C1	3253	U
1	C1	3256	A
1	C1	3257	U
1	C1	3258	G
1	C1	3259	U
1	C1	3260	G
1	C1	3275	A
1	C1	3280	G
1	C1	3281	U
1	C1	3282	A
1	C1	3291	U
1	C1	3293	G
1	C1	3294	U
1	C1	3295	U
1	C1	3296	G
1	C1	3298	U
1	C1	3309	G
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3325	U
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
2	C2	23	U
2	C2	34	U
2	C2	35	C
2	C2	39	G

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Mol	Chain	Res	Type
2	C2	49	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	103	G
2	C2	104	A
2	C2	106	C
2	C2	110	C
2	C2	111	A
2	C2	112	U
2	C2	113	U
2	C2	125	U
2	C2	148	G
2	C2	157	U
2	C2	158	U
2	C2	159	C
2	C2	163	C
2	C2	164	A
2	C2	165	U
2	C2	166	C
2	C2	170	C
2	C2	173	U
2	C2	181	U
2	C2	183	U
2	C2	189	A
2	C2	196	G
2	C2	203	G
2	C2	206	G
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	216	A
2	C2	219	A
2	C2	221	U

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Mol	Chain	Res	Type
2	C2	222	G
2	C2	225	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	294	A
2	C2	295	G
2	C2	300	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	445	A
1	C1	799	C
1	C1	897	G
1	C1	1046	A
1	C1	1063	C
1	C1	1077	U
1	C1	1489	G
1	C1	1949	G
1	C1	2173	U
1	C1	2176	A
1	C1	2327	C
1	C1	3078	U
1	C1	3131	A
1	C1	3162	A
1	C1	3209	U
1	C1	3216	U
1	C1	3229	G
1	C1	3257	U
1	C1	3281	U
1	C1	3297	U
1	C1	3321	U
2	C2	102	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	TPO	CC	163	5	8,10,11	1.65	1 (12%)	10,14,16	1.12	1 (10%)
5	SEP	CC	160	5	8,9,10	1.52	1 (12%)	8,12,14	1.51	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TPO	CC	163	5	-	7/9/11/13	-
5	SEP	CC	160	5	-	0/5/8/10	-

All (2) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	N-CA-CB-CG2
5	CC	163	TPO	N-CA-CB-OG1
5	CC	163	TPO	C-CA-CB-CG2
5	CC	163	TPO	O-C-CA-CB
5	CC	163	TPO	CG2-CB-OG1-P
5	CC	163	TPO	CB-OG1-P-O3P

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Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
66	ADP	CW	1001	67	24,29,29	0.68	0	29,45,45	0.82	1 (3%)
64	GTP	CH	1001	-	26,34,34	1.14	2 (7%)	32,54,54	1.49	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	ADP	CW	1001	67	-	5/12/32/32	0/3/3/3
64	GTP	CH	1001	-	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

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

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	CH	1001	GTP	C5-C6-N1	3.26	119.70	113.95
64	CH	1001	GTP	C8-N7-C5	3.04	108.78	102.99
64	CH	1001	GTP	C2-N1-C6	-2.83	119.88	125.10
64	CH	1001	GTP	PA-O3A-PB	-2.71	123.53	132.83
64	CH	1001	GTP	PB-O3B-PG	-2.69	123.60	132.83
64	CH	1001	GTP	C3'-C2'-C1'	2.61	104.91	100.98
66	CW	1001	ADP	C5-C6-N6	2.28	123.81	120.35
64	CH	1001	GTP	O6-C6-C5	-2.12	120.23	124.37

There are no chirality outliers.

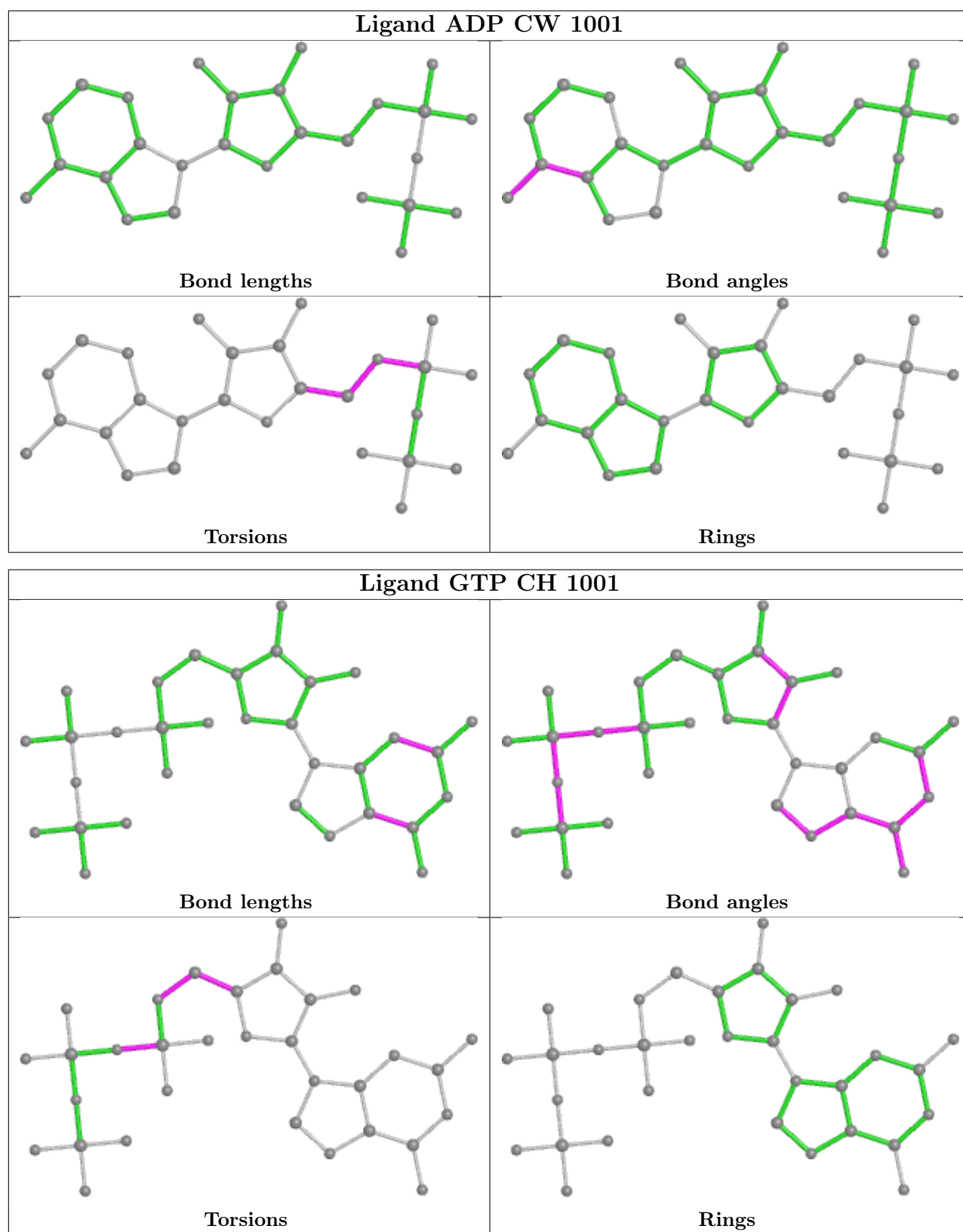
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	CW	1001	ADP	C4'-C5'-O5'-PA
66	CW	1001	ADP	O4'-C4'-C5'-O5'
66	CW	1001	ADP	C3'-C4'-C5'-O5'
64	CH	1001	GTP	PB-O3A-PA-O1A
64	CH	1001	GTP	C3'-C4'-C5'-O5'
66	CW	1001	ADP	C5'-O5'-PA-O3A
66	CW	1001	ADP	C5'-O5'-PA-O2A
64	CH	1001	GTP	O4'-C4'-C5'-O5'
64	CH	1001	GTP	C4'-C5'-O5'-PA
64	CH	1001	GTP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.