Full wwPDB EM Validation Report ⓘ

May 21, 2024 – 10:19 AM JST

PDB ID	:	8I9P
EMDB ID	:	EMD-35279
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - State Mak16
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	3.00 Å(reported)

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

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

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

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

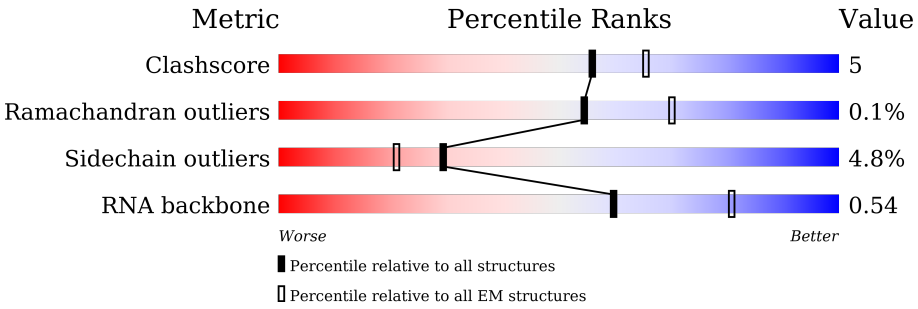
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	C1	3341	25% 12% • 61%
2	C2	306	52% 27% • 16%
3	CA	316	60% 20% • 18%
4	CB	391	56% 13% 31%
5	CC	801	24% 7% • 68%
6	CE	598	66% 11% • 23%
7	CI	414	26% 8% • 65%
8	CJ	679	40% 15% • 44%

Continued on next page...

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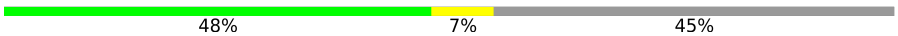
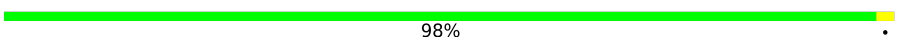
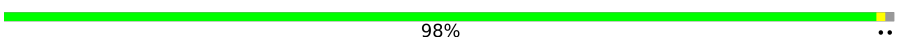
Mol	Chain	Length	Quality of chain
9	CM	249	
9	LF	249	
10	CR	237	
11	CU	451	
12	LC	365	
13	LE	200	
14	LG	262	
15	LL	213	
16	LM	142	
17	LN	203	
18	LO	204	
19	LP	187	
20	LQ	213	
21	LS	174	
22	LT	160	
23	LX	156	
24	LY	138	
25	Le	131	
26	Lf	109	
27	Lh	935	
28	Li	110	
29	Lj	95	
30	Cc	282	
31	Cd	436	
32	Ce	336	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 80799 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	1307	27990	12490	5103	9090	1307	0	0

- Molecule 2 is a RNA chain called RNA (306-MER).

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	269	2140	1370	377	390	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CC	258	2159	1378	362	412	7	0	0

- Molecule 6 is a protein called RNA helicase.

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

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
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 7 is a protein called Putative RNA-binding protein.

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

- Molecule 8 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CJ	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

- Molecule 9 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CM	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
9	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	3		

- Molecule 10 is a protein called Nucleolar protein 16.

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

- Molecule 11 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CU	116	Total	C	N	O	S	0	0
			924	576	169	176	3		

- Molecule 12 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 13 is a protein called 60S ribosomal protein L6.

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

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	185	Total	C	N	O	S	0	0
			1482	958	265	254	5		

- Molecule 15 is a protein called 60S ribosomal protein L13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	128	Total	C	N	O	S	0	0
			1037	661	201	174	1		

- Molecule 17 is a protein called Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 19 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LP	154	Total	C	N	O	S	0	0
			1212	758	233	218	3		

- Molecule 20 is a protein called Ribosomal protein L18-like protein.

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

- Molecule 21 is a protein called 60S ribosomal protein L20.

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

- Molecule 22 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 23 is a protein called 60S ribosomal protein L25-like protein.

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

- Molecule 24 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 25 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 26 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 27 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 28 is a protein called 60S ribosomal protein L36.

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

- Molecule 29 is a protein called Ribosomal protein L37.

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

- Molecule 30 is a protein called Ribosomal RNA-processing protein 1.

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

- Molecule 31 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Cd	343	Total	C	N	O	S	0	0
			2768	1746	534	484	4		

- Molecule 32 is a protein called Protein MAK16.

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

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

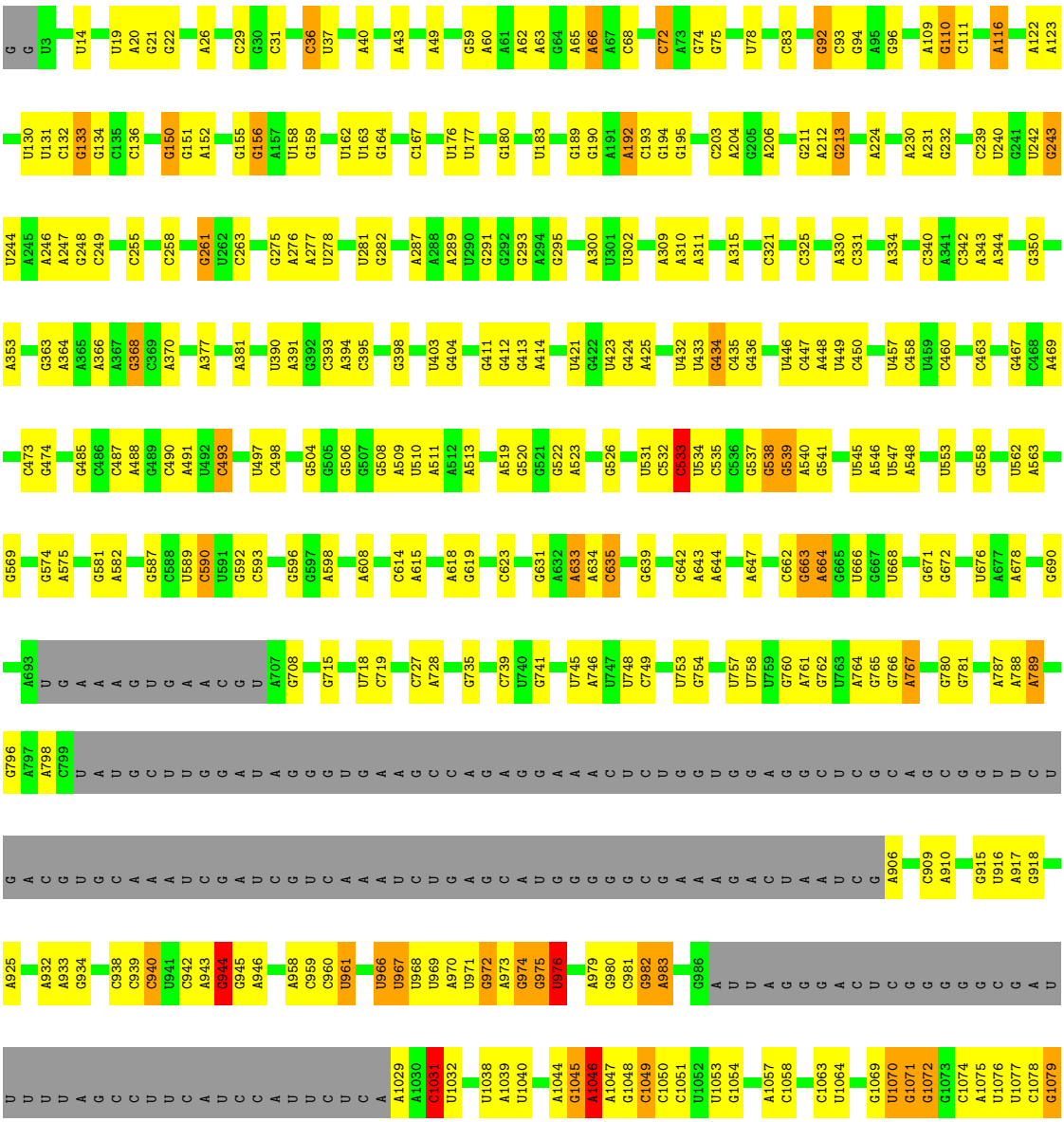
Mol	Chain	Residues	Atoms		AltConf
33	Lj	1	Total	Zn	0
			1	1	
33	Ce	1	Total	Zn	0
			1	1	

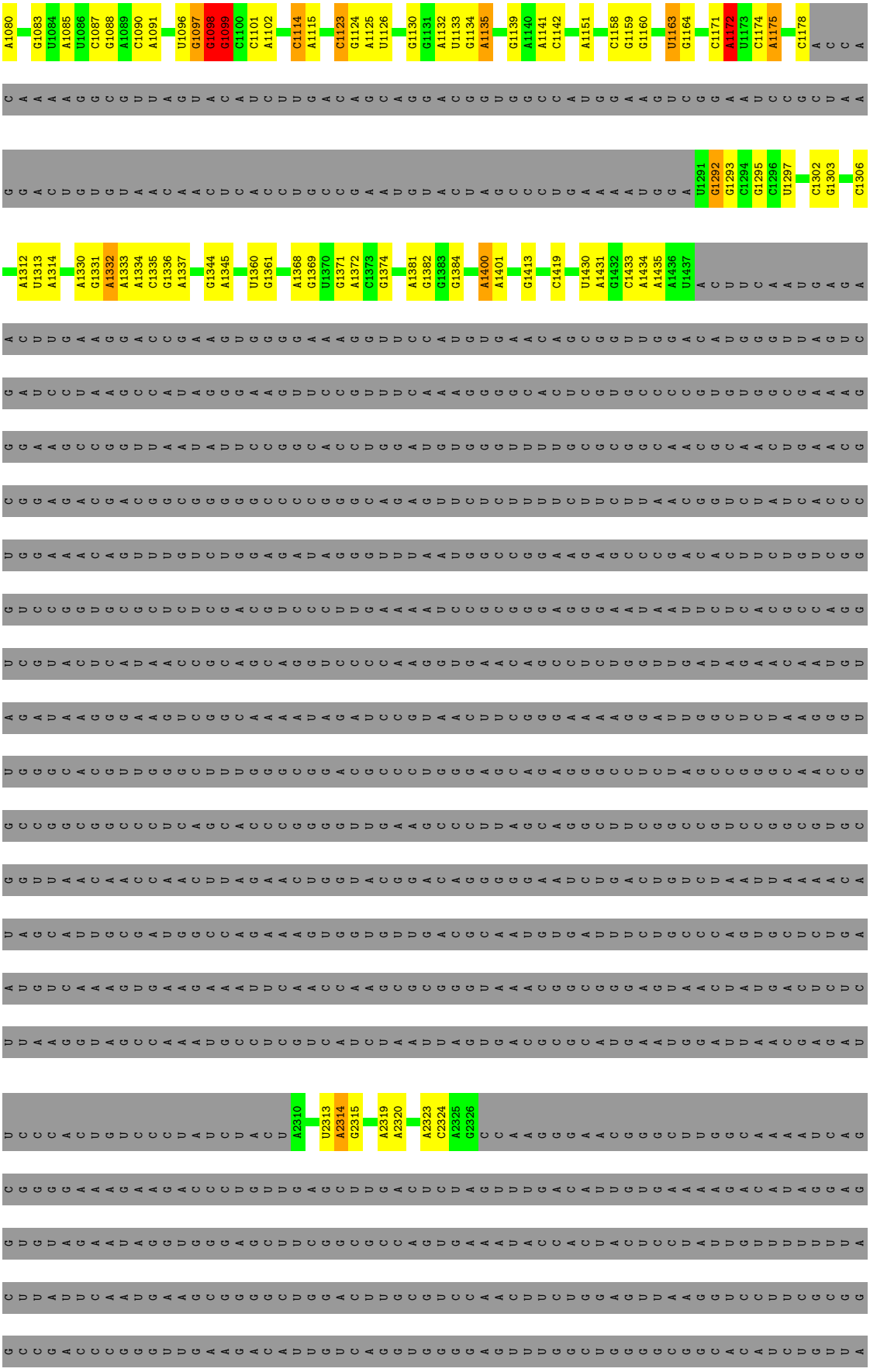
3 Residue-property plots (i)

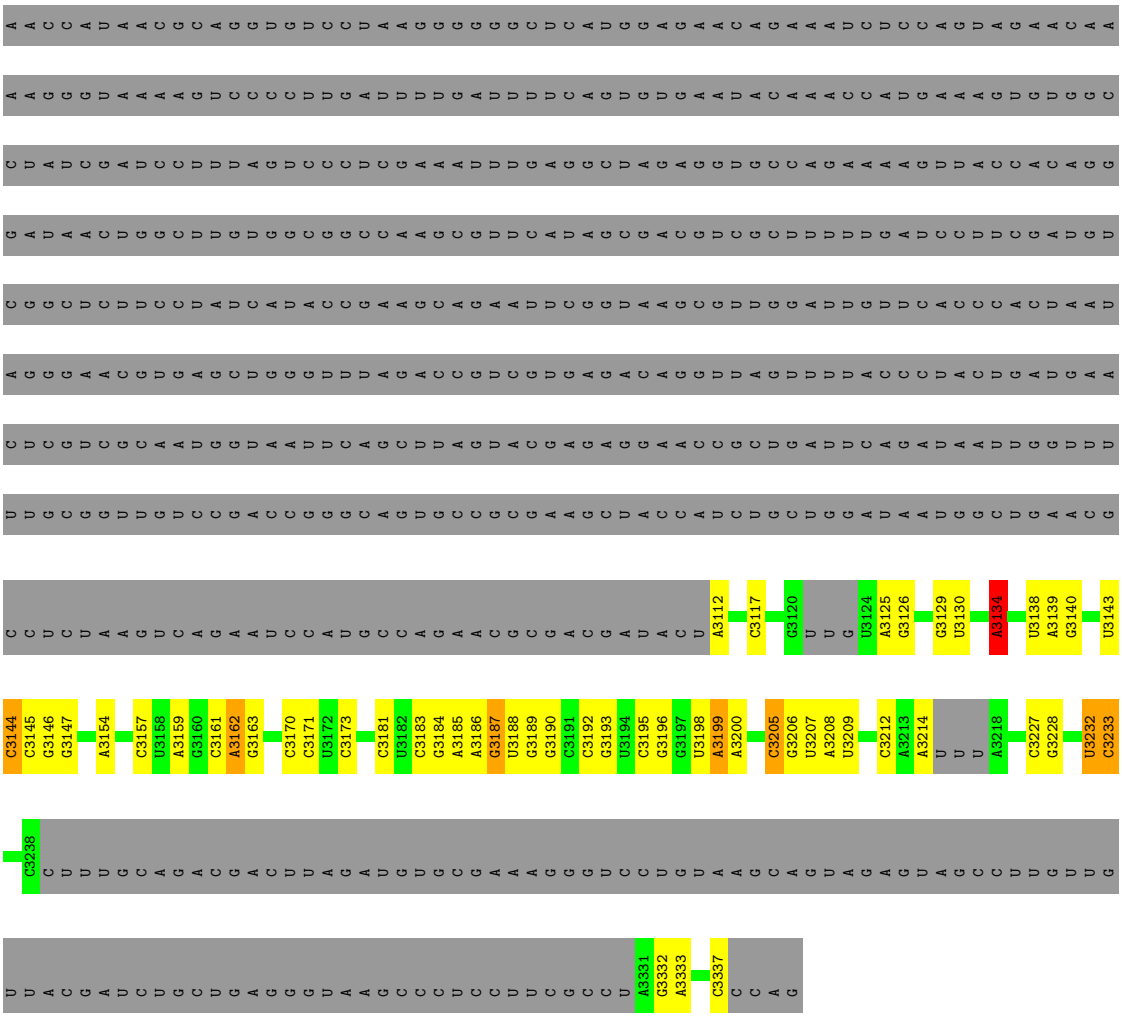
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA (3341-MER)

Chain C1: 25% 12% 61%

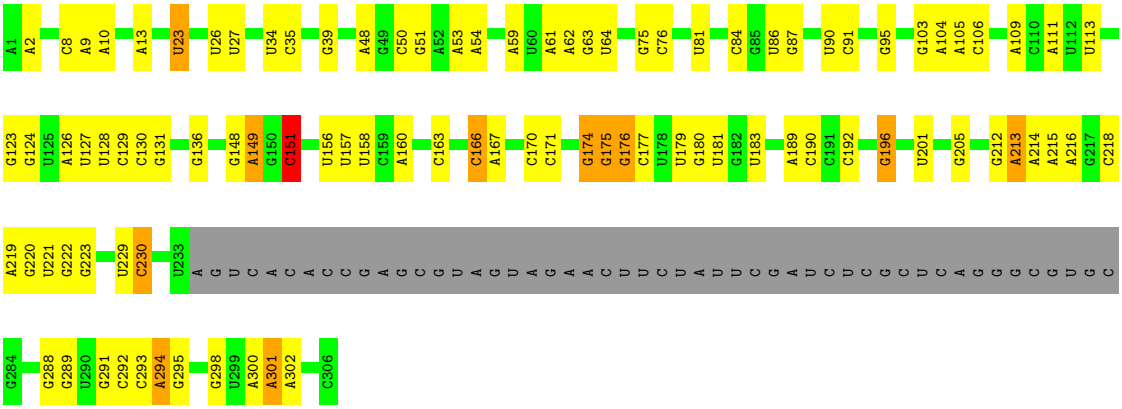



A1080 G1083 U1084 A1085 U1086 C1087 G1088 A1089 C1090 A1091 U1096 G1097 G1098 G1099 C1100 C1101 A1102 C1114 A1115 C1123 G1124 A1125 U1126 G1130 G1131 A1132 U1133 G1134 A1135 G1139 A1140 A1141 C1142 A1151 C1158 G1159 G1160 U1163 G1164 C1171 A1172 U1173 C1174 A1175 C1178
U1291 G1292 G1293 C1294 G1295 C1296 U1297 C1302 G1303 C1306
A1312 U1313 A1314 A1330 G1331 A1332 A1333 A1334 C1335 G1336 A1337 G1344 A1345 U1360 G1361 A1368 G1369 U1370 G1371 A1372 C1373 G1374 A1381 G1382 G1383 G1384 A1400 A1401 G1413 C1419 U1430 A1431 G1432 C1433 A1434 A1435 A1436 U1437
A2310 U2313 A2314 G2315 A2319 A2320 A2323 C2324 A2325 G2326



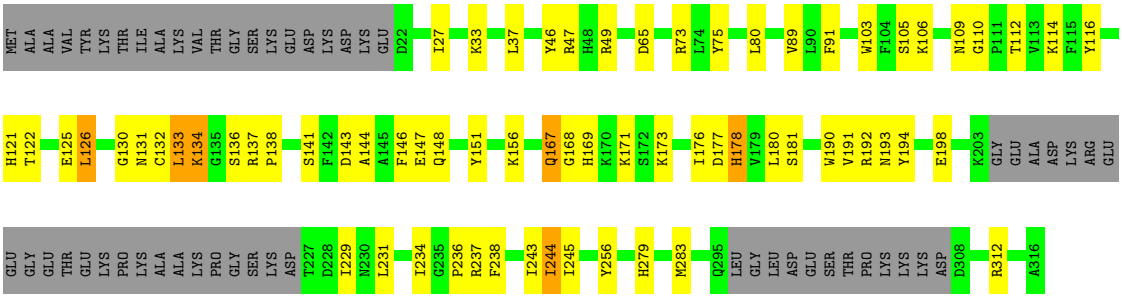
• Molecule 2: RNA (306-MER)

Chain C2:



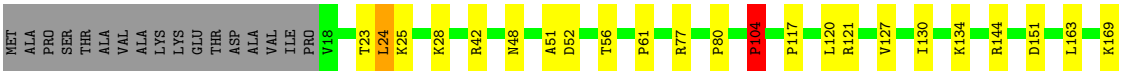
• Molecule 3: Brix domain-containing protein

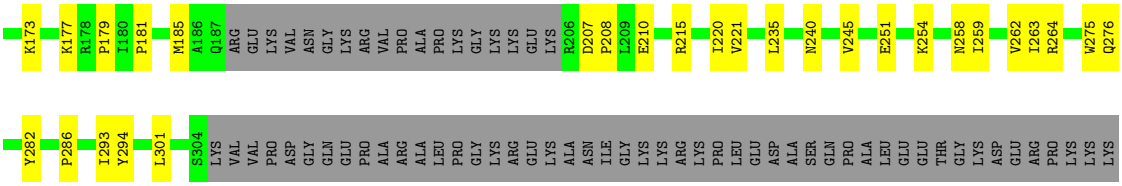
Chain CA:



• Molecule 4: Ribosome biogenesis protein C8F11.04

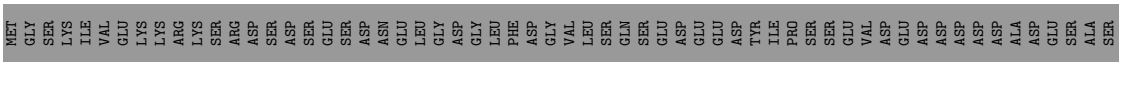
Chain CB:

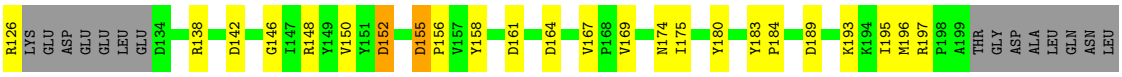


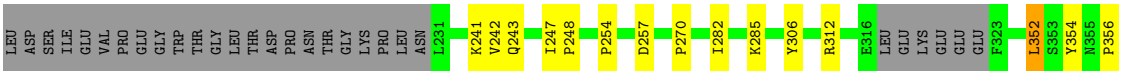


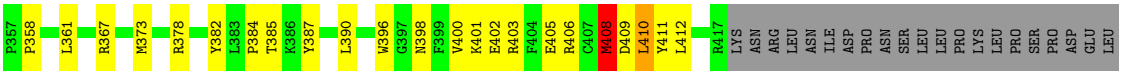
• Molecule 5: Ribosome biogenesis protein ERB1

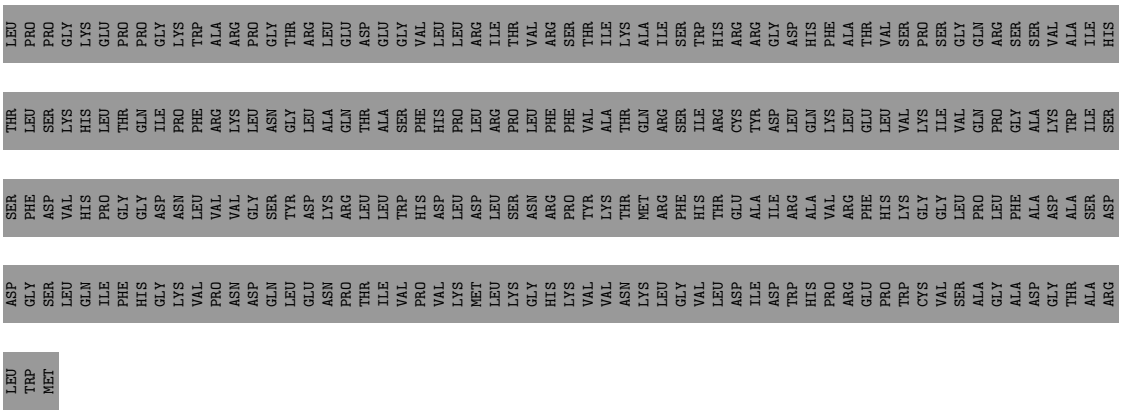
Chain CC:





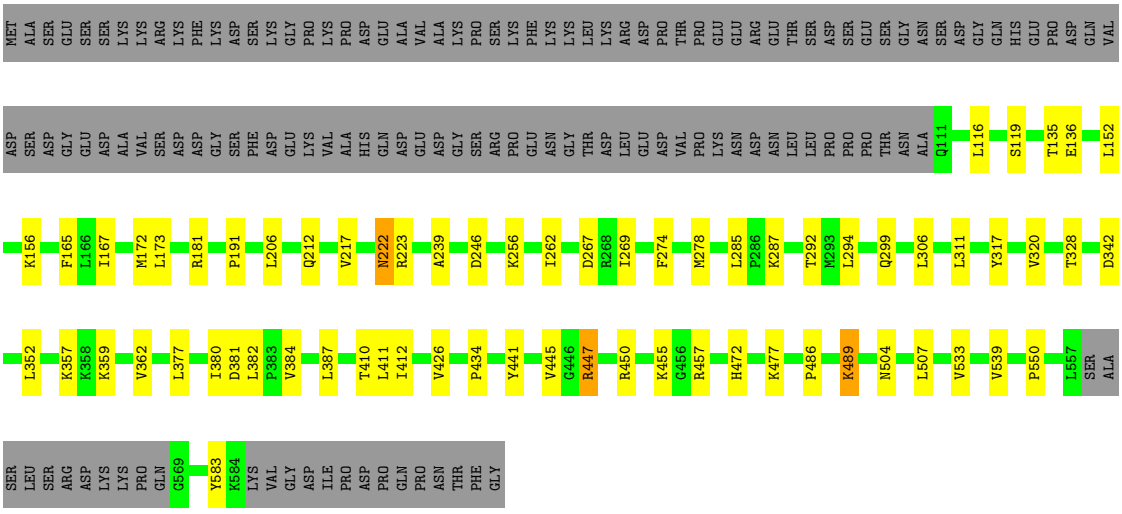






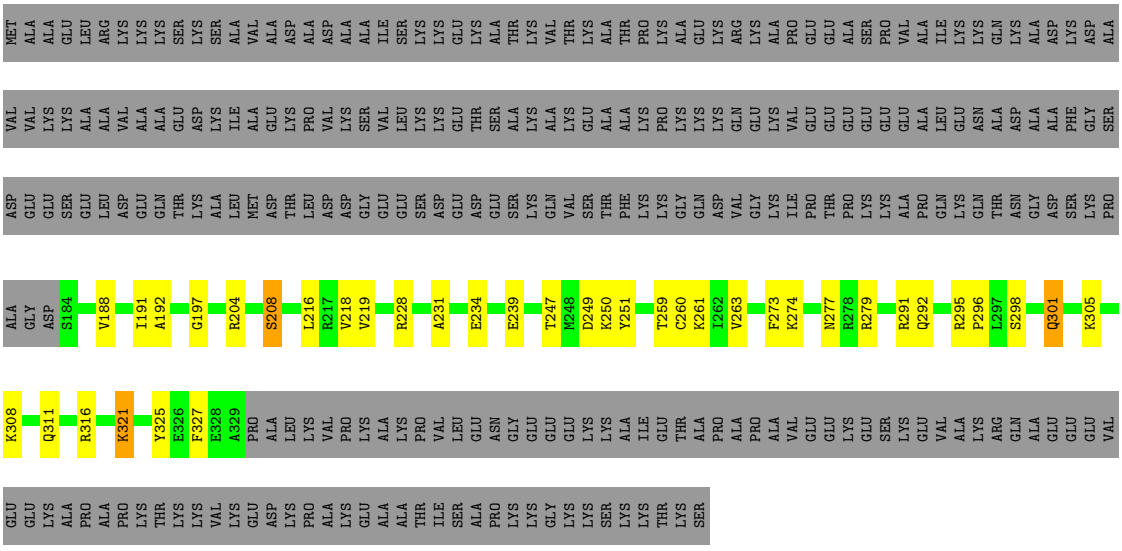
- Molecule 6: RNA helicase

Chain CE:



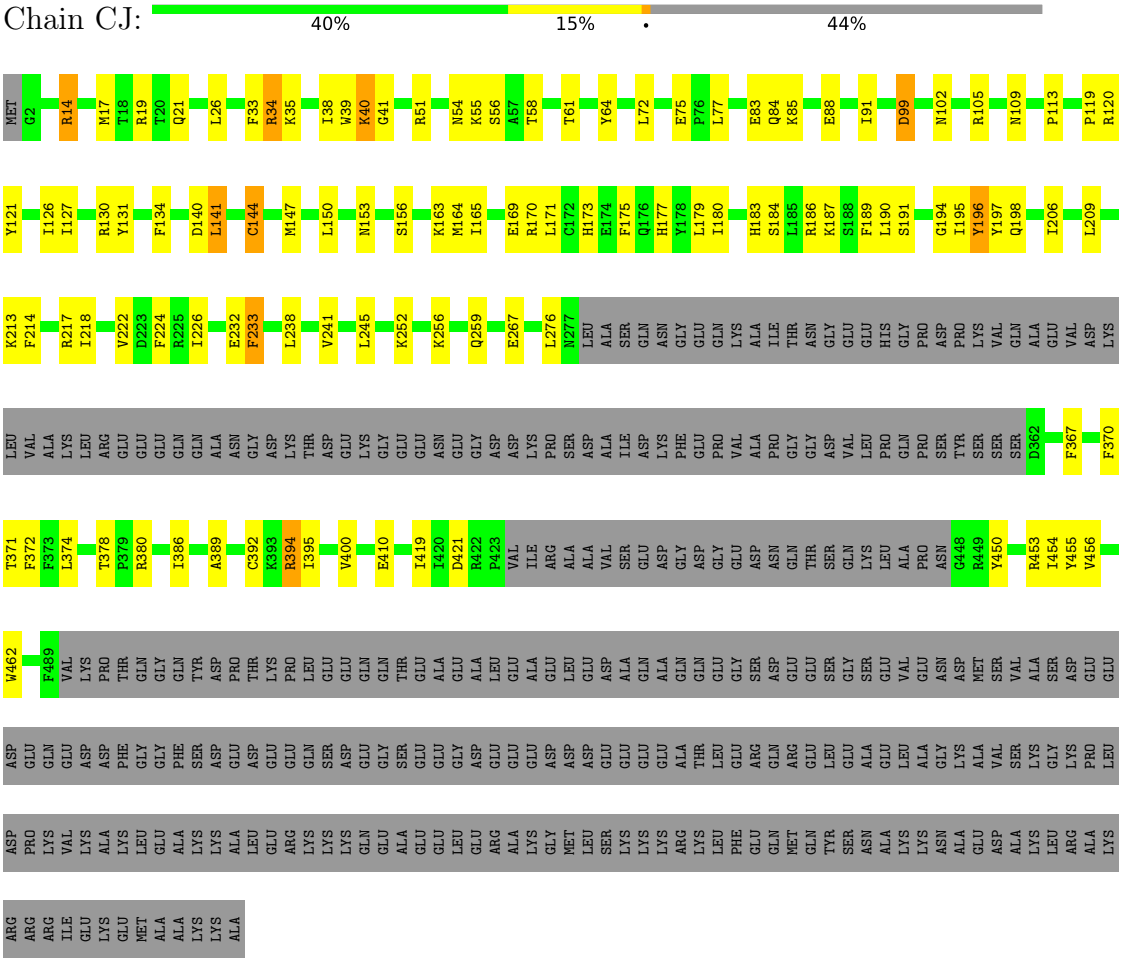
- Molecule 7: Putative RNA-binding protein

Chain CI:



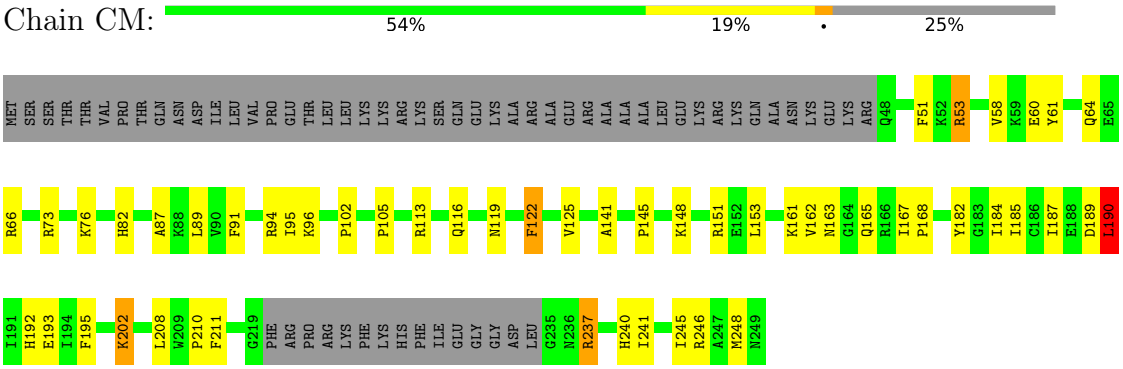
• Molecule 8: Pescadillo homolog

Chain CJ:



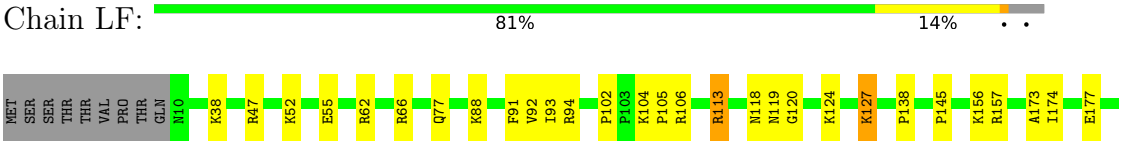
• Molecule 9: 60S ribosomal protein l7-like protein

Chain CM:



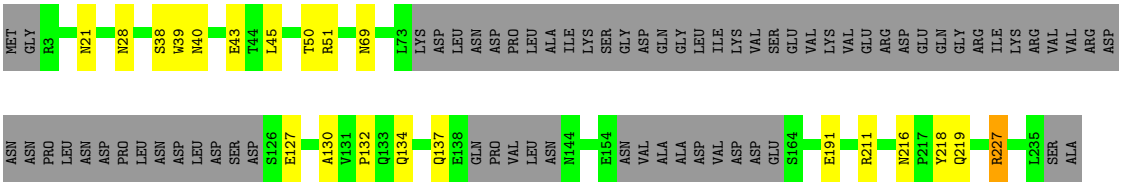
• Molecule 9: 60S ribosomal protein l7-like protein

Chain LF:



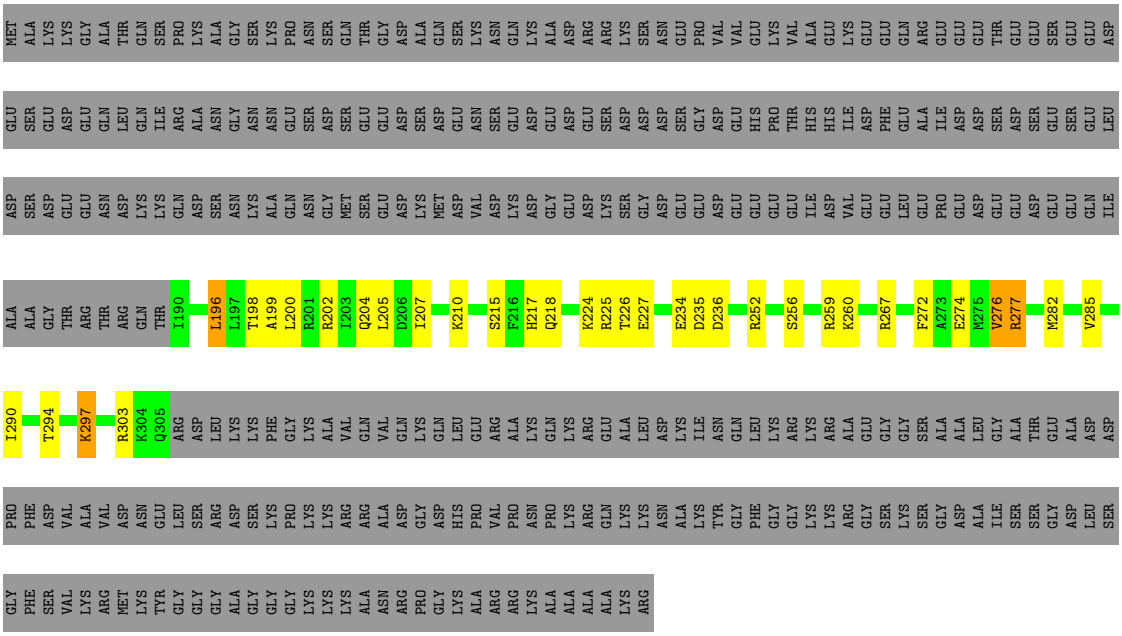
• Molecule 10: Nucleolar protein 16

Chain CR:



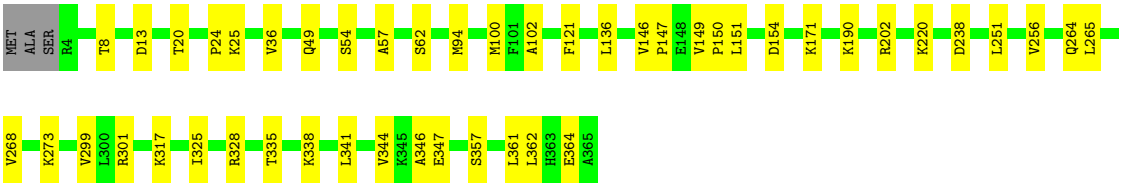
• Molecule 11: rRNA-processing protein EBP2

Chain CU:



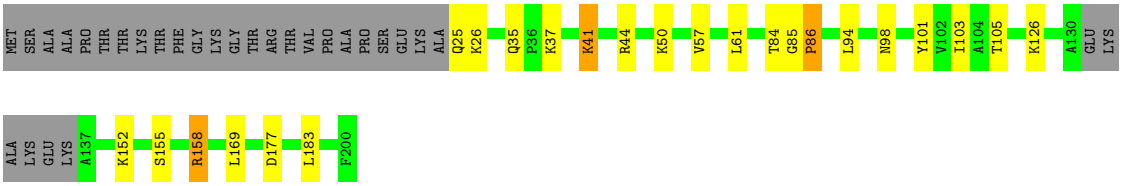
• Molecule 12: 60S ribosomal protein L4-like protein

Chain LC:



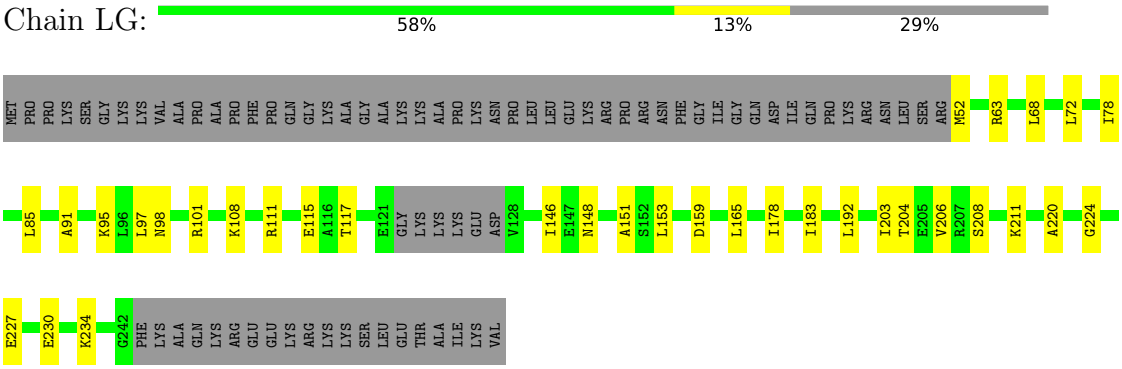
• Molecule 13: 60S ribosomal protein L6

Chain LE:



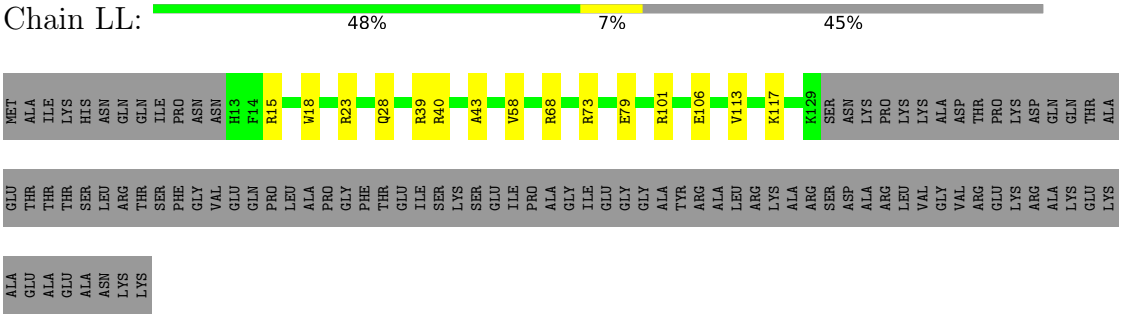
• Molecule 14: 60S ribosomal protein L8

Chain LG:



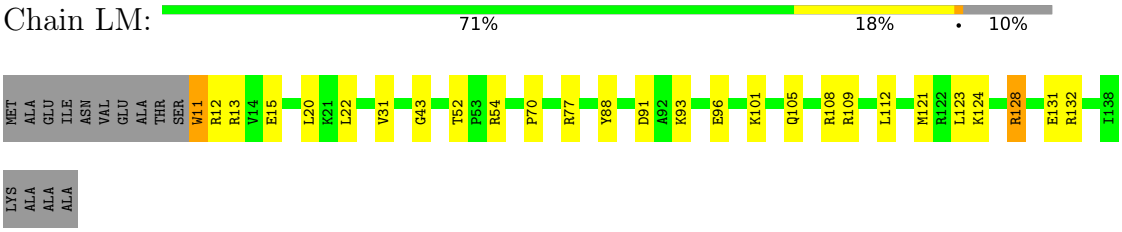
• Molecule 15: 60S ribosomal protein L13

Chain LL:



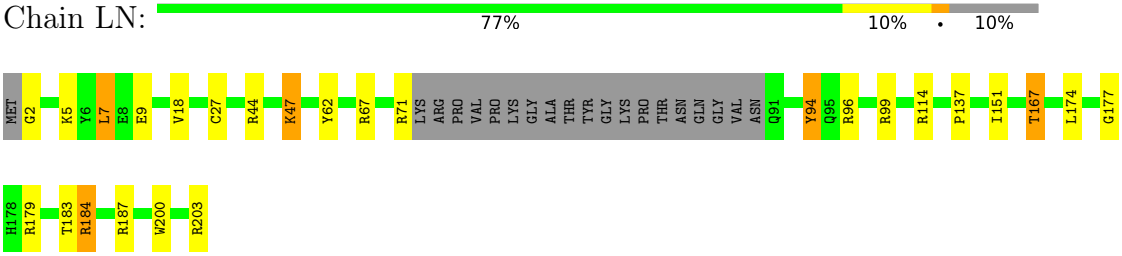
• Molecule 16: 60S ribosomal protein L14-like protein

Chain LM:



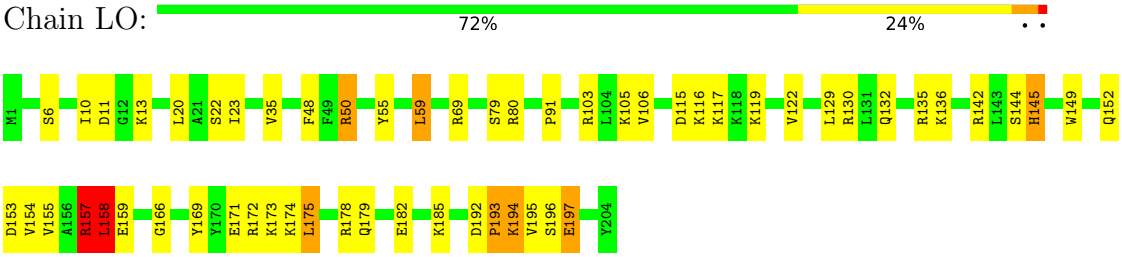
• Molecule 17: Ribosomal protein L15

Chain LN:



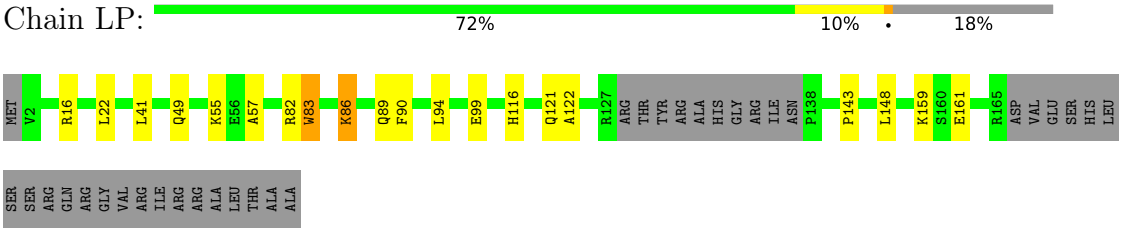
• Molecule 18: 60S ribosomal protein L16-like protein

Chain LO:



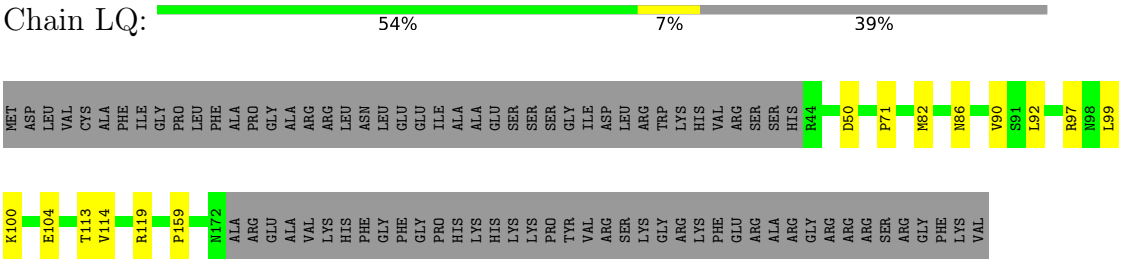
• Molecule 19: 60S ribosomal protein l17-like protein

Chain LP:



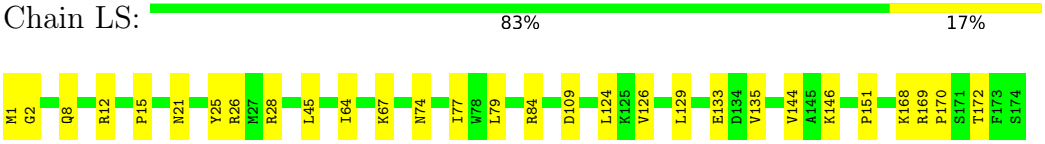
• Molecule 20: Ribosomal protein L18-like protein

Chain LQ:



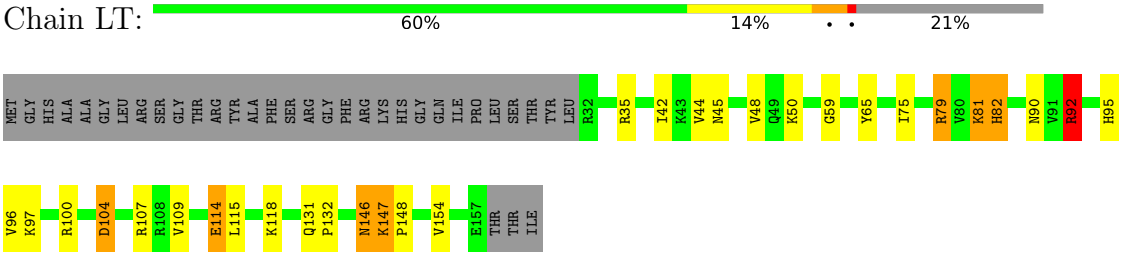
• Molecule 21: 60S ribosomal protein L20

Chain LS:



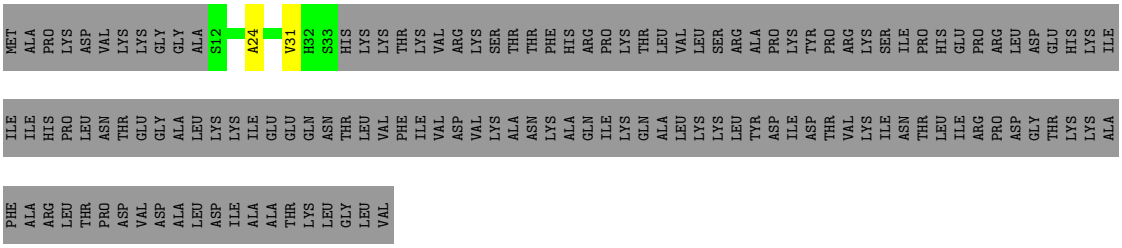
• Molecule 22: 60S ribosomal protein l21-like protein

Chain LT:



• Molecule 23: 60S ribosomal protein L25-like protein

Chain LX:

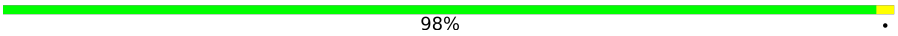


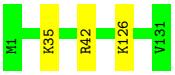
• Molecule 24: 60S ribosomal protein L26-like protein

Chain LY:

• Molecule 25: 60S ribosomal protein L32-like protein

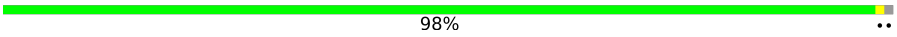
Chain Le:

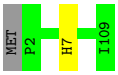




• Molecule 26: 60S ribosomal protein l33-like protein

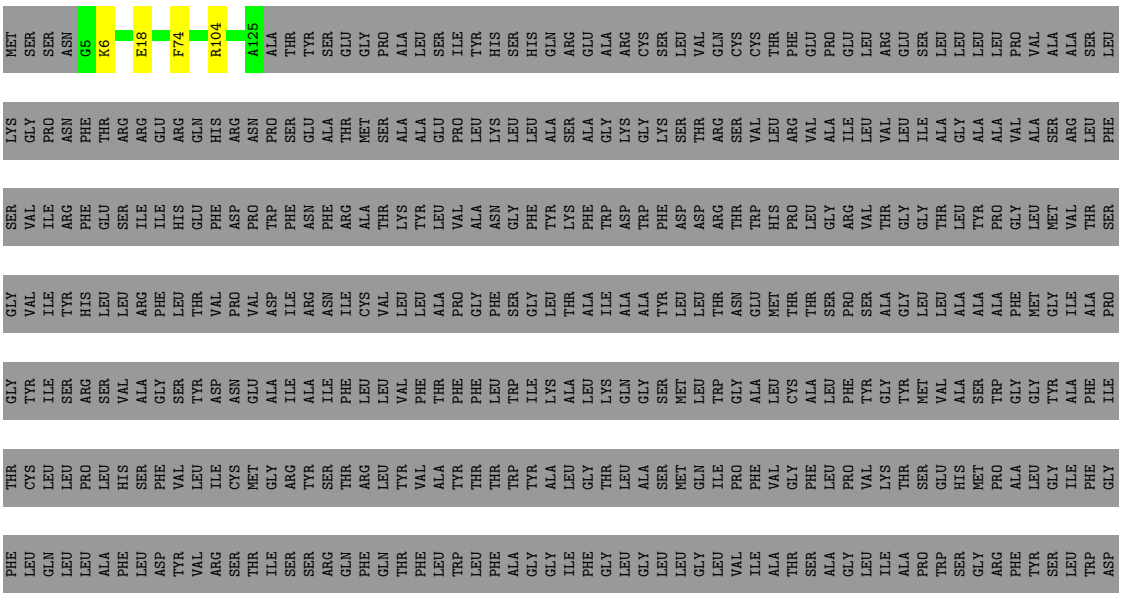
Chain Lf:

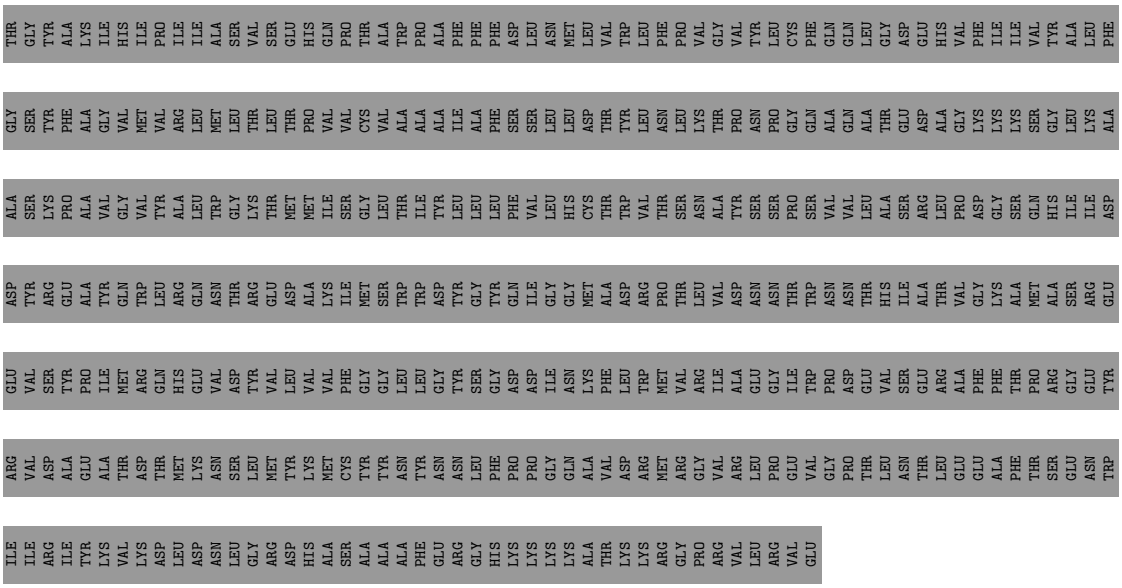




• Molecule 27: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:



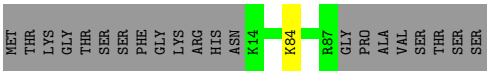


• Molecule 28: 60S ribosomal protein L36

Chain Li:

• Molecule 29: Ribosomal protein L37

Chain Lj:

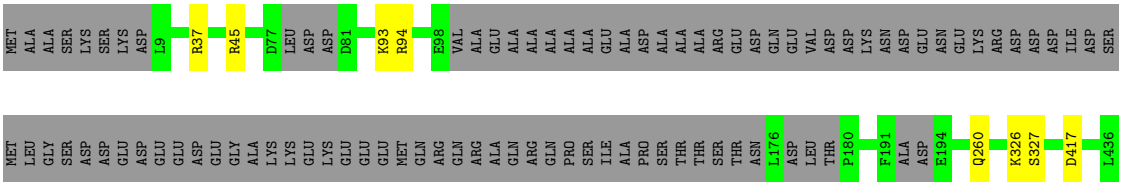


• Molecule 30: Ribosomal RNA-processing protein 1

Chain Cc:

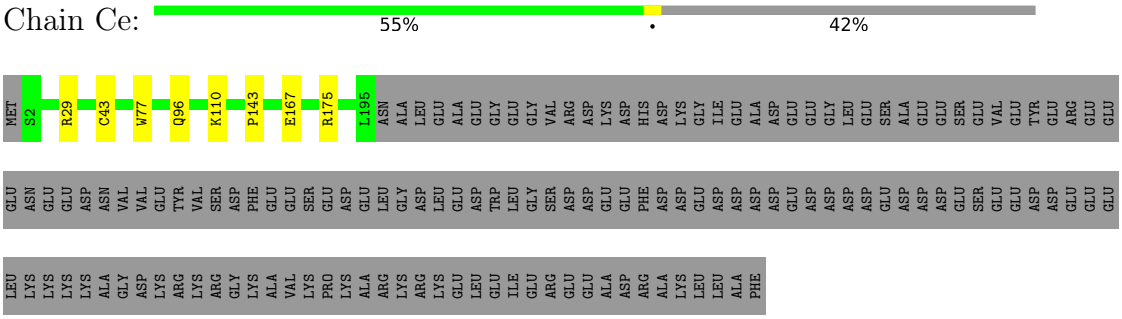
• Molecule 31: Brix domain-containing protein

Chain Cd:



• Molecule 32: Protein MAK16

Chain Ce:


55%
42%
MET S2 R29 C43 W77 Q96 K110 P143 E167 R175 L195 ASN ALA LEU GLU ALA GLU GLY GLU GLY VAL ARG ASP LYS ASP HIS ASP LYS GLY ILE GLU ALA ASP GLU GLU GLY LEU GLU SER ALA GLU GLU SER GLU VAL GLU TYR GLU ARG GLU GLU
GLU ASN GLU GLU ASP ASN VAL VAL GLU TYR VAL SER ASP PHE GLU GLU SER GLU ASP GLU LEU GLY ASP LEU GLU ASP TRP LEU GLY SER ASP ASP GLU GLU PHE ASP ASP GLU ASP ASP ASP GLU ASP ASP ASP ASP GLU ASP ASP ASP GLU SER GLU GLU ASP ASP GLU GLU GLU
LEU LYS LYS LYS LYS ALA GLY ASP LYS ARG LYS ARG GLY LYS ALA VAL LYS PRO LYS ALA ARG LYS ARG LYS GLU LEU GLU ILE GLU ARG GLU ALA ASP ARG ALA LYS LEU LEU ALA PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C1	0.34	1/31321 (0.0%)	0.96	75/48825 (0.2%)
2	C2	0.31	0/6097	0.93	8/9499 (0.1%)
3	CA	0.38	0/2190	0.65	1/2940 (0.0%)
4	CB	0.38	0/2188	0.65	3/2975 (0.1%)
5	CC	0.32	0/2224	0.67	6/3024 (0.2%)
6	CE	0.32	0/3743	0.56	1/5045 (0.0%)
7	CI	0.38	0/1225	0.75	2/1645 (0.1%)
8	CJ	0.30	0/3189	0.70	4/4309 (0.1%)
9	CM	0.32	0/1555	0.74	2/2091 (0.1%)
9	LF	0.35	0/2004	0.60	0/2686
10	CR	0.37	0/1369	0.57	0/1828
11	CU	0.39	0/935	0.79	0/1256
12	LC	0.35	0/2809	0.58	0/3787
13	LE	0.47	0/1363	0.64	1/1833 (0.1%)
14	LG	0.34	0/1504	0.57	0/2018
15	LL	0.31	0/983	0.61	0/1318
16	LM	0.40	0/1056	0.70	1/1419 (0.1%)
17	LN	0.41	0/1595	0.60	0/2132
18	LO	0.32	0/1652	0.81	8/2215 (0.4%)
19	LP	0.32	0/1231	0.60	0/1658
20	LQ	0.38	0/1033	0.64	0/1391
21	LS	0.50	0/1468	0.63	1/1975 (0.1%)
22	LT	0.32	0/1033	0.75	2/1389 (0.1%)
23	LX	0.25	0/148	0.36	0/194
24	LY	0.32	0/1079	0.60	0/1443
25	Le	0.39	0/1073	0.58	0/1431
26	Lf	0.51	0/883	0.63	0/1187
27	Lh	0.30	0/1006	0.61	0/1338
28	Li	0.37	0/738	0.65	0/971
29	Lj	0.29	0/606	0.64	0/803
30	Cc	0.27	0/1934	0.59	1/2614 (0.0%)
31	Cd	0.31	0/2822	0.62	1/3790 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	Ce	0.28	0/1638	0.55	0/2196
All	All	0.34	1/85694 (0.0%)	0.81	117/123225 (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
18	LO	0	1
22	LT	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1098	G	C6-N1	-8.16	1.33	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1098	G	N1-C6-O6	-27.47	103.42	119.90
1	C1	1123	C	N3-C4-N4	-25.91	99.86	118.00
1	C1	1098	G	C5-C6-O6	23.89	142.94	128.60
1	C1	1123	C	C5-C4-N4	20.27	134.38	120.20
1	C1	1050	C	N3-C2-O2	-11.16	114.08	121.90
1	C1	939	C	N3-C2-O2	-10.06	114.86	121.90
18	LO	175	LEU	CA-CB-CG	9.64	137.46	115.30
1	C1	1049	C	N1-C2-O2	9.11	124.37	118.90
22	LT	115	LEU	CA-CB-CG	9.09	136.21	115.30
1	C1	1049	C	N3-C2-O2	-9.07	115.55	121.90
18	LO	59	LEU	CA-CB-CG	9.04	136.10	115.30
1	C1	1123	C	N3-C4-C5	8.87	125.45	121.90
8	CJ	147	MET	CA-CB-CG	8.58	127.88	113.30
18	LO	193	PRO	CA-N-CD	-8.21	100.01	111.50
1	C1	533	C	N1-C2-O2	8.03	123.72	118.90
1	C1	1050	C	N1-C2-O2	7.93	123.66	118.90
1	C1	83	C	C2-N3-C4	-7.91	115.95	119.90
9	CM	190	LEU	CA-CB-CG	7.90	133.46	115.30
1	C1	398	G	O4'-C1'-N9	7.87	114.50	108.20
8	CJ	147	MET	CB-CG-SD	7.81	135.84	112.40
13	LE	177	ASP	CB-CG-OD1	7.68	125.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	590	C	N1-C2-O2	7.61	123.46	118.90
30	Cc	252	ASP	CB-CG-OD1	7.58	125.12	118.30
5	CC	352	LEU	CA-CB-CG	7.56	132.68	115.30
1	C1	590	C	C6-N1-C2	-7.50	117.30	120.30
1	C1	36	C	N1-C2-O2	7.48	123.39	118.90
2	C2	170	C	N1-C2-O2	7.48	123.39	118.90
1	C1	72	C	C2-N3-C4	-7.43	116.19	119.90
1	C1	263	C	N1-C2-O2	7.21	123.22	118.90
2	C2	171	C	N3-C2-O2	-7.18	116.88	121.90
18	LO	158	LEU	CA-CB-CG	7.17	131.79	115.30
1	C1	1051	C	N3-C2-O2	-7.09	116.93	121.90
1	C1	1123	C	C4-C5-C6	-7.05	113.88	117.40
9	CM	210	PRO	CA-N-CD	-6.98	101.73	111.50
1	C1	961	U	C2-N1-C1'	6.97	126.07	117.70
8	CJ	374	LEU	CA-CB-CG	6.94	131.26	115.30
1	C1	162	U	N3-C2-O2	-6.83	117.42	122.20
1	C1	1098	G	C4-N9-C1'	6.79	135.33	126.50
1	C1	590	C	N3-C2-O2	-6.73	117.19	121.90
1	C1	961	U	N1-C2-O2	6.72	127.50	122.80
4	CB	24	LEU	CA-CB-CG	6.70	130.71	115.30
2	C2	230	C	N3-C2-O2	-6.70	117.21	121.90
18	LO	171	GLU	CA-CB-CG	6.61	127.95	113.40
1	C1	463	C	C2-N1-C1'	6.47	125.92	118.80
1	C1	939	C	C6-N1-C2	-6.46	117.71	120.30
1	C1	249	C	N3-C2-O2	-6.41	117.41	121.90
1	C1	533	C	N3-C2-O2	-6.39	117.43	121.90
1	C1	1098	G	O4'-C1'-N9	6.36	113.29	108.20
1	C1	635	C	N1-C2-O2	6.32	122.69	118.90
1	C1	961	U	N3-C2-O2	-6.32	117.78	122.20
1	C1	83	C	N1-C2-N3	6.30	123.61	119.20
1	C1	78	U	N3-C2-O2	-6.26	117.81	122.20
3	CA	126	LEU	CA-CB-CG	6.21	129.59	115.30
5	CC	410	LEU	CA-CB-CG	6.21	129.59	115.30
1	C1	967	U	C5-C6-N1	6.15	125.78	122.70
1	C1	1050	C	C6-N1-C2	-6.14	117.84	120.30
5	CC	408	MET	CA-CB-CG	6.11	123.68	113.30
6	CE	381	ASP	CB-CG-OD1	6.10	123.79	118.30
1	C1	1098	G	C8-N9-C1'	-6.03	119.16	127.00
31	Cd	417	ASP	CB-CG-OD1	6.03	123.73	118.30
21	LS	109	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C1	1072	G	N1-C2-N2	-5.90	110.89	116.20
1	C1	473	C	C2-N1-C1'	5.86	125.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	243	G	C4-N9-C1'	5.85	134.11	126.50
1	C1	263	C	N3-C2-O2	-5.84	117.81	121.90
1	C1	976	U	N1-C2-O2	5.73	126.81	122.80
2	C2	174	G	P-O3'-C3'	5.71	126.55	119.70
1	C1	1099	G	N1-C6-O6	-5.69	116.49	119.90
1	C1	1051	C	C6-N1-C2	-5.67	118.03	120.30
1	C1	36	C	N3-C2-O2	-5.66	117.94	121.90
2	C2	288	G	C5-C6-O6	5.66	131.99	128.60
1	C1	263	C	C2-N1-C1'	5.64	125.00	118.80
1	C1	1031	C	N3-C2-O2	-5.62	117.97	121.90
1	C1	590	C	C2-N1-C1'	5.61	124.97	118.80
5	CC	155	ASP	CB-CG-OD1	5.58	123.33	118.30
1	C1	590	C	C5-C6-N1	5.57	123.79	121.00
5	CC	196	MET	CB-CG-SD	5.57	129.10	112.40
1	C1	3233	C	N1-C2-O2	5.55	122.23	118.90
7	CI	311	GLN	CA-CB-CG	5.54	125.59	113.40
1	C1	243	G	N3-C4-C5	-5.53	125.83	128.60
1	C1	939	C	N1-C2-O2	5.51	122.21	118.90
1	C1	1071	G	N1-C2-N2	-5.48	111.27	116.20
1	C1	133	G	N3-C4-C5	-5.46	125.87	128.60
22	LT	115	LEU	CB-CG-CD1	5.43	120.23	111.00
1	C1	249	C	N1-C2-O2	5.40	122.14	118.90
1	C1	741	G	O4'-C1'-N9	5.38	112.51	108.20
1	C1	162	U	N1-C2-O2	5.35	126.55	122.80
1	C1	976	U	N3-C2-O2	-5.33	118.47	122.20
1	C1	1098	G	N3-C4-N9	5.33	129.19	126.00
1	C1	1098	G	N1-C2-N3	-5.31	120.72	123.90
1	C1	940	C	N3-C2-O2	-5.30	118.19	121.90
1	C1	243	G	N3-C4-N9	5.30	129.18	126.00
1	C1	944	G	N1-C6-O6	-5.24	116.75	119.90
18	LO	59	LEU	CB-CG-CD2	5.24	119.91	111.00
1	C1	938	C	N1-C2-O2	5.24	122.04	118.90
2	C2	170	C	N3-C2-O2	-5.23	118.24	121.90
4	CB	301	LEU	CA-CB-CG	5.22	127.30	115.30
1	C1	3233	C	C2-N1-C1'	5.21	124.53	118.80
1	C1	940	C	C6-N1-C2	-5.21	118.22	120.30
7	CI	216	LEU	CA-CB-CG	5.17	127.19	115.30
16	LM	112	LEU	CA-CB-CG	5.15	127.14	115.30
1	C1	3162	A	P-O3'-C3'	5.14	125.87	119.70
18	LO	157	ARG	CA-CB-CG	5.12	124.67	113.40
18	LO	11	ASP	CB-CG-OD1	5.11	122.90	118.30
4	CB	104	PRO	CA-N-CD	-5.10	104.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	167	C	C2-N1-C1'	5.10	124.41	118.80
1	C1	1031	C	N1-C2-O2	5.09	121.95	118.90
2	C2	288	G	N1-C6-O6	-5.09	116.85	119.90
1	C1	239	C	C2-N1-C1'	5.08	124.38	118.80
8	CJ	141	LEU	CA-CB-CG	5.08	126.97	115.30
1	C1	1046	A	P-O3'-C3'	5.07	125.79	119.70
2	C2	151	C	C2-N1-C1'	5.06	124.36	118.80
1	C1	3205	C	N1-C2-O2	5.05	121.93	118.90
1	C1	150	G	P-O3'-C3'	5.04	125.75	119.70
1	C1	3134	A	C8-N9-C4	-5.02	103.79	105.80
5	CC	118	LEU	CA-CB-CG	5.02	126.84	115.30
1	C1	1172	A	C4-N9-C1'	5.01	135.31	126.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	LO	192	ASP	Peptide
22	LT	92	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	27990	0	14115	200	0
2	C2	5456	0	2762	36	0
3	CA	2144	0	2178	43	0
4	CB	2140	0	2195	27	0
5	CC	2159	0	2081	48	0
6	CE	3673	0	3778	33	0
7	CI	1196	0	1202	23	0
8	CJ	3109	0	3122	71	0
9	CM	1525	0	1604	34	0
9	LF	1967	0	2080	22	0
10	CR	1354	0	1400	13	0
11	CU	924	0	951	27	0
12	LC	2752	0	2878	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	LE	1338	0	1423	12	0
14	LG	1482	0	1610	22	0
15	LL	964	0	1041	14	0
16	LM	1037	0	1110	12	0
17	LN	1563	0	1618	17	0
18	LO	1618	0	1714	35	0
19	LP	1212	0	1250	10	0
20	LQ	1021	0	1118	6	0
21	LS	1433	0	1496	18	0
22	LT	1014	0	1073	20	0
23	LX	148	0	163	2	0
24	LY	1065	0	1156	10	0
25	Le	1055	0	1133	0	0
26	Lf	862	0	891	0	0
27	Lh	995	0	1110	0	0
28	Li	731	0	797	0	0
29	Lj	595	0	625	0	0
30	Cc	1898	0	1931	0	0
31	Cd	2768	0	2860	0	0
32	Ce	1609	0	1682	0	0
33	Ce	1	0	0	0	0
33	Lj	1	0	0	0	0
All	All	80799	0	66147	654	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (654) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:788:A:N6	1:C1:915:G:H1	1.49	1.10
2:C2:223:G:H21	2:C2:301:A:H61	1.11	0.93
2:C2:196:G:H1	2:C2:201:U:H3	0.94	0.91
1:C1:788:A:H62	1:C1:915:G:H1	0.87	0.86
2:C2:223:G:N2	2:C2:301:A:H61	1.73	0.86
6:CE:136:GLU:HG2	6:CE:320:VAL:HG22	1.58	0.84
9:CM:87:ALA:HA	9:CM:125:VAL:O	1.83	0.77
1:C1:1053:U:H3	1:C1:1069:G:H1	1.32	0.77
1:C1:3112:A:N7	1:C1:3232:U:O2	2.19	0.76
6:CE:136:GLU:HG2	6:CE:320:VAL:CG2	2.15	0.76
5:CC:169:VAL:O	5:CC:169:VAL:HG12	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CC:406:ARG:O	5:CC:409:ASP:HB2	1.86	0.73
7:CI:204:ARG:O	7:CI:208:SER:HB2	1.89	0.71
5:CC:396:TRP:HE1	5:CC:398:ASN:HB3	1.57	0.69
3:CA:105:SER:HB2	3:CA:112:THR:HG23	1.75	0.69
1:C1:788:A:N6	1:C1:915:G:N1	2.32	0.69
3:CA:137:ARG:O	11:CU:218:GLN:NE2	2.26	0.69
3:CA:143:ASP:H	3:CA:146:PHE:HD2	1.40	0.68
1:C1:66:A:N6	1:C1:75:G:N2	2.40	0.68
21:LS:8:GLN:HG3	21:LS:26:ARG:HE	1.59	0.68
1:C1:553:U:OP1	21:LS:67:LYS:NZ	2.28	0.67
3:CA:171:LYS:HG2	5:CC:167:VAL:HG11	1.77	0.67
6:CE:384:VAL:HG12	6:CE:410:THR:CG2	2.25	0.66
18:LO:175:LEU:HD23	18:LO:179:GLN:HE22	1.60	0.66
10:CR:38:SER:O	10:CR:51:ARG:NH2	2.28	0.65
1:C1:1083:G:H5"	9:LF:113:ARG:HD3	1.78	0.65
6:CE:352:LEU:HB3	6:CE:382:LEU:HD21	1.78	0.65
6:CE:377:LEU:HA	6:CE:380:ILE:HG22	1.79	0.65
2:C2:223:G:H21	2:C2:301:A:N6	1.90	0.65
5:CC:306:TYR:H	14:LG:117:THR:HG21	1.60	0.64
9:CM:113:ARG:NH2	9:CM:208:LEU:O	2.30	0.64
11:CU:282:MET:HA	11:CU:285:VAL:HG22	1.80	0.64
19:LP:94:LEU:HB3	19:LP:148:LEU:HD21	1.78	0.64
9:CM:167:ILE:HG23	9:CM:168:PRO:HD2	1.80	0.64
7:CI:321:LYS:NZ	7:CI:325:TYR:O	2.27	0.63
1:C1:281:U:H2'	1:C1:282:G:H8	1.63	0.63
4:CB:25:LYS:HA	4:CB:28:LYS:HG2	1.79	0.63
1:C1:974:G:H1	1:C1:1038:U:H3	1.47	0.62
22:LT:42:ILE:HG22	22:LT:96:VAL:HG12	1.80	0.62
13:LE:61:LEU:HD11	13:LE:103:ILE:HG13	1.80	0.62
1:C1:493:C:O2	13:LE:41:LYS:NZ	2.32	0.62
1:C1:255:C:OP2	6:CE:222:ASN:ND2	2.33	0.62
8:CJ:169:GLU:OE1	8:CJ:170:ARG:NH1	2.33	0.61
1:C1:14:U:H3	2:C2:136:G:H21	1.48	0.61
3:CA:109:ASN:O	5:CC:148:ARG:NH2	2.32	0.61
18:LO:132:GLN:HB3	18:LO:135:ARG:HG2	1.81	0.61
10:CR:39:TRP:HE1	15:LL:40:ARG:HH12	1.49	0.61
3:CA:136:SER:HB3	3:CA:176:ILE:HA	1.83	0.60
9:CM:167:ILE:HG22	9:CM:168:PRO:O	2.01	0.60
10:CR:43:GLU:O	15:LL:40:ARG:NH2	2.34	0.60
17:LN:177:GLY:O	17:LN:184:ARG:NH2	2.33	0.60
1:C1:796:G:H1	1:C1:906:A:H61	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LN:99:ARG:HB3	17:LN:167:THR:HG21	1.84	0.60
1:C1:672:G:OP1	15:LL:39:ARG:NH2	2.34	0.60
4:CB:24:LEU:HD13	4:CB:28:LYS:HD3	1.83	0.60
1:C1:281:U:H2'	1:C1:282:G:C8	2.38	0.59
14:LG:165:LEU:HA	17:LN:7:LEU:HD11	1.84	0.59
8:CJ:378:THR:HG21	8:CJ:419:ILE:HG22	1.83	0.59
8:CJ:419:ILE:HD13	8:CJ:456:VAL:HG23	1.85	0.59
1:C1:3173:C:N3	1:C1:3198:U:O2	2.36	0.59
8:CJ:77:LEU:HD22	8:CJ:126:ILE:HD11	1.84	0.59
11:CU:276:VAL:HG12	11:CU:277:ARG:HG2	1.84	0.59
16:LM:93:LYS:HA	16:LM:96:GLU:HG3	1.85	0.58
3:CA:91:PHE:HB3	3:CA:103:TRP:HB2	1.84	0.58
3:CA:73:ARG:NH1	3:CA:75:TYR:OH	2.36	0.58
3:CA:245:ILE:HB	3:CA:256:TYR:HB3	1.84	0.58
5:CC:408:MET:O	5:CC:412:LEU:N	2.37	0.58
7:CI:298:SER:N	7:CI:301:GLN:OE1	2.37	0.58
1:C1:116:A:OP2	17:LN:2:GLY:N	2.36	0.58
4:CB:120:LEU:HD22	4:CB:221:VAL:HG13	1.85	0.58
5:CC:242:VAL:HG23	14:LG:72:LEU:HD21	1.84	0.58
1:C1:189:G:N1	1:C1:192:A:OP2	2.35	0.58
1:C1:403:U:H2'	1:C1:404:G:H8	1.69	0.57
1:C1:3138:U:HO2'	21:LS:172:THR:HG1	1.38	0.57
9:CM:245:ILE:HA	9:CM:248:MET:HB2	1.85	0.57
1:C1:1098:G:H1	1:C1:1123:C:H42	1.50	0.57
12:LC:36:VAL:HG21	12:LC:251:LEU:HD21	1.85	0.57
1:C1:1046:A:N1	1:C1:1074:C:N3	2.52	0.57
1:C1:1071:G:H2'	1:C1:1072:G:C8	2.40	0.57
22:LT:92:ARG:HD3	22:LT:92:ARG:H	1.70	0.57
1:C1:780:G:HO2'	15:LL:18:TRP:HE1	1.46	0.57
8:CJ:421:ASP:OD1	8:CJ:421:ASP:N	2.37	0.57
9:CM:165:GLN:OE1	9:CM:167:ILE:HG13	2.05	0.57
9:LF:124:LYS:HG3	9:LF:197:VAL:HG11	1.86	0.57
1:C1:3189:G:H2'	1:C1:3190:G:H8	1.69	0.57
8:CJ:84:GLN:OE1	8:CJ:120:ARG:NH2	2.38	0.57
8:CJ:189:PHE:HA	8:CJ:462:TRP:HE1	1.70	0.57
1:C1:1124:G:N2	1:C1:1125:A:O2'	2.38	0.57
9:LF:156:LYS:HG2	9:LF:157:ARG:HG3	1.86	0.57
18:LO:35:VAL:HG12	18:LO:105:LYS:HB2	1.86	0.57
2:C2:39:G:C2	2:C2:105:A:C2	2.92	0.56
1:C1:671:G:OP2	15:LL:28:GLN:NE2	2.36	0.56
1:C1:972:G:N2	1:C1:1040:U:O2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CJ:141:LEU:HA	8:CJ:144:CYS:HB3	1.86	0.56
8:CJ:163:LYS:HA	9:CM:246:ARG:HH22	1.69	0.56
11:CU:274:GLU:N	11:CU:274:GLU:OE1	2.38	0.56
12:LC:299:VAL:HG21	20:LQ:159:PRO:HB2	1.86	0.56
3:CA:106:LYS:HB2	3:CA:110:GLY:HA3	1.87	0.56
2:C2:151:C:O2	14:LG:63:ARG:NH2	2.39	0.56
19:LP:41:LEU:HD21	19:LP:99:GLU:HG3	1.86	0.56
1:C1:533:C:C2	1:C1:539:G:C2	2.93	0.56
2:C2:128:U:O4'	8:CJ:14:ARG:NH2	2.39	0.56
5:CC:358:PRO:HA	5:CC:361:LEU:HG	1.86	0.56
1:C1:972:G:C2	1:C1:1040:U:O2	2.58	0.56
1:C1:975:G:N2	1:C1:976:U:O4	2.39	0.56
1:C1:261:G:OP1	17:LN:47:LYS:NZ	2.37	0.56
1:C1:533:C:O2	1:C1:539:G:C2	2.59	0.56
13:LE:84:THR:HB	13:LE:94:LEU:HD23	1.87	0.56
6:CE:441:TYR:O	6:CE:445:VAL:HB	2.06	0.55
9:CM:91:PHE:HB2	9:CM:145:PRO:HG3	1.88	0.55
2:C2:103:G:OP2	2:C2:105:A:O2'	2.22	0.55
4:CB:245:VAL:O	4:CB:258:ASN:ND2	2.39	0.55
16:LM:43:GLY:HA3	16:LM:52:THR:HB	1.87	0.55
6:CE:181:ARG:NH2	10:CR:137:GLN:OE1	2.35	0.55
1:C1:538:G:H2'	1:C1:539:G:H8	1.72	0.55
5:CC:411:TYR:HE1	8:CJ:41:GLY:HA2	1.70	0.55
1:C1:642:C:H2'	1:C1:643:A:H8	1.71	0.55
1:C1:780:G:O2'	15:LL:18:TRP:NE1	2.37	0.55
1:C1:1029:A:OP2	1:C1:1031:C:N4	2.39	0.55
5:CC:142:ASP:OD1	5:CC:146:GLY:N	2.36	0.55
2:C2:163:C:O2	9:CM:73:ARG:NH2	2.40	0.55
6:CE:342:ASP:OD1	6:CE:342:ASP:N	2.40	0.55
6:CE:450:ARG:HG2	6:CE:455:LYS:HD2	1.88	0.55
3:CA:27:ILE:H	3:CA:168:GLY:HA3	1.72	0.55
3:CA:151:TYR:HA	11:CU:196:LEU:HD22	1.89	0.55
12:LC:54:SER:HB2	12:LC:57:ALA:HB2	1.89	0.55
1:C1:3134:A:H1'	18:LO:166:GLY:HA3	1.88	0.55
5:CC:248:PRO:HG2	5:CC:254:PRO:HB3	1.88	0.55
12:LC:364:GLU:O	21:LS:28:ARG:NH1	2.40	0.55
9:LF:91:PHE:HB2	9:LF:145:PRO:HG3	1.88	0.54
17:LN:200:TRP:O	17:LN:203:ARG:NH1	2.40	0.54
1:C1:295:G:OP1	17:LN:179:ARG:NH2	2.40	0.54
1:C1:381:A:OP1	19:LP:16:ARG:NH1	2.40	0.54
4:CB:77:ARG:HB3	4:CB:235:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:196:G:O6	2:C2:201:U:O4	2.26	0.54
7:CI:249:ASP:HA	7:CI:260:CYS:HB2	1.89	0.54
1:C1:1175:A:N6	1:C1:1297:U:N3	2.56	0.54
3:CA:229:ILE:O	11:CU:252:ARG:NH2	2.38	0.54
4:CB:104:PRO:HD3	4:CB:208:PRO:HB3	1.89	0.54
6:CE:387:LEU:HD13	6:CE:411:LEU:HD11	1.90	0.54
8:CJ:371:THR:HG22	8:CJ:394:ARG:HH21	1.73	0.54
21:LS:74:ASN:HD22	21:LS:135:VAL:HG11	1.73	0.54
14:LG:151:ALA:HA	14:LG:204:THR:HG22	1.90	0.54
1:C1:981:C:H5"	1:C1:982:G:H5'	1.89	0.54
14:LG:97:LEU:HB3	14:LG:192:LEU:HD21	1.90	0.54
1:C1:92:G:H5'	1:C1:93:C:H5"	1.89	0.53
1:C1:3134:A:OP2	18:LO:173:LYS:NZ	2.42	0.53
3:CA:33:LYS:HE2	5:CC:156:PRO:HD2	1.90	0.53
18:LO:175:LEU:HD23	18:LO:179:GLN:NE2	2.24	0.53
1:C1:796:G:H1	1:C1:906:A:N6	2.06	0.53
16:LM:128:ARG:HA	16:LM:131:GLU:HG2	1.91	0.53
1:C1:246:A:OP2	5:CC:285:LYS:NZ	2.41	0.53
12:LC:149:VAL:HG13	12:LC:150:PRO:HD3	1.89	0.53
9:CM:184:ILE:HG23	9:CM:189:ASP:HB3	1.90	0.53
1:C1:533:C:N3	1:C1:539:G:N1	2.58	0.52
3:CA:144:ALA:HB3	11:CU:225:ARG:HA	1.90	0.52
12:LC:24:PRO:HG2	12:LC:265:LEU:HD23	1.92	0.52
16:LM:13:ARG:HA	21:LS:151:PRO:HA	1.91	0.52
1:C1:735:G:C6	1:C1:760:G:C2	2.98	0.52
1:C1:764:A:H5"	1:C1:765:G:H5'	1.91	0.52
7:CI:192:ALA:HB3	7:CI:259:THR:HB	1.90	0.52
4:CB:151:ASP:HA	4:CB:177:LYS:HE3	1.91	0.52
5:CC:400:VAL:HG22	8:CJ:150:LEU:HD11	1.91	0.52
6:CE:173:LEU:HB3	6:CE:212:GLN:HG2	1.91	0.52
12:LC:136:LEU:HD22	12:LC:149:VAL:HG23	1.92	0.52
1:C1:36:C:H4'	1:C1:789:A:H2	1.73	0.52
1:C1:1045:G:C6	22:LT:109:VAL:HG12	2.45	0.52
5:CC:174:ASN:OD1	5:CC:174:ASN:N	2.41	0.52
8:CJ:39:TRP:NE1	8:CJ:232:GLU:OE2	2.38	0.52
11:CU:294:THR:HA	11:CU:297:LYS:HG3	1.92	0.52
1:C1:781:G:H22	12:LC:102:ALA:HA	1.74	0.52
14:LG:208:SER:HA	14:LG:211:LYS:HG3	1.91	0.52
24:LY:54:GLU:HB2	24:LY:107:LYS:HB3	1.91	0.52
1:C1:975:G:H4'	1:C1:976:U:H5'	1.91	0.52
18:LO:117:LYS:O	18:LO:119:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LO:182:GLU:HA	18:LO:185:LYS:HE2	1.92	0.52
3:CA:121:HIS:HB2	3:CA:237:ARG:HB2	1.92	0.52
19:LP:122:ALA:HB3	19:LP:143:PRO:HB2	1.91	0.52
1:C1:230:A:H2'	1:C1:231:A:C8	2.44	0.52
2:C2:220:G:OP2	7:CI:274:LYS:NZ	2.43	0.52
1:C1:562:U:H2'	1:C1:563:A:H8	1.75	0.52
1:C1:1171:C:N4	1:C1:1297:U:O2'	2.40	0.52
5:CC:189:ASP:HB3	5:CC:195:ILE:HD11	1.91	0.52
1:C1:1114:C:H2'	1:C1:1115:A:H8	1.74	0.51
1:C1:631:G:H5'	1:C1:1099:G:H1'	1.92	0.51
6:CE:359:LYS:HG2	6:CE:426:VAL:HG12	1.91	0.51
6:CE:377:LEU:HD22	6:CE:382:LEU:HD23	1.91	0.51
1:C1:63:A:H5"	17:LN:174:LEU:HD13	1.93	0.51
1:C1:522:G:H2'	1:C1:523:A:C8	2.45	0.51
1:C1:3144:C:O5'	18:LO:178:ARG:NH1	2.44	0.51
5:CC:169:VAL:O	5:CC:169:VAL:CG1	2.54	0.51
6:CE:362:VAL:HB	6:CE:412:ILE:HG22	1.93	0.51
9:CM:102:PRO:HB2	9:CM:105:PRO:HD2	1.91	0.51
18:LO:153:ASP:O	18:LO:157:ARG:HD2	2.09	0.51
3:CA:234:ILE:O	11:CU:277:ARG:NH2	2.44	0.51
9:CM:237:ARG:HG3	9:CM:240:HIS:HB2	1.93	0.51
11:CU:234:GLU:OE1	11:CU:234:GLU:N	2.43	0.51
22:LT:79:ARG:NH2	22:LT:81:LYS:O	2.43	0.51
1:C1:642:C:H2'	1:C1:643:A:C8	2.45	0.51
1:C1:735:G:C5	1:C1:760:G:N2	2.79	0.51
1:C1:2313:U:H2'	1:C1:2314:A:H8	1.75	0.51
18:LO:154:VAL:O	18:LO:158:LEU:HD23	2.11	0.51
1:C1:2315:G:OP2	19:LP:82:ARG:NH2	2.44	0.50
3:CA:137:ARG:NH2	11:CU:215:SER:O	2.43	0.50
18:LO:129:LEU:HD11	21:LS:170:PRO:HG2	1.93	0.50
5:CC:270:PRO:HB3	14:LG:148:ASN:HA	1.93	0.50
8:CJ:54:ASN:ND2	8:CJ:56:SER:O	2.43	0.50
9:CM:116:GLN:HG2	9:CM:119:ASN:HD21	1.76	0.50
14:LG:91:ALA:O	14:LG:95:LYS:HG3	2.11	0.50
5:CC:138:ARG:HB2	5:CC:150:VAL:HB	1.94	0.50
8:CJ:131:TYR:OH	8:CJ:140:ASP:OD2	2.26	0.50
8:CJ:141:LEU:HD21	8:CJ:238:LEU:HD23	1.94	0.50
8:CJ:410:GLU:O	8:CJ:453:ARG:NH1	2.44	0.50
3:CA:133:LEU:HA	3:CA:134:LYS:HZ3	1.76	0.50
8:CJ:19:ARG:HE	8:CJ:64:TYR:HE2	1.58	0.50
21:LS:21:ASN:OD1	22:LT:146:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CC:242:VAL:HG11	14:LG:68:LEU:HD21	1.92	0.50
8:CJ:41:GLY:HA3	8:CJ:130:ARG:HH12	1.75	0.50
8:CJ:169:GLU:HG2	8:CJ:173:HIS:CE1	2.47	0.50
1:C1:370:A:H4'	24:LY:90:THR:HG22	1.94	0.50
1:C1:3112:A:N6	1:C1:3232:U:H3	2.10	0.50
3:CA:131:ASN:OD1	3:CA:132:CYS:N	2.44	0.50
4:CB:251:GLU:H	4:CB:254:LYS:HE2	1.77	0.50
12:LC:328:ARG:O	9:LF:47:ARG:NH1	2.43	0.50
1:C1:3129:G:N1	1:C1:3157:C:O2	2.45	0.50
4:CB:163:LEU:HD23	4:CB:179:PRO:HG2	1.93	0.50
22:LT:79:ARG:HH21	22:LT:82:HIS:HA	1.76	0.50
1:C1:19:U:H2'	1:C1:20:A:C8	2.47	0.50
1:C1:676:U:OP1	12:LC:220:LYS:NZ	2.45	0.50
1:C1:1049:C:H4'	22:LT:109:VAL:HG21	1.94	0.49
12:LC:238:ASP:OD1	12:LC:238:ASP:N	2.43	0.49
17:LN:114:ARG:NH1	17:LN:151:ILE:O	2.45	0.49
1:C1:3188:U:H2'	1:C1:3189:G:C8	2.47	0.49
8:CJ:184:SER:HA	8:CJ:186:ARG:HH21	1.75	0.49
1:C1:531:U:N3	1:C1:541:G:N1	2.60	0.49
1:C1:969:U:O4	1:C1:970:A:N6	2.45	0.49
2:C2:176:G:H2'	2:C2:177:C:H6	1.78	0.49
5:CC:354:TYR:HD2	5:CC:387:TYR:HB2	1.76	0.49
2:C2:175:G:H2'	2:C2:176:G:O4'	2.11	0.49
5:CC:401:LYS:O	5:CC:405:GLU:N	2.43	0.49
9:CM:162:VAL:O	9:CM:165:GLN:NE2	2.45	0.49
4:CB:48:ASN:HB3	4:CB:51:ALA:HB3	1.95	0.49
1:C1:1046:A:N6	1:C1:1074:C:C2	2.80	0.49
6:CE:486:PRO:HB2	6:CE:489:LYS:HG3	1.94	0.49
8:CJ:180:ILE:HA	8:CJ:389:ALA:HA	1.95	0.49
1:C1:3195:C:H2'	1:C1:3196:G:H8	1.78	0.49
5:CC:282:ILE:HG22	10:CR:219:GLN:HE21	1.77	0.49
4:CB:215:ARG:HG3	4:CB:220:ILE:HG13	1.94	0.49
1:C1:538:G:H2'	1:C1:539:G:C8	2.47	0.49
2:C2:179:U:OP1	4:CB:77:ARG:NH2	2.46	0.49
13:LE:155:SER:HB3	13:LE:158:ARG:HB3	1.95	0.49
1:C1:971:U:H4'	22:LT:100:ARG:HG3	1.94	0.48
1:C1:1302:C:H2'	1:C1:1303:G:H8	1.78	0.48
8:CJ:187:LYS:HB2	8:CJ:198:GLN:HB3	1.95	0.48
18:LO:145:HIS:NE2	18:LO:152:GLN:HG3	2.28	0.48
21:LS:12:ARG:HH22	21:LS:15:PRO:HG3	1.78	0.48
1:C1:581:G:O2'	13:LE:35:GLN:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:972:G:H2'	1:C1:973:A:C8	2.48	0.48
5:CC:396:TRP:NE1	5:CC:398:ASN:HB3	2.27	0.48
7:CI:247:THR:HG21	23:LX:24:ALA:HB1	1.95	0.48
8:CJ:177:HIS:HA	8:CJ:180:ILE:HG12	1.95	0.48
12:LC:361:LEU:HD11	22:LT:148:PRO:HG2	1.94	0.48
1:C1:190:G:N2	1:C1:364:A:C8	2.81	0.48
8:CJ:218:ILE:HG22	8:CJ:222:VAL:HG21	1.95	0.48
3:CA:126:LEU:HD23	11:CU:285:VAL:HG12	1.95	0.48
3:CA:130:GLY:O	11:CU:277:ARG:NH2	2.46	0.48
3:CA:194:TYR:HB3	3:CA:231:LEU:HB3	1.94	0.48
11:CU:236:ASP:OD1	11:CU:236:ASP:N	2.40	0.48
16:LM:124:LYS:O	16:LM:128:ARG:HB2	2.14	0.48
1:C1:403:U:H2'	1:C1:404:G:C8	2.47	0.48
3:CA:114:LYS:HB3	3:CA:244:ILE:HG13	1.95	0.48
9:CM:162:VAL:HG23	9:CM:165:GLN:HE22	1.78	0.48
13:LE:85:GLY:O	13:LE:86:PRO:C	2.50	0.48
1:C1:66:A:N6	1:C1:75:G:C2	2.81	0.48
1:C1:231:A:H2'	1:C1:232:G:C8	2.49	0.48
1:C1:247:A:H2'	1:C1:248:G:C8	2.49	0.48
1:C1:788:A:H61	1:C1:915:G:H22	1.61	0.48
1:C1:3173:C:H42	1:C1:3198:U:H3	1.61	0.48
7:CI:219:VAL:HG23	7:CI:228:ARG:HB2	1.95	0.48
8:CJ:400:VAL:HG21	9:CM:192:HIS:HB3	1.96	0.48
1:C1:966:U:H5"	9:LF:104:LYS:HG3	1.95	0.48
2:C2:26:U:H2'	2:C2:27:U:C6	2.48	0.48
8:CJ:198:GLN:HA	8:CJ:206:ILE:O	2.13	0.48
8:CJ:372:PHE:O	8:CJ:394:ARG:NH2	2.45	0.48
14:LG:159:ASP:N	14:LG:159:ASP:OD1	2.46	0.48
22:LT:65:TYR:HB3	22:LT:75:ILE:HD11	1.95	0.48
2:C2:13:A:O2'	19:LP:121:GLN:O	2.28	0.48
6:CE:384:VAL:HG12	6:CE:410:THR:HG23	1.95	0.48
14:LG:230:GLU:O	14:LG:234:LYS:NZ	2.47	0.48
1:C1:247:A:H2'	1:C1:248:G:H8	1.78	0.48
1:C1:1045:G:H1	1:C1:1079:G:HO2'	1.62	0.48
8:CJ:173:HIS:O	8:CJ:177:HIS:ND1	2.42	0.48
24:LY:43:ASN:HB3	24:LY:122:LYS:HG3	1.95	0.47
1:C1:37:U:O2	15:LL:15:ARG:NH2	2.47	0.47
1:C1:3125:A:O2'	18:LO:103:ARG:NH1	2.47	0.47
13:LE:98:ASN:HB3	13:LE:101:TYR:HD1	1.79	0.47
1:C1:423:U:H2'	1:C1:424:G:C8	2.49	0.47
1:C1:3184:G:H5'	1:C1:3187:G:H21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CI:239:GLU:OE1	7:CI:239:GLU:N	2.47	0.47
8:CJ:179:LEU:HD22	8:CJ:184:SER:HB2	1.95	0.47
1:C1:75:G:H5"	15:LL:58:VAL:HB	1.95	0.47
8:CJ:190:LEU:HB2	8:CJ:195:ILE:HG12	1.97	0.47
2:C2:166:C:H2'	2:C2:167:A:H8	1.79	0.47
8:CJ:51:ARG:HH22	8:CJ:55:LYS:HA	1.80	0.47
8:CJ:113:PRO:HG3	8:CJ:120:ARG:HB2	1.96	0.47
12:LC:8:THR:HA	12:LC:20:THR:HG22	1.96	0.47
5:CC:180:TYR:OH	11:CU:272:PHE:N	2.45	0.47
8:CJ:197:TYR:HE2	8:CJ:386:ILE:HD11	1.80	0.47
1:C1:1372:A:N6	1:C1:1400:A:O2'	2.47	0.47
2:C2:48:A:O2'	2:C2:51:G:N2	2.48	0.47
17:LN:71:ARG:HB2	17:LN:94:TYR:HB2	1.97	0.47
2:C2:9:A:H2'	2:C2:10:A:C8	2.49	0.47
5:CC:142:ASP:HB3	5:CC:148:ARG:HB2	1.97	0.47
7:CI:250:LYS:NZ	14:LG:227:GLU:OE2	2.47	0.47
9:CM:185:ILE:HG22	9:CM:185:ILE:O	2.15	0.47
9:LF:93:ILE:HA	9:LF:119:ASN:O	2.15	0.47
5:CC:152:ASP:OD1	5:CC:152:ASP:N	2.48	0.47
24:LY:36:LYS:HZ1	24:LY:39:ARG:HH11	1.63	0.47
1:C1:1158:C:H4'	18:LO:91:PRO:HD3	1.97	0.46
4:CB:245:VAL:HG12	4:CB:262:VAL:HG21	1.96	0.46
9:CM:153:LEU:HD13	9:CM:245:ILE:HD11	1.97	0.46
18:LO:174:LYS:O	18:LO:178:ARG:HG2	2.14	0.46
1:C1:639:G:H2'	1:C1:2323:A:H5'	1.96	0.46
1:C1:1163:U:O4	18:LO:22:SER:OG	2.23	0.46
4:CB:282:TYR:OH	7:CI:316:ARG:NH1	2.47	0.46
6:CE:269:ILE:HG22	6:CE:274:PHE:HB2	1.97	0.46
21:LS:124:LEU:HD22	22:LT:154:VAL:HG22	1.98	0.46
1:C1:20:A:H2'	1:C1:21:G:C8	2.50	0.46
1:C1:3157:C:OP1	16:LM:132:ARG:NH2	2.48	0.46
1:C1:424:G:H2'	1:C1:425:A:C8	2.51	0.46
1:C1:539:G:H2'	1:C1:540:A:H8	1.80	0.46
1:C1:966:U:H2'	1:C1:967:U:C6	2.51	0.46
1:C1:1087:C:H2'	1:C1:1088:G:H8	1.80	0.46
8:CJ:88:GLU:HA	8:CJ:91:ILE:HG22	1.97	0.46
1:C1:3189:G:H2'	1:C1:3190:G:C8	2.50	0.46
2:C2:167:A:O2'	9:CM:82:HIS:NE2	2.48	0.46
3:CA:148:GLN:OE1	11:CU:225:ARG:NE	2.47	0.46
3:CA:180:LEU:HD12	3:CA:193:ASN:HB3	1.98	0.46
6:CE:135:THR:OG1	6:CE:136:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CR:28:ASN:OD1	15:LL:40:ARG:NH1	2.49	0.46
19:LP:22:LEU:HD13	19:LP:90:PHE:HD2	1.80	0.46
20:LQ:99:LEU:HG	20:LQ:104:GLU:HA	1.96	0.46
1:C1:1134:G:H3'	1:C1:1135:A:H8	1.80	0.46
4:CB:207:ASP:HB3	4:CB:210:GLU:HG3	1.98	0.46
16:LM:105:GLN:NE2	16:LM:109:ARG:HH21	2.13	0.46
16:LM:123:LEU:HG	18:LO:195:VAL:HG23	1.97	0.46
1:C1:1151:A:H4'	9:LF:224:LYS:HD3	1.98	0.46
1:C1:1371:G:O6	12:LC:190:LYS:NZ	2.46	0.46
3:CA:137:ARG:NH1	3:CA:167:GLN:OE1	2.49	0.46
13:LE:57:VAL:O	13:LE:105:THR:OG1	2.31	0.46
9:LF:66:ARG:HA	9:LF:66:ARG:HD2	1.67	0.46
22:LT:147:LYS:HD3	22:LT:148:PRO:HD2	1.97	0.46
11:CU:235:ASP:OD1	11:CU:235:ASP:N	2.47	0.46
9:LF:184:ILE:HG23	9:LF:189:ASP:HB2	1.97	0.46
1:C1:715:G:H5"	20:LQ:71:PRO:HB2	1.97	0.45
1:C1:916:U:H2'	1:C1:917:A:H8	1.81	0.45
1:C1:68:C:OP2	1:C1:293:G:N2	2.42	0.45
1:C1:909:C:H2'	1:C1:910:A:C8	2.50	0.45
1:C1:506:G:H5"	12:LC:346:ALA:HB2	1.98	0.45
1:C1:663:G:H2'	1:C1:767:A:H61	1.80	0.45
1:C1:972:G:OP1	22:LT:100:ARG:NH2	2.40	0.45
6:CE:217:VAL:O	6:CE:239:ALA:HA	2.16	0.45
6:CE:357:LYS:HE2	6:CE:357:LYS:HB2	1.81	0.45
8:CJ:58:THR:HB	8:CJ:61:THR:HG23	1.98	0.45
8:CJ:400:VAL:O	9:CM:151:ARG:NH1	2.50	0.45
12:LC:264:GLN:O	12:LC:268:VAL:HG13	2.17	0.45
1:C1:959:C:H4'	1:C1:961:U:C2	2.52	0.45
1:C1:1430:U:H2'	1:C1:1431:A:H8	1.82	0.45
5:CC:390:LEU:HD23	5:CC:390:LEU:HA	1.81	0.45
8:CJ:392:CYS:HB3	8:CJ:395:ILE:HD11	1.98	0.45
1:C1:1332:A:H2'	1:C1:1333:A:C8	2.51	0.45
1:C1:3143:U:OP1	18:LO:174:LYS:NZ	2.39	0.45
5:CC:352:LEU:HD23	5:CC:382:TYR:CG	2.52	0.45
6:CE:191:PRO:HB3	6:CE:269:ILE:HG12	1.98	0.45
8:CJ:119:PRO:HB3	8:CJ:232:GLU:HB2	1.99	0.45
1:C1:532:C:N4	1:C1:540:A:H61	2.14	0.45
1:C1:664:A:N1	1:C1:690:G:O2'	2.41	0.45
2:C2:293:C:H4'	2:C2:294:A:H2	1.82	0.45
5:CC:164:ASP:O	5:CC:167:VAL:HG23	2.17	0.45
24:LY:28:VAL:O	24:LY:31:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:66:A:H61	1:C1:75:G:N2	2.11	0.45
1:C1:618:A:H2'	1:C1:619:G:C8	2.51	0.45
1:C1:1172:A:N3	18:LO:50:ARG:NH2	2.65	0.45
2:C2:130:C:H2'	2:C2:131:G:C8	2.52	0.45
3:CA:169:HIS:NE2	5:CC:158:TYR:OH	2.40	0.45
3:CA:181:SER:O	3:CA:191:VAL:HA	2.17	0.45
3:CA:198:GLU:HG2	3:CA:229:ILE:HG22	1.99	0.45
11:CU:290:ILE:O	11:CU:294:THR:HG23	2.17	0.45
9:LF:102:PRO:HB2	9:LF:105:PRO:HD2	1.99	0.45
18:LO:55:TYR:O	18:LO:59:LEU:HD22	2.17	0.45
8:CJ:453:ARG:NH2	8:CJ:455:TYR:OH	2.50	0.45
9:CM:185:ILE:O	9:CM:185:ILE:CG2	2.65	0.45
20:LQ:82:MET:HE3	20:LQ:86:ASN:HB3	1.99	0.45
1:C1:155:G:H2'	1:C1:156:G:C8	2.52	0.45
1:C1:662:C:O2'	1:C1:666:U:OP1	2.33	0.45
18:LO:155:VAL:O	18:LO:159:GLU:HB2	2.17	0.45
21:LS:168:LYS:HB2	21:LS:168:LYS:HE3	1.67	0.45
1:C1:1172:A:H2'	18:LO:50:ARG:HH21	1.82	0.44
1:C1:3195:C:H2'	1:C1:3196:G:C8	2.52	0.44
10:CR:50:THR:OG1	10:CR:69:ASN:O	2.22	0.44
1:C1:31:C:H4'	17:LN:96:ARG:HG2	2.00	0.44
1:C1:1046:A:N6	1:C1:1074:C:O2	2.50	0.44
2:C2:148:G:H2'	2:C2:149:A:H8	1.82	0.44
11:CU:207:ILE:HD12	11:CU:217:HIS:HB3	2.00	0.44
13:LE:152:LYS:HB2	13:LE:152:LYS:HE3	1.76	0.44
16:LM:96:GLU:O	16:LM:101:LYS:NZ	2.50	0.44
19:LP:86:LYS:HA	19:LP:89:GLN:HG3	1.99	0.44
3:CA:131:ASN:OD1	11:CU:276:VAL:HB	2.18	0.44
6:CE:285:LEU:O	6:CE:287:LYS:NZ	2.49	0.44
1:C1:447:C:N4	1:C1:448:A:N6	2.64	0.44
1:C1:1070:U:H2'	1:C1:1071:G:C8	2.52	0.44
2:C2:205:G:N3	4:CB:240:ASN:ND2	2.63	0.44
6:CE:267:ASP:OD1	6:CE:267:ASP:N	2.49	0.44
9:CM:241:ILE:HD12	9:CM:241:ILE:H	1.83	0.44
11:CU:200:LEU:O	11:CU:204:GLN:N	2.50	0.44
12:LC:151:LEU:HD23	12:LC:256:VAL:HG22	1.99	0.44
17:LN:114:ARG:HG2	17:LN:137:PRO:HG3	2.00	0.44
18:LO:179:GLN:HA	18:LO:182:GLU:HG3	1.98	0.44
2:C2:75:G:H2'	2:C2:76:C:C6	2.53	0.44
6:CE:165:PHE:HB2	6:CE:262:ILE:HG12	2.00	0.44
14:LG:98:ASN:HA	14:LG:101:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:966:U:H2'	1:C1:967:U:H6	1.83	0.44
2:C2:8:C:H2'	2:C2:9:A:H8	1.82	0.44
2:C2:23:U:H5"	24:LY:12:ARG:HG3	2.00	0.44
5:CC:367:ARG:HH22	5:CC:385:THR:HA	1.83	0.44
8:CJ:130:ARG:HD3	8:CJ:131:TYR:CZ	2.53	0.44
10:CR:132:PRO:HG2	15:LL:106:GLU:HB3	2.00	0.44
1:C1:522:G:H2'	1:C1:523:A:H8	1.83	0.44
1:C1:979:A:H2'	1:C1:980:G:C8	2.53	0.44
1:C1:1292:G:H2'	1:C1:1293:G:C8	2.52	0.44
1:C1:3192:C:H2'	1:C1:3193:G:H8	1.82	0.44
7:CI:218:VAL:HG22	7:CI:231:ALA:HB2	2.00	0.44
8:CJ:84:GLN:HG3	8:CJ:121:TYR:HE1	1.83	0.44
9:CM:190:LEU:HA	9:CM:193:GLU:HB2	1.99	0.44
18:LO:142:ARG:HA	18:LO:145:HIS:HB2	2.00	0.44
22:LT:104:ASP:HA	22:LT:107:ARG:HG2	2.00	0.44
12:LC:49:GLN:HE21	12:LC:49:GLN:HB3	1.64	0.43
22:LT:42:ILE:O	22:LT:59:GLY:HA2	2.18	0.43
5:CC:356:PRO:HG3	5:CC:384:PRO:HB2	2.00	0.43
7:CI:234:GLU:HB2	7:CI:273:PHE:CZ	2.53	0.43
7:CI:251:TYR:OH	9:CM:53:ARG:NH1	2.51	0.43
1:C1:29:C:H4'	1:C1:62:A:H4'	1.99	0.43
1:C1:423:U:H2'	1:C1:424:G:H8	1.82	0.43
4:CB:80:PRO:HD2	4:CB:181:PRO:HD3	1.99	0.43
8:CJ:191:SER:N	8:CJ:194:GLY:O	2.50	0.43
16:LM:11:TRP:HE1	21:LS:151:PRO:HB2	1.83	0.43
4:CB:117:PRO:HA	4:CB:121:ARG:HB3	2.00	0.43
6:CE:539:VAL:HG22	6:CE:550:PRO:HG3	2.01	0.43
9:LF:113:ARG:HB3	9:LF:210:PRO:HG3	2.01	0.43
18:LO:194:LYS:H	18:LO:194:LYS:HD3	1.82	0.43
1:C1:350:G:N2	1:C1:353:A:OP2	2.40	0.43
2:C2:148:G:H2'	2:C2:149:A:C8	2.54	0.43
5:CC:148:ARG:HE	11:CU:202:ARG:HH22	1.66	0.43
8:CJ:34:ARG:HH21	8:CJ:35:LYS:HG3	1.84	0.43
12:LC:344:VAL:HG11	9:LF:62:ARG:HH11	1.84	0.43
9:LF:173:ALA:O	9:LF:177:GLU:HG3	2.18	0.43
1:C1:231:A:H2'	1:C1:232:G:H8	1.84	0.43
1:C1:340:C:O2	1:C1:344:A:O2'	2.35	0.43
1:C1:581:G:H1'	13:LE:37:LYS:HG3	1.99	0.43
5:CC:184:PRO:HA	5:CC:197:ARG:HH12	1.83	0.43
7:CI:197:GLY:HA3	9:CM:58:VAL:HG13	1.98	0.43
8:CJ:99:ASP:OD1	8:CJ:99:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LF:189:ASP:OD1	9:LF:189:ASP:N	2.51	0.43
18:LO:79:SER:HB2	18:LO:106:VAL:HB	2.01	0.43
1:C1:363:G:N1	1:C1:366:A:OP2	2.41	0.43
1:C1:765:G:H2'	20:LQ:97:ARG:HH11	1.84	0.43
1:C1:1344:G:H2'	1:C1:1345:A:C8	2.53	0.43
8:CJ:187:LYS:HB3	8:CJ:187:LYS:HE3	1.89	0.43
16:LM:31:VAL:HG11	16:LM:54:ARG:NH2	2.34	0.43
1:C1:278:U:O2'	17:LN:179:ARG:O	2.35	0.43
1:C1:532:C:H42	1:C1:540:A:N6	2.16	0.43
1:C1:366:A:HO2'	1:C1:368:G:H8	1.65	0.43
1:C1:574:G:H2'	1:C1:575:A:H8	1.84	0.43
1:C1:910:A:OP1	12:LC:62:SER:OG	2.26	0.43
3:CA:177:ASP:OD1	3:CA:177:ASP:N	2.51	0.43
4:CB:61:PRO:HD2	4:CB:286:PRO:HG3	2.00	0.43
4:CB:169:LYS:HG2	4:CB:173:LYS:HB2	1.99	0.43
4:CB:259:ILE:O	4:CB:263:ILE:HG13	2.19	0.43
9:CM:162:VAL:HG23	9:CM:165:GLN:NE2	2.34	0.43
11:CU:198:THR:O	11:CU:202:ARG:HD3	2.19	0.43
18:LO:193:PRO:HA	18:LO:196:SER:OG	2.18	0.43
1:C1:1096:U:H2'	1:C1:1097:G:C8	2.54	0.43
5:CC:175:ILE:HG12	11:CU:274:GLU:OE2	2.19	0.43
10:CR:216:ASN:ND2	10:CR:218:TYR:O	2.52	0.43
14:LG:111:ARG:O	14:LG:115:GLU:HG2	2.19	0.43
18:LO:130:ARG:HD2	18:LO:130:ARG:HA	1.77	0.43
1:C1:243:G:N2	10:CR:191:GLU:OE1	2.52	0.42
2:C2:50:C:OP2	2:C2:51:G:N2	2.47	0.42
3:CA:279:HIS:O	3:CA:283:MET:HG2	2.19	0.42
5:CC:406:ARG:O	5:CC:410:LEU:HD12	2.18	0.42
6:CE:152:LEU:HG	6:CE:317:TYR:HD1	1.84	0.42
9:CM:89:LEU:HD21	9:CM:122:PHE:HB3	2.01	0.42
12:LC:317:LYS:HB2	12:LC:325:ILE:HG13	2.00	0.42
14:LG:206:VAL:HG23	14:LG:211:LYS:HG2	2.01	0.42
8:CJ:245:LEU:HD23	8:CJ:245:LEU:HA	1.89	0.42
21:LS:25:TYR:HB2	21:LS:45:LEU:HD21	1.99	0.42
7:CI:295:ARG:HA	7:CI:296:PRO:HD3	1.87	0.42
8:CJ:72:LEU:HD12	8:CJ:72:LEU:HA	1.92	0.42
12:LC:335:THR:HA	12:LC:338:LYS:HB3	2.02	0.42
18:LO:13:LYS:O	21:LS:169:ARG:NH2	2.43	0.42
1:C1:574:G:H2'	1:C1:575:A:C8	2.54	0.42
1:C1:942:C:H41	11:CU:303:ARG:HH22	1.67	0.42
1:C1:1306:C:H5'	21:LS:2:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CE:167:ILE:HD13	6:CE:206:LEU:HD21	2.01	0.42
11:CU:199:ALA:HA	11:CU:202:ARG:HD3	2.01	0.42
9:LF:174:ILE:H	9:LF:174:ILE:HG13	1.65	0.42
2:C2:48:A:H61	2:C2:54:A:N6	2.17	0.42
3:CA:116:TYR:HB2	3:CA:243:ILE:HD11	2.02	0.42
5:CC:155:ASP:HA	5:CC:156:PRO:HD3	1.89	0.42
5:CC:402:GLU:O	5:CC:405:GLU:HB2	2.19	0.42
8:CJ:134:PHE:HE1	8:CJ:241:VAL:HG22	1.84	0.42
9:LF:52:LYS:O	9:LF:55:GLU:HB2	2.18	0.42
1:C1:497:U:H2'	1:C1:498:C:C6	2.54	0.42
6:CE:278:MET:HG2	6:CE:306:LEU:HD11	2.01	0.42
14:LG:85:LEU:HD12	14:LG:183:ILE:HD12	2.02	0.42
17:LN:44:ARG:NH2	17:LN:47:LYS:HG2	2.35	0.42
1:C1:493:C:O5'	13:LE:44:ARG:NH1	2.52	0.42
1:C1:618:A:H2'	1:C1:619:G:H8	1.84	0.42
9:LF:138:PRO:HA	9:LF:234:LEU:HD13	2.02	0.42
19:LP:57:ALA:HA	19:LP:83:TRP:CD1	2.55	0.42
21:LS:77:ILE:HG12	21:LS:126:VAL:HG13	2.01	0.42
22:LT:114:GLU:O	22:LT:118:LYS:HG2	2.19	0.42
7:CI:191:ILE:HG23	7:CI:231:ALA:HB3	2.01	0.42
18:LO:193:PRO:O	18:LO:197:GLU:HG3	2.19	0.42
1:C1:614:C:H2'	1:C1:615:A:C8	2.55	0.42
1:C1:2313:U:H2'	1:C1:2314:A:C8	2.55	0.42
3:CA:122:THR:OG1	3:CA:125:GLU:OE1	2.29	0.42
8:CJ:40:LYS:HE3	8:CJ:75:GLU:HG3	2.01	0.42
8:CJ:367:PHE:HA	8:CJ:370:PHE:HD2	1.84	0.42
12:LC:362:LEU:HG	21:LS:64:ILE:HG23	2.02	0.42
14:LG:78:ILE:HD11	17:LN:18:VAL:HG13	2.02	0.42
14:LG:220:ALA:O	14:LG:224:GLY:N	2.53	0.42
1:C1:123:A:OP1	14:LG:108:LYS:NZ	2.42	0.42
4:CB:23:THR:HG22	4:CB:293:ILE:HD12	2.01	0.42
8:CJ:26:LEU:HD23	8:CJ:33:PHE:HD1	1.84	0.42
8:CJ:102:ASN:OD1	8:CJ:105:ARG:NH2	2.52	0.42
16:LM:70:PRO:HD3	16:LM:88:TYR:CD2	2.54	0.42
1:C1:434:G:H2'	1:C1:435:C:C6	2.55	0.41
1:C1:487:C:H2'	1:C1:488:A:H8	1.85	0.41
1:C1:983:A:N1	1:C1:1032:U:O2'	2.53	0.41
1:C1:1087:C:H2'	1:C1:1088:G:C8	2.55	0.41
1:C1:1302:C:H2'	1:C1:1303:G:C8	2.55	0.41
1:C1:3117:C:OP2	19:LP:159:LYS:NZ	2.45	0.41
8:CJ:34:ARG:HH21	8:CJ:35:LYS:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LL:79:GLU:OE1	15:LL:101:ARG:NH2	2.53	0.41
24:LY:130:LYS:HA	24:LY:130:LYS:HD3	1.83	0.41
1:C1:945:G:H2'	1:C1:946:A:H8	1.85	0.41
1:C1:1046:A:N1	1:C1:1074:C:C4	2.89	0.41
2:C2:8:C:H2'	2:C2:9:A:C8	2.55	0.41
2:C2:229:U:H2'	2:C2:230:C:C6	2.55	0.41
7:CI:197:GLY:HA2	9:CM:61:TYR:CD2	2.55	0.41
9:CM:51:PHE:HB3	23:LX:31:VAL:HG21	2.02	0.41
9:CM:184:ILE:HD11	9:CM:193:GLU:HG3	2.01	0.41
20:LQ:90:VAL:O	20:LQ:114:VAL:HA	2.20	0.41
1:C1:194:G:H2'	1:C1:195:G:H8	1.86	0.41
1:C1:490:C:H2'	1:C1:491:A:C8	2.55	0.41
1:C1:944:G:H2'	1:C1:945:G:C8	2.55	0.41
2:C2:213:A:OP2	4:CB:144:ARG:NH2	2.50	0.41
6:CE:223:ARG:NE	6:CE:246:ASP:OD2	2.51	0.41
8:CJ:171:LEU:HB3	8:CJ:238:LEU:HD12	2.01	0.41
15:LL:113:VAL:O	15:LL:117:LYS:HG3	2.20	0.41
24:LY:30:MET:HE3	24:LY:100:PRO:HG3	2.01	0.41
3:CA:138:PRO:HB3	3:CA:178:HIS:CE1	2.55	0.41
5:CC:312:ARG:HD2	5:CC:312:ARG:HA	1.89	0.41
5:CC:403:ARG:HG2	8:CJ:150:LEU:HD22	2.02	0.41
8:CJ:34:ARG:HD3	8:CJ:226:ILE:HG22	2.03	0.41
8:CJ:127:ILE:HG22	8:CJ:233:PHE:HE1	1.85	0.41
22:LT:45:ASN:H	22:LT:95:HIS:CE1	2.38	0.41
1:C1:1098:G:O6	1:C1:1123:C:N3	2.53	0.41
1:C1:1139:G:O2'	1:C1:1151:A:N3	2.45	0.41
2:C2:298:G:H5"	7:CI:291:ARG:HH22	1.85	0.41
3:CA:37:LEU:HB3	3:CA:89:VAL:HG12	2.03	0.41
7:CI:305:LYS:HD2	7:CI:305:LYS:HA	1.89	0.41
10:CR:45:LEU:HD13	15:LL:43:ALA:HB2	2.03	0.41
1:C1:968:U:O3'	9:LF:127:LYS:NZ	2.43	0.41
1:C1:1053:U:H2'	1:C1:1054:G:H8	1.85	0.41
1:C1:1360:U:H2'	1:C1:1361:G:H8	1.86	0.41
5:CC:411:TYR:CE1	8:CJ:41:GLY:HA2	2.54	0.41
9:CM:76:LYS:HB3	9:CM:76:LYS:HE2	1.89	0.41
10:CR:40:ASN:HB3	10:CR:43:GLU:HB2	2.02	0.41
12:LC:171:LYS:HE2	12:LC:171:LYS:HB3	1.89	0.41
9:LF:94:ARG:O	9:LF:118:ASN:N	2.54	0.41
17:LN:47:LYS:HA	17:LN:47:LYS:HD2	1.82	0.41
1:C1:72:C:N3	1:C1:74:G:C5	2.89	0.41
1:C1:159:G:OP2	10:CR:227:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CB:104:PRO:HG2	4:CB:208:PRO:O	2.21	0.41
6:CE:292:THR:HB	6:CE:311:LEU:HG	2.02	0.41
7:CI:188:VAL:HG22	7:CI:234:GLU:HG3	2.03	0.41
8:CJ:156:SER:HB2	8:CJ:165:ILE:HD12	2.03	0.41
9:CM:141:ALA:HB1	9:CM:237:ARG:HH22	1.86	0.41
18:LO:23:ILE:HD13	18:LO:122:VAL:HG11	2.01	0.41
18:LO:144:SER:HB3	18:LO:149:TRP:HB2	2.02	0.41
1:C1:436:G:H5"	13:LE:26:LYS:HE3	2.03	0.41
1:C1:727:C:H2'	1:C1:728:A:H8	1.85	0.41
1:C1:3159:A:N6	1:C1:3199:A:H2'	2.36	0.41
3:CA:236:PRO:HB2	3:CA:238:PHE:CE1	2.55	0.41
5:CC:175:ILE:HG23	11:CU:274:GLU:HG3	2.01	0.41
22:LT:131:GLN:HA	22:LT:132:PRO:HD3	1.81	0.41
1:C1:158:U:H2'	1:C1:159:G:C8	2.55	0.41
1:C1:643:A:H2'	1:C1:644:A:C8	2.56	0.41
1:C1:662:C:H2'	1:C1:663:G:O4'	2.21	0.41
1:C1:2319:A:H2'	1:C1:2320:A:H8	1.85	0.41
3:CA:131:ASN:HA	3:CA:234:ILE:HG23	2.02	0.41
3:CA:137:ARG:HE	3:CA:137:ARG:HB3	1.37	0.41
8:CJ:35:LYS:O	8:CJ:38:ILE:HG22	2.20	0.41
8:CJ:190:LEU:HA	8:CJ:195:ILE:HA	2.03	0.41
9:CM:202:LYS:HB2	9:CM:202:LYS:HE2	1.89	0.41
12:LC:154:ASP:N	12:LC:154:ASP:OD1	2.54	0.41
9:LF:92:VAL:O	9:LF:120:GLY:HA2	2.21	0.41
18:LO:10:ILE:HG21	18:LO:20:LEU:HD11	2.03	0.41
22:LT:48:VAL:HG12	22:LT:50:LYS:H	1.86	0.41
24:LY:71:SER:HB3	24:LY:80:HIS:HB2	2.01	0.41
1:C1:533:C:C2	1:C1:539:G:N1	2.89	0.41
4:CB:104:PRO:CD	4:CB:208:PRO:HB3	2.50	0.41
4:CB:130:ILE:O	4:CB:134:LYS:HG3	2.21	0.41
7:CI:301:GLN:CD	7:CI:301:GLN:H	2.23	0.41
8:CJ:267:GLU:HB3	8:CJ:380:ARG:NH2	2.36	0.41
21:LS:146:LYS:HA	21:LS:146:LYS:HD2	1.89	0.41
24:LY:75:LEU:HD23	24:LY:75:LEU:HA	1.79	0.41
1:C1:753:U:H2'	1:C1:754:G:C8	2.57	0.40
1:C1:1090:C:H2'	1:C1:1091:A:H8	1.86	0.40
2:C2:216:A:H2	7:CI:263:VAL:HG22	1.84	0.40
5:CC:241:LYS:HE2	5:CC:241:LYS:HB3	1.81	0.40
5:CC:243:GLN:HG3	5:CC:247:ILE:HD11	2.03	0.40
9:LF:239:GLU:H	9:LF:239:GLU:HG2	1.66	0.40
22:LT:79:ARG:HA	22:LT:79:ARG:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:745:U:O2	1:C1:749:C:N3	2.54	0.40
3:CA:173:LYS:HA	3:CA:173:LYS:HD3	1.79	0.40
4:CB:52:ASP:O	4:CB:56:THR:OG1	2.34	0.40
5:CC:126:ARG:HA	5:CC:126:ARG:HD2	1.99	0.40
6:CE:504:ASN:HB3	6:CE:507:LEU:HB2	2.02	0.40
17:LN:183:THR:HG22	17:LN:187:ARG:HB2	2.03	0.40
3:CA:190:TRP:HE3	3:CA:192:ARG:HH22	1.68	0.40
5:CC:180:TYR:HA	5:CC:183:TYR:HD1	1.86	0.40
8:CJ:17:MET:HG2	8:CJ:21:GLN:HB2	2.03	0.40
8:CJ:196:TYR:CD1	8:CJ:209:LEU:HD13	2.56	0.40
14:LG:146:ILE:HG23	14:LG:178:ILE:HD13	2.03	0.40
1:C1:110:G:OP2	15:LL:73:ARG:NH2	2.35	0.40
1:C1:194:G:OP1	1:C1:213:G:O2'	2.32	0.40
1:C1:411:G:H2'	1:C1:412:G:C8	2.57	0.40
1:C1:633:A:H3'	1:C1:634:A:H8	1.86	0.40
1:C1:1101:C:H2'	1:C1:1102:A:H8	1.85	0.40
3:CA:146:PHE:HB3	3:CA:156:LYS:HD2	2.03	0.40
6:CE:328:THR:HB	6:CE:447:ARG:HH22	1.86	0.40
8:CJ:51:ARG:O	8:CJ:51:ARG:NE	2.54	0.40
8:CJ:183:HIS:ND1	8:CJ:389:ALA:O	2.55	0.40
8:CJ:367:PHE:HA	8:CJ:370:PHE:CD2	2.56	0.40
8:CJ:419:ILE:HD13	8:CJ:419:ILE:HA	1.92	0.40
18:LO:185:LYS:HE2	18:LO:185:LYS:HB2	1.96	0.40
1:C1:1045:G:H1'	1:C1:1048:G:H1'	2.04	0.40
8:CJ:454:ILE:HG22	8:CJ:456:VAL:HG13	2.04	0.40
9:CM:187:ILE:O	9:CM:190:LEU:HD12	2.22	0.40
12:LC:146:VAL:HA	12:LC:147:PRO:HD3	1.95	0.40
14:LG:153:LEU:HB3	14:LG:203:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

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	254/316 (80%)	238 (94%)	16 (6%)	0	100	100
4	CB	265/391 (68%)	252 (95%)	12 (4%)	1 (0%)	34	72
5	CC	250/801 (31%)	241 (96%)	9 (4%)	0	100	100
6	CE	459/598 (77%)	440 (96%)	19 (4%)	0	100	100
7	CI	144/414 (35%)	131 (91%)	13 (9%)	0	100	100
8	CJ	374/679 (55%)	359 (96%)	15 (4%)	0	100	100
9	CM	183/249 (74%)	175 (96%)	8 (4%)	0	100	100
9	LF	238/249 (96%)	229 (96%)	9 (4%)	0	100	100
10	CR	159/237 (67%)	152 (96%)	6 (4%)	1 (1%)	25	64
11	CU	114/451 (25%)	113 (99%)	1 (1%)	0	100	100
12	LC	360/365 (99%)	351 (98%)	9 (2%)	0	100	100
13	LE	166/200 (83%)	152 (92%)	13 (8%)	1 (1%)	25	64
14	LG	181/262 (69%)	178 (98%)	3 (2%)	0	100	100
15	LL	115/213 (54%)	113 (98%)	2 (2%)	0	100	100
16	LM	126/142 (89%)	120 (95%)	5 (4%)	1 (1%)	19	57
17	LN	179/203 (88%)	175 (98%)	4 (2%)	0	100	100
18	LO	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
19	LP	150/187 (80%)	148 (99%)	2 (1%)	0	100	100
20	LQ	127/213 (60%)	122 (96%)	5 (4%)	0	100	100
21	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
22	LT	124/160 (78%)	115 (93%)	7 (6%)	2 (2%)	9	40
23	LX	20/156 (13%)	20 (100%)	0	0	100	100
24	LY	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
25	Le	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
26	Lf	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
27	Lh	119/935 (13%)	116 (98%)	3 (2%)	0	100	100
28	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
29	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
30	Cc	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
31	Cd	334/436 (77%)	317 (95%)	17 (5%)	0	100	100
32	Ce	192/336 (57%)	188 (98%)	4 (2%)	0	100	100
All	All	5764/9436 (61%)	5534 (96%)	224 (4%)	6 (0%)	54	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	104	PRO
10	CR	130	ALA
16	LM	22	LEU
13	LE	86	PRO
22	LT	44	VAL
22	LT	81	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	CA	231/276 (84%)	218 (94%)	13 (6%)	21 56
4	CB	231/329 (70%)	223 (96%)	8 (4%)	36 71
5	CC	240/710 (34%)	231 (96%)	9 (4%)	33 69
6	CE	398/517 (77%)	382 (96%)	16 (4%)	31 68
7	CI	121/336 (36%)	112 (93%)	9 (7%)	13 44
8	CJ	332/579 (57%)	309 (93%)	23 (7%)	15 48
9	CM	161/215 (75%)	144 (89%)	17 (11%)	6 26
9	LF	206/215 (96%)	197 (96%)	9 (4%)	28 65
10	CR	144/206 (70%)	139 (96%)	5 (4%)	36 71
11	CU	99/376 (26%)	86 (87%)	13 (13%)	4 18
12	LC	283/285 (99%)	272 (96%)	11 (4%)	32 69
13	LE	143/166 (86%)	136 (95%)	7 (5%)	25 61
14	LG	158/222 (71%)	157 (99%)	1 (1%)	86 95
15	LL	99/176 (56%)	97 (98%)	2 (2%)	55 83
16	LM	108/117 (92%)	99 (92%)	9 (8%)	11 39
17	LN	164/180 (91%)	154 (94%)	10 (6%)	18 53
18	LO	163/163 (100%)	148 (91%)	15 (9%)	9 34
19	LP	125/152 (82%)	119 (95%)	6 (5%)	25 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	LQ	110/178 (62%)	105 (96%)	5 (4%)	27 64
21	LS	154/154 (100%)	148 (96%)	6 (4%)	32 69
22	LT	109/135 (81%)	99 (91%)	10 (9%)	9 34
23	LX	12/129 (9%)	12 (100%)	0	100 100
24	LY	117/119 (98%)	112 (96%)	5 (4%)	29 66
25	Le	114/114 (100%)	111 (97%)	3 (3%)	46 78
26	Lf	89/90 (99%)	88 (99%)	1 (1%)	73 90
27	Lh	108/781 (14%)	104 (96%)	4 (4%)	34 70
28	Li	75/93 (81%)	71 (95%)	4 (5%)	22 58
29	Lj	61/78 (78%)	60 (98%)	1 (2%)	62 86
30	Cc	204/244 (84%)	202 (99%)	2 (1%)	76 91
31	Cd	291/367 (79%)	284 (98%)	7 (2%)	49 79
32	Ce	173/297 (58%)	165 (95%)	8 (5%)	27 64
All	All	5023/7999 (63%)	4784 (95%)	239 (5%)	29 62

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	46	TYR
3	CA	47	ARG
3	CA	49	ARG
3	CA	65	ASP
3	CA	80	LEU
3	CA	133	LEU
3	CA	134	LYS
3	CA	141	SER
3	CA	147	GLU
3	CA	167	GLN
3	CA	178	HIS
3	CA	244	ILE
3	CA	312	ARG
4	CB	42	ARG
4	CB	104	PRO
4	CB	127	VAL
4	CB	185	MET
4	CB	264	ARG
4	CB	275	TRP

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Mol	Chain	Res	Type
4	CB	276	GLN
4	CB	294	TYR
5	CC	118	LEU
5	CC	119	GLU
5	CC	152	ASP
5	CC	161	ASP
5	CC	193	LYS
5	CC	257	ASP
5	CC	373	MET
5	CC	378	ARG
5	CC	408	MET
6	CE	116	LEU
6	CE	119	SER
6	CE	156	LYS
6	CE	172	MET
6	CE	222	ASN
6	CE	256	LYS
6	CE	294	LEU
6	CE	299	GLN
6	CE	434	PRO
6	CE	447	ARG
6	CE	457	ARG
6	CE	472	HIS
6	CE	477	LYS
6	CE	489	LYS
6	CE	533	VAL
6	CE	583	TYR
7	CI	208	SER
7	CI	261	LYS
7	CI	277	ASN
7	CI	279	ARG
7	CI	292	GLN
7	CI	301	GLN
7	CI	308	LYS
7	CI	321	LYS
7	CI	327	PHE
8	CJ	14	ARG
8	CJ	34	ARG
8	CJ	40	LYS
8	CJ	83	GLU
8	CJ	85	LYS
8	CJ	99	ASP

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Mol	Chain	Res	Type
8	CJ	109	ASN
8	CJ	144	CYS
8	CJ	153	ASN
8	CJ	164	MET
8	CJ	175	PHE
8	CJ	196	TYR
8	CJ	213	LYS
8	CJ	214	PHE
8	CJ	217	ARG
8	CJ	224	PHE
8	CJ	233	PHE
8	CJ	252	LYS
8	CJ	256	LYS
8	CJ	259	GLN
8	CJ	276	LEU
8	CJ	394	ARG
8	CJ	450	TYR
9	CM	53	ARG
9	CM	60	GLU
9	CM	64	GLN
9	CM	66	ARG
9	CM	94	ARG
9	CM	95	ILE
9	CM	96	LYS
9	CM	122	PHE
9	CM	148	LYS
9	CM	161	LYS
9	CM	163	ASN
9	CM	182	TYR
9	CM	190	LEU
9	CM	195	PHE
9	CM	202	LYS
9	CM	211	PHE
9	CM	237	ARG
10	CR	21	ASN
10	CR	127	GLU
10	CR	134	GLN
10	CR	211	ARG
10	CR	227	ARG
11	CU	196	LEU
11	CU	205	LEU
11	CU	210	LYS

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Mol	Chain	Res	Type
11	CU	224	LYS
11	CU	226	THR
11	CU	227	GLU
11	CU	256	SER
11	CU	259	ARG
11	CU	260	LYS
11	CU	267	ARG
11	CU	276	VAL
11	CU	277	ARG
11	CU	297	LYS
12	LC	13	ASP
12	LC	25	LYS
12	LC	94	MET
12	LC	100	MET
12	LC	121	PHE
12	LC	202	ARG
12	LC	273	LYS
12	LC	301	ARG
12	LC	341	LEU
12	LC	347	GLU
12	LC	357	SER
13	LE	25	GLN
13	LE	41	LYS
13	LE	50	LYS
13	LE	126	LYS
13	LE	158	ARG
13	LE	169	LEU
13	LE	183	LEU
9	LF	38	LYS
9	LF	77	GLN
9	LF	88	LYS
9	LF	106	ARG
9	LF	113	ARG
9	LF	127	LYS
9	LF	189	ASP
9	LF	223	ARG
9	LF	246	ARG
14	LG	52	MET
15	LL	23	ARG
15	LL	68	ARG
16	LM	11	TRP
16	LM	12	ARG

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Mol	Chain	Res	Type
16	LM	15	GLU
16	LM	20	LEU
16	LM	77	ARG
16	LM	91	ASP
16	LM	108	ARG
16	LM	121	MET
16	LM	128	ARG
17	LN	5	LYS
17	LN	7	LEU
17	LN	9	GLU
17	LN	27	CYS
17	LN	47	LYS
17	LN	62	TYR
17	LN	67	ARG
17	LN	94	TYR
17	LN	167	THR
17	LN	184	ARG
18	LO	6	SER
18	LO	48	PHE
18	LO	50	ARG
18	LO	69	ARG
18	LO	80	ARG
18	LO	115	ASP
18	LO	116	LYS
18	LO	136	LYS
18	LO	145	HIS
18	LO	157	ARG
18	LO	158	LEU
18	LO	169	TYR
18	LO	172	ARG
18	LO	194	LYS
18	LO	197	GLU
19	LP	49	GLN
19	LP	55	LYS
19	LP	83	TRP
19	LP	86	LYS
19	LP	116	HIS
19	LP	161	GLU
20	LQ	50	ASP
20	LQ	92	LEU
20	LQ	100	LYS
20	LQ	113	THR

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Mol	Chain	Res	Type
20	LQ	119	ARG
21	LS	1	MET
21	LS	79	LEU
21	LS	84	ARG
21	LS	129	LEU
21	LS	133	GLU
21	LS	144	VAL
22	LT	35	ARG
22	LT	79	ARG
22	LT	82	HIS
22	LT	90	ASN
22	LT	92	ARG
22	LT	97	LYS
22	LT	104	ASP
22	LT	114	GLU
22	LT	146	ASN
22	LT	147	LYS
24	LY	15	ARG
24	LY	45	ARG
24	LY	73	TYR
24	LY	75	LEU
24	LY	114	ARG
25	Le	35	LYS
25	Le	42	ARG
25	Le	126	LYS
26	Lf	7	HIS
27	Lh	6	LYS
27	Lh	18	GLU
27	Lh	74	PHE
27	Lh	104	ARG
28	Li	44	LYS
28	Li	52	LEU
28	Li	64	ARG
28	Li	65	ARG
29	Lj	84	LYS
30	Cc	203	ASP
30	Cc	244	ARG
31	Cd	37	ARG
31	Cd	45	ARG
31	Cd	93	LYS
31	Cd	94	ARG
31	Cd	260	GLN

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Mol	Chain	Res	Type
31	Cd	326	LYS
31	Cd	327	SER
32	Ce	29	ARG
32	Ce	43	CYS
32	Ce	77	TRP
32	Ce	96	GLN
32	Ce	110	LYS
32	Ce	143	PRO
32	Ce	167	GLU
32	Ce	175	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
6	CE	222	ASN
9	CM	119	ASN
10	CR	134	GLN
11	CU	218	GLN
11	CU	246	GLN
13	LE	116	GLN
21	LS	74	ASN
21	LS	122	HIS
27	Lh	37	GLN
32	Ce	93	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	1297/3341 (38%)	255 (19%)	10 (0%)
2	C2	254/306 (83%)	59 (23%)	3 (1%)
All	All	1551/3647 (42%)	314 (20%)	13 (0%)

All (314) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	22	G
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A

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Mol	Chain	Res	Type
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	109	A
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	130	U
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	136	C
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	163	U
1	C1	164	G
1	C1	176	U
1	C1	177	U
1	C1	180	G
1	C1	183	U
1	C1	192	A
1	C1	193	C
1	C1	203	C
1	C1	204	A
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	242	U
1	C1	244	U
1	C1	258	C
1	C1	261	G

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Mol	Chain	Res	Type
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	289	A
1	C1	291	G
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	311	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	330	A
1	C1	331	C
1	C1	334	A
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	377	A
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	413	G
1	C1	414	A
1	C1	421	U
1	C1	432	U
1	C1	433	U
1	C1	434	G
1	C1	446	U
1	C1	449	U
1	C1	450	C
1	C1	457	U
1	C1	458	C
1	C1	460	C
1	C1	467	G
1	C1	469	A
1	C1	474	G
1	C1	485	G

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Mol	Chain	Res	Type
1	C1	493	C
1	C1	504	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	537	G
1	C1	538	G
1	C1	539	G
1	C1	545	U
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	558	G
1	C1	569	G
1	C1	582	A
1	C1	587	G
1	C1	589	U
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G
1	C1	598	A
1	C1	608	A
1	C1	623	C
1	C1	633	A
1	C1	635	C
1	C1	647	A
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	739	C
1	C1	746	A

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Mol	Chain	Res	Type
1	C1	748	U
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	766	G
1	C1	767	A
1	C1	787	A
1	C1	789	A
1	C1	798	A
1	C1	918	G
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	940	C
1	C1	943	A
1	C1	944	G
1	C1	958	A
1	C1	960	C
1	C1	966	U
1	C1	972	G
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	1039	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1070	U
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G

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Mol	Chain	Res	Type
1	C1	1080	A
1	C1	1085	A
1	C1	1097	G
1	C1	1098	G
1	C1	1099	G
1	C1	1114	C
1	C1	1126	U
1	C1	1130	G
1	C1	1132	A
1	C1	1133	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1160	G
1	C1	1163	U
1	C1	1164	G
1	C1	1172	A
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1292	G
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1368	A
1	C1	1369	G
1	C1	1374	G
1	C1	1381	A
1	C1	1382	G
1	C1	1384	G
1	C1	1400	A
1	C1	1401	A
1	C1	1413	G
1	C1	1419	C

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Mol	Chain	Res	Type
1	C1	1433	C
1	C1	1434	A
1	C1	1435	A
1	C1	2314	A
1	C1	2324	C
1	C1	3126	G
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3144	C
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3181	C
1	C1	3183	C
1	C1	3185	A
1	C1	3186	A
1	C1	3187	G
1	C1	3199	A
1	C1	3200	A
1	C1	3205	C
1	C1	3206	G
1	C1	3208	A
1	C1	3209	U
1	C1	3212	C
1	C1	3214	A
1	C1	3227	C
1	C1	3228	G
1	C1	3232	U
1	C1	3233	C
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	2	A
2	C2	23	U

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Mol	Chain	Res	Type
2	C2	34	U
2	C2	35	C
2	C2	53	A
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	64	U
2	C2	81	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	91	C
2	C2	95	G
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	111	A
2	C2	113	U
2	C2	124	G
2	C2	126	A
2	C2	127	U
2	C2	129	C
2	C2	149	A
2	C2	151	C
2	C2	156	U
2	C2	157	U
2	C2	158	U
2	C2	160	A
2	C2	166	C
2	C2	174	G
2	C2	175	G
2	C2	176	G
2	C2	180	G
2	C2	181	U
2	C2	183	U
2	C2	189	A
2	C2	190	C
2	C2	192	C
2	C2	196	G
2	C2	212	G

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Mol	Chain	Res	Type
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	218	C
2	C2	219	A
2	C2	221	U
2	C2	222	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
2	C2	301	A
2	C2	302	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	432	U
1	C1	510	U
1	C1	519	A
1	C1	538	G
1	C1	1044	A
1	C1	1046	A
1	C1	1159	G
1	C1	3162	A
1	C1	3207	U
2	C2	123	G
2	C2	174	G
2	C2	175	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.