



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 9, 2019 – 07:52 PM EST

PDB ID : 6CB1
EMDB ID: : EMD-7445
Title : Yeast nucleolar pre-60S ribosomal subunit (state 3)
Authors : Sanghai, Z.A.; Miller, L.; Barandun, J.; Hunziker, M.; Chaker-Margot, M.;
Klinge, S.
Deposited on : 2018-02-01
Resolution : 4.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

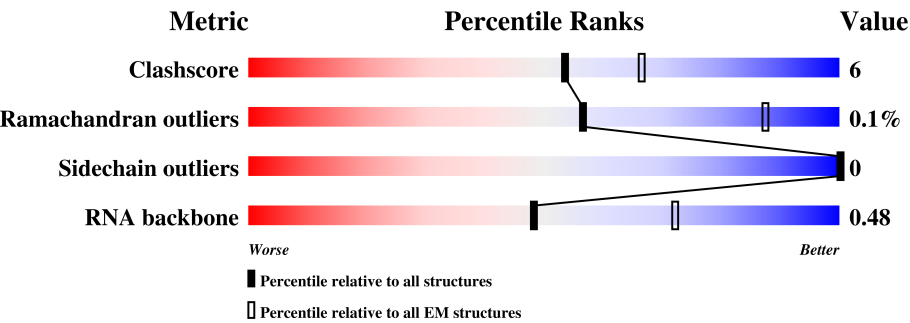
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 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.



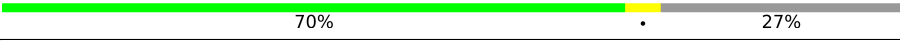















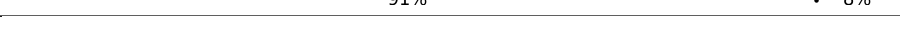
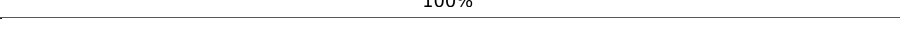
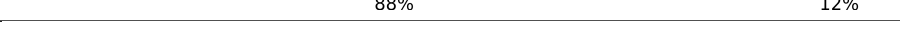
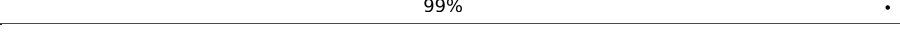

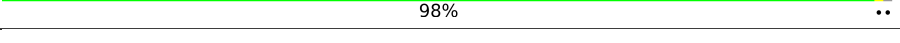


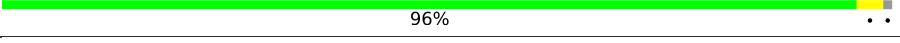
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	3396	21% 15% . 60%
2	2	158	51% 41% 6% .
3	6	232	14% 13% 9% . 62%
4	A	463	78% 7% 15%
5	C	362	85% . 13%
6	D	306	60% . 38%
7	E	176	94% . .
8	F	244	95% . .

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Mol	Chain	Length	Quality of chain
9	G	256	
10	I	295	
11	K	376	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	S	172	
19	X	142	
20	Y	127	
21	Z	136	
22	7	231	
23	b	291	
24	c	105	
25	d	465	
26	e	130	
27	f	107	
28	g	121	
29	h	120	
30	i	100	
31	j	88	
32	k	78	
33	m	102	

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Mol	Chain	Length	Quality of chain
34	n	605	<div><div></div><div>56%</div><div>44%</div></div>
35	o	220	<div><div></div><div>60%</div><div>40%</div></div>
36	p	505	<div><div></div><div>87%</div><div>13%</div></div>
37	s	569	<div><div></div><div>90%</div><div>10%</div></div>
38	t	322	<div><div></div><div>86%</div><div>12%</div></div>
39	x	28	<div><div></div><div>100%</div><div></div></div>
40	z	278	<div><div></div><div>87%</div><div>13%</div></div>

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 69945 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 35S pre-ribosomal RNA miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1370	Total	C	N	O	P	0	0
			29343	13096	5306	9571	1370		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	87	Total	C	N	O	P	0	0
			1838	823	309	619	87		

- Molecule 4 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	394	Total	C	N	O	0	0
			1946	1158	394	394		

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	314	Total	C	N	O	0	0
			1553	925	314	314		

- Molecule 6 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	190	Total	C	N	O	S	0	0
			948	564	190	190	4		

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	170	Total	C	N	O	0	0
			843	503	170	170		

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	242	Total	C	N	O	0	0
			1195	711	242	242		

- Molecule 9 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	187	Total	C	N	O	0	0
			926	552	187	187		

- Molecule 10 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	288	Total	C	N	O	0	0
			1428	852	288	288		

- Molecule 11 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	260	Total	C	N	O	0	0
			1293	773	260	260		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	106	Total	C	N	O	0	0
			525	313	106	106		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	128	Total	C	N	O	0	0
			633	377	128	128		

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	176	Total	C	N	O	0	0
			871	519	176	176		

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	184	Total	C	N	O	0	0
			908	540	184	184		

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	124	Total	C	N	O	0	0
			616	368	124	124		

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	132	Total	C	N	O	0	0
			653	389	132	132		

- Molecule 18 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	171	Total	C	N	O	0	0
			851	509	171	171		

- Molecule 19 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	141	Total	C	N	O	0	0
			700	418	141	141		

- Molecule 20 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	126	Total	C	N	O	0	0
			623	371	126	126		

- Molecule 21 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Z	135	Total	C	N	O	0	0
			667	397	135	135		

- Molecule 22 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	7	156	Total	C	N	O	0	0
			773	461	156	156		

- Molecule 23 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	b	242	Total	C	N	O	0	0
			1201	717	242	242		

- Molecule 24 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	c	97	Total	C	N	O	0	0
			476	282	97	97		

- Molecule 25 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	d	465	Total	C	N	O	0	0
			2288	1358	465	465		

- Molecule 26 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	e	114	Total	C	N	O	0	0
			564	336	114	114		

- Molecule 27 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	f	106	Total	C	N	O	0	0
			522	310	106	106		

- Molecule 28 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	101	Total	C	N	O	0	0
			498	296	101	101		

- Molecule 29 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	119	Total	C	N	O	0	0
			593	355	119	119		

- Molecule 30 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 31 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	72	Total	C	N	O	S	0	0
			357	209	72	72	4		

- Molecule 32 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	k	77	Total	C	N	O	0	0
			382	228	77	77		

- Molecule 33 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 34 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	341	Total	C	N	O	0	0
			1693	1011	341	341		

- Molecule 35 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	o	133	Total	C	N	O	0	0
			656	390	133	133		

- Molecule 36 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	p	437	Total	C	N	O	0	0
			2158	1284	437	437		

- Molecule 37 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	s	512	Total	C	N	O	0	0
			2537	1513	512	512		

- Molecule 38 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	t	282	Total	C	N	O	0	0
			1397	833	282	282		

- Molecule 39 is a protein called BRX1 associated peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	x	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 40 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	z	243	Total	C	N	O	0	0
			1209	723	243	243		

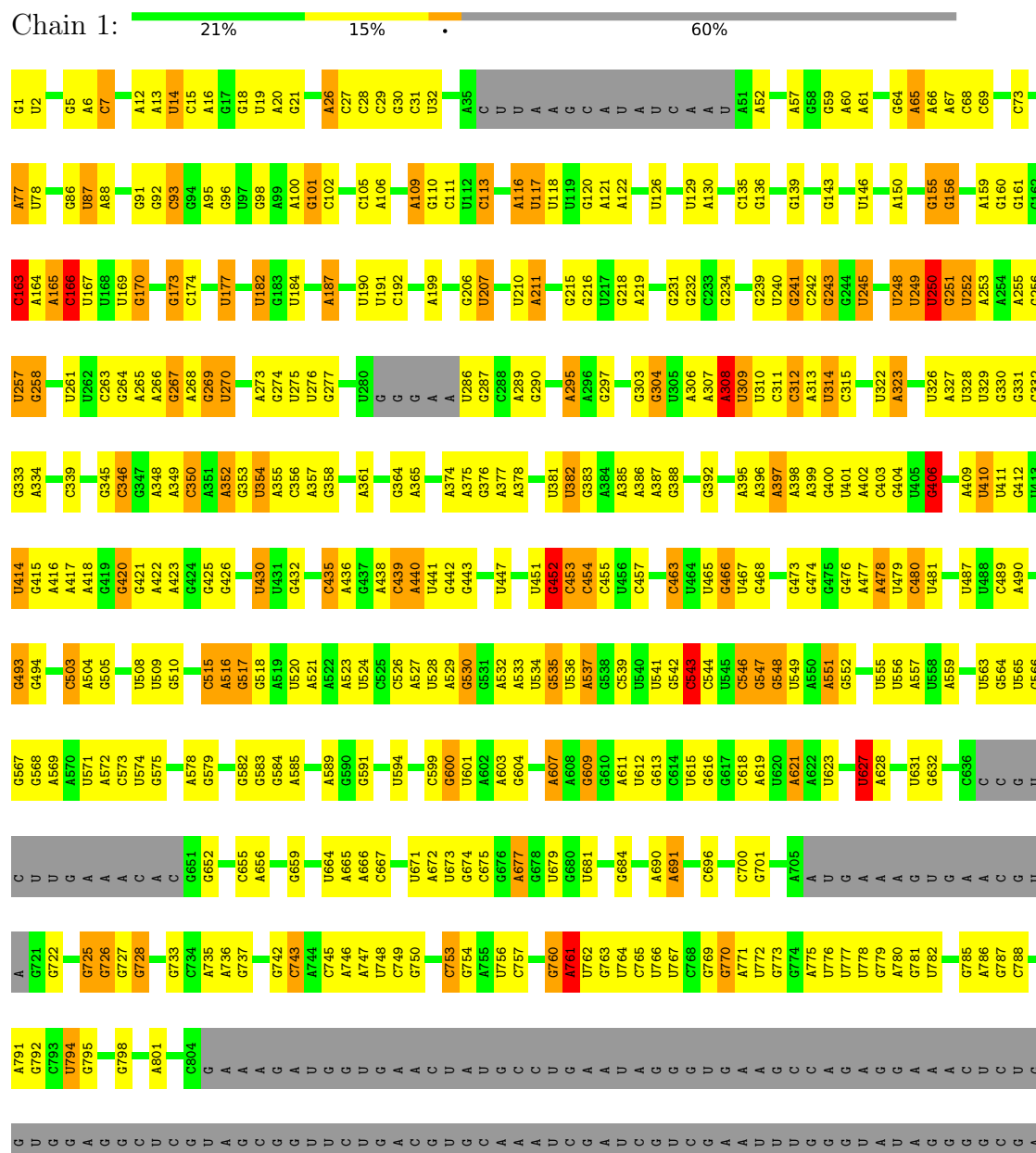
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	j	1	Total	Zn	0
			1	1	
41	D	1	Total	Zn	0
			1	1	

3 Residue-property plots

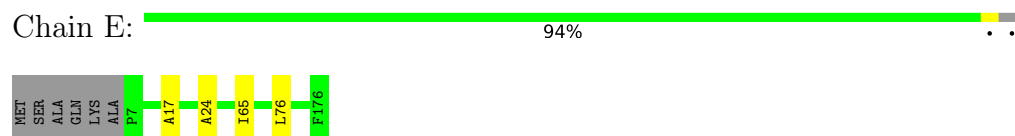
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 35S pre-ribosomal RNA miscRNA

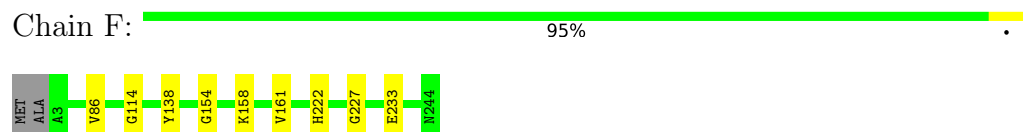




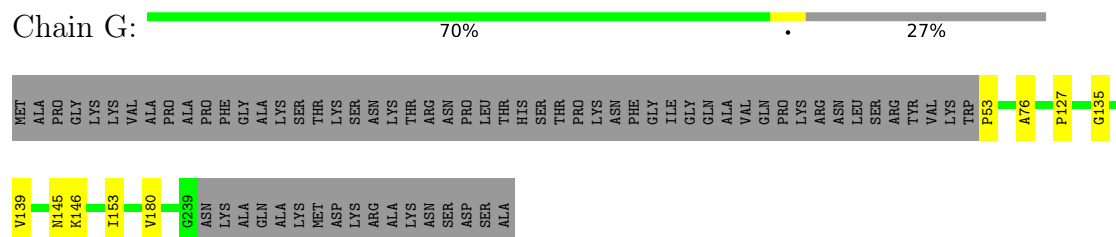

- Molecule 7: 60S ribosomal protein L6-A



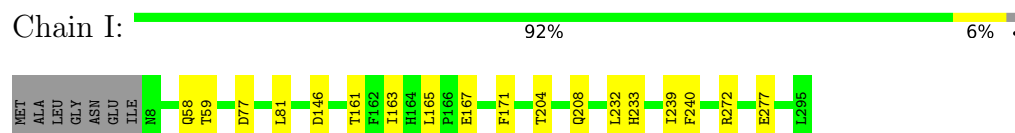
- Molecule 8: 60S ribosomal protein L7-A



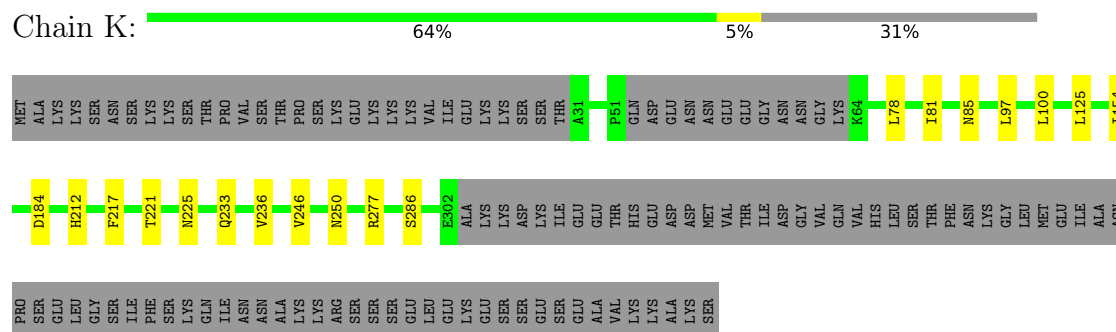
- Molecule 9: 60S ribosomal protein L8-A



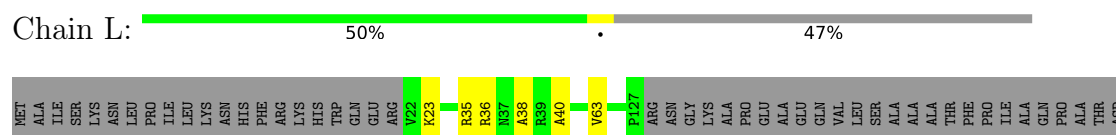
- Molecule 10: Ribosome production factor 1



- Molecule 11: Proteasome-interacting protein CIC1



- Molecule 12: 60S ribosomal protein L13-A




VAL
GLU
ALA
ARG
ALA
VAL
GLN
ASP
ASN
GLY
GLU
SER
ALA
PHE
ARG
THR
LEU
ARG
LEU
ALA
ARG
SER
GLU
LYS
LYS
PHE
ARG
GLY
ILE
ARG
GLU
LYS
ARG
ALA
GLU
GLU
ALA
ALA
GLU
LYS
LYS

- Molecule 13: 60S ribosomal protein L14-A

Chain M:  91% 7%

MET
SER
THR
ASP
SER
ILE
VAL
LYS
ALA
SER
N11
I23
G30
A138

- Molecule 14: 60S ribosomal protein L15-A

Chain N:  83% 14%

MET
G2
R68
GLY
ASN
ARG
LYS
ARG
PRO
VAL
PRO
LYS
GLY
ALA
THR
TVR
GLY
LYS
PRO
THR
ASN
GLN
GLY
VAL
ASN
GLU
LEU
LYS
TVR
G196
D124
Y127
N149
H178
T183
R187
L197
K204

- Molecule 15: 60S ribosomal protein L16-A

Chain O:  88% 8%

MET
SER
Y3
A38
I442
R59
LYS
ALA
THR
PHE
ASN
LYS
THR
ARG
GLY
PRO
PHE
HIS
F73
A83
E106
T136
L194
G198
Y199

- Molecule 16: 60S ribosomal protein L17-A

Chain P:  67% 33%

MET
ALA
ARG
TYR
GLY
ALA
THR
SER
THR
N10
I64
SER
SER
ILE
GLY
ARG
THR
ALA
GLN
GLY
LYS
GLU
PHE
GLY
VAL
THR
R80
R126
ARG
ARG
THR
TYR
ARG
ALA
HIS
GLY
ILE
ARG
ASN
LYS
TYR
E140
A161
GLU
LYS
LYS
VAL
VAL
ARG
LEU
THR
SER
ARG
GLN
ARG
GLY
ARG

ILE
ALA
ALA
GLN
LYS
ILE
ALA
ALA

- Molecule 17: 60S ribosomal protein L18-A

Chain Q:  71% 29%

MET
GLY
ILE
ASP
HIS
THR
SER
LYS
GLN
HIS
LYS
ARG
SER
GLY
H15
S146
ARG
GLU
ALA
VAL
ARG
HIS
PHE
GLY
MET
GLY
PRO
HIS
LYS
GLY
LYS
ALA
PRO
ARG
ILE
LEU
SER
THR
GLY
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ALA
ARG
GLY
ARG
ARG
ARG
LYS
GLY
PHE
LYS
VAL

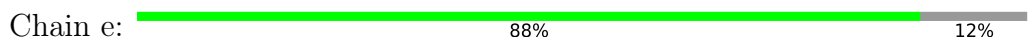
- Molecule 18: 60S ribosomal protein L20-A

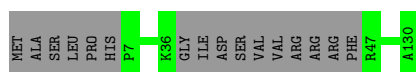
Chain S:  92% 7%

MET
A2
Y7
G11
R12
R13
P22
F25
R28
N62
N74
F75
S83
E93
I129
Y172

- Molecule 19: 60S ribosomal protein L25

Chain X:  89% 11%





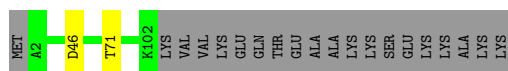
- Molecule 27: 60S ribosomal protein L33-A

Chain f: 99%



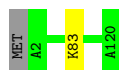
- Molecule 28: 60S ribosomal protein L34-A

Chain g: 82% 17%



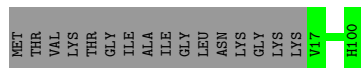
- Molecule 29: 60S ribosomal protein L35-A

Chain h: 98%



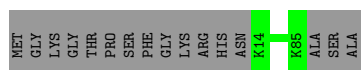
- Molecule 30: 60S ribosomal protein L36-A

Chain i: 84% 16%



- Molecule 31: 60S ribosomal protein L37-A

Chain j: 82% 18%



- Molecule 32: 60S ribosomal protein L38

Chain k: 96%

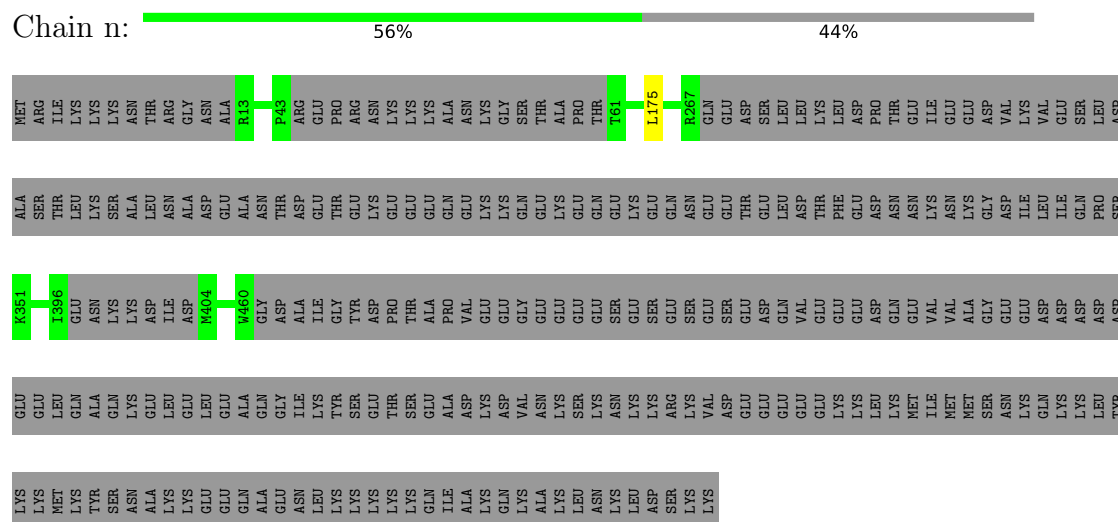


- Molecule 33: rRNA-processing protein EBP2

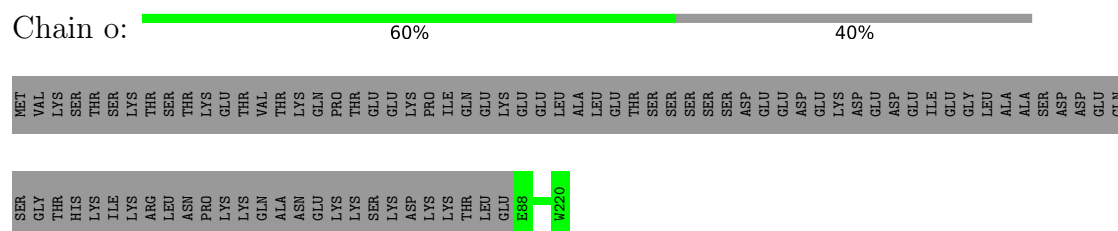
Chain m: 73% 27%



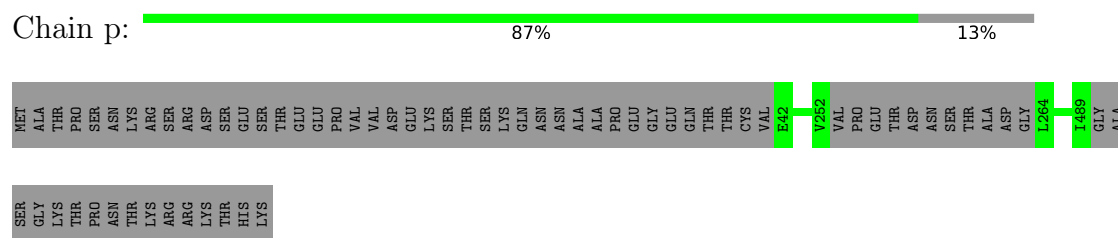
- Molecule 34: Pescadillo homolog



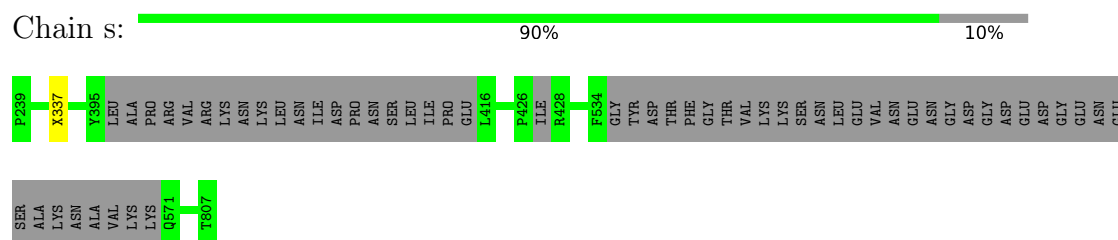
- Molecule 35: Ribosome biogenesis protein 15



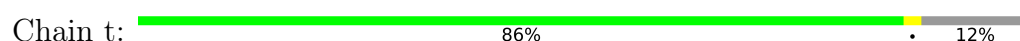
- Molecule 36: ATP-dependent RNA helicase HAS1



- Molecule 37: Ribosome biogenesis protein ERB1



- Molecule 38: Ribosome biogenesis protein RLP7





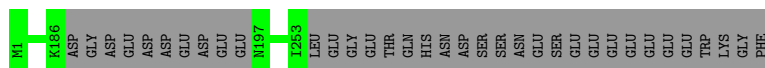
- Molecule 39: BRX1 associated peptide

Chain x: 100%

There are no outlier residues recorded for this chain.

- Molecule 40: Ribosomal RNA-processing protein 1

Chain z: 87% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31419	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.69	0/32836	1.06	172/51180 (0.3%)
10	I	0.35	0/1427	0.55	0/1989
11	K	0.30	0/1291	0.53	0/1800
12	L	0.33	0/524	0.57	0/729
13	M	0.31	0/632	0.50	0/879
14	N	0.34	0/869	0.51	0/1208
15	O	0.32	0/906	0.47	0/1258
16	P	0.31	0/613	0.49	0/851
17	Q	0.34	0/652	0.50	0/907
18	S	0.32	0/850	0.60	1/1186 (0.1%)
19	X	0.33	0/699	0.47	0/974
2	2	0.71	0/3746	1.09	13/5832 (0.2%)
20	Y	0.35	0/622	0.54	0/865
21	Z	0.33	0/666	0.48	0/926
22	7	0.34	0/771	0.55	0/1072
23	b	0.32	0/1107	0.56	0/1538
24	c	0.35	0/475	0.47	0/658
26	e	0.33	0/562	0.52	0/780
27	f	0.37	0/521	0.56	0/723
28	g	0.35	0/497	0.56	0/690
29	h	0.30	0/592	0.55	0/826
3	6	0.63	0/2050	1.33	34/3186 (1.1%)
30	i	0.31	0/415	0.50	0/577
31	j	0.34	0/356	0.53	0/491
32	k	0.34	0/381	0.44	0/530
34	n	0.31	0/1689	0.51	0/2351
35	o	0.34	0/655	0.54	0/910
36	p	0.31	0/2156	0.52	0/2999
37	s	0.30	0/2167	0.52	0/3012
38	t	0.30	0/1225	0.61	0/1704
4	A	0.34	0/1944	0.58	0/2704
40	z	0.32	0/1207	0.47	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	C	0.34	0/1551	0.57	0/2158
6	D	0.37	0/947	0.51	0/1319
7	E	0.31	0/842	0.54	0/1173
8	F	0.33	0/1194	0.56	0/1661
9	G	0.33	0/925	0.64	0/1288
All	All	0.55	0/70562	0.89	220/104617 (0.2%)

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	S	0	4
19	X	0	2
21	Z	0	2
28	g	0	1
29	h	0	1
32	k	0	2
34	n	0	1
37	s	0	1
38	t	0	5
4	A	0	2
6	D	0	1
8	F	0	1
9	G	0	1
All	All	0	24

There are no bond length outliers.

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3217	C	N1-C2-O2	13.26	126.85	118.90
1	1	3217	C	N3-C2-O2	-10.75	114.38	121.90
1	1	3217	C	C2-N1-C1'	10.51	130.36	118.80
1	1	406	G	O4'-C1'-N9	9.94	116.15	108.20
1	1	117	U	N1-C2-O2	9.83	129.68	122.80
1	1	117	U	C2-N1-C1'	9.77	129.42	117.70
1	1	102	C	N1-C2-O2	9.71	124.73	118.90
1	1	117	U	N3-C2-O2	-9.58	115.49	122.20
3	6	223	U	C2-N1-C1'	9.15	128.68	117.70
1	1	312	C	N3-C2-O2	-8.72	115.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3181	C	C2-N1-C1'	8.58	128.24	118.80
1	1	463	C	N1-C2-O2	8.49	123.99	118.90
1	1	1364	C	N1-C2-O2	8.43	123.96	118.90
3	6	223	U	N3-C2-O2	-8.40	116.32	122.20
1	1	250	U	N1-C2-O2	8.37	128.66	122.80
3	6	223	U	N1-C2-O2	8.36	128.65	122.80
1	1	249	U	N1-C2-O2	8.33	128.63	122.80
1	1	249	U	C2-N1-C1'	8.33	127.69	117.70
1	1	270	U	N3-C2-O2	-8.33	116.37	122.20
1	1	102	C	N3-C2-O2	-8.29	116.09	121.90
1	1	466	G	N3-C4-N9	8.25	130.95	126.00
1	1	457	C	N3-C2-O2	-8.14	116.20	121.90
1	1	270	U	N1-C2-O2	7.97	128.38	122.80
1	1	166	C	N1-C2-O2	7.83	123.60	118.90
1	1	3181	C	N1-C2-O2	7.81	123.59	118.90
1	1	3214	U	N3-C2-O2	-7.79	116.75	122.20
1	1	78	U	N3-C2-O2	-7.72	116.80	122.20
1	1	466	G	C4-N9-C1'	7.55	136.32	126.50
1	1	250	U	N3-C2-O2	-7.53	116.93	122.20
3	6	38	U	N3-C2-O2	-7.46	116.98	122.20
1	1	667	C	C2-N1-C1'	7.44	126.99	118.80
1	1	250	U	C2-N1-C1'	7.41	126.59	117.70
3	6	40	U	N1-C2-O2	7.34	127.94	122.80
1	1	3217	C	C6-N1-C1'	-7.31	112.03	120.80
3	6	38	U	N1-C2-O2	7.30	127.91	122.80
1	1	1328	C	N1-C2-O2	7.28	123.27	118.90
1	1	1364	C	N3-C2-O2	-7.25	116.82	121.90
1	1	439	C	N1-C2-O2	7.23	123.24	118.90
3	6	37	C	N1-C2-O2	7.21	123.23	118.90
1	1	7	C	N1-C2-O2	7.18	123.21	118.90
1	1	251	G	N3-C4-N9	7.17	130.30	126.00
1	1	439	C	C2-N1-C1'	7.02	126.52	118.80
1	1	3214	U	C2-N1-C1'	7.01	126.11	117.70
1	1	3214	U	N1-C2-O2	7.00	127.70	122.80
1	1	1425	U	N3-C2-O2	-6.99	117.30	122.20
1	1	1328	C	N3-C2-O2	-6.98	117.01	121.90
1	1	3217	C	C6-N1-C2	-6.93	117.53	120.30
3	6	37	C	C6-N1-C2	-6.90	117.54	120.30
2	2	21	C	N1-C2-O2	6.86	123.02	118.90
1	1	667	C	C6-N1-C2	-6.80	117.58	120.30
1	1	3169	U	OP1-P-O3'	6.75	120.06	105.20
1	1	7	C	C2-N1-C1'	6.74	126.21	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	549	U	N1-C2-O2	6.72	127.51	122.80
3	6	7	C	O4'-C1'-N1	6.71	113.57	108.20
3	6	232	A	O4'-C1'-N9	6.69	113.55	108.20
1	1	251	G	N9-C4-C5	-6.68	102.73	105.40
1	1	3169	U	P-O3'-C3'	6.67	127.70	119.70
1	1	249	U	N3-C2-O2	-6.67	117.53	122.20
1	1	439	C	N3-C2-O2	-6.66	117.24	121.90
1	1	463	C	C2-N1-C1'	6.64	126.10	118.80
1	1	7	C	N3-C2-O2	-6.60	117.28	121.90
3	6	16	U	P-O3'-C3'	6.60	127.62	119.70
1	1	113	C	C2-N1-C1'	6.59	126.05	118.80
1	1	760	G	O4'-C1'-N9	6.59	113.48	108.20
18	S	13	ARG	C-N-CA	6.59	138.17	121.70
1	1	539	C	C5-C6-N1	6.55	124.28	121.00
1	1	1364	C	C2-N1-C1'	6.54	125.99	118.80
1	1	549	U	N3-C2-O2	-6.53	117.63	122.20
1	1	466	G	N3-C4-C5	-6.51	125.34	128.60
1	1	466	G	C6-C5-N7	-6.47	126.52	130.40
1	1	466	G	C8-N9-C1'	-6.46	118.60	127.00
1	1	410	U	N3-C2-O2	-6.46	117.68	122.20
1	1	117	U	C6-N1-C1'	-6.45	112.18	121.20
1	1	3275	U	OP1-P-O3'	6.44	119.37	105.20
1	1	78	U	N1-C2-O2	6.43	127.30	122.80
3	6	1	C	N1-C2-O2	6.41	122.75	118.90
1	1	3168	A	OP2-P-O3'	6.37	119.20	105.20
1	1	466	G	C4-C5-N7	6.36	113.34	110.80
1	1	1339	C	N3-C2-O2	-6.35	117.45	121.90
3	6	41	G	N3-C4-N9	6.34	129.81	126.00
1	1	3181	C	C6-N1-C1'	-6.32	113.21	120.80
1	1	257	U	N3-C2-O2	-6.30	117.79	122.20
3	6	56	U	C2-N1-C1'	6.29	125.25	117.70
1	1	743	C	C6-N1-C2	-6.26	117.79	120.30
1	1	270	U	C2-N1-C1'	6.26	125.21	117.70
1	1	480	C	N1-C2-O2	6.25	122.65	118.90
1	1	250	U	C6-N1-C1'	-6.23	112.47	121.20
3	6	16	U	C2-N1-C1'	6.21	125.15	117.70
1	1	1168	U	N1-C2-O2	6.21	127.14	122.80
1	1	3181	C	N3-C2-O2	-6.19	117.57	121.90
1	1	524	U	N1-C2-O2	6.18	127.13	122.80
2	2	21	C	N3-C2-O2	-6.16	117.59	121.90
1	1	1816	A	C2'-C3'-O3'	6.15	123.54	113.70
1	1	245	U	N1-C2-O2	6.14	127.10	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	249	U	C6-N1-C1'	-6.14	112.61	121.20
1	1	1425	U	N1-C2-O2	6.11	127.08	122.80
1	1	1437	C	C6-N1-C2	-6.09	117.86	120.30
3	6	40	U	N3-C2-O2	-6.08	117.95	122.20
3	6	45	U	N1-C2-O2	6.04	127.03	122.80
3	6	45	U	N3-C2-O2	-6.03	117.98	122.20
1	1	1339	C	N1-C2-O2	6.01	122.51	118.90
3	6	37	C	C5-C6-N1	6.01	124.00	121.00
3	6	59	C	N1-C2-O2	6.00	122.50	118.90
1	1	667	C	N1-C2-O2	5.99	122.49	118.90
2	2	156	U	C2-N1-C1'	5.97	124.86	117.70
1	1	573	C	C5-C6-N1	5.96	123.98	121.00
2	2	36	G	N7-C8-N9	5.96	116.08	113.10
1	1	308	A	C4-N9-C1'	5.95	137.02	126.30
3	6	26	U	O4'-C1'-N1	5.94	112.95	108.20
1	1	463	C	N3-C2-O2	-5.93	117.75	121.90
1	1	3168	A	P-O3'-C3'	5.91	126.79	119.70
1	1	166	C	C2-N1-C1'	5.90	125.29	118.80
1	1	794	U	N1-C2-O2	5.85	126.89	122.80
1	1	3166	C	P-O3'-C3'	5.84	126.70	119.70
1	1	163	C	C6-N1-C2	-5.83	117.97	120.30
1	1	761	A	P-O3'-C3'	5.81	126.67	119.70
3	6	37	C	N3-C2-O2	-5.79	117.85	121.90
1	1	251	G	C8-N9-C1'	-5.77	119.50	127.00
3	6	223	U	C6-N1-C1'	-5.75	113.15	121.20
1	1	267	G	O4'-C1'-N9	-5.75	103.60	108.20
1	1	312	C	C5-C4-N4	5.67	124.17	120.20
1	1	623	U	N3-C2-O2	-5.67	118.23	122.20
1	1	1399	A	C4-N9-C1'	5.66	136.49	126.30
1	1	263	C	C2-N1-C1'	5.64	125.01	118.80
1	1	1388	U	N3-C2-O2	-5.64	118.25	122.20
1	1	1190	A	C2-N3-C4	5.64	113.42	110.60
2	2	157	U	N3-C2-O2	-5.64	118.25	122.20
1	1	87	U	N1-C2-O2	5.63	126.74	122.80
1	1	537	A	C5-C6-N6	-5.62	119.20	123.70
3	6	229	U	N3-C2-O2	-5.62	118.27	122.20
1	1	87	U	N3-C2-O2	-5.58	118.29	122.20
1	1	312	C	N3-C4-N4	-5.58	114.09	118.00
1	1	182	U	N1-C2-O2	5.58	126.70	122.80
1	1	166	C	N3-C2-O2	-5.57	118.00	121.90
1	1	549	U	C2-N1-C1'	5.56	124.37	117.70
1	1	1168	U	N3-C2-O2	-5.55	118.31	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	41	G	C5-C6-O6	-5.53	125.28	128.60
1	1	257	U	N1-C2-O2	5.53	126.67	122.80
1	1	430	U	N3-C2-O2	-5.51	118.34	122.20
3	6	56	U	N1-C2-O2	5.49	126.64	122.80
1	1	537	A	N9-C4-C5	-5.48	103.61	105.80
2	2	100	U	N1-C2-O2	5.47	126.63	122.80
1	1	207	U	N1-C2-O2	5.44	126.61	122.80
2	2	21	C	C2-N1-C1'	5.44	124.79	118.80
1	1	782	U	C2-N1-C1'	5.43	124.22	117.70
1	1	252	U	C5-C6-N1	5.43	125.41	122.70
1	1	7	C	C6-N1-C2	-5.41	118.14	120.30
2	2	36	G	C4-C5-N7	5.41	112.96	110.80
1	1	667	C	C5-C6-N1	5.39	123.70	121.00
1	1	1190	A	N3-C4-N9	5.39	131.71	127.40
3	6	16	U	N1-C2-O2	5.39	126.57	122.80
1	1	382	U	N3-C2-O2	-5.38	118.44	122.20
3	6	59	C	C2-N1-C1'	5.37	124.70	118.80
2	2	11	C	N1-C2-O2	5.37	122.12	118.90
3	6	229	U	N1-C2-O2	5.35	126.55	122.80
2	2	102	U	N3-C2-O2	-5.35	118.45	122.20
1	1	457	C	C6-N1-C2	-5.34	118.17	120.30
1	1	166	C	C5-C6-N1	5.33	123.67	121.00
1	1	174	C	N1-C2-O2	5.33	122.10	118.90
1	1	696	C	N3-C2-O2	-5.33	118.17	121.90
1	1	308	A	N7-C8-N9	5.32	116.46	113.80
1	1	753	C	C6-N1-C2	-5.32	118.17	120.30
1	1	1190	A	C4-N9-C1'	5.32	135.87	126.30
1	1	1437	C	C5-C6-N1	5.30	123.65	121.00
1	1	548	G	N1-C6-O6	5.30	123.08	119.90
3	6	223	U	C5-C6-N1	5.30	125.35	122.70
3	6	1	C	N3-C2-O2	-5.30	118.19	121.90
1	1	102	C	C2-N1-C1'	5.29	124.62	118.80
1	1	480	C	C6-N1-C2	-5.29	118.19	120.30
1	1	466	G	C5-C6-O6	-5.28	125.43	128.60
1	1	3190	C	C5-C6-N1	5.28	123.64	121.00
1	1	3173	G	N3-C4-N9	5.26	129.16	126.00
1	1	452	G	C4-C5-N7	5.26	112.90	110.80
1	1	939	U	N1-C2-O2	5.26	126.48	122.80
2	2	36	G	C5-N7-C8	-5.26	101.67	104.30
1	1	430	U	N1-C2-O2	5.25	126.47	122.80
1	1	493	G	P-O3'-C3'	5.25	125.99	119.70
1	1	1399	A	C8-N9-C1'	-5.24	118.27	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	463	C	C5-C6-N1	5.23	123.62	121.00
2	2	139	U	N3-C2-O2	-5.22	118.55	122.20
1	1	304	G	C5-C6-O6	5.22	131.73	128.60
1	1	1452	A	N3-C4-N9	5.21	131.57	127.40
1	1	1399	A	N3-C4-N9	5.21	131.57	127.40
1	1	251	G	C4-C5-N7	5.20	112.88	110.80
1	1	308	A	C8-N9-C1'	-5.20	118.34	127.70
1	1	480	C	N3-C2-O2	-5.20	118.26	121.90
1	1	539	C	C6-N1-C2	-5.19	118.22	120.30
3	6	56	U	N3-C2-O2	-5.19	118.57	122.20
1	1	414	U	C5-C6-N1	5.18	125.29	122.70
1	1	101	G	C4-N9-C1'	5.18	133.23	126.50
1	1	2359	C	C5-C6-N1	5.18	123.59	121.00
1	1	753	C	C5-C6-N1	5.17	123.59	121.00
1	1	113	C	C5-C6-N1	5.17	123.58	121.00
2	2	102	U	N1-C2-O2	5.16	126.41	122.80
1	1	1452	A	N9-C4-C5	-5.14	103.74	105.80
1	1	743	C	N3-C2-O2	-5.13	118.31	121.90
1	1	113	C	N1-C2-O2	5.13	121.98	118.90
1	1	543	C	C5-C6-N1	5.12	123.56	121.00
1	1	126	U	N3-C2-O2	-5.12	118.61	122.20
1	1	3265	C	C2-N1-C1'	5.12	124.43	118.80
3	6	5	C	C2-N1-C1'	5.11	124.42	118.80
1	1	782	U	C5-C6-N1	5.11	125.25	122.70
1	1	439	C	C6-N1-C1'	-5.08	114.70	120.80
3	6	41	G	N3-C4-C5	-5.08	126.06	128.60
1	1	251	G	C4-N9-C1'	5.07	133.09	126.50
1	1	627	U	N3-C2-O2	-5.06	118.66	122.20
1	1	207	U	N3-C2-O2	-5.05	118.66	122.20
1	1	515	C	C6-N1-C2	-5.05	118.28	120.30
1	1	3181	C	O4'-C1'-N1	5.04	112.24	108.20
1	1	3217	C	C5-C6-N1	5.04	123.52	121.00
1	1	177	U	C5-C6-N1	5.04	125.22	122.70
1	1	251	G	C6-C5-N7	-5.04	127.38	130.40
1	1	435	C	N3-C2-O2	-5.04	118.38	121.90
1	1	3173	G	C4-N9-C1'	5.02	133.03	126.50
1	1	1333	C	C2-N1-C1'	5.02	124.32	118.80
1	1	1396	C	N1-C2-O2	5.01	121.91	118.90
1	1	309	U	P-O3'-C3'	5.01	125.71	119.70
1	1	466	G	N7-C8-N9	5.01	115.60	113.10
1	1	1168	U	C2-N1-C1'	5.01	123.71	117.70
1	1	548	G	C5-C6-O6	-5.00	125.60	128.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	185	ALA	Peptide
4	A	53	ILE	Peptide
6	D	56	ASP	Peptide
8	F	158	LYS	Peptide
9	G	76	ALA	Peptide
18	S	12	ARG	Peptide
18	S	13	ARG	Peptide
18	S	22	PRO	Peptide
18	S	83	SER	Peptide
19	X	17	GLY	Peptide
19	X	65	GLN	Peptide
21	Z	31	GLU	Peptide
21	Z	8	GLY	Peptide
28	g	71	THR	Peptide
29	h	83	LYS	Peptide
32	k	18	ALA	Peptide
32	k	33	LYS	Peptide
34	n	175	LEU	Peptide
37	s	337	UNK	Peptide
38	t	150	PRO	Peptide
38	t	223	GLU	Peptide
38	t	53	UNK	Peptide
38	t	54	LYS	Peptide
38	t	55	PHE	Peptide

5.2 Too-close contacts

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	1	29343	0	14746	312	0
2	2	3353	0	1695	71	0
3	6	1838	0	927	21	0
4	A	1946	0	856	16	0
5	C	1553	0	748	5	0
6	D	948	0	426	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	843	0	380	3	0
8	F	1195	0	556	4	0
9	G	926	0	452	12	0
10	I	1428	0	590	10	0
11	K	1293	0	551	10	0
12	L	525	0	259	3	0
13	M	633	0	321	1	0
14	N	871	0	397	5	0
15	O	908	0	437	5	0
16	P	616	0	304	0	0
17	Q	653	0	314	0	0
18	S	851	0	374	5	0
19	X	700	0	336	41	0
20	Y	623	0	283	3	0
21	Z	667	0	307	0	0
22	7	773	0	339	3	0
23	b	1201	0	497	0	0
24	c	476	0	222	0	0
25	d	2288	0	471	0	0
26	e	564	0	262	0	0
27	f	522	0	239	0	0
28	g	498	0	228	0	0
29	h	593	0	274	0	0
30	i	416	0	198	0	0
31	j	357	0	172	0	0
32	k	382	0	171	0	0
33	m	370	0	76	0	0
34	n	1693	0	731	0	0
35	o	656	0	289	0	0
36	p	2158	0	965	0	0
37	s	2537	0	1013	0	0
38	t	1397	0	583	0	0
39	x	140	0	34	0	0
40	z	1209	0	522	0	0
41	D	1	0	0	0	0
41	j	1	0	0	0	0
All	All	69945	0	32545	440	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 6.

All (440) 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)
1:1:1558:A:P	9:G:53:PRO:HA	1.32	1.64
1:1:1558:A:P	9:G:53:PRO:CA	2.11	1.38
1:1:1558:A:C4'	19:X:33:ARG:O	1.68	1.37
1:1:1558:A:OP1	9:G:53:PRO:HA	1.08	1.25
2:2:133:G:O3'	19:X:55:ASN:HA	1.37	1.24
1:1:1558:A:O2'	19:X:34:LEU:CB	1.73	1.24
1:1:14:U:O2'	19:X:42:ARG:N	1.70	1.21
2:2:134:G:C4'	19:X:53:HIS:O	1.87	1.20
2:2:151:C:C4	19:X:24:LEU:CB	2.27	1.18
1:1:1558:A:OP2	9:G:53:PRO:N	1.77	1.17
2:2:133:G:H4'	19:X:55:ASN:CB	1.75	1.17
2:2:134:G:H4'	19:X:53:HIS:O	1.00	1.17
1:1:15:C:C5'	19:X:42:ARG:HA	1.77	1.15
1:1:16:A:OP1	19:X:44:PRO:HA	1.41	1.14
1:1:1558:A:OP1	9:G:53:PRO:CA	1.94	1.09
2:2:151:C:N4	19:X:24:LEU:CB	2.17	1.06
1:1:1831:U:H1'	2:2:114:G:OP1	1.58	1.03
1:1:15:C:H5''	19:X:42:ARG:CA	1.91	0.98
1:1:1558:A:OP2	9:G:53:PRO:CA	2.08	0.98
1:1:182:U:H3	1:1:234:G:H1	1.07	0.97
1:1:160:G:H1	1:1:261:U:H3	1.09	0.97
1:1:16:A:OP1	19:X:44:PRO:CA	2.11	0.96
1:1:509:U:H3	1:1:582:G:H1	1.10	0.95
1:1:528:U:H3	1:1:564:G:H1	1.09	0.95
1:1:1831:U:O2'	2:2:113:U:H5'	1.68	0.92
1:1:15:C:H5''	19:X:42:ARG:HA	0.94	0.91
1:1:3222:U:H3	1:1:3263:G:H1	1.17	0.91
1:1:129:U:H3	1:1:139:G:H1	0.93	0.90
1:1:1831:U:C2'	2:2:113:U:H5'	2.04	0.88
1:1:1558:A:H4'	19:X:33:ARG:O	0.84	0.87
1:1:600:G:N2	1:1:603:A:OP2	2.08	0.85
1:1:173:G:H1	1:1:245:U:H3	1.23	0.84
2:2:134:G:H4'	19:X:53:HIS:C	1.97	0.84
1:1:297:G:N2	1:1:297:G:OP2	2.11	0.83
1:1:1558:A:H1'	19:X:35:PRO:N	1.94	0.81
1:1:1447:G:N2	1:1:2356:A:OP2	2.12	0.81
1:1:761:A:OP2	1:1:769:G:N2	2.13	0.81
1:1:1558:A:P	9:G:53:PRO:N	2.50	0.81
1:1:14:U:HO2'	19:X:42:ARG:H	1.26	0.81
1:1:177:U:O2	1:1:241:G:N1	2.12	0.80
1:1:726:G:N1	1:1:743:C:OP2	2.14	0.80
1:1:518:G:N2	1:1:518:G:OP2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:91:G:OP2	1:1:93:C:N4	2.15	0.79
1:1:15:C:H5'	19:X:41:ALA:O	1.83	0.79
1:1:91:G:N2	1:1:95:A:OP2	2.16	0.79
1:1:727:G:OP2	1:1:742:G:N2	2.11	0.78
1:1:951:A:OP2	1:1:1367:G:N1	2.14	0.78
1:1:21:G:OP2	2:2:36:G:N1	2.16	0.78
1:1:1831:U:O2'	2:2:113:U:H3'	1.84	0.78
1:1:722:G:H1	1:1:748:U:H3	1.29	0.77
1:1:358:G:N2	1:1:361:A:OP2	2.14	0.77
1:1:346:C:N4	1:1:349:A:OP2	2.19	0.76
3:6:5:C:N4	3:6:24:A:OP2	2.19	0.76
1:1:1:G:N2	1:1:1:G:OP2	2.18	0.75
1:1:533:A:O2'	1:1:535:G:OP2	2.03	0.75
8:F:138:TYR:H	8:F:233:GLU:HA	1.52	0.75
2:2:134:G:C5'	19:X:53:HIS:O	2.36	0.74
1:1:1831:U:H2'	2:2:113:U:H5'	1.69	0.73
1:1:1832:C:O4'	2:2:113:U:H5''	1.88	0.73
1:1:3189:G:H1	1:1:3203:U:H3	1.37	0.73
1:1:508:U:H3	1:1:583:G:H1	1.35	0.73
1:1:420:G:H1	2:2:3:A:H61	1.34	0.73
2:2:103:G:OP2	2:2:105:A:O2'	2.10	0.70
2:2:121:U:H3	2:2:132:G:H1	1.38	0.70
4:A:50:MET:HA	4:A:59:ILE:O	1.92	0.70
1:1:733:G:N2	1:1:736:A:OP2	2.24	0.68
1:1:432:G:H1	1:1:627:U:H3	1.40	0.68
1:1:3195:U:O2'	1:1:3197:G:N2	2.26	0.68
2:2:134:G:OP1	19:X:56:ARG:N	2.26	0.68
1:1:544:C:H2'	1:1:547:G:H1	1.60	0.67
1:1:1830:G:H22	2:2:114:G:H5''	1.60	0.67
1:1:528:U:O2	1:1:564:G:N2	2.26	0.67
1:1:1404:G:N2	1:1:1407:A:OP2	2.25	0.66
1:1:1831:U:O2'	2:2:113:U:C5'	2.44	0.66
1:1:754:G:N2	1:1:778:U:O2	2.28	0.66
1:1:1399:A:N7	2:2:8:C:O2'	2.28	0.65
7:E:65:ILE:O	7:E:76:LEU:HA	1.97	0.65
2:2:134:G:O2'	19:X:52:PRO:CB	2.44	0.65
1:1:1558:A:OP2	9:G:53:PRO:HA	1.79	0.65
18:S:7:TYR:HA	18:S:62:ASN:O	1.97	0.64
4:A:248:PRO:HA	4:A:274:THR:HA	1.79	0.64
1:1:155:G:H4'	1:1:156:G:H2'	1.80	0.63
1:1:353:G:N2	1:1:365:A:OP2	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:39:G:O2'	2:2:105:A:N1	2.32	0.63
1:1:16:A:H5''	19:X:45:LYS:N	2.14	0.62
1:1:1159:A:N3	1:1:1160:C:N4	2.47	0.62
1:1:3222:U:O2	1:1:3263:G:N2	2.30	0.62
1:1:563:U:H2'	1:1:564:G:H8	1.65	0.62
1:1:571:U:H2'	1:1:572:A:H8	1.65	0.61
1:1:312:C:H2'	1:1:313:A:H8	1.66	0.61
4:A:278:HIS:HA	4:A:294:ILE:O	2.00	0.61
1:1:591:G:N2	1:1:612:U:OP1	2.34	0.60
1:1:14:U:O2'	19:X:42:ARG:CB	2.50	0.60
1:1:664:U:H3	1:1:798:G:H1	1.50	0.59
2:2:133:G:C3'	19:X:55:ASN:HA	2.31	0.59
1:1:1189:C:N3	1:1:1315:U:O2'	2.34	0.59
1:1:14:U:O2'	19:X:42:ARG:CA	2.49	0.59
1:1:700:C:H2'	1:1:701:G:H8	1.67	0.59
1:1:1558:A:HO2'	19:X:34:LEU:CB	2.05	0.59
1:1:508:U:O2	1:1:583:G:N2	2.33	0.59
1:1:728:G:N7	1:1:742:G:N2	2.50	0.59
1:1:383:G:O2'	1:1:386:A:N6	2.37	0.58
1:1:348:A:N3	1:1:352:A:O2'	2.35	0.58
1:1:447:U:H3	1:1:487:U:H3	1.51	0.58
4:A:219:ILE:HA	4:A:226:LEU:HA	1.85	0.58
1:1:691:A:N1	2:2:28:C:O2'	2.37	0.58
15:O:194:LEU:O	15:O:199:TYR:N	2.37	0.58
1:1:722:G:N2	1:1:748:U:O2	2.36	0.58
1:1:1558:A:N1	2:2:149:A:H1'	2.19	0.58
1:1:509:U:O2	1:1:582:G:N2	2.31	0.57
1:1:32:U:H3	1:1:52:A:H61	1.53	0.57
2:2:134:G:O3'	19:X:53:HIS:CB	2.53	0.57
1:1:19:U:H3	2:2:140:G:H1	1.53	0.57
2:2:128:U:OP1	2:2:129:C:N4	2.33	0.56
3:6:33:U:O2'	11:K:286:SER:O	2.22	0.56
10:I:233:HIS:O	10:I:239:ILE:HA	2.06	0.56
1:1:105:C:HO2'	1:1:684:G:HO2'	1.53	0.56
1:1:618:C:O2'	1:1:621:A:N3	2.37	0.56
1:1:64:G:H22	1:1:322:U:H2'	1.70	0.56
4:A:57:GLU:HA	4:A:70:VAL:O	2.05	0.56
1:1:679:U:H3	1:1:701:G:H1	1.52	0.56
1:1:1556:C:O2	1:1:1556:C:O4'	2.24	0.56
1:1:173:G:O6	1:1:245:U:O4	2.24	0.56
4:A:14:LYS:HA	4:A:36:ALA:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:28:C:O2'	1:1:61:A:N3	2.39	0.55
3:6:38:U:O2	3:6:41:G:O6	2.25	0.55
1:1:675:C:O2'	1:1:679:U:OP1	2.24	0.55
1:1:1168:U:H2'	1:1:1169:A:H8	1.72	0.55
13:M:23:ILE:O	13:M:30:GLY:N	2.37	0.55
1:1:1831:U:C1'	2:2:114:G:OP1	2.45	0.54
1:1:170:G:H1	1:1:248:U:H3	1.53	0.54
3:6:231:A:H1'	3:6:232:A:H5'	1.89	0.54
15:O:42:ASN:HA	15:O:136:THR:O	2.08	0.54
4:A:49:ARG:H	4:A:61:ALA:HB3	1.73	0.54
1:1:655:C:H2'	1:1:656:A:H8	1.72	0.54
11:K:212:HIS:HA	11:K:217:PHE:HA	1.89	0.54
2:2:36:G:O2'	2:2:104:A:N1	2.37	0.54
1:1:1362:G:H2'	1:1:1363:A:H8	1.72	0.54
1:1:16:A:O3'	19:X:45:LYS:CB	2.56	0.54
1:1:5:G:H2'	1:1:6:A:H8	1.72	0.54
1:1:754:G:C2	1:1:778:U:O2	2.61	0.54
1:1:451:U:H2'	1:1:452:G:C8	2.44	0.53
1:1:109:A:N1	1:1:322:U:O2'	2.35	0.53
1:1:627:U:H4'	1:1:1399:A:H1'	1.91	0.53
11:K:85:ASN:HA	11:K:277:ARG:H	1.73	0.53
1:1:1558:A:C2	2:2:149:A:H1'	2.43	0.53
1:1:182:U:O4	1:1:234:G:O6	2.27	0.53
1:1:532:A:H2'	1:1:533:A:C8	2.44	0.53
1:1:1419:A:OP1	2:2:20:U:O2'	2.26	0.53
1:1:184:U:H3	1:1:232:G:H1	1.58	0.52
1:1:2357:A:H2'	1:1:2358:A:H8	1.74	0.52
1:1:406:G:OP1	1:1:1415:U:O2'	2.26	0.52
3:6:53:A:O2'	3:6:55:A:N6	2.42	0.52
2:2:26:U:O2'	5:C:51:ALA:O	2.26	0.52
10:I:272:ARG:N	10:I:277:GLU:O	2.38	0.52
1:1:67:A:O2'	1:1:315:C:O2	2.26	0.52
1:1:655:C:H2'	1:1:656:A:C8	2.45	0.52
1:1:345:G:O2'	2:2:25:G:N3	2.42	0.52
1:1:1168:U:O2	1:1:1330:A:N7	2.43	0.52
1:1:1381:A:H2'	1:1:1382:G:H8	1.75	0.52
1:1:15:C:H2'	1:1:16:A:H8	1.74	0.52
1:1:1362:G:H2'	1:1:1363:A:C8	2.45	0.52
18:S:74:ASN:O	18:S:129:ILE:N	2.41	0.52
1:1:411:U:H2'	1:1:412:G:H8	1.75	0.51
1:1:425:G:H2'	1:1:426:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:79:A:H8	2:2:79:A:OP2	1.92	0.51
1:1:591:G:O2'	7:E:17:ALA:O	2.25	0.51
1:1:275:U:H3	1:1:290:G:H1	1.57	0.51
3:6:65:U:O2'	3:6:222:A:N6	2.40	0.51
1:1:1724:U:H1'	1:1:1725:C:C6	2.46	0.51
1:1:664:U:H2'	1:1:665:A:H8	1.76	0.51
2:2:134:G:H5''	19:X:54:TYR:O	2.11	0.51
1:1:14:U:H3	2:2:118:C:H1'	1.76	0.51
2:2:40:A:OP2	2:2:103:G:N1	2.44	0.51
1:1:1434:G:OP1	1:1:1437:C:N4	2.43	0.51
4:A:71:LYS:N	4:A:109:GLU:O	2.37	0.50
4:A:17:LEU:O	4:A:33:PHE:N	2.44	0.50
1:1:160:G:N2	1:1:261:U:O2	2.33	0.50
2:2:107:G:H4'	2:2:138:A:H5'	1.92	0.50
2:2:9:A:H2'	2:2:10:A:H8	1.76	0.50
1:1:16:A:H5''	19:X:44:PRO:HA	1.94	0.50
1:1:1178:G:N3	1:1:1328:C:O2'	2.44	0.50
1:1:1831:U:O2'	2:2:113:U:C3'	2.57	0.50
20:Y:70:ILE:HA	20:Y:82:VAL:HA	1.92	0.50
3:6:38:U:O2	3:6:41:G:C6	2.65	0.50
9:G:135:GLY:O	9:G:139:VAL:N	2.44	0.50
1:1:19:U:H2'	1:1:20:A:C8	2.46	0.49
14:N:183:THR:O	14:N:187:ARG:N	2.42	0.49
1:1:16:A:H5''	19:X:45:LYS:H	1.75	0.49
4:A:334:ILE:HA	4:A:343:PHE:O	2.13	0.49
12:L:36:ARG:O	12:L:40:ALA:N	2.40	0.49
8:F:86:VAL:O	8:F:114:GLY:HA2	2.13	0.49
11:K:97:LEU:HA	11:K:236:VAL:O	2.11	0.49
2:2:130:C:H2'	2:2:131:A:H8	1.77	0.49
20:Y:86:THR:HA	20:Y:96:PRO:HA	1.94	0.49
1:1:129:U:H2'	1:1:130:A:C8	2.48	0.49
1:1:761:A:OP2	1:1:770:G:N2	2.45	0.49
2:2:151:C:N3	19:X:24:LEU:CB	2.71	0.49
2:2:154:C:H2'	2:2:155:A:C8	2.48	0.49
1:1:377:A:N6	1:1:400:G:O2'	2.46	0.49
1:1:86:G:N2	1:1:87:U:O4	2.44	0.49
1:1:100:A:H3'	1:1:101:G:H21	1.78	0.49
1:1:27:C:O2'	1:1:327:A:N3	2.39	0.49
1:1:722:G:N1	1:1:748:U:N3	2.49	0.49
2:2:8:C:H2'	2:2:9:A:H8	1.78	0.49
1:1:760:G:N2	1:1:770:G:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:268:A:H61	1:1:295:A:H3'	1.77	0.48
1:1:477:A:H1'	1:1:480:C:H41	1.78	0.48
1:1:671:U:H2'	1:1:672:A:H8	1.78	0.48
1:1:600:G:H5'	1:1:601:U:OP2	2.13	0.48
11:K:100:LEU:O	11:K:233:GLN:HA	2.13	0.48
1:1:477:A:H5''	1:1:478:A:H5'	1.94	0.48
1:1:1448:U:H2'	1:1:1449:A:H8	1.78	0.48
1:1:677:A:N6	1:1:786:A:O4'	2.46	0.48
2:2:8:C:H2'	2:2:9:A:C8	2.48	0.48
1:1:353:G:O2'	1:1:364:G:O6	2.24	0.48
1:1:397:A:HO2'	1:1:400:G:H8	1.60	0.48
3:6:22:G:N2	11:K:184:ASP:O	2.45	0.48
9:G:153:ILE:O	9:G:180:VAL:N	2.46	0.48
1:1:1336:U:H2'	1:1:1337:A:H8	1.79	0.48
1:1:440:A:OP2	1:1:441:U:H5	1.97	0.48
11:K:81:ILE:N	11:K:246:VAL:O	2.41	0.48
1:1:1183:C:H2'	1:1:1184:A:H8	1.78	0.48
1:1:326:U:H2'	1:1:327:A:H8	1.79	0.48
2:2:27:U:H4'	5:C:51:ALA:HB3	1.96	0.48
3:6:42:G:H2'	3:6:43:A:C8	2.49	0.48
2:2:134:G:OP1	19:X:56:ARG:CB	2.62	0.47
2:2:42:G:H1	2:2:102:U:H3	1.62	0.47
1:1:1327:C:H2'	1:1:1328:C:H6	1.79	0.47
18:S:11:GLY:O	18:S:25:PHE:N	2.44	0.47
1:1:105:C:H2'	1:1:106:A:H8	1.79	0.47
1:1:306:A:H2'	1:1:308:A:C8	2.49	0.47
1:1:612:U:H2'	1:1:613:G:H8	1.80	0.47
2:2:134:G:HO2'	19:X:52:PRO:CB	2.26	0.47
1:1:1312:C:O2'	15:O:83:ALA:O	2.33	0.47
2:2:134:G:P	19:X:56:ARG:H	2.37	0.47
1:1:303:G:H2'	1:1:304:G:C8	2.49	0.47
1:1:615:U:H2'	1:1:616:G:H8	1.78	0.47
2:2:154:C:H2'	2:2:155:A:H8	1.79	0.47
1:1:565:U:H2'	1:1:566:G:H8	1.77	0.47
1:1:584:G:H2'	1:1:585:A:H8	1.80	0.47
1:1:1831:U:O2'	2:2:113:U:H6	1.97	0.47
2:2:134:G:C5'	19:X:54:TYR:O	2.62	0.47
1:1:1195:A:H1'	1:1:1319:G:H4'	1.96	0.47
1:1:454:C:OP2	1:1:455:C:OP2	2.33	0.47
1:1:546:C:H5''	1:1:547:G:C5	2.48	0.47
1:1:21:G:P	2:2:36:G:H1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:9:A:H2'	2:2:10:A:C8	2.50	0.47
3:6:9:A:H2'	3:6:10:A:H8	1.80	0.47
1:1:1448:U:H2'	1:1:1449:A:C8	2.50	0.47
9:G:145:ASN:H	9:G:146:LYS:HA	1.80	0.47
10:I:204:THR:O	10:I:208:GLN:N	2.41	0.47
1:1:5:G:H2'	1:1:6:A:C8	2.50	0.47
3:6:24:A:H5'	3:6:217:G:H22	1.80	0.47
6:D:51:ALA:HA	6:D:63:TYR:O	2.14	0.47
11:K:221:THR:O	11:K:225:ASN:CB	2.63	0.47
1:1:3170:A:OP2	1:1:3174:A:N6	2.48	0.47
4:A:70:VAL:HA	4:A:110:ILE:HA	1.97	0.47
3:6:219:A:H8	3:6:219:A:OP2	1.98	0.46
1:1:182:U:O2	1:1:234:G:N2	2.38	0.46
1:1:530:G:OP2	1:1:530:G:H8	1.99	0.46
10:I:146:ASP:HA	10:I:163:ILE:O	2.15	0.46
1:1:392:G:H5'	10:I:59:THR:HA	1.96	0.46
1:1:26:A:N3	1:1:328:U:O2'	2.44	0.46
1:1:129:U:O4	1:1:139:G:O6	2.34	0.46
1:1:330:G:H2'	1:1:331:G:H8	1.80	0.46
1:1:378:A:N1	10:I:58:GLN:N	2.57	0.46
1:1:411:U:H2'	1:1:412:G:C8	2.50	0.46
1:1:541:U:H2'	1:1:542:G:C8	2.50	0.46
1:1:746:A:H2'	1:1:747:A:C8	2.51	0.46
15:O:38:ALA:H	15:O:106:GLU:HA	1.80	0.46
1:1:417:A:H2'	1:1:418:A:C8	2.50	0.46
1:1:535:G:N2	1:1:536:U:O4	2.46	0.46
12:L:23:LYS:N	14:N:197:LEU:O	2.45	0.46
1:1:664:U:H2'	1:1:665:A:C8	2.51	0.46
1:1:589:A:O2'	1:1:1338:C:OP1	2.34	0.46
1:1:163:C:H2'	1:1:164:A:C8	2.51	0.46
1:1:745:C:H2'	1:1:746:A:H8	1.79	0.46
1:1:515:C:O2'	5:C:342:LYS:O	2.31	0.46
1:1:441:U:H5''	1:1:442:G:H5'	1.97	0.45
1:1:1558:A:C1'	19:X:35:PRO:N	2.73	0.45
1:1:165:A:H5'	1:1:166:C:OP2	2.15	0.45
1:1:504:A:H2'	1:1:505:G:H8	1.81	0.45
1:1:69:C:OP1	14:N:178:HIS:N	2.48	0.45
1:1:1:G:O5'	3:6:232:A:O2'	2.26	0.45
1:1:551:A:H2'	1:1:551:A:OP2	2.16	0.45
1:1:794:U:H2'	1:1:795:G:H8	1.80	0.45
1:1:1361:U:H2'	1:1:1362:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:U:H2'	1:1:88:A:H8	1.82	0.45
1:1:250:U:O4	22:7:176:SER:N	2.50	0.45
1:1:255:A:H2'	1:1:256:G:H8	1.81	0.45
1:1:3183:A:N1	1:1:3188:G:O2'	2.48	0.45
1:1:417:A:H2'	1:1:418:A:H8	1.82	0.45
1:1:671:U:H2'	1:1:672:A:C8	2.51	0.45
1:1:269:G:N2	1:1:270:U:O4	2.38	0.45
4:A:206:ALA:HA	4:A:215:LYS:O	2.17	0.45
1:1:187:A:N1	1:1:211:A:O2'	2.39	0.45
1:1:1880:U:H2'	1:1:1881:A:H8	1.82	0.45
2:2:47:C:H1'	2:2:61:A:H2'	1.99	0.45
1:1:354:U:H2'	1:1:355:A:H8	1.82	0.45
1:1:489:C:H2'	1:1:490:A:C8	2.52	0.45
1:1:547:G:H2'	1:1:547:G:OP2	2.17	0.45
1:1:565:U:H2'	1:1:566:G:C8	2.51	0.45
2:2:59:A:H3'	2:2:59:A:OP2	2.16	0.45
3:6:222:A:H4'	3:6:223:U:OP1	2.15	0.45
1:1:15:C:H2'	1:1:16:A:C8	2.51	0.44
1:1:551:A:H8	1:1:551:A:OP2	2.00	0.44
1:1:612:U:H2'	1:1:613:G:C8	2.52	0.44
1:1:1558:A:OP1	9:G:53:PRO:CB	2.61	0.44
1:1:3192:U:H2'	1:1:3193:C:C6	2.52	0.44
1:1:65:A:H61	1:1:323:A:H62	1.65	0.44
1:1:16:A:OP1	19:X:44:PRO:N	2.50	0.44
3:6:41:G:N2	3:6:42:G:N3	2.66	0.44
10:I:77:ASP:O	10:I:81:LEU:CB	2.65	0.44
11:K:78:LEU:HA	11:K:250:ASN:HA	1.98	0.44
1:1:387:A:OP2	1:1:387:A:H8	2.01	0.44
1:1:722:G:O6	1:1:748:U:O4	2.35	0.44
1:1:745:C:H2'	1:1:746:A:C8	2.52	0.44
1:1:86:G:O2'	1:1:98:G:O6	2.32	0.44
20:Y:34:PRO:HA	20:Y:47:ALA:HA	2.00	0.44
1:1:1571:A:C6	14:N:149:ASN:C	58.14	0.44
1:1:1832:C:H1'	2:2:113:U:OP1	2.18	0.44
1:1:536:U:H2'	1:1:537:A:H8	1.83	0.44
1:1:64:G:O2'	1:1:77:A:N3	2.42	0.44
1:1:415:G:H2'	1:1:416:A:C8	2.53	0.44
1:1:516:A:H2'	1:1:517:G:C8	2.53	0.44
1:1:673:U:H2'	1:1:674:G:C8	2.53	0.44
1:1:1831:U:O2'	2:2:113:U:C6	2.68	0.44
1:1:1390:A:N6	1:1:1418:A:O2'	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:124:ASP:N	14:N:127:TYR:O	2.41	0.43
1:1:1448:U:O2	1:1:2356:A:N7	2.51	0.43
1:1:350:C:O2'	1:1:352:A:OP1	2.35	0.43
1:1:476:G:H2'	1:1:477:A:C8	2.53	0.43
1:1:354:U:H2'	1:1:355:A:C8	2.54	0.43
1:1:753:C:H2'	1:1:754:G:C8	2.54	0.43
1:1:1832:C:H1'	2:2:113:U:P	2.58	0.43
1:1:1348:U:H1'	1:1:1350:A:H1'	2.01	0.43
1:1:1404:G:H5'	1:1:1405:U:OP2	2.18	0.43
1:1:772:U:H2'	1:1:773:G:C8	2.54	0.43
1:1:791:A:H2'	1:1:792:G:C8	2.54	0.43
1:1:517:G:H8	1:1:517:G:OP2	2.01	0.43
18:S:75:PHE:O	18:S:93:GLU:HA	2.19	0.43
1:1:1381:A:H2'	1:1:1382:G:C8	2.53	0.43
1:1:1176:C:H2'	1:1:1177:G:C2	2.54	0.43
1:1:584:G:H2'	1:1:585:A:C8	2.53	0.43
6:D:104:PHE:O	6:D:108:CYS:CB	2.67	0.43
1:1:257:U:H2'	1:1:258:G:H8	1.84	0.43
1:1:631:U:H2'	1:1:632:G:C8	2.54	0.43
1:1:273:A:H2'	1:1:274:G:C8	2.54	0.43
1:1:627:U:H2'	1:1:628:A:C8	2.54	0.43
5:C:193:LYS:HA	5:C:198:ARG:HA	2.01	0.43
1:1:15:C:C5'	19:X:42:ARG:CA	2.71	0.42
1:1:452:G:H2'	1:1:453:C:H5''	2.01	0.42
1:1:737:G:H8	1:1:737:G:OP2	2.02	0.42
1:1:753:C:N4	1:1:754:G:O6	2.53	0.42
1:1:659:G:N1	1:1:1434:G:OP2	2.45	0.42
1:1:177:U:O2	1:1:241:G:C6	2.70	0.42
1:1:526:C:H2'	1:1:527:A:H8	1.83	0.42
1:1:409:A:H61	2:2:15:G:H1'	1.84	0.42
4:A:247:TRP:O	4:A:275:ARG:N	2.50	0.42
3:6:9:A:H2'	3:6:10:A:C8	2.53	0.42
1:1:1185:C:H2'	1:1:1186:G:C8	2.55	0.42
4:A:2:ARG:HA	4:A:16:VAL:O	2.19	0.42
1:1:116:A:N1	1:1:264:G:H4'	2.34	0.42
1:1:326:U:H2'	1:1:327:A:C8	2.55	0.42
4:A:367:ILE:HA	4:A:376:LEU:O	2.19	0.42
1:1:1183:C:H2'	1:1:1184:A:C8	2.53	0.42
1:1:435:C:H2'	1:1:436:A:C8	2.55	0.42
1:1:594:U:P	1:1:609:G:H1	2.42	0.42
10:I:232:LEU:HA	10:I:240:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1193:A:N6	1:1:1317:A:H62	2.17	0.42
1:1:276:U:H2'	1:1:277:G:C8	2.54	0.42
4:A:385:ARG:HA	4:A:396:VAL:O	2.19	0.42
15:O:194:LEU:O	15:O:198:GLY:N	2.53	0.42
1:1:950:G:N2	1:1:1368:U:OP2	2.51	0.42
1:1:381:U:H2'	1:1:382:U:H6	1.84	0.42
2:2:126:A:H4'	2:2:127:U:OP2	2.17	0.42
11:K:125:LEU:O	11:K:154:ILE:HA	2.20	0.42
1:1:946:U:H2'	1:1:947:G:C8	2.55	0.42
1:1:1438:U:H1'	5:C:94:CYS:HA	2.01	0.42
1:1:2357:A:H2'	1:1:2358:A:C8	2.54	0.41
1:1:3183:A:H2	1:1:3188:G:H4'	1.85	0.41
1:1:725:G:H3'	1:1:726:G:C8	2.55	0.41
1:1:425:G:H2'	1:1:426:G:C8	2.54	0.41
1:1:1168:U:H2'	1:1:1169:A:C8	2.54	0.41
3:6:54:A:H3'	3:6:55:A:C8	2.55	0.41
18:S:7:TYR:O	18:S:28:ARG:HA	2.20	0.41
1:1:3218:A:H5''	1:1:3219:G:C5	2.55	0.41
1:1:473:G:H2'	1:1:474:G:C8	2.56	0.41
1:1:791:A:H2'	1:1:792:G:H8	1.84	0.41
1:1:377:A:H1'	1:1:392:G:N2	2.35	0.41
1:1:442:G:H2'	1:1:443:G:H8	1.85	0.41
1:1:607:A:OP1	7:E:24:ALA:N	2.48	0.41
1:1:665:A:H2'	1:1:666:A:C8	2.56	0.41
2:2:121:U:O2	2:2:132:G:N2	2.36	0.41
2:2:133:G:H4'	19:X:55:ASN:CA	2.46	0.41
8:F:222:HIS:O	8:F:227:GLY:N	2.50	0.41
1:1:242:C:O2'	1:1:243:G:H8	2.04	0.41
1:1:503:C:H2'	1:1:504:A:C8	2.55	0.41
1:1:946:U:H2'	1:1:947:G:H8	1.84	0.41
1:1:215:G:H2'	1:1:216:G:H8	1.86	0.41
1:1:3189:G:N2	1:1:3203:U:O2	2.48	0.41
1:1:356:C:H2'	1:1:357:A:H8	1.86	0.41
1:1:504:A:H2'	1:1:505:G:C8	2.56	0.41
1:1:1439:U:H2'	1:1:1440:G:C8	2.56	0.41
1:1:574:U:H2'	1:1:575:G:C8	2.56	0.41
2:2:27:U:H2'	2:2:28:C:C6	2.56	0.41
3:6:226:U:H2'	3:6:226:U:H6	1.75	0.41
1:1:528:U:H2'	1:1:529:A:C8	2.55	0.41
1:1:541:U:H2'	1:1:542:G:H8	1.86	0.41
1:1:725:G:H3'	1:1:726:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:787:G:H2'	1:1:788:C:C6	2.55	0.41
1:1:215:G:H2'	1:1:216:G:C8	2.55	0.41
1:1:665:A:H2'	1:1:666:A:H8	1.85	0.41
3:6:220:C:H5'	3:6:221:A:OP1	2.21	0.41
12:L:35:ARG:O	12:L:38:ALA:HB3	2.21	0.41
1:1:1384:U:H2'	1:1:1385:C:C6	2.56	0.40
1:1:29:C:H2'	1:1:30:G:H8	1.85	0.40
1:1:542:G:H2'	1:1:543:C:C6	2.57	0.40
1:1:563:U:H2'	1:1:564:G:C8	2.51	0.40
10:I:161:THR:HA	10:I:171:PHE:O	2.21	0.40
1:1:289:A:H2'	1:1:290:G:H8	1.87	0.40
1:1:68:C:N4	1:1:314:U:O2'	2.46	0.40
1:1:489:C:H2'	1:1:490:A:H8	1.86	0.40
10:I:165:LEU:O	10:I:167:GLU:N	2.52	0.40
2:2:100:U:OP2	2:2:101:U:OP2	2.37	0.40
2:2:149:A:H2'	2:2:150:G:C8	2.56	0.40
22:7:45:THR:O	22:7:49:ASN:CB	2.69	0.40
1:1:159:A:H2'	1:1:160:G:H8	1.86	0.40
1:1:273:A:H2'	1:1:274:G:H8	1.86	0.40
1:1:567:G:H2'	1:1:568:G:C8	2.57	0.40
3:6:231:A:O2'	3:6:232:A:N3	2.44	0.40
22:7:164:GLU:O	22:7:168:ARG:N	2.55	0.40
1:1:1427:U:H2'	1:1:1428:A:C8	2.56	0.40
1:1:1605:A:O2'	1:1:1607:U:OP2	2.36	0.40
1:1:286:U:H2'	1:1:287:G:C8	2.56	0.40
1:1:414:U:H2'	1:1:415:G:C8	2.57	0.40
2:2:142:C:H2'	2:2:143:U:C6	2.56	0.40
3:6:8:A:H2'	3:6:9:A:C8	2.57	0.40
8:F:154:GLY:O	8:F:161:VAL:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	390/463 (84%)	368 (94%)	22 (6%)	0	100	100
5	C	310/362 (86%)	285 (92%)	23 (7%)	2 (1%)	27	69
6	D	188/306 (61%)	177 (94%)	11 (6%)	0	100	100
7	E	168/176 (96%)	158 (94%)	10 (6%)	0	100	100
8	F	240/244 (98%)	225 (94%)	15 (6%)	0	100	100
9	G	185/256 (72%)	170 (92%)	14 (8%)	1 (0%)	31	73
10	I	286/295 (97%)	272 (95%)	14 (5%)	0	100	100
11	K	256/376 (68%)	243 (95%)	13 (5%)	0	100	100
12	L	104/199 (52%)	96 (92%)	7 (7%)	1 (1%)	17	58
13	M	126/138 (91%)	123 (98%)	3 (2%)	0	100	100
14	N	172/204 (84%)	162 (94%)	10 (6%)	0	100	100
15	O	180/199 (90%)	173 (96%)	7 (4%)	0	100	100
16	P	118/184 (64%)	113 (96%)	5 (4%)	0	100	100
17	Q	130/186 (70%)	128 (98%)	2 (2%)	0	100	100
18	S	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
19	X	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
20	Y	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
21	Z	133/136 (98%)	124 (93%)	8 (6%)	1 (1%)	21	64
22	7	152/231 (66%)	137 (90%)	15 (10%)	0	100	100
23	b	220/291 (76%)	207 (94%)	13 (6%)	0	100	100
24	c	95/105 (90%)	93 (98%)	1 (1%)	1 (1%)	16	57
26	e	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
27	f	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
28	g	99/121 (82%)	96 (97%)	2 (2%)	1 (1%)	17	58
29	h	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
30	i	82/100 (82%)	78 (95%)	4 (5%)	0	100	100
31	j	70/88 (80%)	66 (94%)	4 (6%)	0	100	100
32	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
34	n	333/605 (55%)	322 (97%)	11 (3%)	0	100	100
35	o	131/220 (60%)	123 (94%)	8 (6%)	0	100	100
36	p	433/505 (86%)	422 (98%)	11 (2%)	0	100	100
37	s	431/569 (76%)	416 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	t	245/322 (76%)	229 (94%)	14 (6%)	2 (1%)	21	64
40	z	239/278 (86%)	228 (95%)	11 (5%)	0	100	100
All	All	6354/8035 (79%)	6024 (95%)	321 (5%)	9 (0%)	56	88

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	c	100	ILE
38	t	54	LYS
28	g	46	ASP
38	t	56	VAL
5	C	268	ALA
5	C	292	SER
21	Z	59	ALA
12	L	63	VAL
9	G	127	PRO

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	
6	D	4/274 (2%)	4 (100%)	0	100	100
31	j	4/71 (6%)	4 (100%)	0	100	100
All	All	8/345 (2%)	8 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1358/3396 (39%)	339 (24%)	42 (3%)
2	2	157/158 (99%)	35 (22%)	3 (1%)
3	6	85/232 (36%)	44 (51%)	5 (5%)
All	All	1600/3786 (42%)	418 (26%)	50 (3%)

All (418) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	7	C
1	1	12	A
1	1	13	A
1	1	14	U
1	1	18	G
1	1	26	A
1	1	31	C
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	77	A
1	1	92	G
1	1	93	C
1	1	96	G
1	1	109	A
1	1	110	G
1	1	111	C
1	1	113	C
1	1	116	A
1	1	117	U
1	1	118	U
1	1	120	G
1	1	121	A
1	1	122	A
1	1	135	C
1	1	136	G
1	1	143	G
1	1	146	U
1	1	150	A
1	1	155	G
1	1	156	G

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Mol	Chain	Res	Type
1	1	161	G
1	1	163	C
1	1	165	A
1	1	166	C
1	1	167	U
1	1	169	U
1	1	170	G
1	1	173	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	192	C
1	1	199	A
1	1	206	G
1	1	207	U
1	1	210	U
1	1	211	A
1	1	218	G
1	1	219	A
1	1	231	G
1	1	240	U
1	1	241	G
1	1	243	G
1	1	248	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	258	G
1	1	265	A
1	1	266	A
1	1	267	G
1	1	269	G
1	1	295	A
1	1	307	A
1	1	308	A
1	1	309	U
1	1	310	U
1	1	311	C
1	1	314	U
1	1	323	A

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Mol	Chain	Res	Type
1	1	329	U
1	1	332	C
1	1	333	G
1	1	334	A
1	1	339	C
1	1	346	C
1	1	350	C
1	1	352	A
1	1	354	U
1	1	374	A
1	1	375	A
1	1	376	G
1	1	385	A
1	1	388	G
1	1	395	A
1	1	396	A
1	1	397	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	410	U
1	1	421	G
1	1	422	A
1	1	423	A
1	1	430	U
1	1	438	A
1	1	439	C
1	1	440	A
1	1	453	C
1	1	454	C
1	1	463	C
1	1	465	U
1	1	466	G
1	1	467	U
1	1	468	G
1	1	478	A
1	1	479	U
1	1	481	U
1	1	494	G

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Mol	Chain	Res	Type
1	1	503	C
1	1	510	G
1	1	516	A
1	1	517	G
1	1	520	U
1	1	521	A
1	1	523	A
1	1	530	G
1	1	534	U
1	1	535	G
1	1	543	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	551	A
1	1	552	G
1	1	555	U
1	1	556	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	599	C
1	1	600	G
1	1	604	G
1	1	607	A
1	1	609	G
1	1	611	A
1	1	619	A
1	1	621	A
1	1	627	U
1	1	652	G
1	1	677	A
1	1	681	U
1	1	690	A
1	1	691	A
1	1	725	G
1	1	726	G
1	1	728	G
1	1	735	A
1	1	749	C

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Mol	Chain	Res	Type
1	1	750	G
1	1	756	U
1	1	757	C
1	1	762	U
1	1	763	G
1	1	764	U
1	1	765	C
1	1	766	U
1	1	767	U
1	1	770	G
1	1	771	A
1	1	775	A
1	1	776	U
1	1	777	U
1	1	779	G
1	1	780	A
1	1	781	G
1	1	785	G
1	1	801	A
1	1	944	C
1	1	951	A
1	1	1158	A
1	1	1159	A
1	1	1172	G
1	1	1178	G
1	1	1179	A
1	1	1180	A
1	1	1181	U
1	1	1185	C
1	1	1192	C
1	1	1193	A
1	1	1313	G
1	1	1316	C
1	1	1330	A
1	1	1331	U
1	1	1345	G
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U

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Mol	Chain	Res	Type
1	1	1354	G
1	1	1355	A
1	1	1386	A
1	1	1391	C
1	1	1392	G
1	1	1399	A
1	1	1400	G
1	1	1404	G
1	1	1408	G
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1434	G
1	1	1435	A
1	1	1436	U
1	1	1437	C
1	1	1446	A
1	1	1448	U
1	1	1452	A
1	1	1453	A
1	1	1454	A
1	1	1523	U
1	1	1527	C
1	1	1531	C
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1549	U
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1570	U
1	1	1571	A
1	1	1573	G

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Mol	Chain	Res	Type
1	1	1575	A
1	1	1577	G
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1593	A
1	1	1607	U
1	1	1608	C
1	1	1620	U
1	1	1622	U
1	1	1629	U
1	1	1631	C
1	1	1632	A
1	1	1639	C
1	1	1641	U
1	1	1642	A
1	1	1643	A
1	1	1645	U
1	1	1657	C
1	1	1658	G
1	1	1662	G
1	1	1683	A
1	1	1701	C
1	1	1703	U
1	1	1716	U
1	1	1717	U
1	1	1718	G
1	1	1724	U
1	1	1725	C
1	1	1741	A
1	1	1746	U
1	1	1750	A
1	1	1751	G
1	1	1759	C
1	1	1760	A
1	1	1762	C
1	1	1763	U
1	1	1765	U
1	1	1766	G

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Mol	Chain	Res	Type
1	1	1770	G
1	1	1775	G
1	1	1780	G
1	1	1794	G
1	1	1797	A
1	1	1810	A
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1820	U
1	1	1821	U
1	1	1822	C
1	1	1837	U
1	1	1879	A
1	1	1880	U
1	1	1885	U
1	1	1887	A
1	1	2361	A
1	1	3167	A
1	1	3168	A
1	1	3169	U
1	1	3170	A
1	1	3171	U
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3175	U
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3186	A
1	1	3187	A
1	1	3188	G
1	1	3195	U
1	1	3196	U
1	1	3199	G
1	1	3204	C
1	1	3207	U
1	1	3217	C

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Mol	Chain	Res	Type
1	1	3218	A
1	1	3219	G
1	1	3263	G
1	1	3264	G
1	1	3265	C
1	1	3269	U
1	1	3270	U
1	1	3273	A
1	1	3275	U
1	1	3276	G
2	2	16	G
2	2	25	G
2	2	34	U
2	2	35	C
2	2	36	G
2	2	37	A
2	2	39	G
2	2	51	G
2	2	59	A
2	2	62	C
2	2	63	G
2	2	80	A
2	2	81	U
2	2	82	U
2	2	83	C
2	2	84	C
2	2	85	G
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	100	U
2	2	104	A
2	2	106	C
2	2	111	A
2	2	113	U
2	2	124	G
2	2	125	U
2	2	126	A
2	2	127	U
2	2	138	A
2	2	148	G

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Mol	Chain	Res	Type
2	2	151	C
2	2	152	G
2	2	158	U
3	6	2	C
3	6	4	U
3	6	5	C
3	6	6	U
3	6	7	C
3	6	8	A
3	6	13	U
3	6	14	U
3	6	15	C
3	6	16	U
3	6	17	G
3	6	23	U
3	6	24	A
3	6	25	G
3	6	26	U
3	6	27	G
3	6	33	U
3	6	37	C
3	6	40	U
3	6	41	G
3	6	42	G
3	6	52	G
3	6	53	A
3	6	54	A
3	6	55	A
3	6	56	U
3	6	57	U
3	6	58	G
3	6	59	C
3	6	60	U
3	6	61	G
3	6	63	C
3	6	218	A
3	6	219	A
3	6	220	C
3	6	221	A
3	6	223	U
3	6	224	G
3	6	225	U

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Mol	Chain	Res	Type
3	6	226	U
3	6	228	U
3	6	230	A
3	6	231	A
3	6	232	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	239	G
1	1	250	U
1	1	307	A
1	1	309	U
1	1	406	G
1	1	420	G
1	1	452	G
1	1	465	U
1	1	493	G
1	1	761	A
1	1	765	C
1	1	1329	U
1	1	1525	G
1	1	1554	U
1	1	1556	C
1	1	1560	G
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1570	U
1	1	1573	G
1	1	1574	C
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1606	U
1	1	1607	U
1	1	1630	U
1	1	1641	U
1	1	1643	A
1	1	1657	C
1	1	1716	U

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Mol	Chain	Res	Type
1	1	1814	A
1	1	1816	A
1	1	1820	U
1	1	1886	A
1	1	3166	C
1	1	3168	A
1	1	3169	U
1	1	3218	A
1	1	3269	U
2	2	36	G
2	2	123	G
2	2	126	A
3	6	16	U
3	6	25	G
3	6	60	U
3	6	222	A
3	6	225	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	d	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	272:UNK	C	283:UNK	N	25.28
1	d	379:UNK	C	381:UNK	N	6.01