

Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 13, 2018 – 11:28 AM EDT

PDB ID : 6DNC
EMDB ID: : EMD-7970
Title : E.coli RF1 bound to E.coli 70S ribosome in response to UAU sense A-site codon
Authors : Svidritskiy, E.; Demo, G.; Korostelev, A.A.
Deposited on : 2018-06-06
Resolution : 3.70 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-20031172

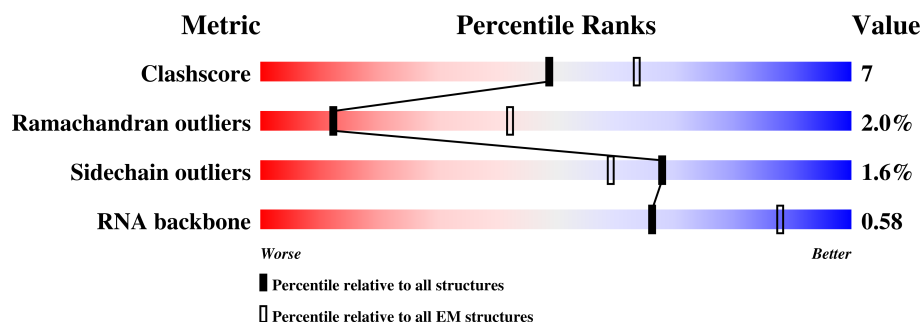
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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

















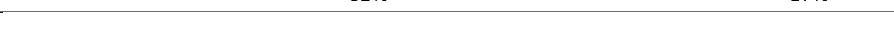




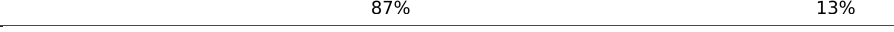





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	A	1539	64% 33% .
2	B	2903	66% 30% .
3	C	120	62% 36% .
4	D	77	45% 49% 5%
4	LA	77	69% 27% .
5	E	234	70% 24% 6%
6	F	273	79% 19% .
7	G	209	81% 18% .

















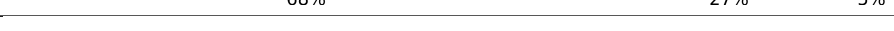
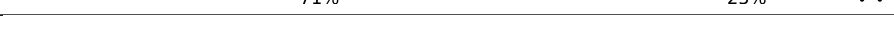
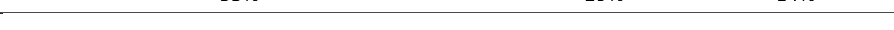
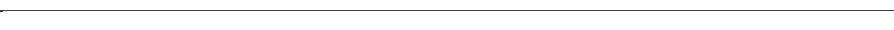
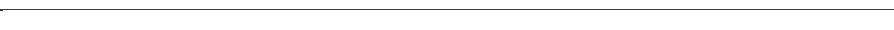




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Mol	Chain	Length	Quality of chain
8	H	201	 83% 16% .
9	I	179	 77% 22% .
10	J	177	 79% 19% ..
11	K	149	 69% 30% .
12	L	165	 52% 24% .. 21%
13	M	142	 68% 29% ..
14	N	142	 83% 16% .
15	O	123	 79% 18% ..
16	P	144	 81% 17% ..
17	Q	136	 89% 10% .
18	R	127	 66% 28% . 6%
19	S	117	 79% 19% ..
20	T	115	 81% 18% .
21	U	118	 82% 17% .
22	V	103	 79% 19% .
23	W	110	 83% 15% .
24	X	100	 87% 6% 7%
25	Y	104	 83% 15% .
26	Z	94	 87% 13%
27	AA	85	 74% 14% 12%
28	BA	78	 91% 8% .
29	CA	63	 86% 14%
30	DA	59	 81% 17% .
31	EA	70	 74% 19% . 6%
32	FA	57	 79% 19% .

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Mol	Chain	Length	Quality of chain
33	GA	55	 89% 9%
34	HA	46	 76% 22%
35	IA	65	 82% 15%
36	JA	38	 74% 24%
37	KA	27	 41% 30% 30%
38	MA	362	 73% 20% 5%
39	OA	241	 77% 15% 7%
40	PA	233	 67% 20% 12%
41	QA	206	 77% 21%
42	RA	167	 71% 22% 6%
43	SA	131	 53% 19% 24%
44	TA	156	 90% 7%
45	UA	130	 81% 18%
46	VA	130	 72% 25%
47	WA	103	 61% 32% 5%
48	XA	129	 73% 16% 10%
49	YA	124	 68% 27% 5%
50	ZA	118	 71% 25%
51	AB	102	 53% 29% 14%
52	BB	89	 83% 16%
53	CB	82	 71% 27%
54	DB	84	 70% 23% 5%
55	EB	75	 75% 11% 13%
56	FB	92	 61% 24% 14%
57	GB	87	 87% 10%

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Mol	Chain	Length	Quality of chain
58	HB	71	<div><div></div><div>55%</div><div>32%</div><div>• 8%</div></div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 152438 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2903	Total	C	N	O	P	0	0
			62318	27801	11468	20147	2902		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	747	C	U	conflict	GB 1036415628
B	1847	G	A	conflict	GB 1036415628

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	A	-	expression tag	GB 1370526515

- Molecule 4 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
4	LA	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 5 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	220	Total	C	N	O	S	0	0
			1637	1023	298	310	6		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AA	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CA	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DA	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	EA	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 32 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FA	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	GA	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 34 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	HA	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 35 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	IA	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 36 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JA	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	KA	19	Total	C	N	O	P	0	0
			412	186	83	125	18		

- Molecule 38 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	MA	344	Total	C	N	O	S	0	0
			2714	1656	507	538	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	361	LEU	-	expression tag	UNP B7MKB3
MA	362	GLU	-	expression tag	UNP B7MKB3

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	OA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	PA	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	QA	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	RA	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SA	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	TA	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	UA	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	VA	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	WA	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	XA	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	YA	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	ZA	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AB	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	35	ALA	-	insertion	UNP B7MCS2

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BB	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CB	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DB	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EB	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FB	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GB	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

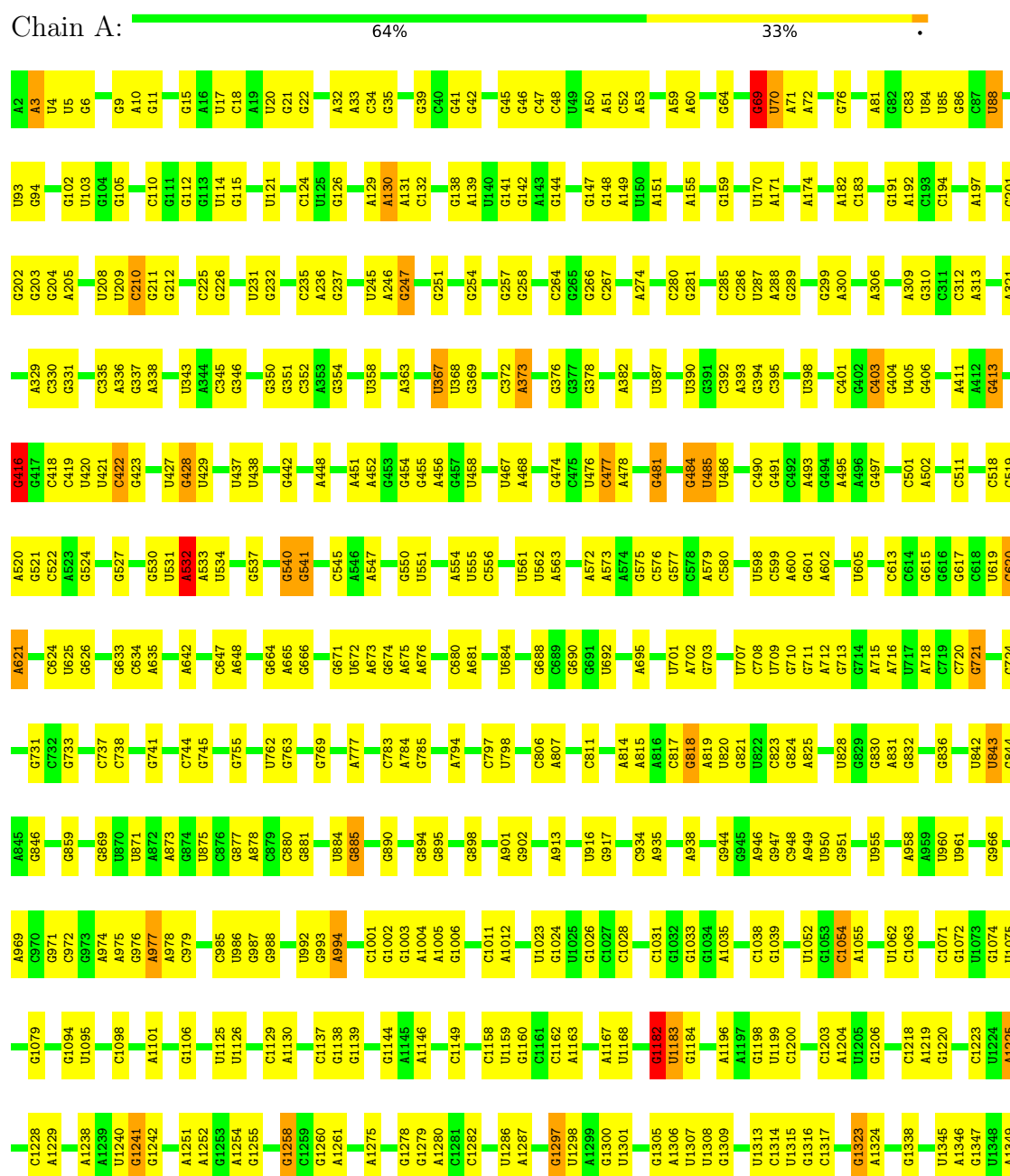
- Molecule 58 is a protein called 30S ribosomal protein S21.

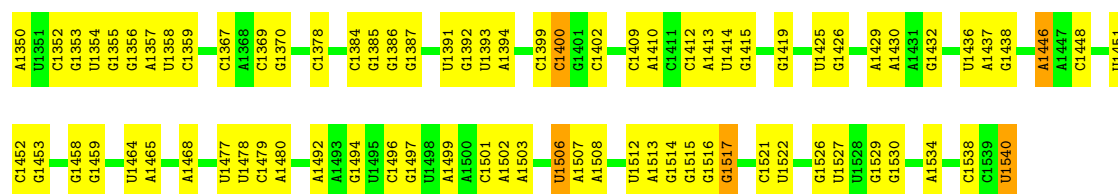
Mol	Chain	Residues	Atoms					AltConf	Trace
58	HB	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

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.

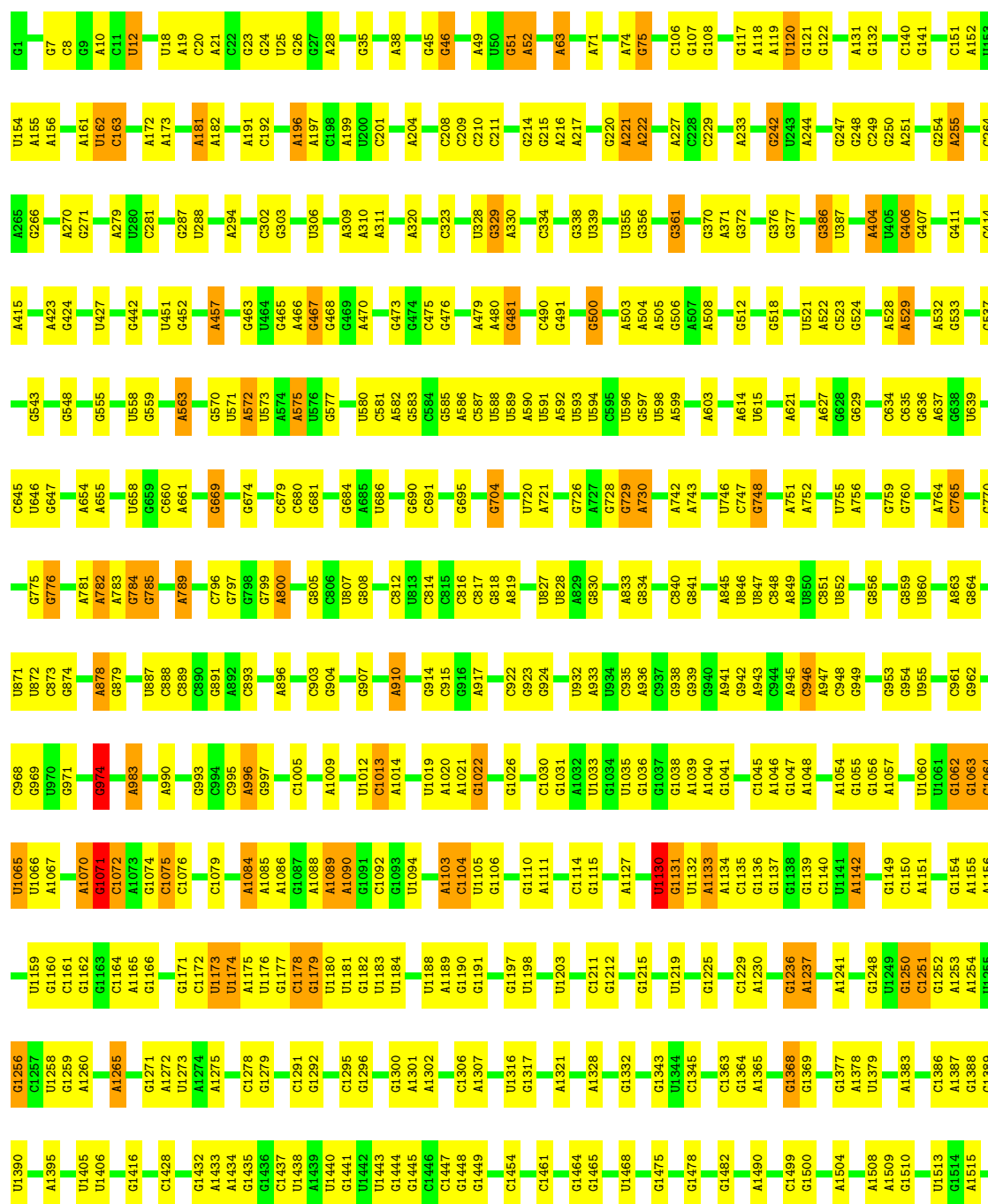
• Molecule 1: 16S ribosomal RNA

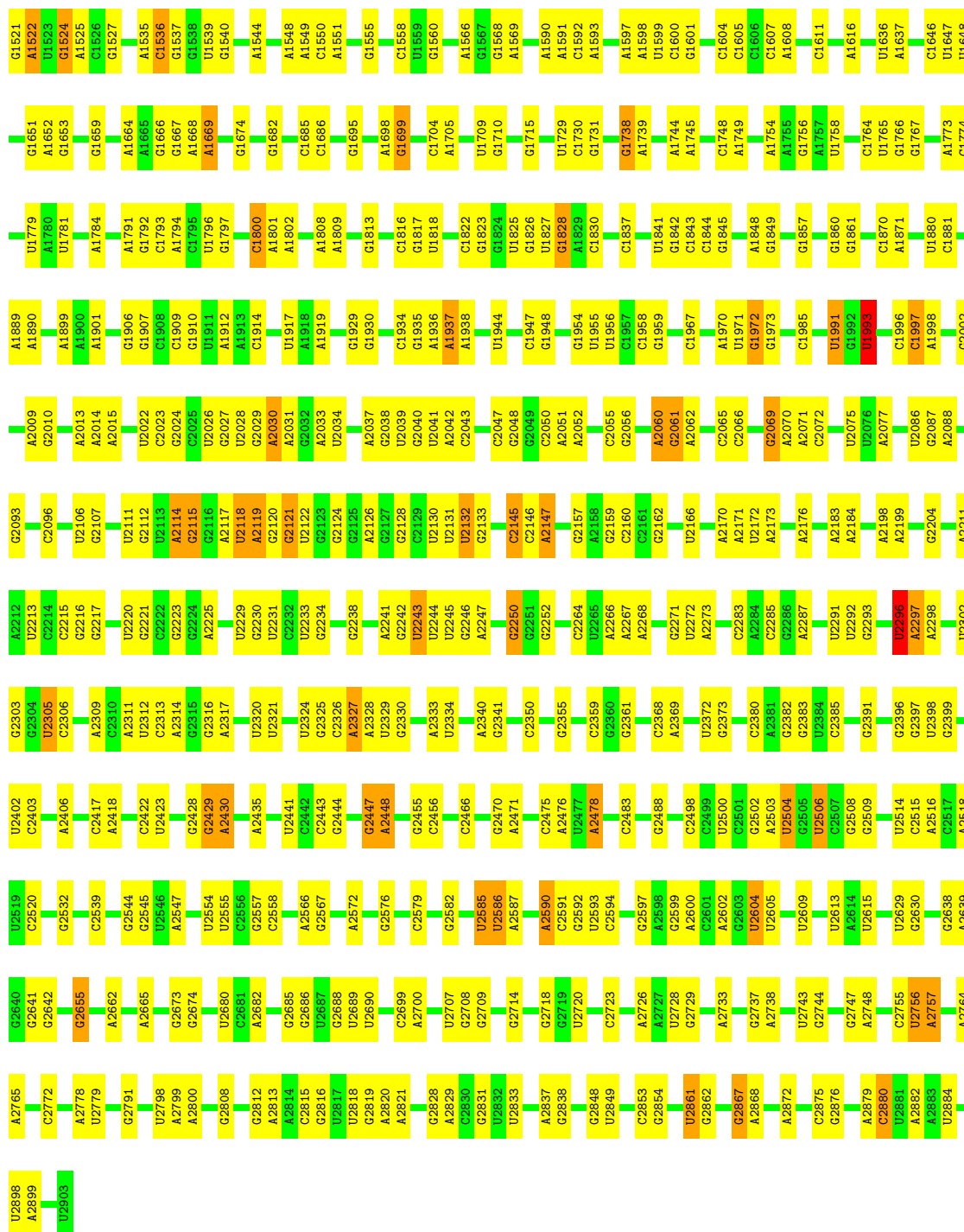




• Molecule 2: 23S ribosomal RNA

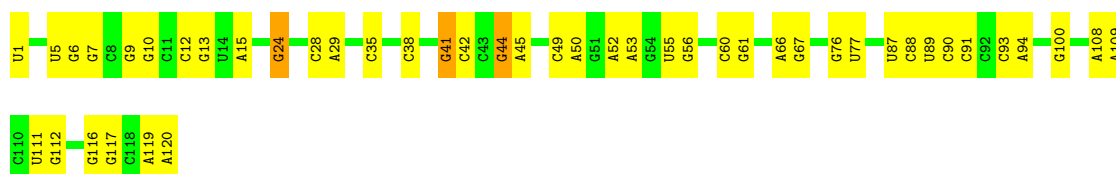
Chain B: 66% 30% •



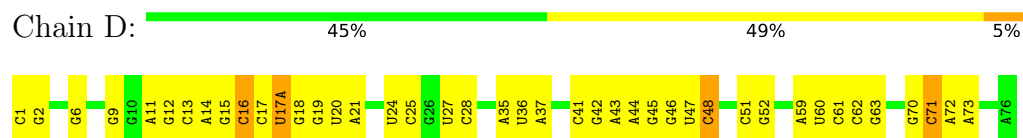


• Molecule 3: 5S ribosomal RNA

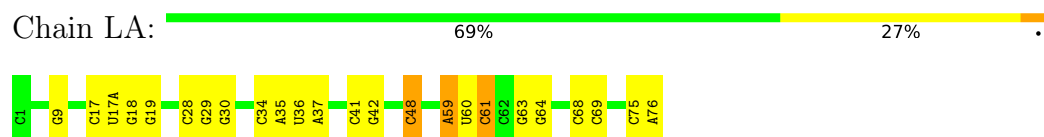
Chain C: 62% 36%



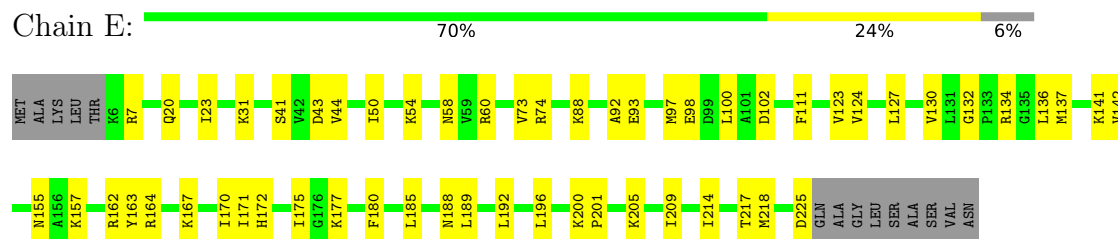
- Molecule 4: tRNA(fMet)



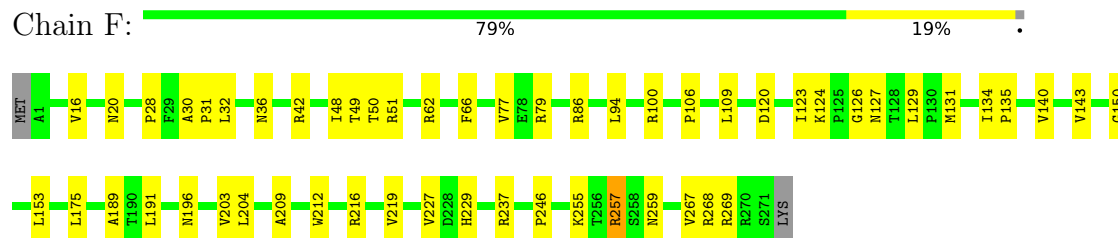
- Molecule 4: tRNA(fMet)



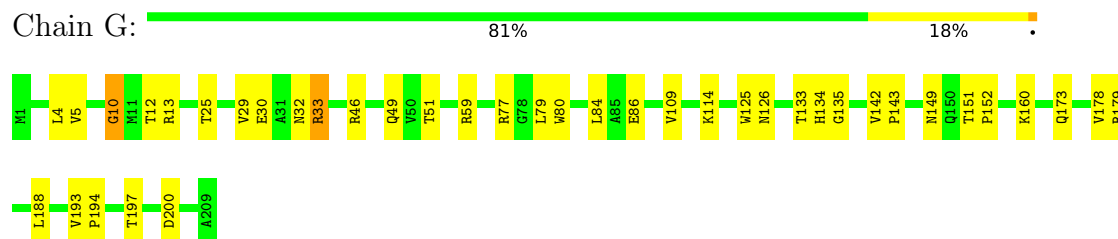
- Molecule 5: 50S ribosomal protein L1



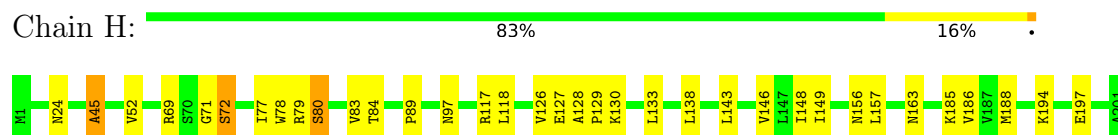
- Molecule 6: 50S ribosomal protein L2



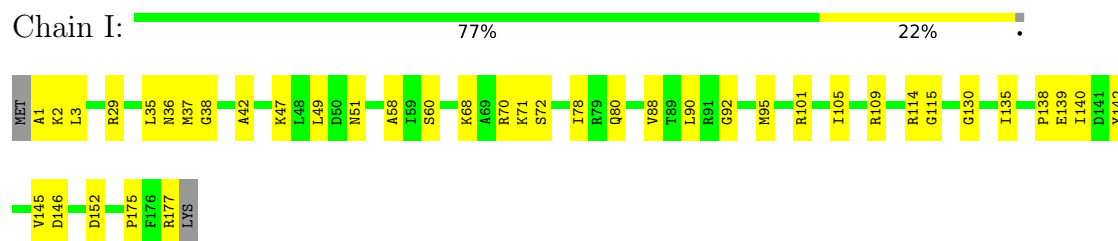
- Molecule 7: 50S ribosomal protein L3



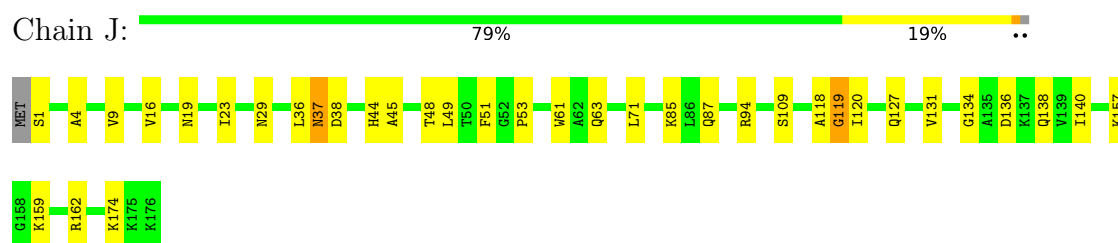
- Molecule 8: 50S ribosomal protein L4



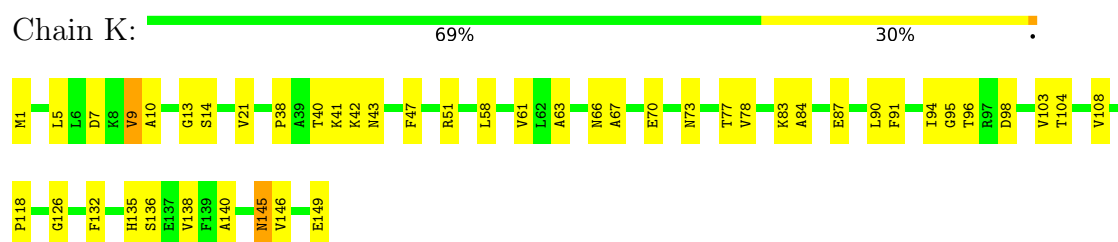
- Molecule 9: 50S ribosomal protein L5



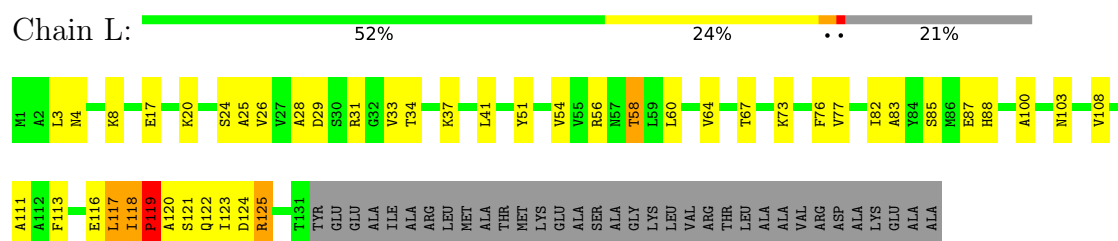
- Molecule 10: 50S ribosomal protein L6



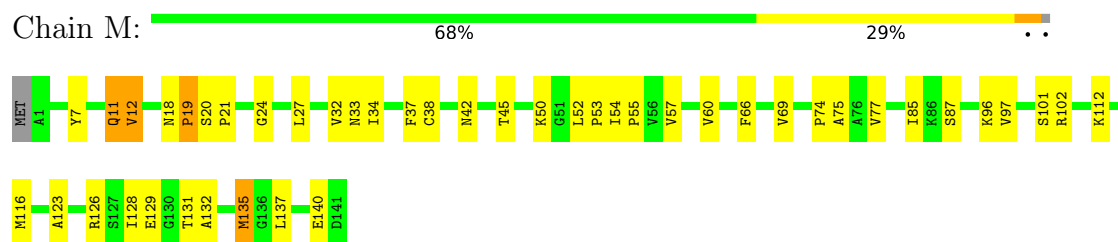
- Molecule 11: 50S ribosomal protein L9



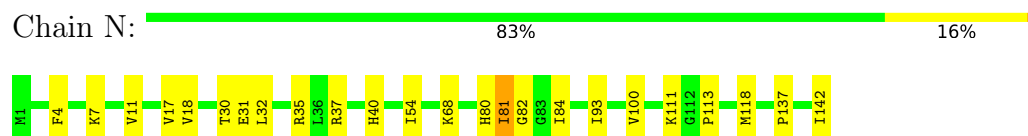
- Molecule 12: 50S ribosomal protein L10



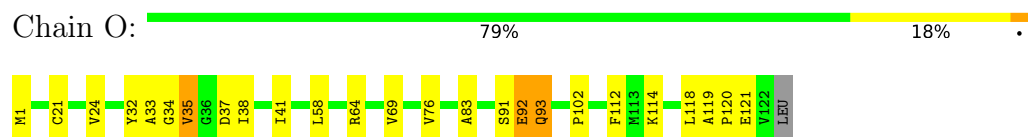
- Molecule 13: 50S ribosomal protein L11



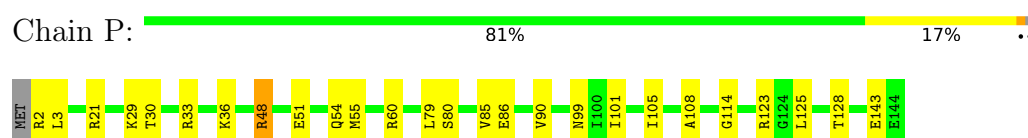
- Molecule 14: 50S ribosomal protein L13



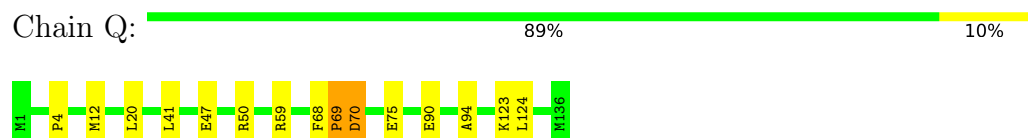
- Molecule 15: 50S ribosomal protein L14



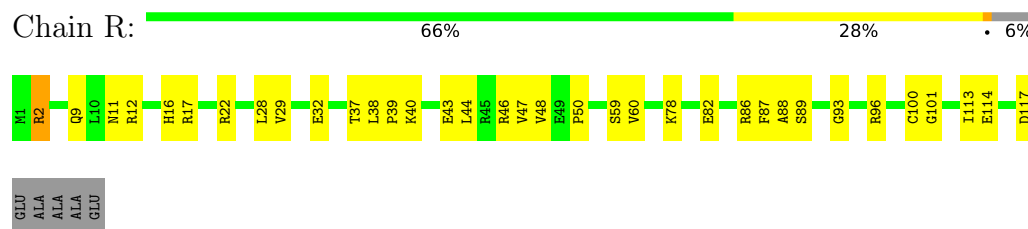
- Molecule 16: 50S ribosomal protein L15



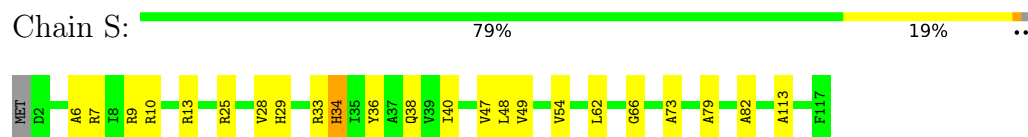
- Molecule 17: 50S ribosomal protein L16



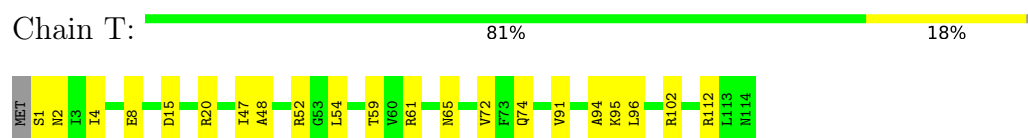
- Molecule 18: 50S ribosomal protein L17




- Molecule 19: 50S ribosomal protein L18



- Molecule 20: 50S ribosomal protein L19




- Molecule 21: 50S ribosomal protein L20

Chain U:  82% 17%




- Molecule 22: 50S ribosomal protein L21

Chain V:  79% 19%



- Molecule 23: 50S ribosomal protein L22

Chain W:  83% 15%




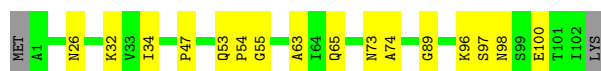
- Molecule 24: 50S ribosomal protein L23

Chain X:  87% 6% 7%




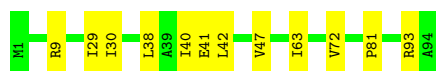
- Molecule 25: 50S ribosomal protein L24

Chain Y:  83% 15%



- Molecule 26: 50S ribosomal protein L25

Chain Z:  87% 13%



- Molecule 27: 50S ribosomal protein L27

Chain AA:  74% 14% 12%



- Molecule 28: 50S ribosomal protein L28

Chain BA:  91% 8%



- Molecule 29: 50S ribosomal protein L29

Chain CA: 86% 14%



- Molecule 30: 50S ribosomal protein L30

Chain DA: 81% 17%



- Molecule 31: 50S ribosomal protein L31

Chain EA: 74% 19% 6%



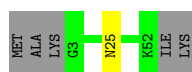
- Molecule 32: 50S ribosomal protein L32

Chain FA: 79% 19%



- Molecule 33: 50S ribosomal protein L33

Chain GA: 89% 9%



- Molecule 34: 50S ribosomal protein L34

Chain HA: 76% 22%



- Molecule 35: 50S ribosomal protein L35

Chain IA: 82% 15%



- Molecule 36: 50S ribosomal protein L36

Chain JA:  74% 24% .




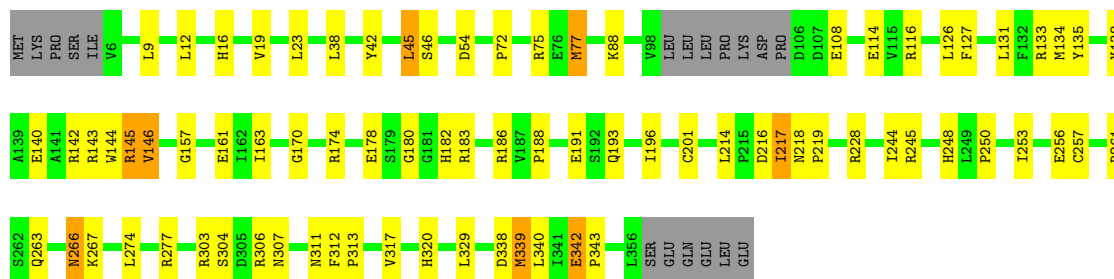
- Molecule 37: mRNA

Chain KA:  41% 30% 30%




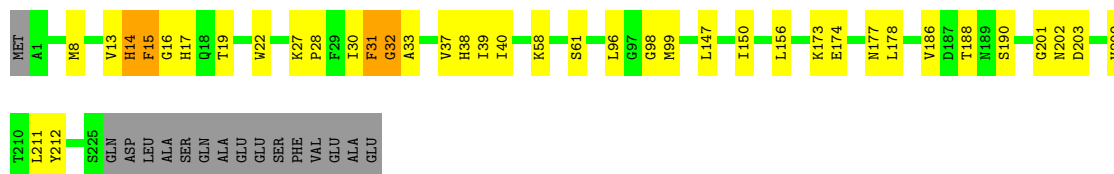
- Molecule 38: Peptide chain release factor 1

Chain MA:  73% 20% . 5%



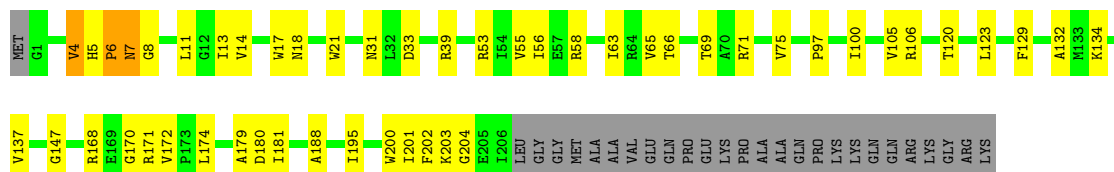
- Molecule 39: 30S ribosomal protein S2

Chain OA:  77% 15% . 7%




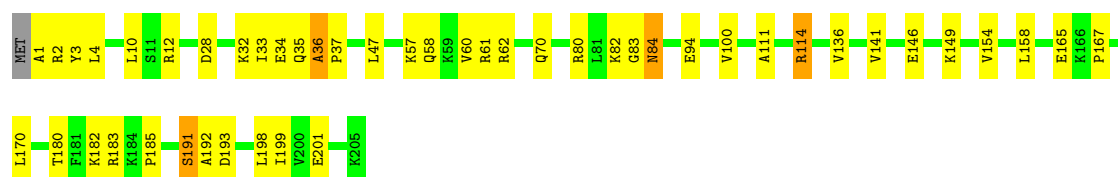
- Molecule 40: 30S ribosomal protein S3

Chain PA:  67% 20% . 12%



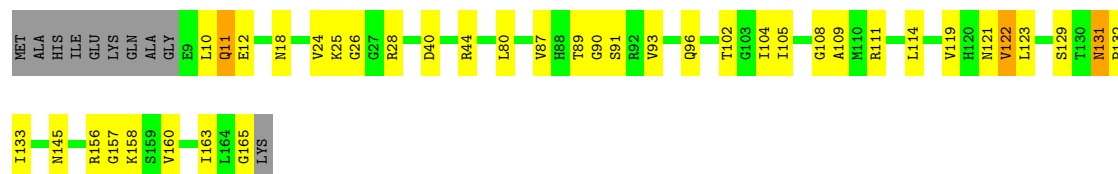
- Molecule 41: 30S ribosomal protein S4

Chain QA:  77% 21% .



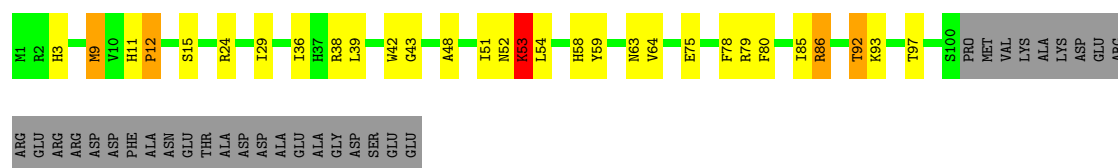
- Molecule 42: 30S ribosomal protein S5

Chain RA: 71% 22% 6%



- Molecule 43: 30S ribosomal protein S6

Chain SA: 53% 19% 24%



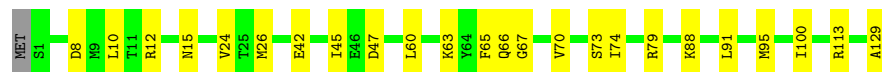
- Molecule 44: 30S ribosomal protein S7

Chain TA: 90% 7%



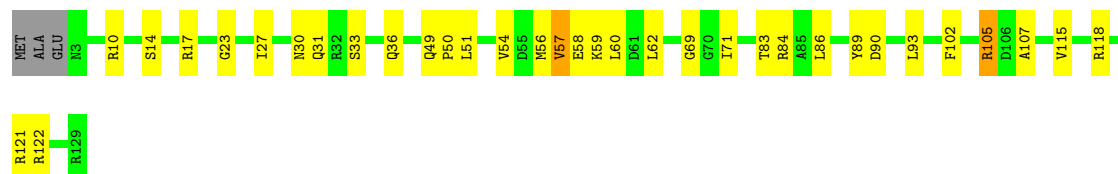
- Molecule 45: 30S ribosomal protein S8

Chain UA: 81% 18%



- Molecule 46: 30S ribosomal protein S9

Chain VA: 72% 25%



- Molecule 47: 30S ribosomal protein S10

Chain WA:  61% 32% 5%



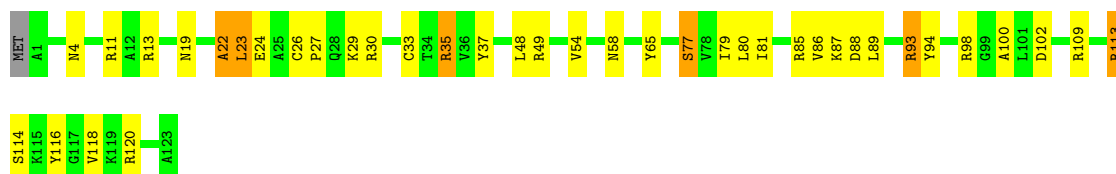
- Molecule 48: 30S ribosomal protein S11

Chain XA:  73% 16% 10%



- Molecule 49: 30S ribosomal protein S12

Chain YA:  68% 27% 5%



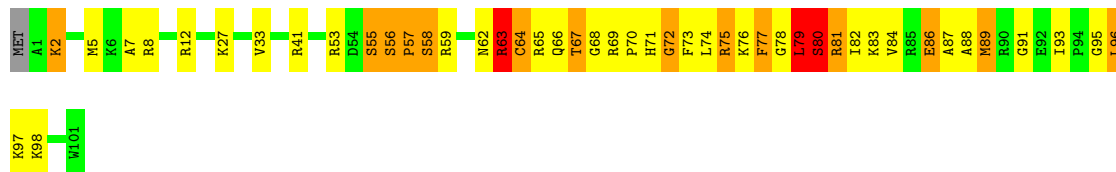
- Molecule 50: 30S ribosomal protein S13

Chain ZA:  71% 25% 2%




- Molecule 51: 30S ribosomal protein S14

Chain AB:  53% 29% 14%



- Molecule 52: 30S ribosomal protein S15

Chain BB:  83% 16% 1%



- Molecule 53: 30S ribosomal protein S16

Chain CB:  71% 27% .




- Molecule 54: 30S ribosomal protein S17

Chain DB:  70% 23% . 5%



- Molecule 55: 30S ribosomal protein S18

Chain EB:  75% 11% . 13%




- Molecule 56: 30S ribosomal protein S19

Chain FB:  61% 24% . 14%



- Molecule 57: 30S ribosomal protein S20

Chain GB:  87% 10% .



- Molecule 58: 30S ribosomal protein S21

Chain HB:  55% 32% . 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	639088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	22000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.43	0/36963	0.70	4/57662 (0.0%)
10	J	0.35	0/1343	0.64	1/1816 (0.1%)
11	K	0.45	0/1122	0.73	0/1515
12	L	0.51	0/1001	0.81	2/1350 (0.1%)
13	M	0.47	0/1046	0.69	0/1410
14	N	0.33	0/1152	0.60	0/1551
15	O	0.34	0/947	0.66	0/1268
16	P	0.34	0/1054	0.64	0/1403
17	Q	0.37	0/1093	0.66	0/1460
18	R	0.38	0/973	0.70	0/1301
19	S	0.35	0/902	0.59	0/1209
2	B	0.42	1/69797 (0.0%)	0.70	11/108890 (0.0%)
20	T	0.35	0/929	0.65	0/1242
21	U	0.39	0/960	0.65	0/1278
22	V	0.37	0/829	0.71	1/1107 (0.1%)
23	W	0.36	0/864	0.70	1/1156 (0.1%)
24	X	0.37	0/744	0.61	0/994
25	Y	0.36	0/787	0.66	0/1051
26	Z	0.34	0/766	0.57	0/1025
27	AA	0.35	0/582	0.61	0/769
28	BA	0.35	0/635	0.64	0/848
29	CA	0.36	0/510	0.69	0/677
3	C	0.41	0/2872	0.71	1/4479 (0.0%)
30	DA	0.32	0/453	0.63	0/605
31	EA	0.45	0/531	0.64	0/709
32	FA	0.33	0/450	0.61	0/599
33	GA	0.34	0/416	0.59	0/554
34	HA	0.37	0/380	0.65	0/498
35	IA	0.34	0/513	0.66	0/676
36	JA	0.45	0/303	0.74	0/397
37	KA	0.40	0/464	0.69	0/723
38	MA	0.85	0/2751	0.67	1/3703 (0.0%)
39	OA	0.55	1/1787 (0.1%)	0.80	3/2408 (0.1%)
4	D	0.40	0/1832	0.68	0/2855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	LA	0.39	0/1832	0.67	0/2855
40	PA	0.45	1/1651 (0.1%)	0.68	1/2225 (0.0%)
41	QA	0.38	0/1665	0.66	0/2227
42	RA	0.45	0/1169	0.78	1/1573 (0.1%)
43	SA	0.40	0/835	0.77	1/1128 (0.1%)
44	TA	0.36	0/1195	0.60	0/1602
45	UA	0.33	0/989	0.63	0/1326
46	VA	0.40	0/1034	0.66	0/1375
47	WA	0.36	0/796	0.70	0/1077
48	XA	0.35	0/885	0.65	0/1195
49	YA	0.38	0/969	0.76	1/1300 (0.1%)
5	E	0.37	0/1652	0.60	0/2227
50	ZA	0.40	0/892	0.66	0/1193
51	AB	0.88	4/822 (0.5%)	1.12	4/1095 (0.4%)
52	BB	0.37	0/722	0.65	0/964
53	CB	0.36	0/659	0.67	0/884
54	DB	0.34	0/657	0.67	0/881
55	EB	0.42	0/544	0.62	0/731
56	FB	0.38	0/652	0.64	0/877
57	GB	0.34	0/671	0.52	0/888
58	HB	0.49	0/550	0.78	0/728
6	F	0.34	0/2121	0.69	0/2852
7	G	0.35	0/1586	0.64	0/2134
8	H	0.36	0/1571	0.65	0/2113
9	I	0.39	0/1434	0.64	0/1926
All	All	0.43	7/165304 (0.0%)	0.70	33/246564 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
2	B	0	33
3	C	0	1
4	D	0	1
All	All	0	45

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	OA	31	PHE	C-O	7.44	1.37	1.23
51	AB	77	PHE	CB-CG	7.04	1.63	1.51
51	AB	63	ARG	CB-CG	6.01	1.68	1.52
40	PA	97	PRO	N-CD	5.77	1.55	1.47
51	AB	86	GLU	C-O	5.27	1.33	1.23
2	B	2590	A	C5-C6	5.14	1.45	1.41
51	AB	77	PHE	C-O	5.04	1.32	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	OA	32	GLY	N-CA-C	12.97	145.52	113.10
51	AB	79	LEU	CA-CB-CG	12.43	143.88	115.30
39	OA	31	PHE	C-N-CA	-9.34	102.70	122.30
12	L	119	PRO	N-CA-C	-8.80	89.22	112.10
2	B	974	G	N9-C1'-C2'	7.74	124.07	114.00
22	V	50	GLY	N-CA-C	-7.62	94.04	113.10
2	B	669	G	N9-C1'-C2'	7.60	123.88	114.00
3	C	41	G	N9-C1'-C2'	7.49	123.74	114.00
38	MA	342	GLU	C-N-CD	7.16	143.44	128.40
2	B	12	U	N1-C1'-C2'	6.47	122.42	114.00
51	AB	55	SER	N-CA-C	-6.39	93.75	111.00
2	B	729	G	N9-C1'-C2'	6.08	121.90	114.00
1	A	1225	A	N9-C1'-C2'	6.04	121.86	114.00
2	B	1130	U	C2'-C3'-O3'	5.95	123.22	113.70
1	A	1297	G	C2'-C3'-O3'	5.56	122.60	113.70
39	OA	16	GLY	C-N-CA	-5.48	108.00	121.70
1	A	1301	U	N1-C1'-C2'	5.40	121.02	114.00
2	B	933	A	N9-C1'-C2'	5.39	121.01	114.00
51	AB	63	ARG	CA-CB-CG	5.39	125.26	113.40
2	B	2430	A	N9-C1'-C2'	5.34	120.95	114.00
43	SA	53	LYS	N-CA-C	-5.34	96.58	111.00
2	B	2296	U	N1-C1'-C2'	5.22	120.78	114.00
40	PA	17	TRP	C-N-CA	-5.21	108.69	121.70
23	W	63	GLY	N-CA-C	5.19	126.08	113.10
1	A	69	G	C2'-C3'-O3'	5.19	122.00	113.70
2	B	1071	G	N9-C1'-C2'	5.17	120.72	114.00
10	J	119	GLY	N-CA-C	5.15	125.98	113.10
42	RA	121	ASN	N-CA-C	5.12	124.81	111.00
51	AB	72	GLY	N-CA-C	5.10	125.84	113.10
49	YA	22	ALA	N-CA-C	-5.09	97.25	111.00
2	B	51	G	C2'-C3'-O3'	5.08	121.83	113.70
2	B	1343	G	N9-C1'-C2'	5.04	120.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	117	LEU	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1167	A	Sidechain
1	A	1182	G	Sidechain
1	A	1316	G	Sidechain
1	A	159	G	Sidechain
1	A	350	G	Sidechain
1	A	416	G	Sidechain
1	A	532	A	Sidechain
1	A	563	A	Sidechain
1	A	898	G	Sidechain
1	A	938	A	Sidechain
2	B	1063	G	Sidechain
2	B	1154	G	Sidechain
2	B	1171	G	Sidechain
2	B	1215	G	Sidechain
2	B	1241	A	Sidechain
2	B	1328	A	Sidechain
2	B	1377	G	Sidechain
2	B	1666	G	Sidechain
2	B	1817	G	Sidechain
2	B	1828	G	Sidechain
2	B	1857	G	Sidechain
2	B	1937	A	Sidechain
2	B	196	A	Sidechain
2	B	1985	C	Sidechain
2	B	1993	U	Sidechain
2	B	201	C	Sidechain
2	B	2061	G	Sidechain
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	2266	A	Sidechain
2	B	2273	A	Sidechain
2	B	2447	G	Sidechain
2	B	2475	C	Sidechain
2	B	2532	G	Sidechain
2	B	26	G	Sidechain
2	B	2604	U	Sidechain

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Mol	Chain	Res	Type	Group
2	B	2662	A	Sidechain
2	B	370	G	Sidechain
2	B	481	G	Sidechain
2	B	500	G	Sidechain
2	B	506	G	Sidechain
2	B	512	G	Sidechain
2	B	75	G	Sidechain
3	C	1	U	Sidechain
4	D	71	C	Sidechain

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	A	33012	0	16618	278	0
2	B	62318	0	31346	532	0
3	C	2568	0	1303	25	0
4	D	1640	0	837	28	0
4	LA	1640	0	837	15	0
5	E	1637	0	1719	40	0
6	F	2082	0	2157	36	0
7	G	1565	0	1616	32	0
8	H	1552	0	1619	27	0
9	I	1410	0	1447	24	0
10	J	1323	0	1374	22	0
11	K	1111	0	1148	24	0
12	L	988	0	1025	37	0
13	M	1032	0	1088	32	0
14	N	1129	0	1162	18	0
15	O	938	0	1012	16	0
16	P	1045	0	1117	16	0
17	Q	1074	0	1157	12	0
18	R	960	0	1000	26	0
19	S	892	0	923	16	0
20	T	917	0	965	16	0
21	U	947	0	1022	20	0
22	V	816	0	839	17	0
23	W	857	0	922	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	738	0	807	5	0
25	Y	779	0	834	8	0
26	Z	753	0	780	9	0
27	AA	575	0	592	8	0
28	BA	625	0	655	3	0
29	CA	509	0	543	5	0
30	DA	449	0	491	6	0
31	EA	522	0	524	9	0
32	FA	444	0	461	8	0
33	GA	409	0	440	1	0
34	HA	377	0	418	8	0
35	IA	504	0	574	11	0
36	JA	302	0	343	10	0
37	KA	412	0	207	7	0
38	MA	2714	0	2636	60	0
39	OA	1756	0	1787	27	0
40	PA	1624	0	1699	37	0
41	QA	1643	0	1710	35	0
42	RA	1156	0	1199	24	0
43	SA	817	0	808	22	0
44	TA	1181	0	1240	4	0
45	UA	979	0	1034	14	0
46	VA	1022	0	1070	21	0
47	WA	786	0	828	25	0
48	XA	869	0	878	16	0
49	YA	955	0	1019	30	0
50	ZA	883	0	944	21	0
51	AB	810	0	852	57	0
52	BB	714	0	737	6	0
53	CB	649	0	666	18	0
54	DB	648	0	691	13	0
55	EB	535	0	552	7	0
56	FB	637	0	665	16	0
57	GB	665	0	714	5	0
58	HB	544	0	579	18	0
All	All	152438	0	104230	1687	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 7.

All (1687) 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)
38:MA:77:MET:CE	38:MA:77:MET:SD	2.04	1.45
39:OA:32:GLY:O	39:OA:38:HIS:HA	1.51	1.08
39:OA:33:ALA:HA	39:OA:37:VAL:O	1.52	1.08
51:AB:73:PHE:HA	51:AB:78:GLY:HA2	1.07	1.03
12:L:119:PRO:CD	12:L:120:ALA:H	1.63	1.03
51:AB:79:LEU:O	51:AB:80:SER:O	1.76	1.01
51:AB:73:PHE:CA	51:AB:78:GLY:HA2	1.90	1.01
12:L:24:SER:O	12:L:116:GLU:HB2	1.64	0.98
39:OA:31:PHE:O	39:OA:39:ILE:HB	1.63	0.98
51:AB:55:SER:O	51:AB:56:SER:C	2.06	0.92
40:PA:4:VAL:HG13	40:PA:5:HIS:H	1.33	0.91
12:L:119:PRO:HD2	12:L:120:ALA:H	1.34	0.89
51:AB:73:PHE:HA	51:AB:78:GLY:CA	2.00	0.88
47:WA:57:VAL:HG22	47:WA:58:ASN:H	1.38	0.88
39:OA:13:VAL:O	39:OA:14:HIS:O	1.91	0.87
12:L:119:PRO:HG2	12:L:121:SER:H	1.39	0.87
4:D:71:C:H2'	4:D:72:A:C8	2.09	0.86
51:AB:56:SER:O	51:AB:58:SER:N	2.08	0.86
1:A:1399:C:H4'	1:A:1400:C:H5'	1.58	0.86
29:CA:19:LEU:O	29:CA:23:ARG:HB2	1.76	0.85
12:L:119:PRO:CD	12:L:120:ALA:N	2.38	0.85
51:AB:80:SER:O	51:AB:82:ILE:N	2.08	0.85
9:I:1:ALA:O	9:I:3:LEU:N	2.08	0.85
43:SA:3:HIS:H	43:SA:92:THR:HG22	1.42	0.85
13:M:11:GLN:O	13:M:54:ILE:O	1.95	0.85
1:A:376:G:H5''	53:CB:5:ARG:HB2	1.59	0.84
39:OA:14:HIS:CG	39:OA:15:PHE:H	1.93	0.84
2:B:962:G:H21	2:B:2250:G:H22	1.24	0.84
2:B:1668:A:H4'	2:B:1669:A:H5'	1.59	0.83
4:LA:75:C:OP2	38:MA:261:ARG:NH2	2.12	0.82
38:MA:16:HIS:O	38:MA:19:VAL:HG12	1.80	0.81
1:A:484:G:H4'	1:A:485:U:H5'	1.61	0.81
9:I:142:TYR:O	9:I:145:VAL:HG22	1.79	0.80
47:WA:64:GLN:O	51:AB:98:LYS:HA	1.82	0.79
18:R:87:PHE:O	18:R:89:SER:N	2.15	0.78
51:AB:87:ALA:O	51:AB:91:GLY:N	2.18	0.77
39:OA:30:ILE:HG22	39:OA:32:GLY:H	1.48	0.77
2:B:1019:U:H3	2:B:1142:A:H62	1.33	0.77
55:EB:11:ARG:HG3	55:EB:14:ALA:HB3	1.67	0.77
41:QA:33:ILE:HG13	41:QA:34:GLU:H	1.49	0.77
51:AB:79:LEU:O	51:AB:80:SER:C	2.23	0.76
13:M:101:SER:HA	13:M:140:GLU:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:G:H22	1:A:1035:A:H2	1.32	0.76
13:M:54:ILE:HG23	13:M:55:PRO:HD2	1.68	0.76
12:L:118:ILE:N	12:L:119:PRO:CD	2.49	0.76
13:M:54:ILE:CG2	13:M:55:PRO:HD2	2.17	0.75
2:B:1912:A:H62	2:B:1917:U:H5	1.34	0.75
2:B:1521:G:H3'	2:B:1522:A:H5''	1.68	0.74
38:MA:339:MET:O	38:MA:343:PRO:HD3	1.87	0.74
51:AB:77:PHE:HB3	51:AB:79:LEU:HD23	1.70	0.74
51:AB:78:GLY:O	51:AB:80:SER:N	2.21	0.73
44:TA:55:LYS:HB3	44:TA:59:GLU:HG3	1.70	0.73
1:A:537:G:H5''	49:YA:109:ARG:HH12	1.53	0.73
48:XA:87:GLY:H	48:XA:113:THR:HG22	1.54	0.73
51:AB:79:LEU:HB2	51:AB:83:LYS:HB2	1.69	0.73
7:G:142:VAL:HG22	7:G:143:PRO:HD2	1.70	0.73
1:A:413:G:H1'	1:A:428:G:H22	1.53	0.72
12:L:118:ILE:O	12:L:118:ILE:HG22	1.86	0.72
43:SA:11:HIS:HD2	43:SA:12:PRO:HD2	1.53	0.72
11:K:63:ALA:HA	11:K:66:ASN:HD22	1.55	0.72
49:YA:22:ALA:O	49:YA:23:LEU:HB2	1.90	0.72
3:C:38:C:H42	3:C:44:G:H1	1.38	0.71
49:YA:33:CYS:H	49:YA:54:VAL:HG13	1.55	0.71
1:A:3:A:H5''	1:A:4:U:H5'	1.73	0.71
38:MA:214:LEU:HG	38:MA:216:ASP:H	1.56	0.70
2:B:807:U:H2'	2:B:808:G:H8	1.57	0.70
53:CB:79:ASN:HB2	53:CB:82:ALA:HB3	1.71	0.70
15:O:21:CYS:HA	15:O:41:ILE:HG22	1.73	0.70
43:SA:38:ARG:HD3	43:SA:97:THR:HA	1.74	0.70
2:B:955:U:H5	2:B:962:G:H1	1.39	0.69
41:QA:36:ALA:H	41:QA:37:PRO:HD3	1.57	0.69
9:I:92:GLY:O	9:I:95:MET:HG2	1.92	0.69
49:YA:54:VAL:HG21	49:YA:79:ILE:HD11	1.74	0.69
8:H:45:ALA:HB2	8:H:89:PRO:HD3	1.74	0.69
38:MA:183:ARG:HE	38:MA:306:ARG:HD3	1.56	0.69
39:OA:30:ILE:HG22	39:OA:32:GLY:N	2.08	0.69
2:B:2478:A:H5'	36:JA:32:LYS:HD2	1.74	0.69
46:VA:83:THR:HG21	46:VA:102:PHE:HB3	1.74	0.68
2:B:1278:C:H2'	2:B:1279:G:H8	1.58	0.68
2:B:2443:C:H2'	2:B:2444:G:H8	1.59	0.68
51:AB:8:ARG:HB3	51:AB:12:ARG:HH12	1.58	0.68
13:M:20:SER:HB3	13:M:21:PRO:HD3	1.76	0.68
51:AB:93:ILE:HB	51:AB:96:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:G:H2'	2:B:954:G:H8	1.57	0.68
2:B:1064:C:O2'	2:B:1065:U:H5'	1.93	0.67
41:QA:36:ALA:N	41:QA:37:PRO:HD3	2.09	0.67
38:MA:217:ILE:HD12	38:MA:218:ASN:H	1.60	0.67
7:G:179:ARG:HB2	7:G:188:LEU:HD12	1.77	0.67
51:AB:79:LEU:HD12	51:AB:83:LYS:HB3	1.77	0.66
58:HB:40:PRO:HA	58:HB:43:GLU:HG2	1.77	0.66
1:A:367:U:C4	1:A:393:A:N1	2.63	0.66
2:B:1796:U:H2'	2:B:1797:G:H8	1.59	0.66
57:GB:65:LEU:HD13	57:GB:66:ILE:HG12	1.77	0.66
12:L:118:ILE:N	12:L:119:PRO:HD2	2.10	0.66
18:R:37:THR:HG22	18:R:39:PRO:HD2	1.78	0.66
49:YA:49:ARG:HG3	49:YA:89:LEU:HD21	1.78	0.66
40:PA:65:VAL:HB	40:PA:100:ILE:HG22	1.77	0.66
49:YA:113:ARG:HH12	49:YA:120:ARG:HA	1.60	0.66
2:B:833:A:H2'	2:B:834:G:H8	1.60	0.66
38:MA:145:ARG:HG2	38:MA:146:VAL:H	1.61	0.66
17:Q:4:PRO:HG3	17:Q:68:PHE:HE2	1.60	0.65
10:J:87:GLN:HE21	10:J:162:ARG:HD2	1.61	0.65
48:XA:23:HIS:HB3	48:XA:30:ILE:HG23	1.78	0.65
2:B:1934:C:H2'	2:B:1935:G:H8	1.60	0.65
1:A:1540:U:O4	37:KA:5:A:H2	1.80	0.64
39:OA:17:HIS:HB2	39:OA:188:THR:OG1	1.97	0.64
47:WA:6:ILE:HG22	47:WA:102:LEU:HG	1.79	0.64
23:W:82:MET:HB2	23:W:98:LYS:HB2	1.79	0.64
8:H:126:VAL:HG23	8:H:133:LEU:HD22	1.80	0.64
47:WA:22:THR:HG21	47:WA:39:PRO:HB3	1.80	0.64
2:B:1636:U:H2'	2:B:1637:A:H8	1.63	0.64
6:F:135:PRO:HG2	43:SA:80:PHE:HD1	1.63	0.64
1:A:413:G:H1'	1:A:428:G:N2	2.13	0.63
2:B:1265:A:H61	2:B:2013:A:H5''	1.62	0.63
1:A:617:G:H4'	53:CB:46:LYS:HE3	1.80	0.63
34:HA:18:PHE:HA	34:HA:43:THR:HG21	1.78	0.63
15:O:38:ILE:HD11	15:O:112:PHE:HZ	1.63	0.63
1:A:76:G:H1	1:A:93:U:H3	1.46	0.63
42:RA:108:GLY:O	42:RA:109:ALA:HB3	1.96	0.63
10:J:23:ILE:HD13	10:J:36:LEU:HD13	1.80	0.63
40:PA:174:LEU:HD23	40:PA:181:ILE:HD13	1.80	0.63
2:B:764:A:O2'	2:B:765:C:H5'	1.99	0.63
2:B:1316:U:H2'	2:B:1317:G:H8	1.63	0.63
2:B:270:A:H5'	2:B:271:G:H5''	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:83:LYS:HA	11:K:149:GLU:HB2	1.81	0.63
15:O:64:ARG:HB2	15:O:83:ALA:HB3	1.81	0.63
46:VA:89:TYR:HB2	46:VA:93:LEU:HG	1.80	0.63
4:D:17:C:H2'	4:D:17(A):U:H5	1.63	0.63
1:A:403:C:OP2	41:QA:70:GLN:NE2	2.32	0.63
2:B:586:A:H5'	8:H:84:THR:HG21	1.81	0.62
16:P:48:ARG:NH2	35:IA:4:LYS:O	2.32	0.62
2:B:910:A:H62	17:Q:12:MET:HA	1.63	0.62
2:B:581:C:H2'	2:B:582:A:C8	2.34	0.62
54:DB:46:HIS:HB2	54:DB:70:LYS:HE2	1.82	0.62
20:T:59:THR:HG22	20:T:72:VAL:HG12	1.80	0.62
47:WA:92:LEU:HD12	47:WA:92:LEU:H	1.64	0.62
49:YA:113:ARG:HB3	49:YA:118:VAL:O	1.99	0.62
2:B:962:G:N2	2:B:2250:G:H22	1.96	0.62
50:ZA:15:VAL:HG23	50:ZA:16:ILE:HD12	1.81	0.62
1:A:454:G:H22	1:A:478:A:H2	1.47	0.62
27:AA:36:GLN:HE21	27:AA:38:GLY:H	1.47	0.62
5:E:23:ILE:HG23	5:E:189:LEU:HD22	1.82	0.62
1:A:231:U:H2'	1:A:232:G:H8	1.64	0.62
30:DA:40:THR:HG22	30:DA:42:ALA:H	1.65	0.62
13:M:7:TYR:HE1	13:M:57:VAL:HG13	1.65	0.62
46:VA:118:ARG:HB3	46:VA:122:ARG:HB3	1.82	0.61
50:ZA:3:ILE:HD11	50:ZA:21:ILE:HD11	1.82	0.61
1:A:1386:G:H2'	1:A:1387:G:H8	1.65	0.61
2:B:1070:A:OP2	2:B:1072:C:H5''	2.00	0.61
2:B:1744:A:H3'	2:B:1745:A:H8	1.65	0.61
2:B:2246:G:H2'	2:B:2247:A:C8	2.35	0.61
56:FB:50:VAL:HG21	56:FB:70:LEU:HB3	1.82	0.61
38:MA:304:SER:HB2	49:YA:48:LEU:HD11	1.83	0.61
39:OA:14:HIS:CG	39:OA:15:PHE:N	2.68	0.61
2:B:1652:A:H62	18:R:11:ASN:HD21	1.47	0.61
2:B:242:G:N2	2:B:255:A:OP2	2.33	0.61
1:A:1279:G:N7	47:WA:45:ARG:NH2	2.48	0.61
1:A:1005:A:H3'	1:A:1006:G:H8	1.64	0.61
2:B:962:G:H21	2:B:2250:G:N2	1.98	0.61
6:F:267:VAL:HG12	6:F:268:ARG:HG2	1.83	0.61
7:G:4:LEU:HD21	7:G:29:VAL:HG11	1.82	0.61
2:B:2121:G:H21	5:E:170:ILE:HD13	1.64	0.61
2:B:2267:A:H5''	2:B:2268:A:H5'	1.82	0.61
7:G:4:LEU:HG	7:G:32:ASN:HD22	1.66	0.61
20:T:1:SER:O	20:T:4:ILE:HG22	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:VA:56:MET:HA	46:VA:59:LYS:HE2	1.84	0.60
10:J:118:ALA:O	10:J:120:ILE:N	2.34	0.60
39:OA:202:ASN:OD1	39:OA:203:ASP:N	2.33	0.60
36:JA:4:ARG:O	36:JA:37:GLN:O	2.19	0.60
38:MA:339:MET:O	38:MA:343:PRO:CD	2.49	0.60
2:B:807:U:H2'	2:B:808:G:C8	2.36	0.60
2:B:1386:C:H2'	2:B:1387:A:H8	1.67	0.60
2:B:2246:G:H2'	2:B:2247:A:H8	1.66	0.60
1:A:1429:A:H2'	1:A:1430:A:H8	1.67	0.60
39:OA:96:LEU:O	39:OA:99:MET:HG3	2.00	0.60
2:B:2743:U:OP2	2:B:2755:C:N4	2.35	0.60
1:A:1218:C:H2'	1:A:1219:A:C8	2.37	0.60
42:RA:160:VAL:O	42:RA:163:ILE:HG13	2.02	0.60
2:B:1368:G:H2'	2:B:1369:G:H8	1.66	0.59
4:D:35:A:H2'	4:D:36:U:C6	2.37	0.59
6:F:16:VAL:HB	6:F:203:VAL:HG22	1.84	0.59
38:MA:144:TRP:O	38:MA:145:ARG:HB2	2.02	0.59
45:UA:95:MET:SD	45:UA:129:ALA:HB1	2.42	0.59
1:A:818:G:H2'	1:A:820:U:H5	1.66	0.59
2:B:2709:G:H5'	18:R:22:ARG:HH22	1.67	0.59
38:MA:127:PHE:HD2	38:MA:201:CYS:HG	1.51	0.59
15:O:114:LYS:HE3	15:O:118:LEU:HD11	1.85	0.59
43:SA:12:PRO:O	43:SA:15:SER:HB3	2.02	0.59
1:A:151:A:H62	1:A:170:U:H3	1.51	0.59
1:A:501:C:OP1	49:YA:113:ARG:NH2	2.36	0.59
1:A:540:G:H3'	1:A:541:G:H8	1.67	0.59
1:A:690:G:OP2	48:XA:28:ASN:ND2	2.33	0.59
51:AB:55:SER:O	51:AB:57:PRO:N	2.35	0.59
2:B:309:A:N3	2:B:329:G:O2'	2.35	0.59
12:L:17:GLU:O	12:L:88:HIS:NE2	2.33	0.59
2:B:2500:U:O2'	2:B:2504:U:OP1	2.21	0.59
1:A:257:G:H2'	1:A:258:G:H8	1.68	0.59
1:A:880:C:H2'	1:A:881:G:H8	1.68	0.59
56:FB:62:THR:H	56:FB:65:MET:HE3	1.68	0.59
2:B:2673:G:H2'	2:B:2674:G:H8	1.68	0.59
2:B:2638:G:HO2'	2:B:2639:A:H8	1.49	0.58
40:PA:147:GLY:HA3	40:PA:171:ARG:O	2.03	0.58
2:B:1173:U:H2'	2:B:1174:U:H4'	1.85	0.58
2:B:2396:G:H2'	2:B:2397:G:H8	1.68	0.58
16:P:80:SER:HB3	16:P:114:GLY:HA3	1.84	0.58
56:FB:77:ARG:H	56:FB:77:ARG:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA:3:HIS:HB2	43:SA:92:THR:HA	1.86	0.58
4:D:1:C:H42	4:D:73:A:H61	1.49	0.58
30:DA:6:ILE:HD13	30:DA:47:ILE:HD11	1.85	0.58
2:B:2130:U:H1'	2:B:2159:G:H22	1.68	0.58
37:KA:8:A:H2'	37:KA:9:G:H8	1.69	0.58
23:W:2:GLU:O	23:W:3:THR:O	2.22	0.58
2:B:306:U:H3	2:B:310:A:H62	1.52	0.58
5:E:185:LEU:HA	5:E:188:ASN:HB2	1.86	0.58
4:D:70:G:O2'	4:D:71:C:H5'	2.04	0.58
22:V:76:LYS:HB2	22:V:85:LYS:HB3	1.86	0.58
13:M:18:ASN:ND2	13:M:38:CYS:SG	2.76	0.57
19:S:33:ARG:O	19:S:34:HIS:CB	2.52	0.57
49:YA:22:ALA:O	49:YA:23:LEU:CB	2.51	0.57
51:AB:86:GLU:O	51:AB:87:ALA:C	2.43	0.57
2:B:1159:U:H2'	2:B:1160:G:H8	1.69	0.57
2:B:1664:A:H61	2:B:1996:C:H42	1.52	0.57
2:B:2642:G:H5'	14:N:80:HIS:CD2	2.39	0.57
17:Q:4:PRO:HG3	17:Q:68:PHE:CE2	2.38	0.57
6:F:77:VAL:HG21	6:F:109:LEU:HD11	1.87	0.57
45:UA:45:ILE:HD11	45:UA:60:LEU:HB3	1.86	0.57
2:B:1252:G:H22	21:U:36:GLN:NE2	2.02	0.57
2:B:465:G:H21	2:B:684:G:H1'	1.68	0.57
1:A:1492:A:H2	37:KA:21:U:H5''	1.68	0.57
12:L:60:LEU:HD12	12:L:64:VAL:HG21	1.85	0.57
2:B:12:U:O2	2:B:12:U:H2'	2.05	0.57
40:PA:4:VAL:HG13	40:PA:5:HIS:N	2.10	0.57
46:VA:27:ILE:HG12	46:VA:62:LEU:HD12	1.87	0.57
41:QA:33:ILE:HG13	41:QA:34:GLU:N	2.20	0.57
1:A:674:G:H2'	1:A:675:A:H8	1.69	0.57
51:AB:81:ARG:HA	51:AB:84:VAL:HB	1.87	0.57
56:FB:30:LEU:HB2	56:FB:48:ILE:HG22	1.87	0.57
58:HB:9:GLU:HB3	58:HB:10:PRO:HD3	1.85	0.57
14:N:81:ILE:HG23	14:N:82:GLY:H	1.69	0.57
39:OA:40:ILE:HD13	39:OA:201:GLY:N	2.18	0.57
2:B:2443:C:H2'	2:B:2444:G:C8	2.38	0.57
43:SA:92:THR:OG1	43:SA:93:LYS:N	2.33	0.57
1:A:18:C:H1'	1:A:1079:G:H21	1.69	0.57
6:F:94:LEU:HD12	6:F:100:ARG:HE	1.70	0.57
1:A:64:G:OP1	1:A:382:A:N6	2.38	0.57
4:D:36:U:H2'	4:D:37:A:O4'	2.05	0.57
38:MA:174:ARG:NH2	38:MA:338:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:4:PRO:HG2	17:Q:70:ASP:HA	1.86	0.57
42:RA:80:LEU:HD13	42:RA:122:VAL:HG11	1.86	0.57
44:TA:11:ILE:HD11	44:TA:20:GLU:HB3	1.87	0.57
1:A:913:A:OP2	49:YA:87:LYS:NZ	2.33	0.56
6:F:28:PRO:HG3	6:F:62:ARG:HH21	1.70	0.56
47:WA:49:PHE:HZ	51:AB:76:LYS:HD3	1.69	0.56
2:B:1651:G:H4'	18:R:39:PRO:HG2	1.87	0.56
36:JA:36:ARG:HG2	36:JA:37:GLN:H	1.70	0.56
13:M:12:VAL:O	13:M:53:PRO:HA	2.05	0.56
19:S:33:ARG:O	19:S:34:HIS:HB2	2.05	0.56
2:B:1390:U:H3	2:B:1395:A:H62	1.52	0.56
2:B:1447:C:H2'	2:B:1448:G:H8	1.70	0.56
34:HA:24:THR:HG23	34:HA:27:GLY:H	1.69	0.56
1:A:69:G:H4'	1:A:70:U:OP1	2.05	0.56
2:B:1013:C:H2'	2:B:1014:A:H8	1.70	0.56
42:RA:114:LEU:HD12	42:RA:119:VAL:HG21	1.88	0.56
49:YA:85:ARG:HA	49:YA:93:ARG:HA	1.87	0.56
1:A:112:G:H21	1:A:354:G:H5'	1.69	0.56
53:CB:44:SER:H	53:CB:46:LYS:NZ	2.04	0.56
2:B:1165:A:H2'	2:B:1166:G:H8	1.69	0.56
2:B:2688:G:N1	2:B:2720:U:OP2	2.37	0.56
2:B:680:C:H2'	2:B:681:G:H8	1.70	0.56
5:E:7:ARG:HH22	5:E:218:MET:HB3	1.70	0.56
43:SA:42:TRP:HB2	43:SA:59:TYR:HB2	1.86	0.56
45:UA:63:LYS:O	45:UA:70:VAL:HG23	2.04	0.56
27:AA:33:ILE:HG22	27:AA:34:VAL:HG23	1.88	0.56
51:AB:55:SER:O	51:AB:56:SER:O	2.22	0.56
2:B:2508:G:H2'	2:B:2509:G:H8	1.71	0.56
2:B:376:G:H2'	2:B:377:G:H8	1.70	0.56
4:D:51:C:H2'	4:D:52:G:C8	2.41	0.56
7:G:142:VAL:CG2	7:G:143:PRO:HD2	2.36	0.56
2:B:1997:C:H2'	2:B:1998:A:H8	1.71	0.56
10:J:85:LYS:HG3	10:J:131:VAL:HG22	1.88	0.56
18:R:47:VAL:O	18:R:50:PRO:HD2	2.05	0.56
2:B:1086:A:H1'	2:B:1103:A:H61	1.71	0.56
2:B:162:U:O2'	2:B:163:C:H5'	2.06	0.56
2:B:2233:U:H2'	2:B:2234:G:H8	1.71	0.56
2:B:2470:G:H2'	2:B:2471:A:H8	1.69	0.56
2:B:591:U:H1'	35:IA:1:PRO:HD2	1.88	0.56
5:E:88:LYS:HA	5:E:92:ALA:HB3	1.87	0.56
32:FA:52:LYS:HE3	32:FA:55:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1278:C:H2'	2:B:1279:G:C8	2.41	0.56
2:B:1386:C:H2'	2:B:1387:A:C8	2.41	0.56
2:B:2747:G:H21	2:B:2757:A:H62	1.52	0.56
58:HB:13:VAL:HB	58:HB:15:LEU:HG	1.88	0.56
10:J:44:HIS:HA	10:J:49:LEU:HD23	1.87	0.56
38:MA:306:ARG:HE	38:MA:320:HIS:CE1	2.23	0.56
1:A:1352:C:H2'	1:A:1353:G:C8	2.41	0.56
2:B:743:A:O2'	2:B:1659:G:OP1	2.24	0.56
2:B:996:A:H2'	2:B:997:G:H8	1.70	0.56
8:H:79:ARG:HG2	8:H:80:SER:N	2.20	0.56
58:HB:16:ARG:HH21	58:HB:19:LYS:HG2	1.71	0.56
11:K:132:PHE:HB2	11:K:140:ALA:HB3	1.87	0.56
46:VA:51:LEU:HB3	46:VA:56:MET:HG2	1.88	0.56
2:B:1072:C:H42	2:B:1092:C:H41	1.53	0.55
2:B:2131:U:H5'	2:B:2132:U:H5''	1.89	0.55
42:RA:131:ASN:HD22	42:RA:132:PRO:HD2	1.71	0.55
5:E:74:ARG:HG3	5:E:93:GLU:HG2	1.88	0.55
31:EA:28:VAL:HG11	31:EA:32:LEU:HD13	1.88	0.55
39:OA:13:VAL:O	39:OA:14:HIS:C	2.44	0.55
40:PA:13:ILE:HG22	40:PA:14:VAL:HG23	1.88	0.55
48:XA:71:ASP:O	48:XA:72:ALA:HB3	2.06	0.55
1:A:1414:U:H2'	1:A:1415:G:H8	1.72	0.55
1:A:416:G:H22	1:A:427:U:H1'	1.71	0.55
2:B:1738:G:HO2'	2:B:1739:A:H8	1.54	0.55
2:B:592:A:O2'	35:IA:63:TYR:OH	2.23	0.55
38:MA:312:PHE:HD1	38:MA:329:LEU:HD21	1.71	0.55
17:Q:69:PRO:HA	17:Q:94:ALA:HB2	1.88	0.55
2:B:1464:G:H2'	2:B:1465:G:H8	1.72	0.55
14:N:35:ARG:HB2	14:N:54:ILE:HD11	1.89	0.55
5:E:74:ARG:HD3	5:E:111:PHE:HA	1.88	0.55
40:PA:123:LEU:HD21	40:PA:129:PHE:HB3	1.88	0.55
43:SA:38:ARG:HB2	43:SA:63:ASN:HB2	1.88	0.55
1:A:246:A:H4'	1:A:247:G:OP1	2.05	0.55
1:A:843:U:H5'	1:A:844:G:C8	2.42	0.55
4:LA:48:C:H2'	4:LA:59:A:H4'	1.88	0.55
1:A:692:U:H5''	48:XA:126:ARG:HH22	1.72	0.55
1:A:1506:U:O2'	1:A:1507:A:H5'	2.06	0.55
1:A:235:C:H2'	1:A:236:A:C8	2.42	0.55
2:B:2305:U:H5''	9:I:130:GLY:HA3	1.89	0.55
2:B:2506:U:N3	2:B:2585:U:O4	2.33	0.55
2:B:2723:C:OP1	7:G:114:LYS:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2882:A:H5'	18:R:96:ARG:HG3	1.89	0.55
48:XA:22:ILE:HG21	48:XA:95:THR:HG21	1.88	0.55
2:B:2818:U:H2'	2:B:2819:G:H8	1.72	0.55
4:D:62:C:O2'	5:E:54:LYS:HG2	2.07	0.55
47:WA:65:TYR:HB3	51:AB:96:LEU:HD12	1.89	0.54
2:B:1447:C:H2'	2:B:1448:G:C8	2.42	0.54
9:I:35:LEU:HB3	9:I:88:VAL:HB	1.89	0.54
4:LA:28:C:H2'	4:LA:29:G:H8	1.72	0.54
46:VA:10:ARG:O	46:VA:105:ARG:NH2	2.40	0.54
2:B:1188:U:H2'	2:B:1189:A:H8	1.71	0.54
2:B:2122:U:H2'	5:E:172:HIS:HE1	1.72	0.54
12:L:77:VAL:HG13	12:L:82:ILE:HD12	1.89	0.54
13:M:132:ALA:HA	13:M:137:LEU:HD12	1.90	0.54
14:N:37:ARG:HA	14:N:118:MET:HE3	1.89	0.54
18:R:87:PHE:C	18:R:89:SER:H	2.10	0.54
1:A:1129:C:H4'	46:VA:17:ARG:HH12	1.72	0.54
1:A:877:G:H2'	1:A:878:A:H8	1.73	0.54
27:AA:61:GLY:HA2	27:AA:81:GLU:HG2	1.90	0.54
2:B:1997:C:H2'	2:B:1998:A:C8	2.43	0.54
2:B:20:C:H2'	2:B:21:A:H8	1.72	0.54
2:B:2292:U:H2'	2:B:2293:G:H8	1.72	0.54
2:B:704:G:H2'	2:B:726:G:N2	2.23	0.54
2:B:974:G:H8	2:B:990:A:H62	1.55	0.54
4:D:41:C:H2'	4:D:42:G:C8	2.43	0.54
40:PA:69:THR:O	40:PA:105:VAL:HG12	2.07	0.54
51:AB:63:ARG:O	51:AB:64:CYS:SG	2.62	0.54
2:B:558:U:OP1	14:N:113:PRO:HD2	2.07	0.54
51:AB:64:CYS:O	51:AB:65:ARG:HB2	2.07	0.54
51:AB:77:PHE:HB3	51:AB:79:LEU:CD2	2.38	0.54
56:FB:10:ILE:HD13	56:FB:40:PHE:HE2	1.72	0.54
10:J:120:ILE:HG21	10:J:140:ILE:HG22	1.89	0.54
11:K:73:ASN:HB2	11:K:108:VAL:HG23	1.88	0.54
38:MA:131:LEU:O	38:MA:134:MET:HG2	2.08	0.54
40:PA:6:PRO:HG2	40:PA:200:TRP:HE1	1.73	0.54
1:A:1240:U:OP1	44:TA:115:MET:HB2	2.08	0.54
47:WA:6:ILE:HG13	47:WA:76:ILE:HB	1.90	0.54
2:B:1048:A:OP2	2:B:1110:G:N2	2.38	0.54
2:B:2297:A:N1	2:B:2321:U:H5	2.05	0.54
8:H:146:VAL:HG12	8:H:185:LYS:HB2	1.89	0.54
29:CA:17:GLU:HB3	29:CA:53:VAL:HG11	1.90	0.54
40:PA:201:ILE:HG22	40:PA:203:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA:36:ILE:HA	43:SA:64:VAL:HG23	1.90	0.54
2:B:570:G:C4	2:B:2030:A:N7	2.76	0.54
2:B:782:A:N7	6:F:219:VAL:HG21	2.23	0.54
47:WA:52:LEU:HB2	51:AB:81:ARG:NE	2.23	0.54
47:WA:8:ILE:HB	47:WA:74:VAL:HB	1.90	0.54
2:B:1709:U:H2'	2:B:1710:G:H8	1.72	0.54
5:E:44:VAL:HA	5:E:214:ILE:HA	1.89	0.54
13:M:74:PRO:HG2	13:M:77:VAL:HG22	1.90	0.54
38:MA:188:PRO:HG2	38:MA:191:GLU:HB2	1.89	0.54
41:QA:141:VAL:HG12	41:QA:180:THR:HG22	1.89	0.54
3:C:111:U:H2'	3:C:112:G:H8	1.72	0.54
5:E:41:SER:HA	5:E:177:LYS:HG2	1.90	0.54
1:A:948:C:H2'	1:A:949:A:H8	1.73	0.53
1:A:974:A:OP2	51:AB:81:ARG:NH1	2.41	0.53
2:B:1548:A:H2'	2:B:1549:A:H8	1.73	0.53
2:B:2837:A:H2'	2:B:2838:G:H8	1.73	0.53
2:B:537:G:H22	2:B:555:G:H2'	1.73	0.53
53:CB:18:GLN:NE2	53:CB:35:ARG:HH11	2.06	0.53
7:G:151:THR:HB	7:G:152:PRO:HD3	1.90	0.53
10:J:120:ILE:HD12	10:J:134:GLY:HA3	1.90	0.53
11:K:66:ASN:HB3	11:K:138:VAL:HG21	1.89	0.53
11:K:78:VAL:HG21	11:K:103:VAL:HG22	1.88	0.53
38:MA:45:LEU:HD23	38:MA:46:SER:N	2.23	0.53
47:WA:57:VAL:HG22	47:WA:58:ASN:N	2.17	0.53
2:B:2861:U:H2'	2:B:2862:G:H8	1.73	0.53
2:B:751:A:N7	2:B:789:A:N6	2.56	0.53
56:FB:24:SER:HB2	56:FB:27:LYS:HD2	1.90	0.53
7:G:46:ARG:HB3	7:G:84:LEU:HD12	1.88	0.53
2:B:2329:U:H2'	2:B:2330:G:H8	1.72	0.53
2:B:596:U:H2'	2:B:597:G:H8	1.73	0.53
31:EA:37:CYS:H	31:EA:40:CYS:HB3	1.73	0.53
6:F:66:PHE:HZ	6:F:86:ARG:HH12	1.57	0.53
15:O:35:VAL:HG13	15:O:69:VAL:HG11	1.91	0.53
16:P:30:THR:HB	16:P:33:ARG:HB2	1.89	0.53
18:R:38:LEU:HB3	18:R:39:PRO:HD3	1.90	0.53
50:ZA:89:ARG:HH22	50:ZA:101:THR:HG21	1.73	0.53
2:B:1796:U:H2'	2:B:1797:G:C8	2.42	0.53
10:J:157:LYS:HG2	10:J:159:LYS:HE3	1.90	0.53
11:K:5:LEU:HD22	11:K:13:GLY:HA3	1.89	0.53
1:A:884:U:H4'	1:A:885:G:H5''	1.89	0.53
2:B:2039:U:H2'	2:B:2040:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2514:U:H2'	2:B:2515:C:C6	2.44	0.53
2:B:2422:C:H41	35:IA:30:HIS:HE2	1.57	0.53
38:MA:257:CYS:SG	38:MA:266:ASN:ND2	2.82	0.53
2:B:197:A:H4'	2:B:2069:G:OP2	2.09	0.53
2:B:2861:U:H2'	2:B:2862:G:C8	2.44	0.53
5:E:60:ARG:HB2	5:E:141:LYS:HG3	1.90	0.53
55:EB:62:ARG:HB3	55:EB:69:TYR:CE1	2.43	0.53
47:WA:53:ILE:HG22	47:WA:61:ALA:O	2.08	0.53
1:A:312:C:H2'	1:A:313:A:C8	2.43	0.53
2:B:210:C:H2'	2:B:211:C:C6	2.44	0.53
8:H:148:ILE:HG21	8:H:157:LEU:HD21	1.90	0.53
40:PA:55:VAL:HG13	40:PA:66:THR:HB	1.90	0.53
40:PA:8:GLY:HA2	40:PA:11:LEU:HG	1.90	0.53
48:XA:84:MET:HG2	48:XA:110:THR:HB	1.91	0.53
1:A:1412:C:H2'	1:A:1413:A:C8	2.44	0.53
2:B:2243:U:H2'	2:B:2244:U:C6	2.44	0.53
2:B:121:G:H2'	2:B:122:G:H8	1.74	0.52
53:CB:19:VAL:HG21	53:CB:52:LEU:HD21	1.89	0.52
40:PA:56:ILE:HG23	40:PA:63:ILE:HD11	1.90	0.52
42:RA:96:GLN:HB3	42:RA:123:LEU:HB2	1.90	0.52
1:A:1308:U:H2'	1:A:1309:G:H8	1.75	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.44	0.52
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.52
7:G:25:THR:HG21	7:G:193:VAL:HG22	1.91	0.52
2:B:1054:A:H4'	12:L:31:ARG:HA	1.90	0.52
2:B:1005:C:O2'	14:N:30:THR:HG21	2.09	0.52
1:A:182:A:H62	1:A:194:C:H42	1.57	0.52
2:B:2329:U:H2'	2:B:2330:G:C8	2.44	0.52
2:B:759:G:H2'	2:B:760:G:H8	1.73	0.52
5:E:43:ASP:N	5:E:43:ASP:OD1	2.42	0.52
7:G:33:ARG:H	7:G:33:ARG:HD2	1.74	0.52
58:HB:6:ARG:O	58:HB:7:GLU:C	2.48	0.52
18:R:100:CYS:SG	18:R:101:GLY:N	2.82	0.52
1:A:149:A:H1'	1:A:1446:A:H2	1.75	0.52
5:E:50:ILE:HG12	5:E:205:LYS:H	1.74	0.52
35:IA:30:HIS:ND1	35:IA:31:ILE:HG13	2.24	0.52
19:S:29:HIS:HB3	19:S:36:TYR:HB2	1.90	0.52
1:A:1429:A:H2'	1:A:1430:A:C8	2.45	0.52
51:AB:64:CYS:SG	51:AB:66:GLN:HB3	2.50	0.52
2:B:581:C:H2'	2:B:582:A:H8	1.75	0.52
1:A:1540:U:O4	37:KA:5:A:C2	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:G:H2'	2:B:954:G:C8	2.40	0.52
25:Y:47:PRO:HG3	25:Y:55:GLY:HA3	1.92	0.52
2:B:244:A:H62	2:B:254:G:H21	1.58	0.52
32:FA:30:ASP:HB3	32:FA:34:GLY:H	1.73	0.52
12:L:118:ILE:O	12:L:118:ILE:CG2	2.55	0.52
16:P:55:MET:O	16:P:60:ARG:NH2	2.42	0.52
49:YA:81:ILE:HG23	49:YA:94:TYR:HB3	1.91	0.52
1:A:490:C:H2'	1:A:491:G:H8	1.75	0.52
2:B:1259:G:H2'	2:B:1260:A:H8	1.75	0.52
2:B:1841:U:H2'	2:B:1842:G:H8	1.74	0.52
2:B:1848:A:H2'	2:B:1849:G:H8	1.74	0.52
2:B:2070:A:H2'	2:B:2071:A:H8	1.74	0.52
2:B:38:A:H4'	8:H:45:ALA:HB3	1.92	0.52
2:B:523:C:H2'	2:B:524:G:H8	1.75	0.52
10:J:9:VAL:HA	10:J:48:THR:HG22	1.91	0.52
38:MA:245:ARG:HG2	38:MA:256:GLU:HG2	1.92	0.52
38:MA:312:PHE:CD1	38:MA:329:LEU:HD21	2.44	0.52
18:R:44:LEU:HD23	18:R:113:ILE:HD13	1.92	0.52
45:UA:42:GLU:HG2	45:UA:100:ILE:HD13	1.92	0.52
51:AB:69:ARG:O	51:AB:71:HIS:N	2.36	0.52
2:B:2215:C:H2'	2:B:2216:G:H8	1.75	0.52
9:I:114:ARG:HD3	31:EA:47:LYS:HE2	1.92	0.52
2:B:1432:G:H2'	2:B:1433:A:C8	2.45	0.52
2:B:2070:A:H2'	2:B:2071:A:C8	2.45	0.52
2:B:582:A:H2'	2:B:583:G:H8	1.75	0.52
2:B:1568:G:OP2	6:F:62:ARG:NH2	2.43	0.52
15:O:24:VAL:HG13	15:O:33:ALA:HB2	1.91	0.52
1:A:1356:G:H2'	1:A:1357:A:C8	2.45	0.51
1:A:502:A:OP1	49:YA:114:SER:N	2.41	0.51
2:B:1197:G:H2'	2:B:1198:U:H6	1.75	0.51
2:B:1826:G:H2'	2:B:1827:U:C6	2.45	0.51
2:B:1934:C:H2'	2:B:1935:G:C8	2.43	0.51
2:B:2050:C:N4	2:B:2051:A:N1	2.58	0.51
5:E:175:ILE:HG12	5:E:188:ASN:HB3	1.92	0.51
8:H:79:ARG:HG2	8:H:80:SER:H	1.75	0.51
12:L:33:VAL:HG12	12:L:34:THR:H	1.76	0.51
39:OA:33:ALA:CA	39:OA:37:VAL:O	2.43	0.51
2:B:585:G:N7	21:U:5:ARG:NH1	2.57	0.51
12:L:56:ARG:HD3	12:L:83:ALA:HB2	1.92	0.51
14:N:84:ILE:O	14:N:84:ILE:HG23	2.10	0.51
1:A:59:A:H3'	1:A:331:G:H22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:ASN:HB3	9:I:152:ASP:HB3	1.93	0.51
4:LA:41:C:H2'	4:LA:42:G:H8	1.75	0.51
41:QA:84:ASN:HA	42:RA:102:THR:HG21	1.92	0.51
42:RA:10:LEU:O	42:RA:11:GLN:O	2.28	0.51
2:B:1539:U:H2'	2:B:1540:G:H8	1.75	0.51
5:E:73:VAL:HG11	5:E:157:LYS:HA	1.93	0.51
8:H:194:LYS:O	8:H:197:GLU:HB3	2.10	0.51
2:B:1203:U:H5'	16:P:3:LEU:HD23	1.92	0.51
41:QA:60:VAL:HG21	41:QA:199:ILE:HD11	1.92	0.51
19:S:49:VAL:HG21	19:S:82:ALA:HA	1.91	0.51
2:B:2118:U:O2	2:B:2145:C:N4	2.44	0.51
2:B:45:G:H5''	2:B:46:G:H5'	1.91	0.51
57:GB:34:VAL:HG11	57:GB:78:LEU:HD21	1.91	0.51
10:J:49:LEU:HD12	10:J:71:LEU:HD21	1.93	0.51
18:R:32:GLU:HB3	18:R:118:ARG:HD2	1.92	0.51
50:ZA:3:ILE:HG12	50:ZA:7:ASN:HB2	1.92	0.51
1:A:451:A:H4'	1:A:452:A:N3	2.26	0.51
12:L:51:TYR:HE2	12:L:87:GLU:HA	1.75	0.51
26:Z:30:ILE:HD11	26:Z:63:ILE:HD13	1.92	0.51
1:A:337:G:H2'	1:A:338:A:C8	2.46	0.51
51:AB:87:ALA:O	51:AB:91:GLY:CA	2.58	0.51
2:B:1251:C:O2'	2:B:1252:G:H3'	2.11	0.51
6:F:66:PHE:HB3	6:F:150:GLY:O	2.11	0.51
8:H:71:GLY:O	8:H:72:SER:HB2	2.11	0.51
38:MA:340:LEU:O	38:MA:343:PRO:HD2	2.11	0.51
41:QA:146:GLU:O	41:QA:149:LYS:HG2	2.09	0.51
42:RA:105:ILE:HG21	42:RA:123:LEU:HD23	1.93	0.51
1:A:1228:C:H2'	1:A:1229:A:H8	1.76	0.51
2:B:2828:G:H2'	2:B:2829:A:H8	1.75	0.51
2:B:580:U:H2'	2:B:581:C:H6	1.76	0.51
28:BA:2:ARG:HD2	28:BA:29:LEU:HD22	1.93	0.51
4:D:59:A:H2'	4:D:60:U:H5'	1.92	0.51
1:A:1144:G:H21	1:A:1146:A:H62	1.58	0.51
1:A:1517:G:N3	2:B:1919:A:O2'	2.43	0.51
2:B:1250:G:OP2	16:P:21:ARG:NH2	2.44	0.51
2:B:799:G:H5''	2:B:800:A:H2'	1.92	0.51
6:F:143:VAL:HB	6:F:153:LEU:HB2	1.92	0.51
10:J:94:ARG:NH1	10:J:127:GLN:OE1	2.41	0.51
15:O:76:VAL:H	20:T:72:VAL:HG22	1.76	0.51
1:A:1437:A:H2'	1:A:1438:G:H8	1.74	0.50
1:A:916:U:H2'	1:A:917:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1837:C:H2'	2:B:1899:A:H61	1.76	0.50
2:B:2183:A:H2'	2:B:2184:A:C8	2.46	0.50
2:B:946:C:H2'	2:B:947:A:H8	1.76	0.50
39:OA:14:HIS:CD2	39:OA:15:PHE:H	2.29	0.50
21:U:43:GLN:HE21	22:V:77:PHE:HB3	1.75	0.50
48:XA:62:ALA:HB1	48:XA:95:THR:HB	1.93	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.45	0.50
1:A:715:A:H2'	1:A:716:A:H8	1.76	0.50
2:B:679:C:H2'	2:B:680:C:C6	2.47	0.50
2:B:878:A:H3'	2:B:879:G:H8	1.75	0.50
8:H:149:ILE:HG23	8:H:188:MET:HA	1.93	0.50
19:S:79:ALA:HB3	19:S:113:ALA:HB3	1.94	0.50
1:A:1369:C:H2'	1:A:1370:G:C8	2.47	0.50
2:B:2183:A:H2'	2:B:2184:A:H8	1.77	0.50
2:B:23:G:H2'	2:B:24:G:H8	1.76	0.50
2:B:720:U:H2'	2:B:721:A:H8	1.76	0.50
15:O:34:GLY:N	15:O:37:ASP:OD2	2.42	0.50
40:PA:179:ALA:HB1	40:PA:202:PHE:HE1	1.76	0.50
1:A:1241:G:H2'	1:A:1242:G:H8	1.76	0.50
1:A:1323:G:H2'	1:A:1324:A:H8	1.76	0.50
1:A:312:C:H2'	1:A:313:A:H8	1.76	0.50
2:B:1548:A:H2'	2:B:1549:A:C8	2.46	0.50
3:C:38:C:N4	3:C:44:G:H1	2.07	0.50
2:B:1057:A:H1'	12:L:34:THR:HG21	1.93	0.50
1:A:208:U:H2'	1:A:210:C:H1'	1.94	0.50
2:B:1130:U:O2'	2:B:1131:G:H2'	2.11	0.50
2:B:1434:A:H2'	2:B:1435:G:H8	1.76	0.50
2:B:2815:C:H2'	2:B:2816:G:H8	1.76	0.50
2:B:467:G:OP2	34:HA:34:ARG:HD3	2.12	0.50
1:A:624:C:H4'	53:CB:10:GLY:HA2	1.93	0.50
4:D:16:C:H5'	4:D:59:A:C2	2.46	0.50
38:MA:244:ILE:HD11	38:MA:263:GLN:HG3	1.93	0.50
14:N:32:LEU:HD22	14:N:54:ILE:HG21	1.92	0.50
39:OA:186:VAL:HG13	39:OA:190:SER:HB2	1.93	0.50
41:QA:94:GLU:HG2	41:QA:185:PRO:HG3	1.93	0.50
18:R:78:LYS:O	18:R:82:GLU:HB2	2.11	0.50
2:B:2115:G:O2'	2:B:2117:A:N6	2.45	0.50
5:E:132:GLY:HA2	5:E:137:MET:HB2	1.94	0.50
38:MA:16:HIS:HA	38:MA:45:LEU:HD11	1.92	0.50
2:B:587:C:OP2	16:P:21:ARG:NH1	2.45	0.50
1:A:1158:C:C4	1:A:1160:G:C8	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1219:U:OP2	21:U:18:LYS:NZ	2.44	0.50
2:B:1258:U:H2'	2:B:1259:G:H8	1.77	0.50
5:E:142:VAL:HG11	5:E:162:ARG:HH21	1.77	0.50
10:J:136:ASP:OD2	10:J:138:GLN:HB3	2.11	0.50
45:UA:8:ASP:OD2	45:UA:12:ARG:NH1	2.44	0.50
46:VA:56:MET:C	46:VA:56:MET:SD	2.90	0.50
2:B:1464:G:H2'	2:B:1465:G:C8	2.47	0.50
2:B:1682:G:OP2	2:B:1699:G:N2	2.44	0.50
2:B:2114:A:H62	2:B:2119:A:H61	1.59	0.50
29:CA:21:LEU:HA	29:CA:25:GLN:HB3	1.92	0.50
8:H:79:ARG:NH1	8:H:80:SER:OG	2.45	0.50
12:L:25:ALA:HB3	12:L:85:SER:HB2	1.92	0.50
1:A:335:C:H2'	1:A:336:A:C8	2.46	0.50
51:AB:53:ARG:HB3	51:AB:59:ARG:HH12	1.76	0.50
2:B:18:U:H2'	2:B:19:A:H8	1.76	0.50
2:B:770:G:OP2	34:HA:11:LYS:HE3	2.11	0.50
10:J:51:PHE:HZ	10:J:71:LEU:HD22	1.75	0.50
38:MA:135:TYR:OH	38:MA:178:GLU:OE1	2.30	0.50
2:B:1387:A:H2'	2:B:1388:G:H8	1.77	0.49
2:B:1779:U:OP2	2:B:1784:A:N6	2.44	0.49
2:B:923:G:H2'	2:B:924:G:H8	1.77	0.49
4:D:42:G:H2'	4:D:43:A:C8	2.47	0.49
54:DB:63:CYS:SG	54:DB:64:ARG:N	2.81	0.49
9:I:60:SER:HB2	9:I:90:LEU:HD21	1.94	0.49
13:M:57:VAL:HB	13:M:69:VAL:HB	1.94	0.49
42:RA:108:GLY:O	42:RA:109:ALA:CB	2.60	0.49
19:S:40:ILE:HG13	19:S:47:VAL:HG12	1.94	0.49
46:VA:49:GLN:HB3	46:VA:50:PRO:HD3	1.93	0.49
1:A:1358:U:OP1	51:AB:75:ARG:HB2	2.12	0.49
2:B:2685:G:H2'	2:B:2686:G:H8	1.77	0.49
2:B:2812:G:H2'	2:B:2813:A:C8	2.47	0.49
2:B:320:A:OP1	8:H:130:LYS:NZ	2.41	0.49
2:B:563:A:OP2	22:V:79:ARG:NH2	2.43	0.49
13:M:52:LEU:O	13:M:54:ILE:HG13	2.12	0.49
17:Q:20:LEU:HD13	26:Z:81:PRO:HG2	1.94	0.49
1:A:254:G:O3'	54:DB:70:LYS:NZ	2.44	0.49
1:A:419:C:H2'	1:A:420:U:O4'	2.12	0.49
2:B:2313:C:H2'	2:B:2314:A:C8	2.48	0.49
2:B:457:A:H61	2:B:470:A:H5''	1.77	0.49
2:B:598:U:H2'	2:B:599:A:H8	1.76	0.49
1:A:110:C:O2'	53:CB:25:ARG:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1754:A:O2'	20:T:102:ARG:NH2	2.46	0.49
1:A:1512:U:H2'	1:A:1513:A:C8	2.47	0.49
2:B:1164:C:H2'	2:B:1165:A:H8	1.78	0.49
2:B:1860:G:H5''	5:E:205:LYS:HD2	1.94	0.49
2:B:2126:A:H2'	2:B:2162:G:N2	2.27	0.49
4:D:24:U:H2'	4:D:25:C:C6	2.46	0.49
39:OA:156:LEU:HD13	39:OA:178:LEU:HD13	1.95	0.49
39:OA:58:LYS:O	39:OA:61:SER:HB3	2.13	0.49
53:CB:44:SER:H	53:CB:46:LYS:HZ2	1.61	0.49
4:D:51:C:H2'	4:D:52:G:H8	1.77	0.49
2:B:2124:G:H21	5:E:217:THR:HA	1.78	0.49
1:A:958:A:C2	56:FB:54:ARG:HB3	2.47	0.49
56:FB:44:ILE:HD13	56:FB:63:ASP:HA	1.94	0.49
38:MA:138:TYR:OH	38:MA:142:ARG:NH2	2.40	0.49
41:QA:36:ALA:H	41:QA:37:PRO:CD	2.25	0.49
52:BB:48:ASP:OD2	52:BB:51:SER:HB2	2.13	0.49
14:N:31:GLU:HG2	14:N:142:ILE:HG12	1.93	0.49
1:A:147:G:H2'	1:A:148:G:C8	2.48	0.49
1:A:530:G:H22	1:A:1492:A:H61	1.61	0.49
2:B:1443:U:H2'	2:B:1444:G:H8	1.78	0.49
54:DB:16:MET:HG3	54:DB:19:SER:OG	2.13	0.49
2:B:2615:U:C2	32:FA:3:GLN:HA	2.47	0.49
47:WA:33:GLY:HA3	47:WA:83:THR:OG1	2.13	0.49
1:A:1098:C:O2'	58:HB:66:ARG:HG3	2.12	0.49
51:AB:72:GLY:O	51:AB:74:LEU:HD23	2.12	0.49
2:B:181:A:H2'	2:B:182:A:C8	2.48	0.49
56:FB:76:THR:OG1	56:FB:77:ARG:N	2.46	0.49
7:G:125:TRP:CD1	7:G:160:LYS:HB3	2.48	0.49
14:N:18:VAL:HG21	14:N:32:LEU:HD21	1.93	0.49
1:A:946:A:H2'	1:A:947:G:H8	1.76	0.49
1:A:950:U:H2'	1:A:951:G:C8	2.47	0.49
2:B:2026:U:H2'	2:B:2027:G:C8	2.48	0.49
3:C:5:U:H2'	3:C:6:G:H8	1.78	0.49
29:CA:22:LEU:HD12	29:CA:23:ARG:HE	1.76	0.49
5:E:130:VAL:O	5:E:134:ARG:NH1	2.46	0.49
11:K:94:ILE:HG23	11:K:98:ASP:HB2	1.95	0.49
13:M:112:LYS:O	13:M:116:MET:N	2.46	0.49
7:G:13:ARG:HH22	20:T:74:GLN:HE21	1.59	0.49
1:A:1149:C:OP2	46:VA:10:ARG:NH2	2.45	0.49
48:XA:28:ASN:HB3	48:XA:56:LYS:HG2	1.95	0.49
1:A:1203:C:H2'	1:A:1204:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:G:N1	1:A:1338:G:OP2	2.46	0.49
1:A:52:C:H2'	1:A:53:A:H8	1.78	0.49
1:A:674:G:H2'	1:A:675:A:C8	2.48	0.49
2:B:1161:C:H2'	2:B:1162:G:H8	1.76	0.49
2:B:1592:C:H2'	2:B:1593:A:H8	1.77	0.49
2:B:863:A:H2'	2:B:864:G:H8	1.77	0.49
30:DA:52:PHE:CE2	30:DA:53:MET:HG3	2.47	0.49
6:F:131:MET:HG2	6:F:134:ILE:HD12	1.95	0.49
8:H:127:GLU:HG2	8:H:128:ALA:H	1.77	0.49
2:B:1260:A:OP1	23:W:83:LYS:NZ	2.46	0.49
2:B:172:A:H2'	2:B:173:A:H8	1.78	0.48
2:B:328:U:O3'	25:Y:65:GLN:HG3	2.13	0.48
2:B:917:A:H5''	2:B:2268:A:H61	1.78	0.48
4:D:2:G:N2	4:D:72:A:C2	2.81	0.48
5:E:164:ARG:H	5:E:171:ILE:HD13	1.78	0.48
11:K:104:THR:HA	11:K:108:VAL:O	2.12	0.48
13:M:27:LEU:HD13	13:M:34:ILE:HA	1.95	0.48
38:MA:317:VAL:HB	38:MA:329:LEU:HD13	1.93	0.48
39:OA:27:LYS:HB3	39:OA:28:PRO:HD3	1.94	0.48
19:S:28:VAL:O	19:S:28:VAL:HG22	2.13	0.48
1:A:1538:C:O2'	58:HB:20:ARG:NH2	2.46	0.48
1:A:264:C:H4'	54:DB:64:ARG:HD2	1.94	0.48
1:A:299:G:C6	1:A:300:A:C6	3.01	0.48
1:A:416:G:C6	1:A:427:U:O2	2.67	0.48
51:AB:66:GLN:O	51:AB:67:THR:OG1	2.27	0.48
2:B:1181:U:H2'	2:B:1182:G:C8	2.48	0.48
40:PA:7:ASN:O	40:PA:8:GLY:C	2.50	0.48
41:QA:191:SER:O	41:QA:193:ASP:N	2.45	0.48
43:SA:9:MET:HG3	43:SA:59:TYR:CE1	2.48	0.48
20:T:8:GLU:HA	20:T:54:LEU:HD22	1.94	0.48
25:Y:73:ASN:O	25:Y:74:ALA:HB3	2.13	0.48
1:A:562:U:H1'	49:YA:11:ARG:HD2	1.93	0.48
2:B:7:G:H2'	2:B:8:C:C6	2.49	0.48
36:JA:36:ARG:O	36:JA:37:GLN:O	2.30	0.48
11:K:103:VAL:HG12	11:K:108:VAL:HB	1.96	0.48
1:A:1492:A:H2'	38:MA:303:ARG:HH12	1.79	0.48
1:A:367:U:N3	1:A:393:A:C2	2.81	0.48
2:B:161:A:C5	2:B:162:U:H5	2.32	0.48
2:B:742:A:H2'	2:B:743:A:C8	2.48	0.48
7:G:77:ARG:NH2	7:G:200:ASP:OD1	2.46	0.48
2:B:2726:A:H4'	15:O:32:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2002:G:OP2	18:R:9:GLN:NE2	2.46	0.48
7:G:13:ARG:HH12	20:T:74:GLN:HE21	1.62	0.48
2:B:107:G:H2'	2:B:108:G:H8	1.77	0.48
2:B:1958:C:H2'	2:B:1959:G:H8	1.79	0.48
2:B:2313:C:H2'	2:B:2314:A:H8	1.78	0.48
2:B:816:C:H2'	2:B:817:C:C6	2.49	0.48
2:B:873:C:H2'	2:B:874:G:H8	1.78	0.48
36:JA:33:HIS:O	36:JA:35:GLN:HG3	2.14	0.48
38:MA:311:ASN:OD1	38:MA:313:PRO:HD2	2.13	0.48
16:P:29:LYS:O	16:P:30:THR:OG1	2.28	0.48
1:A:126:G:OP1	1:A:605:U:O2'	2.28	0.48
1:A:555:U:H2'	1:A:556:C:C6	2.49	0.48
2:B:1590:A:H2'	2:B:1591:A:H8	1.78	0.48
2:B:598:U:H2'	2:B:599:A:C8	2.48	0.48
35:IA:44:ARG:HB3	35:IA:45:PRO:HD3	1.94	0.48
12:L:26:VAL:HG21	12:L:113:PHE:HA	1.95	0.48
1:A:769:G:H4'	1:A:1513:A:H4'	1.94	0.48
2:B:2853:C:H2'	2:B:2854:G:H8	1.79	0.48
2:B:848:C:H2'	2:B:849:A:C8	2.49	0.48
6:F:255:LYS:HD2	6:F:269:ARG:HH22	1.79	0.48
1:A:1182:G:H5'	1:A:1183:U:OP1	2.14	0.48
1:A:34:C:H2'	1:A:35:G:C8	2.48	0.48
2:B:155:A:H2'	2:B:156:A:H8	1.79	0.48
2:B:1791:A:N6	2:B:1828:G:O2'	2.45	0.48
2:B:784:G:H5'	2:B:785:G:OP1	2.12	0.48
50:ZA:8:ILE:N	50:ZA:9:PRO:HD2	2.29	0.48
1:A:880:C:H2'	1:A:881:G:C8	2.48	0.48
2:B:2039:U:H2'	2:B:2040:G:H8	1.77	0.48
2:B:817:C:H2'	2:B:818:G:H8	1.79	0.48
4:D:21:A:H2'	4:D:46:G:O6	2.13	0.48
13:M:123:ALA:HA	13:M:126:ARG:HD2	1.95	0.48
16:P:85:VAL:HG11	16:P:90:VAL:HG22	1.96	0.48
26:Z:40:ILE:HG21	26:Z:63:ILE:HD11	1.96	0.48
1:A:367:U:O4	1:A:393:A:C6	2.67	0.48
2:B:1499:C:H2'	2:B:1500:G:H8	1.79	0.48
2:B:2230:G:H2'	2:B:2231:U:C6	2.49	0.48
2:B:2122:U:H4'	5:E:164:ARG:HH12	1.78	0.48
6:F:48:ILE:HG23	6:F:48:ILE:O	2.13	0.48
7:G:109:VAL:HG11	7:G:193:VAL:HB	1.96	0.48
12:L:119:PRO:CG	12:L:120:ALA:N	2.76	0.48
39:OA:209:VAL:HA	39:OA:212:TYR:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:WA:67:ILE:HG22	51:AB:95:GLY:O	2.13	0.48
25:Y:98:ASN:O	25:Y:100:GLU:HG3	2.14	0.48
1:A:599:C:H2'	1:A:600:A:C8	2.49	0.47
1:A:720:C:H5''	1:A:721:G:H2'	1.96	0.47
2:B:2215:C:H2'	2:B:2216:G:C8	2.49	0.47
2:B:2327:A:H2'	2:B:2328:A:C8	2.49	0.47
2:B:2728:U:H2'	2:B:2729:G:H8	1.79	0.47
3:C:55:U:H2'	3:C:56:G:C8	2.49	0.47
4:D:11:A:H2'	4:D:12:G:C8	2.48	0.47
6:F:257:ARG:HH12	6:F:259:ASN:HB2	1.78	0.47
2:B:210:C:OP1	34:HA:29:GLN:NE2	2.47	0.47
7:G:12:THR:HG23	20:T:4:ILE:HD11	1.95	0.47
22:V:68:ARG:HH11	22:V:90:ARG:HB2	1.79	0.47
47:WA:36:VAL:HG23	47:WA:76:ILE:HA	1.96	0.47
25:Y:73:ASN:HD21	25:Y:98:ASN:HD22	1.60	0.47
1:A:1512:U:H2'	1:A:1513:A:H8	1.78	0.47
2:B:1056:G:H5''	2:B:1057:A:O4'	2.15	0.47
2:B:2241:A:H2'	2:B:2242:G:C8	2.49	0.47
2:B:729:G:O6	2:B:1774:C:N4	2.47	0.47
56:FB:4:LEU:HD12	56:FB:9:PHE:HZ	1.78	0.47
15:O:102:PRO:HB3	15:O:121:GLU:HB2	1.95	0.47
40:PA:69:THR:HG21	40:PA:75:VAL:HG21	1.96	0.47
22:V:59:ILE:HG12	22:V:101:ILE:HG22	1.96	0.47
1:A:1005:A:H3'	1:A:1006:G:C8	2.48	0.47
2:B:468:G:OP2	34:HA:37:LYS:NZ	2.37	0.47
2:B:521:U:H2'	2:B:522:A:H8	1.79	0.47
58:HB:23:GLU:O	58:HB:25:ALA:N	2.40	0.47
9:I:36:ASN:OD1	9:I:37:MET:N	2.47	0.47
10:J:51:PHE:CZ	10:J:71:LEU:HD22	2.49	0.47
38:MA:9:LEU:O	38:MA:12:LEU:HB3	2.14	0.47
17:Q:41:LEU:HD22	17:Q:124:LEU:HD22	1.96	0.47
26:Z:42:LEU:HD23	26:Z:47:VAL:HG21	1.97	0.47
1:A:950:U:H2'	1:A:951:G:H8	1.79	0.47
2:B:406:G:H2'	2:B:407:G:H8	1.80	0.47
39:OA:19:THR:HG22	39:OA:38:HIS:CD2	2.48	0.47
39:OA:22:TRP:CE2	39:OA:38:HIS:HE1	2.31	0.47
40:PA:31:ASN:OD1	40:PA:58:ARG:NH2	2.46	0.47
21:U:87:VAL:HG13	22:V:49:ILE:HD11	1.94	0.47
22:V:68:ARG:HB2	22:V:90:ARG:HH21	1.80	0.47
46:VA:54:VAL:O	46:VA:59:LYS:NZ	2.48	0.47
24:X:11:LEU:HD22	24:X:32:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2244:U:N3	2:B:2245:U:O2	2.47	0.47
54:DB:18:LYS:HA	54:DB:50:ASN:HD21	1.80	0.47
8:H:77:ILE:HG13	8:H:78:TRP:HD1	1.79	0.47
13:M:97:VAL:HB	13:M:137:LEU:HA	1.96	0.47
13:M:38:CYS:SG	13:M:42:ASN:ND2	2.87	0.47
40:PA:129:PHE:HA	40:PA:132:ALA:HB3	1.97	0.47
41:QA:35:GLN:O	41:QA:36:ALA:HB2	2.15	0.47
42:RA:87:VAL:HA	42:RA:91:SER:O	2.14	0.47
15:O:76:VAL:HG12	20:T:72:VAL:HG22	1.97	0.47
50:ZA:113:LYS:HA	50:ZA:114:PRO:HD3	1.72	0.47
1:A:680:C:H2'	1:A:681:A:H8	1.80	0.47
2:B:2316:G:H2'	2:B:2317:A:C8	2.48	0.47
3:C:49:C:H2'	3:C:50:A:C8	2.50	0.47
41:QA:154:VAL:HG12	41:QA:158:LEU:HD23	1.97	0.47
25:Y:96:LYS:O	25:Y:97:SER:HB2	2.14	0.47
49:YA:109:ARG:HB3	49:YA:118:VAL:HG21	1.97	0.47
2:B:1600:C:H2'	2:B:1601:G:H8	1.79	0.47
2:B:1302:A:H5'	2:B:1608:A:OP1	2.14	0.47
2:B:2831:G:OP2	7:G:59:ARG:NH1	2.45	0.47
1:A:741:G:OP1	52:BB:1:SER:N	2.47	0.47
2:B:2060:A:N6	8:H:69:ARG:HH21	2.13	0.47
9:I:109:ARG:HH21	9:I:138:PRO:HG3	1.79	0.47
40:PA:8:GLY:O	40:PA:11:LEU:HG	2.15	0.47
41:QA:12:ARG:HD3	41:QA:36:ALA:O	2.15	0.47
1:A:235:C:H2'	1:A:236:A:H8	1.80	0.47
51:AB:73:PHE:O	51:AB:78:GLY:N	2.47	0.47
2:B:2544:G:H2'	2:B:2545:G:H8	1.80	0.47
3:C:9:G:H2'	3:C:10:G:H8	1.79	0.47
54:DB:45:VAL:HG22	54:DB:72:TRP:HB2	1.96	0.47
32:FA:30:ASP:OD2	32:FA:33:SER:N	2.42	0.47
2:B:452:G:OP1	8:H:52:VAL:HG13	2.14	0.47
2:B:674:G:H5'	8:H:71:GLY:H	1.79	0.47
11:K:126:GLY:O	11:K:145:ASN:ND2	2.47	0.47
13:M:45:THR:HB	13:M:50:LYS:HG2	1.97	0.47
49:YA:33:CYS:N	49:YA:54:VAL:HG13	2.25	0.47
1:A:81:A:H2	1:A:88:U:H3	1.63	0.47
2:B:20:C:H2'	2:B:21:A:C8	2.49	0.47
45:UA:10:LEU:HD13	45:UA:74:ILE:HD11	1.97	0.47
2:B:2599:G:H2'	2:B:2600:A:H8	1.79	0.47
2:B:404:A:H1'	2:B:406:G:C4	2.50	0.47
2:B:814:C:H1'	2:B:1225:G:H21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:833:A:H2'	2:B:834:G:C8	2.46	0.47
2:B:948:C:H2'	2:B:949:G:H8	1.80	0.47
6:F:30:ALA:HB3	6:F:31:PRO:HD3	1.97	0.47
2:B:1265:A:N6	2:B:2013:A:H5''	2.28	0.47
2:B:2087:G:H2'	2:B:2088:A:H8	1.80	0.47
2:B:2166:U:O4	2:B:2170:A:N6	2.48	0.47
2:B:355:U:H2'	2:B:356:G:H8	1.80	0.47
53:CB:78:VAL:HG13	53:CB:78:VAL:O	2.14	0.47
6:F:229:HIS:CD2	6:F:246:PRO:HG3	2.50	0.47
8:H:118:LEU:HD12	8:H:186:VAL:O	2.15	0.47
13:M:32:VAL:HG21	13:M:60:VAL:HG21	1.96	0.47
41:QA:36:ALA:N	41:QA:37:PRO:CD	2.77	0.47
1:A:1254:A:OP1	47:WA:47:GLU:HG2	2.15	0.47
50:ZA:104:ASN:O	50:ZA:105:ALA:HB3	2.14	0.47
1:A:711:G:H2'	1:A:712:A:H8	1.81	0.46
2:B:660:C:H2'	2:B:661:A:H8	1.79	0.46
9:I:72:SER:HB3	9:I:80:GLN:HB2	1.98	0.46
35:IA:30:HIS:O	35:IA:31:ILE:C	2.54	0.46
13:M:87:SER:HB3	13:M:97:VAL:HG22	1.96	0.46
40:PA:134:LYS:O	40:PA:137:VAL:HG12	2.14	0.46
1:A:783:C:H2'	1:A:784:A:H8	1.80	0.46
2:B:1089:A:H2	2:B:1090:A:H62	1.62	0.46
2:B:161:A:H3'	2:B:162:U:H5''	1.97	0.46
2:B:2417:C:H2'	2:B:2418:A:H8	1.79	0.46
2:B:2848:G:H2'	2:B:2867:G:N2	2.30	0.46
12:L:122:GLN:O	12:L:124:ASP:N	2.48	0.46
1:A:1054:C:H42	38:MA:196:ILE:HB	1.80	0.46
41:QA:2:ARG:HG3	41:QA:3:TYR:N	2.30	0.46
20:T:47:ILE:HD11	20:T:61:ARG:HD2	1.97	0.46
2:B:2014:A:H2'	2:B:2015:A:C8	2.50	0.46
2:B:2340:A:H2'	2:B:2341:G:H8	1.80	0.46
2:B:2508:G:H2'	2:B:2509:G:C8	2.51	0.46
2:B:2591:C:H2'	2:B:2592:G:H8	1.80	0.46
11:K:84:ALA:HB2	11:K:90:LEU:HD23	1.96	0.46
16:P:101:ILE:HB	16:P:105:ILE:HG13	1.97	0.46
40:PA:180:ASP:HB3	40:PA:204:GLY:HA3	1.97	0.46
17:Q:75:GLU:HB3	17:Q:90:GLU:HG3	1.97	0.46
2:B:121:G:H2'	2:B:122:G:C8	2.50	0.46
2:B:18:U:H2'	2:B:19:A:C8	2.51	0.46
2:B:1909:C:H2'	2:B:1910:G:H8	1.80	0.46
58:HB:36:PHE:HB3	58:HB:39:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:IA:55:GLY:O	35:IA:58:ILE:HG22	2.16	0.46
38:MA:114:GLU:HG2	38:MA:163:ILE:HG12	1.97	0.46
14:N:7:LYS:O	14:N:11:VAL:HG23	2.16	0.46
2:B:2296:U:OP2	19:S:9:ARG:NH2	2.49	0.46
1:A:1367:C:H5''	46:VA:115:VAL:HG23	1.97	0.46
1:A:1436:U:H2'	1:A:1437:A:C8	2.50	0.46
51:AB:55:SER:HB3	51:AB:56:SER:H	1.51	0.46
2:B:2220:U:H2'	2:B:2221:G:H8	1.81	0.46
2:B:2470:G:H2'	2:B:2471:A:C8	2.50	0.46
2:B:2699:C:H2'	2:B:2700:A:H8	1.81	0.46
2:B:759:G:H2'	2:B:760:G:C8	2.50	0.46
52:BB:66:LEU:HD23	52:BB:66:LEU:HA	1.76	0.46
12:L:20:LYS:HB2	12:L:88:HIS:HD2	1.79	0.46
40:PA:168:ARG:NH2	40:PA:170:GLY:O	2.48	0.46
46:VA:56:MET:O	46:VA:58:GLU:N	2.48	0.46
49:YA:98:ARG:HB2	49:YA:116:TYR:HA	1.98	0.46
1:A:647:C:H2'	1:A:648:A:H8	1.80	0.46
2:B:254:G:O2'	2:B:255:A:O4'	2.33	0.46
2:B:938:G:H2'	2:B:939:G:H8	1.80	0.46
53:CB:78:VAL:O	53:CB:78:VAL:HG22	2.16	0.46
14:N:17:VAL:HG23	14:N:137:PRO:HB2	1.97	0.46
14:N:93:ILE:HD13	14:N:100:VAL:HG21	1.98	0.46
45:UA:88:LYS:O	45:UA:91:LEU:HD23	2.16	0.46
22:V:7:SER:OG	22:V:8:GLY:N	2.49	0.46
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.46
1:A:673:A:H2'	1:A:674:G:C8	2.50	0.46
1:A:875:U:H1'	45:UA:15:ASN:HD21	1.81	0.46
47:WA:49:PHE:CZ	51:AB:76:LYS:HD3	2.49	0.46
40:PA:8:GLY:HA3	51:AB:89:MET:HE2	1.97	0.46
2:B:1114:C:H2'	2:B:1115:G:C8	2.51	0.46
2:B:2880:C:O2	18:R:93:GLY:N	2.47	0.46
5:E:163:TYR:HB2	5:E:171:ILE:HG12	1.98	0.46
55:EB:71:ASP:OD1	55:EB:72:ARG:N	2.49	0.46
37:KA:8:A:H2'	37:KA:9:G:C8	2.48	0.46
39:OA:173:LYS:O	39:OA:177:ASN:ND2	2.49	0.46
17:Q:47:GLU:OE2	17:Q:50:ARG:NH1	2.48	0.46
43:SA:59:TYR:HE2	55:EB:66:LEU:HD21	1.81	0.46
1:A:52:C:H2'	1:A:53:A:C8	2.50	0.46
2:B:1190:G:H2'	2:B:1191:G:H8	1.79	0.46
2:B:1527:G:N1	2:B:1544:A:OP2	2.48	0.46
2:B:2009:A:H2'	2:B:2010:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2087:G:H2'	2:B:2088:A:C8	2.50	0.46
2:B:2483:C:N3	17:Q:123:LYS:NZ	2.62	0.46
3:C:41:G:H1	9:I:68:LYS:HE2	1.80	0.46
7:G:4:LEU:HG	7:G:32:ASN:ND2	2.30	0.46
2:B:2359:C:O2'	35:IA:53:ASP:OD2	2.34	0.46
11:K:40:THR:O	11:K:42:LYS:N	2.48	0.46
18:R:28:LEU:HD23	18:R:48:VAL:HG21	1.98	0.46
42:RA:40:ASP:OD2	42:RA:44:ARG:HB3	2.15	0.46
1:A:599:C:H2'	1:A:600:A:H8	1.81	0.46
1:A:601:G:H2'	1:A:602:A:C8	2.51	0.46
1:A:59:A:H5'	1:A:60:A:H5''	1.98	0.46
51:AB:73:PHE:C	51:AB:78:GLY:HA2	2.35	0.46
2:B:1074:G:H3'	2:B:1075:C:H5''	1.97	0.46
2:B:1440:U:H2'	2:B:1441:G:C8	2.51	0.46
2:B:2146:C:H4'	2:B:2147:A:N7	2.31	0.46
2:B:636:G:H3'	16:P:128:THR:HG21	1.97	0.46
2:B:2591:C:OP1	6:F:237:ARG:HD2	2.16	0.46
23:W:15:GLN:HE22	32:FA:16:ARG:HH22	1.62	0.46
37:KA:20:A:O2'	38:MA:303:ARG:NH2	2.49	0.46
38:MA:248:HIS:CE1	38:MA:250:PRO:HD2	2.50	0.46
41:QA:58:GLN:OE1	41:QA:62:ARG:NH1	2.49	0.46
43:SA:12:PRO:O	43:SA:15:SER:CB	2.64	0.46
24:X:8:LEU:HD23	24:X:50:LEU:HD21	1.98	0.46
1:A:363:A:H5'	49:YA:30:ARG:HB2	1.97	0.46
6:F:123:ILE:HG23	6:F:191:LEU:HD13	1.97	0.46
13:M:75:ALA:HB3	13:M:131:THR:HG21	1.97	0.46
38:MA:42:TYR:HA	38:MA:45:LEU:HB3	1.98	0.46
41:QA:10:LEU:HD13	41:QA:62:ARG:HD3	1.99	0.46
2:B:28:A:H2	21:U:10:ARG:HH12	1.63	0.46
1:A:1513:A:H2'	1:A:1514:G:H8	1.81	0.45
1:A:5:U:H3	41:QA:83:GLY:N	2.14	0.45
51:AB:64:CYS:HB3	51:AB:79:LEU:N	2.31	0.45
51:AB:89:MET:HE1	51:AB:98:LYS:HD2	1.98	0.45
2:B:2398:U:H2'	2:B:2399:G:H8	1.81	0.45
28:BA:27:ARG:HE	28:BA:29:LEU:HD21	1.80	0.45
5:E:31:LYS:HD2	5:E:185:LEU:HD12	1.98	0.45
6:F:48:ILE:HD11	6:F:51:ARG:HA	1.97	0.45
21:U:51:GLN:OE1	21:U:54:ARG:NH1	2.48	0.45
46:VA:30:ASN:O	46:VA:31:GLN:HB2	2.16	0.45
26:Z:72:VAL:HG12	26:Z:93:ARG:HA	1.98	0.45
2:B:1791:A:H5''	6:F:204:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2041:U:H2'	2:B:2042:A:H8	1.81	0.45
2:B:2328:A:H2'	2:B:2329:U:C6	2.51	0.45
2:B:2875:C:H2'	2:B:2876:G:H8	1.81	0.45
2:B:796:C:H2'	2:B:797:G:C8	2.51	0.45
53:CB:75:ILE:O	53:CB:79:ASN:ND2	2.50	0.45
54:DB:56:ASP:OD1	54:DB:56:ASP:N	2.49	0.45
58:HB:13:VAL:HG12	58:HB:14:ALA:H	1.81	0.45
14:N:4:PHE:O	21:U:63:ARG:NH2	2.49	0.45
40:PA:8:GLY:HA3	51:AB:89:MET:CE	2.46	0.45
50:ZA:16:ILE:O	50:ZA:19:THR:OG1	2.26	0.45
2:B:1190:G:H2'	2:B:1191:G:C8	2.51	0.45
2:B:1444:G:H2'	2:B:1445:G:H8	1.82	0.45
2:B:155:A:H2'	2:B:156:A:C8	2.52	0.45
2:B:1704:C:H2'	2:B:1705:A:C8	2.51	0.45
30:DA:23:LEU:HD11	30:DA:53:MET:SD	2.57	0.45
5:E:180:PHE:HB2	5:E:185:LEU:HG	1.97	0.45
18:R:114:GLU:OE1	18:R:118:ARG:NH2	2.49	0.45
1:A:10:A:H2'	1:A:11:G:H8	1.82	0.45
1:A:1386:G:H2'	1:A:1387:G:C8	2.49	0.45
1:A:418:C:H2'	1:A:419:C:C6	2.51	0.45
2:B:2368:C:H2'	2:B:2369:A:H8	1.80	0.45
2:B:629:G:N3	2:B:639:U:O2'	2.49	0.45
5:E:175:ILE:HG13	5:E:192:LEU:HD23	1.97	0.45
7:G:10:GLY:H	7:G:197:THR:HG23	1.82	0.45
40:PA:11:LEU:HD11	51:AB:88:ALA:O	2.16	0.45
3:C:7:G:H5'	19:S:29:HIS:ND1	2.31	0.45
20:T:15:ASP:N	20:T:15:ASP:OD1	2.46	0.45
1:A:675:A:H2'	1:A:676:A:H8	1.81	0.45
2:B:2875:C:H2'	2:B:2876:G:C8	2.52	0.45
2:B:302:C:H2'	2:B:303:G:H8	1.82	0.45
2:B:742:A:H2'	2:B:743:A:H8	1.82	0.45
2:B:781:A:OP1	6:F:216:ARG:NH2	2.50	0.45
3:C:76:G:H2'	3:C:77:U:C6	2.51	0.45
3:C:93:C:H2'	3:C:94:A:H8	1.81	0.45
54:DB:57:VAL:HB	54:DB:78:VAL:HG21	1.97	0.45
5:E:98:GLU:HB3	5:E:123:VAL:HG11	1.99	0.45
6:F:120:ASP:HB2	11:K:91:PHE:HE1	1.80	0.45
2:B:1062:G:H21	13:M:135:MET:HE3	1.81	0.45
13:M:34:ILE:H	13:M:34:ILE:HD12	1.82	0.45
43:SA:48:ALA:H	55:EB:65:SER:HG	1.64	0.45
1:A:1354:U:H2'	1:A:1355:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:C:H2'	1:A:1410:A:H8	1.81	0.45
1:A:710:G:H2'	1:A:711:G:H8	1.82	0.45
1:A:859:G:OP2	1:A:869:G:N1	2.44	0.45
2:B:1178:C:H2'	2:B:1179:G:C8	2.51	0.45
2:B:1765:U:H2'	2:B:1766:G:H8	1.81	0.45
2:B:1792:G:O2'	2:B:1830:C:OP1	2.35	0.45
2:B:2026:U:H2'	2:B:2027:G:H8	1.82	0.45
2:B:2417:C:H2'	2:B:2418:A:C8	2.52	0.45
2:B:2455:G:H2'	2:B:2456:C:C6	2.52	0.45
2:B:2586:U:H2'	2:B:2587:A:C8	2.51	0.45
10:J:120:ILE:HG23	10:J:134:GLY:HA3	1.98	0.45
1:A:1106:G:H5''	40:PA:171:ARG:HG2	1.99	0.45
1:A:519:C:N4	1:A:520:A:C6	2.85	0.45
51:AB:87:ALA:HB1	51:AB:93:ILE:HG13	1.99	0.45
2:B:1136:G:H2'	2:B:1137:G:H8	1.81	0.45
2:B:1251:C:OP2	21:U:5:ARG:NH2	2.48	0.45
2:B:1550:C:H2'	2:B:1551:A:H8	1.82	0.45
2:B:2126:A:H2'	2:B:2162:G:H22	1.80	0.45
2:B:2229:U:H2'	2:B:2230:G:H8	1.82	0.45
2:B:242:G:N7	35:IA:4:LYS:HG2	2.31	0.45
2:B:2466:C:OP1	36:JA:4:ARG:HB3	2.17	0.45
53:CB:22:ALA:HA	53:CB:33:ILE:HD12	1.98	0.45
5:E:124:VAL:HG12	5:E:124:VAL:O	2.16	0.45
5:E:97:MET:HB3	5:E:100:LEU:HB3	1.97	0.45
11:K:87:GLU:OE1	43:SA:24:ARG:NH1	2.44	0.45
22:V:5:PHE:HB3	22:V:59:ILE:HD12	1.98	0.45
1:A:1479:C:H2'	1:A:1480:A:H8	1.81	0.45
27:AA:55:LEU:HD22	27:AA:76:ILE:HD12	1.99	0.45
2:B:1295:C:H2'	2:B:1296:G:H8	1.82	0.45
2:B:1368:G:H2'	2:B:1369:G:C8	2.49	0.45
2:B:2230:G:H2'	2:B:2231:U:H6	1.82	0.45
54:DB:75:VAL:HG12	54:DB:76:ARG:HG3	1.98	0.45
5:E:20:GLN:HG2	5:E:225:ASP:HB3	1.99	0.45
38:MA:54:ASP:HB3	38:MA:88:LYS:CE	2.46	0.45
19:S:33:ARG:O	19:S:34:HIS:CG	2.70	0.45
21:U:20:ALA:O	21:U:23:TYR:HD2	1.99	0.45
23:W:107:VAL:HG22	23:W:108:SER:H	1.82	0.45
23:W:24:ILE:HD13	23:W:36:LEU:HD11	1.99	0.45
26:Z:9:ARG:HG2	26:Z:41:GLU:HB2	1.99	0.45
50:ZA:80:MET:O	50:ZA:91:ARG:NH1	2.49	0.45
50:ZA:86:ARG:HG3	50:ZA:96:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AB:33:VAL:HA	51:AB:41:ARG:HH22	1.82	0.45
2:B:2124:G:N2	5:E:217:THR:HA	2.31	0.45
2:B:2298:A:OP1	9:I:70:ARG:NH2	2.48	0.45
3:C:9:G:H2'	3:C:10:G:C8	2.51	0.45
4:D:12:G:H2'	4:D:13:C:C6	2.52	0.45
12:L:29:ASP:H	12:L:56:ARG:NH2	2.15	0.45
2:B:621:A:OP2	16:P:99:ASN:ND2	2.49	0.45
45:UA:65:PHE:O	45:UA:67:GLY:N	2.50	0.45
1:A:1305:G:HO2'	1:A:1306:A:H8	1.64	0.45
1:A:1507:A:H2'	1:A:1508:A:C8	2.52	0.45
1:A:1521:C:H2'	1:A:1522:U:C6	2.52	0.45
1:A:545:C:OP2	41:QA:61:ARG:NH1	2.50	0.45
1:A:562:U:H2'	49:YA:13:ARG:HD3	1.99	0.45
1:A:987:G:H2'	1:A:988:G:H8	1.82	0.45
2:B:1072:C:H42	2:B:1092:C:N4	2.15	0.45
2:B:1105:U:H2'	2:B:1106:G:H8	1.82	0.45
2:B:1440:U:H2'	2:B:1441:G:H8	1.81	0.45
2:B:2330:G:H21	27:AA:38:GLY:HA2	1.81	0.45
2:B:2756:U:H4'	2:B:2757:A:OP1	2.15	0.45
2:B:2898:U:H2'	2:B:2899:A:C8	2.52	0.45
2:B:2898:U:H2'	2:B:2899:A:H8	1.82	0.45
15:O:41:ILE:HG13	15:O:58:LEU:O	2.17	0.45
1:A:1496:C:O2	1:A:1517:G:N2	2.43	0.44
1:A:532:A:H62	1:A:1206:G:H21	1.65	0.44
2:B:1291:C:H2'	2:B:1292:G:H8	1.82	0.44
2:B:2555:U:O2	38:MA:228:ARG:HB2	2.17	0.44
2:B:2557:G:H2'	2:B:2558:C:C6	2.51	0.44
2:B:2590:A:C2	2:B:2604:U:H5	2.35	0.44
2:B:52:A:OP2	2:B:117:G:N1	2.46	0.44
54:DB:24:ILE:HD11	54:DB:60:ILE:HD11	1.99	0.44
31:EA:45:THR:O	31:EA:48:GLN:HB2	2.17	0.44
4:LA:63:G:H2'	4:LA:64:G:H8	1.81	0.44
40:PA:18:ASN:O	40:PA:39:ARG:NH2	2.50	0.44
41:QA:165:GLU:OE2	41:QA:167:PRO:HD3	2.16	0.44
19:S:62:LEU:HD21	19:S:73:ALA:HB2	1.99	0.44
1:A:1307:U:OP1	50:ZA:99:GLN:NE2	2.50	0.44
1:A:131:A:H2'	1:A:132:C:C6	2.51	0.44
1:A:141:G:H2'	1:A:142:G:H8	1.83	0.44
1:A:830:G:H2'	1:A:831:A:C8	2.52	0.44
1:A:977:A:H2'	1:A:978:A:H5''	1.98	0.44
51:AB:62:ASN:HB2	51:AB:73:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1604:C:H2'	2:B:1605:C:C6	2.53	0.44
55:EB:62:ARG:HB3	55:EB:69:TYR:HE1	1.82	0.44
1:A:823:C:H2'	1:A:824:G:C8	2.52	0.44
2:B:2086:U:H2'	2:B:2087:G:H8	1.82	0.44
2:B:658:U:O2'	8:H:97:ASN:ND2	2.51	0.44
3:C:24:G:C6	3:C:56:G:C2	3.06	0.44
6:F:140:VAL:HG11	6:F:189:ALA:HB1	1.99	0.44
6:F:140:VAL:HG22	6:F:191:LEU:HD23	2.00	0.44
56:FB:66:VAL:HG23	56:FB:67:GLY:H	1.82	0.44
4:LA:17:C:OP1	4:LA:60:U:O2'	2.35	0.44
41:QA:146:GLU:HA	41:QA:149:LYS:HG2	1.99	0.44
49:YA:80:LEU:HD13	49:YA:100:ALA:HB1	2.00	0.44
1:A:1384:C:H2'	1:A:1385:G:C8	2.53	0.44
2:B:1954:G:N2	2:B:1956:U:H3	2.16	0.44
2:B:2655:G:N2	2:B:2665:A:OP2	2.49	0.44
2:B:596:U:H2'	2:B:597:G:C8	2.53	0.44
3:C:49:C:H2'	3:C:50:A:H8	1.83	0.44
3:C:5:U:H2'	3:C:6:G:C8	2.51	0.44
2:B:1993:U:H4'	7:G:133:THR:HG22	1.99	0.44
1:A:545:C:OP1	41:QA:57:LYS:NZ	2.50	0.44
18:R:59:SER:OG	18:R:60:VAL:N	2.50	0.44
42:RA:104:ILE:O	42:RA:104:ILE:HG23	2.17	0.44
47:WA:83:THR:O	47:WA:87:LEU:N	2.48	0.44
1:A:1062:U:H2'	1:A:1063:C:C6	2.52	0.44
1:A:1219:A:H2'	1:A:1220:G:C8	2.53	0.44
1:A:708:C:H2'	1:A:709:U:H6	1.83	0.44
2:B:1165:A:H2'	2:B:1166:G:C8	2.50	0.44
2:B:572:A:OP2	22:V:79:ARG:NH1	2.50	0.44
5:E:60:ARG:HG2	5:E:164:ARG:HA	1.99	0.44
15:O:92:GLU:O	15:O:93:GLN:C	2.56	0.44
41:QA:201:GLU:OE1	42:RA:111:ARG:NH1	2.50	0.44
21:U:104:ALA:HA	22:V:46:GLU:HG3	2.00	0.44
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.63	0.44
1:A:522:C:OP2	49:YA:65:TYR:OH	2.32	0.44
2:B:1055:G:H1	2:B:1104:C:H42	1.64	0.44
2:B:1363:C:H2'	2:B:1364:G:H8	1.82	0.44
2:B:1539:U:H2'	2:B:1540:G:C8	2.53	0.44
2:B:1889:A:H2'	2:B:1890:A:H8	1.83	0.44
2:B:24:G:C2	2:B:25:U:C2	3.05	0.44
2:B:680:C:H2'	2:B:681:G:C8	2.52	0.44
6:F:106:PRO:HD2	6:F:109:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:67:THR:O	12:L:67:THR:OG1	2.31	0.44
24:X:50:LEU:HD12	24:X:50:LEU:N	2.33	0.44
1:A:105:G:OP2	57:GB:12:GLN:NE2	2.51	0.44
1:A:1313:U:OP1	56:FB:5:LYS:HB3	2.18	0.44
1:A:45:G:H2'	1:A:46:G:H8	1.82	0.44
1:A:708:C:H2'	1:A:709:U:C6	2.53	0.44
1:A:737:C:H2'	1:A:738:C:C6	2.53	0.44
51:AB:97:LYS:O	51:AB:98:LYS:C	2.55	0.44
2:B:1013:C:H2'	2:B:1014:A:C8	2.51	0.44
2:B:1509:A:H2'	2:B:1510:G:C8	2.52	0.44
2:B:647:G:N2	2:B:2350:C:O2'	2.48	0.44
2:B:247:G:H4'	2:B:386:G:C2	2.52	0.44
2:B:2590:A:H2'	2:B:2591:C:C6	2.53	0.44
2:B:2591:C:H2'	2:B:2592:G:C8	2.52	0.44
2:B:376:G:C2	2:B:377:G:N7	2.86	0.44
2:B:690:G:H2'	2:B:691:C:H6	1.83	0.44
2:B:971:G:O2'	2:B:983:A:N3	2.50	0.44
11:K:7:ASP:HB3	11:K:9:VAL:HG23	2.00	0.44
12:L:29:ASP:H	12:L:56:ARG:HH22	1.64	0.44
38:MA:54:ASP:HB3	38:MA:88:LYS:NZ	2.33	0.44
18:R:47:VAL:C	18:R:50:PRO:HD2	2.38	0.44
2:B:2720:U:H5''	20:T:52:ARG:NH2	2.32	0.44
23:W:72:THR:HG22	23:W:73:LYS:HG3	1.99	0.44
48:XA:126:ARG:HB3	58:HB:33:ARG:CZ	2.48	0.44
48:XA:126:ARG:O	58:HB:33:ARG:NH2	2.51	0.44
48:XA:83:VAL:HG11	48:XA:96:ILE:HG22	1.98	0.44
26:Z:38:LEU:HG	26:Z:40:ILE:HD11	2.00	0.44
1:A:1198:G:H2'	1:A:1199:U:C6	2.53	0.44
1:A:455:G:H2'	1:A:456:A:C8	2.52	0.44
1:A:797:C:H2'	1:A:798:U:C6	2.53	0.44
51:AB:56:SER:C	51:AB:58:SER:N	2.70	0.44
2:B:1259:G:H2'	2:B:1260:A:C8	2.52	0.44
2:B:2010:G:OP1	23:W:41:LYS:HG3	2.18	0.44
2:B:2884:U:C6	32:FA:49:ARG:HG2	2.52	0.44
9:I:139:GLU:N	9:I:139:GLU:OE1	2.50	0.44
3:C:7:G:O2'	19:S:38:GLN:NE2	2.51	0.44
45:UA:24:VAL:HG12	45:UA:26:MET:HE3	2.00	0.44
1:A:715:A:H2'	1:A:716:A:C8	2.51	0.44
1:A:828:U:N3	1:A:859:G:N3	2.66	0.44
2:B:1030:C:H2'	2:B:1031:G:H8	1.83	0.44
2:B:1306:C:H2'	2:B:1307:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2641:G:H2'	2:B:2642:G:H8	1.83	0.44
2:B:463:G:N2	2:B:466:A:OP2	2.45	0.44
6:F:153:LEU:HB3	6:F:175:LEU:HD11	2.00	0.44
11:K:135:HIS:CG	11:K:136:SER:H	2.36	0.44
21:U:94:LEU:HD23	21:U:94:LEU:HA	1.80	0.44
1:A:501:C:H2'	1:A:502:A:H8	1.83	0.43
1:A:784:A:H2'	1:A:785:G:C8	2.53	0.43
1:A:824:G:H2'	1:A:825:A:H8	1.83	0.43
2:B:2024:G:OP2	2:B:2034:U:H4'	2.17	0.43
2:B:914:G:H5'	2:B:915:C:OP2	2.18	0.43
2:B:968:C:H2'	2:B:969:G:C8	2.53	0.43
31:EA:44:PHE:CD2	31:EA:45:THR:HG23	2.53	0.43
2:B:2772:C:H5'	7:G:173:GLN:HE21	1.82	0.43
7:G:178:VAL:HG12	7:G:179:ARG:HG3	2.00	0.43
58:HB:11:PHE:HB2	58:HB:15:LEU:HD12	1.99	0.43
58:HB:17:ARG:HB3	58:HB:20:ARG:HH21	1.81	0.43
10:J:37:ASN:HD22	10:J:38:ASP:H	1.65	0.43
40:PA:4:VAL:CG1	40:PA:5:HIS:H	2.17	0.43
47:WA:67:ILE:HG13	47:WA:67:ILE:O	2.18	0.43
1:A:1436:U:H2'	1:A:1437:A:H8	1.82	0.43
1:A:204:G:H2'	1:A:205:A:C8	2.53	0.43
1:A:520:A:OP1	49:YA:48:LEU:HB2	2.19	0.43
1:A:707:U:H2'	1:A:708:C:C6	2.53	0.43
51:AB:63:ARG:O	51:AB:65:ARG:N	2.52	0.43
2:B:1592:C:H2'	2:B:1593:A:C8	2.52	0.43
2:B:1843:C:H2'	2:B:1844:C:C6	2.52	0.43
2:B:776:G:N2	2:B:2241:A:OP1	2.47	0.43
30:DA:9:THR:HG22	30:DA:53:MET:O	2.19	0.43
31:EA:24:ILE:HG22	31:EA:25:ARG:N	2.34	0.43
7:G:133:THR:O	7:G:134:HIS:HB2	2.18	0.43
2:B:1022:G:N7	14:N:68:LYS:HD3	2.33	0.43
44:TA:67:ASN:O	44:TA:137:ARG:NH1	2.51	0.43
23:W:36:LEU:HD23	23:W:36:LEU:HA	1.79	0.43
49:YA:77:SER:HB2	49:YA:102:ASP:HB3	2.00	0.43
1:A:613:C:P	41:QA:80:ARG:HH21	2.42	0.43
27:AA:21:ARG:HB3	27:AA:25:GLU:HG2	2.01	0.43
2:B:1161:C:H2'	2:B:1162:G:C8	2.53	0.43
2:B:1437:C:H2'	2:B:1438:U:C6	2.54	0.43
2:B:871:U:H2'	2:B:872:U:C6	2.53	0.43
6:F:32:LEU:HD11	6:F:100:ARG:O	2.18	0.43
32:FA:2:VAL:HG12	32:FA:3:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:LEU:HD22	8:H:185:LYS:HG3	1.99	0.43
38:MA:108:GLU:HB2	38:MA:170:GLY:HA2	2.00	0.43
2:B:2555:U:O2'	38:MA:228:ARG:NH2	2.51	0.43
14:N:35:ARG:HD3	14:N:40:HIS:CD2	2.53	0.43
39:OA:40:ILE:HD12	39:OA:201:GLY:HA2	2.00	0.43
17:Q:68:PHE:HA	17:Q:69:PRO:HD3	1.89	0.43
17:Q:70:ASP:C	17:Q:70:ASP:OD1	2.56	0.43
49:YA:86:VAL:HG23	49:YA:89:LEU:HB2	1.99	0.43
1:A:1349:A:H3'	1:A:1350:A:H8	1.84	0.43
1:A:1477:U:H2'	1:A:1478:U:C6	2.53	0.43
2:B:1709:U:H2'	2:B:1710:G:C8	2.53	0.43
2:B:1822:C:H2'	2:B:1823:G:H8	1.84	0.43
2:B:2291:U:OP1	2:B:2380:C:O2'	2.36	0.43
2:B:2296:U:O2'	2:B:2297:A:O5'	2.33	0.43
2:B:947:A:H2'	2:B:948:C:C6	2.54	0.43
38:MA:191:GLU:HG3	38:MA:193:GLN:H	1.83	0.43
38:MA:217:ILE:HD13	38:MA:219:PRO:HD3	1.99	0.43
40:PA:120:THR:HG23	40:PA:188:ALA:HB2	2.00	0.43
18:R:29:VAL:O	18:R:29:VAL:HG12	2.18	0.43
3:C:7:G:H5'	19:S:29:HIS:CE1	2.53	0.43
46:VA:86:LEU:HD23	46:VA:86:LEU:HA	1.87	0.43
26:Z:40:ILE:HG22	26:Z:42:LEU:HD12	2.00	0.43
1:A:1106:G:O2'	40:PA:168:ARG:NH2	2.52	0.43
1:A:979:C:OP1	1:A:1223:C:N4	2.51	0.43
1:A:1251:A:O2'	1:A:1370:G:H5'	2.19	0.43
1:A:1425:U:H2'	1:A:1426:G:H8	1.83	0.43
1:A:1521:C:H2'	1:A:1522:U:H6	1.84	0.43
1:A:335:C:H2'	1:A:336:A:H8	1.83	0.43
1:A:537:G:H5''	49:YA:109:ARG:NH1	2.27	0.43
1:A:806:C:H2'	1:A:807:A:C8	2.53	0.43
2:B:1133:A:H4'	2:B:1134:A:H5''	2.00	0.43
2:B:1316:U:H2'	2:B:1317:G:C8	2.50	0.43
2:B:1825:U:H2'	2:B:1826:G:C8	2.54	0.43
2:B:2271:G:C5	2:B:2272:U:C4	3.06	0.43
2:B:840:C:H2'	2:B:841:G:H8	1.84	0.43
13:M:54:ILE:CG2	13:M:55:PRO:CD	2.91	0.43
38:MA:304:SER:HB2	49:YA:48:LEU:CD1	2.49	0.43
43:SA:39:LEU:HD12	43:SA:39:LEU:HA	1.91	0.43
2:B:2848:G:C8	20:T:94:ALA:HB2	2.54	0.43
2:B:993:G:OP2	21:U:50:ARG:NH2	2.51	0.43
1:A:1526:G:H2'	1:A:1527:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:C:H2'	1:A:392:C:O2	2.19	0.43
1:A:477:C:H2'	1:A:478:A:C8	2.53	0.43
1:A:634:C:H2'	1:A:635:A:C8	2.54	0.43
51:AB:2:LYS:O	51:AB:5:MET:HB2	2.18	0.43
2:B:2106:U:H2'	2:B:2107:G:C8	2.54	0.43
2:B:63:A:H4'	24:X:77:ARG:NH1	2.33	0.43
3:C:93:C:H2'	3:C:94:A:C8	2.54	0.43
1:A:390:U:H4'	53:CB:28:ARG:HH11	1.83	0.43
53:CB:4:ILE:HD13	53:CB:67:ILE:HG12	2.01	0.43
2:B:1256:G:N2	8:H:77:ILE:O	2.50	0.43
9:I:58:ALA:O	9:I:139:GLU:HG2	2.19	0.43
13:M:54:ILE:HG22	13:M:55:PRO:HD2	1.97	0.43
38:MA:214:LEU:HD23	38:MA:214:LEU:H	1.83	0.43
16:P:123:ARG:NH1	16:P:143:GLU:OE2	2.52	0.43
41:QA:111:ALA:O	41:QA:114:ARG:HG3	2.19	0.43
22:V:46:GLU:OE2	22:V:48:LYS:HB3	2.18	0.43
1:A:202:G:H2'	1:A:203:G:H8	1.84	0.43
1:A:797:C:OP1	48:XA:125:LYS:HB2	2.19	0.43
1:A:948:C:H2'	1:A:949:A:C8	2.53	0.43
2:B:1155:A:O2'	2:B:1156:A:H2'	2.18	0.43
2:B:1800:C:HO2'	2:B:1818:U:H3	1.65	0.43
7:G:5:VAL:HG21	7:G:80:TRP:CG	2.53	0.43
46:VA:23:GLY:H	46:VA:60:LEU:HA	1.83	0.43
47:WA:40:ILE:HB	47:WA:73:LEU:HB3	2.00	0.43
1:A:20:U:H2'	1:A:21:G:O4'	2.19	0.43
1:A:20:U:OP2	42:RA:129:SER:OG	2.27	0.43
51:AB:63:ARG:HA	51:AB:68:GLY:O	2.19	0.43
2:B:1071:G:H1'	2:B:1089:A:C5	2.53	0.43
2:B:1387:A:H2'	2:B:1388:G:C8	2.53	0.43
2:B:1448:G:H2'	2:B:1449:G:H8	1.82	0.43
2:B:572:A:H61	2:B:2029:G:H21	1.65	0.43
2:B:660:C:H2'	2:B:661:A:C8	2.54	0.43
2:B:2680:U:H5'	7:G:194:PRO:HA	2.01	0.43
9:I:71:LYS:HG2	9:I:72:SER:H	1.83	0.43
15:O:119:ALA:HA	15:O:120:PRO:HD3	1.89	0.43
20:T:91:VAL:HG21	20:T:96:LEU:HD11	2.00	0.43
1:A:878:A:OP1	45:UA:79:ARG:HB2	2.19	0.43
46:VA:33:SER:H	46:VA:36:GLN:HE21	1.66	0.43
1:A:684:U:O2'	48:XA:39:ASN:HB3	2.19	0.43
50:ZA:79:LEU:HD12	50:ZA:86:ARG:HB3	1.99	0.43
1:A:1414:U:H2'	1:A:1415:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:G:H5'	53:CB:31:ARG:HB2	2.01	0.43
1:A:634:C:H2'	1:A:635:A:H8	1.83	0.43
2:B:2685:G:H2'	2:B:2686:G:C8	2.54	0.43
2:B:817:C:H2'	2:B:818:G:C8	2.53	0.43
4:D:16:C:H4'	4:D:60:U:H1'	2.00	0.43
4:D:24:U:H2'	4:D:25:C:H6	1.83	0.43
6:F:124:LYS:HB3	6:F:127:ASN:OD1	2.19	0.43
57:GB:54:GLN:N	57:GB:55:PRO:HD2	2.33	0.43
34:HA:4:THR:OG1	34:HA:5:PHE:N	2.51	0.43
9:I:135:ILE:HA	9:I:140:ILE:HG21	2.01	0.43
35:IA:29:ARG:HA	35:IA:29:ARG:HD3	1.92	0.43
11:K:145:ASN:HD22	11:K:146:VAL:N	2.17	0.43
13:M:112:LYS:HD2	13:M:128:ILE:HD11	2.00	0.43
38:MA:126:LEU:HA	38:MA:157:GLY:O	2.19	0.43
16:P:108:ALA:HB3	16:P:125:LEU:HD22	2.00	0.43
18:R:40:LYS:O	18:R:44:LEU:N	2.50	0.43
45:UA:73:SER:HB2	45:UA:129:ALA:HB3	2.01	0.43
50:ZA:28:ARG:HH21	50:ZA:62:PHE:HB2	1.84	0.43
1:A:1011:C:H2'	1:A:1012:A:C8	2.54	0.43
1:A:45:G:H2'	1:A:46:G:C8	2.54	0.43
2:B:151:C:H2'	2:B:152:A:H8	1.84	0.43
2:B:2599:G:H2'	2:B:2600:A:C8	2.54	0.43
2:B:582:A:H2'	2:B:583:G:C8	2.53	0.43
56:FB:4:LEU:HB3	56:FB:5:LYS:H	1.63	0.43
19:S:34:HIS:CE1	19:S:54:VAL:HA	2.54	0.43
2:B:1248:G:C2	21:U:2:ARG:HD2	2.54	0.43
25:Y:32:LYS:HB3	25:Y:63:ALA:HB1	2.01	0.43
26:Z:29:ILE:HG13	26:Z:30:ILE:N	2.34	0.43
1:A:1255:G:O2'	1:A:1258:G:N3	2.43	0.42
2:B:106:C:H2'	2:B:107:G:C8	2.54	0.42
2:B:131:A:H2'	2:B:132:G:H8	1.84	0.42
2:B:1667:G:H22	2:B:1991:U:H3'	1.85	0.42
2:B:2699:C:H2'	2:B:2700:A:C8	2.53	0.42
2:B:2818:U:H2'	2:B:2819:G:C8	2.53	0.42
2:B:521:U:H2'	2:B:522:A:C8	2.53	0.42
2:B:851:C:H2'	2:B:852:U:C6	2.54	0.42
4:D:59:A:C2'	4:D:60:U:H5'	2.48	0.42
4:D:62:C:H2'	4:D:63:G:C8	2.54	0.42
11:K:58:LEU:O	11:K:61:VAL:HG22	2.19	0.42
11:K:67:ALA:O	11:K:70:GLU:HB3	2.19	0.42
4:LA:36:U:H2'	4:LA:37:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:ZA:44:ILE:HD12	50:ZA:47:LEU:HD13	1.99	0.42
1:A:1125:U:HO2'	1:A:1126:U:H6	1.67	0.42
2:B:1229:C:H2'	2:B:1230:A:H8	1.83	0.42
2:B:1766:G:H2'	2:B:1767:G:H8	1.83	0.42
9:I:78:ILE:O	9:I:78:ILE:HG13	2.19	0.42
19:S:6:ALA:O	19:S:9:ARG:HG3	2.20	0.42
49:YA:23:LEU:HD12	49:YA:58:ASN:ND2	2.33	0.42
1:A:1052:U:H2'	1:A:1200:C:H41	1.85	0.42
1:A:309:A:H2'	1:A:310:G:H8	1.85	0.42
2:B:1183:U:H2'	2:B:1184:U:C6	2.53	0.42
2:B:154:U:H2'	2:B:155:A:H8	1.84	0.42
2:B:1550:C:H2'	2:B:1551:A:C8	2.54	0.42
2:B:2086:U:H2'	2:B:2087:G:C8	2.53	0.42
2:B:945:A:C5	2:B:2448:A:C2	3.07	0.42
28:BA:6:VAL:HG21	28:BA:58:ILE:HD11	2.01	0.42
12:L:41:LEU:HA	12:L:41:LEU:HD23	1.89	0.42
39:OA:98:GLY:N	39:OA:174:GLU:OE2	2.42	0.42
18:R:43:GLU:OE2	18:R:46:ARG:NH2	2.51	0.42
50:ZA:86:ARG:HG3	50:ZA:96:VAL:CG1	2.50	0.42
1:A:1074:G:H2'	1:A:1075:U:C6	2.55	0.42
1:A:129:A:H1'	1:A:130:A:N7	2.34	0.42
1:A:1412:C:H2'	1:A:1413:A:H8	1.84	0.42
1:A:451:A:H4'	1:A:452:A:C4	2.54	0.42
51:AB:97:LYS:O	51:AB:98:LYS:HB2	2.18	0.42
2:B:2576:G:O2'	2:B:2579:C:OP2	2.26	0.42
2:B:338:G:C2	2:B:339:U:C2	3.07	0.42
2:B:593:U:H2'	2:B:594:U:C6	2.55	0.42
2:B:784:G:C2	6:F:227:VAL:HG11	2.54	0.42
2:B:968:C:H2'	2:B:969:G:H8	1.83	0.42
4:D:44:A:H2'	4:D:45:G:O4'	2.20	0.42
5:E:127:LEU:O	5:E:127:LEU:HD23	2.19	0.42
8:H:129:PRO:HG3	8:H:156:ASN:HA	2.01	0.42
13:M:102:ARG:N	13:M:140:GLU:O	2.53	0.42
39:OA:8:MET:HG2	39:OA:211:LEU:HD21	2.01	0.42
25:Y:26:ASN:HB2	25:Y:34:ILE:HD11	2.01	0.42
50:ZA:2:ARG:HA	50:ZA:7:ASN:O	2.19	0.42
1:A:405:U:O4	41:QA:1:ALA:N	2.46	0.42
1:A:420:U:O2'	1:A:422:C:OP1	2.32	0.42
1:A:672:U:H2'	1:A:673:A:C8	2.55	0.42
2:B:1791:A:H4'	6:F:204:LEU:HB2	2.01	0.42
2:B:1972:G:H2'	2:B:1973:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:746:U:H1'	2:B:748:G:H21	1.84	0.42
7:G:5:VAL:HG21	7:G:80:TRP:CD2	2.55	0.42
41:QA:170:LEU:O	41:QA:170:LEU:HD12	2.19	0.42
22:V:34:GLU:HG2	22:V:60:LYS:HG2	2.01	0.42
23:W:74:ILE:HD13	23:W:105:VAL:HG22	2.02	0.42
1:A:1071:C:H2'	1:A:1072:G:H8	1.84	0.42
1:A:458:U:H3	1:A:474:G:H1	1.68	0.42
2:B:1164:C:H2'	2:B:1165:A:C8	2.54	0.42
2:B:1229:C:H2'	2:B:1230:A:C8	2.55	0.42
2:B:1793:C:H2'	2:B:1794:A:H8	1.84	0.42
2:B:2291:U:H2'	2:B:2292:U:C6	2.55	0.42
2:B:2306:C:N4	9:I:38:GLY:O	2.52	0.42
2:B:571:U:N3	2:B:575:A:N7	2.67	0.42
2:B:674:G:H1'	8:H:69:ARG:NH1	2.34	0.42
10:J:37:ASN:OD1	10:J:63:GLN:NE2	2.53	0.42
10:J:37:ASN:HD22	10:J:38:ASP:N	2.17	0.42
12:L:26:VAL:HA	12:L:82:ILE:HG23	2.01	0.42
12:L:28:ALA:HB2	12:L:111:ALA:HB2	2.01	0.42
38:MA:145:ARG:HG2	38:MA:146:VAL:N	2.31	0.42
40:PA:5:HIS:O	40:PA:7:ASN:N	2.52	0.42
41:QA:3:TYR:CD2	41:QA:10:LEU:HD11	2.54	0.42
46:VA:14:SER:OG	46:VA:69:GLY:HA3	2.19	0.42
49:YA:26:CYS:SG	49:YA:29:LYS:HD3	2.60	0.42
50:ZA:6:ILE:HG22	50:ZA:8:ILE:HG12	2.00	0.42
1:A:1515:G:H2'	1:A:1516:G:H8	1.85	0.42
1:A:579:A:H2'	1:A:580:C:C6	2.55	0.42
1:A:811:C:O2'	1:A:901:A:N1	2.52	0.42
2:B:181:A:H2'	2:B:182:A:H8	1.84	0.42
2:B:922:C:H2'	2:B:923:G:H8	1.83	0.42
3:C:52:A:O2'	3:C:53:A:N7	2.41	0.42
30:DA:11:SER:OG	30:DA:12:ALA:N	2.53	0.42
10:J:53:PRO:HG2	10:J:61:TRP:CD2	2.54	0.42
11:K:47:PHE:HA	11:K:51:ARG:HB2	2.02	0.42
13:M:126:ARG:O	13:M:129:GLU:HB3	2.19	0.42
2:B:1653:G:H3'	18:R:2:ARG:HG2	2.01	0.42
42:RA:165:GLY:HA3	45:UA:113:ARG:HD2	2.01	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.42
1:A:1432:G:H1'	1:A:1468:A:H62	1.84	0.42
1:A:1458:G:H2'	1:A:1459:G:H8	1.85	0.42
2:B:1685:C:H2'	2:B:1686:C:C6	2.54	0.42
2:B:2316:G:H2'	2:B:2317:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2590:A:H2'	2:B:2591:C:H6	1.85	0.42
2:B:414:C:H2'	2:B:415:A:C8	2.53	0.42
2:B:948:C:H2'	2:B:949:G:C8	2.53	0.42
4:D:14:A:H2'	4:D:15:G:O4'	2.19	0.42
5:E:175:ILE:O	5:E:188:ASN:ND2	2.53	0.42
12:L:33:VAL:HG12	12:L:34:THR:N	2.35	0.42
19:S:7:ARG:HA	19:S:10:ARG:HH11	1.84	0.42
21:U:20:ALA:HA	21:U:23:TYR:CE2	2.54	0.42
22:V:27:ILE:HG13	22:V:33:VAL:HG22	2.01	0.42
1:A:1228:C:P	50:ZA:106:ARG:HH12	2.43	0.42
1:A:986:U:H2'	1:A:987:G:C8	2.54	0.42
51:AB:8:ARG:HB3	51:AB:12:ARG:NH1	2.28	0.42
2:B:1019:U:OP1	2:B:1035:U:O2'	2.29	0.42
2:B:1405:U:H2'	2:B:1406:U:C6	2.55	0.42
2:B:2002:G:OP1	18:R:17:ARG:NH2	2.53	0.42
2:B:910:A:N3	2:B:2264:C:O2'	2.53	0.42
52:BB:49:HIS:O	52:BB:52:ARG:HB3	2.20	0.42
36:JA:18:LYS:HG2	36:JA:18:LYS:O	2.20	0.42
1:A:1492:A:C2	37:KA:21:U:H5''	2.52	0.42
41:QA:100:VAL:HG21	41:QA:136:VAL:HG21	2.01	0.42
41:QA:12:ARG:HG2	41:QA:37:PRO:HA	2.02	0.42
47:WA:12:ALA:HB3	47:WA:18:ILE:HD13	2.02	0.42
1:A:554:A:H2'	1:A:555:U:C6	2.55	0.42
3:C:12:C:H42	27:AA:70:PRO:HD3	1.85	0.42
2:B:1748:C:H2'	2:B:1749:A:H8	1.84	0.42
2:B:1954:G:H21	2:B:1956:U:H3	1.68	0.42
2:B:2159:G:H2'	2:B:2160:C:C6	2.55	0.42
2:B:1127:A:H62	2:B:2488:G:H1'	1.84	0.42
2:B:2515:C:H2'	2:B:2516:A:H8	1.84	0.42
2:B:287:G:H2'	2:B:288:U:C6	2.55	0.42
2:B:279:A:H61	2:B:361:G:H1'	1.84	0.42
2:B:728:G:O2'	2:B:730:A:H8	2.02	0.42
10:J:1:SER:HA	10:J:4:ALA:HB3	2.02	0.42
11:K:95:GLY:C	11:K:96:THR:HG1	2.22	0.42
4:LA:17:C:H5'	4:LA:61:C:OP1	2.20	0.42
38:MA:23:LEU:HD11	38:MA:38:LEU:HB3	2.02	0.42
38:MA:263:GLN:O	38:MA:267:LYS:N	2.49	0.42
40:PA:33:ASP:OD2	51:AB:65:ARG:NH1	2.53	0.42
40:PA:21:TRP:CB	40:PA:58:ARG:HB3	2.49	0.42
43:SA:43:GLY:HA2	43:SA:58:HIS:CE1	2.55	0.42
20:T:20:ARG:HD3	20:T:112:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:20:ALA:HA	21:U:23:TYR:HE2	1.85	0.42
22:V:38:VAL:O	22:V:54:VAL:HG23	2.19	0.42
1:A:1464:U:H2'	1:A:1465:A:H8	1.84	0.41
1:A:625:U:H2'	1:A:626:G:H8	1.85	0.41
2:B:1140:C:OP2	14:N:68:LYS:NZ	2.45	0.41
2:B:1258:U:H2'	2:B:1259:G:C8	2.55	0.41
2:B:191:A:H2'	2:B:192:C:C6	2.54	0.41
2:B:528:A:C2	2:B:2042:A:H2'	2.55	0.41
2:B:720:U:H2'	2:B:721:A:C8	2.54	0.41
7:G:125:TRP:O	7:G:126:ASN:HB2	2.19	0.41
21:U:29:ARG:HD2	32:FA:9:ARG:HH12	1.85	0.41
47:WA:17:LEU:HD13	47:WA:17:LEU:O	2.20	0.41
1:A:1023:U:H2'	1:A:1024:G:C8	2.55	0.41
1:A:1464:U:H2'	1:A:1465:A:C8	2.54	0.41
1:A:1513:A:H2'	1:A:1514:G:C8	2.55	0.41
1:A:287:U:H2'	1:A:288:A:C8	2.55	0.41
1:A:34:C:H2'	1:A:35:G:H8	1.86	0.41
1:A:598:U:H2'	1:A:599:C:C6	2.55	0.41
1:A:986:U:H2'	1:A:987:G:H8	1.84	0.41
2:B:1103:A:H5''	2:B:1104:C:C5	2.56	0.41
2:B:1434:A:H2'	2:B:1435:G:C8	2.54	0.41
2:B:250:G:C6	2:B:251:A:C6	3.09	0.41
2:B:589:U:H2'	2:B:590:A:C8	2.55	0.41
2:B:591:U:H2'	2:B:592:A:H8	1.84	0.41
8:H:71:GLY:O	8:H:72:SER:CB	2.68	0.41
12:L:119:PRO:O	12:L:120:ALA:HB3	2.20	0.41
38:MA:191:GLU:HG3	38:MA:193:GLN:N	2.36	0.41
40:PA:123:LEU:HD13	40:PA:195:ILE:HG21	2.00	0.41
43:SA:29:ILE:HD13	43:SA:64:VAL:HG21	2.01	0.41
1:A:1515:G:H2'	1:A:1516:G:C8	2.55	0.41
1:A:420:U:H2'	1:A:422:C:H1'	2.02	0.41
1:A:671:G:O2'	43:SA:79:ARG:NH2	2.52	0.41
2:B:1388:G:H2'	2:B:1389:G:H8	1.85	0.41
2:B:2593:U:H2'	2:B:2594:C:C6	2.55	0.41
2:B:2707:U:H2'	2:B:2708:G:H8	1.85	0.41
2:B:923:G:H2'	2:B:924:G:C8	2.56	0.41
58:HB:36:PHE:HD1	58:HB:39:LYS:HD3	1.85	0.41
9:I:42:ALA:HB2	9:I:49:LEU:HB2	2.01	0.41
11:K:1:MET:N	11:K:21:VAL:O	2.53	0.41
4:LA:68:C:H2'	4:LA:69:C:C6	2.56	0.41
38:MA:214:LEU:C	38:MA:216:ASP:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA:51:ILE:C	43:SA:53:LYS:H	2.24	0.41
21:U:90:ASP:OD1	21:U:90:ASP:N	2.51	0.41
22:V:58:VAL:HG13	22:V:58:VAL:O	2.20	0.41
1:A:236:A:H2'	1:A:237:G:H8	1.85	0.41
2:B:2355:G:O2'	27:AA:20:LYS:NZ	2.53	0.41
2:B:2047:C:H2'	2:B:2048:G:H8	1.86	0.41
2:B:942:G:H2'	2:B:943:A:H8	1.86	0.41
52:BB:17:ASP:HB2	52:BB:20:ASP:HB2	2.01	0.41
53:CB:44:SER:OG	53:CB:45:GLU:N	2.53	0.41
4:D:41:C:H2'	4:D:42:G:H8	1.83	0.41
38:MA:186:ARG:HH11	38:MA:312:PHE:HE2	1.68	0.41
39:OA:147:LEU:HD22	39:OA:150:ILE:HD11	2.02	0.41
40:PA:4:VAL:O	40:PA:5:HIS:HB2	2.20	0.41
18:R:117:ASP:HB3	18:R:118:ARG:H	1.48	0.41
42:RA:24:VAL:O	42:RA:26:GLY:N	2.53	0.41
1:A:1001:C:H2'	1:A:1002:G:H8	1.86	0.41
1:A:1308:U:H2'	1:A:1309:G:C8	2.54	0.41
2:B:1084:A:N6	2:B:1085:A:N1	2.68	0.41
2:B:1597:A:H5''	2:B:1598:A:H5'	2.01	0.41
2:B:518:G:O5'	23:W:18:ARG:NH1	2.53	0.41
3:C:116:G:H2'	3:C:117:G:H8	1.86	0.41
54:DB:18:LYS:HA	54:DB:50:ASN:ND2	2.35	0.41
36:JA:18:LYS:NZ	36:JA:21:GLY:HA2	2.35	0.41
11:K:38:PRO:O	11:K:43:ASN:ND2	2.50	0.41
12:L:118:ILE:N	12:L:119:PRO:HD3	2.32	0.41
4:LA:34:C:H2'	4:LA:35:A:C8	2.56	0.41
4:LA:41:C:H2'	4:LA:42:G:C8	2.53	0.41
42:RA:87:VAL:O	42:RA:87:VAL:HG13	2.19	0.41
20:T:48:ALA:CB	20:T:95:LYS:HG3	2.50	0.41
1:A:762:U:H2'	1:A:763:G:C8	2.55	0.41
2:B:1086:A:N6	12:L:37:LYS:HZ1	2.18	0.41
2:B:1880:U:H2'	2:B:1881:C:C6	2.55	0.41
2:B:2065:C:H2'	2:B:2066:C:C6	2.56	0.41
2:B:2673:G:H2'	2:B:2674:G:C8	2.52	0.41
2:B:903:C:H2'	2:B:904:G:H8	1.85	0.41
3:C:28:C:H2'	3:C:29:A:C8	2.56	0.41
54:DB:44:HIS:HB2	54:DB:69:THR:O	2.21	0.41
5:E:97:MET:HB3	5:E:100:LEU:CB	2.50	0.41
6:F:106:PRO:HG2	6:F:126:GLY:HA2	2.02	0.41
56:FB:65:MET:HG2	56:FB:73:PHE:CZ	2.55	0.41
4:LA:34:C:H2'	4:LA:35:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:MA:72:PRO:O	38:MA:75:ARG:HB2	2.19	0.41
18:R:12:ARG:HD3	18:R:16:HIS:ND1	2.35	0.41
42:RA:156:ARG:NH1	45:UA:42:GLU:OE2	2.54	0.41
23:W:107:VAL:HG22	23:W:108:SER:N	2.35	0.41
2:B:1599:U:OP1	24:X:40:LYS:HG3	2.21	0.41
2:B:1038:G:H2'	2:B:1039:A:C8	2.55	0.41
2:B:577:G:O2'	2:B:1254:A:OP1	2.39	0.41
2:B:2037:A:H2'	2:B:2038:G:H8	1.86	0.41
2:B:208:C:H2'	2:B:209:C:H6	1.86	0.41
2:B:2737:G:H2'	2:B:2738:A:C8	2.56	0.41
2:B:755:U:H2'	2:B:756:A:C8	2.55	0.41
7:G:149:ASN:O	7:G:152:PRO:HD2	2.21	0.41
57:GB:8:LYS:NZ	57:GB:12:GLN:OE1	2.53	0.41
48:XA:92:ARG:HE	58:HB:24:LYS:HE2	1.85	0.41
9:I:105:ILE:HD12	9:I:138:PRO:HG2	2.02	0.41
12:L:73:LYS:HB2	12:L:117:LEU:HD11	2.02	0.41
42:RA:156:ARG:O	42:RA:158:LYS:N	2.48	0.41
22:V:49:ILE:HG22	22:V:54:VAL:HA	2.03	0.41
50:ZA:53:ASP:OD1	50:ZA:53:ASP:N	2.53	0.41
1:A:191:G:H2'	1:A:192:A:C8	2.56	0.41
1:A:680:C:H2'	1:A:681:A:C8	2.56	0.41
2:B:1508:A:H2'	2:B:1509:A:O4'	2.21	0.41
2:B:154:U:H2'	2:B:155:A:C8	2.56	0.41
2:B:2037:A:H2'	2:B:2038:G:C8	2.56	0.41
2:B:220:G:N2	2:B:427:U:C2	2.89	0.41
2:B:2285:C:OP1	33:GA:25:ASN:ND2	2.54	0.41
2:B:2302:U:H2'	2:B:2303:G:H8	1.85	0.41
2:B:500:G:N1	2:B:503:A:OP2	2.52	0.41
2:B:634:C:H2'	2:B:635:C:C6	2.56	0.41
3:C:111:U:H2'	3:C:112:G:C8	2.53	0.41
4:D:42:G:H2'	4:D:43:A:H8	1.82	0.41
55:EB:11:ARG:HG2	55:EB:12:PHE:N	2.36	0.41
4:LA:68:C:H2'	4:LA:69:C:H6	1.86	0.41
13:M:132:ALA:HA	13:M:137:LEU:HB2	2.02	0.41
38:MA:131:LEU:HD11	38:MA:182:HIS:ND1	2.36	0.41
40:PA:8:GLY:HA2	40:PA:11:LEU:CG	2.50	0.41
41:QA:28:ASP:N	41:QA:28:ASP:OD1	2.52	0.41
1:A:1409:C:H2'	1:A:1410:A:C8	2.56	0.41
1:A:373:A:O4'	1:A:481:G:H5'	2.20	0.41
1:A:550:G:H2'	1:A:551:U:C6	2.55	0.41
1:A:675:A:H2'	1:A:676:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:G:H2'	1:A:831:A:H8	1.86	0.41
1:A:894:G:H2'	1:A:895:G:H8	1.86	0.41
1:A:994:A:O2'	51:AB:7:ALA:HB1	2.21	0.41
2:B:1236:G:O2'	2:B:1237:A:O5'	2.35	0.41
2:B:1536:C:O2'	2:B:1537:G:N2	2.54	0.41
2:B:2297:A:H8	2:B:2297:A:OP2	2.03	0.41
2:B:2075:U:H1'	2:B:2597:G:H21	1.86	0.41
2:B:558:U:H2'	2:B:559:G:H8	1.86	0.41
3:C:76:G:H2'	3:C:77:U:H6	1.85	0.41
58:HB:28:LEU:HA	58:HB:28:LEU:HD23	1.85	0.41
58:HB:34:ARG:HB3	58:HB:36:PHE:CE1	2.56	0.41
9:I:101:ARG:HB3	31:EA:24:ILE:HG21	2.03	0.41
4:LA:29:G:H2'	4:LA:30:G:H8	1.86	0.41
38:MA:253:ILE:HD11	38:MA:277:ARG:HD2	2.03	0.41
38:MA:306:ARG:HE	38:MA:320:HIS:HE1	1.66	0.41
38:MA:180:GLY:HA3	38:MA:307:ASN:OD1	2.21	0.41
42:RA:114:LEU:O	42:RA:119:VAL:HG22	2.21	0.41
1:A:1345:U:OP1	46:VA:121:ARG:NH1	2.53	0.41
48:XA:19:VAL:HG22	48:XA:82:GLU:HB2	2.03	0.41
50:ZA:86:ARG:HH22	56:FB:68:HIS:HE1	1.67	0.41
1:A:1002:G:C2	1:A:1003:G:H1'	2.56	0.41
1:A:114:U:H2'	1:A:115:G:C8	2.56	0.41
1:A:285:C:H2'	1:A:286:C:C6	2.56	0.41
1:A:955:U:OP2	38:MA:133:ARG:NH2	2.54	0.41
2:B:1151:A:H4'	21:U:80:ASN:ND2	2.35	0.41
2:B:1468:U:H2'	2:B:1522:A:N6	2.36	0.41
2:B:1947:C:H2'	2:B:1948:G:C8	2.56	0.41
2:B:2027:G:H2'	2:B:2028:U:C6	2.55	0.41
4:D:48:C:OP2	4:D:59:A:H5'	2.21	0.41
7:G:109:VAL:HG21	7:G:193:VAL:HG12	2.02	0.41
8:H:138:LEU:HD23	8:H:138:LEU:HA	1.91	0.41
9:I:115:GLY:HA3	9:I:177:ARG:HG3	2.03	0.41
12:L:4:ASN:OD1	12:L:8:LYS:NZ	2.52	0.41
42:RA:133:ILE:H	42:RA:133:ILE:HD12	1.85	0.41
50:ZA:8:ILE:HG13	50:ZA:9:PRO:HD3	2.03	0.41
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.41
1:A:664:G:H22	1:A:741:G:H1	1.68	0.41
51:AB:88:ALA:O	51:AB:89:MET:HE3	2.20	0.41
2:B:1035:U:H2'	2:B:1036:G:H8	1.86	0.41
2:B:1448:G:H2'	2:B:1449:G:C8	2.56	0.41
2:B:691:C:OP1	6:F:216:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:935:C:H2'	2:B:936:A:H8	1.86	0.41
7:G:49:GLN:NE2	7:G:79:LEU:HD13	2.36	0.41
12:L:100:ALA:O	12:L:103:ASN:HB3	2.21	0.41
4:LA:28:C:H2'	4:LA:29:G:C8	2.55	0.41
13:M:18:ASN:HA	13:M:19:PRO:HD3	1.81	0.41
13:M:85:ILE:HG13	13:M:85:ILE:H	1.77	0.41
38:MA:140:GLU:O	38:MA:143:ARG:HD2	2.21	0.41
38:MA:342:GLU:O	38:MA:343:PRO:C	2.54	0.41
42:RA:12:GLU:HG2	42:RA:12:GLU:O	2.20	0.41
1:A:15:G:H4'	42:RA:28:ARG:HH12	1.86	0.40
1:A:287:U:H2'	1:A:288:A:H8	1.86	0.40
1:A:806:C:H2'	1:A:807:A:H8	1.86	0.40
1:A:823:C:H2'	1:A:824:G:H8	1.86	0.40
2:B:1844:C:H2'	2:B:1845:G:H8	1.86	0.40
2:B:214:G:O2'	2:B:217:A:H5'	2.22	0.40
2:B:2837:A:H2'	2:B:2838:G:C8	2.53	0.40
2:B:690:G:H2'	2:B:691:C:C6	2.56	0.40
2:B:863:A:H2'	2:B:864:G:C8	2.54	0.40
3:C:60:C:H2'	3:C:61:G:C8	2.56	0.40
29:CA:19:LEU:HD23	29:CA:19:LEU:HA	1.87	0.40
53:CB:76:LYS:O	53:CB:79:ASN:OD1	2.38	0.40
4:D:27:U:H2'	4:D:28:C:C6	2.56	0.40
31:EA:46:GLY:HA2	31:EA:49:ARG:NE	2.36	0.40
10:J:45:ALA:HB3	10:J:48:THR:O	2.21	0.40
13:M:37:PHE:HA	13:M:66:PHE:CZ	2.55	0.40
15:O:35:VAL:HG22	15:O:69:VAL:HG12	2.03	0.40
43:SA:75:GLU:HA	43:SA:78:PHE:HD2	1.86	0.40
23:W:74:ILE:O	23:W:74:ILE:HG23	2.22	0.40
47:WA:5:ARG:N	47:WA:77:VAL:O	2.54	0.40
2:B:2292:U:H2'	2:B:2293:G:C8	2.52	0.40
2:B:2428:G:H5''	2:B:2429:G:OP1	2.22	0.40
2:B:2590:A:N1	2:B:2604:U:C5	2.89	0.40
2:B:873:C:H2'	2:B:874:G:C8	2.56	0.40
52:BB:2:LEU:HB2	52:BB:34:GLN:NE2	2.37	0.40
31:EA:20:ASN:ND2	31:EA:40:CYS:HB2	2.35	0.40
6:F:204:LEU:HB3	6:F:209:ALA:HB3	2.03	0.40
7:G:51:THR:HB	7:G:79:LEU:HD23	2.02	0.40
34:HA:43:THR:OG1	34:HA:44:VAL:N	2.55	0.40
10:J:16:VAL:HG11	10:J:49:LEU:HD11	2.02	0.40
12:L:125:ARG:HD3	12:L:125:ARG:N	2.36	0.40
38:MA:116:ARG:HB3	38:MA:161:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:PA:123:LEU:HD23	40:PA:123:LEU:HA	1.92	0.40
2:B:1252:G:H4'	21:U:32:ARG:HH11	1.86	0.40
47:WA:42:LEU:HB2	47:WA:71:LEU:HB2	2.03	0.40
1:A:1038:C:H2'	1:A:1039:G:H8	1.86	0.40
1:A:102:G:H2'	1:A:103:U:H6	1.85	0.40
1:A:41:G:H2'	1:A:42:G:H8	1.87	0.40
1:A:620:C:O2'	1:A:621:A:H8	2.05	0.40
1:A:985:C:H2'	1:A:986:U:C6	2.57	0.40
2:B:1149:G:H2'	2:B:1150:C:C6	2.56	0.40
2:B:935:C:H2'	2:B:936:A:C8	2.56	0.40
5:E:196:LEU:HD23	5:E:209:ILE:HG21	2.04	0.40
6:F:42:ARG:N	6:F:42:ARG:HD2	2.35	0.40
15:O:91:SER:O	15:O:92:GLU:C	2.59	0.40
1:A:711:G:H2'	1:A:712:A:C8	2.56	0.40
2:B:1478:G:H1	2:B:1513:U:H3	1.68	0.40
2:B:1524:G:H2'	2:B:1525:A:C8	2.56	0.40
2:B:172:A:H2'	2:B:173:A:C8	2.54	0.40
2:B:476:G:N1	2:B:479:A:OP2	2.53	0.40
2:B:743:A:OP1	7:G:135:GLY:HA2	2.21	0.40
2:B:903:C:H2'	2:B:904:G:C8	2.56	0.40
5:E:136:LEU:HA	5:E:162:ARG:HH12	1.87	0.40
56:FB:3:SER:HB3	56:FB:9:PHE:HE2	1.86	0.40
8:H:117:ARG:HH22	16:P:2:ARG:HB2	1.86	0.40
36:JA:7:VAL:HG11	36:JA:36:ARG:O	2.22	0.40
12:L:29:ASP:H	12:L:56:ARG:HH12	1.69	0.40
2:B:529:A:OP2	14:N:113:PRO:HG3	2.21	0.40
16:P:51:GLU:HG3	16:P:54:GLN:HE21	1.86	0.40
41:QA:198:LEU:O	41:QA:201:GLU:HG2	2.21	0.40
43:SA:85:ILE:O	43:SA:86:ARG:O	2.40	0.40
49:YA:35:ARG:HG2	49:YA:37:TYR:HD1	1.87	0.40
1:A:1162:C:H2'	1:A:1163:A:H8	1.86	0.40
1:A:744:C:H2'	1:A:745:G:H8	1.87	0.40
2:B:1040:A:H2'	2:B:1041:G:H8	1.87	0.40
2:B:119:A:H4'	2:B:120:U:H5'	2.03	0.40
2:B:1363:C:H2'	2:B:1364:G:C8	2.55	0.40
2:B:1889:A:H2'	2:B:1890:A:C8	2.56	0.40
2:B:2216:G:H2'	2:B:2217:G:H8	1.85	0.40
2:B:2372:U:H2'	2:B:2373:G:H8	1.86	0.40
2:B:751:A:H62	2:B:789:A:H62	1.68	0.40
5:E:200:LYS:HA	5:E:201:PRO:HD3	1.91	0.40
2:B:1861:G:P	5:E:205:LYS:HZ2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:THR:OG1	6:F:50:THR:N	2.55	0.40
9:I:51:ASN:ND2	9:I:146:ASP:OD2	2.55	0.40
2:B:2539:C:H4'	36:JA:3:VAL:HG21	2.04	0.40
41:QA:4:LEU:HD13	41:QA:4:LEU:HA	1.87	0.40
46:VA:56:MET:O	46:VA:57:VAL:C	2.60	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	
5	E	218/234 (93%)	185 (85%)	32 (15%)	1 (0%)	31	71
6	F	269/273 (98%)	229 (85%)	40 (15%)	0	100	100
7	G	207/209 (99%)	177 (86%)	27 (13%)	3 (1%)	12	52
8	H	199/201 (99%)	176 (88%)	19 (10%)	4 (2%)	8	46
9	I	175/179 (98%)	150 (86%)	23 (13%)	2 (1%)	16	58
10	J	174/177 (98%)	151 (87%)	20 (12%)	3 (2%)	10	49
11	K	147/149 (99%)	123 (84%)	19 (13%)	5 (3%)	4	36
12	L	129/165 (78%)	88 (68%)	34 (26%)	7 (5%)	2	24
13	M	139/142 (98%)	114 (82%)	21 (15%)	4 (3%)	5	39
14	N	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	24	66
15	O	120/123 (98%)	97 (81%)	20 (17%)	3 (2%)	6	41
16	P	141/144 (98%)	120 (85%)	19 (14%)	2 (1%)	12	52
17	Q	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	11	51
18	R	118/127 (93%)	92 (78%)	24 (20%)	2 (2%)	10	49
19	S	114/117 (97%)	103 (90%)	8 (7%)	3 (3%)	6	40
20	T	112/115 (97%)	92 (82%)	19 (17%)	1 (1%)	19	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	115/118 (98%)	101 (88%)	13 (11%)	1 (1%)	19	61
22	V	101/103 (98%)	85 (84%)	14 (14%)	2 (2%)	8	46
23	W	108/110 (98%)	90 (83%)	15 (14%)	3 (3%)	5	39
24	X	91/100 (91%)	81 (89%)	10 (11%)	0	100	100
25	Y	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	5	38
26	Z	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
27	AA	73/85 (86%)	65 (89%)	8 (11%)	0	100	100
28	BA	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
29	CA	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	11	50
30	DA	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
31	EA	64/70 (91%)	52 (81%)	11 (17%)	1 (2%)	11	50
32	FA	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
33	GA	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
34	HA	44/46 (96%)	34 (77%)	9 (20%)	1 (2%)	7	43
35	IA	62/65 (95%)	50 (81%)	11 (18%)	1 (2%)	11	50
36	JA	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	39
38	MA	340/362 (94%)	292 (86%)	45 (13%)	3 (1%)	19	61
39	OA	223/241 (92%)	202 (91%)	19 (8%)	2 (1%)	19	61
40	PA	204/233 (88%)	177 (87%)	25 (12%)	2 (1%)	17	59
41	QA	203/206 (98%)	174 (86%)	21 (10%)	8 (4%)	3	31
42	RA	155/167 (93%)	121 (78%)	27 (17%)	7 (4%)	3	28
43	SA	98/131 (75%)	73 (74%)	20 (20%)	5 (5%)	2	25
44	TA	149/156 (96%)	125 (84%)	21 (14%)	3 (2%)	8	46
45	UA	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	11	50
46	VA	125/130 (96%)	98 (78%)	23 (18%)	4 (3%)	4	37
47	WA	96/103 (93%)	73 (76%)	19 (20%)	4 (4%)	3	29
48	XA	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	19	61
49	YA	121/124 (98%)	96 (79%)	19 (16%)	6 (5%)	2	25
50	ZA	112/118 (95%)	97 (87%)	13 (12%)	2 (2%)	9	48
51	AB	99/102 (97%)	64 (65%)	25 (25%)	10 (10%)	0	10
52	BB	86/89 (97%)	71 (83%)	13 (15%)	2 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	CB	80/82 (98%)	63 (79%)	16 (20%)	1 (1%)	13	54
54	DB	78/84 (93%)	63 (81%)	12 (15%)	3 (4%)	3	32
55	EB	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
56	FB	77/92 (84%)	63 (82%)	14 (18%)	0	100	100
57	GB	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
58	HB	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	15
All	All	6412/6790 (94%)	5417 (84%)	868 (14%)	127 (2%)	12	46

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	83	VAL
9	I	2	LYS
10	J	119	GLY
11	K	9	VAL
11	K	10	ALA
11	K	41	LYS
12	L	118	ILE
12	L	119	PRO
12	L	123	ILE
13	M	11	GLN
14	N	81	ILE
15	O	35	VAL
18	R	88	ALA
19	S	34	HIS
22	V	54	VAL
29	CA	24	GLU
35	IA	31	ILE
36	JA	37	GLN
39	OA	14	HIS
39	OA	15	PHE
40	PA	4	VAL
41	QA	36	ALA
41	QA	191	SER
41	QA	192	ALA
42	RA	11	GLN
42	RA	25	LYS
42	RA	89	THR
42	RA	93	VAL
42	RA	122	VAL

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Mol	Chain	Res	Type
43	SA	86	ARG
43	SA	92	THR
45	UA	66	GLN
46	VA	57	VAL
47	WA	92	LEU
49	YA	23	LEU
49	YA	24	GLU
50	ZA	4	ALA
50	ZA	65	GLU
51	AB	64	CYS
51	AB	79	LEU
51	AB	80	SER
51	AB	81	ARG
7	G	30	GLU
8	H	72	SER
10	J	109	SER
11	K	14	SER
12	L	58	THR
18	R	86	ARG
23	W	3	THR
23	W	63	GLY
34	HA	44	VAL
41	QA	84	ASN
43	SA	54	LEU
44	TA	56	SER
44	TA	64	ALA
45	UA	47	ASP
46	VA	90	ASP
49	YA	35	ARG
51	AB	57	PRO
51	AB	75	ARG
54	DB	17	GLU
54	DB	50	ASN
58	HB	8	ASN
58	HB	24	LYS
5	E	102	ASP
8	H	45	ALA
10	J	174	LYS
12	L	54	VAL
12	L	108	VAL
17	Q	70	ASP
19	S	13	ARG

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Mol	Chain	Res	Type
20	T	65	ASN
23	W	64	ALA
31	EA	29	GLY
38	MA	145	ARG
43	SA	52	ASN
46	VA	107	ALA
47	WA	29	ALA
48	XA	125	LYS
51	AB	67	THR
54	DB	15	LYS
58	HB	12	ASP
58	HB	64	ALA
7	G	10	GLY
8	H	80	SER
9	I	175	PRO
13	M	12	VAL
15	O	92	GLU
15	O	93	GLN
17	Q	69	PRO
21	U	25	GLY
41	QA	47	LEU
43	SA	53	LYS
47	WA	14	ASP
47	WA	33	GLY
51	AB	2	LYS
58	HB	34	ARG
7	G	86	GLU
16	P	36	LYS
16	P	86	GLU
25	Y	54	PRO
41	QA	32	LYS
52	BB	74	VAL
11	K	118	PRO
12	L	76	PHE
13	M	24	GLY
25	Y	89	GLY
38	MA	45	LEU
38	MA	146	VAL
41	QA	82	LYS
41	QA	182	LYS
49	YA	77	SER
49	YA	88	ASP

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Mol	Chain	Res	Type
19	S	66	GLY
51	AB	70	PRO
40	PA	6	PRO
42	RA	90	GLY
46	VA	71	ILE
25	Y	53	GLN
49	YA	27	PRO
51	AB	56	SER
53	CB	30	GLY
13	M	19	PRO
42	RA	157	GLY
44	TA	15	PRO
52	BB	85	GLY
22	V	8	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	171/181 (94%)	168 (98%)	3 (2%)	62	84
6	F	216/218 (99%)	209 (97%)	7 (3%)	42	73
7	G	164/164 (100%)	163 (99%)	1 (1%)	87	94
8	H	165/165 (100%)	163 (99%)	2 (1%)	74	89
9	I	148/150 (99%)	146 (99%)	2 (1%)	69	87
10	J	137/138 (99%)	134 (98%)	3 (2%)	55	80
11	K	114/114 (100%)	112 (98%)	2 (2%)	62	84
12	L	100/123 (81%)	97 (97%)	3 (3%)	44	75
13	M	109/110 (99%)	106 (97%)	3 (3%)	47	76
14	N	116/116 (100%)	115 (99%)	1 (1%)	81	91
15	O	103/104 (99%)	102 (99%)	1 (1%)	78	90
16	P	102/103 (99%)	100 (98%)	2 (2%)	58	82
17	Q	109/109 (100%)	108 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	100/104 (96%)	99 (99%)	1 (1%)	78	90
19	S	86/87 (99%)	84 (98%)	2 (2%)	53	80
20	T	99/100 (99%)	98 (99%)	1 (1%)	78	90
21	U	89/90 (99%)	89 (100%)	0	100	100
22	V	84/84 (100%)	84 (100%)	0	100	100
23	W	93/93 (100%)	92 (99%)	1 (1%)	76	89
24	X	80/84 (95%)	80 (100%)	0	100	100
25	Y	83/85 (98%)	83 (100%)	0	100	100
26	Z	78/78 (100%)	78 (100%)	0	100	100
27	AA	57/63 (90%)	57 (100%)	0	100	100
28	BA	67/68 (98%)	66 (98%)	1 (2%)	67	86
29	CA	55/55 (100%)	54 (98%)	1 (2%)	62	84
30	DA	48/49 (98%)	48 (100%)	0	100	100
31	EA	59/62 (95%)	58 (98%)	1 (2%)	63	85
32	FA	47/48 (98%)	46 (98%)	1 (2%)	56	81
33	GA	45/49 (92%)	45 (100%)	0	100	100
34	HA	38/38 (100%)	38 (100%)	0	100	100
35	IA	51/52 (98%)	51 (100%)	0	100	100
36	JA	34/34 (100%)	34 (100%)	0	100	100
38	MA	284/302 (94%)	279 (98%)	5 (2%)	62	84
39	OA	186/199 (94%)	186 (100%)	0	100	100
40	PA	170/190 (90%)	165 (97%)	5 (3%)	45	75
41	QA	172/173 (99%)	170 (99%)	2 (1%)	74	89
42	RA	119/126 (94%)	116 (98%)	3 (2%)	50	78
43	SA	87/112 (78%)	85 (98%)	2 (2%)	53	80
44	TA	124/129 (96%)	123 (99%)	1 (1%)	83	92
45	UA	104/105 (99%)	104 (100%)	0	100	100
46	VA	105/107 (98%)	103 (98%)	2 (2%)	60	83
47	WA	86/90 (96%)	85 (99%)	1 (1%)	74	89
48	XA	89/99 (90%)	87 (98%)	2 (2%)	55	80
49	YA	103/104 (99%)	99 (96%)	4 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	ZA	92/96 (96%)	91 (99%)	1 (1%)	76	89
51	AB	83/84 (99%)	76 (92%)	7 (8%)	12	46
52	BB	76/77 (99%)	74 (97%)	2 (3%)	49	77
53	CB	65/65 (100%)	61 (94%)	4 (6%)	20	57
54	DB	74/78 (95%)	73 (99%)	1 (1%)	69	87
55	EB	56/65 (86%)	55 (98%)	1 (2%)	62	84
56	FB	70/79 (89%)	69 (99%)	1 (1%)	69	87
57	GB	65/66 (98%)	64 (98%)	1 (2%)	67	86
58	HB	55/61 (90%)	54 (98%)	1 (2%)	62	84
All	All	5312/5525 (96%)	5226 (98%)	86 (2%)	68	86

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	58	ASN
5	E	155	ASN
5	E	167	LYS
6	F	20	ASN
6	F	36	ASN
6	F	79	ARG
6	F	129	LEU
6	F	196	ASN
6	F	212	TRP
6	F	257	ARG
7	G	33	ARG
8	H	24	ASN
8	H	163	ASN
9	I	29	ARG
9	I	47	LYS
10	J	19	ASN
10	J	29	ASN
10	J	37	ASN
11	K	77	THR
11	K	145	ASN
12	L	3	LEU
12	L	58	THR
12	L	125	ARG
13	M	33	ASN
13	M	96	LYS

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Mol	Chain	Res	Type
13	M	135	MET
14	N	111	LYS
15	O	1	MET
16	P	48	ARG
16	P	79	LEU
17	Q	59	ARG
18	R	2	ARG
19	S	25	ARG
19	S	48	LEU
20	T	2	ASN
23	W	62	ASP
28	BA	10	ARG
29	CA	2	LYS
31	EA	49	ARG
32	FA	8	THR
38	MA	77	MET
38	MA	217	ILE
38	MA	266	ASN
38	MA	274	LEU
38	MA	339	MET
40	PA	7	ASN
40	PA	53	ARG
40	PA	71	ARG
40	PA	106	ARG
40	PA	172	VAL
41	QA	114	ARG
41	QA	183	ARG
42	RA	18	ASN
42	RA	131	ASN
42	RA	145	ASN
43	SA	9	MET
43	SA	12	PRO
44	TA	121	ASN
46	VA	84	ARG
46	VA	105	ARG
47	WA	89	ARG
48	XA	30	ILE
48	XA	124	LYS
49	YA	4	ASN
49	YA	19	ASN
49	YA	93	ARG
49	YA	113	ARG

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Mol	Chain	Res	Type
50	ZA	47	LEU
51	AB	27	LYS
51	AB	58	SER
51	AB	63	ARG
51	AB	79	LEU
51	AB	80	SER
51	AB	89	MET
51	AB	96	LEU
52	BB	19	ASN
52	BB	88	ARG
53	CB	25	ARG
53	CB	35	ARG
53	CB	40	ASN
53	CB	74	LEU
54	DB	69	THR
55	EB	11	ARG
56	FB	77	ARG
57	GB	2	ASN
58	HB	40	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	58	ASN
5	E	155	ASN
5	E	172	HIS
5	E	188	ASN
5	E	203	GLN
6	F	20	ASN
6	F	36	ASN
6	F	52	HIS
6	F	141	HIS
6	F	196	ASN
6	F	225	ASN
7	G	32	ASN
7	G	173	GLN
8	H	24	ASN
8	H	30	GLN
8	H	92	HIS
8	H	97	ASN
8	H	163	ASN
8	H	165	HIS

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Mol	Chain	Res	Type
9	I	4	HIS
9	I	126	ASN
10	J	19	ASN
10	J	29	ASN
10	J	37	ASN
10	J	63	GLN
10	J	87	GLN
10	J	114	HIS
11	K	145	ASN
13	M	18	ASN
13	M	33	ASN
13	M	42	ASN
14	N	40	HIS
17	Q	88	ASN
18	R	3	HIS
18	R	11	ASN
19	S	38	GLN
19	S	100	HIS
20	T	2	ASN
20	T	74	GLN
21	U	36	GLN
21	U	43	GLN
23	W	9	HIS
25	Y	53	GLN
25	Y	73	ASN
27	AA	36	GLN
27	AA	72	ASN
30	DA	19	HIS
31	EA	20	ASN
31	EA	41	HIS
32	FA	5	ASN
38	MA	79	GLN
38	MA	156	HIS
38	MA	193	GLN
38	MA	236	HIS
38	MA	266	ASN
38	MA	320	HIS
39	OA	38	HIS
39	OA	177	ASN
40	PA	7	ASN
41	QA	88	ASN
41	QA	115	GLN

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Mol	Chain	Res	Type
42	RA	18	ASN
42	RA	131	ASN
42	RA	145	ASN
43	SA	11	HIS
44	TA	121	ASN
45	UA	15	ASN
46	VA	36	GLN
47	WA	56	HIS
48	XA	39	ASN
49	YA	19	ASN
50	ZA	99	GLN
52	BB	19	ASN
52	BB	34	GLN
53	CB	18	GLN
53	CB	40	ASN
54	DB	30	HIS
54	DB	50	ASN
55	EB	51	GLN
56	FB	51	HIS
56	FB	68	HIS
57	GB	2	ASN
57	GB	60	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1538/1539 (99%)	222 (14%)	5 (0%)
2	B	2902/2903 (99%)	387 (13%)	8 (0%)
3	C	119/120 (99%)	18 (15%)	1 (0%)
37	KA	18/27 (66%)	3 (16%)	0
4	D	76/77 (98%)	10 (13%)	0
4	LA	76/77 (98%)	8 (10%)	0
All	All	4729/4743 (99%)	648 (13%)	14 (0%)

All (648) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	6	G
1	A	9	G
1	A	22	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	70	U
1	A	71	A
1	A	72	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	88	U
1	A	94	G
1	A	121	U
1	A	124	C
1	A	130	A
1	A	138	G
1	A	139	A
1	A	144	G
1	A	155	A
1	A	171	A
1	A	174	A
1	A	183	C
1	A	197	A
1	A	201	G
1	A	209	U
1	A	210	C
1	A	211	G
1	A	212	G
1	A	225	C
1	A	226	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	274	A
1	A	280	C
1	A	281	G

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Mol	Chain	Res	Type
1	A	289	G
1	A	306	A
1	A	321	A
1	A	329	A
1	A	330	C
1	A	343	U
1	A	345	C
1	A	346	G
1	A	351	G
1	A	352	C
1	A	358	U
1	A	367	U
1	A	368	U
1	A	369	G
1	A	372	C
1	A	373	A
1	A	378	G
1	A	387	U
1	A	394	G
1	A	395	C
1	A	398	U
1	A	401	C
1	A	403	C
1	A	404	G
1	A	406	G
1	A	411	A
1	A	413	G
1	A	416	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	437	U
1	A	438	U
1	A	442	G
1	A	448	A
1	A	467	U
1	A	468	A
1	A	476	U
1	A	477	C
1	A	481	G

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Mol	Chain	Res	Type
1	A	484	G
1	A	485	U
1	A	486	U
1	A	493	A
1	A	495	A
1	A	497	G
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	540	G
1	A	541	G
1	A	547	A
1	A	561	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	615	G
1	A	619	U
1	A	620	C
1	A	621	A
1	A	633	G
1	A	642	A
1	A	665	A
1	A	666	G
1	A	688	G
1	A	695	A
1	A	701	U
1	A	702	A
1	A	703	G
1	A	713	G
1	A	718	A
1	A	721	G
1	A	724	G
1	A	731	G

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Mol	Chain	Res	Type
1	A	733	G
1	A	755	G
1	A	777	A
1	A	794	A
1	A	814	A
1	A	815	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	821	G
1	A	832	G
1	A	836	G
1	A	842	U
1	A	843	U
1	A	846	G
1	A	871	U
1	A	873	A
1	A	885	G
1	A	890	G
1	A	902	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1028	C
1	A	1031	C
1	A	1033	G
1	A	1054	C
1	A	1055	A
1	A	1094	G
1	A	1095	U

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Mol	Chain	Res	Type
1	A	1101	A
1	A	1130	A
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1159	U
1	A	1168	U
1	A	1183	U
1	A	1184	G
1	A	1196	A
1	A	1225	A
1	A	1238	A
1	A	1241	G
1	A	1258	G
1	A	1260	G
1	A	1261	A
1	A	1275	A
1	A	1278	G
1	A	1280	A
1	A	1282	C
1	A	1286	U
1	A	1287	A
1	A	1298	U
1	A	1300	G
1	A	1317	C
1	A	1323	G
1	A	1346	A
1	A	1347	G
1	A	1359	C
1	A	1378	C
1	A	1394	A
1	A	1400	C
1	A	1402	C
1	A	1419	G
1	A	1446	A
1	A	1448	C
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1494	G
1	A	1497	G
1	A	1499	A

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Mol	Chain	Res	Type
1	A	1502	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1534	A
1	A	1540	U
2	B	10	A
2	B	35	G
2	B	46	G
2	B	49	A
2	B	52	A
2	B	63	A
2	B	71	A
2	B	74	A
2	B	75	G
2	B	118	A
2	B	120	U
2	B	140	C
2	B	141	G
2	B	162	U
2	B	163	C
2	B	181	A
2	B	196	A
2	B	199	A
2	B	204	A
2	B	215	G
2	B	216	A
2	B	221	A
2	B	222	A
2	B	227	A
2	B	229	C
2	B	233	A
2	B	242	G
2	B	248	G
2	B	249	C
2	B	255	A
2	B	264	C
2	B	266	G
2	B	281	C
2	B	294	A

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Mol	Chain	Res	Type
2	B	311	A
2	B	323	C
2	B	329	G
2	B	330	A
2	B	334	C
2	B	361	G
2	B	371	A
2	B	372	G
2	B	386	G
2	B	387	U
2	B	404	A
2	B	406	G
2	B	411	G
2	B	423	A
2	B	424	G
2	B	442	G
2	B	451	U
2	B	457	A
2	B	467	G
2	B	473	G
2	B	475	C
2	B	480	A
2	B	481	G
2	B	490	C
2	B	491	G
2	B	504	A
2	B	505	A
2	B	508	A
2	B	529	A
2	B	532	A
2	B	533	G
2	B	543	G
2	B	548	G
2	B	563	A
2	B	572	A
2	B	573	U
2	B	575	A
2	B	588	U
2	B	603	A
2	B	614	A
2	B	615	U
2	B	627	A

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Mol	Chain	Res	Type
2	B	637	A
2	B	645	C
2	B	646	U
2	B	654	A
2	B	655	A
2	B	669	G
2	B	686	U
2	B	695	G
2	B	704	G
2	B	730	A
2	B	747	C
2	B	748	G
2	B	752	A
2	B	765	C
2	B	775	G
2	B	776	G
2	B	782	A
2	B	783	A
2	B	784	G
2	B	785	G
2	B	789	A
2	B	800	A
2	B	805	G
2	B	812	C
2	B	819	A
2	B	827	U
2	B	828	U
2	B	830	G
2	B	845	A
2	B	846	U
2	B	847	U
2	B	856	G
2	B	860	U
2	B	878	A
2	B	887	U
2	B	888	C
2	B	889	C
2	B	891	G
2	B	893	C
2	B	896	A
2	B	907	G
2	B	910	A

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Mol	Chain	Res	Type
2	B	932	U
2	B	941	A
2	B	946	C
2	B	961	C
2	B	974	G
2	B	983	A
2	B	995	C
2	B	996	A
2	B	1009	A
2	B	1012	U
2	B	1013	C
2	B	1021	A
2	B	1022	G
2	B	1026	G
2	B	1033	U
2	B	1045	C
2	B	1046	A
2	B	1047	G
2	B	1060	U
2	B	1062	G
2	B	1063	G
2	B	1064	C
2	B	1065	U
2	B	1066	U
2	B	1067	A
2	B	1070	A
2	B	1071	G
2	B	1072	C
2	B	1075	C
2	B	1076	C
2	B	1079	C
2	B	1084	A
2	B	1088	A
2	B	1089	A
2	B	1090	A
2	B	1094	U
2	B	1103	A
2	B	1104	C
2	B	1111	A
2	B	1130	U
2	B	1131	G
2	B	1132	U

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Mol	Chain	Res	Type
2	B	1133	A
2	B	1135	C
2	B	1139	G
2	B	1142	A
2	B	1172	C
2	B	1173	U
2	B	1174	U
2	B	1175	A
2	B	1176	U
2	B	1177	G
2	B	1178	C
2	B	1179	G
2	B	1180	U
2	B	1211	C
2	B	1212	G
2	B	1237	A
2	B	1250	G
2	B	1251	C
2	B	1253	A
2	B	1256	G
2	B	1265	A
2	B	1271	G
2	B	1272	A
2	B	1273	U
2	B	1275	A
2	B	1300	G
2	B	1301	A
2	B	1321	A
2	B	1332	G
2	B	1345	C
2	B	1365	A
2	B	1368	G
2	B	1378	A
2	B	1379	U
2	B	1383	A
2	B	1416	G
2	B	1428	C
2	B	1454	C
2	B	1461	C
2	B	1475	G
2	B	1482	G
2	B	1490	A

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Mol	Chain	Res	Type
2	B	1504	A
2	B	1515	A
2	B	1522	A
2	B	1524	G
2	B	1535	A
2	B	1536	C
2	B	1555	G
2	B	1558	C
2	B	1560	G
2	B	1566	A
2	B	1569	A
2	B	1607	C
2	B	1611	C
2	B	1616	A
2	B	1646	C
2	B	1647	U
2	B	1648	U
2	B	1669	A
2	B	1674	G
2	B	1695	G
2	B	1698	A
2	B	1699	G
2	B	1715	G
2	B	1729	U
2	B	1730	C
2	B	1731	G
2	B	1738	G
2	B	1756	G
2	B	1758	U
2	B	1764	C
2	B	1773	A
2	B	1781	U
2	B	1800	C
2	B	1801	A
2	B	1802	A
2	B	1808	A
2	B	1809	A
2	B	1813	G
2	B	1816	C
2	B	1870	C
2	B	1871	A
2	B	1901	A

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Mol	Chain	Res	Type
2	B	1906	G
2	B	1907	G
2	B	1914	C
2	B	1929	G
2	B	1930	G
2	B	1936	A
2	B	1937	A
2	B	1938	A
2	B	1944	U
2	B	1955	U
2	B	1967	C
2	B	1970	A
2	B	1971	U
2	B	1972	G
2	B	1991	U
2	B	1993	U
2	B	1997	C
2	B	2022	U
2	B	2023	C
2	B	2030	A
2	B	2031	A
2	B	2033	A
2	B	2043	C
2	B	2052	A
2	B	2055	C
2	B	2056	G
2	B	2060	A
2	B	2061	G
2	B	2062	A
2	B	2069	G
2	B	2072	C
2	B	2077	A
2	B	2093	G
2	B	2096	C
2	B	2111	U
2	B	2112	G
2	B	2114	A
2	B	2115	G
2	B	2118	U
2	B	2119	A
2	B	2120	G
2	B	2121	G

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Mol	Chain	Res	Type
2	B	2128	G
2	B	2132	U
2	B	2133	G
2	B	2145	C
2	B	2147	A
2	B	2157	G
2	B	2171	A
2	B	2172	U
2	B	2173	A
2	B	2176	A
2	B	2198	A
2	B	2199	A
2	B	2204	G
2	B	2211	A
2	B	2213	U
2	B	2223	G
2	B	2225	A
2	B	2238	G
2	B	2243	U
2	B	2250	G
2	B	2252	G
2	B	2283	C
2	B	2287	A
2	B	2297	A
2	B	2305	U
2	B	2309	A
2	B	2311	A
2	B	2312	U
2	B	2320	U
2	B	2324	U
2	B	2325	G
2	B	2327	A
2	B	2333	A
2	B	2334	U
2	B	2361	G
2	B	2382	G
2	B	2383	G
2	B	2385	C
2	B	2391	G
2	B	2402	U
2	B	2403	C
2	B	2406	A

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Mol	Chain	Res	Type
2	B	2423	U
2	B	2429	G
2	B	2430	A
2	B	2435	A
2	B	2441	U
2	B	2447	G
2	B	2448	A
2	B	2476	A
2	B	2478	A
2	B	2498	C
2	B	2502	G
2	B	2503	A
2	B	2504	U
2	B	2506	U
2	B	2518	A
2	B	2520	C
2	B	2547	A
2	B	2554	U
2	B	2566	A
2	B	2567	G
2	B	2572	A
2	B	2582	G
2	B	2585	U
2	B	2586	U
2	B	2602	A
2	B	2605	U
2	B	2609	U
2	B	2613	U
2	B	2629	U
2	B	2630	G
2	B	2655	G
2	B	2682	A
2	B	2689	U
2	B	2690	U
2	B	2714	G
2	B	2718	G
2	B	2733	A
2	B	2744	G
2	B	2748	A
2	B	2757	A
2	B	2764	A
2	B	2765	A

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Mol	Chain	Res	Type
2	B	2778	A
2	B	2779	U
2	B	2791	G
2	B	2798	U
2	B	2799	A
2	B	2800	A
2	B	2808	G
2	B	2820	A
2	B	2821	A
2	B	2833	U
2	B	2849	U
2	B	2861	U
2	B	2867	G
2	B	2868	A
2	B	2872	A
2	B	2879	A
2	B	2880	C
3	C	13	G
3	C	15	A
3	C	24	G
3	C	35	C
3	C	42	C
3	C	44	G
3	C	45	A
3	C	67	G
3	C	87	U
3	C	88	C
3	C	89	U
3	C	90	C
3	C	91	C
3	C	100	G
3	C	108	A
3	C	109	A
3	C	119	A
3	C	120	A
4	D	6	G
4	D	9	G
4	D	16	C
4	D	17(A)	U
4	D	18	G
4	D	19	G
4	D	20	U

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Mol	Chain	Res	Type
4	D	47	U
4	D	48	C
4	D	61	C
37	KA	12	A
37	KA	13	A
37	KA	22	A
4	LA	9	G
4	LA	17(A)	U
4	LA	18	G
4	LA	19	G
4	LA	48	C
4	LA	59	A
4	LA	61	C
4	LA	76	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	69	G
1	A	533	A
1	A	733	G
1	A	1182	G
1	A	1297	G
2	B	51	G
2	B	859	G
2	B	1020	A
2	B	1130	U
2	B	1236	G
2	B	2296	U
2	B	2326	C
2	B	2756	U
3	C	66	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.