



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:24 am GMT

PDB ID : 3DEG
EMDB ID: : EMD-1524
Title : Complex of elongating Escherichia coli 70S ribosome and EF4(LepA)-GMPPNP
Authors : Connell, S.R.; Topf, M.; Qin, Y.; Wilson, D.N.; Mielke, T.; Fucini, P.; Nierhaus, K.H.; Spahn, C.M.T.
Deposited on : 2008-06-10
Resolution : 10.90 Å(reported)
Based on PDB ID : 2i2p, 2i2t, 3cb4, 1gix, 2j01

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

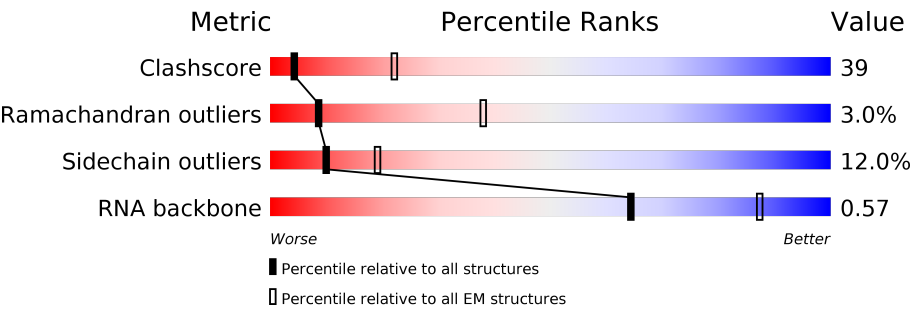
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

1 Overall quality at a glance i

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

The reported resolution of this entry is 10.90 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.




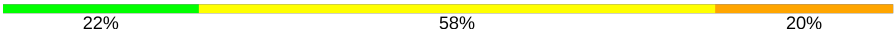
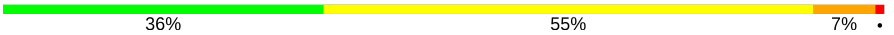
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	76	<div><div>32%</div><div>50%</div><div>13%</div><div>5%</div></div>
2	B	77	<div><div>27%</div><div>48%</div><div>23%</div><div>.</div></div>
3	E	16	<div><div>38%</div><div>56%</div><div>6%</div></div>
4	F	12	<div><div>75%</div><div>25%</div></div>
5	G	70	<div><div>30%</div><div>56%</div><div>10%</div><div>.</div></div>
6	I	29	<div><div>45%</div><div>55%</div></div>
7	J	18	<div><div>44%</div><div>50%</div><div>6%</div></div>
8	K	15	<div><div>33%</div><div>60%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
9	C	545	
10	D	123	
11	H	141	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	M2G	A	26	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12950 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 A/L-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	77	Total	C	N	O	P	0	0
			1645	733	297	538	77		

- Molecule 3 is a RNA chain called 30S RNA helix 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	16	Total	C	N	O	P	0	0
			345	154	65	110	16		

- Molecule 4 is a RNA chain called 30S RNA helix 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	12	Total	C	N	O	P	0	0
			256	114	46	84	12		

- Molecule 5 is a RNA chain called 50S RNA helix 42-44.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	70	Total	C	N	O	P	0	0
			1498	670	276	482	70		

- Molecule 6 is a RNA chain called 50S RNA helix 95.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	29	Total	C	N	O	P	0	0
			625	278	116	202	29		

- Molecule 7 is a RNA chain called 50S RNA helix 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	18	Total	C	N	O	P	0	0
			384	171	67	128	18		

- Molecule 8 is a RNA chain called 50S RNA helix 92.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	15	Total	C	N	O	P	0	0
			316	141	52	108	15		

- Molecule 9 is a protein called GTP-binding protein lepA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	545	Total	C	N	O	S	0	0
			4242	2671	726	824	21		

- Molecule 10 is a protein called 30S ribosomal protein S12.

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

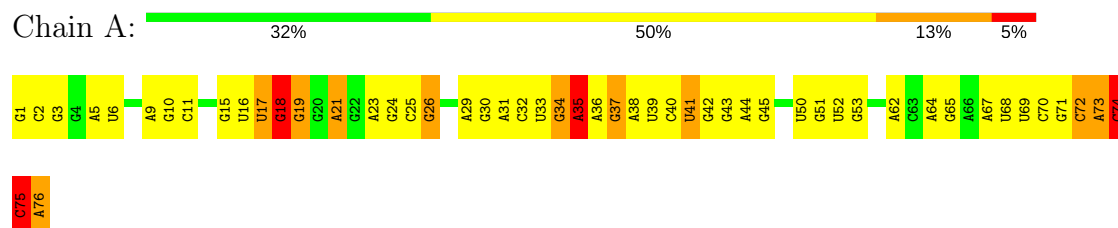
- Molecule 11 is a protein called 50S ribosomal protein L11.

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

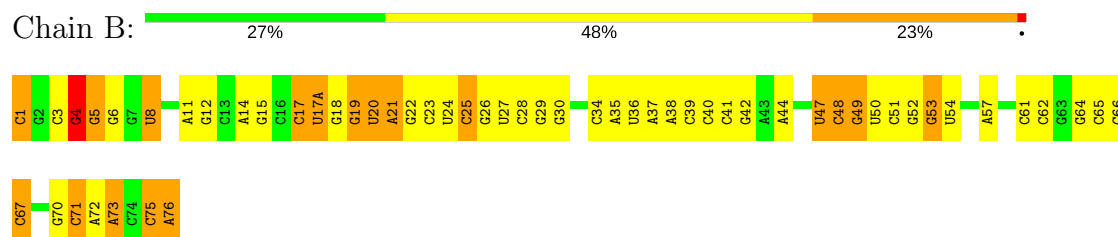
3 Residue-property plots

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.

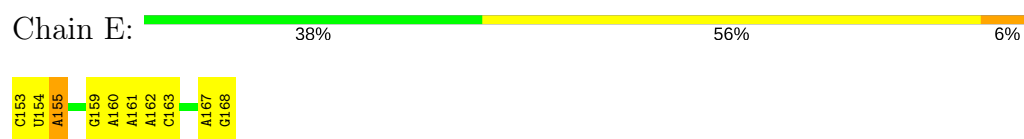
• Molecule 1: A/L-tRNA



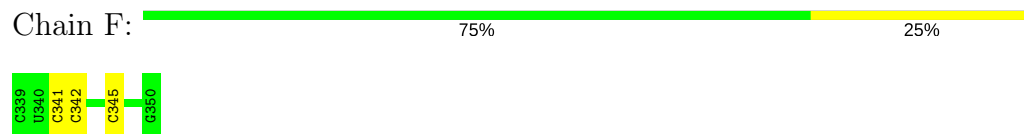
• Molecule 2: P-tRNA



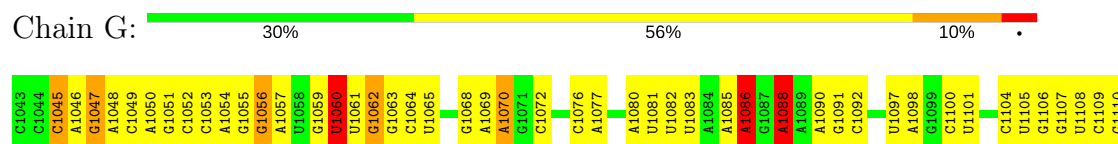
• Molecule 3: 30S RNA helix 8



• Molecule 4: 30S RNA helix 14



• Molecule 5: 50S RNA helix 42-44



A1111
G1112

- Molecule 6: 50S RNA helix 95

Chain I:  45% 55%

C2646 C2649 U2650 C2651 G2655 G2659 A2660 C2661 A2662 C2663 G2664 A2665 C2666 G2667 C2668 G2669 A2670 U2671 U2672 G2673 G2674

- Molecule 7: 50S RNA helix 71

Chain J:  44% 50% 6%

U1944 G1945 U1946 C1947 G1948 G1949 U1955 U1956 C1957 C1958 C1959 A1960 C1961

- Molecule 8: 50S RNA helix 92

Chain K:  33% 60% 7%

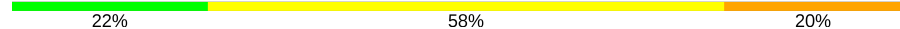
A2547 U2548 U2552 G2553 U2554 U2555 C2556 G2557 C2558 C2559 A2560 U2561

- Molecule 9: GTP-binding protein lepA

Chain C:  57% 34% 7%

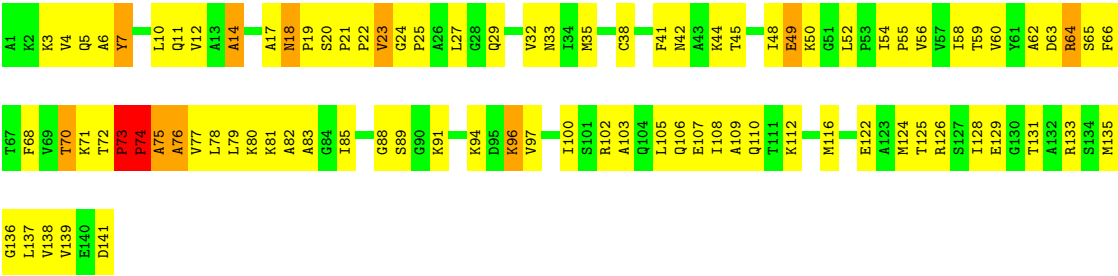
M1 K2 N3 N4 R5 N6 F7 S8 I9 I10 A11 H12 I13 D14 H15 G16 K17 S18 T19 L20 S21 D22 R23 I24 I25 Q26 L27 G28 G29 G30 L31 S32 D33 R34 E35 M36 Q39 V40 L41 D42 S43 M44 D45 L46 E47 R48 E49 R50 G51 I52 T53 I54 K55 A56 G57 S58 E59 Q72 L73 N74 F75 P79 G80 H81 V82 F84 F84 S85 S85 Y86 V101 V102 D103 Q106 E109 A110 Q111 T112 L113 L113 C116 Y117 M120 M120 D123 N131 K132 Y153 I160 L173 L176 P181 P182 P183 E188 L191 Q192 A193 L194 I195 I196 Y203 L204 L210 R211 N214 K219 G220 D221 V225 S227 S227 T228 G229 Q230 A234 T241 R242 K243 D246 T247 T248 C252 G253 E254 V255 L262 I265 H266 G267 A268 T273 L274 L276 L285 K289 K290 V291 K292 P293 Q294 V295 Y296 A297 G298 L299 L317 S318 L319 R320 S323 E327 P328 E329 S330 S331 S332 S333 A334 L334 C340 L343 G344 L345 L346 H347 H348 H348 E349 I350 R354 L355 E358 T365 T366 A367 P368 T369 V370 V371 Y372 E373 V374 V384 L390 N394 L399 R400 R401 P402 L409 L410 P411 A412 Q412 Y414 L415 G416 N417 V418 I419 L421 K425 R426 M431 M432 S432 Y434 M437 Q438 V439 A440 L441 L441 T442 M447 A448 E449 I450 L451 L452 D453 F454 F455 D456 R457 L458 A459 S460 T461 S462 R463 R464 Y465 A466 S467 L468 D469 Y470 F475 Q476 A477 S478 T479 M480 V481 R482 V483 D484 Q485 L486 I487 N488 A494 L495 T499 H500 R501 D502 N503 S504 Q505 N506 R507 L511 K516 T519 P520 R521 Q522 Q523 T526 Q529 T534 H535 A538 R539 S540 T541 V542 K543 Q544 L545

- Molecule 10: 30S ribosomal protein S12

Chain D:  22% 58% 20%



• Molecule 11: 50S ribosomal protein L11



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, OMG, H2U, YG, 2MG, 5MC, 1MA, M2G, 7MG, PSU

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	0.97	2/1486 (0.1%)	1.34	8/2311 (0.3%)
10	D	0.22	0/969	0.46	0/1300
11	H	0.63	5/1046 (0.5%)	0.74	5/1410 (0.4%)
2	B	0.52	1/1814 (0.1%)	0.72	0/2825
3	E	0.21	0/386	0.71	0/600
4	F	0.27	0/285	0.76	0/442
5	G	0.67	5/1677 (0.3%)	0.82	8/2612 (0.3%)
6	I	0.27	0/699	0.74	0/1089
7	J	0.24	0/428	0.72	0/665
8	K	0.23	0/351	0.75	0/544
9	C	0.60	4/4312 (0.1%)	1.04	45/5844 (0.8%)
All	All	0.59	17/13453 (0.1%)	0.92	66/19642 (0.3%)

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	7	3
11	H	0	1
2	B	0	2
5	G	0	4
9	C	1	11
All	All	8	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	OMG	O3'-P	19.74	1.84	1.61
5	G	1086	A	C5-C6	-16.32	1.26	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1088	A	C6-N1	-10.50	1.28	1.35
9	C	480	MET	C-N	8.63	1.53	1.34
5	G	1060	U	C2-N3	7.75	1.43	1.37
9	C	14	ASP	CA-CB	7.67	1.70	1.53
11	H	73	PRO	CA-C	7.39	1.67	1.52
5	G	1086	A	N3-C4	-7.29	1.30	1.34
1	A	1	G	OP3-P	-7.15	1.52	1.61
2	B	1	C	OP3-P	-7.03	1.52	1.61
9	C	14	ASP	CB-CG	6.42	1.65	1.51
5	G	1086	A	N7-C5	-6.20	1.35	1.39
11	H	73	PRO	N-CA	6.00	1.57	1.47
11	H	74	PRO	N-CA	5.98	1.57	1.47
9	C	14	ASP	N-CA	-5.86	1.34	1.46
11	H	72	THR	N-CA	5.15	1.56	1.46
11	H	71	LYS	N-CA	5.01	1.56	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	A	P-O3'-C3'	41.08	168.99	119.70
1	A	34	OMG	O3'-P-O5'	19.74	141.51	104.00
9	C	14	ASP	CB-CA-C	17.60	145.59	110.40
9	C	13	ILE	C-N-CA	-17.05	79.07	121.70
9	C	13	ILE	N-CA-C	12.32	144.26	111.00
1	A	35	A	OP1-P-O3'	11.53	130.55	105.20
9	C	372	TYR	O-C-N	-11.42	104.43	122.70
9	C	476	GLN	O-C-N	-11.17	104.83	122.70
9	C	17	LYS	CB-CA-C	-10.98	88.44	110.40
1	A	34	OMG	OP2-P-O3'	-10.13	82.92	105.20
9	C	372	TYR	C-N-CA	9.13	144.53	121.70
9	C	15	HIS	CA-CB-CG	8.96	128.84	113.60
1	A	35	A	O3'-P-O5'	-8.90	87.09	104.00
5	G	1088	A	N1-C6-N6	-8.46	113.52	118.60
1	A	18	G	C5'-C4'-O4'	-8.40	99.02	109.10
9	C	54	ILE	CA-CB-CG1	8.31	126.80	111.00
9	C	14	ASP	CB-CG-OD1	8.00	125.50	118.30
9	C	488	ASN	CB-CA-C	-7.95	94.51	110.40
9	C	491	ARG	CD-NE-CZ	-7.90	112.55	123.60
9	C	491	ARG	NE-CZ-NH1	-7.84	116.38	120.30
9	C	14	ASP	C-N-CA	7.33	140.03	121.70
5	G	1060	U	C5-C4-O4	-7.31	121.52	125.90
9	C	19	THR	C-N-CA	-7.26	103.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	56	ALA	CB-CA-C	-7.26	99.21	110.10
5	G	1086	A	C4-C5-C6	7.02	120.51	117.00
9	C	291	VAL	C-N-CA	7.02	139.24	121.70
9	C	12	HIS	O-C-N	-6.92	111.62	122.70
9	C	366	THR	N-CA-C	-6.88	92.43	111.00
11	H	75	ALA	N-CA-C	6.86	129.53	111.00
11	H	73	PRO	N-CA-C	6.81	129.81	112.10
9	C	372	TYR	CA-C-N	6.68	131.90	117.20
9	C	56	ALA	N-CA-CB	6.58	119.31	110.10
9	C	17	LYS	N-CA-CB	6.57	122.43	110.60
9	C	367	ALA	O-C-N	-6.55	108.64	121.10
5	G	1088	A	C5-C6-N6	6.54	128.94	123.70
9	C	13	ILE	CA-CB-CG2	6.42	123.73	110.90
9	C	483	VAL	CA-CB-CG1	-6.34	101.39	110.90
9	C	55	LYS	O-C-N	-6.32	112.60	122.70
9	C	294	GLN	N-CA-CB	-6.18	99.47	110.60
9	C	54	ILE	CA-CB-CG2	-6.15	98.60	110.90
9	C	483	VAL	CB-CA-C	-6.11	99.79	111.40
9	C	481	VAL	CA-CB-CG1	-6.11	101.74	110.90
9	C	367	ALA	CA-C-N	6.09	134.16	117.10
5	G	1086	A	C6-C5-N7	-6.09	128.04	132.30
9	C	491	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	15	G	N9-C1'-C2'	-5.97	105.43	112.00
9	C	367	ALA	C-N-CD	-5.95	107.52	120.60
9	C	56	ALA	O-C-N	5.80	131.97	122.70
9	C	14	ASP	N-CA-C	-5.79	95.37	111.00
9	C	54	ILE	CB-CA-C	-5.75	100.09	111.60
9	C	53	THR	N-CA-CB	5.74	121.20	110.30
11	H	70	THR	C-N-CA	5.68	135.90	121.70
5	G	1060	U	N1-C2-O2	-5.67	118.83	122.80
9	C	291	VAL	CA-CB-CG2	-5.62	102.47	110.90
11	H	74	PRO	CA-N-CD	-5.60	103.66	111.50
9	C	14	ASP	CA-CB-CG	5.48	125.46	113.40
9	C	291	VAL	CA-CB-CG1	5.46	119.09	110.90
5	G	1086	A	C2-N3-C4	-5.37	107.92	110.60
11	H	74	PRO	N-CA-C	5.35	126.02	112.10
5	G	1060	U	N3-C2-O2	5.27	125.89	122.20
9	C	53	THR	CA-CB-CG2	-5.27	105.03	112.40
9	C	482	ARG	CD-NE-CZ	-5.26	116.23	123.60
9	C	56	ALA	CA-C-N	-5.25	105.65	117.20
9	C	484	ASP	CA-CB-CG	-5.09	102.20	113.40
1	A	21	A	C5'-C4'-C3'	5.05	124.08	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	182	PRO	N-CA-CB	5.04	109.35	103.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	A	C2'
1	A	74	C	C4',C1'
1	A	75	C	C4',C2',C3'
1	A	76	A	C4'
9	C	13	ILE	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	G	Sidechain
1	A	19	G	Sidechain
1	A	62	A	Sidechain
2	B	25	C	Sidechain
2	B	4	G	Sidechain
9	C	12	HIS	Mainchain,Peptide
9	C	13	ILE	Peptide
9	C	18	SER	Peptide
9	C	289	LYS	Mainchain
9	C	29	GLY	Mainchain
9	C	291	VAL	Peptide
9	C	476	GLN	Mainchain
9	C	482	ARG	Sidechain
9	C	487	ILE	Peptide
9	C	491	ARG	Sidechain
5	G	1060	U	Sidechain
5	G	1086	A	Sidechain
5	G	1088	A	Sidechain
5	G	1111	A	Sidechain
11	H	70	THR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	857	153	0
2	B	1645	0	838	56	0
3	E	345	0	174	12	0
4	F	256	0	131	1	0
5	G	1498	0	757	64	0
6	I	625	0	314	23	0
7	J	384	0	193	27	0
8	K	316	0	161	9	0
9	C	4242	0	4236	417	0
10	D	955	0	1019	126	0
11	H	1032	0	1088	122	0
All	All	12950	0	9768	893	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 39.

All (893) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:G:P	9:C:543:LYS:HE3	1.19	1.65
9:C:110:ALA:HB2	9:C:465:TYR:CD2	1.11	1.63
1:A:69:U:C5'	9:C:539:ARG:HD2	1.22	1.56
9:C:26:GLN:CG	9:C:34:ARG:HB3	1.40	1.47
9:C:26:GLN:CD	9:C:34:ARG:HG2	1.31	1.45
9:C:110:ALA:CB	9:C:465:TYR:CD2	2.02	1.41
9:C:110:ALA:HB2	9:C:465:TYR:CE2	1.53	1.41
1:A:71:G:OP2	9:C:543:LYS:CE	1.71	1.38
1:A:71:G:P	9:C:543:LYS:CE	2.09	1.37
9:C:26:GLN:NE2	9:C:34:ARG:HG2	1.38	1.34
9:C:296:TYR:H	9:C:451:VAL:CG1	1.40	1.33
7:J:1945:G:O2'	9:C:523:GLN:NE2	1.64	1.31
1:A:67:A:H4'	9:C:505:GLN:OE1	1.27	1.30
9:C:26:GLN:CD	9:C:34:ARG:CG	1.99	1.30
9:C:296:TYR:N	9:C:451:VAL:HG13	1.45	1.30
1:A:69:U:C5'	9:C:539:ARG:CD	2.10	1.28
9:C:296:TYR:O	9:C:368:PRO:HB3	1.29	1.25
9:C:26:GLN:NE2	9:C:34:ARG:CG	1.98	1.24
9:C:369:THR:OG1	9:C:452:LEU:HD21	1.35	1.23
1:A:68:U:OP1	9:C:538:ALA:CB	1.86	1.21
1:A:76:A:C2	7:J:1944:U:O3'	1.92	1.21
1:A:69:U:H5'	9:C:539:ARG:CD	1.67	1.20
1:A:33:U:C2	1:A:35:A:H5'	1.77	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:U:OP1	9:C:538:ALA:HB1	1.05	1.19
1:A:25:C:C2'	1:A:26:M2G:H5'	1.72	1.18
1:A:70:C:C5'	9:C:543:LYS:HZ3	1.55	1.17
9:C:368:PRO:HB2	9:C:451:VAL:O	1.44	1.16
1:A:71:G:OP2	9:C:543:LYS:HE3	0.98	1.16
1:A:75:C:C5	7:J:1955:U:C2	2.34	1.15
5:G:1060:U:OP2	11:H:74:PRO:HA	1.46	1.14
9:C:11:ALA:CB	9:C:17:LYS:HB3	1.76	1.13
9:C:26:GLN:CG	9:C:34:ARG:CB	2.27	1.12
9:C:26:GLN:HG2	9:C:34:ARG:HB3	1.18	1.11
1:A:70:C:O3'	9:C:543:LYS:NZ	1.85	1.10
9:C:330:SER:OG	10:D:35:ARG:NH1	1.83	1.09
9:C:369:THR:OG1	9:C:452:LEU:CD2	2.01	1.09
9:C:26:GLN:CD	9:C:34:ARG:CB	2.21	1.08
1:A:75:C:H5	7:J:1955:U:C2	1.69	1.07
9:C:31:LEU:HD13	9:C:243:LYS:HG3	1.22	1.07
1:A:69:U:H5''	9:C:539:ARG:CD	1.76	1.07
9:C:11:ALA:HB2	9:C:17:LYS:HB3	1.34	1.06
9:C:26:GLN:OE1	9:C:34:ARG:HG2	1.55	1.06
1:A:11:C:O5'	9:C:534:THR:HG23	1.29	1.06
1:A:70:C:H5''	9:C:543:LYS:NZ	1.67	1.06
1:A:11:C:O5'	9:C:534:THR:CG2	1.98	1.05
9:C:9:ILE:HG22	9:C:17:LYS:HD2	1.36	1.05
1:A:25:C:C2'	1:A:26:M2G:C5'	2.34	1.05
9:C:18:SER:HA	9:C:21:SER:HB3	1.37	1.04
9:C:22:ASP:OD2	9:C:41:LEU:CD1	2.06	1.03
9:C:297:ALA:HB2	9:C:368:PRO:HG3	1.38	1.02
1:A:70:C:H5''	9:C:543:LYS:HZ3	0.87	1.02
9:C:110:ALA:CB	9:C:465:TYR:CE2	2.35	1.02
5:G:1060:U:OP1	11:H:75:ALA:HB3	1.57	1.02
9:C:23:ARG:HH22	9:C:131:ASN:HD21	1.03	1.01
9:C:11:ALA:HB3	9:C:17:LYS:HD3	1.41	1.01
9:C:50:ARG:HD2	9:C:52:ILE:HB	1.36	1.01
9:C:433:VAL:HA	11:H:25:PRO:CG	1.90	1.01
1:A:25:C:H2'	1:A:26:M2G:C5'	1.91	1.00
9:C:295:VAL:HG13	9:C:451:VAL:O	1.63	0.99
1:A:33:U:O2	1:A:35:A:H5'	1.64	0.98
1:A:76:A:H2	7:J:1944:U:O3'	1.12	0.98
9:C:433:VAL:HA	11:H:25:PRO:HG2	1.44	0.98
9:C:12:HIS:HB3	9:C:13:ILE:HG22	1.46	0.98
2:B:52:G:HO2'	2:B:53:G:H8	1.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:16:GLY:HA3	9:C:131:ASN:OD1	1.64	0.97
9:C:369:THR:HG1	9:C:452:LEU:HD21	1.26	0.96
1:A:67:A:C4'	9:C:505:GLN:OE1	2.13	0.95
9:C:22:ASP:CG	9:C:41:LEU:HD11	1.87	0.95
9:C:26:GLN:NE2	9:C:34:ARG:CB	2.29	0.95
9:C:50:ARG:HB3	9:C:52:ILE:HG22	1.46	0.95
1:A:75:C:H4'	1:A:76:A:OP2	1.63	0.94
1:A:69:U:H5'	9:C:539:ARG:HD2	1.19	0.94
9:C:9:ILE:CG2	9:C:17:LYS:HB2	1.97	0.94
9:C:368:PRO:HB2	9:C:451:VAL:C	1.86	0.94
9:C:22:ASP:OD2	9:C:41:LEU:HD11	1.68	0.93
1:A:10:2MG:O2'	9:C:394:ASN:OD1	1.76	0.93
9:C:26:GLN:HG3	9:C:34:ARG:HB3	1.49	0.93
9:C:370:VAL:HG22	9:C:371:VAL:H	1.32	0.93
11:H:75:ALA:HB2	11:H:112:LYS:HE2	1.51	0.92
9:C:19:THR:O	9:C:23:ARG:HD3	1.70	0.92
9:C:26:GLN:CD	9:C:34:ARG:HB3	1.84	0.91
9:C:345:LEU:HD22	9:C:456:ASP:OD2	1.68	0.91
1:A:68:U:O2'	9:C:539:ARG:HB3	1.67	0.91
1:A:73:A:N3	1:A:73:A:H5''	1.85	0.91
9:C:19:THR:HG22	9:C:23:ARG:HD2	1.53	0.91
5:G:1060:U:OP2	11:H:74:PRO:CA	2.18	0.91
11:H:129:GLU:HB3	11:H:133:ARG:HH12	1.35	0.91
1:A:41:U:H5'	1:A:41:U:H6	1.34	0.90
9:C:45:ASP:HA	9:C:48:ARG:HD3	1.51	0.90
1:A:75:C:O2	7:J:1944:U:C2'	2.09	0.90
1:A:25:C:H2'	1:A:26:M2G:O4'	1.71	0.90
5:G:1060:U:N3	5:G:1088:A:N7	2.20	0.90
9:C:433:VAL:HG13	11:H:25:PRO:HG3	1.51	0.90
9:C:369:THR:HG22	9:C:370:VAL:H	1.34	0.89
9:C:13:ILE:H	9:C:15:HIS:H	1.16	0.89
9:C:1:MET:HG2	9:C:252:CYS:O	1.72	0.89
9:C:369:THR:HG23	9:C:448:ALA:HB1	1.55	0.88
9:C:12:HIS:ND1	9:C:13:ILE:HB	1.89	0.88
9:C:9:ILE:HG22	9:C:17:LYS:CD	2.04	0.87
9:C:349:GLU:OE2	9:C:456:ASP:OD2	1.92	0.87
9:C:4:ILE:HG21	9:C:253:GLY:O	1.73	0.87
10:D:85:ARG:HB3	10:D:93:ARG:HD3	1.55	0.86
9:C:18:SER:HA	9:C:21:SER:CB	2.03	0.86
9:C:345:LEU:H	9:C:455:PHE:HD2	0.93	0.86
9:C:50:ARG:HD2	9:C:52:ILE:CB	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:G:H2'	2:B:71:C:H5'	1.58	0.86
9:C:40:VAL:HG13	9:C:48:ARG:HG2	1.58	0.86
9:C:83:ASP:O	9:C:343:LEU:HD13	1.75	0.85
9:C:46:LEU:HD11	9:C:354:ARG:NE	1.91	0.85
9:C:110:ALA:HB2	9:C:465:TYR:HD2	1.30	0.85
9:C:19:THR:HG22	9:C:23:ARG:CD	2.06	0.85
1:A:75:C:N4	7:J:1944:U:O4'	1.90	0.85
9:C:294:GLN:CA	9:C:470:TYR:OH	1.93	0.84
9:C:345:LEU:N	9:C:455:PHE:HD2	1.73	0.83
10:D:82:ARG:HB2	10:D:97:VAL:HG22	1.60	0.83
2:B:15:G:H22	2:B:48:C:H42	1.23	0.83
11:H:27:LEU:H	11:H:27:LEU:HD23	1.40	0.83
9:C:11:ALA:HB3	9:C:17:LYS:CD	2.08	0.82
1:A:75:C:C6	1:A:76:A:O5'	2.32	0.82
9:C:23:ARG:NH2	9:C:131:ASN:HD21	1.76	0.82
5:G:1060:U:C2	5:G:1088:A:N7	2.48	0.82
10:D:27:PRO:HG2	10:D:28:GLN:HE21	1.43	0.82
9:C:18:SER:CA	9:C:21:SER:HB3	2.09	0.82
1:A:25:C:H2'	1:A:26:M2G:C4'	2.09	0.82
6:I:2660:A:H1'	9:C:459:LYS:O	1.79	0.82
1:A:74:C:O2'	1:A:75:C:P	2.37	0.81
1:A:70:C:C3'	9:C:543:LYS:HZ1	1.92	0.81
5:G:1082:U:C4	5:G:1086:A:C2	2.67	0.81
9:C:368:PRO:CB	9:C:452:LEU:HA	2.11	0.81
1:A:69:U:H5''	9:C:539:ARG:HD2	0.83	0.81
1:A:69:U:OP1	9:C:539:ARG:HG2	1.81	0.81
1:A:69:U:H5'	9:C:539:ARG:NE	1.95	0.81
10:D:35:ARG:NH2	10:D:75:GLU:HB3	1.95	0.80
1:A:68:U:P	9:C:538:ALA:HB1	2.22	0.80
5:G:1060:U:OP1	11:H:75:ALA:CB	2.29	0.80
1:A:68:U:P	9:C:538:ALA:CB	2.69	0.80
1:A:75:C:C4'	1:A:76:A:OP2	2.30	0.80
9:C:433:VAL:HG22	11:H:20:SER:OG	1.81	0.80
9:C:330:SER:CB	10:D:35:ARG:HH12	1.95	0.79
9:C:15:HIS:CD2	9:C:103:ASP:H	1.99	0.79
9:C:9:ILE:HG21	9:C:17:LYS:HB2	1.65	0.79
11:H:21:PRO:HB2	11:H:22:PRO:HD3	1.62	0.79
10:D:43:LYS:H	10:D:44:PRO:HD2	1.47	0.78
10:D:33:CYS:H	10:D:54:VAL:HG13	1.48	0.78
9:C:74:ASN:OD1	9:C:255:VAL:HB	1.83	0.78
1:A:68:U:O2'	9:C:539:ARG:CB	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:C:C3'	9:C:543:LYS:NZ	2.47	0.78
9:C:296:TYR:O	9:C:368:PRO:CB	2.22	0.78
10:D:113:ARG:HB3	10:D:118:VAL:HG23	1.65	0.78
9:C:368:PRO:CA	9:C:452:LEU:HA	2.13	0.77
9:C:296:TYR:H	9:C:451:VAL:HG13	0.61	0.77
9:C:370:VAL:HG11	9:C:447:MET:HB3	1.67	0.77
9:C:86:TYR:OH	9:C:289:LYS:HG2	1.85	0.77
10:D:86:VAL:HG11	10:D:89:LEU:HD23	1.67	0.77
2:B:70:G:C2'	2:B:71:C:H5'	2.14	0.77
1:A:33:U:C2	1:A:35:A:C5'	2.65	0.77
6:I:2660:A:C1'	9:C:459:LYS:O	2.32	0.77
9:C:44:MET:O	9:C:48:ARG:HG3	1.85	0.77
9:C:425:LYS:HD2	9:C:449:GLU:HG3	1.66	0.76
9:C:26:GLN:HE22	9:C:34:ARG:CZ	1.97	0.76
1:A:70:C:C5'	9:C:543:LYS:NZ	2.35	0.76
11:H:33:ASN:HD21	11:H:64:ARG:HH11	1.31	0.76
9:C:372:TYR:HD1	9:C:401:GLU:HA	1.50	0.76
9:C:44:MET:HB2	9:C:47:GLU:OE2	1.85	0.76
9:C:25:ILE:HG22	9:C:30:GLY:O	1.85	0.76
11:H:27:LEU:HD12	11:H:32:VAL:HG11	1.68	0.76
6:I:2660:A:N9	9:C:459:LYS:O	2.18	0.76
10:D:35:ARG:HA	10:D:35:ARG:HE	1.49	0.75
9:C:52:ILE:HG12	9:C:53:THR:O	1.85	0.75
9:C:16:GLY:O	9:C:20:LEU:HB2	1.87	0.75
6:I:2660:A:H1'	9:C:464:GLY:N	2.01	0.75
9:C:296:TYR:HB2	9:C:451:VAL:HG11	1.70	0.74
1:A:25:C:O2'	1:A:26:M2G:H5'	1.85	0.74
1:A:71:G:C6	1:A:72:C:N4	2.55	0.74
1:A:70:C:O3'	9:C:543:LYS:CE	2.26	0.74
9:C:503:ASN:HB2	9:C:507:ARG:HH21	1.51	0.74
1:A:67:A:H4'	9:C:505:GLN:CD	2.07	0.74
6:I:2660:A:H4'	9:C:463:ARG:O	1.86	0.74
10:D:86:VAL:HG12	10:D:87:LYS:H	1.53	0.74
10:D:23:LEU:HD13	10:D:25:ALA:H	1.52	0.74
5:G:1082:U:N3	5:G:1086:A:C2	2.55	0.73
1:A:37:YG:H31	1:A:37:YG:C1'	2.19	0.73
9:C:11:ALA:CB	9:C:17:LYS:CB	2.62	0.73
11:H:106:GLN:O	11:H:110:GLN:HG3	1.89	0.73
9:C:26:GLN:HE22	9:C:34:ARG:HG2	1.45	0.73
9:C:22:ASP:OD1	9:C:41:LEU:HD11	1.87	0.73
9:C:50:ARG:O	9:C:50:ARG:HD3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:45:ASP:HA	9:C:48:ARG:CD	2.18	0.73
1:A:34:OMG:OP2	1:A:34:OMG:H8	1.72	0.73
2:B:20:U:H5'	2:B:21:A:OP2	1.89	0.73
9:C:183:PRO:HB3	9:C:211:ARG:HH22	1.53	0.73
1:A:71:G:OP2	9:C:543:LYS:HE2	1.82	0.72
9:C:294:GLN:C	9:C:470:TYR:OH	2.26	0.72
9:C:333:ALA:CB	9:C:494:ALA:HB2	2.20	0.72
9:C:86:TYR:CZ	9:C:289:LYS:HG2	2.24	0.72
11:H:77:VAL:HA	11:H:80:LYS:HE2	1.70	0.72
9:C:330:SER:HG	10:D:35:ARG:NH1	1.86	0.72
1:A:37:YG:C2'	1:A:37:YG:H31	2.20	0.72
9:C:425:LYS:HD2	9:C:449:GLU:CG	2.19	0.72
9:C:50:ARG:HD2	9:C:52:ILE:CG2	2.20	0.72
9:C:84:PHE:HZ	9:C:350:ILE:HD12	1.55	0.72
1:A:71:G:O6	1:A:72:C:N4	2.22	0.72
9:C:368:PRO:CB	9:C:451:VAL:O	2.31	0.72
5:G:1060:U:C4	5:G:1088:A:N6	2.58	0.72
9:C:11:ALA:CB	9:C:17:LYS:HD3	2.19	0.71
9:C:296:TYR:O	9:C:451:VAL:HG12	1.89	0.71
1:A:75:C:H1'	7:J:1944:U:OP1	1.90	0.71
9:C:368:PRO:N	9:C:452:LEU:HA	2.04	0.71
9:C:183:PRO:HB3	9:C:211:ARG:NH2	2.06	0.71
9:C:265:ILE:HD11	9:C:319:LEU:O	1.90	0.71
9:C:22:ASP:OD1	9:C:41:LEU:HD21	1.90	0.71
11:H:20:SER:HB3	11:H:21:PRO:HD3	1.71	0.71
3:E:154:U:H2'	3:E:155:A:C8	2.26	0.71
5:G:1063:G:O2'	11:H:88:GLY:HA3	1.90	0.70
11:H:122:GLU:O	11:H:126:ARG:HG3	1.90	0.70
9:C:72:GLN:OE1	9:C:254:GLU:HG2	1.90	0.70
11:H:7:TYR:HB3	11:H:59:THR:HA	1.74	0.70
2:B:73:A:H5'	2:B:73:A:H8	1.56	0.70
1:A:44:A:O3'	1:A:45:G:P	2.49	0.70
1:A:67:A:C4'	9:C:505:GLN:CD	2.59	0.70
1:A:69:U:H5'	9:C:539:ARG:HB3	1.74	0.70
9:C:296:TYR:N	9:C:451:VAL:CG1	2.22	0.70
9:C:368:PRO:CD	9:C:452:LEU:HA	2.21	0.70
9:C:434:TYR:HD1	11:H:25:PRO:HB3	1.56	0.70
1:A:75:C:H5	7:J:1955:U:N3	1.89	0.70
9:C:31:LEU:HD13	9:C:243:LYS:CG	2.14	0.69
10:D:20:VAL:HG12	10:D:23:LEU:HB2	1.74	0.69
1:A:37:YG:N20	1:A:37:YG:H101	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:C:H2'	2:B:41:C:H6	1.58	0.69
10:D:64:SER:OG	10:D:96:THR:HG23	1.92	0.69
9:C:46:LEU:CD2	9:C:354:ARG:HD2	2.23	0.69
1:A:37:YG:H31	1:A:37:YG:H1'	1.74	0.69
9:C:26:GLN:HE22	9:C:34:ARG:NH1	1.90	0.68
1:A:75:C:H4'	1:A:75:C:OP2	1.92	0.68
9:C:9:ILE:CG2	9:C:17:LYS:CB	2.72	0.68
11:H:10:LEU:HD13	11:H:12:VAL:HG13	1.75	0.68
2:B:40:C:H2'	2:B:41:C:C6	2.29	0.68
9:C:11:ALA:HB2	9:C:17:LYS:CB	2.18	0.68
10:D:38:THR:HG22	10:D:48:LEU:HB2	1.75	0.68
10:D:29:LYS:H	10:D:81:ILE:HG22	1.59	0.68
11:H:129:GLU:HB3	11:H:133:ARG:NH1	2.09	0.68
9:C:368:PRO:O	9:C:452:LEU:CB	2.14	0.68
2:B:50:U:H2'	2:B:51:C:C6	2.29	0.68
9:C:273:THR:HG21	9:C:285:LEU:H	1.59	0.68
10:D:30:ARG:HG2	10:D:31:GLY:H	1.59	0.68
10:D:42:LYS:HB2	10:D:88:ASP:HA	1.74	0.68
5:G:1060:U:O2	5:G:1088:A:N7	2.27	0.68
9:C:22:ASP:OD2	9:C:41:LEU:HD12	1.93	0.67
6:I:2649:C:H2'	6:I:2650:U:H6	1.58	0.67
1:A:75:C:C2	7:J:1944:U:O5'	2.48	0.67
1:A:73:A:H3'	1:A:73:A:N3	2.09	0.67
9:C:23:ARG:HH22	9:C:131:ASN:ND2	1.85	0.67
9:C:410:LEU:HD13	9:C:418:VAL:HG21	1.76	0.67
9:C:295:VAL:CG1	9:C:451:VAL:O	2.40	0.67
9:C:11:ALA:HB3	9:C:17:LYS:CG	2.24	0.67
9:C:368:PRO:HB2	9:C:452:LEU:HA	1.77	0.67
9:C:481:VAL:HG22	9:C:501:ARG:HA	1.75	0.67
10:D:41:PRO:HD3	10:D:47:ALA:O	1.95	0.67
9:C:343:LEU:H	9:C:347:HIS:CD2	2.13	0.67
9:C:46:LEU:HD21	9:C:358:GLU:OE2	1.95	0.67
9:C:110:ALA:N	9:C:465:TYR:CE2	2.64	0.66
9:C:369:THR:HG22	9:C:370:VAL:N	2.09	0.66
9:C:415:LEU:O	9:C:419:ILE:HD12	1.95	0.66
9:C:13:ILE:N	9:C:15:HIS:H	1.93	0.66
9:C:433:VAL:CG1	11:H:25:PRO:HG3	2.24	0.66
2:B:66:C:H2'	2:B:67:C:C6	2.30	0.65
10:D:3:VAL:HG23	10:D:4:ASN:H	1.59	0.65
10:D:23:LEU:CD1	10:D:25:ALA:H	2.08	0.65
10:D:38:THR:HG21	10:D:48:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:C:C5	7:J:1955:U:O2	2.50	0.65
1:A:26:M2G:HM22	1:A:44:A:C2	2.32	0.65
9:C:110:ALA:CB	9:C:465:TYR:CG	2.76	0.65
9:C:26:GLN:NE2	9:C:34:ARG:NH1	2.45	0.65
9:C:81:HIS:CD2	9:C:82:VAL:H	2.15	0.65
10:D:33:CYS:N	10:D:54:VAL:HG13	2.10	0.65
10:D:49:ARG:HB3	10:D:65:TYR:HE1	1.60	0.65
9:C:81:HIS:CD2	9:C:346:LEU:HD11	2.31	0.65
8:K:2547:A:H2'	8:K:2548:U:C6	2.31	0.65
11:H:25:PRO:O	11:H:29:GLN:HG2	1.97	0.65
9:C:86:TYR:CE1	9:C:289:LYS:HE3	2.32	0.64
9:C:431:ASN:HB3	9:C:442:THR:HG23	1.78	0.64
9:C:84:PHE:HZ	9:C:350:ILE:CD1	2.09	0.64
10:D:27:PRO:CG	10:D:28:GLN:HE21	2.10	0.64
9:C:266:HIS:NE2	9:C:319:LEU:HD23	2.11	0.64
9:C:368:PRO:HB2	9:C:452:LEU:CA	2.28	0.64
1:A:70:C:C4'	9:C:543:LYS:NZ	2.60	0.64
9:C:426:ARG:HE	9:C:480:MET:HE1	1.63	0.64
10:D:62:VAL:HG22	10:D:63:THR:H	1.62	0.64
10:D:74:GLN:NE2	10:D:75:GLU:H	1.94	0.64
2:B:72:A:C3'	2:B:73:A:H5''	2.27	0.64
9:C:26:GLN:NE2	9:C:34:ARG:HB2	2.10	0.64
9:C:9:ILE:CG2	9:C:17:LYS:CG	2.76	0.64
1:A:73:A:C4	1:A:73:A:H5''	2.33	0.64
10:D:23:LEU:HD13	10:D:24:GLU:N	2.12	0.64
6:I:2649:C:H2'	6:I:2650:U:C6	2.32	0.64
9:C:345:LEU:CD2	9:C:456:ASP:OD2	2.40	0.64
11:H:105:LEU:HD11	11:H:139:VAL:HG11	1.78	0.63
9:C:369:THR:OG1	9:C:452:LEU:HD23	1.97	0.63
9:C:333:ALA:HB1	9:C:494:ALA:HB2	1.81	0.63
10:D:36:VAL:HG12	10:D:52:CYS:HB2	1.81	0.63
9:C:16:GLY:CA	9:C:131:ASN:OD1	2.43	0.63
9:C:433:VAL:HA	11:H:25:PRO:HG3	1.79	0.63
1:A:75:C:C6	1:A:76:A:C5'	2.70	0.63
9:C:15:HIS:HD2	9:C:103:ASP:HB2	1.63	0.63
10:D:82:ARG:HB3	10:D:95:HIS:O	1.98	0.63
5:G:1105:U:H2'	5:G:1106:G:H8	1.62	0.63
6:I:2662:A:H2'	6:I:2663:G:O4'	1.99	0.63
9:C:47:GLU:HG3	9:C:54:ILE:H	1.64	0.62
5:G:1060:U:O4	5:G:1088:A:N6	2.31	0.62
10:D:2:THR:HB	10:D:5:GLN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:370:VAL:HG11	9:C:402:PRO:HG2	1.81	0.62
11:H:11:GLN:HA	11:H:55:PRO:HA	1.80	0.62
5:G:1076:C:O3'	11:H:94:LYS:HE3	1.98	0.62
9:C:9:ILE:HG22	9:C:17:LYS:CG	2.29	0.62
10:D:5:GLN:HA	10:D:8:ARG:HH11	1.64	0.62
3:E:154:U:H2'	3:E:155:A:H8	1.64	0.62
5:G:1054:A:H2'	5:G:1055:G:C8	2.35	0.62
5:G:1049:C:H2'	5:G:1050:A:H8	1.65	0.62
9:C:368:PRO:HB2	9:C:452:LEU:N	2.15	0.62
11:H:18:ASN:N	11:H:19:PRO:HD2	2.14	0.62
2:B:17:C:H5''	2:B:17(A):U:C6	2.35	0.62
1:A:75:C:O2	7:J:1944:U:H2'	1.21	0.61
11:H:85:ILE:HD13	11:H:137:LEU:HD21	1.81	0.61
9:C:369:THR:HA	9:C:448:ALA:O	2.01	0.61
5:G:1082:U:N3	5:G:1086:A:C6	2.69	0.61
1:A:72:C:H3'	1:A:72:C:P	2.41	0.61
1:A:9:A:OP1	9:C:535:HIS:NE2	2.33	0.61
9:C:50:ARG:CB	9:C:52:ILE:HG22	2.24	0.61
10:D:48:LEU:HD23	10:D:48:LEU:H	1.66	0.61
1:A:37:YG:H101	1:A:37:YG:C21	2.30	0.61
1:A:72:C:H2'	1:A:73:A:C5	2.36	0.61
9:C:333:ALA:HB2	9:C:494:ALA:HB2	1.83	0.61
10:D:3:VAL:HG23	10:D:4:ASN:N	2.16	0.61
8:K:2557:G:H2'	8:K:2558:C:C6	2.35	0.61
9:C:110:ALA:CA	9:C:465:TYR:CE2	2.83	0.61
11:H:102:ARG:HB2	11:H:141:ASP:OD2	2.01	0.61
1:A:72:C:OP2	1:A:72:C:H3'	2.01	0.61
7:J:1945:G:HO2'	9:C:523:GLN:NE2	1.97	0.61
11:H:20:SER:O	11:H:25:PRO:HD2	2.00	0.61
9:C:46:LEU:HB3	9:C:54:ILE:HD11	1.83	0.60
11:H:89:SER:HA	11:H:97:VAL:HG21	1.82	0.60
10:D:83:GLY:HA2	10:D:94:TYR:HD1	1.66	0.60
5:G:1060:U:C5	11:H:131:THR:HG22	2.37	0.60
1:A:72:C:OP2	1:A:73:A:OP2	2.19	0.60
10:D:74:GLN:HE21	10:D:75:GLU:H	1.47	0.60
1:A:44:A:H3'	1:A:45:G:P	2.41	0.60
9:C:26:GLN:HG3	9:C:34:ARG:CB	2.18	0.60
9:C:26:GLN:OE1	9:C:34:ARG:CG	2.30	0.60
1:A:72:C:C5	1:A:73:A:N6	2.70	0.60
9:C:19:THR:HG22	9:C:23:ARG:HD3	1.84	0.60
10:D:33:CYS:SG	10:D:54:VAL:HG22	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:98:ARG:HB2	10:D:116:TYR:HA	1.84	0.60
1:A:41:U:H5'	1:A:41:U:C6	2.27	0.60
10:D:56:LEU:HD11	10:D:81:ILE:HD12	1.84	0.60
10:D:33:CYS:HB3	10:D:75:GLU:O	2.02	0.59
1:A:74:C:C6	1:A:75:C:OP2	2.55	0.59
9:C:109:GLU:HA	9:C:465:TYR:OH	2.02	0.59
6:I:2660:A:C1'	9:C:464:GLY:N	2.63	0.59
9:C:26:GLN:NE2	9:C:34:ARG:CD	2.65	0.59
5:G:1105:U:H2'	5:G:1106:G:C8	2.37	0.59
8:K:2556:C:H2'	8:K:2557:G:O4'	2.02	0.59
1:A:40:5MC:H2'	1:A:41:U:H5'	1.82	0.59
1:A:41:U:H2'	1:A:42:G:O4'	2.02	0.59
10:D:80:LEU:HB2	10:D:101:LEU:HD22	1.84	0.59
11:H:75:ALA:HB2	11:H:112:LYS:CE	2.30	0.59
9:C:9:ILE:HG21	9:C:17:LYS:CB	2.30	0.59
9:C:343:LEU:H	9:C:347:HIS:HD2	1.49	0.59
9:C:370:VAL:HG22	9:C:371:VAL:N	2.11	0.59
9:C:297:ALA:CB	9:C:368:PRO:HG3	2.24	0.59
1:A:11:C:C5'	9:C:534:THR:HG23	2.31	0.59
10:D:33:CYS:HA	10:D:54:VAL:HA	1.85	0.59
9:C:86:TYR:HE1	9:C:289:LYS:HE3	1.67	0.59
10:D:20:VAL:HG13	10:D:94:TYR:CE1	2.38	0.59
10:D:50:LYS:N	10:D:50:LYS:HD2	2.18	0.59
5:G:1097:U:H2'	5:G:1098:A:H5'	1.84	0.59
11:H:96:LYS:N	11:H:96:LYS:HD2	2.18	0.59
2:B:23:C:H2'	2:B:24:U:C6	2.36	0.59
11:H:27:LEU:CD2	11:H:27:LEU:H	2.15	0.59
9:C:40:VAL:CG1	9:C:48:ARG:HG2	2.31	0.58
10:D:36:VAL:HG12	10:D:52:CYS:CB	2.33	0.58
2:B:15:G:N2	2:B:48:C:H42	1.99	0.58
9:C:265:ILE:CD1	9:C:319:LEU:O	2.50	0.58
9:C:346:LEU:HD13	9:C:346:LEU:H	1.68	0.58
1:A:33:U:O2'	1:A:35:A:N7	2.36	0.58
2:B:17:C:H5''	2:B:17(A):U:C5	2.39	0.58
2:B:72:A:H2'	2:B:73:A:H5''	1.84	0.58
9:C:299:LEU:HD23	9:C:365:THR:HB	1.85	0.58
9:C:46:LEU:HD21	9:C:354:ARG:CD	2.34	0.58
9:C:54:ILE:O	9:C:79:PRO:HB3	2.04	0.58
5:G:1056:G:H4'	5:G:1086:A:H8	1.67	0.58
1:A:64:A:H2'	1:A:65:G:O4'	2.04	0.58
10:D:78:VAL:O	10:D:102:ASP:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:C:HO2'	1:A:75:C:P	2.24	0.58
9:C:17:LYS:HA	9:C:101:VAL:HG11	1.86	0.58
9:C:241:THR:H	9:C:242:PRO:C	2.06	0.58
5:G:1061:U:H4'	5:G:1070:A:O3'	2.04	0.58
5:G:1082:U:C2	5:G:1086:A:C6	2.91	0.57
9:C:434:TYR:H	11:H:25:PRO:HB3	1.69	0.57
9:C:369:THR:CG2	9:C:448:ALA:HB1	2.31	0.57
10:D:54:VAL:HG21	10:D:79:ILE:HD11	1.87	0.57
10:D:98:ARG:HB2	10:D:116:TYR:C	2.25	0.57
9:C:46:LEU:HD21	9:C:354:ARG:HD2	1.86	0.57
5:G:1082:U:O4	5:G:1086:A:C2	2.57	0.57
2:B:37:A:H3'	2:B:38:A:H8	1.70	0.57
9:C:481:VAL:N	9:C:499:THR:O	2.25	0.57
11:H:58:ILE:HD12	11:H:58:ILE:N	2.19	0.57
9:C:19:THR:CG2	9:C:23:ARG:HD2	2.30	0.57
3:E:160:A:H2'	3:E:161:A:O4'	2.04	0.57
3:E:161:A:H2'	3:E:162:A:C8	2.40	0.57
5:G:1076:C:H5''	11:H:94:LYS:HZ1	1.70	0.57
10:D:41:PRO:HG3	10:D:46:SER:CA	2.35	0.57
9:C:265:ILE:CD1	9:C:320:ASN:ND2	2.68	0.56
10:D:79:ILE:HD13	10:D:96:THR:HG22	1.86	0.56
11:H:105:LEU:HD11	11:H:139:VAL:CG1	2.35	0.56
2:B:67:C:O2	2:B:67:C:H2'	2.05	0.56
9:C:30:GLY:HA3	9:C:31:LEU:C	2.26	0.56
11:H:33:ASN:HD21	11:H:64:ARG:NH1	2.03	0.56
10:D:18:SER:C	10:D:20:VAL:H	2.09	0.56
9:C:3:ASN:HD21	9:C:69:GLU:HG2	1.70	0.56
10:D:58:ASN:ND2	10:D:58:ASN:H	2.02	0.56
1:A:73:A:C3'	1:A:73:A:N3	2.68	0.56
9:C:17:LYS:C	9:C:21:SER:H	2.09	0.56
11:H:14:ALA:HB1	11:H:50:LYS:HA	1.87	0.56
9:C:6:ASN:HD22	9:C:211:ARG:NH2	2.04	0.56
9:C:31:LEU:CD1	9:C:243:LYS:HG3	2.16	0.56
9:C:330:SER:HB3	10:D:35:ARG:HH12	1.69	0.56
9:C:529:GLN:HB3	9:C:539:ARG:HG3	1.87	0.56
11:H:10:LEU:O	11:H:10:LEU:HD12	2.05	0.56
11:H:76:ALA:O	11:H:80:LYS:HG3	2.06	0.56
7:J:1948:G:O2'	7:J:1949:G:H5'	2.05	0.56
1:A:72:C:C6	1:A:73:A:N6	2.74	0.56
9:C:13:ILE:HG12	9:C:14:ASP:N	2.20	0.56
10:D:6:LEU:HD21	10:D:11:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:112:LYS:O	11:H:116:MET:HG3	2.06	0.56
2:B:1:C:H42	2:B:72:A:H61	1.53	0.56
9:C:292:LYS:HG2	9:C:293:PRO:N	2.20	0.56
11:H:17:ALA:O	11:H:18:ASN:HB3	2.06	0.56
1:A:29:A:O2'	1:A:30:G:H5'	2.06	0.55
9:C:193:ALA:HB1	9:C:210:ILE:HG23	1.88	0.55
9:C:81:HIS:NE2	9:C:346:LEU:HD11	2.22	0.55
5:G:1061:U:O4'	5:G:1070:A:H1'	2.06	0.55
1:A:25:C:C4	1:A:26:M2G:C8	2.94	0.55
10:D:51:VAL:HG12	10:D:52:CYS:H	1.70	0.55
6:I:2650:U:H2'	6:I:2651:C:C6	2.42	0.55
9:C:480:MET:SD	9:C:500:HIS:N	2.80	0.55
9:C:411:PRO:HG2	9:C:414:TYR:HD2	1.70	0.55
2:B:8:U:H1'	2:B:48:C:O2	2.06	0.55
9:C:11:ALA:HB3	9:C:17:LYS:HB3	1.84	0.55
10:D:73:LEU:HD21	10:D:103:CYS:HB2	1.88	0.55
1:A:44:A:C3'	1:A:45:G:P	2.95	0.55
7:J:1945:G:HO2'	9:C:523:GLN:HE21	1.55	0.55
10:D:113:ARG:CB	10:D:118:VAL:HG23	2.37	0.55
10:D:83:GLY:HA2	10:D:94:TYR:CD1	2.42	0.55
10:D:32:VAL:H	10:D:54:VAL:CG1	2.20	0.55
10:D:64:SER:HG	10:D:96:THR:HG23	1.72	0.55
1:A:25:C:C5	1:A:26:M2G:C8	2.95	0.55
10:D:113:ARG:NH2	10:D:120:ARG:HA	2.22	0.55
5:G:1097:U:C2'	5:G:1098:A:H5'	2.37	0.55
9:C:520:PRO:O	9:C:522:GLN:HG3	2.06	0.54
9:C:273:THR:HG21	9:C:285:LEU:N	2.21	0.54
9:C:345:LEU:N	9:C:455:PHE:CD2	2.53	0.54
9:C:46:LEU:HB2	9:C:47:GLU:OE1	2.08	0.54
10:D:58:ASN:N	10:D:58:ASN:HD22	2.04	0.54
5:G:1060:U:O4	11:H:131:THR:HG22	2.08	0.54
9:C:31:LEU:CD2	9:C:242:PRO:HG2	2.38	0.54
10:D:31:GLY:O	10:D:78:VAL:HG13	2.07	0.54
11:H:81:LYS:HG3	11:H:82:ALA:N	2.23	0.54
2:B:3:C:H2'	2:B:4:G:H5'	1.90	0.54
2:B:72:A:C2'	2:B:73:A:H5''	2.38	0.54
10:D:54:VAL:HG11	10:D:79:ILE:HD11	1.90	0.54
5:G:1108:U:H2'	5:G:1109:C:O4'	2.07	0.54
9:C:434:TYR:N	11:H:25:PRO:HB3	2.23	0.54
9:C:4:ILE:HD13	9:C:253:GLY:C	2.28	0.54
9:C:266:HIS:NE2	9:C:319:LEU:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:31:LEU:CD1	9:C:243:LYS:HE3	2.38	0.54
11:H:77:VAL:HA	11:H:80:LYS:CE	2.38	0.54
1:A:69:U:H5'	9:C:539:ARG:HE	1.72	0.54
9:C:345:LEU:HB2	9:C:455:PHE:CD2	2.43	0.54
10:D:58:ASN:H	10:D:58:ASN:HD22	1.55	0.54
1:A:16:H2U:H1'	1:A:17:H2U:OP2	2.08	0.53
1:A:16:H2U:O2'	1:A:17:H2U:OP2	2.21	0.53
11:H:125:THR:O	11:H:129:GLU:HG3	2.07	0.53
9:C:297:ALA:HB2	9:C:368:PRO:CG	2.26	0.53
10:D:67:GLY:O	10:D:98:ARG:HD2	2.08	0.53
11:H:109:ALA:HB1	11:H:124:MET:HG3	1.89	0.53
11:H:91:LYS:HB2	11:H:94:LYS:HD2	1.91	0.53
2:B:52:G:O2'	2:B:53:G:H8	1.77	0.53
9:C:9:ILE:HG21	9:C:17:LYS:O	2.09	0.53
10:D:32:VAL:H	10:D:54:VAL:HG13	1.74	0.53
1:A:33:U:O2	1:A:35:A:H3'	2.07	0.53
10:D:106:VAL:HG13	10:D:116:TYR:HB3	1.90	0.53
10:D:23:LEU:C	10:D:23:LEU:HD22	2.29	0.53
9:C:46:LEU:HD11	9:C:354:ARG:CD	2.39	0.53
1:A:74:C:C2	1:A:75:C:OP2	2.62	0.53
9:C:329:GLU:C	10:D:76:HIS:NE2	2.61	0.53
4:F:341:C:O2'	4:F:342:C:H5'	2.08	0.53
5:G:1060:U:C4	11:H:131:THR:HG22	2.44	0.53
11:H:18:ASN:N	11:H:19:PRO:CD	2.71	0.53
1:A:69:U:H5'	9:C:539:ARG:CG	2.36	0.53
10:D:86:VAL:HG12	10:D:87:LYS:N	2.21	0.53
11:H:89:SER:HB2	11:H:136:GLY:HA3	1.91	0.53
9:C:26:GLN:HE21	9:C:34:ARG:HB2	1.74	0.53
11:H:100:ILE:O	11:H:139:VAL:HA	2.09	0.53
1:A:75:C:N4	7:J:1944:U:C2	2.51	0.53
9:C:15:HIS:HD2	9:C:103:ASP:H	1.52	0.52
6:I:2671:G:H2'	6:I:2672:U:C6	2.44	0.52
1:A:69:U:H5'	9:C:539:ARG:CB	2.38	0.52
9:C:481:VAL:CG2	9:C:501:ARG:HA	2.39	0.52
5:G:1100:C:H2'	5:G:1101:U:H6	1.73	0.52
5:G:1076:C:H5''	11:H:94:LYS:NZ	2.24	0.52
3:E:154:U:O2'	3:E:155:A:H5'	2.10	0.52
6:I:2666:C:O2	6:I:2666:C:O4'	2.23	0.52
2:B:35:A:O2'	2:B:36:U:H5'	2.09	0.52
1:A:70:C:C3'	9:C:543:LYS:CE	2.86	0.52
1:A:75:C:OP1	1:A:75:C:H3'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1053:C:H2'	5:G:1054:A:H8	1.74	0.52
6:I:2660:A:C4	9:C:459:LYS:O	2.61	0.52
1:A:75:C:O2'	1:A:75:C:C2	2.58	0.52
10:D:106:VAL:HG22	10:D:116:TYR:HB2	1.91	0.52
1:A:75:C:C4	7:J:1955:U:C2	2.96	0.52
1:A:69:U:OP1	9:C:539:ARG:CG	2.55	0.52
1:A:75:C:C6	1:A:76:A:H5''	2.39	0.52
2:B:26:G:H1	2:B:44:A:H61	1.57	0.52
9:C:368:PRO:CA	9:C:452:LEU:CA	2.85	0.52
9:C:47:GLU:OE1	9:C:54:ILE:HG13	2.10	0.52
2:B:5:G:O2'	2:B:6:G:H5'	2.10	0.52
11:H:11:GLN:O	11:H:11:GLN:HG3	2.08	0.52
9:C:13:ILE:H	9:C:15:HIS:N	1.95	0.52
10:D:121:PRO:HG2	10:D:122:LYS:H	1.75	0.52
9:C:296:TYR:CA	9:C:451:VAL:CG1	2.88	0.52
9:C:31:LEU:HD12	9:C:243:LYS:HE3	1.91	0.52
9:C:40:VAL:HG12	9:C:42:ASP:O	2.10	0.52
9:C:44:MET:HB2	9:C:47:GLU:CD	2.31	0.52
11:H:23:VAL:HG23	11:H:24:GLY:N	2.25	0.52
9:C:31:LEU:HG	9:C:32:SER:N	2.25	0.51
9:C:369:THR:HG23	9:C:448:ALA:CB	2.34	0.51
9:C:410:LEU:HD21	9:C:441:LEU:HD12	1.91	0.51
5:G:1045:C:H5''	5:G:1047:G:C1'	2.40	0.51
5:G:1048:A:H1'	5:G:1112:G:N2	2.26	0.51
5:G:1060:U:O2	5:G:1088:A:C8	2.63	0.51
11:H:17:ALA:O	11:H:18:ASN:CB	2.58	0.51
1:A:67:A:O4'	9:C:505:GLN:NE2	2.43	0.51
10:D:105:GLY:HA3	10:D:117:GLY:O	2.11	0.51
3:E:153:C:H2'	3:E:154:U:H6	1.73	0.51
9:C:4:ILE:O	9:C:183:PRO:HD3	2.11	0.51
9:C:27:ILE:HD11	9:C:173:LEU:HD22	1.91	0.51
9:C:292:LYS:O	9:C:343:LEU:HD23	2.11	0.51
7:J:1958:C:O2'	7:J:1959:G:H5'	2.10	0.51
9:C:476:GLN:HG3	9:C:477:ALA:H	1.75	0.51
1:A:74:C:N1	1:A:75:C:OP2	2.43	0.51
9:C:9:ILE:HG21	9:C:17:LYS:CG	2.40	0.51
9:C:31:LEU:HG	9:C:32:SER:H	1.76	0.51
9:C:370:VAL:CG2	9:C:371:VAL:H	2.15	0.51
3:E:159:G:N1	3:E:163:C:N4	2.59	0.51
5:G:1083:U:H2'	5:G:1085:A:OP2	2.11	0.51
11:H:49:GLU:CG	11:H:54:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:U:H6	1:A:41:U:C5'	2.13	0.51
1:A:69:U:H2'	1:A:70:C:C6	2.46	0.51
11:H:23:VAL:HG23	11:H:24:GLY:H	1.75	0.51
7:J:1945:G:H2'	7:J:1946:U:C6	2.46	0.51
1:A:40:5MC:H2'	1:A:41:U:C5'	2.40	0.51
9:C:294:GLN:HA	9:C:470:TYR:OH	2.00	0.51
10:D:8:ARG:HG3	10:D:9:LYS:H	1.75	0.51
11:H:29:GLN:HE21	11:H:29:GLN:HA	1.75	0.51
11:H:3:LYS:HG2	11:H:4:VAL:N	2.25	0.51
9:C:17:LYS:HG3	9:C:17:LYS:O	2.11	0.50
9:C:196:ILE:HD11	9:C:211:ARG:HB2	1.93	0.50
10:D:41:PRO:HG3	10:D:46:SER:O	2.10	0.50
9:C:83:ASP:OD1	9:C:344:GLY:HA3	2.11	0.50
9:C:46:LEU:HD11	9:C:354:ARG:HE	1.72	0.50
9:C:193:ALA:HB3	9:C:274:LEU:HB2	1.93	0.50
11:H:48:ILE:HG22	11:H:49:GLU:HG2	1.93	0.50
1:A:69:U:C5'	9:C:539:ARG:CG	2.86	0.50
9:C:34:ARG:HD2	9:C:34:ARG:O	2.10	0.50
9:C:86:TYR:CZ	9:C:289:LYS:CG	2.95	0.50
1:A:30:G:O2'	1:A:31:A:H5'	2.12	0.50
9:C:15:HIS:C	9:C:132:LYS:HE2	2.32	0.50
9:C:31:LEU:HD22	9:C:242:PRO:HG2	1.94	0.50
9:C:503:ASN:HB2	9:C:507:ARG:NH2	2.24	0.50
10:D:20:VAL:CG1	10:D:23:LEU:HB2	2.41	0.50
2:B:66:C:H2'	2:B:67:C:H6	1.74	0.50
1:A:70:C:C4'	9:C:543:LYS:HZ1	2.22	0.50
10:D:98:ARG:HB2	10:D:116:TYR:CA	2.40	0.50
10:D:9:LYS:HD3	10:D:9:LYS:O	2.11	0.50
11:H:89:SER:HA	11:H:97:VAL:CG2	2.41	0.50
2:B:34:C:H2'	2:B:34:C:O2	2.10	0.50
10:D:27:PRO:HB2	10:D:28:GLN:NE2	2.27	0.50
9:C:434:TYR:CD1	11:H:25:PRO:HB3	2.41	0.50
6:I:2659:G:N2	6:I:2661:G:H5''	2.26	0.50
2:B:52:G:N3	2:B:53:G:C8	2.80	0.49
2:B:73:A:C8	2:B:73:A:H5'	2.41	0.49
10:D:43:LYS:H	10:D:44:PRO:CD	2.23	0.49
9:C:117:TYR:HA	9:C:120:MET:HE2	1.93	0.49
9:C:7:PHE:CZ	9:C:176:LEU:HD11	2.47	0.49
3:E:153:C:H2'	3:E:154:U:C6	2.47	0.49
7:J:1946:U:H2'	7:J:1947:C:C6	2.48	0.49
9:C:333:ALA:HB1	9:C:494:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:84:PHE:CZ	9:C:350:ILE:CD1	2.94	0.49
6:I:2665:A:O2'	6:I:2666:C:H5'	2.12	0.49
1:A:25:C:N4	1:A:26:M2G:C5	2.80	0.49
9:C:219:LYS:O	9:C:234:ALA:O	2.31	0.49
9:C:36:MET:HE3	9:C:39:GLN:HG2	1.95	0.49
9:C:265:ILE:HD11	9:C:319:LEU:C	2.32	0.49
9:C:368:PRO:O	9:C:452:LEU:CA	2.60	0.49
11:H:124:MET:O	11:H:128:ILE:HG12	2.13	0.49
11:H:56:VAL:CG2	11:H:68:PHE:HB2	2.43	0.49
9:C:17:LYS:N	9:C:101:VAL:HG11	2.27	0.49
10:D:6:LEU:HD21	10:D:11:ARG:NE	2.27	0.49
1:A:25:C:C5	1:A:26:M2G:N7	2.80	0.49
1:A:74:C:O2'	1:A:75:C:OP1	2.30	0.49
10:D:5:GLN:HA	10:D:8:ARG:NH1	2.27	0.49
3:E:159:G:H1	3:E:163:C:N4	2.10	0.49
1:A:71:G:P	9:C:543:LYS:NZ	2.64	0.48
9:C:480:MET:SD	9:C:500:HIS:CA	3.01	0.48
10:D:98:ARG:HB2	10:D:116:TYR:O	2.13	0.48
9:C:434:TYR:HD1	11:H:25:PRO:CB	2.23	0.48
9:C:86:TYR:CE1	9:C:289:LYS:CE	2.97	0.48
5:G:1080:A:O2'	5:G:1081:U:H5'	2.13	0.48
9:C:22:ASP:OD2	9:C:41:LEU:CG	2.61	0.48
1:A:9:A:OP1	9:C:535:HIS:CE1	2.67	0.48
10:D:51:VAL:HG12	10:D:52:CYS:N	2.28	0.48
10:D:71:HIS:HA	10:D:98:ARG:HH22	1.78	0.48
1:A:23:A:O2'	1:A:24:G:H5'	2.12	0.48
2:B:64:G:H2'	2:B:65:C:C6	2.48	0.48
1:A:72:C:C3'	1:A:72:C:P	3.01	0.48
2:B:53:G:C8	2:B:54:5MU:H72	2.49	0.48
9:C:46:LEU:CD1	9:C:354:ARG:HD2	2.43	0.48
9:C:480:MET:SD	9:C:500:HIS:HA	2.54	0.48
9:C:521:ARG:HB2	9:C:545:LEU:HD13	1.94	0.48
6:I:2661:G:H2'	6:I:2662:A:O4'	2.13	0.48
1:A:67:A:C5'	9:C:505:GLN:CD	2.82	0.48
11:H:79:LEU:HD11	11:H:131:THR:OG1	2.13	0.48
5:G:1080:A:H2'	5:G:1081:U:H6	1.78	0.47
9:C:241:THR:N	9:C:242:PRO:CA	2.77	0.47
9:C:476:GLN:O	9:C:477:ALA:C	2.53	0.47
5:G:1047:G:H4'	5:G:1047:G:OP1	2.14	0.47
2:B:14:A:C6	2:B:22:G:C5	3.02	0.47
9:C:81:HIS:CD2	9:C:82:VAL:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:2650:U:H2'	6:I:2651:C:H6	1.78	0.47
2:B:25:C:H2'	2:B:26:G:C8	2.50	0.47
9:C:195:ILE:HD11	9:C:274:LEU:HG	1.96	0.47
5:G:1100:C:H2'	5:G:1101:U:C6	2.50	0.47
11:H:52:LEU:N	11:H:52:LEU:HD12	2.29	0.47
9:C:9:ILE:HG23	9:C:17:LYS:HB2	1.92	0.47
5:G:1051:G:H2'	5:G:1052:C:O4'	2.15	0.47
11:H:32:VAL:HG13	11:H:66:PHE:CD2	2.49	0.47
2:B:47:U:H3'	2:B:48:C:C5'	2.44	0.47
2:B:4:G:O2'	2:B:5:G:OP2	2.32	0.47
10:D:107:LYS:HD2	10:D:107:LYS:N	2.29	0.47
1:A:67:A:H5'	9:C:505:GLN:CD	2.35	0.47
2:B:25:C:H2'	2:B:26:G:O4'	2.15	0.47
9:C:17:LYS:C	9:C:20:LEU:H	2.18	0.47
5:G:1110:G:N2	5:G:1111:A:N6	2.63	0.47
11:H:122:GLU:CD	11:H:122:GLU:H	2.18	0.47
8:K:2553:G:H2'	8:K:2554:U:C4'	2.45	0.47
5:G:1048:A:H1'	5:G:1112:G:H21	1.79	0.47
1:A:25:C:C4	1:A:26:M2G:N7	2.83	0.47
6:I:2665:A:H2'	6:I:2666:C:O2	2.14	0.47
7:J:1947:C:O2'	7:J:1948:G:H5'	2.14	0.47
9:C:182:PRO:HA	9:C:183:PRO:HD3	1.49	0.46
9:C:425:LYS:HD2	9:C:449:GLU:HG2	1.96	0.46
10:D:22:ALA:HB1	10:D:56:LEU:CD2	2.45	0.46
1:A:72:C:H6	1:A:72:C:H3'	1.80	0.46
9:C:17:LYS:HB2	9:C:101:VAL:HG21	1.98	0.46
10:D:80:LEU:O	10:D:97:VAL:HG23	2.14	0.46
2:B:75:C:H2'	2:B:76:A:O4'	2.15	0.46
9:C:433:VAL:HG22	11:H:20:SER:HG	1.80	0.46
9:C:412:GLN:HG2	9:C:439:VAL:HG23	1.97	0.46
9:C:17:LYS:HA	9:C:20:LEU:CB	2.46	0.46
9:C:483:VAL:HG12	9:C:484:ASP:O	2.15	0.46
9:C:480:MET:HG3	9:C:499:THR:O	2.15	0.46
9:C:16:GLY:C	9:C:20:LEU:H	2.19	0.46
9:C:193:ALA:HB1	9:C:210:ILE:CG2	2.45	0.46
10:D:106:VAL:HG22	10:D:116:TYR:CB	2.46	0.46
9:C:17:LYS:C	9:C:20:LEU:N	2.69	0.46
11:H:135:MET:HG3	11:H:137:LEU:HG	1.98	0.46
9:C:426:ARG:NH2	9:C:480:MET:HE2	2.31	0.46
5:G:1082:U:C2	5:G:1086:A:N1	2.84	0.46
11:H:19:PRO:HB2	11:H:22:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:431:ASN:HB3	9:C:442:THR:CG2	2.43	0.46
9:C:481:VAL:HG23	9:C:504:SER:HB3	1.97	0.46
10:D:24:GLU:C	10:D:26:CYS:H	2.19	0.46
5:G:1047:G:C2'	5:G:1110:G:H1	2.29	0.46
11:H:103:ALA:O	11:H:107:GLU:HG3	2.16	0.46
11:H:116:MET:SD	11:H:124:MET:HB2	2.56	0.46
11:H:21:PRO:HB2	11:H:22:PRO:CD	2.41	0.46
11:H:62:ALA:C	11:H:64:ARG:H	2.19	0.46
2:B:11:A:O2'	2:B:12:G:H5'	2.16	0.45
2:B:4:G:O2'	2:B:5:G:P	2.74	0.45
10:D:21:PRO:C	10:D:23:LEU:H	2.19	0.45
10:D:41:PRO:HG3	10:D:46:SER:C	2.36	0.45
5:G:1091:G:O2'	5:G:1092:C:H5'	2.16	0.45
8:K:2559:C:O2'	8:K:2560:A:H5'	2.16	0.45
2:B:27:U:H2'	2:B:28:C:H6	1.81	0.45
9:C:112:THR:O	9:C:116:CYS:HB2	2.16	0.45
11:H:44:LYS:O	11:H:48:ILE:HG13	2.16	0.45
9:C:74:ASN:HB3	9:C:255:VAL:HG21	1.97	0.45
9:C:265:ILE:HD12	9:C:320:ASN:ND2	2.31	0.45
1:A:37:YG:O2'	1:A:37:YG:H31	2.15	0.45
2:B:49:G:H1	2:B:65:C:H42	1.63	0.45
11:H:138:VAL:HG12	11:H:139:VAL:N	2.32	0.45
2:B:29:G:O2'	2:B:30:G:H5'	2.17	0.45
9:C:13:ILE:CG2	9:C:15:HIS:CG	2.99	0.45
9:C:367:ALA:O	9:C:452:LEU:CD2	2.65	0.45
1:A:68:U:O2'	9:C:539:ARG:NE	2.50	0.45
10:D:20:VAL:O	10:D:23:LEU:HB3	2.16	0.45
6:I:2661:G:H2'	6:I:2662:A:C8	2.51	0.45
2:B:4:G:O2'	2:B:5:G:C8	2.69	0.45
5:G:1064:C:H2'	5:G:1065:U:O4'	2.17	0.45
5:G:1072:C:N3	5:G:1092:C:N4	2.65	0.45
6:I:2668:G:O2'	6:I:2669:G:H5'	2.16	0.45
8:K:2547:A:H2'	8:K:2548:U:H6	1.79	0.45
8:K:2552:U:C2	8:K:2554:U:H5'	2.52	0.45
1:A:50:U:O2'	1:A:51:G:H5'	2.17	0.45
9:C:13:ILE:N	9:C:15:HIS:N	2.60	0.45
9:C:333:ALA:CB	9:C:494:ALA:CB	2.94	0.45
5:G:1104:C:H2'	5:G:1105:U:C6	2.51	0.45
5:G:1060:U:H5	11:H:131:THR:HG22	1.82	0.45
2:B:39:C:H2'	2:B:40:C:H6	1.82	0.44
9:C:372:TYR:CD1	9:C:401:GLU:HA	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:2660:A:C4	9:C:459:LYS:C	2.90	0.44
10:D:19:ASN:OD1	10:D:20:VAL:HG23	2.17	0.44
11:H:107:GLU:HA	11:H:110:GLN:OE1	2.18	0.44
9:C:370:VAL:CG1	9:C:402:PRO:HG2	2.47	0.44
9:C:476:GLN:CG	9:C:477:ALA:N	2.80	0.44
10:D:35:ARG:HE	10:D:35:ARG:CA	2.24	0.44
5:G:1059:G:H2'	5:G:1060:U:C5	2.52	0.44
10:D:89:LEU:HB3	10:D:92:VAL:HG21	1.98	0.44
9:C:83:ASP:OD1	9:C:455:PHE:CE2	2.71	0.44
9:C:81:HIS:CE1	9:C:346:LEU:HD11	2.53	0.44
10:D:30:ARG:CG	10:D:31:GLY:H	2.28	0.44
11:H:102:ARG:HD3	11:H:141:ASP:OD1	2.17	0.44
7:J:1946:U:H2'	7:J:1947:C:H6	1.82	0.44
1:A:43:G:H2'	1:A:44:A:C8	2.52	0.44
2:B:53:G:C5	2:B:54:5MU:H72	2.53	0.44
3:E:167:A:H2'	3:E:168:G:H8	1.82	0.44
5:G:1076:C:H2'	5:G:1077:A:C8	2.53	0.44
5:G:1076:C:H2'	5:G:1077:A:H8	1.82	0.44
11:H:29:GLN:NE2	11:H:29:GLN:HA	2.31	0.44
11:H:12:VAL:HG23	11:H:41:PHE:CE2	2.53	0.44
7:J:1947:C:H2'	7:J:1948:G:H8	1.83	0.44
1:A:50:U:C2'	1:A:51:G:H5'	2.48	0.44
11:H:19:PRO:HG2	11:H:22:PRO:HB2	2.00	0.44
11:H:85:ILE:CD1	11:H:137:LEU:HD21	2.46	0.44
2:B:39:C:O2'	2:B:40:C:H5'	2.17	0.44
9:C:211:ARG:HG2	9:C:255:VAL:HG22	2.00	0.44
9:C:262:ILE:HD13	9:C:268:ALA:HB2	2.00	0.44
9:C:46:LEU:CD2	9:C:358:GLU:OE2	2.65	0.44
2:B:41:C:C2	2:B:42:G:C8	3.06	0.44
9:C:417:ASN:HB3	9:C:461:THR:OG1	2.18	0.44
1:A:16:H2U:C2'	1:A:17:H2U:OP2	2.65	0.43
1:A:23:A:H2'	1:A:24:G:C8	2.52	0.43
9:C:409:LEU:O	9:C:466:ALA:HA	2.17	0.43
10:D:55:ARG:HA	10:D:61:GLU:HA	1.99	0.43
5:G:1064:C:C5'	11:H:88:GLY:H	2.31	0.43
8:K:2557:G:H2'	8:K:2558:C:H6	1.83	0.43
9:C:36:MET:HE2	9:C:39:GLN:HG3	2.00	0.43
9:C:86:TYR:CE1	9:C:289:LYS:CD	3.02	0.43
2:B:72:A:H3'	2:B:73:A:H5''	1.99	0.43
9:C:374:VAL:HG22	9:C:399:LEU:HD13	2.01	0.43
9:C:41:LEU:O	9:C:41:LEU:HD23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:426:ARG:NE	9:C:480:MET:HE1	2.30	0.43
10:D:89:LEU:N	10:D:89:LEU:HD22	2.33	0.43
11:H:79:LEU:HD23	11:H:108:ILE:CD1	2.48	0.43
1:A:75:C:C1'	7:J:1944:U:OP1	2.64	0.43
1:A:32:OMC:H6	1:A:32:OMC:O5'	2.01	0.43
9:C:516:LYS:HE3	9:C:540:SER:OG	2.18	0.43
10:D:116:TYR:HB2	10:D:117:GLY:H	1.62	0.43
1:A:68:U:O2'	9:C:539:ARG:HB2	2.17	0.43
1:A:73:A:N3	1:A:73:A:C5'	2.72	0.43
1:A:71:G:OP1	9:C:543:LYS:CE	2.61	0.43
10:D:13:ARG:HH11	10:D:13:ARG:HG2	1.82	0.43
10:D:105:GLY:HA3	10:D:117:GLY:HA3	2.01	0.43
10:D:115:LYS:N	10:D:115:LYS:HD2	2.34	0.43
10:D:58:ASN:ND2	10:D:58:ASN:N	2.61	0.43
9:C:81:HIS:NE2	9:C:459:LYS:HE2	2.34	0.43
10:D:49:ARG:HG2	10:D:49:ARG:NH1	2.33	0.43
11:H:14:ALA:HA	11:H:45:THR:HG21	2.01	0.43
11:H:63:ASP:C	11:H:65:SER:H	2.21	0.43
9:C:226:MET:HG3	9:C:273:THR:O	2.18	0.43
1:A:33:U:O2'	1:A:35:A:C8	2.63	0.43
10:D:8:ARG:HG3	10:D:9:LYS:N	2.33	0.43
7:J:1957:C:H2'	7:J:1958:C:C6	2.54	0.43
1:A:75:C:C5	7:J:1955:U:N1	2.85	0.42
2:B:72:A:H3'	2:B:73:A:C5'	2.49	0.42
10:D:71:HIS:HA	10:D:98:ARG:NH2	2.34	0.42
11:H:102:ARG:HB2	11:H:141:ASP:CG	2.40	0.42
11:H:14:ALA:CB	11:H:50:LYS:HA	2.50	0.42
11:H:49:GLU:HG3	11:H:54:ILE:HD11	2.01	0.42
11:H:63:ASP:O	11:H:65:SER:N	2.51	0.42
9:C:225:VAL:HB	9:C:228:THR:CG2	2.49	0.42
9:C:329:GLU:O	10:D:76:HIS:NE2	2.52	0.42
5:G:1064:C:O2'	5:G:1065:U:H5'	2.19	0.42
11:H:63:ASP:C	11:H:65:SER:N	2.73	0.42
9:C:110:ALA:HA	9:C:113:LEU:HD12	2.00	0.42
9:C:370:VAL:HG21	9:C:447:MET:HG2	2.01	0.42
9:C:371:VAL:O	9:C:402:PRO:HD3	2.19	0.42
9:C:81:HIS:NE2	9:C:459:LYS:CE	2.83	0.42
1:A:69:U:C5'	9:C:539:ARG:HB3	2.45	0.42
10:D:74:GLN:HB3	10:D:75:GLU:H	1.65	0.42
9:C:433:VAL:CA	11:H:25:PRO:HG3	2.48	0.42
11:H:5:GLN:HG2	11:H:6:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:C:H2'	2:B:72:A:H8	1.84	0.42
9:C:367:ALA:HB1	9:C:452:LEU:HD12	1.03	0.42
10:D:111:GLN:HB2	10:D:111:GLN:HE21	1.54	0.42
11:H:56:VAL:HG13	11:H:58:ILE:HD11	2.00	0.42
8:K:2553:G:H2'	8:K:2554:U:H4'	2.01	0.42
9:C:241:THR:H	9:C:242:PRO:CA	2.33	0.42
10:D:29:LYS:O	10:D:80:LEU:HD12	2.19	0.42
5:G:1059:G:H2'	5:G:1060:U:C6	2.54	0.42
5:G:1107:G:O2'	5:G:1108:U:H5'	2.20	0.42
1:A:37:YG:H32	1:A:38:A:O4'	2.20	0.42
9:C:369:THR:HA	9:C:452:LEU:HD23	1.81	0.42
9:C:401:GLU:OE1	9:C:478:SER:HA	2.20	0.42
9:C:488:ASN:OD1	9:C:526:ILE:HG23	2.19	0.42
3:E:162:A:H2'	3:E:163:C:O4'	2.18	0.42
5:G:1060:U:C1'	5:G:1062:G:H5'	2.49	0.42
11:H:116:MET:HE1	11:H:124:MET:O	2.20	0.42
11:H:52:LEU:O	11:H:54:ILE:HG13	2.20	0.42
9:C:18:SER:N	9:C:20:LEU:N	2.67	0.42
9:C:457:ARG:HH11	9:C:457:ARG:HG2	1.85	0.42
9:C:491:ARG:HH11	9:C:491:ARG:HD2	1.67	0.42
10:D:49:ARG:HG2	10:D:49:ARG:HH11	1.83	0.42
5:G:1062:G:H2'	5:G:1063:G:H8	1.84	0.42
11:H:83:ALA:N	11:H:100:ILE:HD11	2.35	0.42
11:H:109:ALA:HB1	11:H:124:MET:CG	2.49	0.42
11:H:27:LEU:HB2	11:H:32:VAL:HG21	2.01	0.42
7:J:1957:C:H2'	7:J:1958:C:H6	1.84	0.42
9:C:103:ASP:HB3	9:C:106:GLN:HB2	2.01	0.42
9:C:296:TYR:O	9:C:451:VAL:CG1	2.64	0.42
5:G:1049:C:O2'	5:G:1050:A:H5'	2.20	0.42
11:H:35:MET:SD	11:H:35:MET:C	2.98	0.42
9:C:384:VAL:HG21	9:C:390:LEU:HD12	2.02	0.42
9:C:434:TYR:H	11:H:25:PRO:CB	2.31	0.42
9:C:86:TYR:CE1	9:C:289:LYS:HD2	2.55	0.42
9:C:9:ILE:HG21	9:C:17:LYS:HG3	2.01	0.42
11:H:129:GLU:CB	11:H:133:ARG:HH12	2.19	0.42
11:H:38:CYS:O	11:H:42:ASN:ND2	2.52	0.42
2:B:61:C:O2'	2:B:62:C:H5'	2.20	0.42
9:C:266:HIS:CE1	9:C:319:LEU:HA	2.54	0.42
9:C:368:PRO:CB	9:C:452:LEU:CA	2.86	0.42
9:C:448:ALA:O	9:C:452:LEU:HD23	2.20	0.42
1:A:69:U:C3'	9:C:541:THR:HG22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:49:ARG:NH2	10:D:88:ASP:OD1	2.53	0.42
9:C:296:TYR:HA	9:C:340:CYS:O	2.20	0.41
10:D:120:ARG:HG2	10:D:121:PRO:HD2	2.02	0.41
3:E:167:A:H2'	3:E:168:G:C8	2.55	0.41
6:I:2659:G:H3'	9:C:463:ARG:HD3	1.71	0.41
6:I:2655:G:N2	6:I:2664:G:H2'	2.35	0.41
9:C:203:TYR:CD2	9:C:204:LEU:HD13	2.56	0.41
9:C:368:PRO:HD2	9:C:452:LEU:HA	2.00	0.41
10:D:62:VAL:HG22	10:D:63:THR:N	2.30	0.41
5:G:1064:C:H5''	11:H:88:GLY:H	1.85	0.41
5:G:1068:G:C6	5:G:1069:A:N6	2.89	0.41
9:C:181:PRO:HA	9:C:182:PRO:HD3	1.93	0.41
10:D:18:SER:C	10:D:20:VAL:N	2.73	0.41
10:D:95:HIS:ND1	10:D:96:THR:N	2.68	0.41
9:C:17:LYS:CA	9:C:20:LEU:H	2.34	0.41
9:C:400:ARG:HB3	9:C:475:PHE:HB3	2.02	0.41
10:D:21:PRO:HG2	10:D:22:ALA:H	1.85	0.41
10:D:34:THR:N	10:D:53:ARG:O	2.53	0.41
11:H:21:PRO:CB	11:H:22:PRO:HD3	2.39	0.41
9:C:519:ILE:HG23	9:C:522:GLN:NE2	2.36	0.41
11:H:7:TYR:CB	11:H:59:THR:HA	2.48	0.41
9:C:26:GLN:HE22	9:C:34:ARG:CG	2.11	0.41
9:C:476:GLN:CG	9:C:477:ALA:H	2.33	0.41
10:D:89:LEU:HB3	10:D:92:VAL:CG2	2.51	0.41
1:A:67:A:O3'	9:C:538:ALA:HB2	2.21	0.41
9:C:241:THR:N	9:C:242:PRO:HA	2.34	0.41
10:D:40:THR:HB	10:D:41:PRO:HD2	2.02	0.41
2:B:19:G:C2	2:B:57:A:N3	2.88	0.41
2:B:75:C:H6	2:B:75:C:H5'	1.86	0.41
11:H:102:ARG:HA	11:H:105:LEU:HD12	2.02	0.41
1:A:25:C:C4	1:A:26:M2G:C5	3.09	0.41
1:A:52:U:O2'	1:A:53:G:H5'	2.20	0.41
1:A:5:A:H2'	1:A:6:U:O4'	2.21	0.41
9:C:486:LEU:HD23	9:C:486:LEU:N	2.36	0.41
2:B:52:G:C2	2:B:53:G:C8	3.09	0.41
10:D:9:LYS:HE3	10:D:9:LYS:HB2	1.85	0.41
11:H:91:LYS:HG3	11:H:91:LYS:O	2.21	0.41
9:C:6:ASN:ND2	9:C:211:ARG:NH2	2.67	0.40
5:G:1057:A:H62	5:G:1086:A:H2'	1.85	0.40
9:C:221:ASP:HB3	9:C:276:LEU:CD2	2.51	0.40
9:C:296:TYR:CB	9:C:451:VAL:HG11	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PSU:N1	1:A:40:5MC:HM52	2.36	0.40
1:A:72:C:C6	1:A:72:C:C3'	3.05	0.40
9:C:331:SER:HB2	9:C:334:LEU:HB2	2.02	0.40
10:D:41:PRO:CB	10:D:88:ASP:HB3	2.51	0.40
2:B:41:C:O2'	2:B:42:G:H5'	2.21	0.40
9:C:369:THR:O	9:C:451:VAL:HG11	2.21	0.40
11:H:78:LEU:HD13	11:H:108:ILE:HG23	2.03	0.40
11:H:32:VAL:HG22	11:H:60:VAL:CG2	2.51	0.40
11:H:73:PRO:HB2	11:H:74:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	543/545 (100%)	507 (93%)	31 (6%)	5 (1%)	20	63
10	D	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1	15
11	H	139/141 (99%)	115 (83%)	16 (12%)	8 (6%)	2	24
All	All	803/809 (99%)	702 (87%)	77 (10%)	24 (3%)	9	37

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	488	ASN
10	D	42	LYS
11	H	18	ASN
9	C	291	VAL
9	C	293	PRO
10	D	84	GLY
10	D	92	VAL
11	H	14	ALA

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Mol	Chain	Res	Type
11	H	64	ARG
11	H	73	PRO
11	H	76	ALA
10	D	19	ASN
10	D	47	ALA
11	H	23	VAL
10	D	122	LYS
11	H	74	PRO
9	C	453	ASP
10	D	43	LYS
10	D	120	ARG
10	D	121	PRO
11	H	49	GLU
9	C	241	THR
10	D	15	VAL
10	D	101	LEU

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	
9	C	465/465 (100%)	407 (88%)	58 (12%)	5	26
10	D	103/103 (100%)	83 (81%)	20 (19%)	1	10
11	H	109/109 (100%)	106 (97%)	3 (3%)	49	74
All	All	677/677 (100%)	596 (88%)	81 (12%)	10	27

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	C	13	ILE
9	C	14	ASP
9	C	31	LEU
9	C	32	SER
9	C	34	ARG
9	C	49	GLU

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Mol	Chain	Res	Type
9	C	50	ARG
9	C	53	THR
9	C	54	ILE
9	C	58	SER
9	C	75	PHE
9	C	109	GLU
9	C	123	ASP
9	C	153	ILE
9	C	160	ARG
9	C	188	GLU
9	C	191	LEU
9	C	204	LEU
9	C	214	ASN
9	C	230	GLN
9	C	246	ASP
9	C	248	THR
9	C	273	THR
9	C	291	VAL
9	C	292	LYS
9	C	294	GLN
9	C	317	LEU
9	C	318	SER
9	C	323	SER
9	C	327	GLU
9	C	332	SER
9	C	346	LEU
9	C	355	LEU
9	C	366	THR
9	C	401	GLU
9	C	410	LEU
9	C	415	LEU
9	C	419	ILE
9	C	421	LEU
9	C	437	ASN
9	C	442	THR
9	C	449	GLU
9	C	454	PHE
9	C	458	LEU
9	C	459	LYS
9	C	468	LEU
9	C	482	ARG
9	C	486	LEU

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Mol	Chain	Res	Type
9	C	487	ILE
9	C	491	ARG
9	C	495	LEU
9	C	506	ASN
9	C	507	ARG
9	C	511	LEU
9	C	516	LYS
9	C	540	SER
9	C	541	THR
9	C	545	LEU
10	D	5	GLN
10	D	9	LYS
10	D	23	LEU
10	D	28	GLN
10	D	33	CYS
10	D	35	ARG
10	D	37	TYR
10	D	48	LEU
10	D	49	ARG
10	D	50	LYS
10	D	55	ARG
10	D	58	ASN
10	D	60	PHE
10	D	72	ASN
10	D	74	GLN
10	D	82	ARG
10	D	111	GLN
10	D	115	LYS
10	D	118	VAL
10	D	119	LYS
11	H	7	TYR
11	H	73	PRO
11	H	96	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
9	C	6	ASN
9	C	26	GLN
9	C	81	HIS
9	C	131	ASN
9	C	320	ASN

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Mol	Chain	Res	Type
9	C	347	HIS
9	C	395	ASN
9	C	505	GLN
9	C	523	GLN
10	D	28	GLN
10	D	58	ASN
10	D	72	ASN
10	D	74	GLN
10	D	111	GLN
11	H	29	GLN
11	H	33	ASN
11	H	93	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	74/76 (97%)	16 (21%)	0
2	B	76/77 (98%)	18 (23%)	0
3	E	15/16 (93%)	1 (6%)	0
4	F	11/12 (91%)	1 (9%)	0
5	G	69/70 (98%)	9 (13%)	0
6	I	28/29 (96%)	0	0
7	J	17/18 (94%)	1 (5%)	0
8	K	14/15 (93%)	1 (7%)	0
All	All	304/313 (97%)	47 (15%)	0

All (47) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C
1	A	3	G
1	A	17	H2U
1	A	18	G
1	A	19	G
1	A	21	A
1	A	26	M2G
1	A	35	A
1	A	36	A
1	A	37	YG
1	A	41	U
1	A	72	C

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Mol	Chain	Res	Type
1	A	73	A
1	A	74	C
1	A	75	C
1	A	76	A
2	B	4	G
2	B	5	G
2	B	8	U
2	B	17	C
2	B	17(A)	U
2	B	18	G
2	B	19	G
2	B	20	U
2	B	21	A
2	B	47	U
2	B	48	C
2	B	49	G
2	B	53	G
2	B	67	C
2	B	71	C
2	B	73	A
2	B	75	C
2	B	76	A
3	E	155	A
4	F	345	C
5	G	1045	C
5	G	1046	A
5	G	1047	G
5	G	1056	G
5	G	1062	G
5	G	1070	A
5	G	1088	A
5	G	1090	A
5	G	1112	G
7	J	1955	U
8	K	2554	U

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	A	10	1	19,26,27	1.05	1 (5%)	20,38,41	2.52	4 (20%)
1	H2U	A	16	1	17,21,22	0.78	1 (5%)	21,30,33	1.16	2 (9%)
1	H2U	A	17	1	17,21,22	0.75	0	21,30,33	1.03	2 (9%)
1	M2G	A	26	1	20,27,28	1.22	3 (15%)	21,40,43	2.67	4 (19%)
1	OMC	A	32	1	15,22,23	0.87	0	19,31,34	0.61	0
1	OMG	A	34	1	18,26,27	1.32	2 (11%)	22,38,41	2.56	4 (18%)
1	YG	A	37	1	29,42,43	1.05	2 (6%)	29,62,65	2.23	8 (27%)
1	PSU	A	39	1	16,21,22	1.25	2 (12%)	20,30,33	6.11	4 (20%)
1	5MC	A	40	1	15,22,23	0.98	1 (6%)	17,32,35	1.03	2 (11%)
1	7MG	A	46	1	20,26,27	1.19	2 (10%)	22,39,42	2.12	2 (9%)
1	5MC	A	49	1	15,22,23	0.91	0	17,32,35	1.14	2 (11%)
1	5MU	A	54	1	14,22,23	1.28	2 (14%)	16,32,35	4.39	2 (12%)
1	PSU	A	55	1	16,21,22	1.46	3 (18%)	20,30,33	5.94	6 (30%)
1	1MA	A	58	1	16,25,26	2.74	4 (25%)	13,37,40	1.20	1 (7%)
2	5MU	B	54	2	14,22,23	1.06	2 (14%)	16,32,35	4.20	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	10	1	-	0/5/27/28	0/3/3/3
1	H2U	A	16	1	-	0/7/38/39	0/2/2/2
1	H2U	A	17	1	-	0/7/38/39	0/2/2/2
1	M2G	A	26	1	-	0/7/29/30	0/3/3/3
1	OMC	A	32	1	-	0/5/27/28	0/2/2/2
1	OMG	A	34	1	-	0/5/27/28	0/3/3/3
1	YG	A	37	1	-	0/20/42/43	0/4/4/4
1	PSU	A	39	1	-	0/7/25/26	0/2/2/2
1	5MC	A	40	1	-	0/3/25/26	0/2/2/2
1	7MG	A	46	1	-	0/7/37/38	0/3/3/3
1	5MC	A	49	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	A	54	1	-	0/3/25/26	0/2/2/2
1	PSU	A	55	1	-	0/7/25/26	0/2/2/2
1	1MA	A	58	1	-	0/3/25/26	0/3/3/3
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	PSU	C6-C5	-3.41	1.33	1.38
1	A	55	PSU	C6-C5	-3.07	1.34	1.38
1	A	58	1MA	O5'-C5'	-2.68	1.41	1.44
1	A	54	5MU	O5'-C5'	-2.66	1.41	1.44
1	A	40	5MC	C6-C5	-2.21	1.34	1.40
1	A	26	M2G	C8-N7	-2.18	1.30	1.34
2	B	54	5MU	C6-C5	-2.15	1.34	1.40
1	A	55	PSU	O4'-C1'	-2.14	1.41	1.44
1	A	37	YG	C6-C5	2.00	1.44	1.41
1	A	34	OMG	C2-N1	2.05	1.39	1.35
1	A	26	M2G	C2-N1	2.15	1.38	1.34
1	A	46	7MG	CM7-N7	2.29	1.49	1.46
1	A	16	H2U	C2-N1	2.56	1.39	1.35
1	A	37	YG	C6-N1	2.85	1.42	1.37
1	A	39	PSU	C4-N3	2.95	1.38	1.33
2	B	54	5MU	C4-N3	3.00	1.38	1.33
1	A	46	7MG	C6-N1	3.17	1.38	1.33
1	A	54	5MU	C4-N3	3.24	1.38	1.33
1	A	58	1MA	C6-C5	3.39	1.47	1.41
1	A	26	M2G	C6-N1	3.46	1.39	1.33
1	A	10	2MG	C6-N1	3.65	1.39	1.33
1	A	58	1MA	C2-N3	4.01	1.37	1.30
1	A	55	PSU	C4-N3	4.14	1.40	1.33
1	A	34	OMG	C6-N1	4.15	1.40	1.33
1	A	58	1MA	C6-N6	8.76	1.48	1.27

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	PSU	N1-C2-N3	-19.72	114.22	128.40
1	A	55	PSU	N1-C2-N3	-19.43	114.43	128.40
1	A	39	PSU	C5-C4-N3	-12.86	114.88	125.43
1	A	55	PSU	C5-C4-N3	-12.24	115.39	125.43
1	A	54	5MU	C5-C4-N3	-10.19	114.01	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	-8.93	115.40	125.24
1	A	34	OMG	C5-C6-N1	-8.59	111.25	123.48
1	A	26	M2G	C5-C6-N1	-8.22	111.78	123.48
1	A	10	2MG	C5-C6-N1	-8.17	111.85	123.48
1	A	46	7MG	C5-C6-N1	-7.06	112.30	123.37
1	A	37	YG	C13-C12-C11	-4.14	123.46	130.66
1	A	37	YG	O23-C21-O22	-3.54	119.75	124.60
1	A	58	1MA	C2-N3-C4	-3.06	111.72	116.41
1	A	26	M2G	C2-N3-C4	-3.04	111.64	115.11
1	A	49	5MC	CM5-C5-C4	-3.01	118.56	121.65
1	A	34	OMG	C2-N3-C4	-2.78	111.92	115.16
1	A	10	2MG	C2-N3-C4	-2.77	111.96	115.11
1	A	40	5MC	CM5-C5-C4	-2.68	118.90	121.65
1	A	34	OMG	N3-C2-N1	-2.49	123.82	127.46
1	A	17	H2U	C5-C4-N3	-2.39	114.35	116.72
1	A	55	PSU	C4-C5-C1'	-2.20	116.89	121.15
1	A	55	PSU	O2'-C2'-C1'	-2.19	107.25	112.21
1	A	26	M2G	N3-C2-N2	2.08	119.29	117.15
2	B	54	5MU	C5M-C5-C6	2.13	122.92	118.67
1	A	40	5MC	CM5-C5-C6	2.20	123.07	118.67
1	A	17	H2U	C4-N3-C2	2.24	127.74	125.81
1	A	37	YG	O18-C16-C15	2.29	117.58	111.54
1	A	16	H2U	O3'-C3'-C2'	2.41	119.53	111.83
1	A	49	5MC	CM5-C5-C6	2.48	123.61	118.67
1	A	16	H2U	C4-N3-C2	2.72	128.14	125.81
1	A	37	YG	C19-O18-C16	2.76	122.43	115.97
1	A	37	YG	C3-N3-C2	2.98	122.55	118.31
1	A	10	2MG	N2-C2-N3	3.34	120.20	116.95
1	A	37	YG	O23-C21-N20	4.02	118.53	110.82
1	A	37	YG	C3-N3-C4	5.07	125.53	118.31
1	A	55	PSU	C6-N1-C2	5.21	123.70	115.36
1	A	39	PSU	C6-N1-C2	5.29	123.82	115.36
1	A	10	2MG	C6-N1-C2	5.41	124.86	115.18
1	A	37	YG	C24-O23-C21	5.97	123.05	115.68
1	A	46	7MG	C6-N1-C2	6.01	124.71	116.06
1	A	34	OMG	C6-N1-C2	6.43	125.31	116.06
1	A	26	M2G	C6-N1-C2	7.32	124.90	116.18
1	A	55	PSU	C4-N3-C2	11.30	125.04	115.16
1	A	39	PSU	C4-N3-C2	12.32	125.93	115.16
2	B	54	5MU	C4-N3-C2	13.87	127.29	115.16
1	A	54	5MU	C4-N3-C2	14.00	127.41	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	2MG	1	0
1	A	16	H2U	3	0
1	A	17	H2U	3	0
1	A	26	M2G	13	0
1	A	32	OMC	1	0
1	A	34	OMG	1	0
1	A	37	YG	7	0
1	A	39	PSU	1	0
1	A	40	5MC	3	0
2	B	54	5MU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.