Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:52 pm GMT

PDB ID	:	6I0Y
EMDB ID	:	EMD-0322
Title	:	TnaC-stalled ribosome complex with the titin I27 domain folding close to the ribosomal exit tunnel
Authors	:	Su, T.; Kudva, R.; von Heijne, G.; Beckmann, R.
Deposited on	:	2018-10-26
Resolution	:	3.20 Å(reported)

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

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

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

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

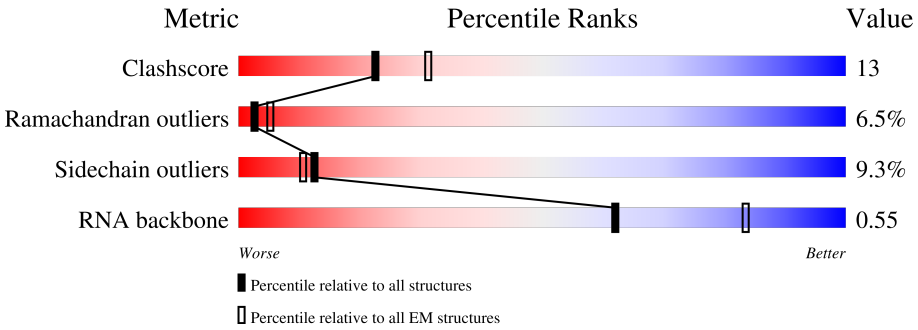
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	h	104	94%
2	0	57	75% 19%
3	1	55	5% 56% 27% 7% 9%
4	2	46	76% 22%
5	3	65	75% 18% 5%
6	4	38	55% 39%
7	5	165	50% 25% 38% 18% 8% 10%

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Mol	Chain	Length	Quality of chain
8	6	121	25% 17% 6% 75%
9	7	24	25% 38% 33%
10	8	94	80% 18%
11	A	2903	57% 31% 9%
12	B	118	68% 25% 8%
13	C	273	69% 26%
14	D	209	66% 28% 5%
15	E	201	70% 24%
16	F	177	43% 67% 29%
17	G	176	65% 27% 7%
18	H	50	10% 58% 36% 6%
19	I	141	61% 51% 43% 6%
20	J	142	59% 29% 11%
21	K	122	55% 35% 8%
22	L	143	71% 23%
23	M	136	63% 29% 7%
24	N	120	66% 31%
25	O	116	68% 28%
26	P	114	66% 25% 8%
27	Q	117	63% 31% 5%
28	R	103	63% 34%
29	S	110	65% 23% 10%
30	T	93	59% 34% 6%
31	V	77	51% 35% 14%
32	W	79	34% 43% 20%

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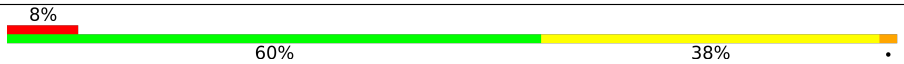
Mol	Chain	Length	Quality of chain
33	X	77	
34	Y	63	
35	Z	58	
36	z	89	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 93619 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 protein called 50S ribosomal protein L24.

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

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0	56	444	269	94	80	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	1	50	409	263	75	71	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	46	377	228	90	57	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	3	64	504	323	105	74	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	4	38	302	185	65	48	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 9 is a protein called Tryptophanase operon leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	7	16	Total	C	N	O	0	0
			139	89	26	24		

- Molecule 10 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	8	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 12 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 13 is a protein called 50S ribosomal protein L2.

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

- Molecule 14 is a protein called 50S ribosomal protein L3.

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

- Molecule 15 is a protein called 50S ribosomal protein L4.

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

- Molecule 16 is a protein called 50S ribosomal protein L5.

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

- Molecule 17 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 19 is a protein called 50S ribosomal protein L11.

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

- Molecule 20 is a protein called 50S ribosomal protein L13.

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

- Molecule 21 is a protein called 50S ribosomal protein L14.

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

- Molecule 22 is a protein called 50S ribosomal protein L15.

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

- Molecule 23 is a protein called 50S ribosomal protein L16.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

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

- Molecule 25 is a protein called 50S ribosomal protein L18.

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

- Molecule 26 is a protein called 50S ribosomal protein L19.

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

- Molecule 27 is a protein called 50S ribosomal protein L20.

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

- Molecule 28 is a protein called 50S ribosomal protein L21.

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

- Molecule 29 is a protein called 50S ribosomal protein L22.

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

- Molecule 30 is a protein called 50S ribosomal protein L23.

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

- Molecule 31 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 33 is a protein called 50S ribosomal protein L28.

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

- Molecule 34 is a protein called 50S ribosomal protein L29.

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

- Molecule 35 is a protein called 50S ribosomal protein L30.

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

- Molecule 36 is a protein called Titin.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	89	Total	C	N	O	S	0	0
			688	439	113	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	3	GLU	LYS	conflict	UNP Q8WZ42

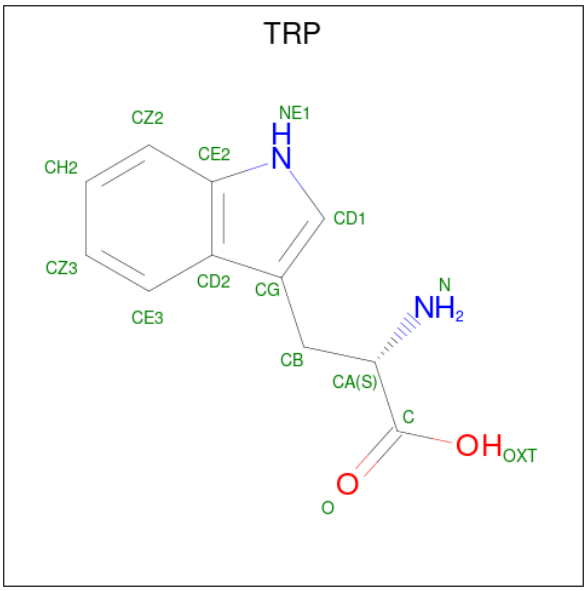
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	Mg	0
			1	1	
37	A	136	Total	Mg	0
			136	136	
37	B	4	Total	Mg	0
			4	4	
37	C	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	4	1	Total	Zn	0
			1	1	

- Molecule 39 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
39	A	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 40 is water.

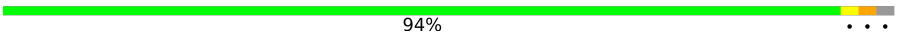
Mol	Chain	Residues	Atoms		AltConf
40	4	1	Total	O	0
			1	1	
40	A	415	Total	O	0
			415	415	
40	B	14	Total	O	0
			14	14	
40	C	2	Total	O	0
			2	2	
40	D	3	Total	O	0
			3	3	
40	E	1	Total	O	0
			1	1	
40	L	3	Total	O	0
			3	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

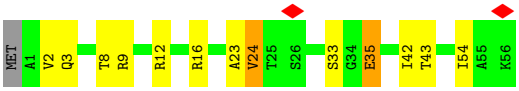
• Molecule 1: 50S ribosomal protein L24

Chain h:



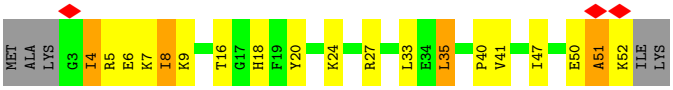
• Molecule 2: 50S ribosomal protein L32

Chain 0:



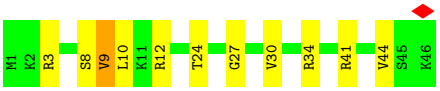
• Molecule 3: 50S ribosomal protein L33

Chain 1:



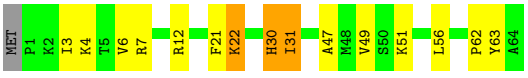
• Molecule 4: 50S ribosomal protein L34

Chain 2:



• Molecule 5: 50S ribosomal protein L35

Chain 3:

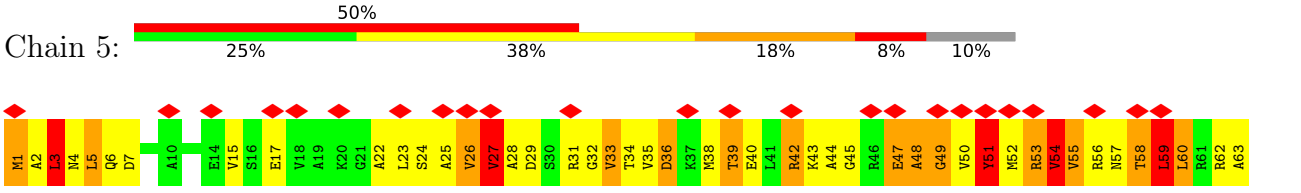


• Molecule 6: 50S ribosomal protein L36

Chain 4:

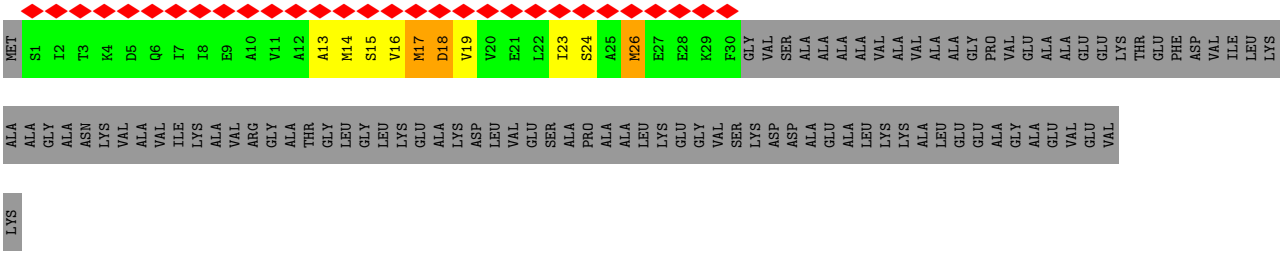
• Molecule 7: 50S ribosomal protein L10

Chain 5:



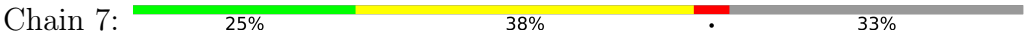
• Molecule 8: 50S ribosomal protein L7/L12

Chain 6:



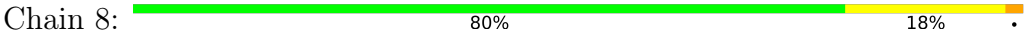
• Molecule 9: Tryptophanase operon leader peptide

Chain 7:



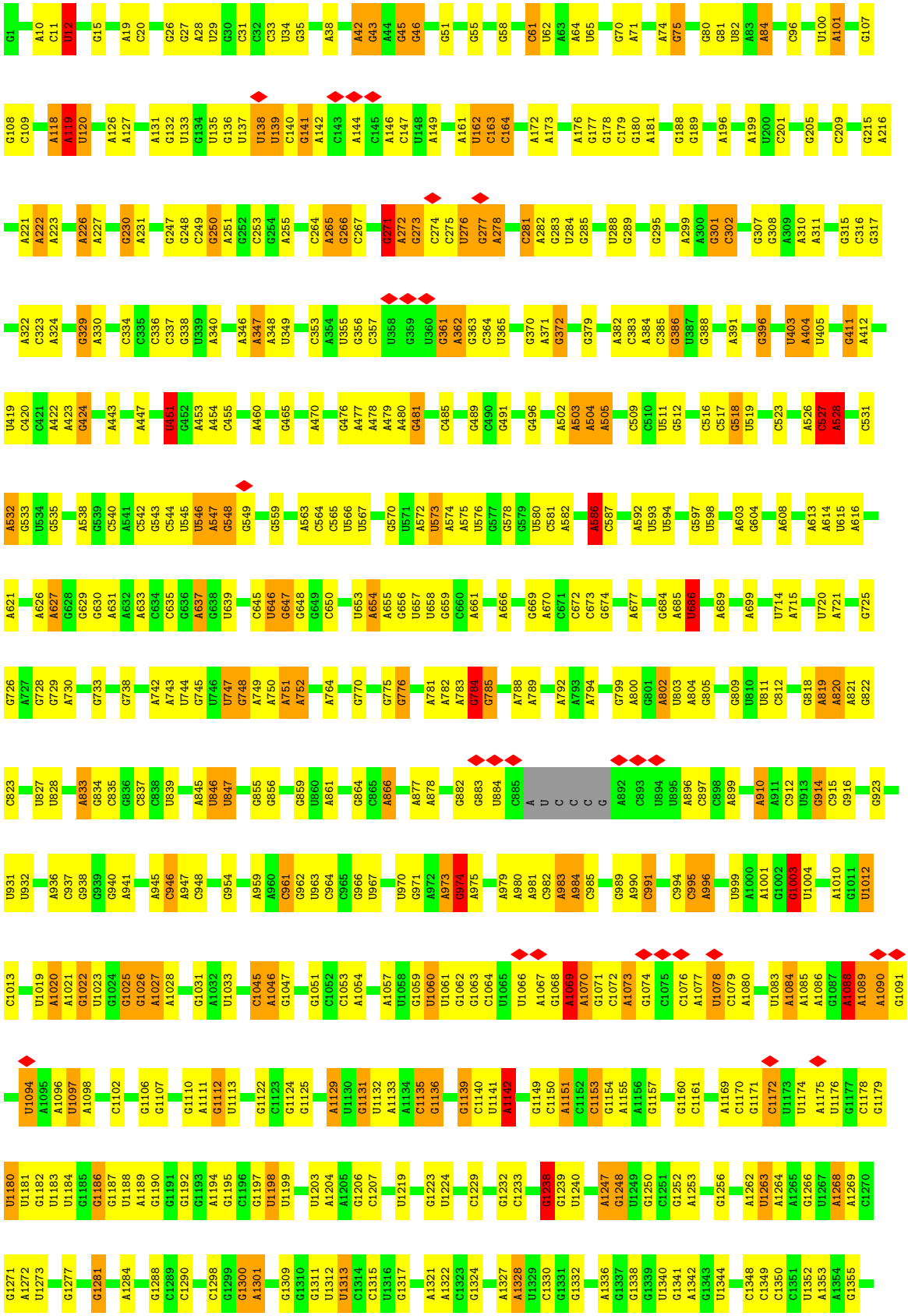
• Molecule 10: 50S ribosomal protein L25

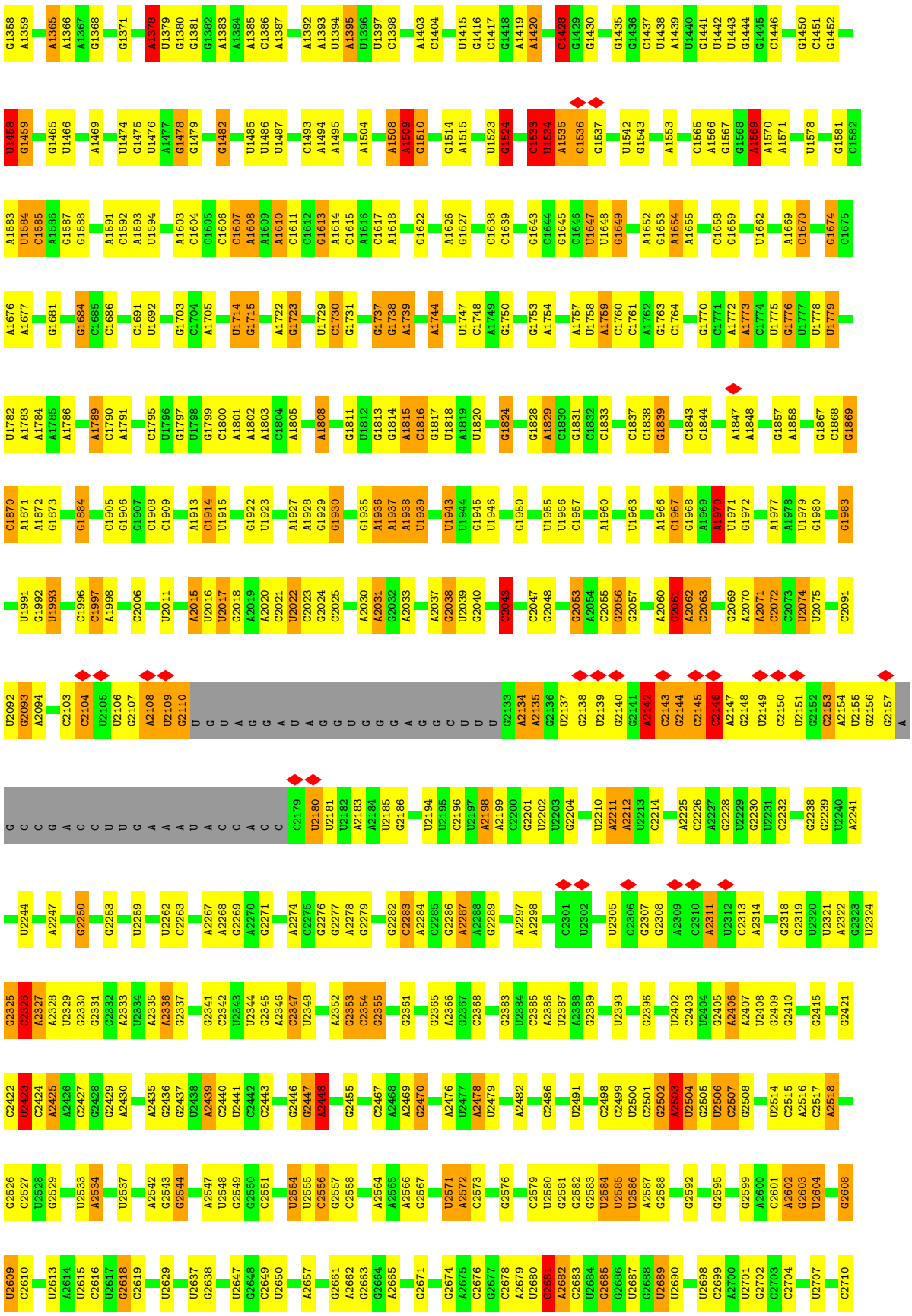
Chain 8:

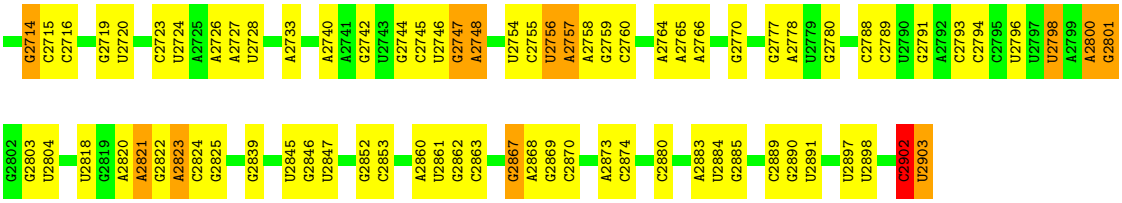


• Molecule 11: 23S ribosomal RNA

Chain A:

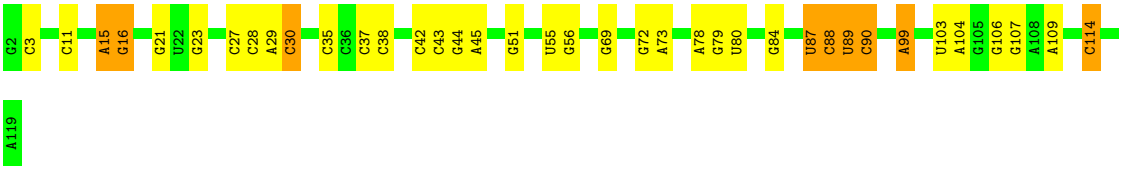






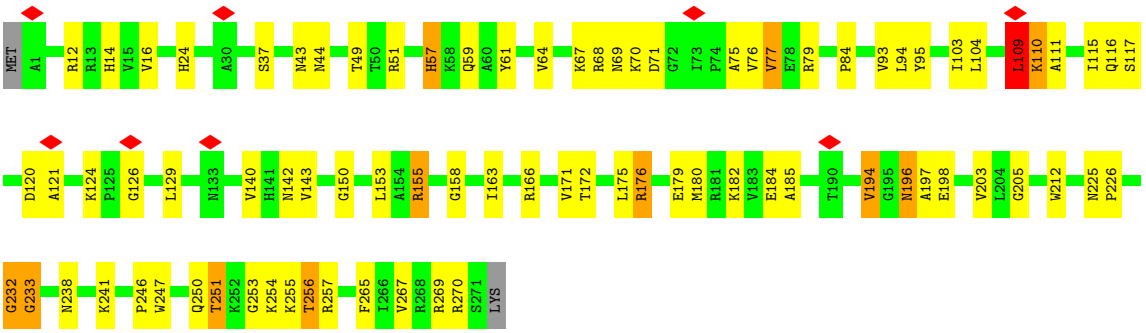
• Molecule 12: 5S ribosomal RNA

Chain B:



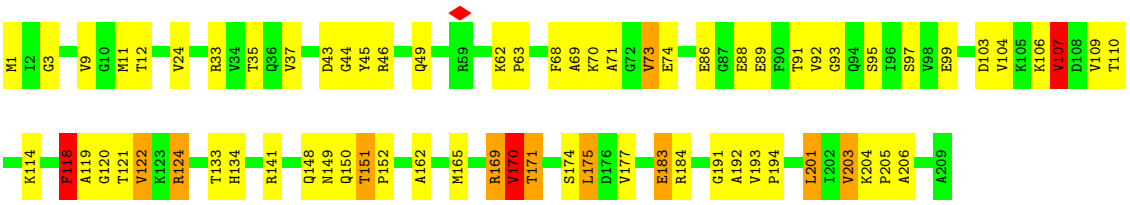
• Molecule 13: 50S ribosomal protein L2

Chain C:



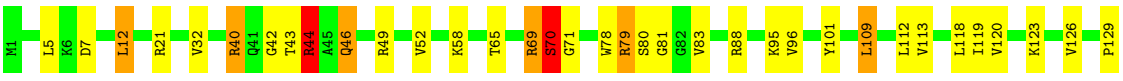
• Molecule 14: 50S ribosomal protein L3

Chain D:

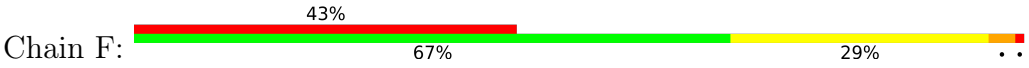


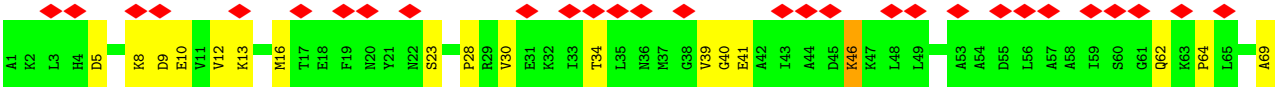
• Molecule 15: 50S ribosomal protein L4

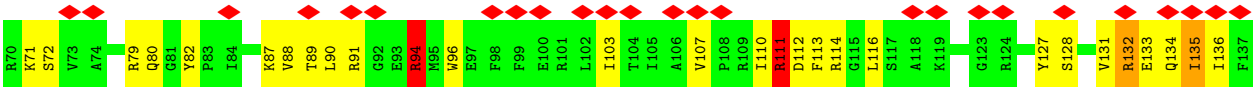
Chain E:

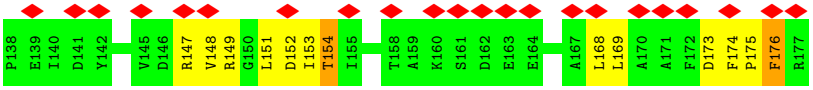


• Molecule 16: 50S ribosomal protein L5

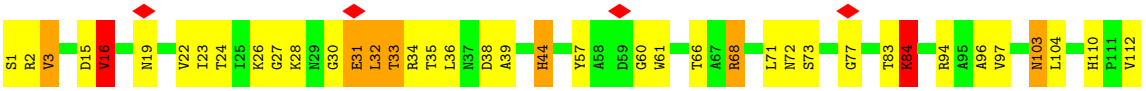


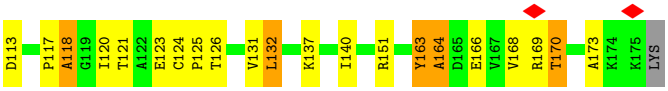




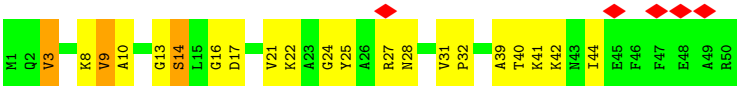


• Molecule 17: 50S ribosomal protein L6

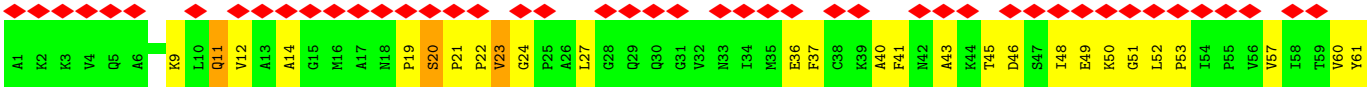


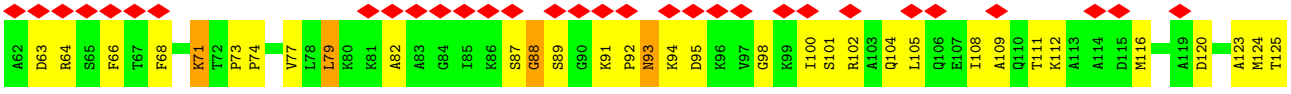


• Molecule 18: 50S ribosomal protein L9



• Molecule 19: 50S ribosomal protein L11



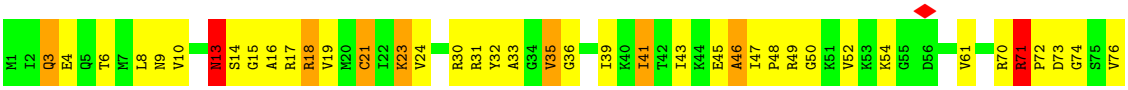


• Molecule 20: 50S ribosomal protein L13

Chain J:

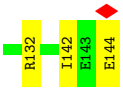
• Molecule 21: 50S ribosomal protein L14

Chain K:



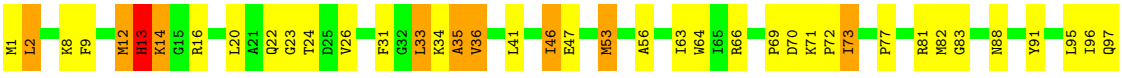
• Molecule 22: 50S ribosomal protein L15

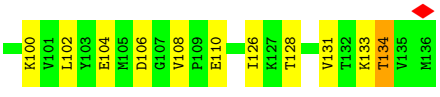
Chain L:



• Molecule 23: 50S ribosomal protein L16

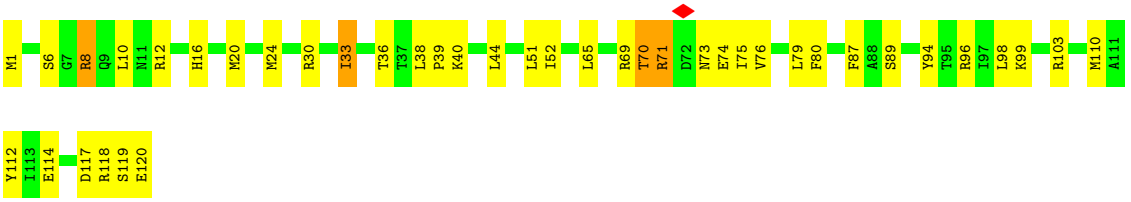
Chain M:





• Molecule 24: 50S ribosomal protein L17

Chain N:



• Molecule 25: 50S ribosomal protein L18

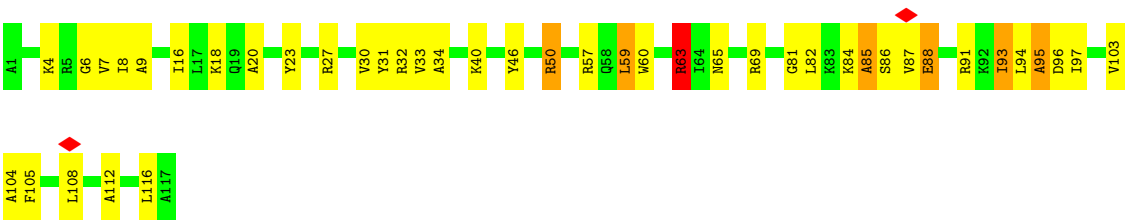
Chain O:

• Molecule 26: 50S ribosomal protein L19

Chain P:

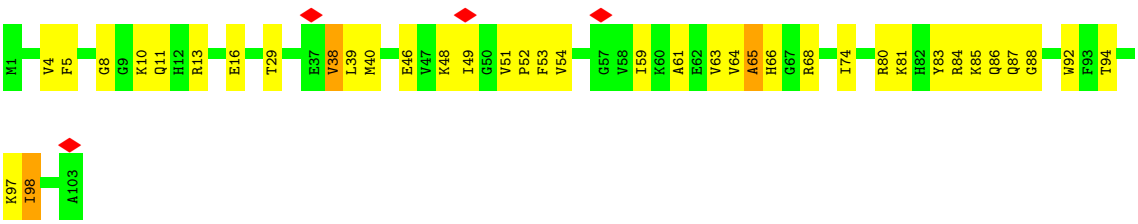
• Molecule 27: 50S ribosomal protein L20

Chain Q:



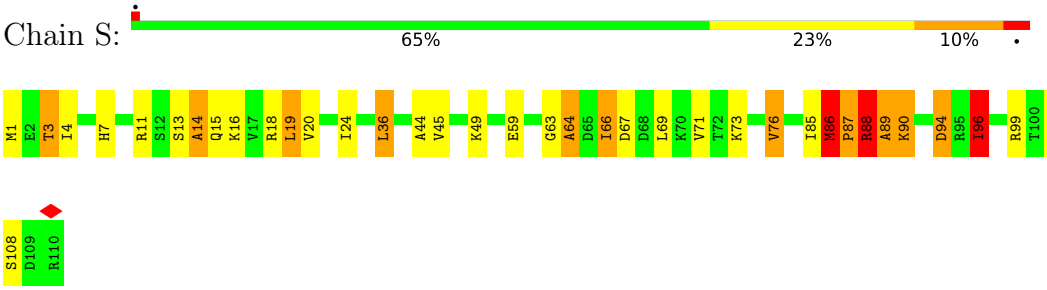
• Molecule 28: 50S ribosomal protein L21

Chain R:



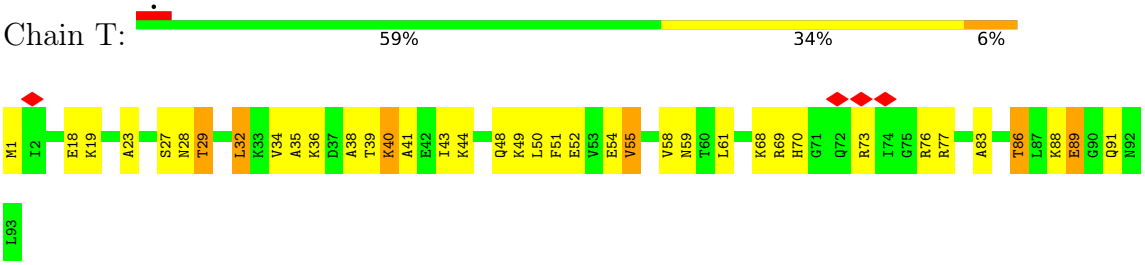
• Molecule 29: 50S ribosomal protein L22

Chain S:



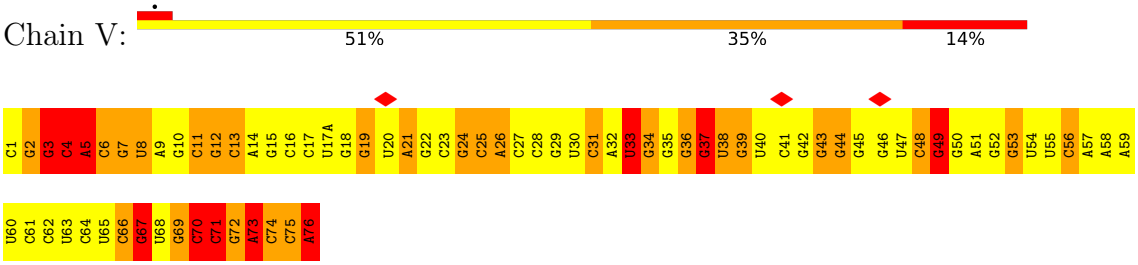
• Molecule 30: 50S ribosomal protein L23

Chain T:



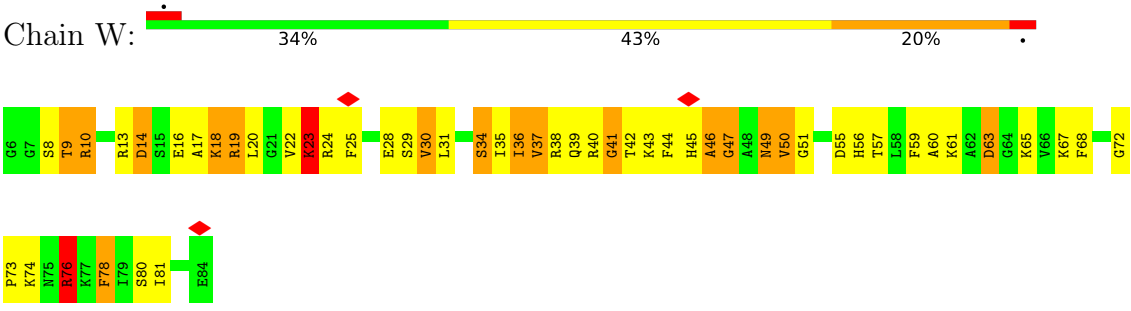
• Molecule 31: Proline tRNA

Chain V:



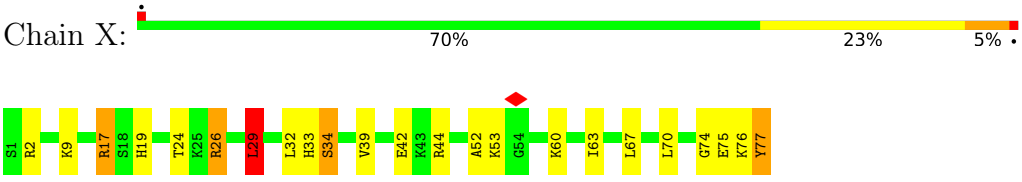
• Molecule 32: 50S ribosomal protein L27

Chain W:



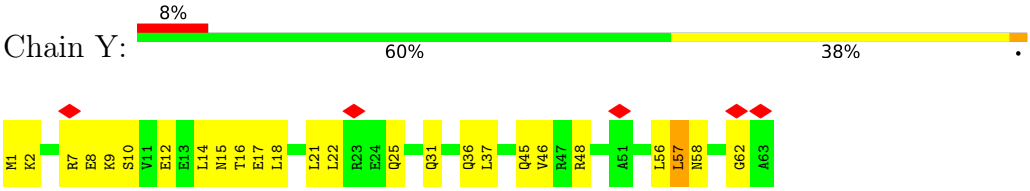
• Molecule 33: 50S ribosomal protein L28

Chain X:



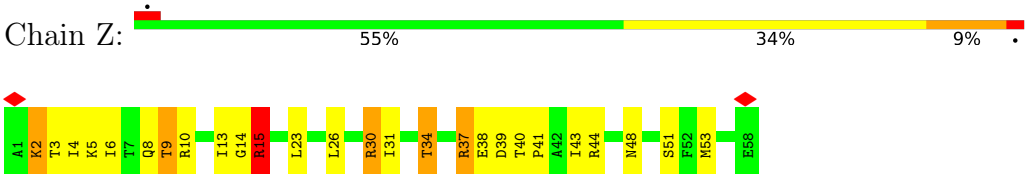
• Molecule 34: 50S ribosomal protein L29

Chain Y:



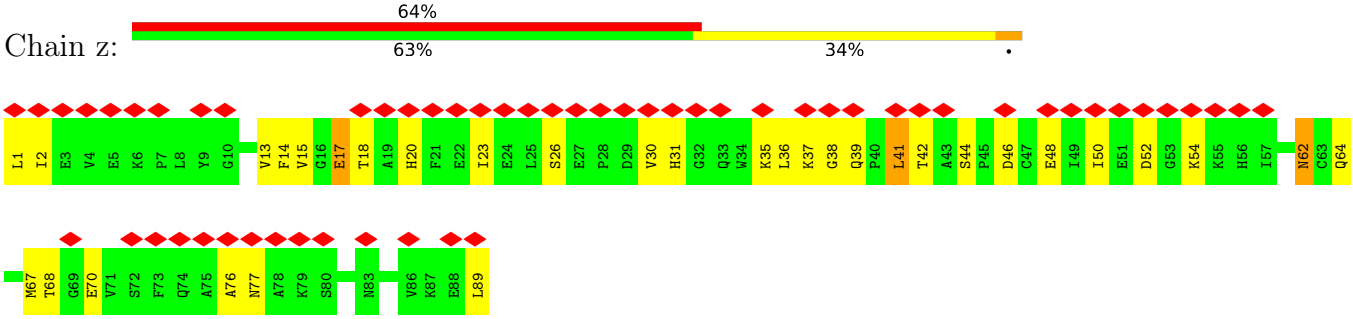
• Molecule 35: 50S ribosomal protein L30

Chain Z:



• Molecule 36: Titin

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.926	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.240	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	394.31998, 394.31998, 394.31998	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	h	0.73	1/787 (0.1%)	0.89	1/1051 (0.1%)
2	0	0.54	0/450	0.70	0/599
3	1	0.53	0/416	0.75	0/554
4	2	0.53	0/380	0.70	0/498
5	3	0.53	0/513	0.75	0/676
6	4	0.59	0/303	0.84	0/397
7	5	0.74	0/1131	1.32	26/1524 (1.7%)
8	6	0.58	0/227	0.65	0/304
9	7	0.52	0/143	0.91	1/193 (0.5%)
10	8	0.48	0/766	0.67	1/1025 (0.1%)
11	A	0.81	19/68626 (0.0%)	1.23	309/107056 (0.3%)
12	B	0.67	0/2828	1.10	3/4410 (0.1%)
13	C	0.54	0/2121	0.80	3/2852 (0.1%)
14	D	0.58	0/1586	0.77	1/2134 (0.0%)
15	E	0.53	0/1571	0.76	2/2113 (0.1%)
16	F	0.50	0/1434	0.71	1/1926 (0.1%)
17	G	0.56	0/1333	0.74	0/1805
18	H	0.53	0/389	0.73	0/523
19	I	0.62	0/1046	0.84	1/1410 (0.1%)
20	J	0.63	1/1152 (0.1%)	0.78	0/1551
21	K	0.65	1/947 (0.1%)	0.77	0/1268
22	L	0.56	0/1054	0.79	2/1403 (0.1%)
23	M	0.61	0/1093	0.77	0/1460
24	N	0.51	0/973	0.69	0/1301
25	O	0.46	0/902	0.70	0/1209
26	P	0.53	0/929	0.78	1/1242 (0.1%)
27	Q	0.62	0/960	0.71	1/1278 (0.1%)
28	R	0.61	1/829 (0.1%)	0.76	0/1107
29	S	0.84	2/864 (0.2%)	1.31	6/1156 (0.5%)
30	T	0.55	0/744	0.85	0/994
31	V	2.38	77/1842 (4.2%)	2.83	255/2870 (8.9%)
32	W	0.69	0/603	1.00	1/797 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	X	0.50	0/635	0.79	1/848 (0.1%)
34	Y	0.46	0/510	0.75	0/677
35	Z	0.54	0/453	0.84	1/605 (0.2%)
36	z	1.05	0/701	1.24	0/946
All	All	0.81	102/101241 (0.1%)	1.19	617/151762 (0.4%)

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
7	5	0	1
13	C	0	1
14	D	0	1
20	J	0	1
21	K	0	1
29	S	0	3
31	V	0	13
All	All	0	21

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	39	G	N9-C4	15.37	1.50	1.38
31	V	69	G	C6-N1	13.06	1.48	1.39
31	V	5	A	C6-N1	12.86	1.44	1.35
31	V	39	G	C2-N3	12.30	1.42	1.32
31	V	39	G	N1-C2	11.24	1.46	1.37
31	V	5	A	C6-N6	10.60	1.42	1.33
31	V	67	G	N9-C4	10.50	1.46	1.38
1	h	68	SER	CB-OG	10.21	1.55	1.42
11	A	2602	A	O3'-P	-10.07	1.49	1.61
31	V	37	G	C2-N3	10.01	1.40	1.32
31	V	67	G	N7-C5	9.99	1.45	1.39
31	V	70	C	N1-C6	9.70	1.43	1.37
31	V	5	A	N7-C5	-9.64	1.33	1.39
31	V	73	A	N7-C5	-9.53	1.33	1.39
31	V	1	C	C2-N3	9.35	1.43	1.35
31	V	69	G	N1-C2	8.79	1.44	1.37
31	V	75	C	N1-C6	8.63	1.42	1.37
31	V	7	G	C8-N7	-8.59	1.25	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	984	A	N9-C4	-8.41	1.32	1.37
31	V	38	U	C2'-C1'	-8.27	1.44	1.53
31	V	32	A	N9-C8	8.13	1.44	1.37
31	V	4	C	C2-N3	8.11	1.42	1.35
31	V	2	G	C8-N7	-8.08	1.26	1.30
31	V	70	C	P-O5'	-7.89	1.51	1.59
31	V	73	A	C5'-C4'	7.83	1.60	1.51
31	V	76	A	C5-C4	-7.76	1.33	1.38
31	V	72	G	C2'-C1'	-7.72	1.44	1.53
31	V	6	C	C4-C5	-7.69	1.36	1.43
31	V	3	G	O3'-P	-7.64	1.51	1.61
31	V	72	G	C2-N2	7.55	1.42	1.34
31	V	3	G	N9-C4	7.51	1.44	1.38
31	V	33	U	C4'-C3'	7.48	1.61	1.53
31	V	32	A	C4'-O4'	-7.23	1.36	1.45
31	V	13	C	C4'-O4'	7.08	1.54	1.45
31	V	75	C	N3-C4	6.94	1.38	1.33
31	V	6	C	C4-N4	6.87	1.40	1.33
31	V	76	A	C6-N6	6.74	1.39	1.33
31	V	37	G	C5-C4	-6.74	1.33	1.38
11	A	528	A	N9-C4	-6.64	1.33	1.37
31	V	3	G	C2'-C1'	-6.60	1.46	1.53
31	V	7	G	N9-C8	6.57	1.42	1.37
31	V	71	C	C4'-O4'	6.52	1.54	1.45
31	V	32	A	O3'-P	-6.49	1.53	1.61
11	A	1142	A	N9-C4	-6.45	1.33	1.37
31	V	38	U	C4'-C3'	-6.38	1.46	1.53
31	V	34	G	C3'-C2'	-6.33	1.45	1.52
31	V	68	U	C4-O4	-6.32	1.18	1.23
31	V	76	A	C6-N1	6.28	1.40	1.35
31	V	5	A	C2-N3	6.20	1.39	1.33
31	V	76	A	C8-N7	-6.17	1.27	1.31
31	V	5	A	C5-C6	6.11	1.46	1.41
11	A	783	A	N9-C4	-6.09	1.34	1.37
11	A	783	A	N3-C4	-6.04	1.31	1.34
11	A	2504	U	C4-O4	6.04	1.28	1.23
31	V	1	C	C2-O2	6.03	1.29	1.24
31	V	2	G	N9-C4	6.00	1.42	1.38
11	A	1569	A	N9-C4	-5.98	1.34	1.37
31	V	32	A	N9-C4	5.94	1.41	1.37
31	V	5	A	N1-C2	-5.94	1.29	1.34
11	A	2504	U	N3-C4	5.86	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1073	A	C5-C6	5.86	1.46	1.41
29	S	88	ARG	CA-C	-5.83	1.37	1.52
31	V	7	G	P-O5'	-5.80	1.53	1.59
31	V	76	A	N9-C4	5.76	1.41	1.37
31	V	70	C	O3'-P	5.75	1.68	1.61
31	V	6	C	C3'-C2'	5.70	1.59	1.52
31	V	1	C	C3'-C2'	-5.69	1.46	1.52
20	J	44	TYR	CD2-CE2	-5.67	1.30	1.39
31	V	76	A	N1-C2	-5.62	1.29	1.34
31	V	2	G	C4'-C3'	-5.62	1.47	1.52
11	A	2504	U	C2-N3	5.61	1.41	1.37
31	V	69	G	C8-N7	-5.61	1.27	1.30
11	A	528	A	N3-C4	-5.58	1.31	1.34
31	V	68	U	C2'-C1'	-5.55	1.47	1.53
31	V	73	A	N3-C4	-5.55	1.31	1.34
11	A	1142	A	C5-C6	-5.53	1.36	1.41
31	V	4	C	C4'-C3'	5.53	1.59	1.53
31	V	32	A	C3'-C2'	5.46	1.58	1.52
31	V	4	C	O4'-C1'	-5.44	1.34	1.41
31	V	69	G	C5-C6	-5.43	1.36	1.42
31	V	38	U	N1-C6	5.43	1.42	1.38
31	V	72	G	O3'-P	-5.43	1.54	1.61
31	V	67	G	P-O5'	-5.41	1.54	1.59
28	R	86	GLN	CB-CG	5.40	1.67	1.52
31	V	36	G	C4'-C3'	-5.39	1.47	1.52
11	A	783	A	N7-C5	-5.37	1.36	1.39
31	V	70	C	O4'-C1'	5.27	1.48	1.41
11	A	2015	A	N3-C4	-5.25	1.31	1.34
31	V	37	G	C2'-C1'	-5.24	1.47	1.53
29	S	86	MET	CA-C	-5.24	1.39	1.52
11	A	783	A	C5-C6	-5.23	1.36	1.41
31	V	67	G	C5-C4	-5.23	1.34	1.38
21	K	21	CYS	CB-SG	-5.16	1.73	1.81
31	V	70	C	C4-C5	-5.13	1.38	1.43
11	A	2053	G	C6-O6	5.12	1.28	1.24
31	V	4	C	C2-O2	5.11	1.29	1.24
31	V	67	G	C6-N1	5.11	1.43	1.39
31	V	68	U	C5-C6	5.09	1.38	1.34
11	A	2478	A	N9-C4	-5.07	1.34	1.37
11	A	1321	A	N9-C4	5.07	1.40	1.37
31	V	73	A	C2-N3	5.07	1.38	1.33
31	V	7	G	C2'-C1'	-5.06	1.47	1.53

All (617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	86	MET	C-N-CD	-30.06	54.47	120.60
31	V	73	A	N1-C6-N6	22.82	132.29	118.60
31	V	69	G	N1-C6-O6	19.95	131.87	119.90
11	A	1073	A	N1-C6-N6	-19.92	106.65	118.60
31	V	69	G	C5-C6-O6	-19.63	116.82	128.60
31	V	73	A	C5-C6-N6	-15.38	111.39	123.70
11	A	2608	G	C4'-C3'-O3'	14.22	141.45	113.00
11	A	1073	A	C5-C6-N6	14.03	134.92	123.70
11	A	2053	G	N1-C6-O6	13.81	128.19	119.90
31	V	2	G	N1-C6-O6	13.60	128.06	119.90
31	V	3	G	C6-C5-N7	-13.53	122.28	130.40
31	V	4	C	N3-C4-N4	13.33	127.33	118.00
31	V	70	C	O4'-C1'-N1	13.14	118.71	108.20
11	A	2504	U	N3-C4-O4	13.12	128.58	119.40
31	V	67	G	N1-C6-O6	13.11	127.77	119.90
31	V	39	G	C8-N9-C4	-12.75	101.30	106.40
31	V	4	C	C5-C4-N4	-12.56	111.41	120.20
31	V	6	C	C6-N1-C2	-12.53	115.29	120.30
31	V	14	A	N1-C6-N6	12.47	126.08	118.60
31	V	21	A	N1-C6-N6	12.43	126.06	118.60
31	V	26	A	N1-C6-N6	12.42	126.05	118.60
31	V	51	A	N1-C6-N6	12.35	126.01	118.60
11	A	984	A	C2-N3-C4	-12.23	104.48	110.60
31	V	5	A	O4'-C1'-N9	12.23	117.98	108.20
31	V	9	A	N1-C6-N6	12.18	125.91	118.60
31	V	57	A	N1-C6-N6	12.12	125.87	118.60
31	V	7	G	N3-C2-N2	11.98	128.28	119.90
31	V	58	A	N1-C6-N6	11.91	125.75	118.60
11	A	961	C	O5'-P-OP2	-11.73	95.14	105.70
11	A	2053	G	C6-C5-N7	-11.59	123.45	130.40
31	V	72	G	P-O3'-C3'	11.47	133.47	119.70
11	A	2053	G	C5-C6-N1	-11.43	105.78	111.50
31	V	32	A	P-O3'-C3'	11.43	133.41	119.70
11	A	1073	A	C6-C5-N7	11.35	140.25	132.30
31	V	59	A	N1-C6-N6	11.35	125.41	118.60
31	V	69	G	O4'-C1'-N9	11.32	117.26	108.20
11	A	751	A	C4'-C3'-O3'	11.24	135.48	113.00
11	A	1073	A	C4-C5-N7	-11.15	105.12	110.70
31	V	5	A	N1-C6-N6	11.14	125.29	118.60
31	V	6	C	C5-C6-N1	11.02	126.51	121.00
31	V	67	G	C5-C6-O6	-10.89	122.06	128.60
11	A	783	A	C5-N7-C8	-10.70	98.55	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2504	U	C5-C6-N1	10.48	127.94	122.70
11	A	974	G	C6-C5-N7	-10.48	124.11	130.40
11	A	2053	G	C4-C5-C6	10.07	124.84	118.80
31	V	37	G	N3-C4-C5	-10.01	123.59	128.60
31	V	33	U	P-O3'-C3'	9.94	131.62	119.70
31	V	4	C	O4'-C1'-N1	9.84	116.07	108.20
11	A	2504	U	C6-N1-C2	-9.78	115.13	121.00
31	V	34	G	P-O5'-C5'	9.78	136.54	120.90
11	A	783	A	N7-C8-N9	9.75	118.67	113.80
31	V	53	G	N1-C6-O6	9.73	125.74	119.90
31	V	7	G	P-O3'-C3'	9.73	131.38	119.70
11	A	974	G	C4-C5-N7	9.67	114.67	110.80
31	V	10	G	N1-C6-O6	9.64	125.68	119.90
7	5	92	ALA	C-N-CA	9.59	145.67	121.70
31	V	32	A	N7-C8-N9	-9.48	109.06	113.80
31	V	65	U	P-O3'-C3'	9.45	131.03	119.70
31	V	22	G	N1-C6-O6	9.41	125.55	119.90
31	V	46	G	N1-C6-O6	9.41	125.55	119.90
11	A	1534	U	C2-N1-C1'	9.38	128.96	117.70
11	A	528	A	C2-N3-C4	-9.37	105.91	110.60
31	V	37	G	C2-N3-C4	9.32	116.56	111.90
29	S	88	ARG	N-CA-C	-9.29	85.93	111.00
31	V	72	G	O4'-C1'-N9	9.24	115.59	108.20
11	A	1073	A	C5-N7-C8	9.19	108.50	103.90
31	V	43	G	N1-C6-O6	9.19	125.42	119.90
31	V	39	G	N3-C4-C5	-9.12	124.04	128.60
31	V	31	C	O4'-C1'-N1	9.11	115.49	108.20
31	V	50	G	N1-C6-O6	9.10	125.36	119.90
31	V	39	G	C6-C5-N7	-9.10	124.94	130.40
7	5	93	ALA	C-N-CA	9.05	144.32	121.70
11	A	1950	G	N1-C6-O6	8.98	125.29	119.90
31	V	42	G	N1-C6-O6	8.89	125.24	119.90
31	V	15	G	N1-C6-O6	8.88	125.22	119.90
31	V	24	G	N1-C6-O6	8.88	125.22	119.90
31	V	74	C	O4'-C1'-N1	8.85	115.28	108.20
31	V	37	G	O4'-C1'-N9	8.79	115.23	108.20
11	A	783	A	C8-N9-C4	-8.77	102.29	105.80
11	A	2061	G	C4'-C3'-O3'	-8.75	91.02	109.40
31	V	29	G	N1-C6-O6	8.75	125.15	119.90
31	V	44	G	N1-C6-O6	8.75	125.15	119.90
11	A	465	G	C8-N9-C4	-8.67	102.93	106.40
31	V	52	G	N1-C6-O6	8.65	125.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1073	A	N9-C4-C5	8.65	109.26	105.80
31	V	39	G	O4'-C1'-N9	8.62	115.10	108.20
31	V	73	A	C5'-C4'-C3'	8.62	129.78	116.00
11	A	2534	A	N1-C6-N6	8.61	123.77	118.60
31	V	45	G	N1-C6-O6	8.61	125.07	119.90
11	A	2074	U	O5'-P-OP2	-8.59	97.97	105.70
31	V	12	G	N1-C6-O6	8.59	125.05	119.90
11	A	2572	A	N1-C6-N6	8.52	123.71	118.60
31	V	2	G	C5-C6-O6	-8.52	123.49	128.60
31	V	18	G	N1-C6-O6	8.51	125.00	119.90
11	A	1533	C	N1-C2-O2	8.48	123.99	118.90
11	A	1533	C	C2-N1-C1'	8.44	128.09	118.80
31	V	19	G	N1-C6-O6	8.44	124.96	119.90
11	A	1936	A	C2-N3-C4	-8.41	106.40	110.60
31	V	3	G	N1-C2-N3	-8.35	118.89	123.90
31	V	34	G	OP1-P-OP2	-8.35	107.08	119.60
11	A	974	G	C4-N9-C1'	8.34	137.34	126.50
11	A	1142	A	C2-N3-C4	-8.30	106.45	110.60
31	V	56	C	O4'-C1'-N1	8.23	114.79	108.20
31	V	39	G	C6-N1-C2	-8.21	120.17	125.10
11	A	1795	C	C6-N1-C2	-8.20	117.02	120.30
7	5	27	VAL	CG1-CB-CG2	8.18	123.99	110.90
31	V	61	C	O4'-C1'-N1	8.13	114.70	108.20
31	V	25	C	O4'-C1'-N1	8.09	114.67	108.20
11	A	586	A	O5'-P-OP1	-8.07	98.44	105.70
31	V	49	G	N1-C6-O6	8.04	124.72	119.90
31	V	39	G	C4-C5-C6	8.02	123.61	118.80
14	D	151	THR	C-N-CD	8.02	145.24	128.40
31	V	65	U	O4'-C1'-N1	7.99	114.59	108.20
31	V	11	C	O4'-C1'-N1	7.99	114.59	108.20
31	V	62	C	O4'-C1'-N1	7.96	114.57	108.20
31	V	53	G	C5-C6-O6	-7.94	123.83	128.60
31	V	23	C	O4'-C1'-N1	7.93	114.55	108.20
11	A	984	A	N3-C4-C5	7.92	132.34	126.80
29	S	86	MET	N-CA-C	-7.91	89.66	111.00
11	A	2609	U	C5'-C4'-O4'	7.86	118.53	109.10
11	A	2609	U	O4'-C1'-N1	7.86	114.49	108.20
31	V	46	G	C5-C6-O6	-7.86	123.89	128.60
31	V	64	C	O4'-C1'-N1	7.83	114.47	108.20
11	A	2504	U	N3-C4-C5	-7.80	109.92	114.60
31	V	27	C	O4'-C1'-N1	7.78	114.42	108.20
31	V	71	C	O4'-C1'-N1	7.76	114.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1533	C	C6-N1-C2	-7.74	117.20	120.30
11	A	783	A	C4-C5-N7	7.74	114.57	110.70
11	A	1478	G	N1-C6-O6	7.71	124.52	119.90
31	V	10	G	C5-C6-O6	-7.71	123.98	128.60
31	V	70	C	N1-C2-O2	7.68	123.51	118.90
7	5	49	GLY	C-N-CA	7.68	140.90	121.70
11	A	2053	G	C4-N9-C1'	7.67	136.47	126.50
7	5	51	TYR	C-N-CA	7.66	140.84	121.70
7	5	123	ILE	CG1-CB-CG2	7.64	128.21	111.40
11	A	2609	U	P-O5'-C5'	7.64	133.12	120.90
11	A	465	G	N3-C4-C5	-7.62	124.79	128.60
11	A	2146	C	N3-C4-C5	-7.62	118.85	121.90
11	A	974	G	C8-N9-C1'	-7.61	117.11	127.00
7	5	119	PRO	C-N-CA	7.60	140.70	121.70
11	A	1839	G	N1-C6-O6	7.60	124.46	119.90
31	V	28	C	O4'-C1'-N1	7.59	114.28	108.20
31	V	30	U	O4'-C1'-N1	7.59	114.28	108.20
31	V	20	U	O4'-C1'-N1	7.58	114.27	108.20
11	A	783	A	N1-C6-N6	7.55	123.13	118.60
31	V	76	A	C8-N9-C4	-7.53	102.79	105.80
11	A	2053	G	C2-N3-C4	-7.51	108.15	111.90
15	E	44	ARG	NE-CZ-NH1	7.50	124.05	120.30
11	A	783	A	C6-C5-N7	-7.43	127.10	132.30
31	V	41	C	O4'-C1'-N1	7.42	114.14	108.20
11	A	776	G	C5-C6-O6	7.42	133.05	128.60
31	V	2	G	C6-N1-C2	7.36	129.52	125.10
7	5	72	LEU	C-N-CA	7.35	140.08	121.70
32	W	76	ARG	NE-CZ-NH1	7.35	123.97	120.30
31	V	17	C	O4'-C1'-N1	7.34	114.07	108.20
11	A	2504	U	C5-C4-O4	-7.34	121.50	125.90
7	5	81	LEU	CB-CG-CD2	7.33	123.46	111.00
31	V	22	G	C5-C6-O6	-7.32	124.21	128.60
11	A	1073	A	O5'-P-OP2	7.29	119.44	110.70
11	A	2501	C	C2-N1-C1'	-7.27	110.80	118.80
11	A	1533	C	N3-C2-O2	-7.26	116.82	121.90
1	h	16	GLY	N-CA-C	7.25	131.24	113.10
11	A	974	G	C5-N7-C8	-7.25	100.67	104.30
31	V	3	G	C2-N3-C4	7.25	115.53	111.90
31	V	43	G	C5-C6-O6	-7.23	124.26	128.60
11	A	1534	U	C6-N1-C1'	-7.23	111.08	121.20
11	A	2602	A	C4'-C3'-O3'	-7.21	94.25	109.40
31	V	3	G	N3-C2-N2	7.21	124.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2447	G	O5'-P-OP1	-7.20	99.22	105.70
31	V	54	U	O4'-C1'-N1	7.19	113.95	108.20
31	V	1	C	N3-C4-N4	7.17	123.02	118.00
31	V	37	G	C4-C5-C6	7.14	123.08	118.80
31	V	37	G	N1-C2-N3	-7.14	119.62	123.90
7	5	28	ALA	C-N-CA	7.13	139.54	121.70
11	A	1950	G	C6-C5-N7	-7.13	126.12	130.40
11	A	2053	G	C8-N9-C1'	-7.13	117.73	127.00
31	V	63	U	O4'-C1'-N1	7.13	113.90	108.20
29	S	94	ASP	N-CA-C	-7.12	91.78	111.00
11	A	2053	G	N1-C2-N3	7.10	128.16	123.90
11	A	2250	G	C6-C5-N7	-7.10	126.14	130.40
11	A	984	A	N3-C4-N9	-7.10	121.72	127.40
31	V	8	U	O4'-C1'-N1	7.10	113.88	108.20
31	V	75	C	N3-C4-C5	-7.10	119.06	121.90
7	5	47	GLU	C-N-CA	7.04	139.30	121.70
11	A	776	G	C5-C6-N1	-7.01	107.99	111.50
7	5	54	VAL	CG1-CB-CG2	7.01	122.12	110.90
11	A	1142	A	N1-C6-N6	7.01	122.80	118.60
31	V	67	G	C4-C5-C6	7.00	123.00	118.80
31	V	50	G	C5-C6-O6	-6.99	124.41	128.60
11	A	2250	G	N1-C6-O6	6.98	124.09	119.90
31	V	2	G	C6-C5-N7	-6.98	126.21	130.40
31	V	15	G	C5-C6-O6	-6.97	124.42	128.60
31	V	7	G	OP1-P-O3'	6.97	120.53	105.20
11	A	2503	A	C5-C6-N6	-6.97	118.13	123.70
11	A	2423	U	P-O3'-C3'	6.96	128.05	119.70
31	V	37	G	C8-N9-C4	-6.95	103.62	106.40
11	A	2448	A	N1-C6-N6	6.95	122.77	118.60
11	A	974	G	N1-C6-O6	6.95	124.07	119.90
31	V	7	G	N1-C2-N3	-6.92	119.75	123.90
31	V	60	U	O4'-C1'-N1	6.92	113.73	108.20
11	A	974	G	N3-C4-N9	6.91	130.14	126.00
11	A	1654	A	O5'-P-OP1	-6.90	99.49	105.70
11	A	1935	G	O5'-P-OP2	-6.90	99.49	105.70
11	A	2602	A	P-O3'-C3'	6.90	127.98	119.70
11	A	1378	A	P-O3'-C3'	6.87	127.95	119.70
31	V	3	G	O4'-C1'-N9	6.87	113.70	108.20
11	A	2681	C	C6-N1-C2	6.87	123.05	120.30
31	V	3	G	N9-C4-C5	-6.87	102.65	105.40
31	V	66	C	N3-C4-C5	-6.87	119.15	121.90
11	A	1284	A	O5'-P-OP2	-6.85	99.53	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	974	G	N9-C4-C5	-6.84	102.66	105.40
11	A	1839	G	C6-C5-N7	-6.84	126.30	130.40
31	V	42	G	C5-C6-O6	-6.82	124.51	128.60
11	A	783	A	C2-N3-C4	-6.80	107.20	110.60
31	V	67	G	C6-C5-N7	-6.80	126.32	130.40
11	A	2504	U	C2-N1-C1'	6.79	125.84	117.70
11	A	1192	G	C8-N9-C4	6.77	109.11	106.40
31	V	14	A	C4-C5-C6	6.76	120.38	117.00
11	A	974	G	C5-C6-O6	-6.75	124.55	128.60
11	A	12	U	N3-C2-O2	-6.74	117.48	122.20
31	V	6	C	C4'-C3'-C2'	-6.72	95.88	102.60
31	V	12	G	C5-C6-O6	-6.72	124.57	128.60
11	A	2823	A	C8-N9-C4	-6.72	103.11	105.80
31	V	36	G	P-O5'-C5'	-6.70	110.17	120.90
22	L	19	LEU	CA-CB-CG	6.70	130.70	115.30
11	A	1815	A	N9-C4-C5	6.69	108.48	105.80
11	A	802	A	N1-C6-N6	-6.67	114.59	118.60
11	A	974	G	N7-C8-N9	6.66	116.43	113.10
31	V	47	U	O4'-C1'-N1	6.66	113.53	108.20
31	V	76	A	N1-C6-N6	6.66	122.59	118.60
11	A	2146	C	C2-N3-C4	6.66	123.23	119.90
11	A	670	A	O4'-C1'-N9	-6.63	102.89	108.20
31	V	48	C	O4'-C1'-N1	6.63	113.50	108.20
11	A	528	A	N1-C6-N6	6.62	122.57	118.60
31	V	1	C	O4'-C1'-N1	6.62	113.50	108.20
16	F	94	ARG	NE-CZ-NH1	6.61	123.61	120.30
31	V	69	G	N3-C4-C5	6.61	131.90	128.60
11	A	503	A	C8-N9-C4	-6.60	103.16	105.80
31	V	45	G	C5-C6-O6	-6.58	124.66	128.60
31	V	44	G	C5-C6-O6	-6.57	124.66	128.60
13	C	233	GLY	N-CA-C	-6.56	96.69	113.10
31	V	40	U	O4'-C1'-N1	6.56	113.44	108.20
31	V	29	G	C5-C6-O6	-6.55	124.67	128.60
31	V	55	U	O4'-C1'-N1	6.55	113.44	108.20
11	A	1311	G	C8-N9-C4	-6.54	103.78	106.40
31	V	52	G	C5-C6-O6	-6.54	124.67	128.60
31	V	58	A	C4-C5-C6	6.54	120.27	117.00
31	V	39	G	N3-C4-N9	6.49	129.90	126.00
11	A	820	A	O5'-P-OP1	-6.49	99.86	105.70
31	V	24	G	C5-C6-O6	-6.48	124.71	128.60
31	V	72	G	N3-C2-N2	6.47	124.43	119.90
31	V	19	G	C5-C6-O6	-6.46	124.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	84	TYR	C-N-CA	6.46	137.85	121.70
31	V	3	G	P-O5'-C5'	-6.46	110.57	120.90
31	V	39	G	N7-C8-N9	6.45	116.33	113.10
11	A	1263	U	N3-C4-C5	-6.45	110.73	114.60
31	V	69	G	N9-C4-C5	-6.43	102.83	105.40
7	5	147	SER	C-N-CA	6.42	137.76	121.70
11	A	404	A	P-O3'-C3'	6.42	127.40	119.70
31	V	18	G	C5-C6-O6	-6.41	124.75	128.60
7	5	40	GLU	C-N-CA	6.41	137.72	121.70
11	A	2551	C	OP2-P-O3'	6.40	119.27	105.20
29	S	94	ASP	CB-CG-OD2	6.38	124.04	118.30
11	A	2689	U	C5-C4-O4	6.36	129.72	125.90
29	S	85	ILE	O-C-N	-6.35	112.54	122.70
31	V	9	A	C4-C5-C6	6.34	120.17	117.00
7	5	50	VAL	C-N-CA	6.33	137.54	121.70
31	V	5	A	C5'-C4'-C3'	6.33	126.14	116.00
11	A	1839	G	C5-C6-O6	-6.33	124.80	128.60
31	V	6	C	C2-N3-C4	6.33	123.06	119.90
15	E	44	ARG	NE-CZ-NH2	-6.33	117.14	120.30
31	V	21	A	C4-C5-C6	6.32	120.16	117.00
11	A	1142	A	N3-C4-C5	6.32	131.22	126.80
11	A	2142	A	OP2-P-O3'	6.31	119.08	105.20
31	V	37	G	N9-C4-C5	6.30	107.92	105.40
31	V	13	C	N3-C4-N4	6.29	122.40	118.00
31	V	70	C	P-O5'-C5'	6.29	130.96	120.90
31	V	66	C	O4'-C1'-N1	6.27	113.21	108.20
31	V	44	G	O4'-C1'-N9	6.26	113.21	108.20
31	V	6	C	O4'-C1'-N1	6.26	113.21	108.20
31	V	26	A	C4-C5-C6	6.26	120.13	117.00
11	A	1125	G	N1-C6-O6	6.25	123.65	119.90
11	A	2754	U	N3-C4-O4	6.24	123.77	119.40
7	5	108	VAL	CG1-CB-CG2	6.24	120.88	110.90
31	V	2	G	N1-C2-N3	-6.24	120.16	123.90
31	V	39	G	C2'-C3'-O3'	6.23	123.67	113.70
31	V	37	G	C5-N7-C8	6.23	107.42	104.30
31	V	69	G	C5-N7-C8	6.22	107.41	104.30
31	V	1	C	C5-C4-N4	-6.22	115.85	120.20
7	5	60	LEU	CB-CG-CD1	6.21	121.56	111.00
11	A	1003	G	O5'-P-OP2	-6.21	100.11	105.70
11	A	2770	G	N1-C6-O6	-6.21	116.18	119.90
11	A	1950	G	C5-C6-O6	-6.20	124.88	128.60
11	A	2447	G	N1-C6-O6	6.19	123.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	66	C	P-O3'-C3'	6.18	127.11	119.70
31	V	21	A	C5-C6-N6	-6.18	118.76	123.70
31	V	49	G	C5-C6-O6	-6.17	124.90	128.60
11	A	748	G	O4'-C1'-N9	6.16	113.13	108.20
7	5	39	THR	C-N-CA	6.16	137.09	121.70
11	A	1815	A	C8-N9-C4	-6.16	103.34	105.80
13	C	109	LEU	CA-CB-CG	6.16	129.46	115.30
11	A	1142	A	C5-N7-C8	-6.15	100.83	103.90
31	V	57	A	C4-C5-C6	6.13	120.07	117.00
31	V	2	G	C5-C6-N1	-6.13	108.44	111.50
11	A	984	A	N1-C6-N6	6.11	122.27	118.60
11	A	528	A	C5-C6-N1	-6.11	114.64	117.70
11	A	784	G	P-O3'-C3'	6.11	127.03	119.70
31	V	52	G	O4'-C1'-N9	6.10	113.08	108.20
22	L	82	LEU	CA-CB-CG	6.09	129.31	115.30
11	A	1142	A	C4-C5-N7	6.09	113.75	110.70
31	V	38	U	C6-N1-C2	-6.09	117.35	121.00
11	A	1670	C	N1-C2-O2	-6.08	115.25	118.90
11	A	2592	G	O5'-P-OP2	-6.08	100.23	105.70
11	A	784	G	O4'-C1'-N9	-6.07	103.34	108.20
11	A	548	G	C8-N9-C4	-6.07	103.97	106.40
11	A	2267	A	C8-N9-C4	-6.07	103.37	105.80
11	A	379	G	N1-C6-O6	6.06	123.54	119.90
31	V	26	A	C5-C6-N6	-6.06	118.85	123.70
11	A	1025	G	P-O3'-C3'	6.06	126.97	119.70
31	V	76	A	C1'-O4'-C4'	6.05	114.74	109.90
31	V	3	G	N3-C4-N9	6.05	129.63	126.00
7	5	59	LEU	C-N-CA	6.04	136.80	121.70
11	A	2250	G	C4-C5-N7	6.04	113.22	110.80
11	A	119	A	O5'-P-OP2	-6.02	100.28	105.70
11	A	1073	A	N7-C8-N9	-6.01	110.80	113.80
31	V	49	G	O4'-C1'-N9	6.00	113.00	108.20
31	V	59	A	O4'-C1'-N9	6.00	113.00	108.20
11	A	1428	C	O5'-P-OP1	-6.00	100.30	105.70
11	A	1069	A	OP2-P-O3'	6.00	118.40	105.20
11	A	2554	U	O5'-P-OP1	-6.00	100.30	105.70
31	V	74	C	C3'-C2'-C1'	-6.00	96.70	101.50
11	A	567	U	N1-C2-O2	-5.99	118.61	122.80
31	V	68	U	C6-N1-C2	-5.99	117.41	121.00
11	A	2534	A	C4-C5-N7	5.96	113.68	110.70
31	V	14	A	C5-C6-N6	-5.96	118.93	123.70
11	A	1328	A	O5'-P-OP2	-5.94	100.35	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2250	G	C5-N7-C8	-5.94	101.33	104.30
31	V	70	C	C5-C4-N4	-5.94	116.05	120.20
31	V	75	C	C2-N3-C4	5.93	122.87	119.90
31	V	29	G	O4'-C1'-N9	5.92	112.94	108.20
11	A	527	C	P-O3'-C3'	5.91	126.80	119.70
7	5	53	ARG	C-N-CA	5.91	136.47	121.70
11	A	1645	G	N3-C4-C5	-5.90	125.65	128.60
31	V	70	C	N3-C2-O2	-5.90	117.77	121.90
11	A	1358	G	C8-N9-C4	-5.90	104.04	106.40
11	A	2241	A	C8-N9-C4	-5.89	103.44	105.80
31	V	51	A	C5-C6-N6	-5.89	118.99	123.70
11	A	2043	C	C6-N1-C2	-5.88	117.95	120.30
31	V	59	A	C4-C5-C6	5.87	119.94	117.00
11	A	2747	G	OP2-P-O3'	5.87	118.12	105.20
11	A	2447	G	C5-C6-O6	-5.86	125.08	128.60
11	A	1779	U	N3-C4-O4	-5.86	115.30	119.40
31	V	51	A	C4-C5-C6	5.85	119.92	117.00
31	V	16	C	N3-C4-N4	5.84	122.09	118.00
11	A	1509	A	O4'-C1'-N9	5.84	112.87	108.20
31	V	76	A	N7-C8-N9	5.84	116.72	113.80
11	A	1094	U	N3-C4-C5	-5.83	111.10	114.60
31	V	36	G	O5'-C5'-C4'	5.83	122.78	111.70
11	A	1837	C	O5'-P-OP1	-5.83	100.46	105.70
11	A	2719	G	C5-C6-N1	-5.82	108.59	111.50
31	V	16	C	N3-C4-C5	-5.82	119.57	121.90
11	A	964	C	O5'-P-OP2	-5.81	100.47	105.70
31	V	48	C	N3-C4-N4	5.80	122.06	118.00
11	A	2715	C	C6-N1-C2	5.80	122.62	120.30
31	V	16	C	O4'-C1'-N1	5.80	112.84	108.20
11	A	516	C	O5'-P-OP1	-5.78	100.50	105.70
31	V	32	A	C5-N7-C8	5.78	106.79	103.90
31	V	58	A	C5-C6-N1	-5.77	114.82	117.70
31	V	7	G	N3-C4-C5	-5.76	125.72	128.60
11	A	1263	U	C6-N1-C2	-5.75	117.55	121.00
31	V	9	A	C5-C6-N6	-5.75	119.10	123.70
11	A	1606	C	C2-N3-C4	-5.74	117.03	119.90
31	V	42	G	O4'-C1'-N9	5.74	112.79	108.20
7	5	117	LEU	C-N-CA	5.73	136.03	121.70
31	V	62	C	N3-C4-N4	5.73	122.01	118.00
11	A	2534	A	C5-N7-C8	-5.72	101.04	103.90
31	V	57	A	C5-C6-N6	-5.72	119.12	123.70
31	V	7	G	P-O5'-C5'	5.71	130.04	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	45	G	O4'-C1'-N9	5.71	112.77	108.20
11	A	1247	A	P-O3'-C3'	5.70	126.55	119.70
11	A	2271	G	C5-C6-O6	-5.70	125.18	128.60
11	A	2604	U	N3-C4-O4	-5.70	115.41	119.40
31	V	61	C	N3-C4-N4	5.70	121.99	118.00
11	A	2544	G	N1-C6-O6	5.69	123.32	119.90
11	A	2448	A	C6-C5-N7	-5.69	128.32	132.30
11	A	1088	A	O4'-C1'-N9	-5.69	103.65	108.20
31	V	27	C	N3-C4-N4	5.69	121.98	118.00
11	A	866	A	N1-C6-N6	5.68	122.01	118.60
31	V	41	C	N3-C4-N4	5.67	121.97	118.00
11	A	1789	A	O5'-P-OP1	-5.66	100.60	105.70
11	A	2719	G	N1-C6-O6	5.66	123.30	119.90
11	A	1979	U	C6-N1-C2	-5.66	117.60	121.00
31	V	31	C	N3-C4-N4	5.66	121.96	118.00
11	A	626	A	N1-C6-N6	5.65	121.99	118.60
11	A	1509	A	P-O3'-C3'	5.65	126.48	119.70
11	A	1534	U	C5-C6-N1	5.65	125.53	122.70
31	V	70	C	N3-C4-C5	5.65	124.16	121.90
11	A	1611	C	N1-C2-O2	-5.65	115.51	118.90
11	A	271	G	OP1-P-O3'	5.64	117.61	105.20
11	A	1066	U	N3-C2-O2	-5.64	118.25	122.20
31	V	11	C	N3-C4-C5	-5.63	119.65	121.90
31	V	12	G	O4'-C1'-N9	5.62	112.69	108.20
11	A	84	A	N1-C6-N6	-5.62	115.23	118.60
11	A	1192	G	N9-C4-C5	-5.61	103.16	105.40
11	A	2053	G	N3-C2-N2	-5.60	115.98	119.90
31	V	22	G	O4'-C1'-N9	5.60	112.68	108.20
31	V	62	C	N3-C4-C5	-5.60	119.66	121.90
11	A	1153	C	N1-C2-O2	-5.60	115.54	118.90
11	A	1446	C	C6-N1-C2	-5.60	118.06	120.30
31	V	48	C	N3-C4-C5	-5.59	119.66	121.90
31	V	2	G	N7-C8-N9	5.59	115.89	113.10
11	A	2355	G	C8-N9-C4	5.58	108.63	106.40
11	A	989	G	O4'-C1'-N9	5.57	112.66	108.20
11	A	1069	A	O4'-C1'-N9	5.57	112.66	108.20
31	V	26	A	O4'-C1'-N9	5.57	112.66	108.20
11	A	1073	A	C4-N9-C1'	-5.57	116.28	126.30
31	V	76	A	OP1-P-OP2	-5.57	111.25	119.60
11	A	1207	C	C6-N1-C2	-5.56	118.08	120.30
12	B	80	U	N1-C2-N3	5.56	118.24	114.90
31	V	3	G	C4-C5-C6	5.56	122.13	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1198	U	O5'-P-OP2	-5.55	100.70	105.70
11	A	2501	C	N3-C4-C5	5.55	124.12	121.90
31	V	2	G	N9-C4-C5	-5.55	103.18	105.40
11	A	672	C	N1-C2-O2	5.54	122.23	118.90
11	A	1025	G	N3-C4-C5	-5.53	125.83	128.60
11	A	2241	A	N9-C4-C5	5.53	108.01	105.80
31	V	50	G	O4'-C1'-N9	5.53	112.62	108.20
11	A	2353	G	N1-C6-O6	-5.52	116.59	119.90
31	V	31	C	N3-C4-C5	-5.51	119.70	121.90
31	V	28	C	N3-C4-C5	-5.50	119.70	121.90
11	A	2439	A	N1-C6-N6	5.50	121.90	118.60
11	A	1129	A	O5'-P-OP1	-5.50	100.75	105.70
31	V	33	U	O3'-P-O5'	5.50	114.45	104.00
31	V	57	A	O4'-C1'-N9	5.50	112.60	108.20
31	V	25	C	N3-C4-N4	5.50	121.85	118.00
11	A	1824	G	N9-C4-C5	5.49	107.60	105.40
11	A	2326	C	C5-C4-N4	-5.49	116.36	120.20
11	A	2271	G	N1-C6-O6	5.49	123.19	119.90
11	A	1565	C	C6-N1-C2	-5.49	118.11	120.30
11	A	1157	G	N1-C6-O6	5.49	123.19	119.90
11	A	2015	A	N1-C6-N6	-5.49	115.31	118.60
31	V	41	C	N3-C4-C5	-5.48	119.71	121.90
11	A	1027	A	O4'-C1'-N9	-5.48	103.81	108.20
31	V	17	C	N3-C4-N4	5.48	121.84	118.00
11	A	2689	U	N3-C4-O4	-5.47	115.57	119.40
11	A	2037	A	N9-C4-C5	5.47	107.99	105.80
11	A	1684	G	N3-C4-C5	-5.47	125.87	128.60
11	A	29	U	OP2-P-O3'	5.46	117.22	105.20
11	A	733	G	C8-N9-C4	-5.46	104.21	106.40
31	V	43	G	O4'-C1'-N9	5.46	112.57	108.20
11	A	1524	G	C8-N9-C4	-5.46	104.22	106.40
11	A	55	G	C5-C6-O6	-5.46	125.33	128.60
11	A	2544	G	C6-C5-N7	-5.45	127.13	130.40
31	V	7	G	C1'-O4'-C4'	5.45	114.26	109.90
31	V	25	C	N3-C4-C5	-5.43	119.73	121.90
11	A	532	A	C8-N9-C4	-5.43	103.63	105.80
11	A	1206	G	N3-C4-C5	-5.43	125.88	128.60
11	A	2250	G	C2-N3-C4	-5.43	109.19	111.90
11	A	2263	C	N3-C4-C5	-5.43	119.73	121.90
31	V	14	A	C5-C6-N1	-5.43	114.99	117.70
31	V	23	C	N3-C4-N4	5.42	121.80	118.00
31	V	69	G	C6-N1-C2	-5.42	121.84	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2446	G	OP2-P-O3'	5.42	117.13	105.20
11	A	1125	G	C6-C5-N7	-5.42	127.15	130.40
11	A	209	C	C6-N1-C2	5.42	122.47	120.30
11	A	2353	G	C2-N3-C4	5.42	114.61	111.90
11	A	2604	U	C5-C4-O4	5.41	129.15	125.90
31	V	73	A	C2'-C3'-O3'	5.41	122.36	113.70
31	V	9	A	C5-C6-N1	-5.41	115.00	117.70
11	A	2609	U	N1-C1'-C2'	5.41	121.03	114.00
31	V	57	A	C5-C6-N1	-5.41	115.00	117.70
11	A	1190	G	C5-N7-C8	-5.41	101.60	104.30
11	A	1430	G	N1-C6-O6	5.41	123.14	119.90
26	P	113	LEU	CA-CB-CG	5.41	127.73	115.30
31	V	51	A	C5-C6-N1	-5.41	115.00	117.70
31	V	28	C	N3-C4-N4	5.40	121.78	118.00
11	A	1069	A	C8-N9-C4	-5.39	103.64	105.80
11	A	598	U	OP2-P-O3'	5.39	117.06	105.20
11	A	1355	G	C8-N9-C4	-5.39	104.24	106.40
11	A	2153	C	O4'-C1'-N1	5.39	112.51	108.20
11	A	2685	G	C5-C6-N1	-5.38	108.81	111.50
11	A	677	A	OP1-P-O3'	5.38	117.03	105.20
11	A	1073	A	C8-N9-C1'	5.38	137.38	127.70
11	A	1950	G	C8-N9-C1'	-5.37	120.02	127.00
31	V	7	G	N7-C8-N9	-5.36	110.42	113.10
11	A	451	U	O4'-C1'-N1	5.36	112.49	108.20
11	A	1420	A	O4'-C1'-N9	5.36	112.49	108.20
11	A	250	G	O5'-P-OP2	-5.36	100.88	105.70
11	A	916	G	C6-C5-N7	-5.34	127.19	130.40
31	V	58	A	C5-C6-N6	-5.34	119.43	123.70
11	A	984	A	C5-C6-N1	-5.34	115.03	117.70
11	A	1229	C	C6-N1-C2	5.33	122.43	120.30
31	V	68	U	C1'-O4'-C4'	5.33	114.16	109.90
11	A	2501	C	C6-N1-C1'	5.32	127.18	120.80
31	V	51	A	O4'-C1'-N9	5.32	112.45	108.20
7	5	131	THR	N-CA-C	-5.31	96.66	111.00
11	A	2146	C	C6-N1-C2	-5.31	118.17	120.30
31	V	53	G	O4'-C1'-N9	5.31	112.45	108.20
11	A	518	G	O5'-P-OP1	-5.31	100.92	105.70
11	A	548	G	N3-C4-C5	-5.31	125.94	128.60
27	Q	63	ARG	NE-CZ-NH2	-5.31	117.65	120.30
7	5	50	VAL	CG1-CB-CG2	5.31	119.39	110.90
11	A	2244	U	C5-C4-O4	-5.31	122.72	125.90
11	A	991	C	C6-N1-C2	-5.30	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2571	U	C2-N1-C1'	-5.30	111.34	117.70
11	A	2518	A	N1-C6-N6	5.29	121.78	118.60
31	V	23	C	N3-C4-C5	-5.29	119.78	121.90
11	A	940	G	N1-C6-O6	5.29	123.07	119.90
11	A	837	C	N1-C2-O2	-5.29	115.73	118.90
31	V	9	A	O4'-C1'-N9	5.29	112.43	108.20
11	A	2470	G	OP2-P-O3'	5.28	116.82	105.20
33	X	29	LEU	CA-CB-CG	5.28	127.45	115.30
11	A	1458	U	P-O3'-C3'	5.28	126.04	119.70
11	A	776	G	C4-N9-C1'	5.28	133.36	126.50
31	V	17	C	N3-C4-C5	-5.28	119.79	121.90
11	A	1264	A	O5'-P-OP1	-5.27	100.95	105.70
7	5	50	VAL	CA-CB-CG1	5.27	118.81	110.90
11	A	2250	G	N7-C8-N9	5.27	115.73	113.10
11	A	1970	A	C8-N9-C4	-5.26	103.69	105.80
31	V	59	A	C5-C6-N6	-5.26	119.49	123.70
11	A	2443	C	N3-C4-N4	5.26	121.68	118.00
31	V	13	C	C1'-O4'-C4'	-5.26	105.69	109.90
11	A	2071	A	OP2-P-O3'	5.26	116.77	105.20
31	V	15	G	O4'-C1'-N9	5.25	112.40	108.20
31	V	5	A	C5-C6-N1	-5.25	115.08	117.70
31	V	61	C	N3-C4-C5	-5.25	119.80	121.90
11	A	2503	A	N1-C6-N6	5.24	121.75	118.60
11	A	833	A	C8-N9-C4	-5.24	103.70	105.80
11	A	2396	G	N9-C4-C5	5.24	107.50	105.40
31	V	7	G	C2-N3-C4	5.24	114.52	111.90
11	A	1131	G	OP1-P-O3'	5.23	116.71	105.20
11	A	2603	G	O4'-C4'-C3'	5.23	110.29	106.10
11	A	1355	G	N3-C2-N2	-5.23	116.24	119.90
11	A	1795	C	N3-C4-C5	-5.22	119.81	121.90
31	V	64	C	N3-C4-N4	5.22	121.65	118.00
11	A	2704	C	C6-N1-C2	5.22	122.39	120.30
11	A	404	A	C8-N9-C4	-5.21	103.72	105.80
11	A	1533	C	C5-C6-N1	5.21	123.61	121.00
11	A	1350	C	C6-N1-C2	5.21	122.38	120.30
11	A	1936	A	N3-C4-C5	5.21	130.45	126.80
31	V	59	A	C5-C6-N1	-5.21	115.10	117.70
31	V	26	A	C5-C6-N1	-5.21	115.10	117.70
11	A	984	A	N1-C2-N3	5.20	131.90	129.30
11	A	2422	C	N1-C2-O2	5.20	122.02	118.90
31	V	10	G	O4'-C1'-N9	5.19	112.35	108.20
7	5	130	PRO	CA-N-CD	-5.19	104.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	22	HIS	N-CA-C	5.19	125.02	111.00
11	A	1659	G	N3-C4-C5	5.19	131.19	128.60
11	A	2618	G	C5-C6-N1	-5.18	108.91	111.50
11	A	1759	A	N1-C6-N6	5.18	121.71	118.60
35	Z	15	ARG	NE-CZ-NH1	5.18	122.89	120.30
31	V	37	G	N1-C6-O6	5.18	123.01	119.90
11	A	748	G	C4-C5-N7	-5.17	108.73	110.80
31	V	71	C	C2-N3-C4	5.17	122.49	119.90
11	A	1983	G	C5-C6-N1	-5.17	108.92	111.50
31	V	24	G	O4'-C1'-N9	5.17	112.33	108.20
11	A	2439	A	C4-C5-N7	5.16	113.28	110.70
11	A	699	A	N1-C6-N6	5.16	121.70	118.60
31	V	17(A)	U	O4'-C1'-N1	5.16	112.33	108.20
11	A	1533	C	C6-N1-C1'	-5.16	114.61	120.80
11	A	2723	C	C6-N1-C2	-5.15	118.24	120.30
11	A	2534	A	C5-C6-N6	-5.15	119.58	123.70
31	V	21	A	O4'-C1'-N9	5.15	112.32	108.20
12	B	80	U	C6-N1-C2	-5.15	117.91	121.00
11	A	1238	G	O5'-P-OP2	-5.15	101.07	105.70
11	A	2015	A	N9-C4-C5	5.14	107.86	105.80
11	A	2448	A	C5-C6-N6	-5.13	119.59	123.70
11	A	2282	G	C8-N9-C4	-5.13	104.35	106.40
11	A	1122	G	N3-C4-N9	-5.12	122.92	126.00
11	A	2198	A	O4'-C1'-N9	5.12	112.30	108.20
31	V	5	A	C5-C6-N6	-5.12	119.61	123.70
31	V	56	C	N3-C4-C5	-5.12	119.85	121.90
11	A	2368	C	C6-N1-C2	5.11	122.34	120.30
11	A	1534	U	N1-C2-O2	5.11	126.38	122.80
11	A	1395	A	O4'-C1'-N9	5.11	112.28	108.20
12	B	114	C	C5-C4-N4	-5.11	116.63	120.20
31	V	38	U	N3-C2-O2	5.11	125.77	122.20
11	A	465	G	C4-C5-C6	5.10	121.86	118.80
11	A	1606	C	P-O3'-C3'	5.10	125.82	119.70
11	A	119	A	P-O3'-C3'	5.10	125.82	119.70
11	A	2602	A	O4'-C1'-N9	5.10	112.28	108.20
11	A	2825	G	N3-C4-N9	5.10	129.06	126.00
31	V	3	G	C5-C6-N1	-5.09	108.95	111.50
11	A	55	G	N1-C6-O6	5.09	122.95	119.90
11	A	1311	G	N7-C8-N9	5.09	115.64	113.10
11	A	1831	G	C8-N9-C4	-5.09	104.36	106.40
11	A	454	A	O5'-P-OP2	-5.09	101.12	105.70
10	8	61	LEU	CA-CB-CG	5.08	126.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	403	U	P-O3'-C3'	5.08	125.80	119.70
11	A	2015	A	C5-C6-N6	5.08	127.76	123.70
11	A	2537	U	N1-C2-N3	5.07	117.94	114.90
11	A	1977	A	C2-N3-C4	-5.07	108.07	110.60
11	A	1928	A	N1-C6-N6	5.06	121.64	118.60
11	A	686	U	C2-N1-C1'	-5.06	111.63	117.70
31	V	56	C	N3-C4-N4	5.06	121.54	118.00
31	V	7	G	N1-C2-N2	-5.05	111.65	116.20
11	A	2551	C	O5'-P-OP1	-5.05	101.16	105.70
11	A	542	C	N3-C4-C5	-5.04	119.88	121.90
31	V	21	A	C5-C6-N1	-5.04	115.18	117.70
19	I	79	LEU	CA-CB-CG	5.04	126.89	115.30
11	A	970	U	N1-C2-O2	-5.03	119.28	122.80
11	A	2253	G	C5-C6-O6	-5.03	125.58	128.60
31	V	32	A	N1-C6-N6	5.03	121.62	118.60
11	A	1649	G	O5'-P-OP1	-5.03	101.18	105.70
11	A	1943	U	C5-C4-O4	5.03	128.92	125.90
11	A	1997	C	O4'-C1'-N1	5.03	112.22	108.20
11	A	2038	G	N1-C6-O6	5.03	122.92	119.90
31	V	11	C	N3-C4-N4	5.02	121.52	118.00
11	A	1639	C	C6-N1-C2	5.02	122.31	120.30
11	A	1815	A	N1-C6-N6	-5.02	115.59	118.60
11	A	2455	G	O5'-P-OP2	-5.02	101.19	105.70
11	A	2902	C	P-O3'-C3'	5.01	125.72	119.70
11	A	1094	U	C6-N1-C2	-5.01	117.99	121.00
31	V	33	U	OP1-P-OP2	-5.01	112.09	119.60
11	A	1025	G	C8-N9-C4	-5.01	104.40	106.40
13	C	155	ARG	CG-CD-NE	5.00	122.31	111.80
11	A	751	A	C2'-C3'-O3'	-5.00	98.50	109.50

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	5	130	PRO	Peptide
13	C	233	GLY	Peptide
14	D	9	VAL	Peptide
20	J	110	PRO	Peptide
21	K	71	ARG	Peptide
29	S	86	MET	Mainchain
29	S	88	ARG	Peptide
29	S	89	ALA	Peptide

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Mol	Chain	Res	Type	Group
31	V	13	C	Sidechain
31	V	3	G	Sidechain
31	V	33	U	Sidechain
31	V	37	G	Sidechain
31	V	39	G	Sidechain
31	V	4	C	Sidechain
31	V	5	A	Sidechain
31	V	66	C	Sidechain
31	V	67	G	Sidechain
31	V	69	G	Sidechain
31	V	70	C	Sidechain
31	V	71	C	Sidechain
31	V	75	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	h	779	0	829	0	0
2	0	444	0	461	17	0
3	1	409	0	440	16	0
4	2	377	0	418	6	0
5	3	504	0	574	11	0
6	4	302	0	340	16	0
7	5	1117	0	1155	124	0
8	6	227	0	237	6	0
9	7	139	0	134	12	0
10	8	753	0	780	11	0
11	A	61274	0	30816	819	0
12	B	2529	0	1281	20	0
13	C	2082	0	2157	53	0
14	D	1565	0	1616	49	0
15	E	1552	0	1619	36	0
16	F	1410	0	1445	44	0
17	G	1313	0	1361	36	0
18	H	384	0	405	13	0
19	I	1032	0	1088	53	0
20	J	1129	0	1162	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	938	0	1012	42	0
22	L	1045	0	1117	35	0
23	M	1074	0	1157	28	0
24	N	960	0	1000	30	0
25	O	892	0	923	21	0
26	P	917	0	965	42	0
27	Q	947	0	1022	49	0
28	R	816	0	839	34	0
29	S	857	0	922	41	0
30	T	738	0	807	34	0
31	V	1649	0	833	53	0
32	W	596	0	610	81	0
33	X	625	0	655	18	0
34	Y	509	0	543	13	0
35	Z	449	0	491	17	0
36	z	688	0	691	0	0
37	4	1	0	0	0	0
37	A	136	0	0	0	0
37	B	4	0	0	0	0
37	C	1	0	0	0	0
37	E	1	0	0	0	0
38	4	1	0	0	0	0
39	A	15	0	9	3	0
40	4	1	0	0	0	0
40	A	415	0	0	77	0
40	B	14	0	0	1	0
40	C	2	0	0	0	0
40	D	3	0	0	0	0
40	E	1	0	0	0	0
40	L	3	0	0	0	0
All	All	93619	0	61914	1673	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 13.

All (1673) 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)
16:F:79:ARG:NH2	31:V:56:C:O2	1.62	1.30
11:A:2062:A:H2'	11:A:2063:C:C6	1.70	1.27
11:A:2062:A:H2'	11:A:2063:C:C5	1.71	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1923:U:H5”	31:V:24:G:O2’	1.04	1.18
9:7:24:PRO:HB2	31:V:76:A:O3’	1.40	1.18
11:A:912:C:OP1	23:M:8:LYS:NZ	1.79	1.14
11:A:1923:U:C5’	31:V:24:G:O2’	1.98	1.10
29:S:88:ARG:NH1	29:S:94:ASP:OD2	1.84	1.09
11:A:1782:U:N3	11:A:2586:U:O4	1.90	1.05
7:5:71:CYS:HB3	7:5:117:LEU:HD12	1.33	1.03
16:F:79:ARG:NH2	31:V:56:C:C2	2.25	1.02
7:5:26:VAL:HG21	7:5:115:GLY:H	1.23	1.02
7:5:3:LEU:O	7:5:7:ASP:OD1	1.79	1.00
11:A:1782:U:C2’	11:A:2608:G:O2’	2.09	0.99
11:A:1923:U:H5”	31:V:24:G:C2’	1.92	0.98
11:A:1782:U:C2	11:A:2586:U:O4	2.17	0.98
11:A:1782:U:H2’	11:A:2608:G:O2’	1.62	0.97
7:5:117:LEU:CD2	7:5:120:ALA:HA	1.97	0.94
11:A:2062:A:O2’	11:A:2063:C:O5’	1.83	0.94
11:A:2062:A:C2’	11:A:2063:C:C6	2.50	0.94
11:A:576:U:OP1	40:A:3201:HOH:O	1.85	0.94
9:7:22:HIS:O	11:A:2506:U:C5	2.21	0.94
11:A:2585:U:O2’	11:A:2586:U:OP2	1.85	0.94
9:7:24:PRO:HB2	31:V:76:A:HO3’	1.22	0.93
11:A:1909:C:H4’	31:V:11:C:H4’	1.49	0.92
7:5:71:CYS:HB3	7:5:117:LEU:CD1	1.99	0.92
11:A:1154:G:OP2	27:Q:57:ARG:NH1	2.03	0.91
7:5:71:CYS:CB	7:5:117:LEU:HD12	2.00	0.91
12:B:43:C:O2	16:F:91:ARG:NH1	2.05	0.90
11:A:2279:G:N7	32:W:10:ARG:NH2	2.20	0.90
11:A:1248:G:OP2	15:E:44:ARG:NH2	2.04	0.90
11:A:1922:G:O2’	31:V:25:C:H1’	1.73	0.89
7:5:71:CYS:CB	7:5:117:LEU:CD1	2.50	0.89
11:A:2608:G:H8	11:A:2608:G:H5”	1.38	0.89
11:A:1923:U:H5”	31:V:24:G:HO2’	1.32	0.89
11:A:1336:A:OP2	30:T:68:LYS:NZ	2.06	0.88
7:5:24:SER:HB2	7:5:116:GLU:HG2	1.53	0.88
11:A:996:A:OP2	27:Q:91:ARG:NH2	2.07	0.87
11:A:2062:A:H2’	11:A:2063:C:H6	1.40	0.86
30:T:39:THR:O	30:T:41:ALA:N	2.09	0.85
11:A:1723:G:O6	11:A:1737:G:O2’	1.94	0.84
7:5:71:CYS:HA	7:5:117:LEU:HD13	1.60	0.84
11:A:1069:A:N3	11:A:1073:A:N6	2.25	0.84
11:A:2608:G:H5”	11:A:2608:G:C8	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:981:A:OP1	40:A:3202:HOH:O	1.95	0.83
11:A:1371:G:N7	40:A:3237:HOH:O	2.13	0.82
7:5:77:VAL:C	7:5:79:PRO:HD2	2.00	0.82
11:A:1909:C:O4'	31:V:11:C:O2'	1.95	0.82
13:C:196:ASN:O	13:C:198:GLU:N	2.12	0.82
7:5:33:VAL:N	7:5:36:ASP:OD2	2.12	0.82
7:5:71:CYS:HA	7:5:117:LEU:CD1	2.09	0.82
11:A:991:C:OP2	40:A:3204:HOH:O	1.98	0.82
11:A:526:A:OP1	40:A:3203:HOH:O	1.97	0.81
11:A:2608:G:H8	11:A:2608:G:C5'	1.93	0.81
9:7:24:PRO:CB	31:V:76:A:O3'	2.27	0.81
11:A:1923:U:OP1	31:V:25:C:H5'	1.79	0.81
11:A:1783:A:OP1	40:A:3207:HOH:O	1.98	0.81
11:A:1922:G:O3'	31:V:25:C:H4'	1.78	0.81
26:P:50:ARG:HB3	26:P:57:ALA:H	1.43	0.81
7:5:103:ASN:ND2	7:5:107:GLU:O	2.13	0.81
11:A:2062:A:H2'	11:A:2063:C:H5	1.45	0.81
25:O:34:HIS:O	25:O:102:ARG:NH2	2.14	0.81
11:A:504:A:O2'	11:A:505:A:OP1	1.98	0.81
11:A:1268:A:OP1	40:A:3208:HOH:O	1.99	0.80
11:A:1908:C:O2'	31:V:12:G:H5'	1.80	0.80
11:A:945:A:OP2	40:A:3206:HOH:O	1.98	0.80
11:A:1647:U:OP2	40:A:3205:HOH:O	1.98	0.80
11:A:1012:U:OP2	27:Q:69:ARG:NH2	2.14	0.80
11:A:1614:A:C6	29:S:87:PRO:HB3	2.17	0.80
11:A:2720:U:OP1	26:P:52:ARG:NH2	2.15	0.80
29:S:88:ARG:HD2	29:S:94:ASP:OD1	1.83	0.79
11:A:975:A:OP2	40:A:3211:HOH:O	2.00	0.79
11:A:2062:A:C2'	11:A:2063:C:H6	1.92	0.79
11:A:2448:A:OP2	40:A:3210:HOH:O	2.00	0.79
7:5:33:VAL:HG12	7:5:34:THR:H	1.48	0.78
34:Y:18:LEU:O	34:Y:22:LEU:N	2.17	0.78
7:5:43:LYS:NZ	7:5:98:GLU:OE1	2.16	0.78
11:A:1509:A:O2'	11:A:1510:G:OP2	2.01	0.78
7:5:117:LEU:HD23	7:5:120:ALA:HA	1.65	0.78
11:A:1799:G:OP2	13:C:269:ARG:NH2	2.16	0.77
7:5:71:CYS:CA	7:5:117:LEU:CD1	2.62	0.77
7:5:91:ALA:C	7:5:93:ALA:H	1.87	0.77
11:A:2062:A:OP2	40:A:3209:HOH:O	2.00	0.77
11:A:2025:C:OP2	40:A:3213:HOH:O	2.03	0.77
14:D:184:ARG:NH2	26:P:6:GLN:OE1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2062:A:HO2'	11:A:2063:C:C5'	1.98	0.77
21:K:105:ARG:NH1	21:K:106:GLU:OE2	2.16	0.77
11:A:1380:G:OP2	40:A:3214:HOH:O	2.04	0.77
11:A:946:C:OP2	40:A:3206:HOH:O	2.02	0.76
13:C:68:ARG:NH2	13:C:126:GLY:O	2.18	0.76
7:5:35:VAL:HA	7:5:38:MET:SD	2.24	0.76
11:A:1922:G:HO2'	31:V:25:C:C2'	1.97	0.76
13:C:69:ASN:O	13:C:71:ASP:N	2.18	0.76
11:A:526:A:OP1	40:A:3212:HOH:O	2.03	0.76
11:A:1153:C:OP2	40:A:3217:HOH:O	2.04	0.75
11:A:1342:A:O2'	11:A:1344:U:OP2	2.04	0.75
11:A:2006:C:OP1	40:A:3208:HOH:O	2.04	0.75
11:A:2331:G:O2'	32:W:39:GLN:O	2.04	0.75
11:A:2503:A:OP1	40:A:3201:HOH:O	2.04	0.75
11:A:1187:G:OP1	28:R:85:LYS:NZ	2.20	0.74
11:A:2579:C:OP1	40:A:3218:HOH:O	2.05	0.74
12:B:23:G:O6	40:B:1301:HOH:O	2.05	0.74
11:A:572:A:OP2	28:R:80:ARG:NH2	2.21	0.74
7:5:131:THR:O	7:5:134:GLU:N	2.20	0.74
14:D:91:THR:O	14:D:93:GLY:N	2.21	0.74
6:4:11:CYS:SG	6:4:14:CYS:N	2.60	0.73
7:5:57:ASN:O	7:5:59:LEU:N	2.21	0.73
11:A:1782:U:O2	11:A:2586:U:O4	2.06	0.73
11:A:2588:G:OP2	40:A:3219:HOH:O	2.05	0.73
11:A:1186:G:OP2	40:A:3216:HOH:O	2.04	0.73
11:A:2707:U:O2	24:N:71:ARG:NH2	2.20	0.73
11:A:1922:G:O2'	31:V:25:C:C1'	2.35	0.73
11:A:1998:A:OP2	14:D:141:ARG:NH2	2.21	0.73
11:A:990:A:OP2	40:A:3221:HOH:O	2.06	0.73
11:A:1782:U:O2	11:A:2608:G:O2'	2.02	0.73
11:A:1782:U:N3	11:A:2586:U:C4	2.49	0.72
11:A:1799:G:O2'	13:C:179:GLU:OE2	2.07	0.72
17:G:22:VAL:HG12	17:G:36:LEU:CD1	2.19	0.72
11:A:2056:G:OP2	40:A:3222:HOH:O	2.06	0.72
11:A:2506:U:C4	11:A:2585:U:O4	2.43	0.72
7:5:106:PHE:O	7:5:108:VAL:N	2.22	0.72
20:J:43:GLU:O	20:J:45:THR:N	2.22	0.72
11:A:1010:A:OP2	40:A:3225:HOH:O	2.08	0.72
11:A:1439:A:OP2	40:A:3224:HOH:O	2.07	0.72
26:P:5:LYS:NZ	26:P:9:GLN:OE1	2.23	0.72
11:A:1970:A:OP2	40:A:3223:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:21:ASP:O	11:A:2062:A:N1	2.23	0.71
11:A:621:A:OP2	40:A:3226:HOH:O	2.08	0.71
11:A:1604:C:OP1	40:A:3228:HOH:O	2.09	0.71
11:A:1993:U:H4'	14:D:133:THR:HG21	1.73	0.71
11:A:2057:G:OP2	40:A:3222:HOH:O	2.08	0.71
11:A:2353:G:H1'	32:W:30:VAL:HG12	1.72	0.70
11:A:1776:G:OP2	40:A:3230:HOH:O	2.09	0.70
11:A:161:A:H3'	11:A:162:U:H5"	1.72	0.70
11:A:971:G:OP2	11:A:974:G:N2	2.25	0.70
11:A:2609:U:C4	39:A:3001:TRP:CE3	2.79	0.70
16:F:116:LEU:N	16:F:176:PHE:O	2.24	0.69
6:4:2:LYS:NZ	11:A:2478:A:OP2	2.23	0.69
11:A:512:G:N7	40:A:3288:HOH:O	2.25	0.69
7:5:1:MET:SD	7:5:2:ALA:N	2.58	0.69
11:A:981:A:OP1	40:A:3227:HOH:O	2.08	0.69
11:A:1332:G:OP1	40:A:3231:HOH:O	2.09	0.69
11:A:2247:A:OP1	40:A:3232:HOH:O	2.11	0.69
11:A:587:C:OP2	22:L:21:ARG:NH2	2.25	0.69
23:M:66:ARG:NH1	23:M:104:GLU:OE2	2.26	0.69
7:5:26:VAL:O	7:5:27:VAL:HB	1.93	0.69
11:A:2324:U:H3'	11:A:2325:G:H5"	1.74	0.69
11:A:2602:A:H4'	11:A:2603:G:H5'	1.74	0.69
11:A:1938:A:OP2	40:A:3229:HOH:O	2.09	0.69
11:A:1805:A:N3	13:C:49:THR:OG1	2.24	0.68
11:A:2506:U:O4	11:A:2585:U:O4	2.12	0.68
11:A:1936:A:N6	11:A:1963:U:O2	2.26	0.68
11:A:1820:U:OP1	13:C:176:ARG:NH1	2.27	0.68
35:Z:8:GLN:O	35:Z:10:ARG:N	2.25	0.68
11:A:2269:G:OP1	40:A:3233:HOH:O	2.11	0.68
11:A:2615:U:OP1	40:A:3235:HOH:O	2.12	0.68
32:W:30:VAL:HG13	32:W:30:VAL:O	1.92	0.68
7:5:24:SER:CB	7:5:116:GLU:HG2	2.24	0.68
12:B:73:A:C4	12:B:104:A:C2	2.82	0.68
21:K:76:VAL:HB	26:P:72:VAL:HG22	1.76	0.68
7:5:129:LEU:O	7:5:131:THR:N	2.25	0.67
11:A:1658:C:OP1	40:A:3234:HOH:O	2.11	0.67
11:A:2091:C:O2	33:X:33:HIS:NE2	2.26	0.67
11:A:1417:C:HO2'	11:A:1587:G:HO2'	1.40	0.67
22:L:93:ASN:O	22:L:95:LEU:N	2.27	0.67
11:A:120:U:OP1	40:A:3236:HOH:O	2.12	0.67
7:5:25:ALA:O	7:5:26:VAL:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:149:ASN:OD1	14:D:150:GLN:N	2.26	0.67
11:A:1614:A:N6	29:S:87:PRO:HB3	2.10	0.67
19:I:100:ILE:HB	19:I:139:VAL:HA	1.76	0.67
11:A:324:A:N6	11:A:338:G:O2'	2.27	0.67
11:A:2602:A:O2'	31:V:74:C:OP1	2.12	0.67
22:L:93:ASN:OD1	22:L:94:THR:N	2.28	0.67
20:J:4:PHE:N	20:J:44:TYR:OH	2.28	0.67
11:A:948:C:O2	11:A:984:A:O2'	2.12	0.66
11:A:2142:A:H4'	11:A:2143:C:OP2	1.96	0.66
11:A:42:A:C2'	11:A:43:G:H5'	2.24	0.66
21:K:18:ARG:HB2	21:K:45:GLU:HB2	1.77	0.66
11:A:1922:G:C2'	31:V:25:C:HO2'	2.04	0.66
21:K:71:ARG:HB3	21:K:72:PRO:HD3	1.78	0.66
24:N:118:ARG:O	24:N:120:GLU:N	2.30	0.65
32:W:37:VAL:HG12	32:W:38:ARG:H	1.61	0.65
11:A:363:G:H2'	11:A:364:C:C6	2.31	0.65
25:O:76:LYS:NZ	25:O:80:GLU:OE2	2.29	0.65
29:S:88:ARG:HB3	29:S:88:ARG:CZ	2.26	0.65
11:A:1199:U:H5'	27:Q:4:LYS:HE3	1.79	0.65
11:A:1669:A:OP2	40:A:3241:HOH:O	2.15	0.65
11:A:999:U:OP2	40:A:3243:HOH:O	2.15	0.65
7:5:39:THR:HA	7:5:42:ARG:HD2	1.78	0.65
11:A:1908:C:O2'	31:V:12:G:C5'	2.45	0.65
17:G:38:ASP:N	17:G:38:ASP:OD1	2.29	0.65
7:5:117:LEU:HD22	7:5:120:ALA:HA	1.76	0.65
11:A:861:A:N3	12:B:79:G:O2'	2.27	0.65
11:A:1670:C:OP1	40:A:3239:HOH:O	2.14	0.65
11:A:2608:G:C8	11:A:2608:G:C5'	2.76	0.65
11:A:2588:G:OP2	40:A:3242:HOH:O	2.15	0.64
15:E:58:LYS:NZ	15:E:70:SER:O	2.31	0.64
20:J:6:ALA:HB3	20:J:45:THR:HG21	1.78	0.64
13:C:43:ASN:OD1	13:C:44:ASN:N	2.30	0.64
20:J:44:TYR:HB2	27:Q:63:ARG:HB3	1.79	0.64
26:P:4:ILE:O	26:P:6:GLN:N	2.31	0.64
11:A:1378:A:O2'	11:A:1380:G:N7	2.27	0.64
11:A:1617:C:OP1	40:A:3244:HOH:O	2.15	0.64
11:A:1614:A:N1	29:S:87:PRO:HB3	2.13	0.64
11:A:1482:G:H1'	11:A:1509:A:H61	1.62	0.63
26:P:50:ARG:HG3	26:P:57:ALA:O	1.97	0.63
11:A:2602:A:H2'	31:V:74:C:H5"	1.80	0.63
17:G:1:SER:O	17:G:3:VAL:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:18:ARG:O	29:S:19:LEU:HB2	1.98	0.63
9:7:22:HIS:O	11:A:2506:U:H5	1.80	0.63
11:A:2061:G:OP2	40:A:3246:HOH:O	2.16	0.63
11:A:1813:G:H1'	13:C:49:THR:HG21	1.81	0.63
11:A:42:A:H2'	11:A:43:G:H5'	1.80	0.63
11:A:511:U:OP2	40:A:3245:HOH:O	2.16	0.63
11:A:923:G:H1'	32:W:23:LYS:HD3	1.81	0.63
19:I:73:PRO:O	19:I:112:LYS:NZ	2.31	0.63
29:S:88:ARG:HG2	29:S:94:ASP:OD2	1.99	0.63
32:W:35:ILE:O	32:W:37:VAL:N	2.31	0.63
6:4:2:LYS:HZ1	11:A:2478:A:P	2.22	0.63
11:A:1385:A:H1'	11:A:1386:C:C6	2.34	0.63
11:A:2346:A:H3'	11:A:2347:C:C5'	2.29	0.62
19:I:131:THR:O	19:I:134:SER:OG	2.16	0.62
29:S:88:ARG:HG2	29:S:88:ARG:HH11	1.64	0.62
32:W:9:THR:OG1	32:W:10:ARG:N	2.31	0.62
11:A:163:C:O2'	11:A:164:C:O5'	2.17	0.62
12:B:87:U:H3'	12:B:88:C:H5'	1.81	0.62
2:0:42:ILE:HD11	24:N:98:LEU:HB3	1.79	0.62
30:T:32:LEU:H	30:T:83:ALA:HB3	1.63	0.62
19:I:108:ILE:O	19:I:111:THR:OG1	2.17	0.62
24:N:73:ASN:HA	24:N:76:VAL:HG12	1.82	0.62
11:A:546:U:O2'	11:A:547:A:H4'	1.99	0.62
11:A:856:G:H21	32:W:19:ARG:NH2	1.97	0.62
11:A:1922:G:O3'	31:V:25:C:C4'	2.46	0.62
11:A:819:A:OP2	11:A:1187:G:N2	2.23	0.62
11:A:1248:G:N7	15:E:46:GLN:NE2	2.48	0.61
11:A:2499:C:O2	40:A:3238:HOH:O	2.13	0.61
7:5:27:VAL:HG13	7:5:83:ALA:HB3	1.83	0.61
26:P:50:ARG:CB	26:P:57:ALA:H	2.12	0.61
11:A:1567:G:H5'	13:C:57:HIS:CD2	2.35	0.61
11:A:1359:A:OP1	40:A:3248:HOH:O	2.16	0.61
11:A:2011:U:OP2	29:S:16:LYS:NZ	2.31	0.61
11:A:1938:A:OP2	40:A:3249:HOH:O	2.16	0.60
6:4:36:ARG:HG2	6:4:37:GLN:H	1.66	0.60
19:I:100:ILE:HG22	19:I:101:SER:N	2.15	0.60
11:A:370:G:O2'	11:A:424:G:OP1	2.14	0.60
11:A:616:A:H4'	15:E:101:TYR:CE2	2.36	0.60
20:J:6:ALA:CB	20:J:45:THR:HG21	2.31	0.60
11:A:276:U:O2'	11:A:278:A:N7	2.34	0.60
24:N:98:LEU:O	24:N:112:TYR:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:105:ALA:O	25:O:107:ALA:N	2.35	0.60
11:A:1338:G:O2'	30:T:18:GLU:OE2	2.20	0.60
11:A:2681:C:OP2	14:D:114:LYS:NZ	2.33	0.60
7:5:15:VAL:HG22	7:5:66:GLY:HA3	1.84	0.60
7:5:26:VAL:HG21	7:5:115:GLY:N	2.06	0.60
11:A:1828:G:OP2	40:A:3250:HOH:O	2.16	0.60
7:5:29:ASP:HA	7:5:108:VAL:HG11	1.82	0.60
14:D:118:PHE:HD1	14:D:119:ALA:H	1.49	0.60
11:A:370:G:OP2	40:A:3251:HOH:O	2.16	0.60
11:A:1782:U:N3	11:A:2586:U:N3	2.46	0.60
11:A:1262:A:OP2	29:S:99:ARG:NH2	2.35	0.60
13:C:16:VAL:N	13:C:203:VAL:HG12	2.17	0.60
32:W:55:ASP:O	32:W:57:THR:N	2.35	0.60
19:I:93:ASN:ND2	19:I:135:MET:O	2.35	0.59
11:A:963:U:OP2	40:A:3247:HOH:O	2.16	0.59
11:A:1803:A:O3'	13:C:256:THR:OG1	2.20	0.59
11:A:2353:G:N3	32:W:30:VAL:CG1	2.65	0.59
11:A:983:A:C6	11:A:984:A:C2	2.90	0.59
8:6:18:ASP:OD1	8:6:18:ASP:N	2.32	0.59
11:A:2800:A:H3'	11:A:2801:G:C5'	2.32	0.59
25:O:89:ASP:HA	25:O:116:GLN:HB3	1.84	0.59
11:A:635:C:OP2	22:L:126:ARG:NH2	2.35	0.59
7:5:62:ARG:NH2	11:A:1106:G:OP1	2.35	0.59
19:I:92:PRO:O	19:I:94:LYS:N	2.36	0.59
11:A:1131:G:OP1	20:J:82:GLY:HA2	2.02	0.59
26:P:63:ILE:HA	26:P:68:GLY:HA2	1.85	0.59
11:A:2062:A:O2'	11:A:2063:C:H6	1.85	0.58
30:T:35:ALA:HB3	30:T:38:ALA:HB2	1.85	0.58
11:A:800:A:OP1	40:A:3252:HOH:O	2.17	0.58
11:A:947:A:HO2'	11:A:984:A:H2	1.50	0.58
11:A:1076:C:H2'	11:A:1077:A:O4'	2.04	0.58
13:C:77:VAL:HG23	13:C:111:ALA:HA	1.85	0.58
27:Q:84:LYS:O	27:Q:86:SER:N	2.36	0.58
11:A:1782:U:O2'	11:A:2608:G:O2'	2.21	0.58
27:Q:63:ARG:NH1	27:Q:95:ALA:O	2.36	0.58
32:W:76:ARG:HH11	32:W:76:ARG:CG	2.17	0.58
11:A:802:A:OP1	40:A:3254:HOH:O	2.17	0.58
32:W:51:GLY:HA3	32:W:59:PHE:CE1	2.38	0.58
30:T:19:LYS:O	30:T:23:ALA:N	2.34	0.58
7:5:45:GLY:HA2	7:5:49:GLY:HA2	1.86	0.58
11:A:784:G:O2'	11:A:785:G:OP2	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1076:C:H1'	19:I:93:ASN:HB3	1.86	0.58
11:A:1359:A:OP1	40:A:3253:HOH:O	2.17	0.58
11:A:1386:C:H2'	11:A:1387:A:C8	2.39	0.58
27:Q:81:GLY:O	27:Q:85:ALA:N	2.37	0.58
30:T:54:GLU:HG3	30:T:88:LYS:HB2	1.86	0.58
11:A:673:C:OP1	15:E:49:ARG:NH1	2.36	0.58
11:A:1923:U:H5'	31:V:25:C:O4'	2.04	0.58
11:A:2780:G:OP2	20:J:120:ARG:NE	2.33	0.58
11:A:1923:U:C5'	31:V:24:G:C2'	2.76	0.57
11:A:2502:G:OP2	40:A:3257:HOH:O	2.17	0.57
11:A:81:G:HO2'	11:A:295:G:HO2'	1.47	0.57
11:A:422:A:C2	11:A:423:A:C4	2.93	0.57
15:E:168:ASP:OD2	15:E:170:ARG:NH1	2.36	0.57
21:K:121:GLU:OE2	26:P:62:LYS:NZ	2.36	0.57
11:A:1936:A:H2	11:A:1943:U:C5	2.22	0.57
11:A:1922:G:O2'	31:V:25:C:C2'	2.47	0.57
27:Q:63:ARG:HH22	27:Q:95:ALA:C	2.08	0.57
26:P:50:ARG:HB3	26:P:57:ALA:N	2.16	0.57
7:5:3:LEU:CD1	7:5:5:LEU:HG	2.35	0.57
11:A:2331:G:O2'	11:A:2336:A:N1	2.38	0.57
11:A:2517:C:C6	11:A:2542:A:N7	2.73	0.57
11:A:2548:U:O2	21:K:23:LYS:NZ	2.37	0.57
19:I:37:PHE:O	19:I:41:PHE:HB3	2.04	0.57
23:M:41:LEU:HD11	23:M:126:ILE:HD13	1.85	0.57
32:W:51:GLY:HA3	32:W:59:PHE:CZ	2.39	0.57
27:Q:105:PHE:O	27:Q:108:LEU:N	2.38	0.56
11:A:31:C:OP1	40:A:3258:HOH:O	2.18	0.56
11:A:1353:A:C8	11:A:1378:A:N6	2.73	0.56
13:C:14:HIS:O	13:C:203:VAL:HG11	2.05	0.56
32:W:28:GLU:HB3	32:W:31:LEU:HD21	1.86	0.56
32:W:39:GLN:HG2	32:W:41:GLY:H	1.69	0.56
11:A:1315:C:OP2	40:A:3260:HOH:O	2.18	0.56
11:A:1324:G:C4	11:A:1328:A:N6	2.74	0.56
19:I:100:ILE:HD11	19:I:137:LEU:HG	1.88	0.56
7:5:58:THR:CG2	11:A:1107:G:H5"	2.36	0.56
26:P:58:PHE:CD1	26:P:75:THR:HG22	2.40	0.56
22:L:85:VAL:CG2	22:L:94:THR:HG22	2.36	0.56
32:W:18:LYS:HG3	32:W:19:ARG:N	2.21	0.56
11:A:910:A:N6	11:A:2277:G:O2'	2.36	0.56
11:A:2439:A:N6	31:V:76:A:OP1	2.39	0.56
15:E:150:THR:HG21	15:E:153:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1908:C:HO2'	31:V:12:G:H5'	1.71	0.56
11:A:2680:U:H5'	14:D:194:PRO:HA	1.88	0.56
7:5:132:TYR:CZ	8:6:23:ILE:HD11	2.40	0.56
11:A:1332:G:OP1	40:A:3260:HOH:O	2.18	0.56
11:A:1773:A:N7	11:A:1829:A:H1'	2.20	0.56
20:J:81:ILE:HG13	20:J:82:GLY:N	2.21	0.56
30:T:59:ASN:O	30:T:83:ALA:O	2.24	0.56
7:5:56:ARG:O	7:5:57:ASN:ND2	2.39	0.56
11:A:100:U:H4'	11:A:101:A:O5'	2.06	0.56
11:A:443:A:N7	15:E:40:ARG:HD3	2.21	0.56
33:X:32:LEU:O	33:X:33:HIS:ND1	2.39	0.56
7:5:129:LEU:C	7:5:131:THR:H	2.10	0.55
3:1:8:ILE:HD11	3:1:24:LYS:N	2.21	0.55
34:Y:56:LEU:O	34:Y:58:ASN:N	2.39	0.55
11:A:283:G:C2	11:A:284:U:H1'	2.41	0.55
11:A:1482:G:C6	11:A:1508:A:C2	2.94	0.55
30:T:32:LEU:N	30:T:83:ALA:HB3	2.21	0.55
2:0:2:VAL:HG22	11:A:2015:A:C2	2.41	0.55
3:1:20:TYR:HH	11:A:2347:C:HO2'	1.55	0.55
11:A:2355:G:H4'	32:W:20:LEU:HD13	1.88	0.55
19:I:116:MET:SD	19:I:124:MET:HE2	2.46	0.55
7:5:43:LYS:HZ3	7:5:98:GLU:HB2	1.72	0.55
7:5:64:VAL:O	7:5:68:PRO:HD2	2.06	0.55
11:A:1019:U:H3	11:A:1142:A:H62	1.52	0.55
11:A:1654:A:O2'	14:D:118:PHE:CG	2.55	0.55
7:5:81:LEU:HA	11:A:1107:G:H4'	1.88	0.55
11:A:1458:U:H4'	11:A:1459:G:O5'	2.07	0.55
11:A:1715:G:N2	11:A:1744:A:OP2	2.36	0.55
28:R:39:LEU:O	28:R:49:ILE:HG23	2.07	0.55
11:A:1909:C:H4'	31:V:11:C:C4'	2.30	0.55
19:I:135:MET:HB3	19:I:137:LEU:HD22	1.88	0.55
24:N:30:ARG:NH1	24:N:74:GLU:OE2	2.40	0.55
11:A:811:U:C4	22:L:21:ARG:NH1	2.75	0.55
16:F:151:LEU:HD12	16:F:152:ASP:N	2.21	0.55
11:A:565:C:O3'	40:A:3262:HOH:O	2.18	0.55
11:A:1824:G:N3	13:C:251:THR:HG21	2.21	0.55
27:Q:93:ILE:O	27:Q:96:ASP:N	2.39	0.55
11:A:277:G:O2'	11:A:278:A:OP2	2.25	0.55
25:O:2:ASP:OD1	25:O:3:LYS:N	2.39	0.55
11:A:834:G:C6	11:A:835:C:C4	2.95	0.54
11:A:2757:A:N1	17:G:66:THR:HG21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:68:ARG:CD	13:C:103:ILE:HD11	2.36	0.54
27:Q:91:ARG:NH1	28:R:10:LYS:HB3	2.22	0.54
4:2:3:ARG:NH2	11:A:752:A:OP1	2.41	0.54
11:A:411:G:OP2	11:A:2406:A:O2'	2.25	0.54
11:A:1397:U:OP2	11:A:1398:C:N4	2.34	0.54
11:A:1754:A:H4'	26:P:102:ARG:NH2	2.22	0.54
11:A:2335:A:C6	11:A:2337:G:H1'	2.42	0.54
14:D:107:VAL:CG2	14:D:203:VAL:HG23	2.38	0.54
26:P:33:GLU:HB2	26:P:38:ARG:HH21	1.71	0.54
11:A:1676:A:OP2	40:A:3259:HOH:O	2.18	0.54
11:A:1786:A:H1'	11:A:1938:A:N6	2.22	0.54
21:K:43:ILE:CD1	21:K:52:VAL:HB	2.37	0.54
2:0:2:VAL:HG11	11:A:2016:U:H1'	1.90	0.54
11:A:163:C:O2'	11:A:164:C:P	2.65	0.54
17:G:84:LYS:HG3	17:G:132:LEU:H	1.73	0.54
20:J:17:VAL:HG23	20:J:139:VAL:HA	1.88	0.54
26:P:50:ARG:CG	26:P:57:ALA:O	2.55	0.54
11:A:686:U:H2'	11:A:788:A:N1	2.21	0.54
11:A:877:A:C2	11:A:899:A:C2	2.96	0.54
11:A:1779:U:H5	11:A:1784:A:N7	2.06	0.54
20:J:32:LEU:HD22	20:J:54:ILE:HD12	1.90	0.54
26:P:4:ILE:HG22	26:P:5:LYS:H	1.72	0.54
32:W:63:ASP:OD1	32:W:63:ASP:N	2.35	0.54
7:5:23:LEU:HG	7:5:24:SER:N	2.22	0.54
9:7:23:ARG:HG3	9:7:23:ARG:O	2.08	0.54
11:A:855:G:H1'	32:W:23:LYS:HE3	1.89	0.54
11:A:1909:C:C4'	31:V:11:C:O2'	2.55	0.54
11:A:1936:A:N6	11:A:1963:U:H3	2.05	0.54
11:A:2415:G:H4'	22:L:66:PHE:HB2	1.90	0.54
14:D:118:PHE:O	14:D:120:GLY:N	2.36	0.54
23:M:33:LEU:HD22	23:M:128:THR:HB	1.90	0.54
11:A:2579:C:OP1	40:A:3256:HOH:O	2.17	0.54
12:B:55:U:O3'	16:F:23:SER:OG	2.21	0.54
22:L:77:ILE:CD1	22:L:108:ALA:HB1	2.38	0.54
7:5:44:ALA:O	7:5:49:GLY:N	2.40	0.54
11:A:384:A:H2'	11:A:385:C:H5'	1.90	0.54
11:A:396:G:OP2	33:X:9:LYS:NZ	2.40	0.54
11:A:674:G:H1'	15:E:69:ARG:HE	1.72	0.54
11:A:1772:A:N1	11:A:1980:G:C6	2.76	0.54
16:F:103:ILE:HG23	16:F:175:PRO:HD3	1.90	0.54
21:K:80:ASP:HB2	26:P:67:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:T:50:LEU:C	30:T:52:GLU:H	2.11	0.54
11:A:299:A:OP2	40:A:3264:HOH:O	2.18	0.54
6:4:36:ARG:NH1	11:A:2742:G:OP1	2.38	0.54
11:A:2698:U:H2'	11:A:2699:C:H6	1.72	0.54
27:Q:81:GLY:HA2	27:Q:116:LEU:CD1	2.38	0.54
35:Z:5:LYS:H	35:Z:5:LYS:HD2	1.72	0.54
2:0:12:ARG:NH1	11:A:1263:U:OP1	2.41	0.53
11:A:1738:G:O2'	11:A:1739:A:O5'	2.25	0.53
21:K:10:VAL:HG11	21:K:16:ALA:HB3	1.90	0.53
28:R:49:ILE:HB	28:R:51:VAL:O	2.08	0.53
6:4:1:MET:N	11:A:2526:G:N3	2.57	0.53
10:8:80:HIS:HD2	10:8:83:LYS:N	2.05	0.53
11:A:630:G:N2	11:A:633:A:OP2	2.37	0.53
11:A:1930:G:O2'	11:A:1968:G:O6	2.17	0.53
14:D:120:GLY:HA2	14:D:162:ALA:CB	2.38	0.53
11:A:27:G:O2'	11:A:28:A:OP2	2.19	0.53
11:A:1001:A:OP2	40:A:3265:HOH:O	2.19	0.53
17:G:84:LYS:HB3	17:G:132:LEU:O	2.09	0.53
29:S:88:ARG:HH11	29:S:88:ARG:CG	2.17	0.53
32:W:46:ALA:HB3	32:W:80:SER:HB3	1.91	0.53
7:5:4:ASN:O	7:5:6:GLN:N	2.41	0.53
7:5:60:LEU:O	7:5:64:VAL:HB	2.08	0.53
9:7:15:ILE:HB	39:A:3001:TRP:CH2	2.43	0.53
11:A:2547:A:H2'	11:A:2548:U:C6	2.43	0.53
14:D:106:LYS:HB3	14:D:206:ALA:HB3	1.89	0.53
29:S:89:ALA:O	29:S:90:LYS:HB2	2.08	0.53
7:5:54:VAL:HA	7:5:84:TYR:O	2.08	0.53
7:5:129:LEU:HB3	7:5:130:PRO:HD2	1.89	0.53
11:A:265:A:H4'	11:A:266:G:OP1	2.07	0.53
27:Q:65:ASN:OD1	27:Q:69:ARG:NH1	2.42	0.53
11:A:1187:G:H5"	28:R:83:TYR:CE2	2.44	0.53
32:W:13:ARG:HG2	32:W:14:ASP:H	1.74	0.53
7:5:25:ALA:HB3	7:5:85:SER:OG	2.09	0.53
11:A:954:G:OP2	23:M:16:ARG:NH2	2.42	0.53
11:A:2425:A:H5"	11:A:2427:C:O4'	2.09	0.53
7:5:58:THR:HB	7:5:82:ILE:HB	1.89	0.53
11:A:1069:A:C4	11:A:1073:A:N7	2.77	0.53
11:A:1080:A:H1'	19:I:127:SER:HA	1.91	0.53
11:A:1759:A:HO2'	11:A:2714:G:HO2'	1.51	0.53
19:I:98:GLY:HA3	19:I:137:LEU:HB3	1.90	0.53
20:J:39:LYS:HA	20:J:43:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:70:ARG:HD3	21:K:76:VAL:HG22	1.90	0.53
28:R:49:ILE:HG22	28:R:54:VAL:HG13	1.89	0.53
30:T:44:LYS:HG3	30:T:55:VAL:HG11	1.90	0.53
30:T:50:LEU:O	30:T:52:GLU:N	2.42	0.53
32:W:37:VAL:HB	32:W:38:ARG:HH11	1.74	0.53
29:S:73:LYS:HB3	29:S:106:VAL:HB	1.90	0.53
32:W:37:VAL:HG13	32:W:55:ASP:C	2.29	0.53
11:A:1535:A:H4'	11:A:1536:C:OP2	2.08	0.53
11:A:2134:A:HO2'	11:A:2135:A:H8	1.56	0.53
11:A:2297:A:N1	11:A:2321:U:H5	2.07	0.53
11:A:189:G:O6	11:A:205:G:O2'	2.19	0.52
11:A:273:G:N2	11:A:365:U:C2	2.78	0.52
25:O:31:THR:HG22	25:O:34:HIS:H	1.74	0.52
26:P:50:ARG:CD	26:P:51:ASN:N	2.72	0.52
27:Q:63:ARG:HH12	27:Q:96:ASP:CA	2.22	0.52
30:T:50:LEU:HD12	30:T:50:LEU:H	1.74	0.52
11:A:1069:A:C5	11:A:1073:A:N7	2.77	0.52
25:O:36:TYR:N	25:O:36:TYR:CD1	2.78	0.52
35:Z:48:ASN:O	35:Z:51:SER:OG	2.27	0.52
7:5:81:LEU:HD23	7:5:82:ILE:N	2.24	0.52
11:A:1288:G:C4	11:A:1327:A:C2	2.98	0.52
11:A:2092:U:H4'	11:A:2093:G:O5'	2.09	0.52
11:A:2232:C:P	33:X:26:ARG:HH22	2.33	0.52
11:A:2502:G:H5'	11:A:2503:A:H5"	1.92	0.52
7:5:36:ASP:O	7:5:39:THR:OG1	2.26	0.52
7:5:118:ILE:HB	7:5:119:PRO:CD	2.39	0.52
11:A:2053:G:H1	11:A:2616:C:H42	1.57	0.52
11:A:2211:A:O2'	11:A:2212:A:OP1	2.25	0.52
27:Q:31:TYR:O	27:Q:34:ALA:N	2.42	0.52
11:A:1328:A:H2'	11:A:1330:C:C5	2.45	0.52
13:C:255:LYS:O	13:C:257:ARG:N	2.43	0.52
24:N:73:ASN:HA	24:N:76:VAL:CG1	2.39	0.52
30:T:89:GLU:O	30:T:91:GLN:N	2.41	0.52
35:Z:6:ILE:O	35:Z:34:THR:HA	2.10	0.52
7:5:43:LYS:NZ	7:5:98:GLU:HB2	2.24	0.52
11:A:2602:A:H4'	11:A:2603:G:C5'	2.39	0.52
11:A:38:A:O2'	15:E:43:THR:HA	2.09	0.52
11:A:974:G:H8	11:A:990:A:H62	1.58	0.52
13:C:256:THR:OG1	13:C:256:THR:O	2.28	0.52
2:0:2:VAL:CG1	11:A:2016:U:H1'	2.40	0.52
7:5:94:ARG:O	7:5:97:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:8:51:GLN:OE1	10:8:57:TYR:OH	2.28	0.52
11:A:1394:U:H4'	11:A:1603:A:H4'	1.91	0.52
20:J:39:LYS:HA	20:J:43:GLU:HB2	1.91	0.52
22:L:91:ASP:OD1	22:L:92:LEU:N	2.43	0.52
28:R:61:ALA:HB2	28:R:98:ILE:HA	1.92	0.52
31:V:33:U:C4	31:V:35:G:OP2	2.63	0.52
14:D:151:THR:HG22	14:D:152:PRO:HD3	1.93	0.51
23:M:8:LYS:HE3	23:M:9:PHE:CE2	2.45	0.51
32:W:16:GLU:O	32:W:17:ALA:HB3	2.10	0.51
17:G:96:ALA:HB3	17:G:103:ASN:HB2	1.92	0.51
23:M:73:ILE:HG21	23:M:91:TYR:CZ	2.45	0.51
26:P:33:GLU:CD	26:P:34:GLY:N	2.63	0.51
3:1:33:LEU:N	3:1:51:ALA:HB3	2.25	0.51
11:A:1783:A:N1	11:A:2587:A:H2'	2.25	0.51
16:F:132:ARG:O	16:F:133:GLU:HB3	2.10	0.51
10:8:44:HIS:HE1	10:8:86:LEU:H	1.59	0.51
11:A:2354:C:H4'	32:W:31:LEU:HD22	1.92	0.51
11:A:2803:G:H2'	11:A:2804:U:C6	2.45	0.51
11:A:460:A:C2	11:A:470:A:C4	2.99	0.51
11:A:729:G:H2'	11:A:1775:U:H1'	1.91	0.51
11:A:1203:U:O2'	22:L:4:ASN:OD1	2.28	0.51
15:E:148:ILE:HA	15:E:187:VAL:HB	1.93	0.51
17:G:83:THR:HA	17:G:84:LYS:CE	2.39	0.51
19:I:36:GLU:HB3	19:I:66:PHE:CE1	2.46	0.51
27:Q:94:LEU:C	27:Q:96:ASP:H	2.14	0.51
32:W:8:SER:O	32:W:9:THR:HG22	2.10	0.51
10:8:9:ARG:NH2	10:8:12:GLN:HA	2.26	0.51
11:A:1797:G:O2'	13:C:256:THR:CG2	2.59	0.51
20:J:55:ILE:HD11	20:J:130:HIS:CG	2.45	0.51
4:2:27:GLY:O	4:2:30:VAL:HB	2.11	0.51
6:4:7:VAL:O	6:4:35:GLN:NE2	2.42	0.51
11:A:565:C:H2'	11:A:566:U:O4'	2.11	0.51
11:A:1509:A:HO2'	11:A:1510:G:P	2.32	0.51
11:A:2313:C:H5"	16:F:87:LYS:HD3	1.92	0.51
11:A:2387:U:O2'	32:W:38:ARG:NH2	2.43	0.51
20:J:49:ASP:OD1	20:J:121:LYS:NZ	2.32	0.51
30:T:29:THR:OG1	30:T:86:THR:N	2.43	0.51
35:Z:41:PRO:HA	35:Z:44:ARG:HB3	1.93	0.51
11:A:1300:G:H4'	11:A:1301:A:H5'	1.92	0.51
11:A:2074:U:H2'	11:A:2075:U:C6	2.46	0.51
14:D:91:THR:O	14:D:91:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:16:VAL:HG21	17:G:44:HIS:CD2	2.46	0.51
28:R:39:LEU:HA	28:R:49:ILE:HG21	1.92	0.51
30:T:69:ARG:CG	30:T:70:HIS:H	2.23	0.51
6:4:3:VAL:HG23	6:4:4:ARG:H	1.74	0.51
7:5:3:LEU:HD12	7:5:5:LEU:H	1.76	0.51
7:5:25:ALA:O	7:5:116:GLU:OE1	2.28	0.51
11:A:27:G:N2	11:A:512:G:H1'	2.26	0.51
11:A:1776:G:OP2	40:A:3267:HOH:O	2.19	0.51
11:A:2504:U:O5'	11:A:2504:U:H6	1.94	0.51
11:A:2506:U:HO2'	11:A:2507:C:P	2.33	0.51
18:H:41:LYS:HA	18:H:44:ILE:HG12	1.93	0.51
11:A:26:G:C6	11:A:27:G:N1	2.79	0.51
11:A:1647:U:OP2	40:A:3269:HOH:O	2.19	0.51
11:A:1753:G:OP1	26:P:92:ARG:NE	2.38	0.51
11:A:1816:C:C5	13:C:61:TYR:CE2	2.99	0.51
11:A:2039:U:H2'	11:A:2040:G:C8	2.45	0.51
11:A:2314:A:OP1	16:F:87:LYS:NZ	2.44	0.51
14:D:62:LYS:HB2	14:D:63:PRO:HD3	1.93	0.50
21:K:9:ASN:O	21:K:83:ALA:HA	2.11	0.50
4:2:34:ARG:NH1	4:2:41:ARG:O	2.45	0.50
11:A:945:A:C5	11:A:2448:A:C2	2.98	0.50
11:A:2094:A:C2	11:A:2196:C:C2	2.99	0.50
16:F:71:LYS:HD3	16:F:72:SER:N	2.26	0.50
23:M:35:ALA:O	23:M:36:VAL:HB	2.11	0.50
27:Q:91:ARG:HE	27:Q:93:ILE:CG2	2.25	0.50
27:Q:94:LEU:C	27:Q:96:ASP:N	2.65	0.50
11:A:391:A:C6	11:A:411:G:C2	3.00	0.50
11:A:1179:G:H2'	11:A:1180:U:O4'	2.12	0.50
11:A:1533:C:C2	11:A:1534:U:C4	2.99	0.50
11:A:1533:C:H2'	11:A:1534:U:C6	2.46	0.50
20:J:81:ILE:CG1	20:J:82:GLY:N	2.74	0.50
32:W:76:ARG:HH11	32:W:76:ARG:HG2	1.76	0.50
11:A:139:U:O2'	30:T:1:MET:HA	2.12	0.50
11:A:1778:U:H2'	11:A:1784:A:N6	2.27	0.50
20:J:44:TYR:O	20:J:45:THR:HB	2.11	0.50
11:A:1028:A:N3	11:A:2486:C:O2'	2.42	0.50
29:S:86:MET:SD	29:S:96:ILE:HG21	2.51	0.50
35:Z:26:LEU:O	35:Z:37:ARG:NH1	2.44	0.50
21:K:19:VAL:CG1	21:K:41:ILE:HG12	2.41	0.50
21:K:107:LEU:O	21:K:109:SER:N	2.38	0.50
24:N:52:ILE:HB	24:N:94:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1322:A:OP1	29:S:11:ARG:NE	2.37	0.50
11:A:1759:A:O2'	11:A:2714:G:O2'	2.25	0.50
11:A:1654:A:H2'	11:A:1655:A:H8	1.77	0.50
11:A:1808:A:O2'	33:X:2:ARG:NH2	2.45	0.50
11:A:2571:U:O2'	14:D:151:THR:CG2	2.60	0.50
19:I:109:ALA:HB2	19:I:128:ILE:HG13	1.93	0.50
34:Y:8:GLU:O	34:Y:12:GLU:HB2	2.12	0.50
11:A:221:A:N1	11:A:265:A:O2'	2.45	0.50
11:A:586:A:N1	11:A:809:G:O2'	2.38	0.50
11:A:748:G:OP2	29:S:88:ARG:HB2	2.12	0.50
11:A:856:G:H21	32:W:19:ARG:HH22	1.58	0.50
11:A:1437:C:H2'	11:A:1438:U:C6	2.46	0.50
11:A:1750:G:O2'	11:A:2860:A:N1	2.37	0.50
22:L:81:ASP:O	22:L:83:ALA:N	2.41	0.50
29:S:88:ARG:NH1	29:S:88:ARG:CG	2.73	0.50
7:5:4:ASN:C	7:5:6:GLN:N	2.66	0.49
11:A:1869:G:H3'	11:A:1870:C:H5"	1.93	0.49
11:A:2329:U:H2'	11:A:2330:G:C8	2.47	0.49
14:D:148:GLN:OE1	14:D:148:GLN:N	2.45	0.49
20:J:21:THR:HG22	20:J:22:GLY:N	2.27	0.49
32:W:9:THR:HG23	32:W:10:ARG:HD3	1.94	0.49
11:A:322:A:H5'	11:A:340:A:H1'	1.94	0.49
29:S:20:VAL:HG11	29:S:44:ALA:HA	1.93	0.49
7:5:71:CYS:CA	7:5:117:LEU:HD13	2.31	0.49
11:A:118:A:N3	11:A:178:G:H1'	2.27	0.49
11:A:443:A:C5	15:E:40:ARG:HD3	2.47	0.49
11:A:1730:C:OP1	11:A:1730:C:H4'	2.12	0.49
11:A:2352:A:C6	32:W:30:VAL:HG11	2.47	0.49
23:M:20:LEU:HD22	23:M:20:LEU:N	2.26	0.49
23:M:106:ASP:O	23:M:108:VAL:N	2.44	0.49
33:X:70:LEU:O	33:X:75:GLU:N	2.45	0.49
35:Z:30:ARG:HB3	35:Z:30:ARG:HH11	1.76	0.49
5:3:30:HIS:HD2	11:A:2421:G:N7	2.10	0.49
11:A:489:G:N7	29:S:49:LYS:NZ	2.58	0.49
11:A:654:A:H3'	11:A:654:A:N3	2.26	0.49
7:5:55:VAL:HG13	11:A:1084:A:H5'	1.93	0.49
7:5:95:LEU:HD22	7:5:95:LEU:H	1.77	0.49
11:A:223:A:C5	11:A:422:A:C8	3.00	0.49
11:A:1475:G:O2'	11:A:1514:G:O6	2.30	0.49
14:D:193:VAL:HG21	14:D:201:LEU:HD21	1.93	0.49
29:S:13:SER:O	29:S:14:ALA:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:88:ARG:NH1	29:S:88:ARG:HB3	2.28	0.49
30:T:54:GLU:CG	30:T:88:LYS:HB2	2.42	0.49
14:D:151:THR:CG2	14:D:152:PRO:HD3	2.43	0.49
19:I:48:ILE:HG13	19:I:49:GLU:H	1.77	0.49
24:N:96:ARG:NH1	24:N:114:GLU:OE2	2.44	0.49
3:1:4:ILE:HG23	3:1:5:ARG:H	1.77	0.49
11:A:250:G:C6	11:A:251:A:C6	3.01	0.49
11:A:2211:A:O2'	11:A:2212:A:P	2.70	0.49
11:A:2228:G:H22	33:X:33:HIS:HE2	1.61	0.49
11:A:2701:U:H3'	11:A:2702:G:C5'	2.42	0.49
16:F:5:ASP:OD1	16:F:8:LYS:NZ	2.46	0.49
11:A:107:G:H2'	11:A:108:G:H8	1.78	0.49
11:A:1199:U:H5'	27:Q:4:LYS:CE	2.42	0.49
11:A:1607:C:H4'	11:A:1608:A:O5'	2.13	0.49
11:A:1778:U:H2'	11:A:1784:A:H62	1.78	0.49
11:A:2109:U:H2'	11:A:2110:G:H5'	1.93	0.49
11:A:2584:U:H2'	11:A:2585:U:O5'	2.13	0.49
15:E:112:LEU:HD13	15:E:186:VAL:HG11	1.94	0.49
17:G:30:GLY:O	17:G:32:LEU:N	2.38	0.49
19:I:123:ALA:HA	19:I:126:ARG:CZ	2.43	0.49
26:P:91:VAL:O	26:P:92:ARG:HG2	2.12	0.49
7:5:68:PRO:HA	7:5:72:LEU:HD11	1.94	0.49
7:5:138:ARG:NH2	8:6:26:MET:HA	2.28	0.49
11:A:2043:C:OP1	11:A:2777:G:O2'	2.24	0.49
11:A:2063:C:O2	11:A:2063:C:H2'	2.10	0.49
11:A:2330:G:C2	11:A:2386:A:C2	3.01	0.49
7:5:4:ASN:C	7:5:6:GLN:H	2.16	0.49
7:5:58:THR:HG23	11:A:1107:G:H5"	1.94	0.49
11:A:923:G:H1'	32:W:23:LYS:CD	2.43	0.49
11:A:1022:G:C5	11:A:1140:C:C4	3.00	0.49
11:A:1277:G:C5'	24:N:20:MET:HE2	2.43	0.49
11:A:1327:A:N6	11:A:1328:A:C2	2.81	0.49
2:0:2:VAL:CG2	11:A:2015:A:C2	2.96	0.48
11:A:995:C:O2	20:J:3:THR:HG23	2.13	0.48
11:A:1567:G:H2'	13:C:84:PRO:HG3	1.95	0.48
11:A:2867:G:O2'	11:A:2868:A:OP2	2.28	0.48
14:D:68:PHE:C	14:D:73:VAL:HG12	2.33	0.48
14:D:174:SER:OG	14:D:175:LEU:N	2.46	0.48
17:G:73:SER:O	17:G:77:GLY:N	2.45	0.48
25:O:51:ALA:HB3	25:O:78:VAL:HG13	1.95	0.48
27:Q:63:ARG:NH1	27:Q:96:ASP:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:49:ILE:HD12	28:R:52:PRO:HA	1.95	0.48
11:A:1922:G:H4'	31:V:25:C:O2'	2.13	0.48
11:A:2016:U:H2'	11:A:2017:U:C6	2.48	0.48
18:H:9:VAL:O	18:H:13:GLY:N	2.46	0.48
30:T:34:VAL:O	30:T:34:VAL:CG2	2.61	0.48
32:W:44:PHE:HD1	32:W:45:HIS:CE1	2.31	0.48
11:A:580:U:H2'	11:A:581:C:H6	1.79	0.48
11:A:749:A:C6	11:A:1618:A:C2	3.01	0.48
11:A:1474:U:H2'	11:A:1475:G:H5'	1.95	0.48
11:A:1996:C:OP1	21:K:31:ARG:NE	2.46	0.48
11:A:2230:G:O3'	33:X:29:LEU:HD23	2.14	0.48
13:C:265:PHE:N	13:C:265:PHE:CD1	2.82	0.48
33:X:70:LEU:O	33:X:74:GLY:N	2.46	0.48
11:A:308:G:O2'	11:A:329:G:N2	2.46	0.48
11:A:564:C:O2	11:A:578:G:N2	2.46	0.48
11:A:1417:C:N3	11:A:1581:G:N2	2.60	0.48
11:A:1760:C:H2'	11:A:1761:C:O4'	2.14	0.48
15:E:32:VAL:HG23	15:E:178:VAL:HG12	1.94	0.48
23:M:1:MET:O	23:M:2:LEU:CB	2.62	0.48
32:W:18:LYS:CG	32:W:19:ARG:N	2.77	0.48
11:A:856:G:O2'	32:W:22:VAL:HG23	2.14	0.48
11:A:2393:U:H5'	22:L:60:ARG:O	2.13	0.48
16:F:110:ILE:O	16:F:112:ASP:N	2.46	0.48
17:G:15:ASP:O	17:G:16:VAL:HG13	2.12	0.48
20:J:43:GLU:O	20:J:45:THR:HG22	2.13	0.48
22:L:19:LEU:HB2	22:L:27:LEU:HB3	1.94	0.48
7:5:77:VAL:O	7:5:79:PRO:HD2	2.13	0.48
11:A:2355:G:H4'	32:W:20:LEU:CD1	2.44	0.48
19:I:14:ALA:HB3	19:I:51:GLY:H	1.79	0.48
32:W:49:ASN:ND2	32:W:49:ASN:C	2.66	0.48
35:Z:38:GLU:O	35:Z:43:ILE:HG12	2.13	0.48
5:3:63:TYR:HH	11:A:592:A:HO2'	1.62	0.48
11:A:995:C:N4	20:J:2:LYS:HB3	2.29	0.48
11:A:2747:G:O2'	17:G:66:THR:HG22	2.14	0.48
16:F:79:ARG:HB3	16:F:82:TYR:CE1	2.48	0.48
23:M:53:MET:HE3	23:M:63:ILE:HD13	1.95	0.48
26:P:19:PHE:N	26:P:19:PHE:CD1	2.82	0.48
29:S:24:ILE:HG22	29:S:71:VAL:HG11	1.95	0.48
29:S:88:ARG:HG2	29:S:94:ASP:CG	2.34	0.48
33:X:39:VAL:HG22	33:X:44:ARG:O	2.14	0.48
11:A:301:G:H1'	11:A:302:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2346:A:H3'	11:A:2347:C:H5"	1.95	0.48
11:A:2678:C:H2'	11:A:2679:A:O4'	2.14	0.48
11:A:2800:A:H3'	11:A:2801:G:H5"	1.96	0.48
13:C:225:ASN:HB3	13:C:226:PRO:HD2	1.95	0.48
15:E:164:LEU:HB3	15:E:167:VAL:CG1	2.44	0.48
16:F:10:GLU:O	16:F:12:VAL:N	2.44	0.48
16:F:79:ARG:HB3	16:F:82:TYR:CZ	2.48	0.48
19:I:87:SER:OG	19:I:88:GLY:N	2.43	0.48
21:K:24:VAL:HG13	21:K:33:ALA:HB2	1.95	0.48
32:W:18:LYS:HA	32:W:36:ILE:HG13	1.95	0.48
32:W:23:LYS:HE2	32:W:24:ARG:H	1.78	0.48
4:2:10:LEU:HD23	11:A:770:G:H5"	1.96	0.48
7:5:110:ALA:HB1	7:5:113:PHE:CZ	2.49	0.48
11:A:1485:U:H2'	11:A:1486:U:C6	2.49	0.48
11:A:2406:A:C2	22:L:69:ARG:NH2	2.82	0.48
19:I:40:ALA:O	19:I:43:ALA:HB3	2.14	0.48
19:I:135:MET:HB3	19:I:137:LEU:CD2	2.43	0.48
23:M:34:LYS:HD2	23:M:131:VAL:HG11	1.95	0.48
7:5:39:THR:HA	7:5:42:ARG:CD	2.43	0.48
11:A:479:A:C2	11:A:480:A:C4	3.01	0.48
11:A:996:A:H4'	27:Q:91:ARG:NE	2.29	0.48
11:A:1022:G:C6	11:A:1140:C:C4	3.01	0.48
11:A:1348:C:H2'	11:A:1349:C:H5'	1.96	0.48
11:A:1814:G:C6	11:A:1815:A:N6	2.82	0.48
11:A:2581:G:C2	11:A:2610:C:C6	3.02	0.48
13:C:232:GLY:H	13:C:241:LYS:HE3	1.79	0.48
14:D:148:GLN:HB2	14:D:152:PRO:HG2	1.96	0.48
17:G:22:VAL:HG23	17:G:22:VAL:O	2.14	0.48
17:G:104:LEU:HB2	17:G:112:VAL:HG21	1.96	0.48
20:J:32:LEU:CD2	20:J:54:ILE:HD12	2.44	0.48
32:W:39:GLN:HG2	32:W:40:ARG:N	2.28	0.48
11:A:11:C:C3'	11:A:12:U:H5'	2.44	0.47
11:A:391:A:C5	11:A:411:G:C2	3.02	0.47
11:A:528:A:C2	11:A:2043:C:H4'	2.49	0.47
19:I:60:VAL:HG22	19:I:66:PHE:HB3	1.95	0.47
20:J:44:TYR:CD1	27:Q:63:ARG:HG2	2.49	0.47
31:V:6:C:H2'	31:V:7:G:H8	1.78	0.47
7:5:15:VAL:HG21	7:5:66:GLY:HA2	1.96	0.47
7:5:51:TYR:C	7:5:51:TYR:CD1	2.86	0.47
11:A:1135:C:N4	11:A:1139:G:C6	2.82	0.47
11:A:1268:A:OP1	40:A:3270:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1799:G:C5	13:C:175:LEU:HD23	2.49	0.47
16:F:134:GLN:O	16:F:136:ILE:N	2.47	0.47
24:N:103:ARG:HD3	24:N:110:MET:HE3	1.96	0.47
29:S:63:GLY:O	29:S:64:ALA:CB	2.62	0.47
31:V:34:G:C2	31:V:35:G:C4	3.02	0.47
32:W:49:ASN:HA	32:W:61:LYS:HB2	1.94	0.47
33:X:39:VAL:HG21	33:X:42:GLU:HB2	1.96	0.47
33:X:67:LEU:HD23	33:X:70:LEU:HD12	1.95	0.47
11:A:747:U:O2'	29:S:88:ARG:NE	2.47	0.47
11:A:954:G:O2'	11:A:2274:A:N1	2.41	0.47
11:A:983:A:N6	11:A:984:A:C2	2.82	0.47
11:A:999:U:OP2	40:A:3268:HOH:O	2.19	0.47
11:A:1327:A:H2'	11:A:1328:A:O4'	2.14	0.47
11:A:2587:A:O5'	11:A:2587:A:H8	1.97	0.47
28:R:68:ARG:HD3	28:R:92:TRP:CZ2	2.49	0.47
3:1:16:THR:HG21	3:1:41:VAL:HG13	1.97	0.47
7:5:51:TYR:HD1	7:5:52:MET:N	2.12	0.47
7:5:110:ALA:HB1	7:5:113:PHE:CE1	2.49	0.47
11:A:451:U:C2	11:A:453:A:N7	2.83	0.47
11:A:2902:C:C2'	11:A:2903:U:O5'	2.63	0.47
17:G:23:ILE:HG21	17:G:71:LEU:HD11	1.95	0.47
17:G:84:LYS:HG3	17:G:132:LEU:N	2.28	0.47
20:J:84:ILE:HG23	20:J:84:ILE:O	2.15	0.47
32:W:42:THR:HG22	32:W:43:LYS:HZ2	1.80	0.47
2:0:9:ARG:NH1	11:A:517:C:OP2	2.48	0.47
11:A:523:C:H5"	11:A:540:C:O2'	2.15	0.47
11:A:1474:U:C2'	11:A:1475:G:H5'	2.44	0.47
11:A:1738:G:HO2'	11:A:1739:A:P	2.38	0.47
11:A:2506:U:O2	11:A:2506:U:H2'	2.14	0.47
7:5:100:ALA:HB2	7:5:125:ARG:HE	1.79	0.47
11:A:478:A:C6	11:A:480:A:C6	3.03	0.47
11:A:587:C:P	22:L:21:ARG:NH2	2.88	0.47
11:A:725:G:C6	11:A:726:G:N1	2.82	0.47
11:A:2425:A:C5'	11:A:2427:C:O4'	2.62	0.47
14:D:35:THR:N	14:D:49:GLN:O	2.41	0.47
17:G:112:VAL:HG23	17:G:113:ASP:N	2.28	0.47
21:K:30:ARG:NH1	21:K:32:TYR:O	2.45	0.47
27:Q:91:ARG:HH21	27:Q:93:ILE:HD13	1.80	0.47
32:W:47:GLY:H	32:W:80:SER:HB3	1.80	0.47
7:5:23:LEU:H	7:5:87:GLU:HB2	1.79	0.47
7:5:60:LEU:HD23	7:5:78:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:419:U:H2'	11:A:420:C:C6	2.50	0.47
11:A:947:A:O2'	11:A:984:A:H2	1.98	0.47
11:A:1010:A:OP2	40:A:3273:HOH:O	2.20	0.47
11:A:1069:A:C1'	11:A:1073:A:H62	2.27	0.47
11:A:1090:A:C2	11:A:1102:C:H1'	2.50	0.47
11:A:1219:U:OP2	27:Q:18:LYS:NZ	2.46	0.47
11:A:2839:G:N2	11:A:2880:C:C4	2.82	0.47
16:F:69:ALA:N	16:F:82:TYR:O	2.47	0.47
17:G:118:ALA:O	17:G:120:ILE:N	2.41	0.47
24:N:12:ARG:CZ	24:N:20:MET:HE1	2.44	0.47
28:R:64:VAL:HG21	28:R:97:LYS:HB2	1.97	0.47
32:W:30:VAL:HG23	32:W:60:ALA:O	2.15	0.47
34:Y:56:LEU:O	34:Y:57:LEU:HB3	2.14	0.47
6:4:6:SER:HB2	11:A:1031:G:H4'	1.95	0.47
7:5:88:HIS:CB	7:5:89:PRO:HD3	2.44	0.47
11:A:479:A:H4'	11:A:480:A:OP1	2.15	0.47
11:A:1923:U:H5"	31:V:24:G:H2'	1.90	0.47
11:A:2335:A:C5	11:A:2337:G:C4	3.02	0.47
11:A:2862:G:C5	11:A:2863:C:C5	3.02	0.47
22:L:82:LEU:CD1	22:L:116:VAL:HG23	2.44	0.47
23:M:46:ILE:HD13	23:M:47:GLU:N	2.30	0.47
30:T:61:LEU:C	30:T:61:LEU:HD12	2.35	0.47
32:W:9:THR:HG23	32:W:10:ARG:N	2.30	0.47
32:W:28:GLU:O	32:W:30:VAL:N	2.48	0.47
3:1:4:ILE:HD11	3:1:27:ARG:HB2	1.96	0.47
7:5:123:ILE:HG12	7:5:124:ASP:N	2.30	0.47
7:5:127:ALA:O	7:5:129:LEU:N	2.48	0.47
11:A:1161:C:H1'	28:R:8:GLY:O	2.15	0.47
11:A:1392:A:N6	11:A:1393:A:N6	2.63	0.47
11:A:2405:G:O2'	11:A:2406:A:OP1	2.26	0.47
11:A:2889:C:N4	11:A:2890:G:C6	2.83	0.47
12:B:29:A:H2'	12:B:30:C:C6	2.50	0.47
21:K:98:ARG:HA	21:K:118:LEU:HD23	1.97	0.47
29:S:88:ARG:CZ	29:S:88:ARG:CB	2.92	0.47
31:V:6:C:H2'	31:V:7:G:C8	2.49	0.47
32:W:9:THR:CG2	32:W:10:ARG:HD3	2.44	0.47
11:A:983:A:N6	11:A:984:A:N1	2.62	0.47
11:A:1079:C:O2	19:I:130:GLY:HA3	2.15	0.47
11:A:1478:G:C2	11:A:1479:G:N7	2.83	0.47
11:A:2318:G:C6	11:A:2319:G:C6	3.03	0.47
13:C:246:PRO:HG2	13:C:247:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:61:TYR:N	19:I:61:TYR:CD1	2.82	0.47
19:I:100:ILE:HD13	19:I:137:LEU:HD12	1.96	0.47
26:P:50:ARG:HG2	26:P:57:ALA:N	2.30	0.47
26:P:105:LYS:HA	26:P:108:ARG:HD2	1.95	0.47
28:R:68:ARG:HD3	28:R:92:TRP:CE2	2.50	0.47
30:T:69:ARG:CD	30:T:70:HIS:H	2.28	0.47
32:W:60:ALA:HA	32:W:81:ILE:HD12	1.97	0.47
11:A:1198:U:O3'	27:Q:4:LYS:HE3	2.15	0.46
11:A:1313:U:H2'	11:A:1610:A:C2	2.51	0.46
11:A:2601:C:O5'	11:A:2601:C:H6	1.98	0.46
15:E:119:ILE:HG13	15:E:119:ILE:O	2.16	0.46
16:F:131:VAL:HG22	16:F:151:LEU:H	1.80	0.46
19:I:14:ALA:HB1	19:I:45:THR:HG23	1.97	0.46
22:L:23:ILE:HD12	28:R:84:ARG:CZ	2.45	0.46
22:L:85:VAL:HG22	22:L:94:THR:HG22	1.97	0.46
11:A:657:U:H2'	11:A:658:U:C6	2.50	0.46
16:F:64:PRO:HA	16:F:88:VAL:HG22	1.95	0.46
29:S:24:ILE:HD11	29:S:36:LEU:HD13	1.96	0.46
2:0:42:ILE:H	2:0:42:ILE:HD12	1.80	0.46
11:A:2365:G:H4'	32:W:59:PHE:CZ	2.51	0.46
11:A:2701:U:H3'	11:A:2702:G:H5"	1.96	0.46
14:D:169:ARG:O	14:D:170:VAL:HG13	2.15	0.46
16:F:39:VAL:HG13	16:F:40:GLY:N	2.31	0.46
19:I:19:PRO:CG	19:I:23:VAL:HG23	2.45	0.46
21:K:72:PRO:O	21:K:74:GLY:N	2.43	0.46
25:O:41:ALA:O	25:O:44:GLY:N	2.41	0.46
27:Q:4:LYS:NZ	27:Q:7:VAL:CG1	2.79	0.46
30:T:54:GLU:N	30:T:54:GLU:OE1	2.48	0.46
7:5:15:VAL:HG22	7:5:66:GLY:CA	2.44	0.46
11:A:973:A:P	28:R:81:LYS:HZ3	2.37	0.46
11:A:1509:A:C4	11:A:1510:G:C8	3.04	0.46
11:A:1782:U:H2'	11:A:2608:G:HO2'	1.77	0.46
18:H:21:VAL:CG2	18:H:25:TYR:CD2	2.98	0.46
11:A:751:A:C6	11:A:789:A:C5	3.04	0.46
11:A:1567:G:C2'	13:C:84:PRO:HG3	2.46	0.46
11:A:1817:G:H2'	11:A:1818:U:H5'	1.97	0.46
11:A:2210:U:H4'	11:A:2211:A:H5'	1.97	0.46
11:A:2585:U:O2'	11:A:2585:U:O2	2.16	0.46
13:C:75:ALA:HB2	13:C:95:TYR:HA	1.97	0.46
17:G:123:GLU:HG2	17:G:124:CYS:N	2.30	0.46
19:I:57:VAL:HG23	19:I:71:LYS:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:68:SER:O	22:L:69:ARG:HB3	2.15	0.46
27:Q:4:LYS:NZ	27:Q:7:VAL:HG11	2.31	0.46
27:Q:63:ARG:HH22	27:Q:96:ASP:N	2.12	0.46
28:R:66:HIS:CG	28:R:94:THR:HG22	2.50	0.46
30:T:29:THR:HB	30:T:86:THR:HG22	1.97	0.46
31:V:70:C:H2'	31:V:71:C:H5'	1.98	0.46
11:A:247:G:H4'	11:A:386:G:C5	2.51	0.46
11:A:750:A:OP1	11:A:1615:C:N4	2.40	0.46
11:A:1939:U:O2	11:A:1967:C:H4'	2.15	0.46
11:A:2062:A:O2'	11:A:2063:C:C5'	2.55	0.46
11:A:2683:C:O2	21:K:70:ARG:NH2	2.38	0.46
11:A:2698:U:H2'	11:A:2699:C:C6	2.50	0.46
11:A:2897:U:H2'	11:A:2898:U:C6	2.51	0.46
15:E:44:ARG:HG3	15:E:44:ARG:HH11	1.80	0.46
22:L:132:ARG:HG3	22:L:142:ILE:HD12	1.98	0.46
25:O:15:ARG:NE	25:O:93:ASP:OD2	2.44	0.46
11:A:141:G:N1	30:T:1:MET:O	2.44	0.46
11:A:959:A:H62	23:M:82:MET:CE	2.28	0.46
11:A:1088:A:HO2'	11:A:1089:A:P	2.38	0.46
11:A:1936:A:N6	11:A:1963:U:C2	2.84	0.46
14:D:193:VAL:HB	14:D:194:PRO:HD2	1.98	0.46
16:F:147:ARG:HG3	16:F:148:VAL:N	2.30	0.46
17:G:23:ILE:HD12	17:G:23:ILE:H	1.81	0.46
17:G:163:TYR:O	17:G:164:ALA:HB2	2.16	0.46
21:K:24:VAL:CG1	21:K:30:ARG:HD3	2.45	0.46
28:R:49:ILE:HG22	28:R:53:PHE:C	2.36	0.46
32:W:72:GLY:N	32:W:73:PRO:CD	2.78	0.46
35:Z:39:ASP:OD2	35:Z:44:ARG:NH2	2.46	0.46
7:5:68:PRO:HA	7:5:72:LEU:CG	2.46	0.46
10:8:80:HIS:HD2	10:8:83:LYS:H	1.62	0.46
11:A:118:A:C8	11:A:119:A:C8	3.04	0.46
11:A:1171:G:C6	11:A:1172:C:C4	3.04	0.46
11:A:1730:C:O2'	11:A:1731:G:C4	2.68	0.46
14:D:1:MET:HG2	14:D:205:PRO:HG3	1.98	0.46
16:F:62:GLN:NE2	16:F:89:THR:O	2.47	0.46
21:K:13:ASN:O	21:K:15:GLY:N	2.43	0.46
7:5:54:VAL:HG22	7:5:83:ALA:HB1	1.97	0.46
11:A:593:U:H2'	11:A:594:U:C6	2.51	0.46
11:A:1057:A:C6	11:A:1086:A:C2	3.04	0.46
13:C:67:LYS:HG2	13:C:150:GLY:HA2	1.97	0.46
16:F:30:VAL:CG1	16:F:96:TRP:CH2	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:89:SER:OG	19:I:135:MET:SD	2.68	0.46
19:I:100:ILE:CG2	19:I:101:SER:N	2.79	0.46
22:L:19:LEU:HD23	22:L:19:LEU:C	2.35	0.46
23:M:22:GLN:O	23:M:24:THR:N	2.48	0.46
25:O:79:ALA:O	25:O:82:ALA:N	2.49	0.46
26:P:58:PHE:CE1	26:P:75:THR:HG22	2.51	0.46
5:3:3:ILE:HG21	5:3:62:PRO:HG3	1.98	0.46
5:3:12:ARG:HD3	22:L:61:LEU:O	2.16	0.46
7:5:71:CYS:CA	7:5:117:LEU:HD11	2.43	0.46
7:5:136:ILE:HG13	7:5:139:LEU:HD12	1.98	0.46
11:A:2740:A:C6	11:A:2764:A:C8	3.04	0.46
11:A:2793:C:H2'	11:A:2794:C:C6	2.50	0.46
11:A:2862:G:C6	11:A:2863:C:C4	3.04	0.46
14:D:86:GLU:CD	14:D:86:GLU:N	2.69	0.46
18:H:8:LYS:O	18:H:9:VAL:HB	2.15	0.46
19:I:137:LEU:HD23	19:I:137:LEU:H	1.81	0.46
20:J:44:TYR:O	20:J:45:THR:CB	2.64	0.46
26:P:91:VAL:HG11	26:P:96:LEU:HD21	1.98	0.46
27:Q:91:ARG:HH21	27:Q:93:ILE:HG21	1.81	0.46
30:T:29:THR:CB	30:T:86:THR:H	2.29	0.46
11:A:728:G:H4'	13:C:12:ARG:HD3	1.98	0.45
11:A:923:G:N3	32:W:23:LYS:HD2	2.31	0.45
11:A:1248:G:C5	15:E:46:GLN:NE2	2.84	0.45
11:A:1838:C:H4'	11:A:1839:G:C8	2.51	0.45
11:A:2024:G:C4	11:A:2040:G:N2	2.84	0.45
11:A:2144:G:H3'	11:A:2144:G:N3	2.30	0.45
11:A:2436:G:C2	11:A:2437:G:C8	3.04	0.45
11:A:2649:C:H2'	11:A:2650:U:C6	2.51	0.45
11:A:2852:G:C6	11:A:2853:C:N3	2.84	0.45
20:J:55:ILE:HD11	20:J:130:HIS:CD2	2.51	0.45
26:P:72:VAL:HG23	26:P:72:VAL:O	2.15	0.45
32:W:17:ALA:O	32:W:18:LYS:CB	2.63	0.45
5:3:21:PHE:O	5:3:22:LYS:O	2.33	0.45
6:4:8:LYS:NZ	11:A:2467:C:OP1	2.48	0.45
11:A:1662:U:O2	11:A:2687:U:H4'	2.17	0.45
12:B:37:C:C5	12:B:38:C:C4	3.04	0.45
13:C:24:HIS:NE2	13:C:79:ARG:NH1	2.65	0.45
19:I:120:ASP:O	19:I:123:ALA:N	2.45	0.45
20:J:37:ARG:HA	20:J:118:MET:CE	2.45	0.45
32:W:19:ARG:CZ	32:W:22:VAL:HB	2.46	0.45
32:W:39:GLN:HG3	32:W:42:THR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:42:ILE:HD11	24:N:98:LEU:CB	2.46	0.45
3:1:6:GLU:OE1	3:1:52:LYS:CE	2.64	0.45
5:3:51:LYS:NZ	11:A:938:G:OP2	2.33	0.45
6:4:36:ARG:O	6:4:37:GLN:C	2.55	0.45
10:8:80:HIS:CD2	10:8:83:LYS:HB2	2.51	0.45
11:A:855:G:H21	32:W:23:LYS:HG2	1.82	0.45
11:A:1569:A:N6	11:A:1570:A:C6	2.84	0.45
11:A:2262:U:H4'	11:A:2328:A:C2	2.52	0.45
16:F:113:PHE:HE1	16:F:116:LEU:HD13	1.81	0.45
18:H:31:VAL:HB	18:H:32:PRO:CD	2.46	0.45
19:I:24:GLY:O	19:I:27:LEU:HG	2.16	0.45
21:K:61:VAL:HG22	21:K:87:LEU:HD11	1.98	0.45
21:K:80:ASP:CB	26:P:67:GLU:HG3	2.47	0.45
26:P:21:PRO:HD3	26:P:49:ILE:HD12	1.98	0.45
7:5:48:ALA:HB3	7:5:51:TYR:HB3	1.98	0.45
7:5:63:ALA:HB3	7:5:84:TYR:CE2	2.52	0.45
11:A:33:C:O2	11:A:447:A:N6	2.50	0.45
11:A:271:G:H4'	11:A:272:A:OP1	2.17	0.45
12:B:11:C:O2'	12:B:15:A:N6	2.50	0.45
13:C:93:VAL:HG12	13:C:94:LEU:N	2.31	0.45
18:H:14:SER:OG	18:H:17:ASP:CG	2.55	0.45
18:H:40:THR:C	18:H:42:LYS:H	2.20	0.45
25:O:43:ASN:O	25:O:45:SER:N	2.50	0.45
2:0:8:THR:HG21	11:A:2021:C:P	2.56	0.45
11:A:799:G:C6	11:A:800:A:C6	3.05	0.45
11:A:1141:U:H4'	11:A:1142:A:O4'	2.17	0.45
11:A:1593:A:H2'	11:A:1594:U:O4'	2.17	0.45
19:I:125:THR:O	19:I:128:ILE:N	2.48	0.45
20:J:12:LYS:O	20:J:13:ARG:HB2	2.15	0.45
21:K:13:ASN:O	21:K:14:SER:OG	2.29	0.45
21:K:13:ASN:OD1	21:K:13:ASN:N	2.48	0.45
11:A:11:C:H2'	11:A:12:U:H5'	1.98	0.45
11:A:800:A:OP1	40:A:3274:HOH:O	2.21	0.45
11:A:980:A:C4	11:A:1136:G:O4'	2.70	0.45
11:A:996:A:H4'	27:Q:91:ARG:CD	2.47	0.45
11:A:1936:A:C2	11:A:1943:U:C5	3.03	0.45
11:A:2022:U:OP1	40:A:3271:HOH:O	2.20	0.45
13:C:163:ILE:HG23	13:C:171:VAL:CG1	2.47	0.45
18:H:8:LYS:O	18:H:13:GLY:HA2	2.16	0.45
20:J:12:LYS:O	20:J:13:ARG:CB	2.64	0.45
21:K:98:ARG:HA	21:K:118:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:118:LEU:O	21:K:119:ALA:HB3	2.17	0.45
29:S:1:MET:O	29:S:108:SER:HB2	2.16	0.45
31:V:34:G:C6	31:V:35:G:C6	3.05	0.45
35:Z:15:ARG:HG2	35:Z:15:ARG:HH11	1.82	0.45
2:0:3:GLN:HA	11:A:2615:U:C2	2.51	0.45
3:1:4:ILE:HG23	3:1:5:ARG:N	2.32	0.45
6:4:6:SER:HB2	11:A:1031:G:C4'	2.47	0.45
7:5:125:ARG:CZ	7:5:125:ARG:HA	2.47	0.45
11:A:597:G:C2	11:A:661:A:C2	3.04	0.45
11:A:1686:C:C2	11:A:1703:G:C2	3.05	0.45
11:A:2326:C:C6	11:A:2326:C:H3'	2.52	0.45
11:A:2407:A:C2	11:A:2408:U:C2	3.05	0.45
16:F:79:ARG:CZ	31:V:56:C:C2	2.87	0.45
35:Z:3:THR:HA	35:Z:37:ARG:O	2.16	0.45
9:7:17:ASN:ND2	11:A:2586:U:H1'	2.32	0.45
11:A:281:C:H2'	11:A:282:A:C8	2.51	0.45
11:A:1150:C:H2'	11:A:1151:A:O5'	2.17	0.45
11:A:1417:C:O2'	11:A:1587:G:O2'	2.19	0.45
11:A:1428:C:C5	11:A:1569:A:H5"	2.52	0.45
11:A:2533:U:OP1	11:A:2665:A:O2'	2.20	0.45
14:D:70:LYS:O	14:D:71:ALA:HB3	2.17	0.45
15:E:154:ASP:OD1	15:E:154:ASP:N	2.50	0.45
20:J:30:THR:HG22	20:J:31:GLU:N	2.31	0.45
24:N:33:ILE:CD1	24:N:118:ARG:NE	2.80	0.45
24:N:103:ARG:CZ	24:N:110:MET:CE	2.94	0.45
27:Q:91:ARG:HH12	28:R:10:LYS:HB3	1.81	0.45
32:W:19:ARG:C	32:W:19:ARG:CD	2.85	0.45
7:5:71:CYS:HA	7:5:117:LEU:HD11	1.96	0.45
7:5:129:LEU:CB	7:5:130:PRO:HD2	2.47	0.45
11:A:315:G:H2'	11:A:316:C:C6	2.52	0.45
11:A:2326:C:H4'	11:A:2327:A:OP1	2.16	0.45
11:A:2758:A:H2'	11:A:2759:G:H5'	1.99	0.45
13:C:265:PHE:N	13:C:265:PHE:HD1	2.15	0.45
24:N:20:MET:HE1	24:N:40:LYS:HE2	1.99	0.45
24:N:70:THR:HB	24:N:75:ILE:CD1	2.46	0.45
29:S:18:ARG:HG3	29:S:76:VAL:HG13	1.98	0.45
31:V:36:G:H2'	31:V:37:G:O4'	2.17	0.45
3:1:33:LEU:N	3:1:51:ALA:CB	2.80	0.45
11:A:277:G:H2'	11:A:361:G:O6	2.17	0.45
11:A:973:A:O4'	11:A:1188:U:C6	2.70	0.45
11:A:1181:U:H2'	11:A:1182:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2478:A:H2'	11:A:2479:U:H5'	1.98	0.45
11:A:2564:A:C2	11:A:2647:U:H4'	2.52	0.45
12:B:51:G:OP2	25:O:64:TYR:HD2	1.98	0.45
17:G:60:GLY:O	17:G:61:TRP:HB2	2.17	0.45
27:Q:7:VAL:HG13	27:Q:8:ILE:N	2.32	0.45
31:V:2:G:C6	31:V:3:G:C5	3.05	0.45
10:8:80:HIS:CD2	10:8:82:TYR:H	2.35	0.44
11:A:272:A:HO2'	11:A:273:G:H8	1.64	0.44
11:A:646:U:H3'	11:A:647:G:H5"	1.99	0.44
11:A:1060:U:H3	11:A:1088:A:H2	1.64	0.44
11:A:1737:G:H5"	11:A:1738:G:OP2	2.17	0.44
11:A:2307:G:N2	11:A:2311:A:C8	2.86	0.44
11:A:2846:G:H2'	11:A:2847:U:O4'	2.17	0.44
14:D:73:VAL:HG23	14:D:74:GLU:H	1.83	0.44
16:F:107:VAL:HG11	16:F:116:LEU:HD21	1.99	0.44
17:G:24:THR:HG23	17:G:34:ARG:HG2	1.99	0.44
21:K:99:ILE:HG21	21:K:119:ALA:HB2	1.98	0.44
26:P:102:ARG:O	26:P:103:THR:HG22	2.17	0.44
27:Q:103:VAL:HG23	27:Q:104:ALA:N	2.32	0.44
30:T:40:LYS:HG2	30:T:58:VAL:HG22	1.99	0.44
31:V:34:G:H2'	31:V:35:G:C8	2.53	0.44
3:1:8:ILE:HG21	3:1:51:ALA:HA	1.98	0.44
11:A:948:C:H1'	11:A:984:A:O2'	2.17	0.44
11:A:979:A:H2'	11:A:982:C:H42	1.82	0.44
11:A:2283:C:H5"	11:A:2389:G:O2'	2.18	0.44
11:A:2747:G:O6	11:A:2755:C:H5"	2.18	0.44
14:D:121:THR:O	14:D:122:VAL:HB	2.17	0.44
16:F:128:SER:HA	16:F:154:THR:HA	1.99	0.44
19:I:109:ALA:CB	19:I:128:ILE:HG13	2.48	0.44
5:3:31:ILE:O	5:3:31:ILE:HG13	2.17	0.44
11:A:1523:U:O2'	11:A:1524:G:H5'	2.18	0.44
11:A:2108:A:C2'	11:A:2109:U:O5'	2.64	0.44
11:A:2108:A:H2'	11:A:2109:U:O5'	2.17	0.44
12:B:51:G:H5"	25:O:64:TYR:CD2	2.52	0.44
13:C:180:MET:O	13:C:267:VAL:N	2.42	0.44
14:D:44:GLY:HA3	14:D:45:TYR:HD1	1.82	0.44
15:E:187:VAL:O	15:E:188:MET:HB3	2.16	0.44
16:F:127:TYR:O	16:F:128:SER:CB	2.65	0.44
20:J:44:TYR:HD1	27:Q:63:ARG:HG2	1.81	0.44
31:V:26:A:H61	31:V:44:G:H1	1.64	0.44
32:W:37:VAL:HG11	32:W:55:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:3:GLN:NE2	11:A:2016:U:O2	2.46	0.44
7:5:100:ALA:HB3	7:5:125:ARG:HD2	1.98	0.44
11:A:278:A:N1	11:A:362:A:C8	2.85	0.44
11:A:820:A:H2'	11:A:821:A:O4'	2.16	0.44
11:A:980:A:C6	11:A:981:A:N1	2.86	0.44
11:A:1443:U:H2'	11:A:1444:G:C8	2.53	0.44
11:A:1584:U:H2'	11:A:1585:C:H5'	1.99	0.44
11:A:2745:C:C4	11:A:2746:U:C4	3.05	0.44
13:C:76:VAL:HG22	13:C:76:VAL:O	2.17	0.44
17:G:83:THR:C	17:G:84:LYS:HD3	2.37	0.44
17:G:104:LEU:HB2	17:G:112:VAL:CG2	2.47	0.44
19:I:46:ASP:HA	19:I:50:LYS:HD2	2.00	0.44
20:J:80:HIS:O	20:J:82:GLY:N	2.49	0.44
29:S:89:ALA:HA	29:S:90:LYS:O	2.18	0.44
32:W:17:ALA:O	32:W:18:LYS:HB2	2.18	0.44
32:W:19:ARG:NH2	32:W:22:VAL:HG21	2.33	0.44
7:5:51:TYR:CE1	7:5:52:MET:HG2	2.53	0.44
11:A:819:A:C4	11:A:1189:A:C2	3.06	0.44
11:A:1387:A:H5'	11:A:1469:A:H1'	2.00	0.44
16:F:72:SER:HB2	16:F:80:GLN:HB2	1.99	0.44
17:G:35:THR:HG22	17:G:36:LEU:N	2.33	0.44
7:5:15:VAL:CG2	7:5:66:GLY:HA2	2.47	0.44
11:A:222:A:N6	11:A:231:A:C2	2.86	0.44
11:A:627:A:C6	11:A:637:A:C8	3.04	0.44
11:A:855:G:H21	32:W:23:LYS:CG	2.31	0.44
11:A:1439:A:C2	11:A:1553:A:C4	3.06	0.44
14:D:45:TYR:N	14:D:45:TYR:CD1	2.86	0.44
16:F:94:ARG:HH11	16:F:94:ARG:CG	2.31	0.44
20:J:44:TYR:HA	27:Q:59:LEU:CD2	2.48	0.44
27:Q:91:ARG:HH11	28:R:11:GLN:H	1.64	0.44
11:A:61:C:H2'	11:A:62:U:H5'	2.00	0.44
11:A:336:C:N3	11:A:337:C:C5	2.86	0.44
11:A:822:G:H2'	11:A:823:C:H6	1.83	0.44
11:A:1186:G:P	40:A:3204:HOH:O	2.75	0.44
11:A:1542:U:H2'	11:A:1543:G:O4'	2.16	0.44
11:A:2031:A:C6	11:A:2498:C:H1'	2.53	0.44
11:A:2423:U:H5'	11:A:2423:U:H6	1.83	0.44
12:B:78:A:H2'	12:B:79:G:O4'	2.18	0.44
14:D:69:ALA:HA	14:D:73:VAL:CG1	2.47	0.44
23:M:102:LEU:N	23:M:102:LEU:HD12	2.33	0.44
7:5:71:CYS:HB3	7:5:74:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:323:C:OP1	11:A:338:G:N2	2.51	0.44
11:A:720:U:H2'	11:A:721:A:C8	2.53	0.44
11:A:818:G:H5'	11:A:839:U:OP1	2.18	0.44
11:A:1045:C:C3'	11:A:1046:A:H5'	2.48	0.44
11:A:2657:A:C2	11:A:2665:A:C4	3.06	0.44
11:A:2788:C:H2'	11:A:2789:C:C6	2.53	0.44
12:B:27:C:C5	12:B:28:C:C5	3.06	0.44
12:B:78:A:C2	12:B:99:A:C4	3.06	0.44
19:I:40:ALA:O	19:I:68:PHE:CZ	2.71	0.44
21:K:47:ILE:HG13	21:K:48:PRO:HD2	2.00	0.44
22:L:122:VAL:CG1	22:L:142:ILE:HG12	2.47	0.44
11:A:132:G:C2'	11:A:133:U:H5'	2.48	0.44
11:A:172:A:H2'	11:A:173:A:C8	2.53	0.44
11:A:748:G:OP2	29:S:88:ARG:CB	2.66	0.44
11:A:792:A:C6	11:A:2440:C:C6	3.05	0.44
11:A:2283:C:C2	11:A:2389:G:C2	3.06	0.44
11:A:2902:C:H2'	11:A:2903:U:O5'	2.18	0.44
19:I:100:ILE:HD11	19:I:137:LEU:CG	2.48	0.44
20:J:44:TYR:O	20:J:44:TYR:CD2	2.71	0.44
20:J:110:PRO:HB2	20:J:111:LYS:HG3	2.00	0.44
21:K:10:VAL:HG21	21:K:17:ARG:H	1.82	0.44
23:M:13:HIS:O	23:M:14:LYS:CB	2.66	0.44
24:N:38:LEU:HB3	24:N:39:PRO:CD	2.48	0.44
30:T:69:ARG:CG	30:T:70:HIS:N	2.81	0.44
32:W:18:LYS:N	32:W:36:ILE:HG13	2.33	0.44
32:W:19:ARG:HA	32:W:34:SER:HA	2.00	0.44
11:A:994:C:H1'	28:R:10:LYS:CE	2.47	0.43
11:A:1232:G:C5	11:A:1233:C:C5	3.06	0.43
11:A:1340:U:H4'	11:A:1341:G:OP2	2.17	0.43
11:A:1779:U:C5	11:A:1784:A:N7	2.86	0.43
11:A:2103:C:H2'	11:A:2104:C:C5'	2.47	0.43
11:A:2180:U:C2	11:A:2181:U:C5	3.06	0.43
11:A:2276:G:P	23:M:83:GLY:O	2.76	0.43
11:A:2344:U:H4'	11:A:2345:G:OP1	2.17	0.43
13:C:24:HIS:CE1	13:C:79:ARG:HH11	2.36	0.43
14:D:12:THR:OG1	26:P:8:GLU:OE2	2.21	0.43
15:E:44:ARG:HH11	15:E:44:ARG:CG	2.31	0.43
15:E:147:LEU:HB3	15:E:186:VAL:HG23	2.00	0.43
22:L:112:LEU:HD23	22:L:114:GLY:H	1.83	0.43
28:R:64:VAL:O	28:R:65:ALA:HB3	2.18	0.43
32:W:36:ILE:HG22	32:W:36:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Z:5:LYS:HD2	35:Z:5:LYS:N	2.32	0.43
3:1:8:ILE:CD1	3:1:24:LYS:HG2	2.48	0.43
8:6:13:ALA:HB1	8:6:17:MET:CE	2.48	0.43
11:A:1003:G:N2	11:A:1004:U:C2	2.86	0.43
11:A:1867:G:C5	11:A:1868:C:C5	3.05	0.43
11:A:2134:A:O2'	11:A:2135:A:O4'	2.36	0.43
11:A:2517:C:C5	11:A:2542:A:C5	3.07	0.43
11:A:2661:G:C6	11:A:2662:A:C2	3.06	0.43
24:N:70:THR:HB	24:N:75:ILE:HD11	2.00	0.43
27:Q:91:ARG:HH11	28:R:11:GLN:N	2.16	0.43
33:X:67:LEU:HD22	33:X:77:TYR:CE1	2.53	0.43
4:2:12:ARG:HH21	4:2:44:VAL:HG11	1.82	0.43
5:3:31:ILE:O	5:3:31:ILE:CG1	2.66	0.43
10:8:29:ILE:HD13	10:8:30:ILE:N	2.33	0.43
11:A:288:U:H2'	11:A:289:G:C8	2.52	0.43
11:A:666:A:H4'	22:L:48:ARG:HD2	1.99	0.43
11:A:936:A:H2'	11:A:937:C:C6	2.54	0.43
11:A:1914:C:H2'	11:A:1915:U:O4'	2.18	0.43
11:A:2602:A:O2'	31:V:74:C:P	2.76	0.43
14:D:3:GLY:HA3	14:D:204:LYS:HG2	1.99	0.43
14:D:133:THR:HG23	14:D:134:HIS:N	2.34	0.43
17:G:36:LEU:N	17:G:36:LEU:HD22	2.33	0.43
22:L:2:ARG:HA	22:L:5:THR:HG21	2.01	0.43
22:L:111:ILE:N	22:L:111:ILE:HD12	2.33	0.43
29:S:66:ILE:HD13	29:S:67:ASP:N	2.33	0.43
29:S:88:ARG:HD2	29:S:94:ASP:CG	2.35	0.43
7:5:17:GLU:HA	7:5:88:HIS:CE1	2.54	0.43
7:5:87:GLU:OE2	7:5:95:LEU:HD23	2.18	0.43
9:7:24:PRO:HD3	11:A:2585:U:C5	2.53	0.43
11:A:580:U:O3'	27:Q:30:VAL:HG13	2.18	0.43
11:A:1171:G:N2	11:A:1179:G:C4	2.86	0.43
11:A:1188:U:H4'	28:R:81:LYS:O	2.19	0.43
11:A:1441:G:H2'	11:A:1442:U:C6	2.53	0.43
11:A:1923:U:C5'	31:V:24:G:H2'	2.48	0.43
11:A:2609:U:C4	39:A:3001:TRP:CZ3	3.06	0.43
12:B:90:C:H6	12:B:90:C:H5"	1.83	0.43
19:I:45:THR:O	19:I:48:ILE:HG13	2.17	0.43
27:Q:27:ARG:HA	27:Q:33:VAL:HG12	1.99	0.43
32:W:24:ARG:HD3	32:W:65:LYS:CD	2.48	0.43
34:Y:21:LEU:HA	34:Y:25:GLN:HB3	2.01	0.43
34:Y:45:GLN:O	34:Y:46:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:54:VAL:O	7:5:55:VAL:C	2.57	0.43
7:5:71:CYS:SG	7:5:117:LEU:HD12	2.58	0.43
11:A:274:C:H2'	11:A:275:C:O4'	2.19	0.43
11:A:348:A:C5	11:A:349:U:C5	3.07	0.43
11:A:545:U:H6	11:A:545:U:O5'	2.02	0.43
11:A:684:G:C2	11:A:794:A:C2	3.06	0.43
11:A:962:G:P	40:A:3285:HOH:O	2.76	0.43
11:A:1509:A:O2'	11:A:1510:G:P	2.76	0.43
11:A:2682:A:C8	14:D:11:MET:HG3	2.53	0.43
12:B:72:G:N2	12:B:103:U:C5	2.86	0.43
15:E:158:PHE:HD2	15:E:159:LEU:HD12	1.83	0.43
15:E:160:ALA:O	15:E:161:ALA:HB3	2.18	0.43
20:J:11:VAL:HG11	20:J:50:THR:HA	2.01	0.43
32:W:49:ASN:ND2	32:W:50:VAL:N	2.66	0.43
7:5:17:GLU:OE2	7:5:53:ARG:NH1	2.51	0.43
11:A:201:C:OP1	33:X:17:ARG:NH2	2.51	0.43
11:A:1482:G:H1'	11:A:1509:A:N6	2.30	0.43
11:A:1843:C:O2'	13:C:253:GLY:O	2.29	0.43
11:A:2603:G:H2'	11:A:2604:U:O4'	2.18	0.43
16:F:103:ILE:HG21	16:F:173:ASP:HB2	2.01	0.43
18:H:8:LYS:O	18:H:9:VAL:CB	2.66	0.43
19:I:82:ALA:HB1	19:I:108:ILE:HG21	2.00	0.43
21:K:13:ASN:O	21:K:14:SER:CB	2.67	0.43
23:M:26:VAL:HB	23:M:133:LYS:HA	2.00	0.43
24:N:8:ARG:HB3	24:N:10:LEU:CD2	2.48	0.43
27:Q:60:TRP:CE2	27:Q:93:ILE:HB	2.54	0.43
28:R:74:ILE:HB	28:R:87:GLN:O	2.18	0.43
30:T:48:GLN:O	30:T:52:GLU:HA	2.17	0.43
5:3:22:LYS:HA	5:3:47:ALA:O	2.19	0.43
7:5:110:ALA:O	7:5:113:PHE:N	2.46	0.43
11:A:635:C:O2'	11:A:639:U:OP1	2.34	0.43
11:A:833:A:OP1	22:L:39:LYS:HE3	2.19	0.43
11:A:975:A:C5	11:A:990:A:N7	2.86	0.43
11:A:1071:G:H1'	11:A:1089:A:C5	2.53	0.43
11:A:1197:G:H2'	11:A:1198:U:H6	1.83	0.43
11:A:1536:C:H1'	11:A:1537:G:N2	2.34	0.43
11:A:2039:U:H2'	11:A:2040:G:H8	1.82	0.43
11:A:2094:A:P	18:H:22:LYS:HD2	2.59	0.43
11:A:2335:A:N6	11:A:2337:G:H1'	2.34	0.43
11:A:2506:U:O2'	11:A:2507:C:O5'	2.28	0.43
14:D:124:ARG:HA	14:D:165:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Q:20:ALA:HA	27:Q:23:TYR:CE2	2.54	0.43
27:Q:94:LEU:CD1	28:R:13:ARG:HB2	2.49	0.43
34:Y:1:MET:H3	34:Y:2:LYS:HD2	1.83	0.43
35:Z:15:ARG:HD3	35:Z:53:MET:SD	2.59	0.43
7:5:67:THR:CG2	7:5:72:LEU:HA	2.49	0.43
11:A:479:A:N3	11:A:481:G:H5"	2.34	0.43
11:A:528:A:P	20:J:116:ARG:HH21	2.42	0.43
11:A:581:C:H2'	11:A:582:A:C8	2.54	0.43
11:A:742:A:H2'	11:A:743:A:C8	2.53	0.43
11:A:744:U:H2'	11:A:745:G:O4'	2.19	0.43
11:A:1096:A:H2'	11:A:1097:U:H5"	2.01	0.43
11:A:1252:G:C2	27:Q:32:ARG:HG2	2.52	0.43
11:A:1782:U:O2	11:A:2608:G:C2'	2.66	0.43
11:A:1857:G:C2	11:A:1884:G:N3	2.86	0.43
11:A:2353:G:N3	32:W:30:VAL:HG12	2.32	0.43
11:A:2516:A:N6	11:A:2517:C:N4	2.67	0.43
11:A:2823:A:C5	11:A:2824:C:C5	3.07	0.43
16:F:134:GLN:OE1	16:F:149:ARG:HB3	2.18	0.43
21:K:3:GLN:HG3	21:K:4:GLU:N	2.34	0.43
21:K:35:VAL:HG12	21:K:36:GLY:N	2.34	0.43
28:R:16:GLU:HA	28:R:98:ILE:HG22	2.01	0.43
30:T:69:ARG:HG3	30:T:70:HIS:H	1.83	0.43
30:T:76:ARG:HG3	30:T:77:ARG:N	2.34	0.43
31:V:37:G:C2	31:V:38:U:H1'	2.53	0.43
3:1:5:ARG:CZ	3:1:24:LYS:HA	2.49	0.43
11:A:146:A:H2'	11:A:147:C:C6	2.54	0.43
11:A:226:A:C6	11:A:227:A:C6	3.07	0.43
11:A:247:G:N7	11:A:249:C:C2	2.86	0.43
11:A:356:G:C6	11:A:357:C:C4	3.07	0.43
11:A:959:A:H62	23:M:82:MET:HE1	1.84	0.43
11:A:1204:A:C2	11:A:1240:U:N3	2.87	0.43
11:A:2595:G:N1	11:A:2599:G:C6	2.87	0.43
34:Y:14:LEU:HA	34:Y:17:GLU:HB3	2.01	0.43
2:0:42:ILE:HG22	2:0:43:THR:O	2.19	0.43
11:A:476:G:H4'	11:A:502:A:N1	2.33	0.43
11:A:959:A:N6	23:M:82:MET:CE	2.82	0.43
19:I:93:ASN:HB2	19:I:135:MET:SD	2.59	0.43
22:L:2:ARG:HA	22:L:5:THR:CG2	2.48	0.43
27:Q:86:SER:O	28:R:51:VAL:HA	2.18	0.43
28:R:5:PHE:HB3	28:R:59:ILE:HD12	2.01	0.43
34:Y:56:LEU:HD22	34:Y:56:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:372:G:C4	33:X:60:LYS:HE2	2.54	0.42
11:A:545:U:H2'	11:A:546:U:O3'	2.18	0.42
11:A:573:U:O2'	11:A:574:A:H3'	2.19	0.42
11:A:1224:U:H4'	28:R:88:GLY:O	2.19	0.42
11:A:1378:A:C4	11:A:1380:G:N7	2.87	0.42
11:A:1494:A:C2	11:A:1495:A:C4	3.06	0.42
11:A:1747:U:H2'	11:A:1748:C:C6	2.54	0.42
14:D:120:GLY:HA2	14:D:162:ALA:HA	2.00	0.42
32:W:37:VAL:HB	32:W:38:ARG:NH1	2.34	0.42
3:1:7:LYS:NZ	11:A:2421:G:P	2.92	0.42
11:A:764:A:C6	11:A:781:A:C2	3.06	0.42
11:A:2070:A:H2'	11:A:2071:A:O4'	2.19	0.42
11:A:2287:A:C8	11:A:2289:G:C8	3.08	0.42
11:A:2557:G:H2'	11:A:2558:C:C6	2.54	0.42
11:A:2661:G:H2'	11:A:2662:A:O4'	2.19	0.42
13:C:109:LEU:HD23	13:C:110:LYS:H	1.83	0.42
15:E:42:GLY:O	15:E:43:THR:OG1	2.35	0.42
17:G:123:GLU:HG2	17:G:125:PRO:HD3	2.01	0.42
19:I:9:LYS:HB3	19:I:71:LYS:NZ	2.34	0.42
20:J:60:ASP:N	20:J:60:ASP:OD1	2.52	0.42
25:O:31:THR:HG22	25:O:34:HIS:N	2.33	0.42
26:P:50:ARG:CB	26:P:57:ALA:N	2.78	0.42
8:6:15:SER:OG	8:6:16:VAL:N	2.53	0.42
11:A:570:G:C4	11:A:2030:A:N7	2.87	0.42
11:A:2062:A:O2'	11:A:2063:C:P	2.74	0.42
13:C:16:VAL:N	13:C:203:VAL:CG1	2.82	0.42
14:D:118:PHE:HZ	24:N:1:MET:HB2	1.85	0.42
20:J:38:GLY:O	20:J:43:GLU:HB2	2.19	0.42
24:N:8:ARG:HB3	24:N:10:LEU:HD22	2.01	0.42
25:O:75:GLY:HA3	25:O:109:ALA:HB3	2.00	0.42
30:T:29:THR:HB	30:T:86:THR:HA	2.01	0.42
32:W:24:ARG:HD3	32:W:65:LYS:HG2	2.00	0.42
7:5:108:VAL:CG1	7:5:109:LYS:N	2.83	0.42
11:A:580:U:H2'	11:A:581:C:C6	2.54	0.42
11:A:803:U:C4	11:A:804:A:N7	2.88	0.42
11:A:864:G:OP2	23:M:22:GLN:NE2	2.52	0.42
11:A:1112:G:C5	11:A:1113:U:C5	3.07	0.42
11:A:1281:G:C2	11:A:1290:C:C2	3.07	0.42
11:A:1476:U:C5	11:A:1514:G:C2	3.07	0.42
11:A:1770:G:C6	11:A:1983:G:C6	3.07	0.42
11:A:1782:U:C1'	11:A:2608:G:O2'	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1814:G:C6	11:A:1815:A:C6	3.08	0.42
11:A:1844:C:O3'	13:C:255:LYS:NZ	2.43	0.42
11:A:1937:A:N7	11:A:1939:U:H2'	2.35	0.42
11:A:2508:G:N1	11:A:2582:G:O6	2.52	0.42
16:F:111:ARG:NE	16:F:111:ARG:HA	2.34	0.42
19:I:91:LYS:HB2	19:I:95:ASP:HB2	2.00	0.42
23:M:8:LYS:CE	23:M:9:PHE:CE2	3.02	0.42
24:N:117:ASP:O	24:N:118:ARG:C	2.57	0.42
32:W:44:PHE:O	32:W:78:PHE:HA	2.19	0.42
34:Y:31:GLN:HG2	34:Y:36:GLN:HB2	2.01	0.42
35:Z:13:ILE:HG22	35:Z:14:GLY:N	2.34	0.42
35:Z:39:ASP:CG	35:Z:44:ARG:HH21	2.23	0.42
7:5:67:THR:C	7:5:69:PHE:N	2.73	0.42
11:A:19:A:H2'	11:A:20:C:O4'	2.20	0.42
11:A:75:G:H4'	34:Y:48:ARG:NH2	2.34	0.42
11:A:996:A:C5	11:A:1160:G:C2	3.08	0.42
11:A:1084:A:C6	11:A:1085:A:C6	3.08	0.42
11:A:1239:G:H2'	11:A:1240:U:O4'	2.19	0.42
11:A:1394:U:OP1	40:A:3277:HOH:O	2.22	0.42
11:A:1923:U:OP1	31:V:25:C:C5'	2.61	0.42
11:A:2526:G:C5	11:A:2527:C:C5	3.07	0.42
11:A:2727:A:C6	11:A:2728:U:O4	2.73	0.42
11:A:2748:A:H1'	17:G:66:THR:CG2	2.49	0.42
12:B:89:U:H3'	12:B:90:C:C5'	2.50	0.42
12:B:106:G:H2'	12:B:107:G:O4'	2.19	0.42
17:G:39:ALA:HB2	17:G:57:TYR:CD2	2.54	0.42
20:J:43:GLU:O	20:J:44:TYR:C	2.58	0.42
26:P:92:ARG:CG	26:P:92:ARG:O	2.68	0.42
5:3:4:LYS:NZ	11:A:253:C:OP2	2.38	0.42
11:A:479:A:C2	11:A:480:A:C5	3.08	0.42
11:A:1171:G:H1	11:A:1178:C:H42	1.66	0.42
11:A:1183:U:H2'	11:A:1184:U:C6	2.55	0.42
11:A:1223:G:P	28:R:68:ARG:HH21	2.41	0.42
11:A:1638:C:H4'	11:A:2710:C:O2	2.18	0.42
11:A:1956:U:H2'	11:A:1957:C:H5'	2.01	0.42
11:A:2586:U:O2	11:A:2586:U:H2'	2.19	0.42
14:D:110:THR:HG23	14:D:171:THR:HG22	2.00	0.42
16:F:107:VAL:HG13	16:F:110:ILE:HD12	2.02	0.42
20:J:4:PHE:CD2	20:J:44:TYR:CE2	3.08	0.42
20:J:88:THR:HG22	20:J:91:GLU:CG	2.49	0.42
24:N:24:MET:HE2	24:N:44:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:79:LEU:O	24:N:80:PHE:HB2	2.19	0.42
27:Q:4:LYS:HZ3	27:Q:7:VAL:CG1	2.33	0.42
28:R:74:ILE:HD12	28:R:74:ILE:N	2.34	0.42
3:1:18:HIS:CE1	3:1:40:PRO:HD3	2.54	0.42
7:5:106:PHE:CG	7:5:107:GLU:N	2.87	0.42
7:5:142:THR:OG1	7:5:143:MET:N	2.52	0.42
11:A:27:G:HO2'	11:A:28:A:P	2.39	0.42
11:A:301:G:H2'	11:A:334:C:H2'	2.01	0.42
11:A:994:C:O2'	11:A:996:A:OP1	2.25	0.42
11:A:1019:U:H3	11:A:1142:A:N6	2.16	0.42
11:A:1312:U:H4'	11:A:1313:U:O5'	2.20	0.42
11:A:1782:U:N3	11:A:2587:A:C6	2.87	0.42
11:A:1936:A:C2	11:A:1943:U:H5	2.38	0.42
11:A:2047:C:O2'	11:A:2048:G:H5'	2.19	0.42
11:A:2071:A:H2'	11:A:2072:C:C6	2.54	0.42
15:E:188:MET:HE3	15:E:196:VAL:HG21	2.01	0.42
19:I:20:SER:HB3	19:I:21:PRO:HD3	2.01	0.42
20:J:64:VAL:HG13	20:J:65:THR:N	2.35	0.42
20:J:81:ILE:CG1	20:J:82:GLY:H	2.33	0.42
29:S:59:GLU:HA	29:S:64:ALA:CB	2.50	0.42
30:T:70:HIS:HB3	30:T:73:ARG:O	2.19	0.42
2:0:42:ILE:HD12	24:N:99:LYS:O	2.20	0.42
7:5:47:GLU:HG2	7:5:95:LEU:HD21	2.01	0.42
10:8:72:VAL:HG12	10:8:93:ARG:HA	2.01	0.42
10:8:75:GLN:HB2	10:8:92:VAL:CG2	2.48	0.42
11:A:518:G:H2'	11:A:519:U:C6	2.55	0.42
11:A:1179:G:C6	11:A:1180:U:C4	3.08	0.42
11:A:1789:A:H2'	11:A:1790:C:O4'	2.20	0.42
11:A:2755:C:O2'	11:A:2756:U:H2'	2.19	0.42
16:F:134:GLN:HG2	16:F:135:ILE:N	2.34	0.42
7:5:3:LEU:HD12	7:5:5:LEU:N	2.35	0.42
7:5:33:VAL:HB	7:5:36:ASP:OD1	2.20	0.42
11:A:866:A:N7	11:A:914:G:C6	2.88	0.42
11:A:1338:G:O2'	11:A:1393:A:N1	2.44	0.42
15:E:52:VAL:HG11	15:E:81:GLY:HA3	2.01	0.42
22:L:77:ILE:HD13	22:L:108:ALA:HB1	2.02	0.42
23:M:53:MET:CE	23:M:63:ILE:HG21	2.50	0.42
25:O:14:ALA:O	25:O:17:LYS:N	2.52	0.42
32:W:24:ARG:HH11	32:W:65:LYS:HG2	1.85	0.42
33:X:52:ALA:O	33:X:53:LYS:CB	2.67	0.42
35:Z:4:ILE:HD13	35:Z:44:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:22:ALA:N	7:5:87:GLU:O	2.53	0.42
7:5:27:VAL:O	7:5:83:ALA:N	2.52	0.42
7:5:88:HIS:CB	7:5:89:PRO:CD	2.97	0.42
11:A:653:U:H5	11:A:654:A:C2	2.38	0.42
11:A:751:A:O4'	29:S:90:LYS:HG3	2.19	0.42
11:A:945:A:C4	11:A:2448:A:C2	3.07	0.42
11:A:966:G:C6	11:A:967:U:C4	3.07	0.42
11:A:1094:U:N3	11:A:1097:U:OP2	2.51	0.42
11:A:1486:U:H2'	11:A:1487:U:C6	2.55	0.42
11:A:2274:A:C5	11:A:2276:G:C8	3.07	0.42
11:A:2602:A:H8	31:V:74:C:OP2	2.03	0.42
11:A:2821:A:C2	11:A:2822:G:C4	3.08	0.42
15:E:187:VAL:O	15:E:188:MET:CB	2.67	0.42
26:P:58:PHE:HD1	26:P:75:THR:HG22	1.83	0.42
28:R:38:VAL:O	28:R:53:PHE:HA	2.20	0.42
30:T:34:VAL:O	30:T:34:VAL:HG22	2.20	0.42
11:A:126:A:C6	11:A:127:A:N1	2.88	0.41
11:A:1485:U:H2'	11:A:1486:U:H6	1.83	0.41
11:A:1691:C:C4	11:A:1692:U:C4	3.08	0.41
11:A:2201:G:C6	11:A:2202:U:C4	3.08	0.41
11:A:2869:G:C6	11:A:2870:C:C4	3.09	0.41
13:C:16:VAL:H	13:C:203:VAL:HG12	1.83	0.41
19:I:11:GLN:OE1	19:I:11:GLN:N	2.43	0.41
21:K:71:ARG:CB	21:K:72:PRO:HD3	2.49	0.41
29:S:96:ILE:O	29:S:96:ILE:HG13	2.20	0.41
7:5:26:VAL:O	7:5:27:VAL:CB	2.64	0.41
11:A:685:A:C2	11:A:689:A:C6	3.08	0.41
11:A:1026:G:H2'	11:A:1027:A:C8	2.55	0.41
11:A:1069:A:C2'	11:A:1070:A:OP2	2.68	0.41
11:A:1268:A:H2'	11:A:1269:A:O4'	2.21	0.41
11:A:1681:G:N2	11:A:1763:G:OP2	2.45	0.41
11:A:2341:G:H2'	11:A:2342:C:C6	2.55	0.41
11:A:2580:U:C5	11:A:2581:G:C6	3.08	0.41
11:A:2676:C:P	21:K:31:ARG:HH12	2.44	0.41
14:D:46:ARG:HB3	14:D:46:ARG:CZ	2.50	0.41
15:E:12:LEU:HD12	15:E:193:VAL:HG11	2.02	0.41
15:E:134:LEU:CD2	15:E:161:ALA:HB2	2.51	0.41
16:F:28:PRO:HB2	16:F:168:LEU:HD22	2.02	0.41
16:F:94:ARG:HH11	16:F:94:ARG:HB2	1.84	0.41
19:I:74:PRO:HG2	19:I:77:VAL:HB	2.02	0.41
20:J:35:ARG:HG2	20:J:40:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:40:SER:O	22:L:41:ARG:CB	2.68	0.41
26:P:92:ARG:HH11	26:P:92:ARG:HB2	1.85	0.41
11:A:833:A:OP2	22:L:39:LYS:NZ	2.45	0.41
11:A:996:A:C6	11:A:1160:G:C2	3.08	0.41
11:A:1298:C:C2	11:A:1643:G:N2	2.88	0.41
11:A:2259:U:H1'	11:A:2427:C:C2	2.55	0.41
11:A:2576:G:H3'	11:A:2576:G:N3	2.35	0.41
11:A:2637:U:C2'	11:A:2638:G:H5'	2.50	0.41
11:A:2685:G:H1	11:A:2724:U:H3	1.68	0.41
11:A:2803:G:H2'	11:A:2804:U:H6	1.84	0.41
13:C:16:VAL:HB	13:C:203:VAL:HG12	2.02	0.41
14:D:24:VAL:HA	14:D:191:GLY:H	1.85	0.41
18:H:39:ALA:HB1	18:H:44:ILE:HG22	2.01	0.41
28:R:80:ARG:O	28:R:81:LYS:HD3	2.20	0.41
6:4:32:LYS:HD3	11:A:2478:A:H5'	2.02	0.41
11:A:45:G:H5'	11:A:46:G:H5'	2.03	0.41
11:A:528:A:H2	11:A:2043:C:H5'	1.85	0.41
11:A:1069:A:N3	11:A:1073:A:C6	2.88	0.41
11:A:1509:A:H1'	11:A:1510:G:O5'	2.20	0.41
11:A:1591:A:H2'	11:A:1592:C:C6	2.55	0.41
11:A:1607:C:H42	11:A:1622:G:P	2.43	0.41
11:A:1674:G:N2	11:A:1677:A:N1	2.69	0.41
11:A:2062:A:O2'	11:A:2063:C:C6	2.68	0.41
11:A:2180:U:N3	11:A:2181:U:C5	2.89	0.41
11:A:2352:A:N1	32:W:30:VAL:HG21	2.35	0.41
11:A:2409:G:H2'	11:A:2410:G:O4'	2.20	0.41
11:A:2478:A:C2'	11:A:2479:U:H5'	2.51	0.41
11:A:2581:G:C4	11:A:2610:C:C5	3.09	0.41
12:B:16:G:C5	12:B:69:G:C2	3.07	0.41
13:C:203:VAL:O	13:C:205:GLY:N	2.53	0.41
15:E:129:PRO:HG3	15:E:156:ASN:OD1	2.21	0.41
16:F:46:LYS:H	16:F:46:LYS:HD3	1.86	0.41
23:M:12:MET:HE3	23:M:71:LYS:HG3	2.03	0.41
11:A:138:U:H5'	11:A:139:U:C5'	2.51	0.41
11:A:301:G:C6	11:A:317:G:C6	3.09	0.41
11:A:485:C:C2	11:A:496:G:N2	2.88	0.41
11:A:527:C:H4'	11:A:528:A:O5'	2.20	0.41
11:A:1020:A:C2	11:A:1141:U:C2	3.09	0.41
11:A:1238:G:O2'	11:A:1239:G:H5'	2.19	0.41
11:A:1381:G:H1'	11:A:1571:A:N1	2.36	0.41
11:A:1403:A:C2	11:A:1404:C:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1494:A:C6	11:A:1495:A:C5	3.08	0.41
11:A:1747:U:H2'	11:A:1748:C:H6	1.85	0.41
11:A:1923:U:H5'	31:V:25:C:C1'	2.50	0.41
11:A:1945:G:C6	11:A:1946:U:C4	3.09	0.41
11:A:2543:G:C6	11:A:2544:G:C6	3.08	0.41
11:A:2618:G:C6	11:A:2619:C:C4	3.09	0.41
11:A:2796:U:C4	11:A:2798:U:C5	3.08	0.41
16:F:151:LEU:CD1	16:F:153:ILE:HG23	2.51	0.41
19:I:19:PRO:HG2	19:I:24:GLY:H	1.85	0.41
20:J:4:PHE:HB3	20:J:44:TYR:CE2	2.55	0.41
32:W:19:ARG:NH1	32:W:22:VAL:CG2	2.83	0.41
9:7:24:PRO:HD3	11:A:2585:U:H5	1.86	0.41
11:A:307:G:N2	11:A:310:A:C8	2.88	0.41
11:A:608:A:C8	11:A:621:A:N6	2.89	0.41
11:A:1063:G:H2'	11:A:1064:C:O4'	2.20	0.41
11:A:1194:A:C2'	11:A:1195:G:O5'	2.68	0.41
11:A:1365:A:N6	11:A:1366:A:C6	2.88	0.41
11:A:1647:U:P	11:A:1647:U:H3'	2.60	0.41
11:A:1992:G:OP1	40:A:3272:HOH:O	2.20	0.41
11:A:2845:U:H5"	26:P:51:ASN:O	2.20	0.41
13:C:143:VAL:HB	13:C:153:LEU:HB2	2.02	0.41
14:D:46:ARG:HH21	14:D:86:GLU:H	1.68	0.41
14:D:104:VAL:HG12	14:D:106:LYS:H	1.85	0.41
15:E:109:LEU:O	15:E:112:LEU:N	2.54	0.41
17:G:26:LYS:CG	17:G:27:GLY:N	2.83	0.41
19:I:52:LEU:HB3	19:I:53:PRO:HD2	2.03	0.41
19:I:100:ILE:CD1	19:I:137:LEU:HD12	2.50	0.41
21:K:15:GLY:O	21:K:46:ALA:HA	2.21	0.41
24:N:12:ARG:HB3	24:N:16:HIS:HB3	2.02	0.41
26:P:50:ARG:CD	26:P:56:SER:HB3	2.51	0.41
27:Q:6:GLY:HA2	27:Q:9:ALA:HB3	2.02	0.41
29:S:18:ARG:HG3	29:S:76:VAL:CG1	2.50	0.41
29:S:63:GLY:O	29:S:64:ALA:HB3	2.21	0.41
2:0:12:ARG:HD2	2:0:16:ARG:NH2	2.36	0.41
7:5:108:VAL:HG12	7:5:109:LYS:N	2.35	0.41
7:5:131:THR:HA	7:5:134:GLU:CG	2.50	0.41
10:8:6:ALA:HB1	10:8:40:ILE:CG2	2.50	0.41
11:A:629:G:H4'	11:A:650:C:O2	2.21	0.41
11:A:846:U:HO2'	11:A:847:U:P	2.43	0.41
11:A:945:A:N7	40:A:3330:HOH:O	2.37	0.41
11:A:1465:G:H2'	11:A:1466:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2038:G:H2'	11:A:2039:U:O4'	2.21	0.41
12:B:114:C:H1'	25:O:47:VAL:HG11	2.03	0.41
14:D:149:ASN:CG	14:D:150:GLN:H	2.21	0.41
17:G:19:ASN:O	17:G:22:VAL:HG22	2.21	0.41
21:K:71:ARG:O	21:K:72:PRO:O	2.39	0.41
21:K:76:VAL:CB	26:P:72:VAL:HG22	2.47	0.41
22:L:29:LYS:HG2	22:L:30:THR:N	2.36	0.41
31:V:3:G:C2	31:V:71:C:C2	3.09	0.41
35:Z:2:LYS:CB	35:Z:39:ASP:HB3	2.51	0.41
11:A:749:A:C5	11:A:1618:A:C2	3.09	0.41
11:A:1613:G:O6	11:A:1617:C:H2'	2.21	0.41
11:A:1817:G:C2'	11:A:1818:U:H5'	2.51	0.41
11:A:2103:C:N4	11:A:2186:G:H1	2.19	0.41
11:A:2145:C:N3	11:A:2146:C:N3	2.69	0.41
11:A:2298:A:C6	11:A:2321:U:C4	3.09	0.41
16:F:10:GLU:HG2	16:F:13:LYS:HD3	2.02	0.41
16:F:169:LEU:O	16:F:174:PHE:HB2	2.21	0.41
17:G:68:ARG:HH21	17:G:72:ASN:ND2	2.18	0.41
20:J:65:THR:HG22	20:J:68:LYS:NZ	2.36	0.41
20:J:88:THR:HG23	20:J:91:GLU:H	1.86	0.41
22:L:127:VAL:HG11	22:L:142:ILE:HG21	2.03	0.41
24:N:87:PHE:O	24:N:89:SER:N	2.54	0.41
26:P:30:TRP:CE3	26:P:39:LEU:HD12	2.56	0.41
27:Q:82:LEU:HD12	27:Q:112:ALA:HB2	2.02	0.41
32:W:19:ARG:HG2	32:W:19:ARG:HH11	1.86	0.41
32:W:60:ALA:CB	32:W:81:ILE:CD1	2.98	0.41
7:5:88:HIS:HB3	7:5:89:PRO:HD3	2.03	0.41
7:5:132:TYR:HE1	8:6:19:VAL:HG13	1.85	0.41
11:A:45:G:C5'	11:A:46:G:H5'	2.51	0.41
11:A:58:G:N2	11:A:70:G:C4	2.89	0.41
11:A:109:C:H4'	11:A:348:A:H4'	2.02	0.41
11:A:347:A:C2	11:A:348:A:C4	3.09	0.41
11:A:535:G:C6	11:A:559:G:C6	3.09	0.41
11:A:1078:U:H5"	11:A:1079:C:OP1	2.20	0.41
11:A:1301:A:N3	11:A:1301:A:H2'	2.35	0.41
11:A:1392:A:C6	11:A:1393:A:C6	3.09	0.41
11:A:1967:C:H2'	11:A:1968:G:H5'	2.03	0.41
11:A:2017:U:H5"	11:A:2018:G:P	2.61	0.41
11:A:2681:C:C2	11:A:2724:U:O4	2.74	0.41
13:C:115:ILE:HG22	13:C:116:GLN:N	2.36	0.41
15:E:79:ARG:HG2	15:E:80:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:178:VAL:HG23	15:E:179:SER:N	2.36	0.41
17:G:31:GLU:O	17:G:33:THR:N	2.52	0.41
17:G:137:LYS:HA	17:G:140:ILE:HG22	2.02	0.41
19:I:52:LEU:HB3	19:I:53:PRO:CD	2.51	0.41
19:I:104:GLN:O	19:I:105:LEU:CB	2.69	0.41
24:N:24:MET:CE	24:N:36:THR:HG21	2.51	0.41
25:O:49:VAL:HG12	25:O:50:ALA:N	2.35	0.41
31:V:72:G:C3'	31:V:73:A:H5"	2.51	0.41
32:W:39:GLN:HG2	32:W:41:GLY:N	2.34	0.41
32:W:39:GLN:OE1	32:W:43:LYS:HB2	2.21	0.41
7:5:23:LEU:HD22	7:5:92:ALA:O	2.21	0.41
7:5:47:GLU:CG	7:5:95:LEU:HD21	2.51	0.41
7:5:51:TYR:CD1	7:5:52:MET:HG2	2.55	0.41
7:5:77:VAL:C	7:5:79:PRO:CD	2.83	0.41
9:7:24:PRO:O	31:V:76:A:O3'	2.39	0.41
11:A:659:G:H4'	15:E:95:LYS:HD3	2.02	0.41
11:A:1068:G:H3'	11:A:1069:A:H5"	2.02	0.41
11:A:1813:G:H1'	13:C:49:THR:CG2	2.49	0.41
11:A:1843:C:H5'	13:C:250:GLN:NE2	2.36	0.41
11:A:2070:A:C2	11:A:2071:A:C4	3.09	0.41
11:A:2581:G:C2	11:A:2610:C:C5	3.09	0.41
11:A:2674:G:H4'	21:K:30:ARG:HG3	2.02	0.41
11:A:2682:A:C8	14:D:11:MET:CG	3.04	0.41
11:A:2766:A:N3	11:A:2766:A:H2'	2.36	0.41
11:A:2868:A:C2	11:A:2869:G:C4	3.09	0.41
15:E:187:VAL:HG12	15:E:188:MET:N	2.36	0.41
23:M:63:ILE:HG22	23:M:64:TRP:N	2.36	0.41
27:Q:46:TYR:CZ	27:Q:50:ARG:NH2	2.89	0.41
7:5:131:THR:HA	7:5:134:GLU:HG3	2.03	0.40
11:A:528:A:H2	11:A:2043:C:C5'	2.34	0.40
11:A:669:G:N3	11:A:669:G:C2'	2.83	0.40
11:A:1494:A:C6	11:A:1495:A:C6	3.08	0.40
11:A:1722:A:C2	11:A:1739:A:N3	2.89	0.40
11:A:1905:C:N4	11:A:1930:G:C2	2.89	0.40
11:A:2347:C:H2'	11:A:2348:U:C6	2.56	0.40
13:C:172:THR:HG22	13:C:182:LYS:HG2	2.02	0.40
13:C:254:LYS:O	13:C:256:THR:N	2.51	0.40
20:J:36:LEU:O	20:J:121:LYS:NZ	2.39	0.40
21:K:39:ILE:HD12	21:K:41:ILE:HD11	2.02	0.40
24:N:51:LEU:HD21	24:N:70:THR:CG2	2.51	0.40
29:S:69:LEU:HG	29:S:107:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:V:7:G:C6	31:V:49:G:C5	3.09	0.40
32:W:19:ARG:NH1	32:W:19:ARG:HG2	2.36	0.40
5:3:30:HIS:ND1	5:3:31:ILE:HG23	2.36	0.40
6:4:32:LYS:CD	11:A:2478:A:H5'	2.51	0.40
6:4:38:GLY:OXT	11:A:1124:G:H1'	2.21	0.40
7:5:59:LEU:HD23	7:5:62:ARG:HE	1.85	0.40
11:A:364:C:H2'	11:A:365:U:H6	1.87	0.40
11:A:1450:G:C6	11:A:1451:C:N4	2.90	0.40
11:A:1587:G:C4	11:A:1588:G:C8	3.09	0.40
11:A:2103:C:H2'	11:A:2104:C:H5"	2.02	0.40
13:C:158:GLY:H	13:C:194:VAL:HG22	1.86	0.40
13:C:184:GLU:O	13:C:185:ALA:HB3	2.20	0.40
18:H:24:GLY:O	18:H:28:ASN:HB2	2.21	0.40
25:O:75:GLY:HA3	25:O:106:LEU:HA	2.04	0.40
26:P:92:ARG:O	26:P:93:LYS:HB2	2.21	0.40
32:W:22:VAL:O	32:W:23:LYS:HG3	2.22	0.40
33:X:67:LEU:HD22	33:X:77:TYR:CZ	2.57	0.40
34:Y:12:GLU:O	34:Y:15:ASN:HB2	2.21	0.40
2:0:33:SER:OG	2:0:35:GLU:HG3	2.21	0.40
3:1:9:LYS:N	3:1:9:LYS:HD2	2.37	0.40
3:1:35:LEU:HD22	3:1:35:LEU:N	2.37	0.40
7:5:31:ARG:NH2	11:A:1054:A:OP1	2.53	0.40
11:A:176:A:N7	11:A:177:G:C6	2.90	0.40
11:A:230:G:N2	11:A:231:A:C4	2.90	0.40
11:A:1096:A:N6	11:A:1097:U:C4	2.89	0.40
11:A:1149:G:H2'	11:A:1150:C:C6	2.57	0.40
11:A:1365:A:C6	11:A:1366:A:C5	3.10	0.40
11:A:1684:G:C2	11:A:1705:A:C2	3.10	0.40
11:A:1714:U:H5'	11:A:1715:G:H5'	2.02	0.40
11:A:2583:G:C2'	11:A:2584:U:H5'	2.50	0.40
13:C:77:VAL:HG23	13:C:77:VAL:O	2.20	0.40
14:D:88:GLU:O	14:D:89:GLU:HG3	2.21	0.40
16:F:112:ASP:N	16:F:112:ASP:OD1	2.54	0.40
21:K:19:VAL:HG13	21:K:41:ILE:HG12	2.02	0.40
21:K:76:VAL:HG12	21:K:77:ILE:N	2.37	0.40
25:O:7:ARG:HA	25:O:10:ARG:NH1	2.36	0.40
26:P:4:ILE:HG22	26:P:8:GLU:HG3	2.04	0.40
11:A:179:C:C2	11:A:180:G:C8	3.08	0.40
11:A:477:A:C6	11:A:478:A:C6	3.10	0.40
11:A:996:A:C5	11:A:1160:G:N2	2.89	0.40
11:A:1669:A:O2'	11:A:2549:G:OP1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1909:C:C1'	31:V:11:C:O2'	2.68	0.40
11:A:2318:G:C5	11:A:2319:G:C6	3.10	0.40
11:A:2447:G:C4	11:A:2500:U:C5	3.09	0.40
16:F:148:VAL:HG23	16:F:149:ARG:N	2.36	0.40
19:I:57:VAL:HG23	19:I:71:LYS:HZ1	1.86	0.40
26:P:33:GLU:HG3	26:P:36:LYS:O	2.22	0.40
32:W:30:VAL:O	32:W:30:VAL:CG1	2.64	0.40
2:0:16:ARG:CZ	29:S:15:GLN:NE2	2.84	0.40
4:2:9:VAL:HG13	11:A:1309:G:OP1	2.21	0.40
6:4:36:ARG:HG2	6:4:37:GLN:N	2.34	0.40
7:5:91:ALA:O	7:5:93:ALA:N	2.51	0.40
7:5:111:ALA:C	7:5:113:PHE:N	2.75	0.40
11:A:64:A:C6	11:A:65:U:C4	3.10	0.40
11:A:528:A:H3'	11:A:528:A:C8	2.57	0.40
11:A:811:U:H2'	22:L:21:ARG:HA	2.04	0.40
11:A:1773:A:N7	11:A:1829:A:C1'	2.85	0.40
11:A:1782:U:N3	11:A:2587:A:N1	2.70	0.40
11:A:2352:A:C4	11:A:2366:A:C2	3.10	0.40
11:A:2469:A:C6	11:A:2482:A:C8	3.10	0.40
11:A:2514:U:H2'	11:A:2515:C:C6	2.57	0.40
11:A:2533:U:H2'	11:A:2534:A:H5'	2.04	0.40
11:A:2555:U:C5	11:A:2556:C:C2	3.09	0.40
18:H:27:ARG:NH2	33:X:63:ILE:HG13	2.36	0.40
20:J:18:VAL:HG22	20:J:140:LEU:HD13	2.04	0.40
20:J:26:GLY:HA2	20:J:29:ALA:HB3	2.02	0.40
20:J:73:VAL:HB	20:J:75:TYR:CE2	2.57	0.40
23:M:64:TRP:HZ3	23:M:106:ASP:HB2	1.86	0.40
30:T:69:ARG:HG3	30:T:70:HIS:N	2.36	0.40
32:W:67:LYS:O	32:W:68:PHE:HB2	2.20	0.40
34:Y:2:LYS:HD2	34:Y:2:LYS:N	2.36	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
1	h	100/104 (96%)	92 (92%)	6 (6%)	2 (2%)	7 38
2	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1 7
3	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1 10
4	2	44/46 (96%)	41 (93%)	3 (7%)	0	100 100
5	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4 26
6	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1 5
7	5	146/165 (88%)	77 (53%)	41 (28%)	28 (19%)	0 0
8	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3 23
9	7	14/24 (58%)	13 (93%)	0	1 (7%)	1 8
10	8	92/94 (98%)	81 (88%)	11 (12%)	0	100 100
13	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2 14
14	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1 9
15	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2 16
16	F	175/177 (99%)	141 (81%)	30 (17%)	4 (2%)	6 34
17	G	173/176 (98%)	126 (73%)	30 (17%)	17 (10%)	0 3
18	H	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0 3
19	I	139/141 (99%)	97 (70%)	33 (24%)	9 (6%)	1 10
20	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1 10
21	K	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1 5
22	L	141/143 (99%)	104 (74%)	32 (23%)	5 (4%)	3 24
23	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1 5
24	N	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	19 58
25	O	114/116 (98%)	95 (83%)	18 (16%)	1 (1%)	17 56
26	P	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1 6
27	Q	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	3 24
28	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4 28
29	S	108/110 (98%)	91 (84%)	10 (9%)	7 (6%)	1 10
30	T	91/93 (98%)	57 (63%)	24 (26%)	10 (11%)	0 2
32	W	77/79 (98%)	39 (51%)	21 (27%)	17 (22%)	0 0
33	X	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1 9
35	Z	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3 23
36	z	87/89 (98%)	60 (69%)	14 (16%)	13 (15%)	0 1
All	All	3484/3678 (95%)	2699 (78%)	558 (16%)	227 (6%)	2 10

All (227) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	23	ALA
5	3	22	LYS
6	4	8	LYS
7	5	27	VAL
7	5	48	ALA
7	5	54	VAL
7	5	55	VAL
7	5	58	THR
7	5	69	PHE
7	5	93	ALA
7	5	107	GLU
7	5	108	VAL
7	5	120	ALA
7	5	124	ASP
7	5	130	PRO
9	7	22	HIS
13	C	70	LYS
13	C	104	LEU
13	C	121	ALA
13	C	140	VAL
14	D	43	ASP
14	D	73	VAL
14	D	170	VAL
15	E	79	ARG
16	F	111	ARG
17	G	2	ARG
17	G	16	VAL
17	G	28	LYS
17	G	31	GLU
17	G	84	LYS
17	G	164	ALA
17	G	168	VAL
18	H	3	VAL

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Mol	Chain	Res	Type
20	J	13	ARG
20	J	21	THR
20	J	44	TYR
20	J	45	THR
20	J	81	ILE
20	J	125	TYR
22	L	66	PHE
23	M	14	LYS
23	M	77	PRO
24	N	119	SER
26	P	50	ARG
26	P	51	ASN
26	P	93	LYS
29	S	3	THR
29	S	14	ALA
29	S	64	ALA
29	S	87	PRO
30	T	27	SER
30	T	29	THR
30	T	40	LYS
32	W	9	THR
32	W	18	LYS
32	W	29	SER
32	W	36	ILE
32	W	56	HIS
35	Z	9	THR
36	z	15	VAL
36	z	17	GLU
36	z	36	LEU
36	z	37	LYS
36	z	41	LEU
36	z	44	SER
36	z	54	LYS
36	z	62	ASN
36	z	67	MET
1	h	16	GLY
2	0	35	GLU
3	1	4	ILE
3	1	50	GLU
7	5	3	LEU
7	5	33	VAL
7	5	88	HIS

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Mol	Chain	Res	Type
7	5	92	ALA
7	5	116	GLU
7	5	119	PRO
13	C	37	SER
13	C	77	VAL
13	C	238	ASN
13	C	256	THR
14	D	92	VAL
14	D	99	GLU
14	D	107	VAL
14	D	118	PHE
16	F	135	ILE
17	G	169	ARG
18	H	9	VAL
18	H	16	GLY
19	I	20	SER
19	I	79	LEU
20	J	111	LYS
21	K	35	VAL
21	K	71	ARG
22	L	111	ILE
23	M	2	LEU
23	M	36	VAL
23	M	56	ALA
28	R	65	ALA
29	S	19	LEU
29	S	96	ILE
30	T	36	LYS
30	T	49	LYS
32	W	14	ASP
32	W	47	GLY
32	W	50	VAL
32	W	74	LYS
34	Y	37	LEU
36	z	30	VAL
1	h	99	ASN
3	1	51	ALA
6	4	4	ARG
7	5	5	LEU
7	5	78	GLY
7	5	118	ILE
8	6	14	MET

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Mol	Chain	Res	Type
13	C	110	LYS
14	D	95	SER
14	D	109	VAL
14	D	192	ALA
15	E	7	ASP
15	E	70	SER
15	E	123	LYS
16	F	176	PHE
17	G	32	LEU
17	G	117	PRO
17	G	170	THR
18	H	10	ALA
19	I	11	GLN
20	J	74	TYR
21	K	13	ASN
21	K	46	ALA
21	K	93	GLN
23	M	69	PRO
25	O	3	LYS
26	P	113	LEU
28	R	98	ILE
32	W	34	SER
33	X	17	ARG
35	Z	34	THR
2	0	54	ILE
6	4	16	ILE
7	5	89	PRO
13	C	59	GLN
13	C	197	ALA
14	D	169	ARG
14	D	175	LEU
16	F	132	ARG
17	G	33	THR
17	G	173	ALA
19	I	64	ARG
21	K	119	ALA
23	M	23	GLY
23	M	134	THR
26	P	4	ILE
26	P	92	ARG
26	P	103	THR
27	Q	87	VAL

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Mol	Chain	Res	Type
27	Q	88	GLU
27	Q	95	ALA
30	T	28	ASN
30	T	51	PHE
30	T	55	VAL
32	W	37	VAL
33	X	34	SER
33	X	76	LYS
34	Y	7	ARG
36	z	38	GLY
36	z	76	ALA
7	5	36	ASP
7	5	72	LEU
7	5	94	ARG
7	5	128	THR
13	C	64	VAL
13	C	120	ASP
13	C	196	ASN
14	D	183	GLU
15	E	46	GLN
15	E	96	VAL
17	G	97	VAL
17	G	163	TYR
17	G	166	GLU
19	I	12	VAL
19	I	71	LYS
20	J	65	THR
21	K	49	ARG
21	K	108	ARG
22	L	5	THR
22	L	29	LYS
22	L	41	ARG
23	M	35	ALA
23	M	73	ILE
26	P	34	GLY
27	Q	85	ALA
29	S	90	LYS
30	T	86	THR
30	T	89	GLU
32	W	46	ALA
34	Y	9	LYS
7	5	59	LEU

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Mol	Chain	Res	Type
15	E	83	VAL
15	E	153	LEU
17	G	118	ALA
18	H	14	SER
19	I	93	ASN
21	K	6	THR
21	K	50	GLY
23	M	13	HIS
28	R	40	MET
32	W	10	ARG
32	W	23	LYS
32	W	76	ARG
32	W	78	PHE
26	P	63	ILE
32	W	41	GLY
36	z	23	ILE
7	5	32	GLY
15	E	148	ILE
5	3	6	VAL
13	C	232	GLY
14	D	122	VAL
19	I	22	PRO
19	I	88	GLY
34	Y	62	GLY
2	0	24	VAL
15	E	71	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
1	h	83/85 (98%)	81 (98%)	2 (2%)	49 77
2	0	47/48 (98%)	46 (98%)	1 (2%)	53 79
3	1	45/49 (92%)	42 (93%)	3 (7%)	16 50
4	2	38/38 (100%)	35 (92%)	3 (8%)	12 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	3	51/52 (98%)	46 (90%)	5 (10%)	8 31
6	4	34/34 (100%)	31 (91%)	3 (9%)	10 36
7	5	112/123 (91%)	93 (83%)	19 (17%)	2 10
8	6	26/85 (31%)	22 (85%)	4 (15%)	2 13
9	7	16/24 (67%)	12 (75%)	4 (25%)	0 2
10	8	78/78 (100%)	75 (96%)	3 (4%)	33 67
13	C	216/218 (99%)	202 (94%)	14 (6%)	17 51
14	D	164/164 (100%)	151 (92%)	13 (8%)	12 43
15	E	165/165 (100%)	146 (88%)	19 (12%)	5 24
16	F	148/148 (100%)	138 (93%)	10 (7%)	16 49
17	G	136/137 (99%)	122 (90%)	14 (10%)	7 29
18	H	40/40 (100%)	39 (98%)	1 (2%)	47 77
19	I	109/109 (100%)	105 (96%)	4 (4%)	34 68
20	J	116/116 (100%)	100 (86%)	16 (14%)	3 16
21	K	103/103 (100%)	92 (89%)	11 (11%)	6 27
22	L	102/102 (100%)	95 (93%)	7 (7%)	15 49
23	M	109/109 (100%)	93 (85%)	16 (15%)	3 14
24	N	100/100 (100%)	93 (93%)	7 (7%)	15 48
25	O	86/86 (100%)	78 (91%)	8 (9%)	9 33
26	P	99/99 (100%)	91 (92%)	8 (8%)	11 42
27	Q	89/89 (100%)	81 (91%)	8 (9%)	9 34
28	R	84/84 (100%)	78 (93%)	6 (7%)	14 47
29	S	93/93 (100%)	83 (89%)	10 (11%)	6 27
30	T	80/80 (100%)	78 (98%)	2 (2%)	47 77
32	W	59/59 (100%)	53 (90%)	6 (10%)	7 29
33	X	67/67 (100%)	61 (91%)	6 (9%)	9 34
34	Y	55/55 (100%)	52 (94%)	3 (6%)	21 57
35	Z	48/48 (100%)	40 (83%)	8 (17%)	2 10
36	z	75/75 (100%)	52 (69%)	23 (31%)	0 0
All	All	2873/2962 (97%)	2606 (91%)	267 (9%)	12 33

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	17	LYS
1	h	68	SER
2	0	24	VAL
3	1	8	ILE
3	1	35	LEU
3	1	47	ILE
4	2	8	SER
4	2	9	VAL
4	2	24	THR
5	3	7	ARG
5	3	30	HIS
5	3	31	ILE
5	3	49	VAL
5	3	56	LEU
6	4	4	ARG
6	4	15	LYS
6	4	27	CYS
7	5	1	MET
7	5	3	LEU
7	5	26	VAL
7	5	42	ARG
7	5	51	TYR
7	5	54	VAL
7	5	59	LEU
7	5	65	GLU
7	5	69	PHE
7	5	70	GLU
7	5	96	PHE
7	5	106	PHE
7	5	107	GLU
7	5	116	GLU
7	5	121	SER
7	5	125	ARG
7	5	130	PRO
7	5	132	TYR
7	5	143	MET
8	6	17	MET
8	6	18	ASP
8	6	24	SER
8	6	26	MET
9	7	10	SER
9	7	11	LYS
9	7	13	PHE

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Mol	Chain	Res	Type
9	7	16	ASP
10	8	29	ILE
10	8	61	LEU
10	8	87	GLN
13	C	51	ARG
13	C	57	HIS
13	C	109	LEU
13	C	117	SER
13	C	124	LYS
13	C	129	LEU
13	C	142	ASN
13	C	155	ARG
13	C	166	ARG
13	C	176	ARG
13	C	194	VAL
13	C	212	TRP
13	C	251	THR
13	C	270	ARG
14	D	33	ARG
14	D	37	VAL
14	D	97	SER
14	D	103	ASP
14	D	107	VAL
14	D	118	PHE
14	D	124	ARG
14	D	170	VAL
14	D	171	THR
14	D	177	VAL
14	D	183	GLU
14	D	201	LEU
14	D	203	VAL
15	E	5	LEU
15	E	12	LEU
15	E	21	ARG
15	E	40	ARG
15	E	44	ARG
15	E	65	THR
15	E	69	ARG
15	E	70	SER
15	E	78	TRP
15	E	88	ARG
15	E	109	LEU

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Mol	Chain	Res	Type
15	E	113	VAL
15	E	118	LEU
15	E	120	VAL
15	E	126	VAL
15	E	131	THR
15	E	149	ILE
15	E	167	VAL
15	E	171	ASP
16	F	9	ASP
16	F	16	MET
16	F	34	THR
16	F	41	GLU
16	F	46	LYS
16	F	90	LEU
16	F	94	ARG
16	F	111	ARG
16	F	114	ARG
16	F	154	THR
17	G	3	VAL
17	G	16	VAL
17	G	44	HIS
17	G	68	ARG
17	G	84	LYS
17	G	94	ARG
17	G	103	ASN
17	G	110	HIS
17	G	121	THR
17	G	126	THR
17	G	131	VAL
17	G	132	LEU
17	G	151	ARG
17	G	170	THR
18	H	3	VAL
19	I	23	VAL
19	I	63	ASP
19	I	102	ARG
19	I	137	LEU
20	J	2	LYS
20	J	17	VAL
20	J	24	THR
20	J	30	THR
20	J	36	LEU

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Mol	Chain	Res	Type
20	J	40	HIS
20	J	54	ILE
20	J	55	ILE
20	J	65	THR
20	J	72	LYS
20	J	73	VAL
20	J	95	ARG
20	J	103	ILE
20	J	129	GLU
20	J	131	ASN
20	J	140	LEU
21	K	3	GLN
21	K	8	LEU
21	K	13	ASN
21	K	18	ARG
21	K	21	CYS
21	K	23	LYS
21	K	41	ILE
21	K	54	LYS
21	K	73	ASP
21	K	93	GLN
21	K	105	ARG
22	L	5	THR
22	L	19	LEU
22	L	82	LEU
22	L	91	ASP
22	L	100	ILE
22	L	121	THR
22	L	144	GLU
23	M	12	MET
23	M	13	HIS
23	M	31	PHE
23	M	33	LEU
23	M	46	ILE
23	M	53	MET
23	M	70	ASP
23	M	72	PRO
23	M	81	ARG
23	M	88	ASN
23	M	95	LEU
23	M	96	ILE
23	M	97	GLN

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Mol	Chain	Res	Type
23	M	100	LYS
23	M	110	GLU
23	M	134	THR
24	N	6	SER
24	N	8	ARG
24	N	33	ILE
24	N	65	LEU
24	N	69	ARG
24	N	70	THR
24	N	71	ARG
25	O	18	LEU
25	O	31	THR
25	O	33	ARG
25	O	36	TYR
25	O	38	GLN
25	O	47	VAL
25	O	106	LEU
25	O	115	LEU
26	P	16	VAL
26	P	19	PHE
26	P	62	LYS
26	P	83	ILE
26	P	85	VAL
26	P	92	ARG
26	P	95	LYS
26	P	103	THR
27	Q	16	ILE
27	Q	40	LYS
27	Q	50	ARG
27	Q	59	LEU
27	Q	63	ARG
27	Q	88	GLU
27	Q	93	ILE
27	Q	97	ILE
28	R	4	VAL
28	R	29	THR
28	R	38	VAL
28	R	46	GLU
28	R	48	LYS
28	R	63	VAL
29	S	3	THR
29	S	4	ILE

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Mol	Chain	Res	Type
29	S	7	HIS
29	S	36	LEU
29	S	45	VAL
29	S	66	ILE
29	S	76	VAL
29	S	88	ARG
29	S	96	ILE
29	S	101	SER
30	T	32	LEU
30	T	43	ILE
32	W	19	ARG
32	W	23	LYS
32	W	25	PHE
32	W	30	VAL
32	W	49	ASN
32	W	63	ASP
33	X	19	HIS
33	X	24	THR
33	X	26	ARG
33	X	29	LEU
33	X	34	SER
33	X	77	TYR
34	Y	10	SER
34	Y	16	THR
34	Y	57	LEU
35	Z	2	LYS
35	Z	9	THR
35	Z	15	ARG
35	Z	23	LEU
35	Z	30	ARG
35	Z	31	ILE
35	Z	37	ARG
35	Z	40	THR
36	z	1	LEU
36	z	2	ILE
36	z	13	VAL
36	z	14	PHE
36	z	17	GLU
36	z	18	THR
36	z	20	HIS
36	z	26	SER
36	z	31	HIS

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Mol	Chain	Res	Type
36	z	35	LYS
36	z	39	GLN
36	z	41	LEU
36	z	42	THR
36	z	46	ASP
36	z	48	GLU
36	z	50	ILE
36	z	52	ASP
36	z	62	ASN
36	z	64	GLN
36	z	68	THR
36	z	70	GLU
36	z	77	ASN
36	z	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
5	3	30	HIS
10	8	44	HIS
10	8	80	HIS
16	F	26	GLN
34	Y	38	GLN
34	Y	41	HIS
36	z	31	HIS
36	z	39	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	2850/2903 (98%)	457 (16%)	40 (1%)
12	B	117/118 (99%)	17 (14%)	0
31	V	76/77 (98%)	15 (19%)	0
All	All	3043/3098 (98%)	489 (16%)	40 (1%)

All (489) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	10	A
11	A	12	U

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Mol	Chain	Res	Type
11	A	15	G
11	A	34	U
11	A	35	G
11	A	42	A
11	A	43	G
11	A	45	G
11	A	46	G
11	A	51	G
11	A	61	C
11	A	71	A
11	A	74	A
11	A	75	G
11	A	80	G
11	A	82	U
11	A	84	A
11	A	96	C
11	A	101	A
11	A	118	A
11	A	119	A
11	A	120	U
11	A	131	A
11	A	135	U
11	A	136	G
11	A	137	U
11	A	138	U
11	A	139	U
11	A	140	C
11	A	141	G
11	A	142	A
11	A	144	A
11	A	149	A
11	A	162	U
11	A	163	C
11	A	164	C
11	A	181	A
11	A	188	G
11	A	196	A
11	A	199	A
11	A	215	G
11	A	216	A
11	A	222	A
11	A	226	A

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Mol	Chain	Res	Type
11	A	230	G
11	A	248	G
11	A	255	A
11	A	264	C
11	A	265	A
11	A	266	G
11	A	267	C
11	A	272	A
11	A	273	G
11	A	276	U
11	A	277	G
11	A	278	A
11	A	281	C
11	A	285	G
11	A	302	C
11	A	311	A
11	A	329	G
11	A	330	A
11	A	346	A
11	A	347	A
11	A	353	C
11	A	355	U
11	A	361	G
11	A	362	A
11	A	371	A
11	A	372	G
11	A	382	A
11	A	383	C
11	A	386	G
11	A	388	G
11	A	396	G
11	A	404	A
11	A	405	U
11	A	411	G
11	A	412	A
11	A	424	G
11	A	451	U
11	A	455	C
11	A	481	G
11	A	491	G
11	A	503	A
11	A	504	A

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Mol	Chain	Res	Type
11	A	505	A
11	A	509	C
11	A	528	A
11	A	531	C
11	A	532	A
11	A	533	G
11	A	538	A
11	A	543	G
11	A	544	C
11	A	546	U
11	A	547	A
11	A	548	G
11	A	549	G
11	A	563	A
11	A	573	U
11	A	575	A
11	A	586	A
11	A	603	A
11	A	604	G
11	A	613	A
11	A	614	A
11	A	615	U
11	A	627	A
11	A	631	A
11	A	637	A
11	A	645	C
11	A	646	U
11	A	647	G
11	A	648	G
11	A	654	A
11	A	655	A
11	A	656	G
11	A	686	U
11	A	714	U
11	A	715	A
11	A	730	A
11	A	738	G
11	A	747	U
11	A	752	A
11	A	775	G
11	A	776	G
11	A	782	A

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Mol	Chain	Res	Type
11	A	784	G
11	A	785	G
11	A	805	G
11	A	812	C
11	A	819	A
11	A	827	U
11	A	828	U
11	A	845	A
11	A	846	U
11	A	847	U
11	A	859	G
11	A	878	A
11	A	883	G
11	A	884	U
11	A	896	A
11	A	897	C
11	A	910	A
11	A	914	G
11	A	915	C
11	A	932	U
11	A	941	A
11	A	946	C
11	A	961	C
11	A	973	A
11	A	974	G
11	A	983	A
11	A	985	C
11	A	995	C
11	A	996	A
11	A	1003	G
11	A	1012	U
11	A	1013	C
11	A	1021	A
11	A	1022	G
11	A	1023	U
11	A	1025	G
11	A	1026	G
11	A	1033	U
11	A	1045	C
11	A	1046	A
11	A	1047	G
11	A	1051	G

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Mol	Chain	Res	Type
11	A	1053	C
11	A	1059	G
11	A	1060	U
11	A	1061	U
11	A	1062	G
11	A	1067	A
11	A	1069	A
11	A	1070	A
11	A	1072	C
11	A	1074	G
11	A	1078	U
11	A	1083	U
11	A	1084	A
11	A	1088	A
11	A	1089	A
11	A	1090	A
11	A	1091	G
11	A	1097	U
11	A	1098	A
11	A	1110	G
11	A	1111	A
11	A	1112	G
11	A	1129	A
11	A	1132	U
11	A	1133	A
11	A	1135	C
11	A	1136	G
11	A	1139	G
11	A	1142	A
11	A	1151	A
11	A	1155	A
11	A	1169	A
11	A	1170	C
11	A	1172	C
11	A	1174	U
11	A	1175	A
11	A	1176	U
11	A	1180	U
11	A	1186	G
11	A	1238	G
11	A	1248	G
11	A	1250	G

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Mol	Chain	Res	Type
11	A	1253	A
11	A	1256	G
11	A	1266	G
11	A	1268	A
11	A	1271	G
11	A	1272	A
11	A	1273	U
11	A	1281	G
11	A	1300	G
11	A	1301	A
11	A	1313	U
11	A	1317	G
11	A	1352	U
11	A	1365	A
11	A	1368	G
11	A	1378	A
11	A	1379	U
11	A	1383	A
11	A	1395	A
11	A	1415	U
11	A	1416	G
11	A	1419	A
11	A	1420	A
11	A	1428	C
11	A	1435	G
11	A	1452	G
11	A	1459	G
11	A	1482	G
11	A	1493	C
11	A	1504	A
11	A	1508	A
11	A	1510	G
11	A	1515	A
11	A	1524	G
11	A	1533	C
11	A	1534	U
11	A	1535	A
11	A	1536	C
11	A	1566	A
11	A	1569	A
11	A	1578	U
11	A	1583	A

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Mol	Chain	Res	Type
11	A	1584	U
11	A	1585	C
11	A	1607	C
11	A	1608	A
11	A	1610	A
11	A	1613	G
11	A	1627	G
11	A	1647	U
11	A	1648	U
11	A	1649	G
11	A	1652	A
11	A	1653	G
11	A	1674	G
11	A	1714	U
11	A	1715	G
11	A	1723	G
11	A	1729	U
11	A	1730	C
11	A	1737	G
11	A	1738	G
11	A	1739	A
11	A	1744	A
11	A	1758	U
11	A	1764	C
11	A	1773	A
11	A	1776	G
11	A	1791	A
11	A	1800	C
11	A	1801	A
11	A	1802	A
11	A	1808	A
11	A	1811	G
11	A	1816	C
11	A	1829	A
11	A	1833	C
11	A	1847	A
11	A	1848	A
11	A	1858	A
11	A	1869	G
11	A	1870	C
11	A	1871	A
11	A	1872	A

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Mol	Chain	Res	Type
11	A	1873	G
11	A	1884	G
11	A	1906	G
11	A	1913	A
11	A	1914	C
11	A	1927	A
11	A	1929	G
11	A	1930	G
11	A	1937	A
11	A	1938	A
11	A	1955	U
11	A	1960	A
11	A	1966	A
11	A	1967	C
11	A	1970	A
11	A	1971	U
11	A	1972	G
11	A	1991	U
11	A	1993	U
11	A	1997	C
11	A	2017	U
11	A	2020	A
11	A	2022	U
11	A	2023	C
11	A	2031	A
11	A	2033	A
11	A	2043	C
11	A	2055	C
11	A	2056	G
11	A	2060	A
11	A	2061	G
11	A	2062	A
11	A	2063	C
11	A	2069	G
11	A	2072	C
11	A	2093	G
11	A	2104	C
11	A	2106	U
11	A	2107	G
11	A	2108	A
11	A	2109	U
11	A	2110	G

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Mol	Chain	Res	Type
11	A	2134	A
11	A	2135	A
11	A	2137	U
11	A	2138	G
11	A	2139	U
11	A	2140	G
11	A	2142	A
11	A	2143	C
11	A	2144	G
11	A	2145	C
11	A	2146	C
11	A	2147	A
11	A	2148	G
11	A	2149	U
11	A	2150	C
11	A	2151	U
11	A	2153	C
11	A	2154	A
11	A	2155	U
11	A	2156	G
11	A	2157	G
11	A	2180	U
11	A	2183	A
11	A	2185	U
11	A	2194	U
11	A	2198	A
11	A	2199	A
11	A	2204	G
11	A	2211	A
11	A	2212	A
11	A	2214	C
11	A	2225	A
11	A	2226	C
11	A	2238	G
11	A	2239	G
11	A	2250	G
11	A	2268	A
11	A	2278	A
11	A	2283	C
11	A	2284	A
11	A	2286	G
11	A	2287	A

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Mol	Chain	Res	Type
11	A	2305	U
11	A	2308	G
11	A	2311	A
11	A	2322	A
11	A	2325	G
11	A	2327	A
11	A	2333	A
11	A	2336	A
11	A	2347	C
11	A	2354	C
11	A	2361	G
11	A	2383	G
11	A	2385	C
11	A	2402	U
11	A	2403	C
11	A	2406	A
11	A	2423	U
11	A	2424	C
11	A	2425	A
11	A	2429	G
11	A	2430	A
11	A	2435	A
11	A	2441	U
11	A	2448	A
11	A	2470	G
11	A	2476	A
11	A	2491	U
11	A	2502	G
11	A	2503	A
11	A	2505	G
11	A	2506	U
11	A	2507	C
11	A	2518	A
11	A	2529	G
11	A	2554	U
11	A	2556	C
11	A	2566	A
11	A	2567	G
11	A	2572	A
11	A	2573	C
11	A	2584	U
11	A	2585	U

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Mol	Chain	Res	Type
11	A	2586	U
11	A	2613	U
11	A	2629	U
11	A	2663	G
11	A	2671	G
11	A	2681	C
11	A	2682	A
11	A	2689	U
11	A	2690	U
11	A	2714	G
11	A	2716	C
11	A	2726	A
11	A	2733	A
11	A	2744	G
11	A	2748	A
11	A	2757	A
11	A	2760	C
11	A	2765	A
11	A	2778	A
11	A	2791	G
11	A	2798	U
11	A	2800	A
11	A	2801	G
11	A	2818	U
11	A	2820	A
11	A	2821	A
11	A	2861	U
11	A	2867	G
11	A	2873	A
11	A	2874	C
11	A	2883	A
11	A	2884	U
11	A	2885	G
11	A	2891	U
11	A	2903	U
12	B	3	C
12	B	15	A
12	B	16	G
12	B	21	G
12	B	30	C
12	B	35	C
12	B	42	C

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Mol	Chain	Res	Type
12	B	44	G
12	B	45	A
12	B	56	G
12	B	84	G
12	B	87	U
12	B	88	C
12	B	89	U
12	B	90	C
12	B	99	A
12	B	109	A
31	V	4	C
31	V	5	A
31	V	8	U
31	V	19	G
31	V	21	A
31	V	31	C
31	V	33	U
31	V	43	G
31	V	48	C
31	V	49	G
31	V	53	G
31	V	67	G
31	V	71	C
31	V	73	A
31	V	76	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	119	A
11	A	271	G
11	A	277	G
11	A	301	G
11	A	403	U
11	A	404	A
11	A	503	A
11	A	527	C
11	A	613	A
11	A	655	A
11	A	784	G
11	A	827	U
11	A	846	U

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Mol	Chain	Res	Type
11	A	882	G
11	A	931	U
11	A	1020	A
11	A	1025	G
11	A	1069	A
11	A	1088	A
11	A	1110	G
11	A	1247	A
11	A	1378	A
11	A	1458	U
11	A	1509	A
11	A	1535	A
11	A	1626	A
11	A	1738	G
11	A	1757	A
11	A	1847	A
11	A	1870	C
11	A	1939	U
11	A	2108	A
11	A	2142	A
11	A	2211	A
11	A	2286	G
11	A	2326	C
11	A	2423	U
11	A	2756	U
11	A	2873	A
11	A	2902	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 145 ligands modelled in this entry, 144 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	TRP	A	3001	-	14,16,16	0.94	0	16,22,22	0.94	0

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
39	TRP	A	3001	-	-	6/7/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	3001	TRP	OXT-C-CA-N
39	A	3001	TRP	OXT-C-CA-CB
39	A	3001	TRP	O-C-CA-CB
39	A	3001	TRP	N-CA-CB-CG
39	A	3001	TRP	O-C-CA-N
39	A	3001	TRP	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	A	3001	TRP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

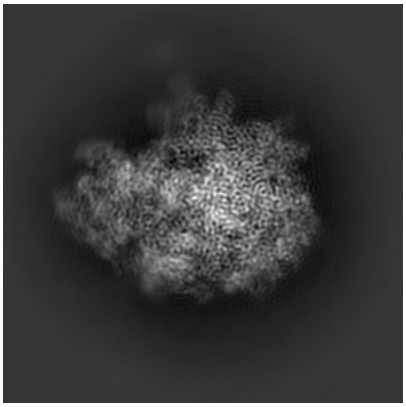
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0322. These allow visual inspection of the internal detail of the map and identification of artifacts.

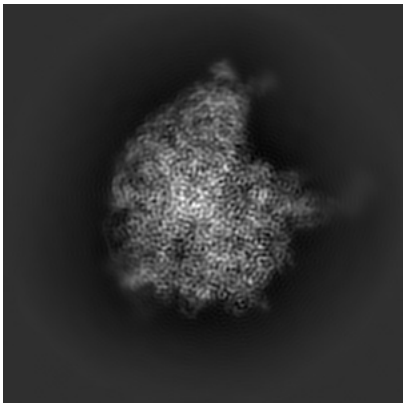
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

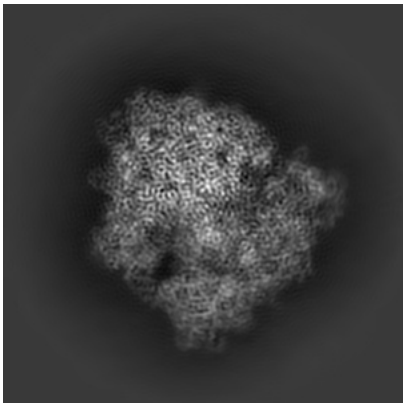
6.1.1 Primary map



X



Y

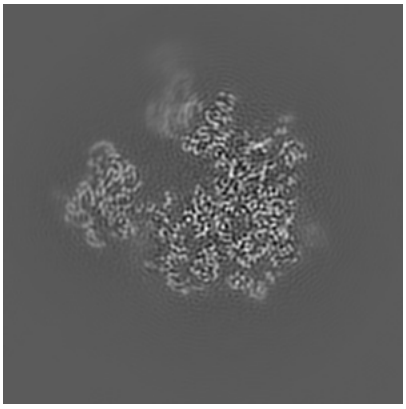


Z

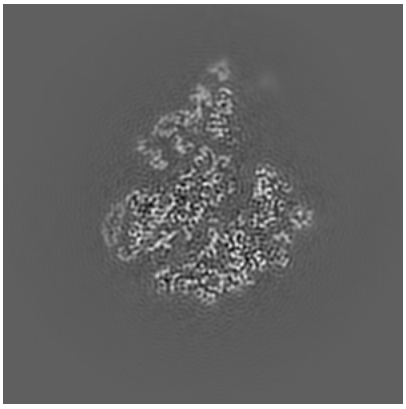
The images above show the map projected in three orthogonal directions.

6.2 Central slices

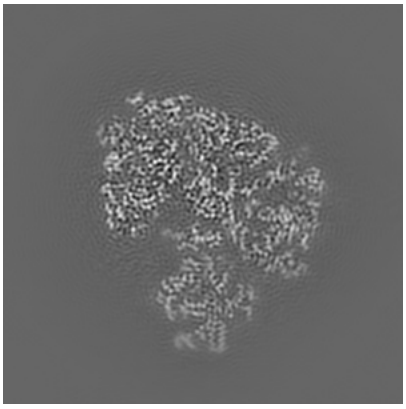
6.2.1 Primary map



X Index: 186



Y Index: 186

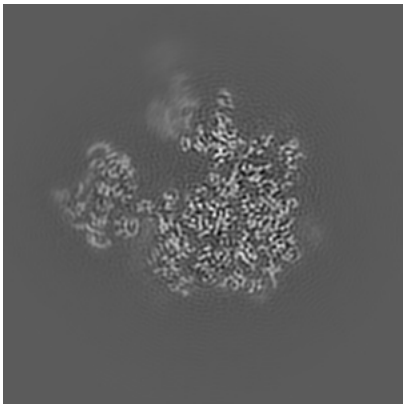


Z Index: 186

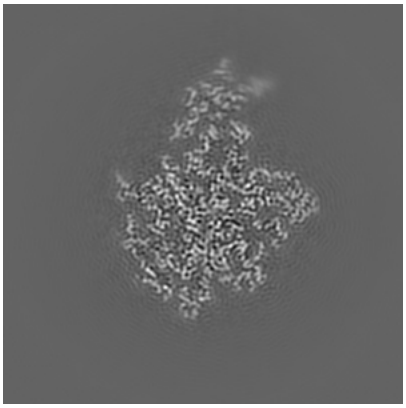
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

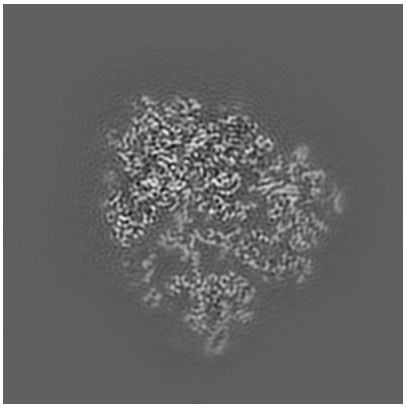
6.3.1 Primary map



X Index: 190



Y Index: 204



Z Index: 194

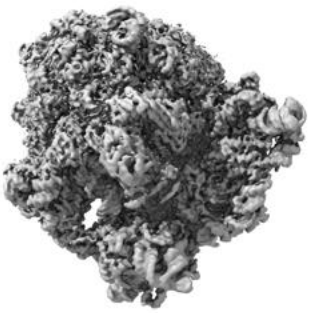
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

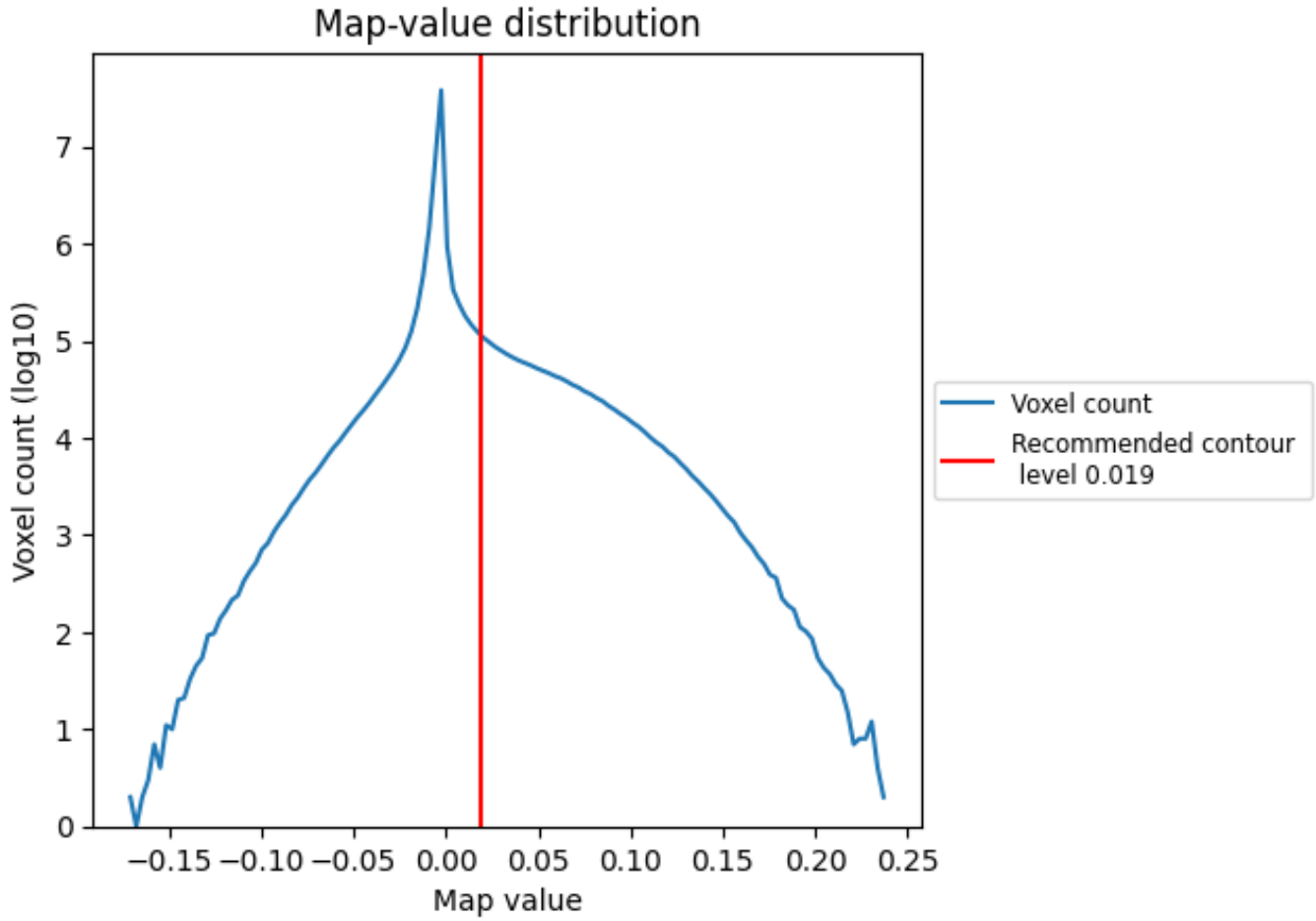
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

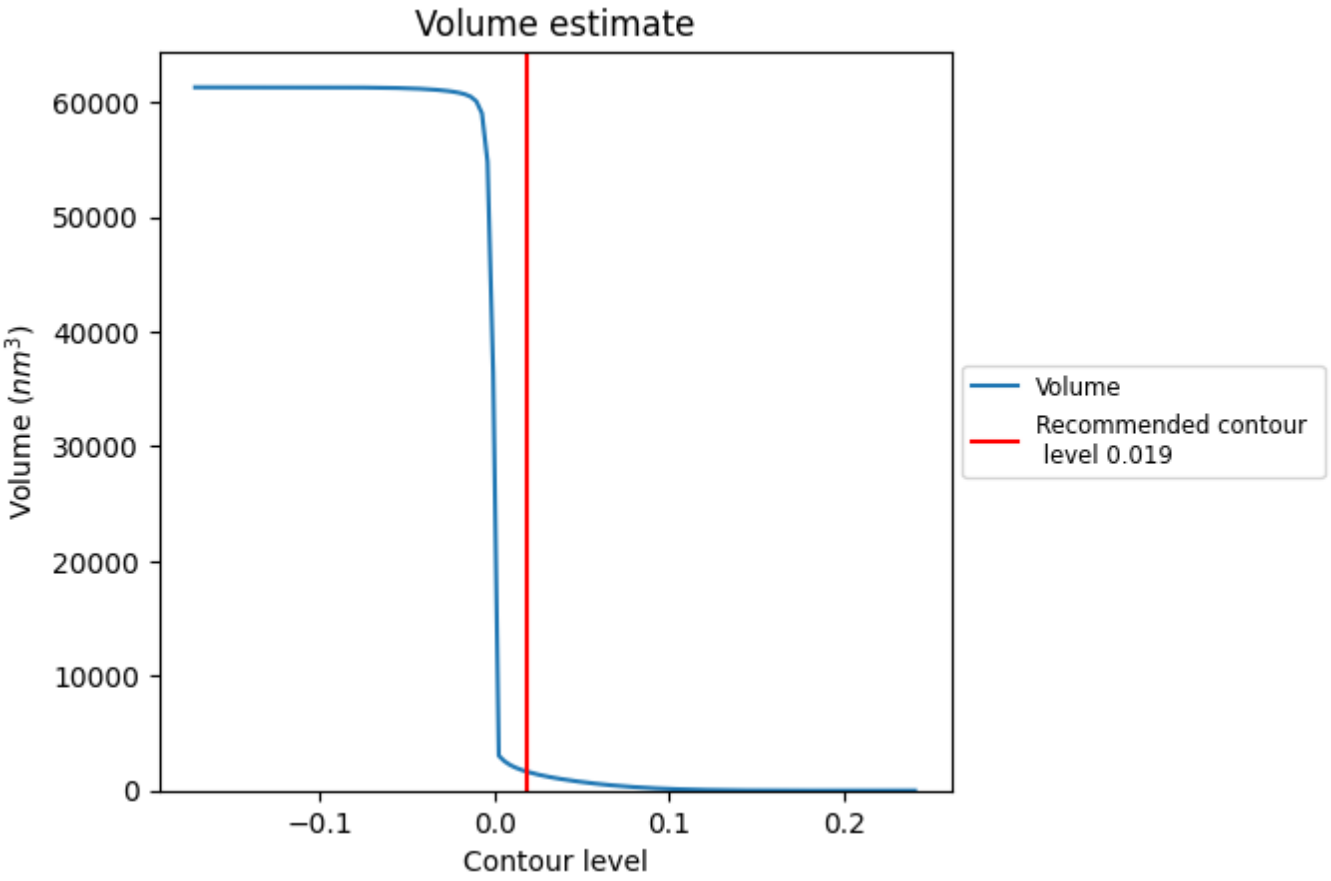
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

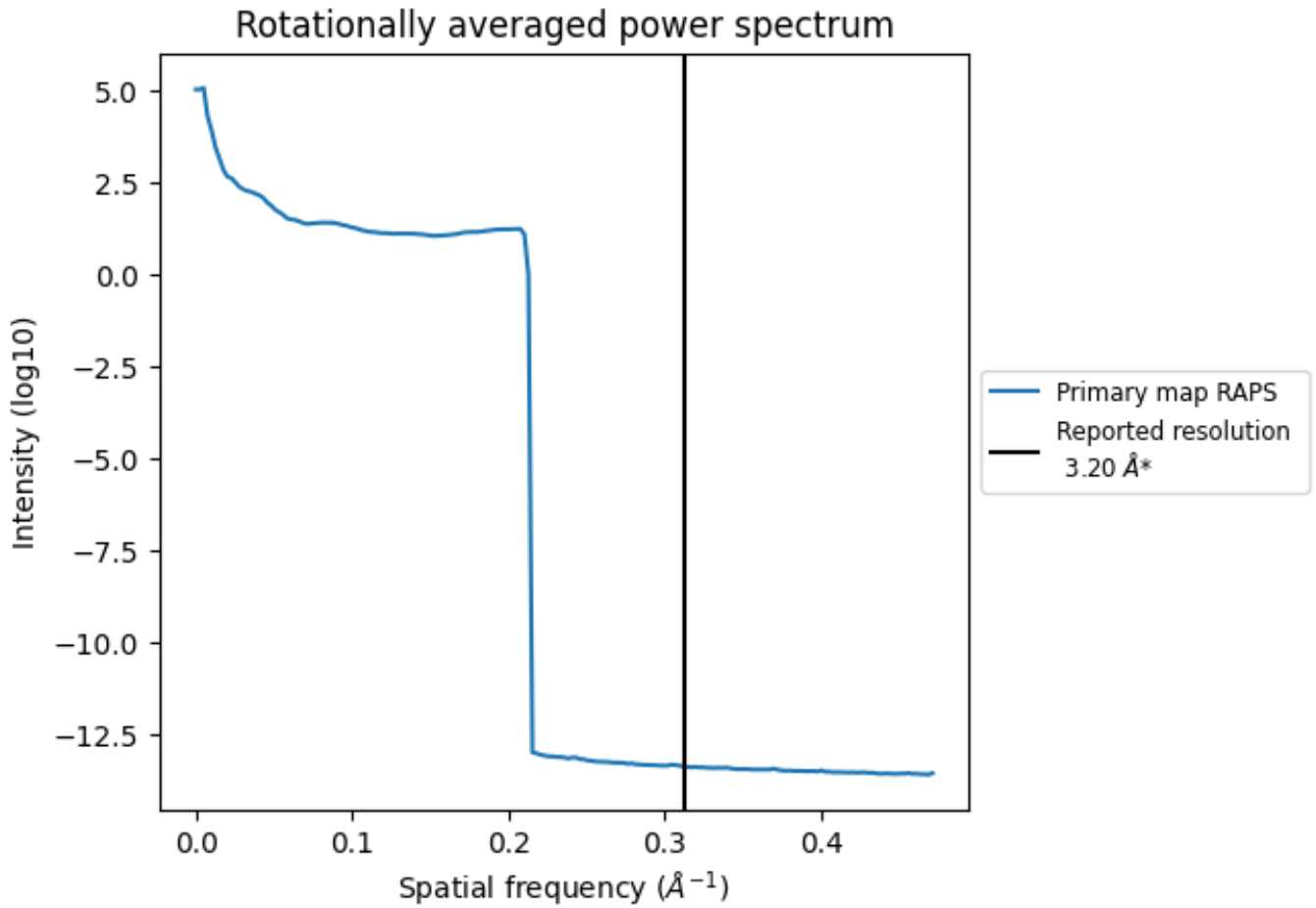
7.2 Volume estimate



The volume at the recommended contour level is 1634 nm^3; this corresponds to an approximate mass of 1476 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

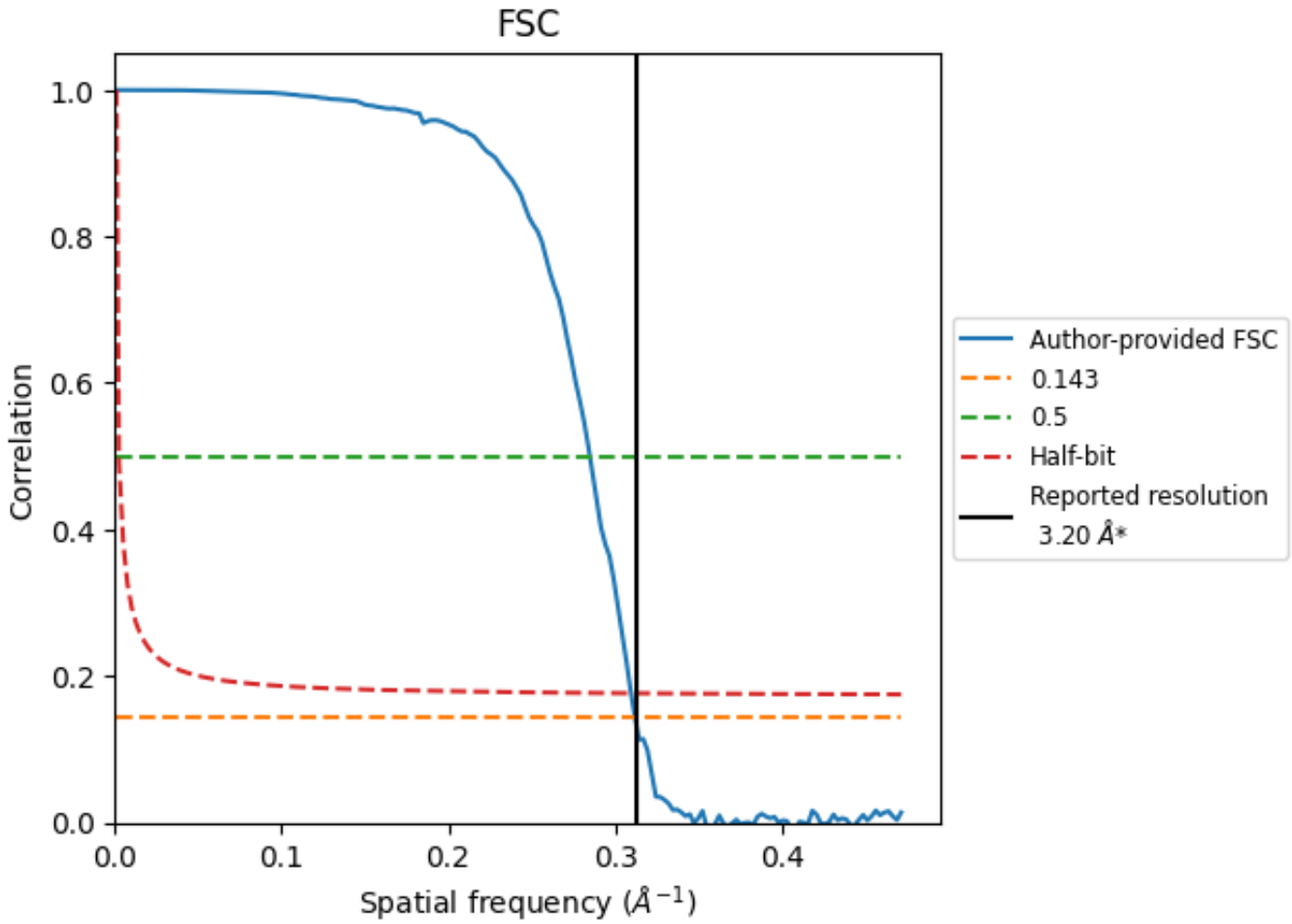


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

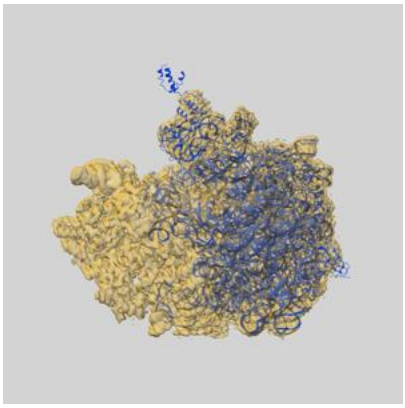
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.51	3.23
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

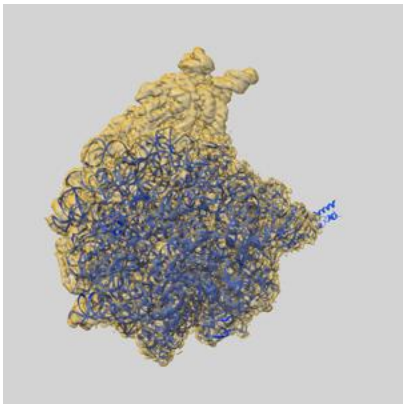
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0322 and PDB model 6I0Y. Per-residue inclusion information can be found in section 3 on page 12.

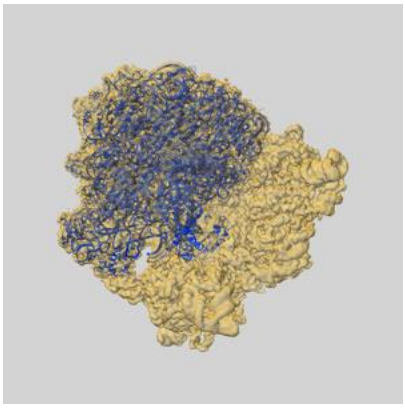
9.1 Map-model overlay



X



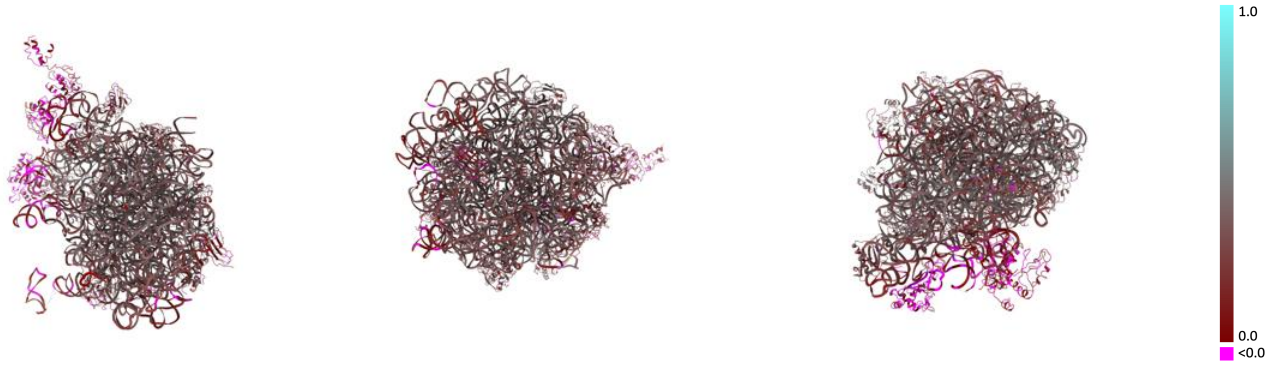
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

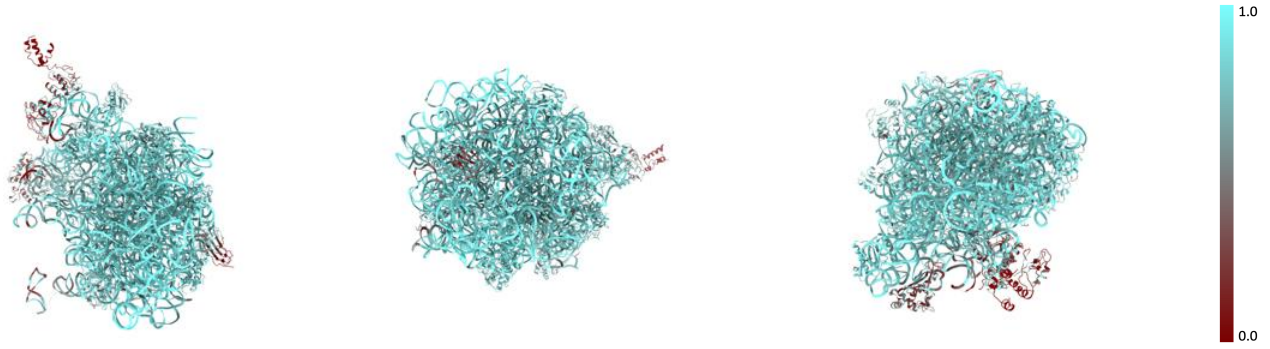
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

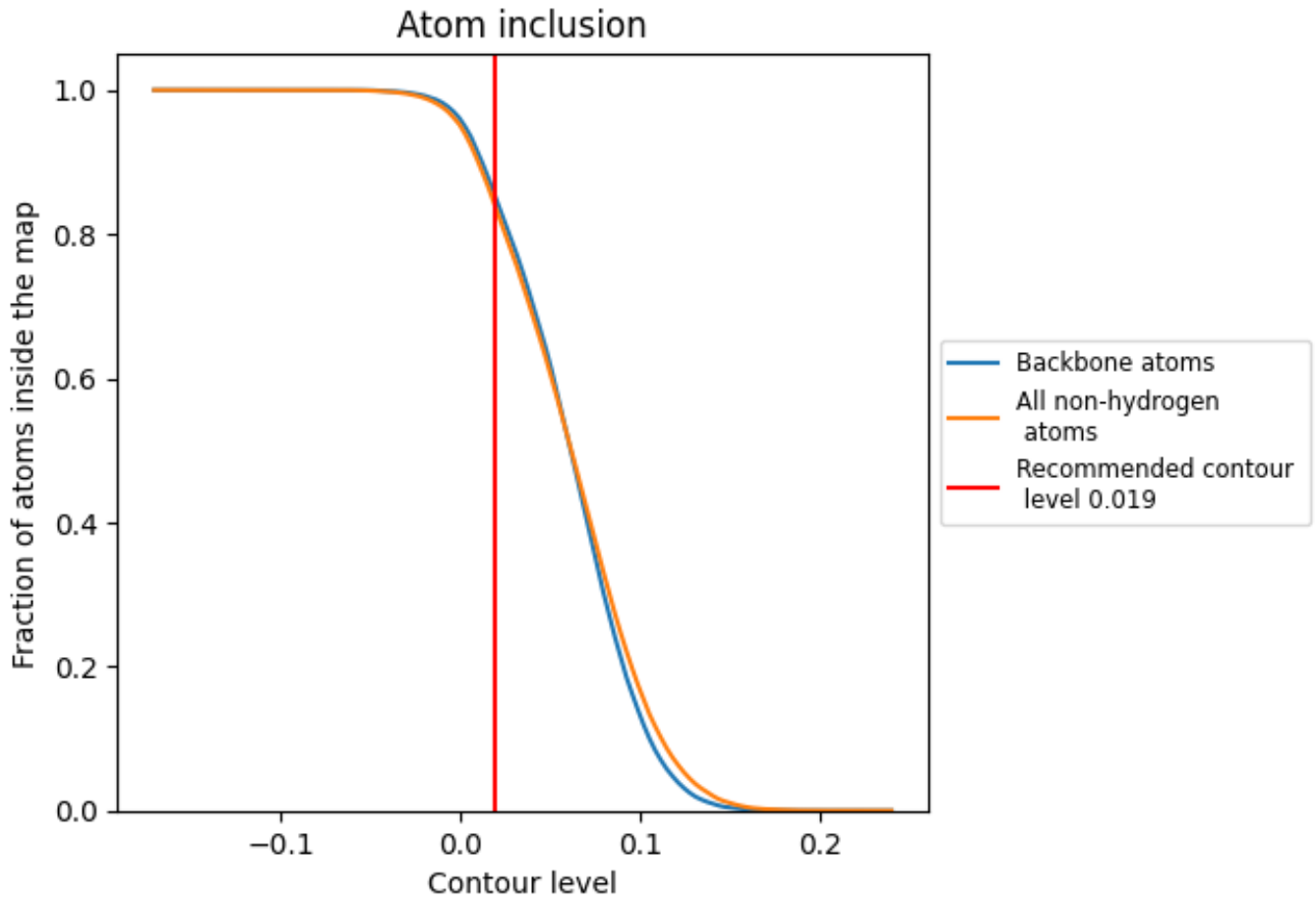
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8408	0.3050
0	0.8154	0.3330
1	0.8155	0.3060
2	0.8282	0.3250
3	0.8656	0.3850
4	0.8129	0.3330
5	0.3821	0.0800
6	0.0000	0.0630
7	0.7206	0.2810
8	0.7967	0.3240
A	0.8934	0.3250
B	0.8796	0.2830
C	0.7868	0.2870
D	0.8257	0.3490
E	0.7922	0.3250
F	0.4676	-0.0220
G	0.7863	0.2640
H	0.6887	0.2060
I	0.3160	0.0540
J	0.8045	0.3010
K	0.8007	0.3460
L	0.8258	0.3420
M	0.8167	0.3460
N	0.8590	0.3490
O	0.8262	0.3090
P	0.7962	0.3310
Q	0.7952	0.2860
R	0.8030	0.3110
S	0.8038	0.3410
T	0.7673	0.3200
V	0.7107	0.1310
W	0.7690	0.2990
X	0.8403	0.3390
Y	0.7887	0.2610
Z	0.7918	0.3030

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Chain	Atom inclusion	Q-score
h	0.7992	0.3170
z	0.3017	0.1300