Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:39 pm GMT

PDB ID	:	5JBH
EMDB ID	:	EMD-8149
Title	:	Cryo-EM structure of a full archaeal ribosomal translation initiation complex in the P-IN conformation
Authors	:	Coureux, P.-D.; Schmitt, E.; Mechulam, Y.
Deposited on	:	2016-04-13
Resolution	:	5.34 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:

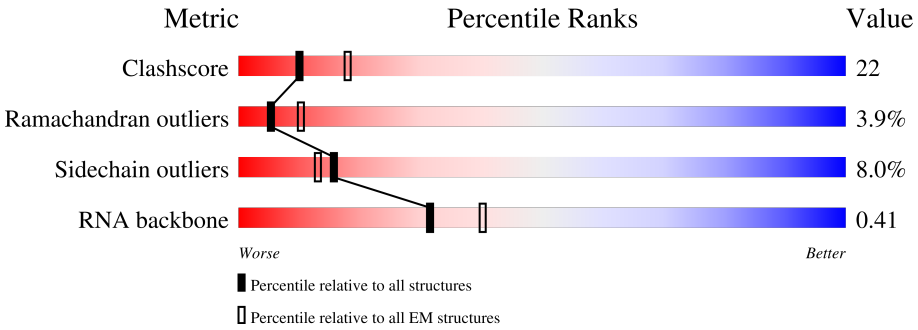
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 5.34 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	2	1518	31% 51% 15%
2	Z	210	79% 9% 11%
3	3	123	20% 85% 14%
4	L	102	6% 67% 25% 7%
5	O	148	10% 86% 13%
6	P	56	80% 16%
7	S	67	85% 13%

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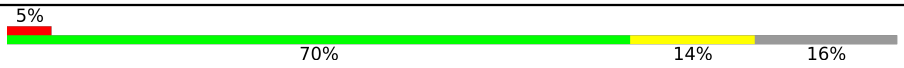
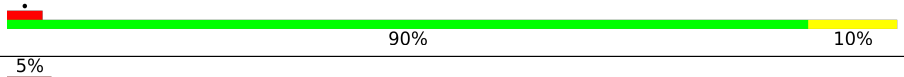
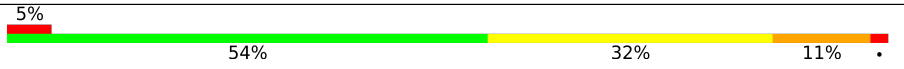
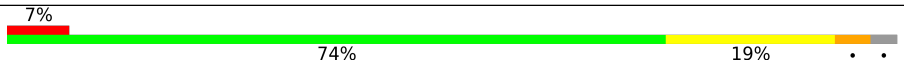
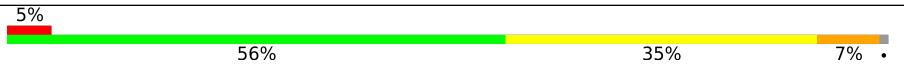
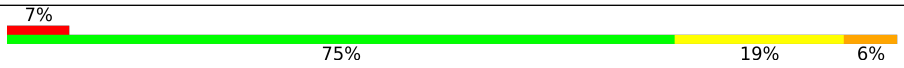
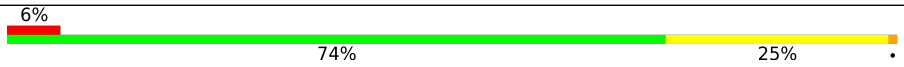
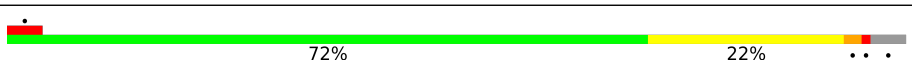
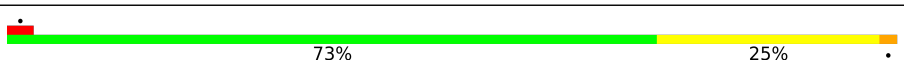
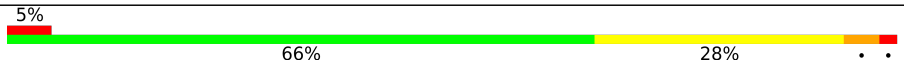
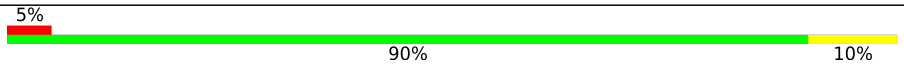
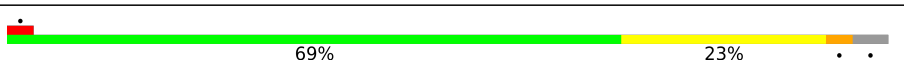
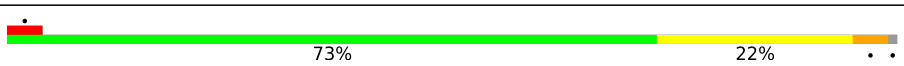
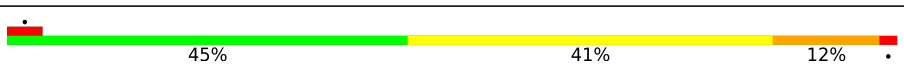
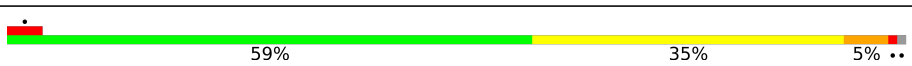
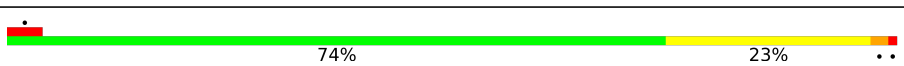
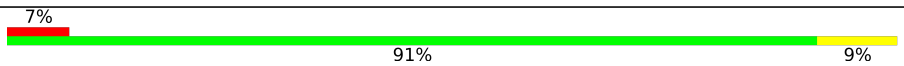
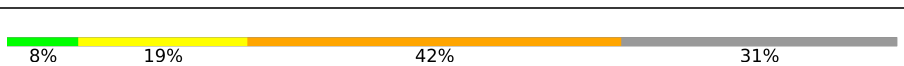
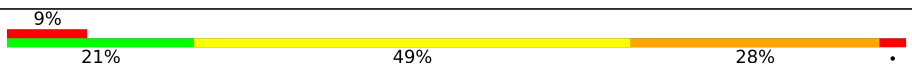
Mol	Chain	Length	Quality of chain
8	T	132	
9	U	150	
10	X	71	
11	Y	50	
12	H	215	
13	K	135	
14	M	137	
15	N	147	
16	Q	158	
17	R	113	
18	A	198	
19	B	202	
20	V	99	
21	W	63	
22	D	180	
23	E	243	
24	F	236	
25	G	125	
26	I	130	
27	J	127	
28	C	57	
29	0	22	
30	5	26	
31	1	102	
32	4	76	

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Mol	Chain	Length	Quality of chain
33	6	113	12% 76% 6% 16%
34	7	415	31% 41% 47% 10%
35	8	139	76% 32% 52% 9% 7%
36	9	266	53% 35% 48% 11% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	MET	4	101	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 70653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1495	32135	14297	5954	10389	1495	0	0

- Molecule 2 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	186	1459	933	271	251	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	123	939	599	155	181	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	102	822	507	159	152	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	O	148	1189	746	237	200	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	P	56	462	292	95	69	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	67	Total	C	N	O	S	0	0
			556	353	105	95	3		

- Molecule 8 is a protein called 30S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	111	Total	C	N	O	S	0	0
			923	594	173	150	6		

- Molecule 9 is a protein called 30S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	144	Total	C	N	O	S	0	0
			1175	758	212	204	1		

- Molecule 10 is a protein called 30S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	71	Total	C	N	O	S	0	0
			568	345	115	107	1		

- Molecule 11 is a protein called 30S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	50	Total	C	N	O	S	0	0
			409	262	75	66	6		

- Molecule 12 is a protein called 30S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 13 is a protein called 30S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	135	Total	C	N	O	S	0	0
			1072	671	205	190	6		

- Molecule 14 is a protein called 30S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	133	Total	C	N	O	S	0	0
			1004	623	200	179	2		

- Molecule 15 is a protein called 30S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	145	Total	C	N	O	S	0	0
			1140	722	222	193	3		

- Molecule 16 is a protein called 30S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	158	Total	C	N	O	S	0	0
			1310	834	250	221	5		

- Molecule 17 is a protein called 30S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	113	Total	C	N	O	S	0	0
			934	592	177	160	5		

- Molecule 18 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	190	Total	C	N	O	S	0	0
			1559	1007	273	274	5		

- Molecule 19 is a protein called 30S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	202	Total	C	N	O	S	0	0
			1623	1046	282	290	5		

- Molecule 20 is a protein called 30S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	99	Total	C	N	O	S	0	0
			823	532	134	154	3		

- Molecule 21 is a protein called 30S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	63	Total	C	N	O	S	0	0
			478	306	85	81	6		

- Molecule 22 is a protein called 30S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	172	Total	C	N	O	S	0	0
			1434	902	273	255	4		

- Molecule 23 is a protein called 30S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	241	Total	C	N	O	S	0	0
			1976	1277	355	339	5		

- Molecule 24 is a protein called 30S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	217	Total	C	N	O	S	0	0
			1716	1084	319	305	8		

- Molecule 25 is a protein called 30S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	125	Total	C	N	O	S	0	0
			984	623	180	179	2		

- Molecule 26 is a protein called 30S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 27 is a protein called 30S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	J	127	Total	C	N	O	S	0	0
			1004	622	207	174	1		

- Molecule 28 is a protein called 30S ribosomal protein SX.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	57	Total	C	N	O	0	0
			286	171	57	58		

- Molecule 29 is a protein called 30S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	0	22	Total	C	N	O	S	0	0
			213	135	52	25	1		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	18	Total	C	N	O	P	0	0
			388	173	70	127	18		

- Molecule 31 is a protein called aIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	80	Total	C	N	O	S	0	0
			632	399	112	117	4		

- Molecule 32 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	76	Total	C	N	O	P	0	0
			1621	723	291	531	76		

- Molecule 33 is a protein called aIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	95	Total	C	N	O	S	2	0
			792	504	150	135	3		

- Molecule 34 is a protein called aIF2-gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	409	Total	C	N	O	S	0	0
			3171	2028	541	590	12		

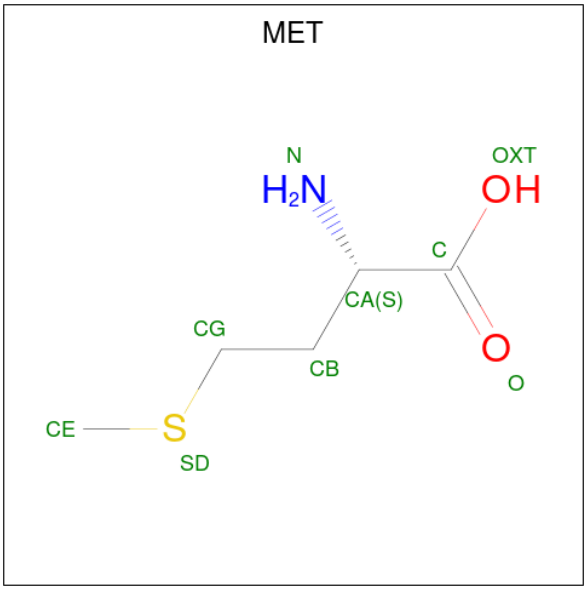
- Molecule 35 is a protein called aIF2-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	129	Total	C	N	O	S	0	0
			1033	659	172	192	10		

- Molecule 36 is a protein called aIF2-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	253	Total	C	N	O	S	0	0
			2025	1296	345	383	1		

- Molecule 37 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

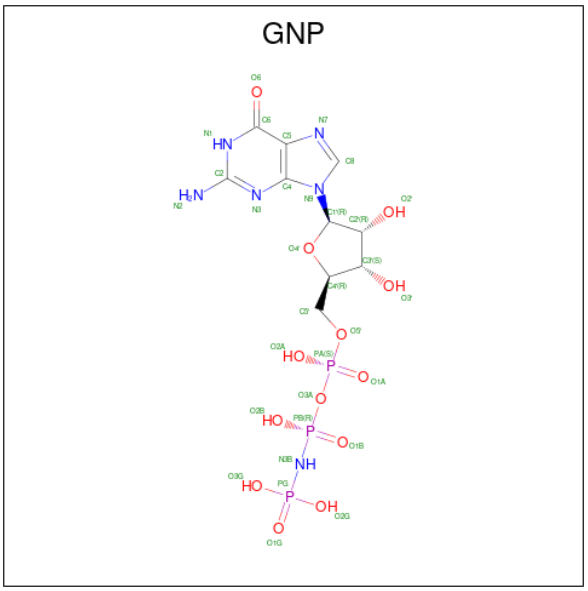


Mol	Chain	Residues	Atoms					AltConf
37	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	7	1	Total	Mg	0
			1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

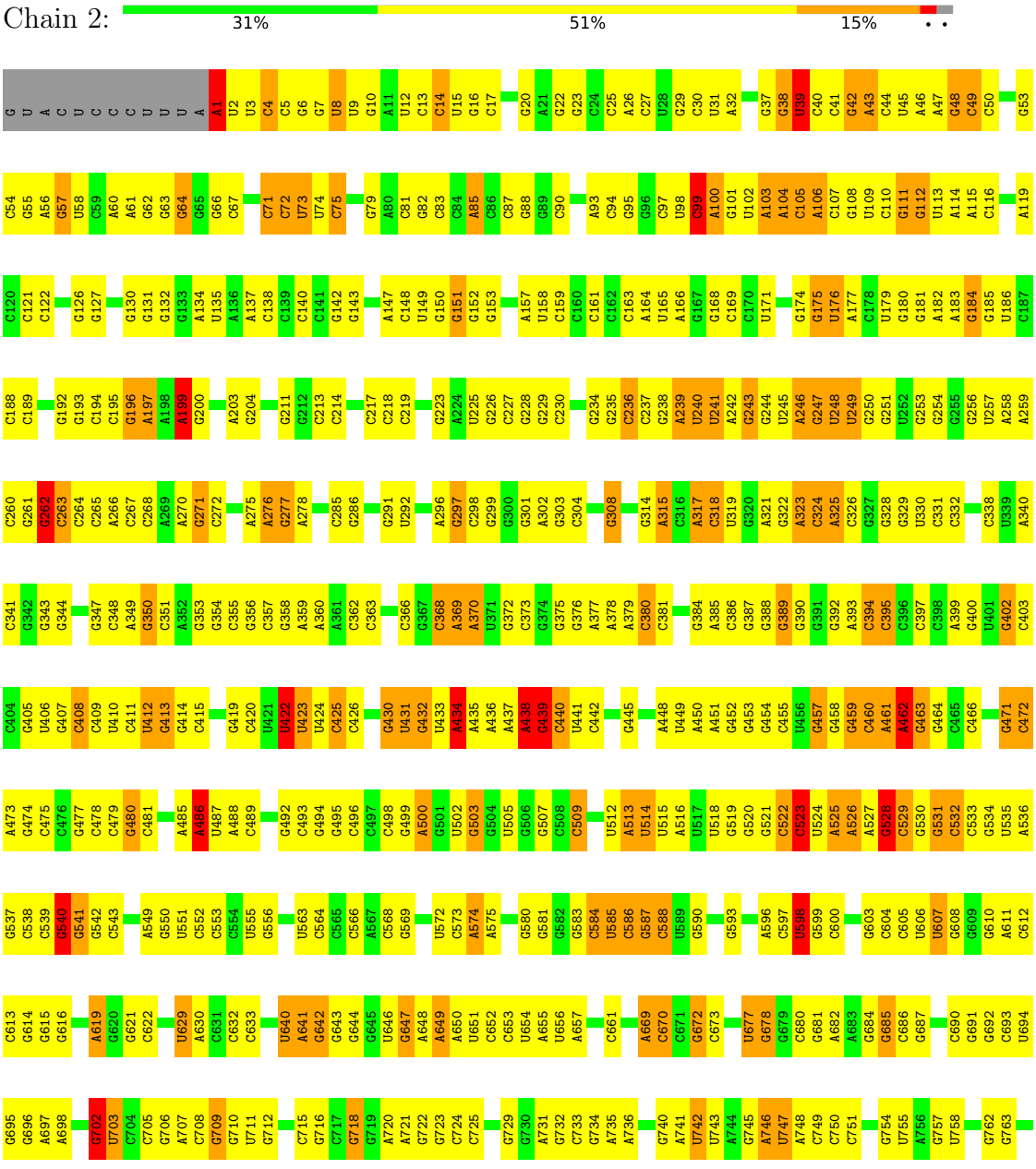
Mol	Chain	Residues	Atoms		AltConf
40	8	1	Total	Zn	0
			1	1	

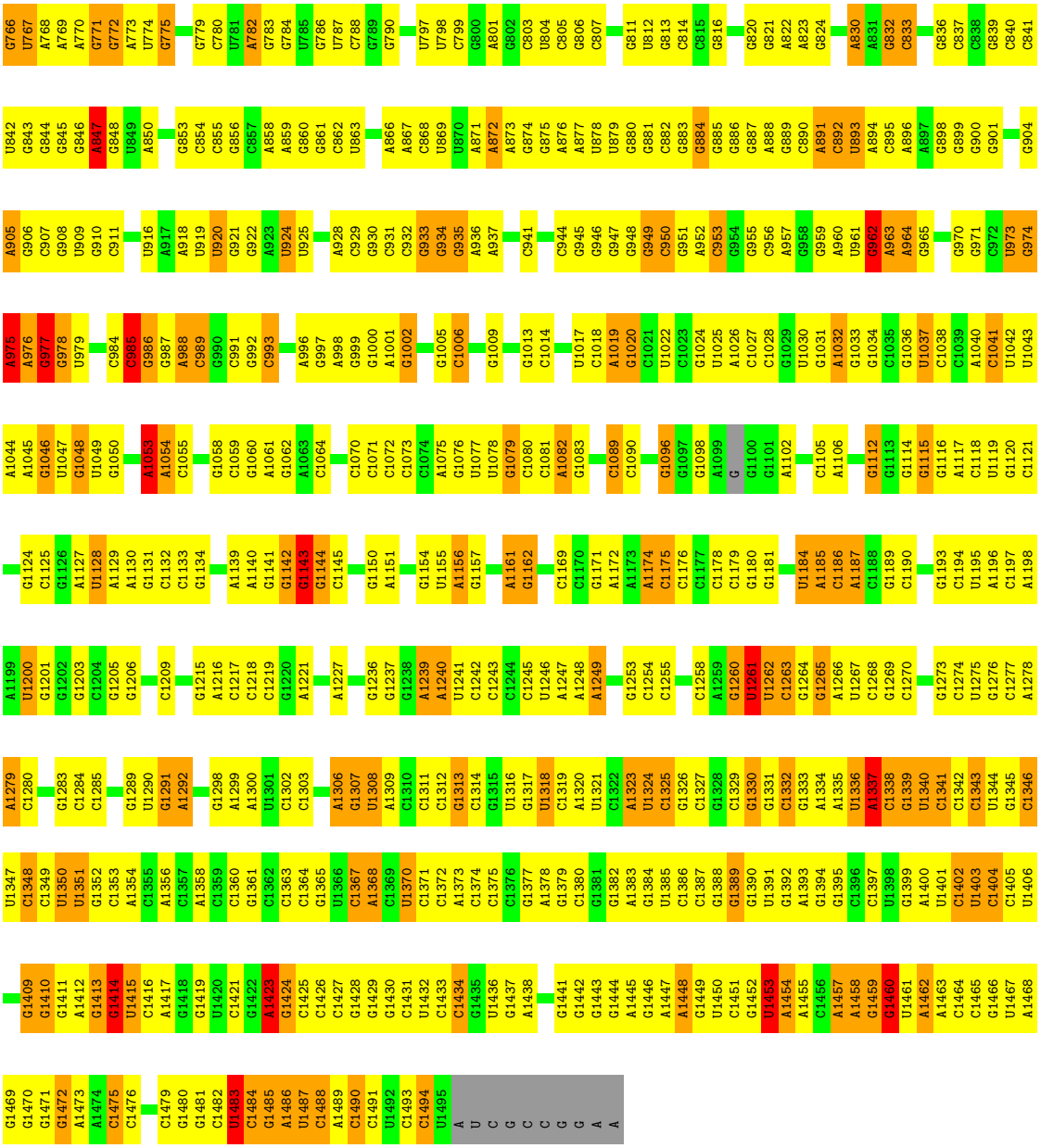
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: 16S ribosomal RNA

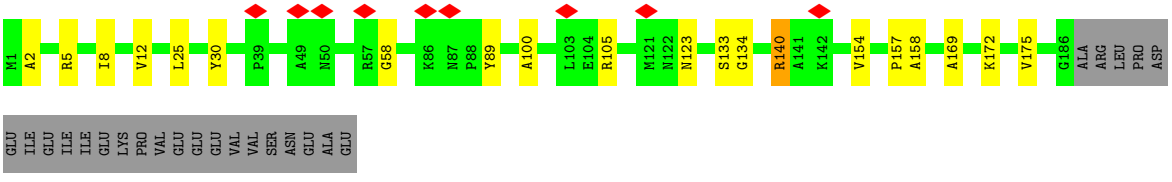
Chain 2:





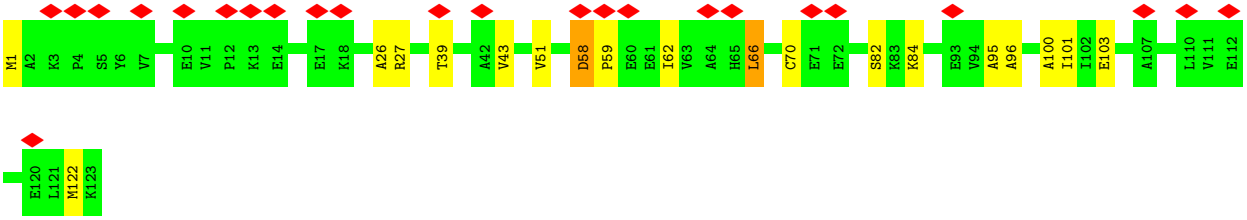
• Molecule 2: 30S ribosomal protein uS3

Chain Z:

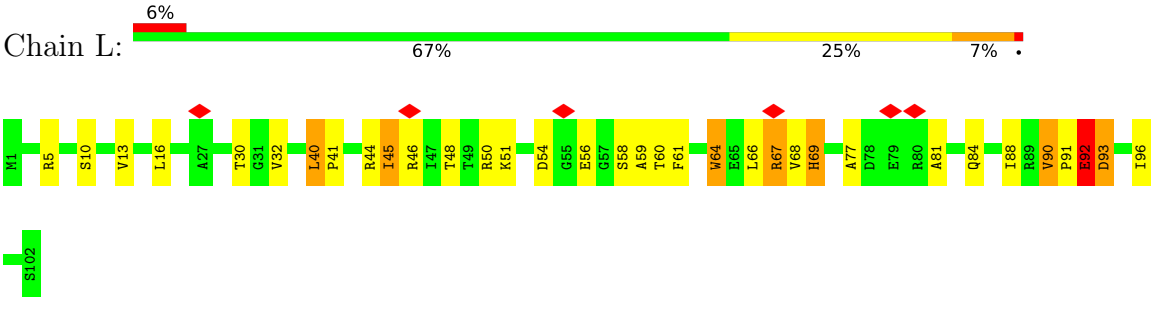


• Molecule 3: 50S ribosomal protein uL30

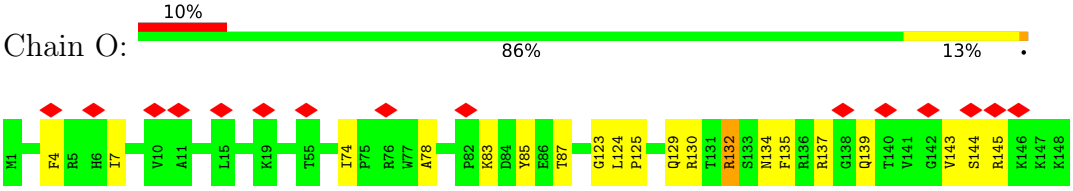
Chain 3:



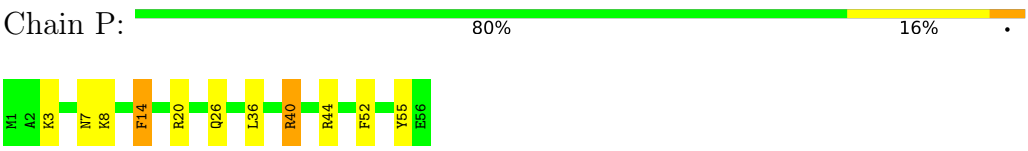
• Molecule 4: 30S ribosomal protein uS10



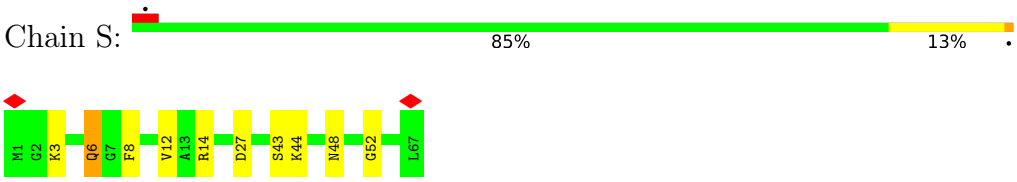
• Molecule 5: 30S ribosomal protein uS13



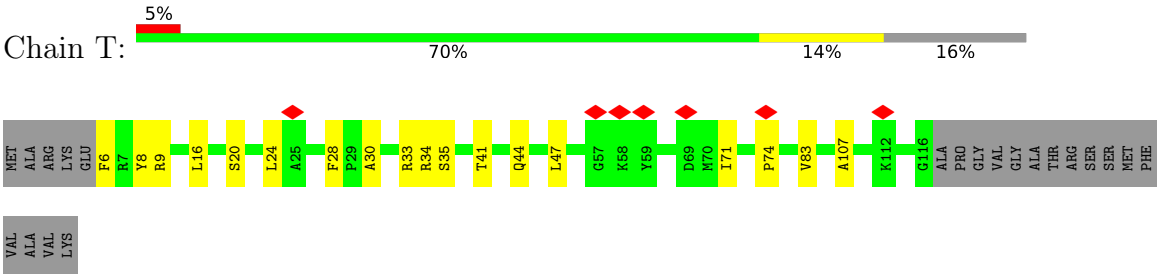
• Molecule 6: 30S ribosomal protein uS14



• Molecule 7: 30S ribosomal protein eS17

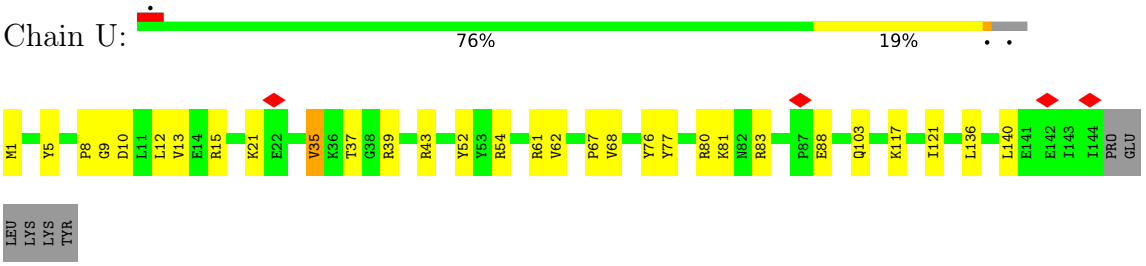


• Molecule 8: 30S ribosomal protein uS19



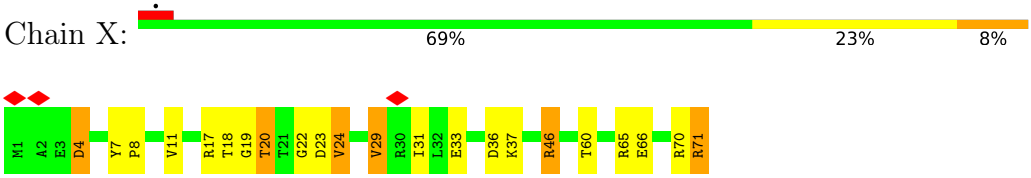
• Molecule 9: 30S ribosomal protein eS19

Chain U:



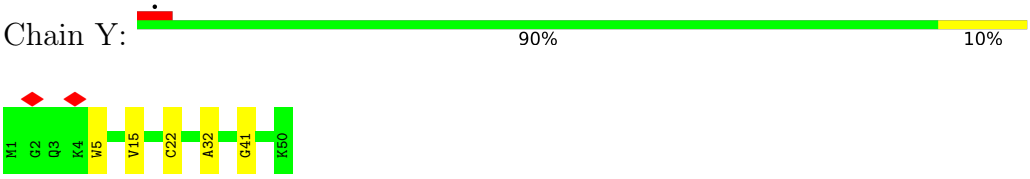
• Molecule 10: 30S ribosomal protein eS28

Chain X:



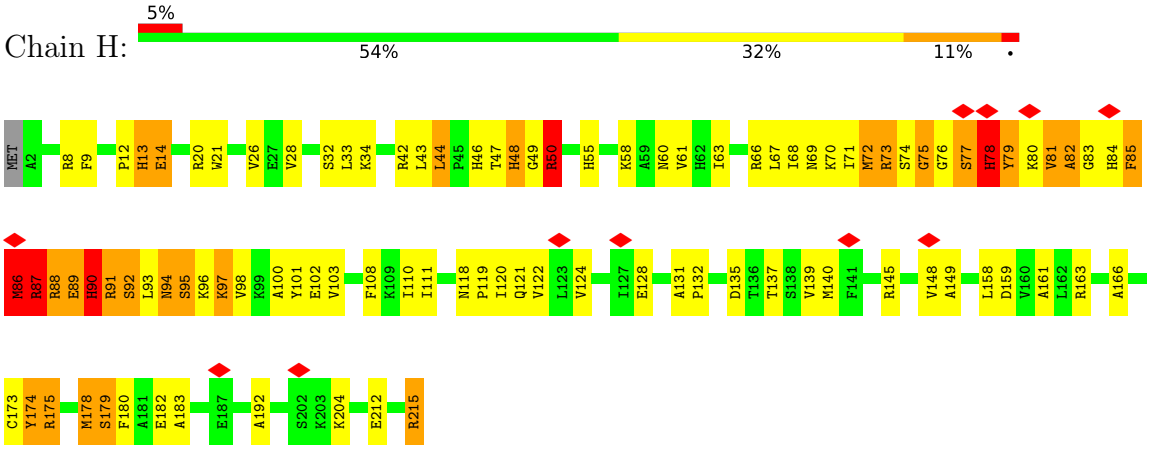
• Molecule 11: 30S ribosomal protein eS27

Chain Y:



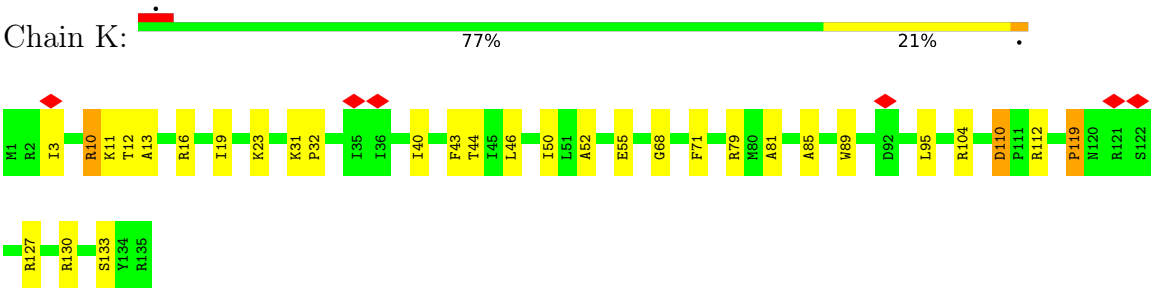
• Molecule 12: 30S ribosomal protein uS7

Chain H:



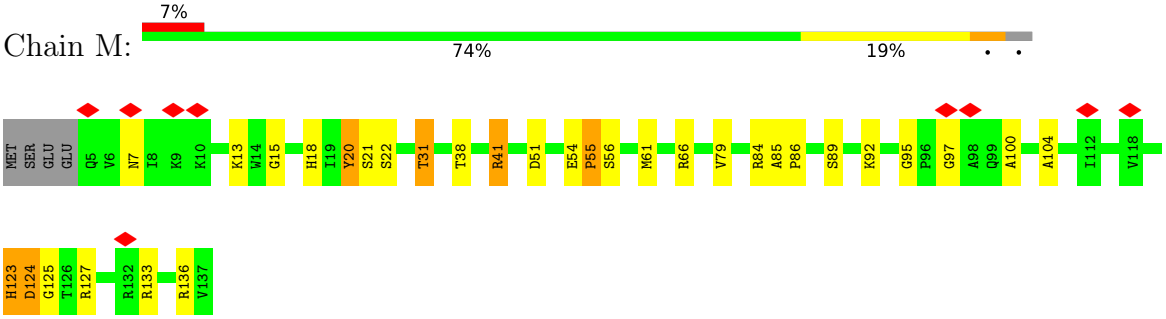
• Molecule 13: 30S ribosomal protein uS9

Chain K:



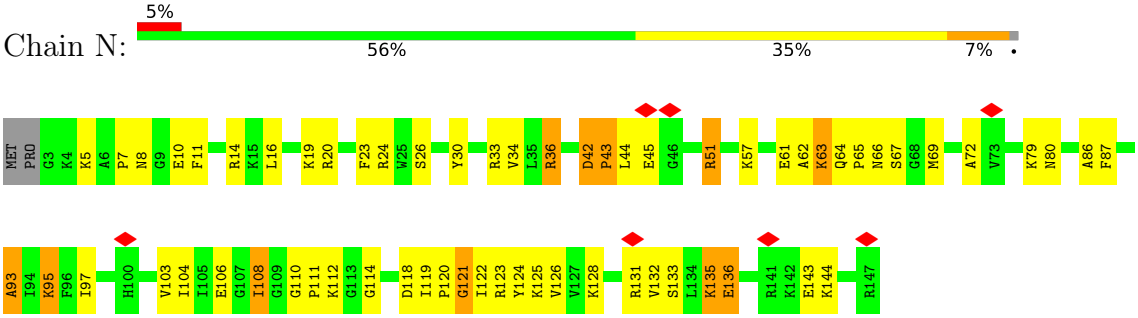
• Molecule 14: 30S ribosomal protein uS11

Chain M:



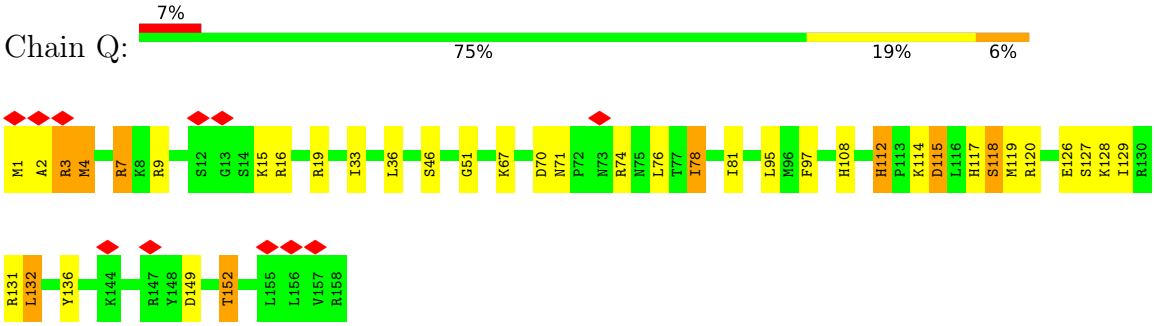
• Molecule 15: 30S ribosomal protein uS12

Chain N:



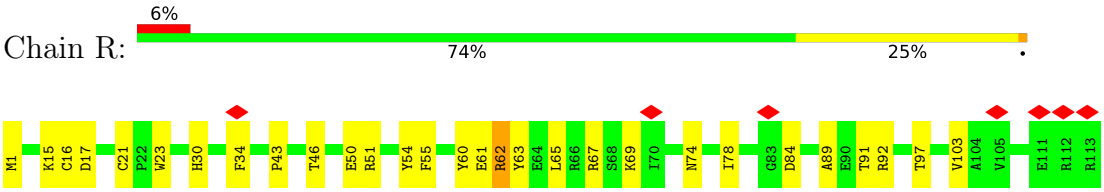
• Molecule 16: 30S ribosomal protein uS15

Chain Q:



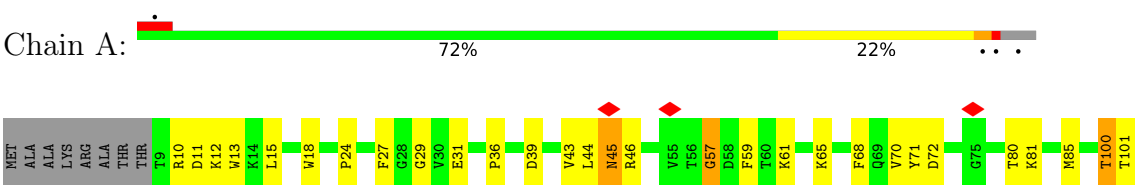
• Molecule 17: 30S ribosomal protein uS17

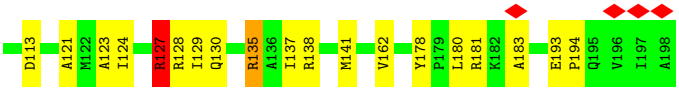
Chain R:



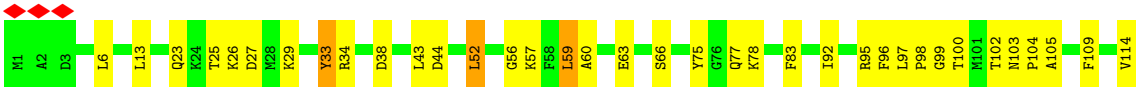
• Molecule 18: 30S ribosomal protein uS3

Chain A:



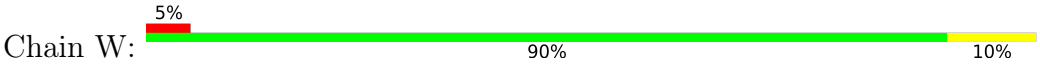


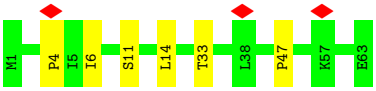
• Molecule 19: 30S ribosomal protein uS2



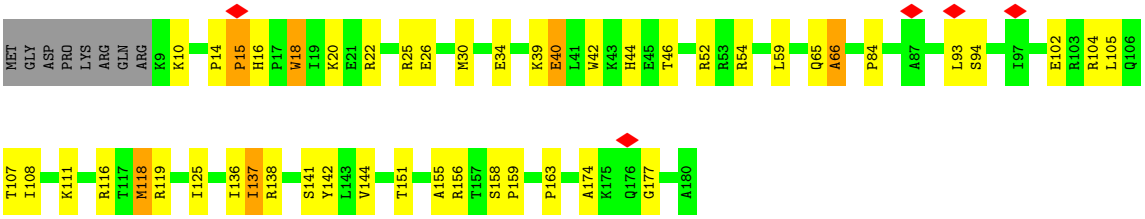
• Molecule 20: 30S ribosomal protein eS24

• Molecule 21: 30S ribosomal protein eS27

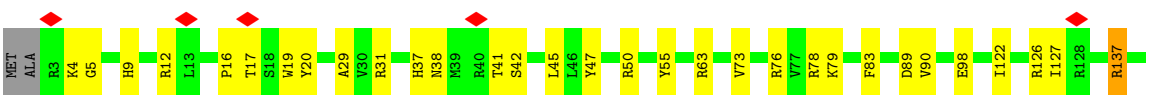


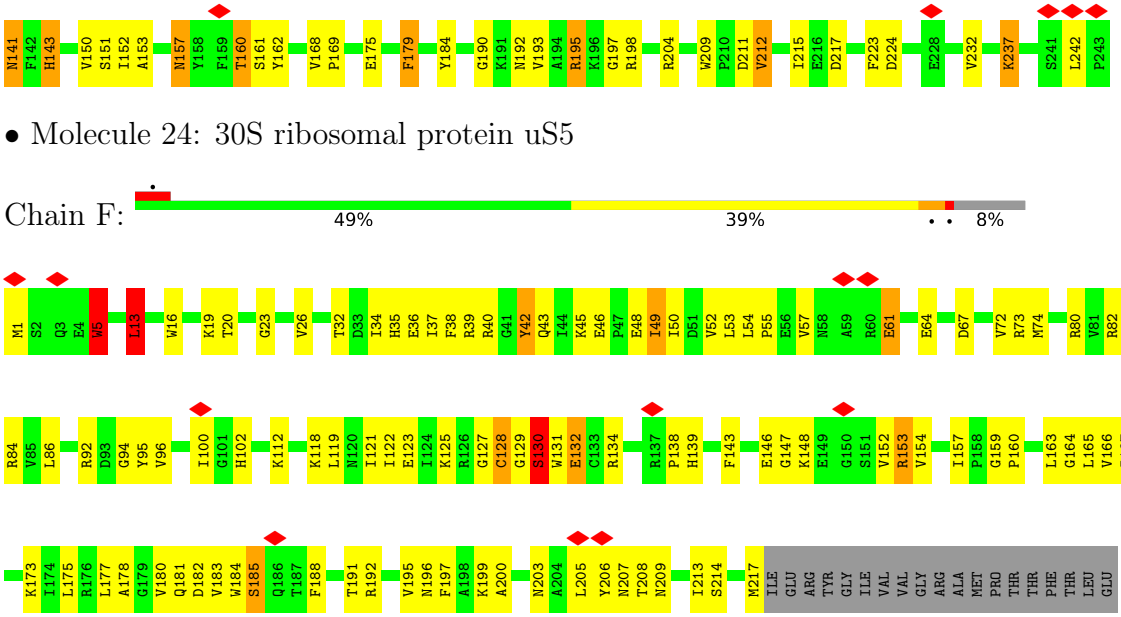


• Molecule 22: 30S ribosomal protein uS4



• Molecule 23: 30S ribosomal protein eS4





• Molecule 24: 30S ribosomal protein uS5

Chain F:

• Molecule 25: 30S ribosomal protein eS6

Chain G:

• Molecule 26: 30S ribosomal protein uS8

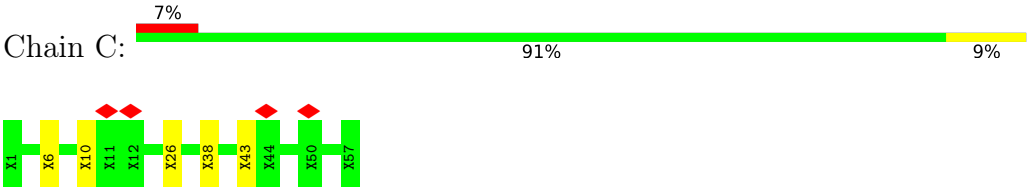
Chain I:

• Molecule 27: 30S ribosomal protein eS8

Chain J:

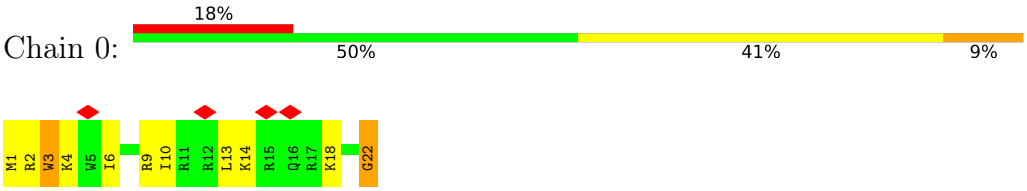
• Molecule 28: 30S ribosomal protein SX

Chain C:



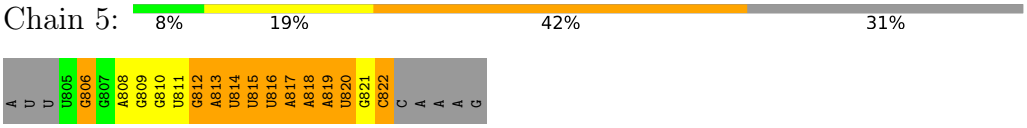
• Molecule 29: 30S ribosomal protein eL41

Chain 0:



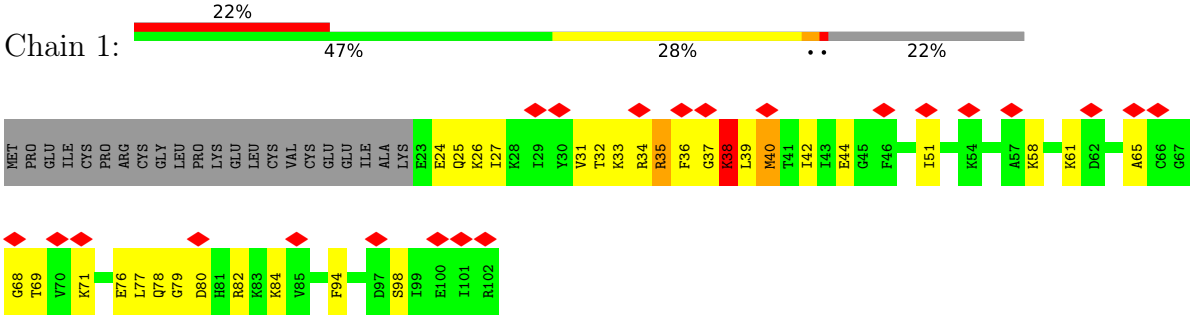
• Molecule 30: mRNA

Chain 5:



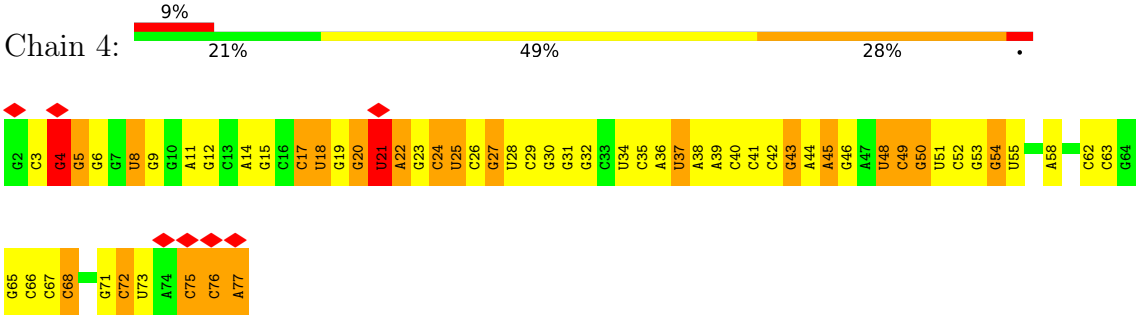
• Molecule 31: aIF1

Chain 1:



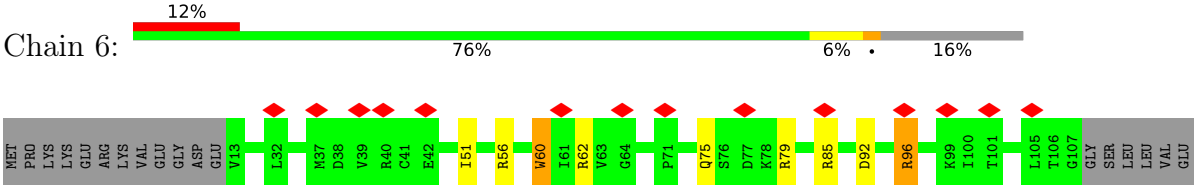
• Molecule 32: initiator Met-tRNA fMet from E. coli (A1U72 variant)

Chain 4:



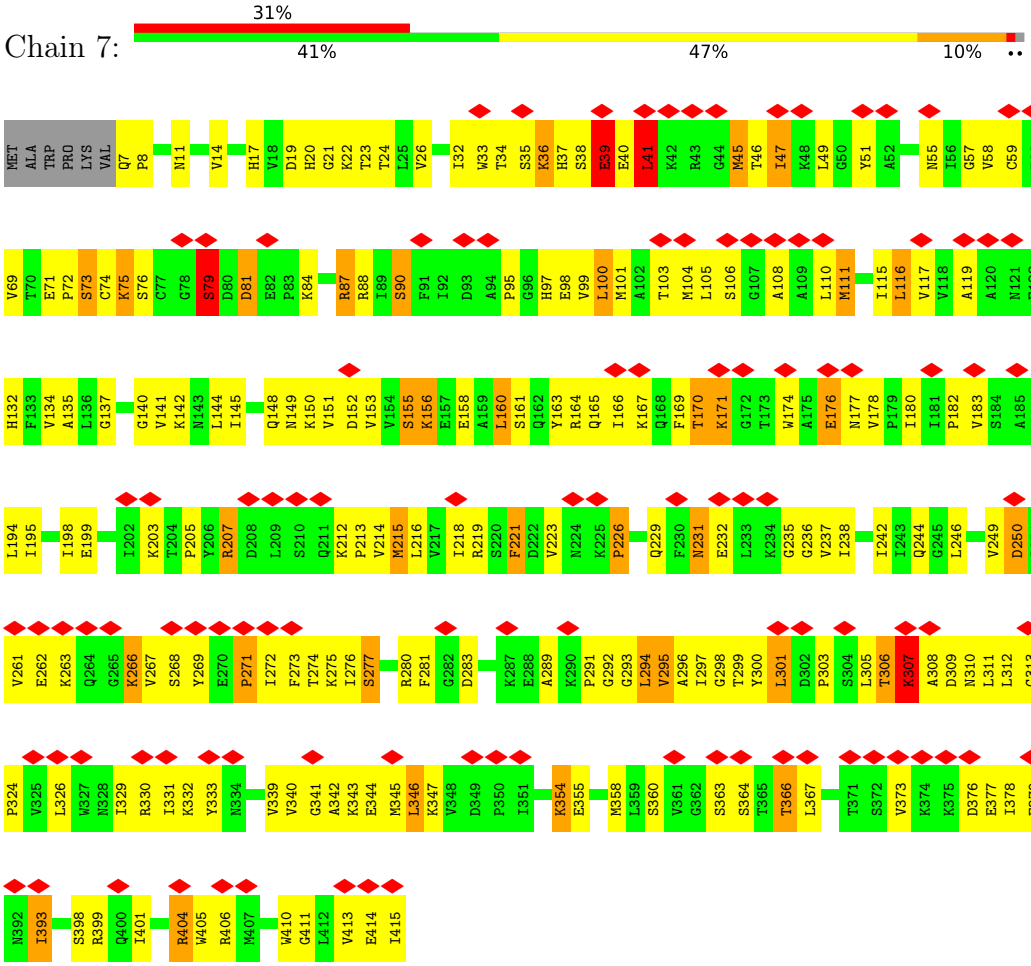
• Molecule 33: aIF1A

Chain 6:



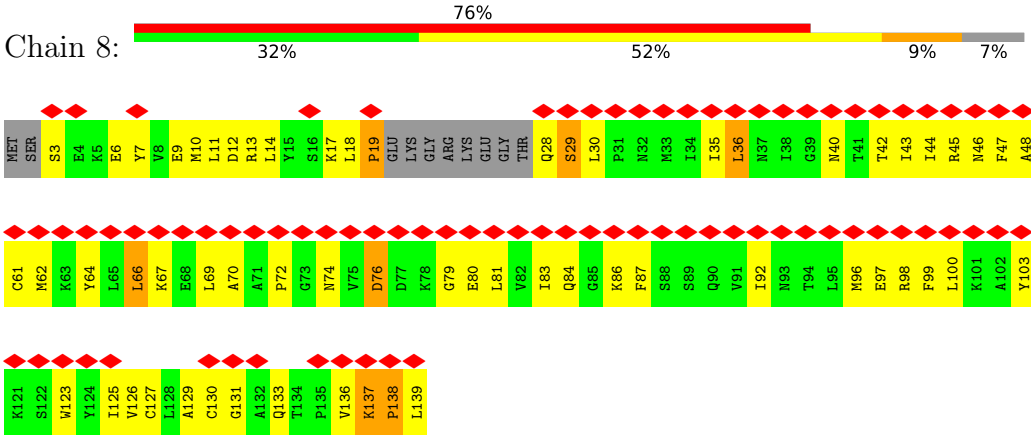
• Molecule 34: aIF2-gamma

Chain 7:



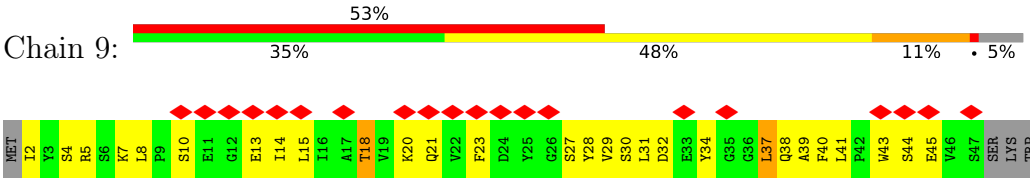
• Molecule 35: aIF2-beta

Chain 8:



• Molecule 36: aIF2-alpha

Chain 9:




N61 R62 K63 V64 I65 V66 K67 V68 I69 R70 V71 D72 R73 R74 K75 G76 T77 V78 D79 V80 S81 L82 K83 K84 V85 T86 D87 D88 E89 R90 R91 K92 K93 N94 L95 Q96 W97 K98 K99 I100 L103 D104 L107 E108 L109 V110 S111 Q112 K113 L114 K115 L116 S117 E118 K119 D120 A121 W122
E123 Q124 V125 A126 W127 E130 A131 K132 Y133 G134 D135 P136 I137 T138 A139 I140 E141 K142 A143 V144 K145 E146 G147 E148 K149 I150 L151 I152 D153 A154 G155 V156 P157 E158 I159 W160 V161 K162 P163 L164 L165 E166 E167 A168 S169 LYS HIS ALA GLU GLU R175 K176 V177 K178 M179 S180 G181 L182 I183
T184 V185 R186 T187 N188 E189 P190 V193 E194 K195 V199 I200 S201 L204 E205 N206 I207 E208 Q209 D210 Y211 E212 S213 L214 L215 N216 I217 K218 I219 Y220 T221 I222 G223 A224 P225 R226 Y227 R228 V229 D230 V231 V232 G233 T234 N235 P236 K237 E238 A239 S240 L243 N244 Q245 I246 I247
L250 I251 K252 I253 G254 K255 E256 E257 N258 V259 D260 I261 S262 V263 V264 LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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, 5MU, H2U, OMC, GNP, 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	2	0.65	17/35964 (0.0%)	0.91	59/56130 (0.1%)
2	Z	0.70	0/1480	0.87	2/1985 (0.1%)
3	3	0.86	0/951	0.90	1/1281 (0.1%)
4	L	0.76	1/830 (0.1%)	1.08	3/1113 (0.3%)
5	O	0.82	0/1208	0.96	2/1619 (0.1%)
6	P	0.73	0/471	1.11	1/620 (0.2%)
7	S	0.80	0/562	0.96	1/744 (0.1%)
8	T	0.84	0/942	0.91	0/1257
9	U	0.86	0/1203	0.95	3/1621 (0.2%)
10	X	0.78	0/570	1.06	2/760 (0.3%)
11	Y	0.76	0/421	0.78	0/558
12	H	0.95	1/1765 (0.1%)	1.19	12/2371 (0.5%)
13	K	0.79	0/1088	0.92	3/1455 (0.2%)
14	M	0.77	0/1022	0.96	3/1375 (0.2%)
15	N	0.81	0/1156	1.07	2/1535 (0.1%)
16	Q	0.76	0/1338	0.99	5/1797 (0.3%)
17	R	0.72	0/956	0.95	2/1287 (0.2%)
18	A	0.68	0/1585	0.89	2/2124 (0.1%)
19	B	0.75	0/1654	0.98	4/2233 (0.2%)
20	V	0.67	0/839	1.00	3/1122 (0.3%)
21	W	0.65	0/485	0.88	0/651
22	D	0.75	2/1457 (0.1%)	0.94	5/1953 (0.3%)
23	E	0.68	0/2025	0.95	7/2732 (0.3%)
24	F	0.77	1/1745 (0.1%)	1.00	3/2350 (0.1%)
25	G	0.75	0/999	1.09	7/1337 (0.5%)
26	I	0.71	1/1049 (0.1%)	0.96	4/1408 (0.3%)
27	J	0.67	0/1013	0.92	0/1349
29	0	1.18	2/216 (0.9%)	1.11	0/279
30	5	0.42	0/434	0.72	0/675
31	1	0.39	0/636	0.50	0/843
32	4	0.41	0/1743	0.68	0/2716
33	6	0.33	0/808	0.54	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	7	0.65	2/3227 (0.1%)	0.80	2/4367 (0.0%)
35	8	0.50	0/1046	0.81	1/1402 (0.1%)
36	9	0.52	0/2050	0.76	1/2760 (0.0%)
All	All	0.68	27/74938 (0.0%)	0.92	140/108902 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Z	0	1
5	O	0	1
10	X	0	3
12	H	4	9
13	K	0	2
15	N	0	2
16	Q	0	1
17	R	0	1
19	B	0	1
20	V	0	3
23	E	0	1
24	F	0	2
25	G	1	7
26	I	0	1
27	J	0	3
32	4	0	1
34	7	0	3
36	9	0	1
All	All	5	43

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1019	A	O3'-P	32.77	2.00	1.61
1	2	1351	U	O3'-P	-26.03	1.29	1.61
34	7	271	PRO	C-N	21.68	1.83	1.34
29	0	3	TRP	CB-CG	-7.26	1.37	1.50
34	7	256	LEU	C-N	7.03	1.47	1.34
1	2	357	C	O3'-P	-6.96	1.52	1.61
1	2	830	A	O3'-P	-6.71	1.53	1.61
1	2	1471	G	O3'-P	-6.43	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	86	MET	N-CA	6.27	1.58	1.46
1	2	833	C	O3'-P	-6.00	1.53	1.61
1	2	1462	A	O3'-P	-5.88	1.54	1.61
29	0	22	GLY	C-O	5.74	1.32	1.23
1	2	596	A	O3'-P	-5.65	1.54	1.61
1	2	523	C	O3'-P	-5.63	1.54	1.61
1	2	395	C	O3'-P	-5.59	1.54	1.61
1	2	629	U	C4-O4	-5.56	1.19	1.23
1	2	847	A	O3'-P	-5.44	1.54	1.61
1	2	522	C	O3'-P	-5.40	1.54	1.61
4	L	64	TRP	CB-CG	-5.40	1.40	1.50
22	D	18	TRP	CB-CG	-5.36	1.40	1.50
1	2	457	G	O3'-P	-5.34	1.54	1.61
24	F	42	TYR	CB-CG	-5.32	1.43	1.51
1	2	598	U	O3'-P	-5.31	1.54	1.61
26	I	5	ASP	CB-CG	5.25	1.62	1.51
22	D	40	GLU	CD-OE1	5.21	1.31	1.25
1	2	271	G	O3'-P	-5.03	1.55	1.61
1	2	850	A	O3'-P	-5.01	1.55	1.61

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1019	A	P-O3'-C3'	21.19	145.13	119.70
1	2	1350	U	P-O3'-C3'	-16.16	100.30	119.70
1	2	1414	G	O5'-P-OP1	-15.24	91.99	105.70
1	2	962	G	O5'-P-OP1	-13.70	93.37	105.70
1	2	1350	U	O3'-P-O5'	11.66	126.15	104.00
1	2	1019	A	O3'-P-O5'	10.25	123.47	104.00
12	H	87	ARG	N-CA-C	9.93	137.80	111.00
1	2	540	G	N9-C1'-C2'	-8.74	102.39	112.00
1	2	985	C	C2'-C3'-O3'	8.40	127.99	109.50
12	H	86	MET	N-CA-C	8.36	133.56	111.00
1	2	1340	U	C2'-C3'-O3'	8.11	127.34	109.50
1	2	962	G	O5'-P-OP2	-8.10	98.41	105.70
24	F	5	TRP	CA-CB-CG	8.04	128.98	113.70
1	2	277	G	C2'-C3'-O3'	8.00	127.11	109.50
35	8	29	SER	N-CA-C	-7.90	89.68	111.00
1	2	975	A	C2'-C3'-O3'	7.82	126.70	109.50
17	R	62	ARG	NE-CZ-NH1	7.46	124.03	120.30
16	Q	3	ARG	NE-CZ-NH1	7.46	124.03	120.30
25	G	86	VAL	CB-CA-C	-7.40	97.33	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1343	C	O5'-P-OP1	7.38	119.56	110.70
1	2	462	A	C2'-C3'-O3'	7.27	125.50	109.50
1	2	408	C	C2'-C3'-O3'	7.24	125.43	109.50
1	2	1460	G	C2'-C3'-O3'	7.20	125.35	109.50
1	2	1261	U	C2'-C3'-O3'	7.14	125.20	109.50
12	H	79	TYR	CA-CB-CG	7.11	126.91	113.40
18	A	135	ARG	NE-CZ-NH2	-6.95	116.83	120.30
6	P	40	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	2	1053	A	C2'-C3'-O3'	6.74	124.48	113.70
1	2	528	G	C2'-C3'-O3'	6.73	124.47	113.70
20	V	85	TYR	CA-CB-CG	6.72	126.16	113.40
1	2	1453	U	C2'-C3'-O3'	6.63	124.31	113.70
23	E	78	ARG	NE-CZ-NH1	6.62	123.61	120.30
22	D	104	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	2	847	A	C2'-C3'-O3'	-6.47	95.27	109.50
26	I	57	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	2	742	U	C2'-C3'-O3'	6.38	123.90	113.70
25	G	109	GLY	N-CA-C	6.35	128.97	113.10
20	V	85	TYR	N-CA-CB	6.35	122.02	110.60
1	2	924	U	C2'-C3'-O3'	6.34	123.85	113.70
1	2	1	A	O5'-P-OP1	-6.34	100.00	105.70
1	2	1306	A	C2'-C3'-O3'	6.32	123.82	113.70
9	U	61	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	2	422	U	N1-C1'-C2'	-6.27	105.10	112.00
1	2	462	A	O4'-C4'-C3'	-6.27	97.73	104.00
19	B	128	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	2	434	A	C2'-C3'-O3'	6.22	123.65	113.70
1	2	99	C	C2'-C3'-O3'	6.12	123.49	113.70
1	2	1483	U	C2'-C3'-O3'	6.12	123.49	113.70
7	S	14	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	2	486	A	C2'-C3'-O3'	6.10	123.46	113.70
22	D	25	ARG	NE-CZ-NH1	6.10	123.35	120.30
19	B	115	LEU	CA-CB-CG	6.08	129.30	115.30
18	A	127	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	Z	140	ARG	NE-CZ-NH1	6.06	123.33	120.30
17	R	51	ARG	NE-CZ-NH1	6.06	123.33	120.30
12	H	86	MET	C-N-CA	6.04	136.81	121.70
1	2	438	A	C4'-C3'-O3'	6.04	125.08	113.00
22	D	25	ARG	NE-CZ-NH2	-6.03	117.28	120.30
24	F	13	LEU	CA-CB-CG	6.02	129.15	115.30
4	L	92	GLU	N-CA-C	6.01	127.22	111.00
1	2	262	G	C2'-C3'-O3'	5.99	123.28	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1368	A	C2'-C3'-O3'	5.95	123.22	113.70
15	N	51	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	2	439	G	C2'-C3'-O3'	5.92	123.16	113.70
25	G	86	VAL	CG1-CB-CG2	5.91	120.36	110.90
25	G	75	ARG	NE-CZ-NH1	5.87	123.24	120.30
10	X	71	ARG	NE-CZ-NH1	5.87	123.23	120.30
26	I	33	LEU	CA-CB-CG	5.84	128.74	115.30
26	I	4	LEU	CA-CB-CG	5.83	128.72	115.30
1	2	196	G	C4'-C3'-O3'	-5.83	97.16	109.40
1	2	1262	U	C2'-C3'-O3'	5.80	122.99	113.70
34	7	41	LEU	CA-CB-CG	5.80	128.64	115.30
12	H	85	PHE	CB-CA-C	5.78	121.96	110.40
26	I	5	ASP	CB-CG-OD2	-5.77	113.11	118.30
14	M	66	ARG	NE-CZ-NH2	-5.75	117.42	120.30
12	H	14	GLU	N-CA-C	5.72	126.44	111.00
25	G	54	GLU	N-CA-CB	5.71	120.89	110.60
4	L	92	GLU	C-N-CA	5.71	135.97	121.70
23	E	63	ARG	NE-CZ-NH1	5.70	123.15	120.30
12	H	215	ARG	NE-CZ-NH1	5.69	123.15	120.30
5	O	132	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	2	1423	A	C2'-C3'-O3'	5.67	122.76	113.70
14	M	41	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	2	1343	C	O5'-P-OP2	5.66	117.50	110.70
12	H	79	TYR	N-CA-CB	-5.66	100.41	110.60
23	E	76	ARG	NE-CZ-NH1	5.64	123.12	120.30
9	U	43	ARG	NE-CZ-NH1	5.62	123.11	120.30
25	G	53	LYS	CB-CA-C	5.62	121.63	110.40
13	K	79	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	2	199	A	P-O3'-C3'	5.56	126.37	119.70
16	Q	3	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	2	977	G	C2'-C3'-O3'	5.53	122.55	113.70
1	2	1249	A	O5'-P-OP1	-5.51	100.74	105.70
4	L	67	ARG	NE-CZ-NH1	5.48	123.04	120.30
22	D	119	ARG	NE-CZ-NH1	5.46	123.03	120.30
9	U	43	ARG	NE-CZ-NH2	-5.45	117.57	120.30
23	E	50	ARG	NE-CZ-NH1	5.44	123.02	120.30
12	H	163	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	2	176	U	C2'-C3'-O3'	5.39	122.33	113.70
1	2	1351	U	P-O3'-C3'	-5.39	113.23	119.70
12	H	8	ARG	NE-CZ-NH1	5.38	122.99	120.30
13	K	127	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	2	1378	A	N9-C1'-C2'	-5.36	106.10	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	7	271	PRO	O-C-N	5.34	131.24	122.70
15	N	36	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	2	438	A	C2'-C3'-O3'	-5.29	97.86	109.50
20	V	33	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	2	962	G	OP1-P-OP2	5.27	127.50	119.60
22	D	52	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	2	669	A	C4-N9-C1'	5.25	135.76	126.30
24	F	42	TYR	CA-CB-CG	-5.25	103.42	113.40
16	Q	74	ARG	NE-CZ-NH2	-5.25	117.68	120.30
13	K	104	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	2	39	U	C5'-C4'-O4'	5.21	115.35	109.10
2	Z	105	ARG	NE-CZ-NH2	-5.20	117.70	120.30
23	E	78	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	2	1351	U	OP2-P-O3'	5.17	116.56	105.20
1	2	1350	U	OP1-P-O3'	-5.15	93.86	105.20
3	3	27	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	2	702	G	N9-C1'-C2'	5.15	120.69	114.00
10	X	71	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	2	111	G	C2'-C3'-O3'	5.13	121.91	113.70
1	2	175	G	C4'-C3'-O3'	5.13	123.26	113.00
16	Q	7	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	2	669	A	C8-N9-C1'	-5.11	118.49	127.70
1	2	1318	U	O4'-C1'-N1	5.11	112.29	108.20
5	O	145	ARG	NE-CZ-NH1	5.10	122.85	120.30
14	M	136	ARG	NE-CZ-NH1	5.10	122.85	120.30
19	B	34	ARG	NE-CZ-NH1	5.09	122.85	120.30
36	9	214	LEU	CA-CB-CG	5.08	126.98	115.30
16	Q	19	ARG	NE-CZ-NH1	5.07	122.83	120.30
25	G	80	GLY	N-CA-C	-5.05	100.47	113.10
1	2	1143	G	C2'-C3'-O3'	5.05	121.78	113.70
12	H	75	GLY	N-CA-C	5.05	125.72	113.10
19	B	34	ARG	NE-CZ-NH2	-5.05	117.78	120.30
23	E	209	TRP	CA-CB-CG	5.03	123.26	113.70
1	2	1458	A	C2'-C3'-O3'	5.03	121.74	113.70
1	2	1337	A	C4'-C3'-O3'	5.01	123.03	113.00
12	H	91	ARG	NE-CZ-NH1	5.01	122.81	120.30
23	E	137	ARG	NE-CZ-NH1	5.01	122.80	120.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	H	85	PHE	CA

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Mol	Chain	Res	Type	Atom
12	H	86	MET	CA
12	H	87	ARG	CA
12	H	96	LYS	CA
25	G	53	LYS	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	4	4	G	Sidechain
34	7	256	LEU	Peptide,Mainchain
34	7	79	SER	Peptide
36	9	212	GLU	Peptide
19	B	6	LEU	Peptide
23	E	143	HIS	Peptide
24	F	130	SER	Peptide
24	F	72	VAL	Peptide
25	G	17	LYS	Peptide
25	G	43	LEU	Peptide
25	G	49	GLU	Peptide
25	G	56	PRO	Peptide
25	G	74	MET	Peptide
25	G	97	LYS	Peptide
25	G	98	GLU	Peptide
12	H	12	PRO	Peptide
12	H	14	GLU	Peptide
12	H	178	MET	Peptide
12	H	42	ARG	Peptide
12	H	78	HIS	Peptide
12	H	84	HIS	Peptide
12	H	86	MET	Peptide
12	H	87	ARG	Peptide
12	H	90	HIS	Peptide
26	I	21	GLY	Peptide
27	J	6	GLY	Peptide
27	J	63	ALA	Peptide
27	J	64	ASN	Peptide
13	K	110	ASP	Peptide
13	K	12	THR	Peptide
15	N	121	GLY	Peptide
15	N	5	LYS	Peptide
5	O	124	LEU	Peptide
16	Q	2	ALA	Peptide

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Mol	Chain	Res	Type	Group
17	R	34	PHE	Peptide
20	V	55	TYR	Peptide
20	V	94	GLU	Peptide
20	V	96	LYS	Peptide
10	X	22	GLY	Peptide
10	X	4	ASP	Peptide
10	X	66	GLU	Peptide
2	Z	157	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32135	0	16232	1511	0
2	Z	1459	0	1549	10	0
3	3	939	0	994	5	0
4	L	822	0	870	25	0
5	O	1189	0	1248	11	0
6	P	462	0	492	6	0
7	S	556	0	604	5	0
8	T	923	0	986	7	0
9	U	1175	0	1216	20	0
10	X	568	0	600	22	0
11	Y	409	0	410	3	0
12	H	1728	0	1775	127	0
13	K	1072	0	1128	16	0
14	M	1004	0	1041	15	0
15	N	1140	0	1235	47	0
16	Q	1310	0	1392	21	0
17	R	934	0	960	19	0
18	A	1559	0	1648	26	0
19	B	1623	0	1682	110	0
20	V	823	0	847	27	0
21	W	478	0	524	3	0
22	D	1434	0	1498	28	0
23	E	1976	0	2046	34	0
24	F	1716	0	1769	108	0
25	G	984	0	1044	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	I	1028	0	1065	44	0
27	J	1004	0	1088	17	0
28	C	286	0	61	3	0
29	0	213	0	250	11	0
30	5	388	0	193	30	0
31	1	632	0	668	125	0
32	4	1621	0	827	168	0
33	6	792	0	815	26	0
34	7	3171	0	3291	290	0
35	8	1033	0	1074	178	0
36	9	2025	0	2130	156	0
37	4	8	0	8	16	0
38	7	1	0	0	0	0
39	7	32	0	13	1	0
40	8	1	0	0	0	0
All	All	70653	0	55273	2703	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 22.

All (2703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1367:C:H1'	31:1:65:ALA:CB	1.17	1.58
1:2:1367:C:C1'	31:1:65:ALA:CB	1.89	1.49
31:1:32:THR:HG21	31:1:42:ILE:CD1	1.40	1.48
1:2:1053:A:C8	19:B:125:GLN:OE1	1.63	1.47
1:2:1053:A:N1	19:B:98:PRO:C	1.71	1.44
1:2:1025:U:H1'	19:B:105:ALA:CB	1.45	1.43
1:2:1448:A:C8	33:6:56:ARG:NE	1.89	1.41
1:2:1027:C:C5'	19:B:102:THR:OG1	1.66	1.39
1:2:1025:U:C1'	19:B:105:ALA:HB3	1.50	1.38
1:2:1053:A:C8	19:B:125:GLN:CD	1.97	1.38
1:2:1026:A:O2'	19:B:99:GLY:CA	1.71	1.37
1:2:8:U:N3	1:2:873:A:N6	1.70	1.36
1:2:1053:A:N7	19:B:125:GLN:NE2	1.68	1.36
1:2:1367:C:C1'	31:1:65:ALA:HB1	1.53	1.34
34:7:190:ASN:CB	35:8:14:LEU:HD12	1.57	1.34
31:1:33:LYS:HB2	32:4:27:G:OP1	1.19	1.34
36:9:98:LYS:NZ	36:9:235:ASN:CG	1.80	1.34
1:2:1448:A:N7	33:6:56:ARG:HG2	1.43	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1:38:LYS:O	31:1:39:LEU:HD12	1.22	1.33
1:2:1054:A:H4'	19:B:95:ARG:NH1	1.42	1.31
34:7:192:ASP:OD2	35:8:13:ARG:NH2	1.63	1.31
34:7:192:ASP:OD2	35:8:13:ARG:CZ	1.78	1.30
34:7:271:PRO:C	34:7:272:ILE:N	1.83	1.30
1:2:1025:U:O2	19:B:103:ASN:ND2	1.68	1.26
1:2:1025:U:C1'	19:B:105:ALA:CB	2.09	1.25
1:2:1367:C:O2'	31:1:65:ALA:HB2	1.31	1.25
36:9:98:LYS:NZ	36:9:235:ASN:ND2	1.85	1.25
31:1:33:LYS:CB	32:4:27:G:OP1	1.84	1.25
35:8:19:PRO:CG	35:8:129:ALA:HB1	1.67	1.25
1:2:1026:A:O2'	19:B:99:GLY:HA2	1.06	1.23
1:2:1298:G:H22	32:4:30:G:N2	1.34	1.23
31:1:32:THR:CG2	31:1:42:ILE:CD1	2.17	1.22
1:2:1451:C:O3'	31:1:78:GLN:OE1	1.57	1.20
34:7:182:PRO:HG3	35:8:7:TYR:CE1	1.76	1.20
1:2:1027:C:H5'	19:B:102:THR:OG1	1.06	1.20
1:2:1367:C:C2'	31:1:65:ALA:HB2	1.72	1.20
1:2:1053:A:OP2	19:B:95:ARG:CD	1.88	1.19
36:9:98:LYS:HD3	36:9:175:ARG:NH1	1.56	1.19
34:7:182:PRO:CG	35:8:7:TYR:HE1	1.56	1.18
34:7:187:HIS:HA	35:8:130:CYS:O	1.43	1.18
1:2:1053:A:H8	19:B:125:GLN:OE1	0.83	1.18
34:7:189:ILE:HB	35:8:14:LEU:HD21	1.26	1.18
1:2:1054:A:C4'	19:B:95:ARG:HH12	1.55	1.18
31:1:32:THR:HB	31:1:42:ILE:CG1	1.73	1.17
1:2:920:U:H3	1:2:1161:A:N6	1.42	1.17
36:9:98:LYS:HZ1	36:9:235:ASN:CG	1.38	1.17
1:2:1019:A:O3'	1:2:1020:G:P	2.00	1.17
34:7:192:ASP:OD2	35:8:13:ARG:NH1	1.78	1.16
34:7:190:ASN:HB2	35:8:14:LEU:HD12	1.16	1.16
34:7:190:ASN:HB2	35:8:14:LEU:CD1	1.75	1.15
31:1:32:THR:HG21	31:1:42:ILE:HD13	1.20	1.15
1:2:1367:C:O2'	31:1:65:ALA:CB	1.94	1.14
1:2:1299:A:H1'	32:4:42:C:C1'	1.77	1.14
1:2:1028:C:OP1	19:B:132:GLU:OE1	1.65	1.14
1:2:1053:A:OP2	19:B:95:ARG:HD2	0.96	1.14
36:9:98:LYS:HD3	36:9:175:ARG:HH12	1.00	1.14
1:2:1028:C:P	19:B:132:GLU:OE1	2.06	1.13
1:2:1448:A:H8	33:6:56:ARG:CZ	1.61	1.13
1:2:1053:A:N7	19:B:125:GLN:CD	1.92	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1053:A:N1	19:B:99:GLY:N	1.97	1.12
36:9:98:LYS:HZ1	36:9:235:ASN:ND2	1.39	1.12
1:2:1448:A:H8	33:6:56:ARG:NE	1.31	1.11
34:7:189:ILE:HG22	35:8:14:LEU:HG	1.18	1.11
1:2:1053:A:P	19:B:95:ARG:HD2	1.90	1.11
1:2:516:A:N6	1:2:842:U:H3	1.48	1.10
1:2:1032:A:C5'	24:F:84:ARG:CZ	2.29	1.10
32:4:77:A:H3'	37:4:101:MET:O	1.48	1.10
1:2:1054:A:O2'	19:B:95:ARG:NH2	1.85	1.09
32:4:75:C:OP1	34:7:226:PRO:HG2	1.49	1.09
1:2:1448:A:C5'	33:6:56:ARG:HH21	1.65	1.09
31:1:38:LYS:C	31:1:39:LEU:HD12	1.71	1.09
1:2:1053:A:C2	19:B:98:PRO:C	2.27	1.07
31:1:32:THR:HG21	31:1:42:ILE:HD11	1.30	1.07
1:2:822:A:H2'	1:2:823:A:C8	1.89	1.07
31:1:32:THR:CG2	31:1:42:ILE:HD11	1.82	1.07
1:2:314:G:O2'	1:2:1424:G:OP1	1.73	1.06
1:2:1367:C:C1'	31:1:65:ALA:HB2	1.73	1.06
32:4:77:A:C3'	37:4:101:MET:O	2.02	1.06
34:7:188:LYS:CE	35:8:131:GLY:O	2.04	1.06
1:2:1402:C:H2'	1:2:1403:U:O4'	1.54	1.06
1:2:1448:A:H5'	33:6:56:ARG:HH21	1.13	1.06
1:2:1026:A:H5"	19:B:102:THR:O	1.55	1.05
34:7:188:LYS:HG3	35:8:131:GLY:HA3	1.34	1.05
29:0:1:MET:SD	29:0:4:LYS:NZ	2.29	1.05
1:2:1299:A:H1'	32:4:42:C:H1'	1.07	1.05
31:1:34:ARG:HD3	31:1:40:MET:CE	1.86	1.05
1:2:6:G:O6	1:2:7:G:O6	1.75	1.04
1:2:315:A:H1'	1:2:1423:A:H1'	1.38	1.03
32:4:42:C:O2'	32:4:43:G:H5'	1.58	1.03
1:2:1367:C:C2'	31:1:65:ALA:CB	2.32	1.03
1:2:1448:A:N7	33:6:56:ARG:CG	2.21	1.03
1:2:1346:C:H2'	1:2:1347:U:C6	1.91	1.03
37:4:101:MET:HE1	34:7:219:ARG:NH2	1.73	1.03
36:9:98:LYS:HZ3	36:9:235:ASN:HA	1.13	1.03
1:2:1452:G:OP1	31:1:78:GLN:NE2	1.91	1.03
1:2:1344:U:H2'	1:2:1345:G:C8	1.95	1.02
31:1:35:ARG:HD3	31:1:36:PHE:H	1.21	1.02
34:7:182:PRO:CD	35:8:7:TYR:HE1	1.73	1.02
34:7:187:HIS:CB	35:8:130:CYS:HA	1.89	1.02
31:1:32:THR:CB	31:1:42:ILE:HD11	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1:25:GLN:OE1	31:1:51:ILE:HD11	1.61	1.01
31:1:32:THR:CB	31:1:42:ILE:CG1	2.38	1.01
34:7:188:LYS:CG	35:8:131:GLY:HA3	1.91	1.01
34:7:190:ASN:HB3	35:8:14:LEU:HD12	1.37	1.01
1:2:1025:U:O2'	19:B:105:ALA:N	1.94	1.00
31:1:32:THR:CG2	31:1:42:ILE:HG12	1.92	1.00
34:7:182:PRO:HG3	35:8:7:TYR:HE1	1.09	1.00
1:2:1448:A:O5'	33:6:56:ARG:NH2	1.95	1.00
34:7:190:ASN:HB2	35:8:14:LEU:CG	1.91	0.99
1:2:1054:A:H4'	19:B:95:ARG:HH12	0.83	0.99
31:1:34:ARG:HG3	31:1:35:ARG:H	1.22	0.99
31:1:33:LYS:HG3	32:4:27:G:C5'	1.91	0.99
34:7:188:LYS:HE2	35:8:131:GLY:O	1.60	0.99
1:2:1054:A:H4'	19:B:95:ARG:CZ	1.92	0.98
36:9:95:LEU:HD11	36:9:237:LYS:HG3	1.45	0.98
34:7:189:ILE:HD12	35:8:18:LEU:HD23	1.46	0.98
1:2:1487:U:H2'	1:2:1488:C:C6	1.98	0.98
31:1:34:ARG:HD3	31:1:40:MET:HE2	1.41	0.98
1:2:648:A:N6	1:2:741:A:O2'	1.96	0.97
1:2:507:G:OP1	15:N:111:PRO:HG3	1.64	0.97
1:2:1346:C:H2'	1:2:1347:U:C5	1.98	0.97
1:2:1350:U:N3	1:2:1351:U:C5	2.33	0.97
36:9:94:ASN:OD1	36:9:236:PRO:CG	2.13	0.97
36:9:94:ASN:OD1	36:9:236:PRO:HG2	1.65	0.97
1:2:1360:C:O4'	30:5:821:G:C6	2.17	0.97
1:2:1298:G:N2	32:4:30:G:N2	2.11	0.96
1:2:1298:G:N2	32:4:43:G:O4'	1.98	0.96
1:2:1448:A:C5'	33:6:56:ARG:NH2	2.27	0.96
35:8:138:PRO:O	35:8:139:LEU:HD12	1.66	0.96
1:2:885:G:N2	1:2:1350:U:O2	1.99	0.96
34:7:189:ILE:HB	35:8:14:LEU:CD2	1.95	0.96
34:7:189:ILE:HG22	35:8:14:LEU:CG	1.96	0.96
1:2:60:A:N1	1:2:64:G:O6	1.97	0.95
1:2:1348:C:H2'	1:2:1349:C:C6	2.01	0.95
31:1:32:THR:CG2	31:1:42:ILE:CG1	2.43	0.95
34:7:189:ILE:CG2	35:8:14:LEU:HG	1.96	0.95
1:2:1022:U:P	24:F:80:ARG:NH1	2.40	0.95
1:2:8:U:C4	1:2:873:A:N6	2.34	0.95
31:1:38:LYS:HA	31:1:38:LYS:HE3	1.49	0.95
34:7:193:SER:HB2	35:8:10:MET:CE	1.96	0.94
1:2:8:U:N3	1:2:873:A:C6	2.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:101:MET:CE	34:7:219:ARG:NH2	2.31	0.94
1:2:1031:G:O3'	24:F:84:ARG:NH1	1.88	0.94
1:2:229:G:C2	1:2:230:C:C5	2.56	0.94
1:2:1403:U:O2'	25:G:110:ASN:ND2	2.00	0.94
37:4:101:MET:HE2	34:7:219:ARG:CZ	1.98	0.94
1:2:516:A:H61	1:2:842:U:H3	0.94	0.93
1:2:1448:A:N6	33:6:51:ILE:HG21	1.83	0.93
32:4:77:A:H2'	34:7:280:ARG:NH2	1.82	0.93
1:2:619:A:N6	1:2:678:G:O6	2.01	0.92
31:1:25:GLN:NE2	31:1:94:PHE:CD1	2.38	0.92
1:2:1414:G:OP1	25:G:86:VAL:HG13	1.70	0.92
31:1:32:THR:HB	31:1:42:ILE:HG12	1.49	0.92
34:7:182:PRO:CG	35:8:7:TYR:CE1	2.44	0.92
34:7:189:ILE:CD1	35:8:18:LEU:HD23	1.99	0.92
1:2:1451:C:OP1	31:1:36:PHE:O	1.87	0.92
35:8:56:ARG:HH12	35:8:104:VAL:HA	1.34	0.92
35:8:137:LYS:HG2	35:8:139:LEU:HD13	1.50	0.92
1:2:920:U:N3	1:2:1161:A:N6	2.09	0.91
31:1:38:LYS:O	31:1:39:LEU:CD1	2.14	0.91
31:1:32:THR:CB	31:1:42:ILE:HG12	2.00	0.91
31:1:25:GLN:OE1	31:1:51:ILE:CD1	2.19	0.91
31:1:32:THR:CB	31:1:42:ILE:CD1	2.48	0.91
1:2:1026:A:H5'	19:B:104:PRO:HD2	1.52	0.91
1:2:1448:A:N7	33:6:56:ARG:NE	2.19	0.91
1:2:1026:A:C5'	19:B:103:ASN:OD1	2.18	0.91
36:9:18:THR:HB	36:9:63:LYS:HG2	1.52	0.91
1:2:229:G:N2	1:2:230:C:C2	2.39	0.91
1:2:1032:A:H5'	24:F:84:ARG:CZ	1.99	0.91
32:4:53:G:HO2'	32:4:54:G:H8	1.00	0.91
31:1:32:THR:HB	31:1:42:ILE:HG13	1.49	0.90
32:4:71:G:H2'	32:4:72:C:H5'	1.53	0.90
36:9:95:LEU:CD1	36:9:237:LYS:HG3	2.01	0.90
1:2:1318:U:H3	1:2:1323:A:N6	1.69	0.90
1:2:1414:G:OP1	25:G:86:VAL:CG1	2.19	0.90
1:2:229:G:C2	1:2:230:C:C4	2.59	0.90
1:2:975:A:H2'	1:2:976:A:H5'	1.54	0.90
36:9:98:LYS:HZ3	36:9:235:ASN:CA	1.83	0.90
1:2:1412:A:O2'	25:G:92:PRO:HG3	1.69	0.90
35:8:19:PRO:CG	35:8:129:ALA:CB	2.48	0.90
1:2:1367:C:H1'	31:1:65:ALA:HB3	1.53	0.90
36:9:98:LYS:HZ2	36:9:235:ASN:ND2	1.65	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1:40:MET:HG2	31:1:77:LEU:O	1.71	0.89
34:7:190:ASN:HB2	35:8:14:LEU:HB2	1.54	0.89
1:2:439:G:H1'	1:2:440:C:C5	2.08	0.89
1:2:151:G:O2'	25:G:64:ARG:NE	2.06	0.89
31:1:35:ARG:NH1	31:1:36:PHE:HB2	1.88	0.89
1:2:1022:U:P	24:F:80:ARG:HH11	1.96	0.89
1:2:1054:A:C5'	19:B:95:ARG:HH12	1.86	0.89
1:2:1022:U:OP1	24:F:80:ARG:NH1	2.05	0.88
34:7:62:CYS:SG	34:7:63:LYS:N	2.45	0.88
34:7:182:PRO:CD	35:8:7:TYR:CE1	2.56	0.88
31:1:34:ARG:HB2	31:1:40:MET:HB2	1.53	0.88
1:2:1298:G:N2	32:4:30:G:H22	1.72	0.88
32:4:43:G:C2	32:4:44:A:C8	2.61	0.88
1:2:1313:G:OP1	12:H:81:VAL:HG23	1.73	0.88
1:2:1025:U:C1'	19:B:105:ALA:HB2	2.03	0.88
1:2:1299:A:C4'	32:4:42:C:H4'	2.03	0.88
34:7:66:GLU:HB3	35:8:13:ARG:NH2	1.89	0.88
1:2:1298:G:H22	32:4:30:G:H21	1.16	0.88
36:9:98:LYS:NZ	36:9:235:ASN:CB	2.36	0.88
34:7:190:ASN:HB2	35:8:14:LEU:CB	2.03	0.87
1:2:8:U:H3	1:2:873:A:N6	1.59	0.87
35:8:115:ILE:HG22	35:8:116:LEU:N	1.89	0.87
1:2:8:U:C2	1:2:873:A:N6	2.42	0.87
34:7:187:HIS:CG	35:8:130:CYS:HA	2.10	0.87
31:1:40:MET:HG2	31:1:78:GLN:HA	1.55	0.87
36:9:98:LYS:NZ	36:9:235:ASN:HA	1.88	0.87
1:2:1026:A:H5'	19:B:103:ASN:OD1	1.73	0.86
31:1:33:LYS:CG	32:4:27:G:OP1	2.22	0.86
34:7:187:HIS:CA	35:8:130:CYS:O	2.21	0.86
36:9:240:SER:HA	36:9:243:LEU:HB3	1.55	0.86
1:2:229:G:N1	1:2:230:C:C4	2.44	0.86
1:2:516:A:N1	1:2:842:U:O4	2.08	0.86
1:2:1448:A:H62	33:6:51:ILE:HG21	1.35	0.86
31:1:34:ARG:HG2	31:1:40:MET:HG3	1.58	0.86
34:7:187:HIS:ND1	35:8:130:CYS:HB2	1.91	0.86
1:2:1345:G:O2'	1:2:1346:C:H5'	1.76	0.85
1:2:368:C:O2'	1:2:369:A:OP2	1.94	0.85
1:2:1298:G:C2	32:4:43:G:O4'	2.29	0.85
1:2:1342:C:H3'	1:2:1343:C:P	2.16	0.85
31:1:34:ARG:CG	31:1:40:MET:HG3	2.07	0.85
29:0:22:GLY:O	34:7:354:LYS:HG2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:87:ARG:HG3	12:H:90:HIS:HA	1.57	0.85
1:2:1448:A:H5'	33:6:56:ARG:NH2	1.90	0.85
1:2:6:G:C6	1:2:7:G:C6	2.65	0.85
30:5:819:A:O2'	30:5:820:U:H5'	1.76	0.85
1:2:1200:U:N3	12:H:180:PHE:HB2	1.92	0.85
31:1:32:THR:HG23	31:1:40:MET:HB3	1.57	0.85
34:7:193:SER:HB2	35:8:10:MET:SD	2.17	0.85
1:2:1350:U:C2	1:2:1351:U:C6	2.65	0.85
31:1:35:ARG:NH2	32:4:38:A:N3	2.25	0.85
1:2:1053:A:C2	19:B:98:PRO:O	2.29	0.84
34:7:17:HIS:O	34:7:22:LYS:NZ	2.10	0.84
34:7:193:SER:OG	35:8:10:MET:SD	2.34	0.84
1:2:460:C:H5'	1:2:461:A:H5"	1.59	0.84
1:2:1195:U:OP1	12:H:79:TYR:HB2	1.76	0.84
1:2:184:G:O2'	1:2:185:G:C8	2.30	0.84
1:2:1026:A:H5'	19:B:104:PRO:CD	2.08	0.83
32:4:36:A:O2'	32:4:37:U:H5'	1.77	0.83
1:2:1298:G:H1'	32:4:43:G:H5"	1.57	0.83
1:2:1298:G:H22	32:4:30:G:H22	1.25	0.83
31:1:33:LYS:HG3	32:4:27:G:H5'	1.61	0.83
31:1:35:ARG:CD	31:1:36:PHE:H	1.90	0.83
25:G:53:LYS:HA	25:G:54:GLU:HB2	1.59	0.83
31:1:32:THR:OG1	31:1:42:ILE:HD11	1.79	0.83
30:5:819:A:N6	32:4:38:A:C6	2.47	0.82
1:2:1338:C:O2	10:X:23:ASP:HA	1.78	0.82
32:4:15:G:H22	32:4:49:C:H42	1.23	0.82
1:2:1190:C:H5'	32:4:31:G:H5"	1.61	0.82
1:2:1032:A:H5"	24:F:84:ARG:CZ	2.10	0.82
35:8:76:ASP:HB2	35:8:80:GLU:HB2	1.61	0.82
1:2:1400:A:H2'	1:2:1401:U:C6	2.14	0.81
1:2:1025:U:O4'	19:B:105:ALA:HB2	1.79	0.81
1:2:1054:A:C2'	19:B:95:ARG:HH22	1.93	0.81
32:4:28:U:H2'	32:4:29:C:H6	1.45	0.81
32:4:43:G:N3	32:4:44:A:C8	2.49	0.81
34:7:193:SER:CB	35:8:10:MET:SD	2.68	0.81
1:2:1392:G:O2'	1:2:1423:A:N6	2.13	0.81
35:8:97:GLU:HA	35:8:100:LEU:HD12	1.61	0.81
1:2:540:G:O2'	1:2:541:G:OP2	1.97	0.81
1:2:1026:A:HO2'	19:B:99:GLY:HA2	1.00	0.81
37:4:101:MET:CE	34:7:219:ARG:CZ	2.59	0.81
1:2:1299:A:C1'	32:4:42:C:C1'	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1413:G:H2'	1:2:1414:G:C8	2.16	0.81
1:2:1026:A:O2'	19:B:99:GLY:HA3	1.76	0.81
32:4:42:C:HO2'	32:4:43:G:H5'	1.41	0.81
34:7:189:ILE:CG2	35:8:14:LEU:CD2	2.59	0.80
34:7:188:LYS:CD	35:8:131:GLY:O	2.28	0.80
36:9:94:ASN:CG	36:9:236:PRO:HG2	2.01	0.80
34:7:187:HIS:HA	35:8:130:CYS:C	2.02	0.80
1:2:459:G:H3'	1:2:460:C:C4'	2.12	0.80
1:2:1451:C:H4'	31:1:78:GLN:HB2	1.62	0.80
1:2:884:G:N2	30:5:818:A:H5"	1.96	0.80
1:2:1347:U:O2'	1:2:1348:C:H5'	1.80	0.80
1:2:1053:A:N1	19:B:98:PRO:CA	2.18	0.80
1:2:1054:A:H4'	19:B:95:ARG:NH2	1.97	0.80
23:E:37:HIS:CE1	23:E:41:THR:HB	2.17	0.80
34:7:193:SER:HB2	35:8:10:MET:HE2	1.64	0.80
34:7:188:LYS:HE2	35:8:131:GLY:C	2.01	0.80
35:8:72:PRO:HG2	35:8:84:GLN:HB2	1.61	0.80
1:2:879:U:O2'	24:F:74:MET:O	2.00	0.80
1:2:1448:A:N6	33:6:51:ILE:HD13	1.96	0.80
20:V:56:ILE:HG13	20:V:67:GLY:HA3	1.63	0.80
36:9:98:LYS:CD	36:9:175:ARG:HH12	1.88	0.80
34:7:187:HIS:HB3	35:8:130:CYS:HA	1.62	0.79
1:2:1311:C:OP1	12:H:76:GLY:C	2.21	0.79
1:2:1333:G:C8	12:H:48:HIS:CE1	2.69	0.79
36:9:179:MET:HG3	36:9:239:ALA:HB1	1.63	0.79
34:7:189:ILE:HG21	35:8:14:LEU:HD23	1.65	0.78
1:2:1248:A:O2'	12:H:81:VAL:HG22	1.84	0.78
1:2:1041:C:H5"	10:X:71:ARG:NE	1.98	0.78
1:2:1350:U:C2	1:2:1351:U:C5	2.72	0.78
1:2:1443:G:H2'	1:2:1444:G:C8	2.18	0.78
32:4:12:G:N2	32:4:25:U:O2	2.16	0.78
34:7:188:LYS:HD2	35:8:131:GLY:O	1.82	0.78
1:2:867:A:O2'	1:2:1374:C:H4'	1.84	0.78
1:2:1360:C:O4'	30:5:821:G:O6	2.00	0.78
1:2:1472:G:P	31:1:58:LYS:HD2	2.23	0.78
1:2:8:U:O2	1:2:873:A:N7	2.17	0.78
1:2:62:G:N7	1:2:63:G:N7	2.32	0.78
1:2:152:G:H2'	1:2:153:G:C8	2.18	0.78
34:7:390:SER:H	34:7:393:ILE:HD11	1.48	0.78
31:1:32:THR:HG21	31:1:42:ILE:CG1	2.10	0.78
1:2:437:A:OP2	1:2:439:G:O6	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1448:A:C8	33:6:56:ARG:CZ	2.51	0.78
21:W:4:PRO:HB3	26:I:28:LYS:HE3	1.66	0.78
12:H:90:HIS:HB2	12:H:94:ASN:HB2	1.66	0.77
34:7:189:ILE:HG23	35:8:17:LYS:HB2	1.66	0.77
35:8:123:TRP:CD1	35:8:138:PRO:HB3	2.19	0.77
1:2:1248:A:O3'	12:H:81:VAL:HG13	1.83	0.77
1:2:1402:C:O2	25:G:79:HIS:HB2	1.83	0.77
1:2:880:G:H2'	1:2:881:G:C8	2.19	0.77
32:4:42:C:C2'	32:4:43:G:H5'	2.15	0.77
1:2:644:G:N2	1:2:651:U:O4	2.18	0.77
1:2:745:G:O2'	31:1:69:THR:HG21	1.84	0.77
1:2:1318:U:N3	1:2:1323:A:N6	2.29	0.77
31:1:33:LYS:HG3	32:4:27:G:OP1	1.84	0.77
1:2:846:G:H4'	1:2:1443:G:H4'	1.64	0.77
1:2:1200:U:H3	12:H:180:PHE:HB2	1.48	0.77
1:2:1037:U:H1'	1:2:1046:G:C6	2.20	0.77
1:2:1025:U:C2	19:B:103:ASN:ND2	2.36	0.76
1:2:1025:U:C2'	19:B:105:ALA:HB3	2.15	0.76
1:2:1053:A:C6	19:B:98:PRO:C	2.54	0.76
25:G:40:ALA:HB3	25:G:59:VAL:HG13	1.67	0.76
35:8:114:THR:HG22	35:8:127:CYS:HA	1.67	0.76
1:2:1053:A:H61	19:B:99:GLY:H	1.31	0.76
36:9:98:LYS:HD3	36:9:175:ARG:CZ	2.14	0.76
1:2:1054:A:C4'	19:B:95:ARG:HH22	1.99	0.76
32:4:24:C:H2'	32:4:25:U:C6	2.21	0.76
34:7:71:GLU:O	34:7:73:SER:N	2.19	0.76
1:2:1299:A:H4'	32:4:42:C:H4'	1.68	0.76
35:8:100:LEU:HA	35:8:104:VAL:HG12	1.67	0.76
1:2:276:A:H4'	15:N:14:ARG:NH2	2.01	0.76
1:2:1448:A:N7	33:6:56:ARG:CD	2.48	0.76
1:2:643:G:C2	1:2:653:C:N3	2.54	0.75
1:2:1042:U:OP1	10:X:70:ARG:NH2	2.19	0.75
34:7:189:ILE:CB	35:8:14:LEU:CD2	2.64	0.75
1:2:1348:C:O2'	1:2:1349:C:H5'	1.85	0.75
34:7:55:ASN:OD1	34:7:88:ARG:NE	2.19	0.75
1:2:1448:A:H8	33:6:56:ARG:NH2	1.83	0.75
25:G:78:ILE:HB	25:G:109:GLY:HA2	1.67	0.75
34:7:205:PRO:O	34:7:207:ARG:NH1	2.19	0.75
1:2:431:U:H4'	20:V:33:ARG:HH21	1.52	0.75
1:2:1041:C:H5"	10:X:71:ARG:CZ	2.16	0.74
1:2:1053:A:OP1	19:B:95:ARG:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:471:G:N2	15:N:65:PRO:O	2.19	0.74
1:2:830:A:C8	1:2:832:G:C8	2.75	0.74
1:2:1451:C:O3'	31:1:78:GLN:CD	2.25	0.74
22:D:59:LEU:HD11	24:F:132:GLU:HG3	1.68	0.74
30:5:821:G:H5'	30:5:822:C:OP1	1.85	0.74
32:4:9:G:C6	32:4:46:G:C6	2.75	0.74
32:4:71:G:C2'	32:4:72:C:H5'	2.16	0.74
36:9:95:LEU:HD11	36:9:237:LYS:CG	2.17	0.74
1:2:324:C:O2'	1:2:325:A:OP2	2.04	0.74
4:L:32:VAL:HG22	4:L:77:ALA:HB2	1.69	0.74
34:7:65:PRO:HB2	35:8:13:ARG:NH1	2.02	0.74
35:8:115:ILE:HG22	35:8:116:LEU:H	1.48	0.74
1:2:1344:U:H2'	1:2:1345:G:H8	1.51	0.74
34:7:189:ILE:CG2	35:8:14:LEU:HD23	2.17	0.74
34:7:66:GLU:HA	35:8:13:ARG:HH22	1.53	0.74
36:9:209:GLN:HA	36:9:212:GLU:HG3	1.70	0.74
1:2:134:A:H2'	1:2:135:U:C6	2.23	0.74
36:9:182:LEU:HD13	36:9:226:ARG:HD3	1.68	0.74
1:2:879:U:H4'	24:F:73:ARG:CZ	2.17	0.73
32:4:77:A:C8	34:7:280:ARG:NH2	2.55	0.73
1:2:642:G:H2'	1:2:643:G:O4'	1.87	0.73
1:2:1096:G:H21	9:U:1:MET:HA	1.51	0.73
35:8:117:LYS:HE3	35:8:126:VAL:HG21	1.70	0.73
1:2:643:G:N2	1:2:653:C:C2	2.57	0.73
1:2:1413:G:N3	25:G:77:ASP:OD2	2.21	0.73
34:7:218:ILE:HD11	34:7:294:LEU:HD11	1.69	0.73
1:2:438:A:H3'	1:2:439:G:H5"	1.70	0.73
1:2:394:C:H2'	1:2:395:C:H6	1.52	0.73
1:2:1299:A:H4'	32:4:42:C:C4'	2.18	0.73
24:F:157:ILE:HB	24:F:184:TRP:HB2	1.70	0.73
1:2:1403:U:C2	25:G:77:ASP:CG	2.62	0.73
1:2:1053:A:N6	19:B:99:GLY:H	1.87	0.73
1:2:1351:U:N3	1:2:1352:G:N7	2.37	0.73
12:H:178:MET:HB3	12:H:183:ALA:HB2	1.71	0.73
1:2:1025:U:HO2'	19:B:105:ALA:H	1.35	0.73
1:2:1413:G:C2	25:G:77:ASP:OD2	2.42	0.73
1:2:433:U:O5'	1:2:433:U:O2	2.07	0.72
32:4:21:H2U:H5'	32:4:22:A:OP2	1.89	0.72
1:2:321:A:H2'	1:2:322:G:O4'	1.89	0.72
23:E:16:PRO:HG2	23:E:19:TRP:NE1	2.04	0.72
1:2:1032:A:H5'	24:F:84:ARG:NH1	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1448:A:C6	33:6:51:ILE:HD13	2.25	0.72
30:5:819:A:C2'	30:5:820:U:H5'	2.19	0.72
1:2:344:G:OP1	25:G:106:THR:HG21	1.90	0.72
1:2:868:C:H5"	1:2:1373:A:O2'	1.88	0.72
31:1:34:ARG:HG3	31:1:35:ARG:N	2.03	0.72
34:7:346:LEU:HD11	34:7:401:ILE:HD13	1.71	0.72
35:8:115:ILE:CG2	35:8:116:LEU:H	2.03	0.72
1:2:359:A:OP1	15:N:51:ARG:N	2.22	0.72
1:2:1053:A:C6	19:B:99:GLY:N	2.58	0.72
1:2:1290:U:O4	1:2:1291:G:C2	2.43	0.72
1:2:1402:C:H42	1:2:1413:G:H22	1.38	0.72
1:2:1403:U:C2	25:G:77:ASP:OD1	2.42	0.72
1:2:892:C:O2'	1:2:894:A:OP2	2.08	0.72
1:2:495:G:N2	1:2:496:C:C2	2.58	0.71
1:2:884:G:C6	1:2:1460:G:C6	2.78	0.71
31:1:35:ARG:NH2	32:4:38:A:H1'	2.03	0.71
32:4:77:A:O3'	37:4:101:MET:C	2.29	0.71
34:7:182:PRO:HD3	35:8:7:TYR:CE1	2.24	0.71
1:2:179:U:H3	1:2:184:G:H1	1.35	0.71
1:2:1025:U:O4'	19:B:105:ALA:CB	2.37	0.71
1:2:1459:G:O2'	1:2:1460:G:OP2	2.06	0.71
1:2:1485:G:H2'	1:2:1486:A:H5"	1.70	0.71
35:8:111:SER:O	35:8:112:LEU:HB2	1.87	0.71
1:2:229:G:N3	1:2:230:C:C6	2.58	0.71
1:2:394:C:H2'	1:2:395:C:C6	2.26	0.71
1:2:1300:A:H4'	32:4:32:G:O2'	1.90	0.71
34:7:190:ASN:CB	35:8:14:LEU:HB2	2.20	0.71
34:7:330:ARG:NH1	34:7:379:GLU:OE2	2.23	0.71
34:7:388:VAL:HG13	34:7:393:ILE:HG13	1.73	0.71
35:8:42:THR:HG21	35:8:92:ILE:HD11	1.71	0.71
1:2:113:U:OP1	17:R:30:HIS:CE1	2.44	0.71
1:2:1347:U:C2'	1:2:1348:C:H5'	2.21	0.71
12:H:71:ILE:HG23	12:H:180:PHE:CE1	2.26	0.71
23:E:12:ARG:HA	23:E:29:ALA:HB2	1.73	0.71
1:2:400:G:O2'	1:2:423:U:O2	2.09	0.71
32:4:77:A:O3'	37:4:101:MET:HA	1.91	0.71
36:9:251:ILE:O	36:9:255:LYS:N	2.24	0.71
1:2:359:A:P	15:N:51:ARG:H	2.14	0.70
1:2:607:U:H4'	26:I:57:ARG:HH21	1.56	0.70
1:2:1404:C:H2'	1:2:1405:C:O4'	1.91	0.70
36:9:109:LEU:HD23	36:9:112:GLN:OE1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:315:A:C1'	1:2:1423:A:H1'	2.20	0.70
1:2:1022:U:OP2	24:F:80:ARG:NH1	2.24	0.70
1:2:1080:C:O2'	1:2:1082:A:OP2	2.05	0.70
1:2:1360:C:C5	32:4:35:C:C5	2.80	0.70
34:7:190:ASN:CB	35:8:14:LEU:CD1	2.45	0.70
1:2:17:C:H4'	1:2:843:G:C8	2.26	0.70
4:L:45:ILE:HG23	4:L:66:LEU:HB3	1.72	0.70
1:2:317:A:O2'	25:G:102:ARG:NH2	2.25	0.70
26:I:11:LEU:O	26:I:14:ILE:HG22	1.92	0.70
1:2:495:G:C2	1:2:496:C:C4	2.80	0.70
1:2:1494:C:O2	30:5:806:G:N2	2.24	0.70
36:9:220:TYR:OH	36:9:228:ARG:HD2	1.92	0.70
1:2:318:C:H4'	25:G:102:ARG:HD3	1.73	0.70
1:2:930:G:C5	1:2:1325:C:H4'	2.27	0.70
1:2:1360:C:C5	32:4:35:C:C4	2.79	0.70
34:7:65:PRO:HB2	35:8:13:ARG:HH12	1.54	0.70
1:2:6:G:N7	24:F:192:ARG:NH2	2.40	0.70
1:2:650:A:N3	1:2:740:G:O2'	2.23	0.70
1:2:1025:U:H1'	19:B:105:ALA:HB3	0.71	0.70
1:2:1028:C:OP2	19:B:132:GLU:OE1	2.09	0.70
12:H:44:LEU:HD13	13:K:44:THR:OG1	1.90	0.70
12:H:87:ARG:C	12:H:88:ARG:HD3	2.12	0.70
34:7:156:LYS:H	34:7:156:LYS:HD2	1.54	0.70
36:9:111:SER:HA	36:9:160:TRP:HZ3	1.54	0.70
1:2:1032:A:C5'	24:F:84:ARG:NH1	2.55	0.69
1:2:1350:U:N3	1:2:1351:U:C4	2.59	0.69
24:F:203:ASN:O	24:F:206:TYR:HB3	1.92	0.69
1:2:642:G:C6	1:2:654:U:N3	2.60	0.69
1:2:909:U:OP2	5:O:130:ARG:HD2	1.92	0.69
1:2:1189:G:O2'	32:4:31:G:OP1	2.10	0.69
1:2:121:C:N3	1:2:122:C:C5	2.61	0.69
1:2:1026:A:O3'	19:B:102:THR:OG1	1.82	0.69
34:7:189:ILE:CB	35:8:14:LEU:HD21	2.14	0.69
32:4:41:C:H2'	32:4:42:C:H6	1.58	0.69
35:8:115:ILE:CG2	35:8:116:LEU:N	2.54	0.69
1:2:229:G:N3	1:2:230:C:C5	2.61	0.69
24:F:129:GLY:HA2	24:F:134:ARG:HB3	1.73	0.69
12:H:87:ARG:HA	12:H:88:ARG:HD3	1.75	0.69
12:H:137:THR:HB	12:H:139:VAL:HG13	1.75	0.69
17:R:1:MET:C	17:R:15:LYS:HG2	2.12	0.69
1:2:251:G:O6	1:2:262:G:O6	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:260:ARG:HD2	34:7:267:VAL:HG13	1.75	0.69
1:2:152:G:H2'	1:2:153:G:H8	1.58	0.69
1:2:229:G:C2	1:2:230:C:C6	2.80	0.69
1:2:1452:G:H2'	1:2:1453:U:H6	1.58	0.69
34:7:33:TRP:HE1	34:7:36:LYS:HD2	1.58	0.69
1:2:1313:G:H5'	12:H:81:VAL:HG21	1.75	0.68
1:2:1424:G:C5	1:2:1425:C:C4	2.81	0.68
36:9:98:LYS:HZ2	36:9:235:ASN:CB	2.05	0.68
34:7:207:ARG:HE	34:7:291:PRO:HB2	1.58	0.68
1:2:507:G:P	15:N:111:PRO:HG3	2.34	0.68
1:2:516:A:N6	1:2:842:U:N3	2.18	0.68
1:2:1118:C:N3	1:2:1141:G:N2	2.41	0.68
12:H:110:ILE:HD13	12:H:182:GLU:HG2	1.74	0.68
1:2:152:G:H4'	25:G:64:ARG:HD2	1.73	0.68
1:2:1299:A:C4'	32:4:42:C:C4'	2.71	0.68
1:2:1413:G:H2'	1:2:1414:G:H8	1.58	0.68
34:7:182:PRO:HG3	35:8:7:TYR:CZ	2.26	0.68
34:7:238:ILE:HG21	34:7:316:ILE:HD11	1.75	0.68
1:2:315:A:H4'	1:2:1423:A:H4'	1.75	0.68
1:2:585:U:H3'	1:2:586:C:H4'	1.74	0.68
26:I:80:PRO:HA	26:I:124:ARG:HA	1.74	0.68
31:1:33:LYS:HE3	32:4:27:G:H5"	1.74	0.68
34:7:235:GLY:HA2	36:9:193:VAL:HG21	1.76	0.68
35:8:100:LEU:HD23	35:8:104:VAL:HG11	1.75	0.68
35:8:100:LEU:O	35:8:104:VAL:HG12	1.93	0.68
36:9:94:ASN:CB	36:9:236:PRO:HG2	2.24	0.68
1:2:1341:C:H2'	1:2:1342:C:C6	2.29	0.68
32:4:34:U:H2'	32:4:36:A:OP2	1.92	0.68
32:4:77:A:O3'	37:4:101:MET:CA	2.41	0.68
36:9:98:LYS:NZ	36:9:235:ASN:CA	2.50	0.68
1:2:460:C:H4'	1:2:460:C:OP1	1.94	0.68
1:2:771:G:C5	1:2:773:A:O4'	2.46	0.68
31:1:32:THR:HG22	31:1:42:ILE:HG12	1.74	0.68
34:7:108:ALA:HA	34:7:111:MET:SD	2.34	0.68
1:2:478:C:H2'	1:2:479:C:C6	2.28	0.68
1:2:1131:G:H2'	1:2:1132:C:C6	2.29	0.68
1:2:112:G:H8	1:2:112:G:O5'	1.77	0.68
1:2:607:U:H4'	26:I:57:ARG:NH2	2.09	0.68
34:7:189:ILE:CG2	35:8:14:LEU:CG	2.65	0.68
1:2:6:G:O6	1:2:7:G:C6	2.47	0.67
1:2:957:A:C2	1:2:991:C:N4	2.61	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1298:G:N3	32:4:43:G:H5'	2.08	0.67
32:4:41:C:H2'	32:4:42:C:C6	2.29	0.67
1:2:1027:C:C5'	19:B:102:THR:CB	2.31	0.67
24:F:203:ASN:O	24:F:207:ASN:ND2	2.28	0.67
1:2:1350:U:C4	1:2:1351:U:C5	2.82	0.67
34:7:187:HIS:CA	35:8:130:CYS:HA	2.23	0.67
1:2:1460:G:O2'	30:5:815:U:O4	2.11	0.67
1:2:127:G:C2	1:2:218:C:C2	2.83	0.67
1:2:884:G:H22	30:5:818:A:H5"	1.58	0.67
1:2:1049:U:O2'	1:2:1129:A:N3	2.27	0.67
32:4:51:U:H2'	32:4:52:C:C6	2.29	0.67
34:7:115:ILE:HG12	34:7:145:ILE:HB	1.76	0.67
23:E:20:TYR:O	23:E:47:TYR:OH	2.13	0.67
1:2:1178:C:H2'	1:2:1179:C:C6	2.28	0.67
1:2:1367:C:O2'	31:1:65:ALA:HB3	1.89	0.67
1:2:513:A:O2'	1:2:514:U:OP2	2.09	0.67
35:8:58:ASP:O	35:8:62:MET:HB2	1.95	0.67
1:2:1451:C:H5"	31:1:78:GLN:HB3	1.77	0.67
1:2:151:G:N3	25:G:64:ARG:NH2	2.42	0.67
1:2:1054:A:C3'	19:B:95:ARG:HH22	2.08	0.67
1:2:1299:A:O4'	32:4:42:C:H4'	1.93	0.67
1:2:1371:C:N4	1:2:1372:C:N4	2.43	0.66
31:1:33:LYS:HG3	32:4:27:G:H5"	1.73	0.66
36:9:94:ASN:HB3	36:9:236:PRO:HG2	1.76	0.66
1:2:643:G:C2	1:2:653:C:C2	2.84	0.66
24:F:165:LEU:HD23	24:F:183:VAL:HG12	1.77	0.66
1:2:1025:U:O2'	19:B:105:ALA:CB	2.44	0.66
34:7:188:LYS:HG3	35:8:131:GLY:CA	2.20	0.66
1:2:1025:U:C4'	19:B:105:ALA:HB2	2.25	0.66
1:2:1346:C:C2'	1:2:1347:U:C6	2.75	0.66
1:2:1345:G:C2'	1:2:1346:C:H5'	2.25	0.66
32:4:67:C:H2'	32:4:68:C:C6	2.30	0.66
1:2:1033:G:OP2	24:F:102:HIS:CD2	2.49	0.66
19:B:104:PRO:HG2	24:F:19:LYS:HE2	1.77	0.66
22:D:26:GLU:O	22:D:30:MET:N	2.29	0.66
24:F:143:PHE:CZ	26:I:96:ALA:HB3	2.31	0.66
1:2:6:G:C6	1:2:7:G:O6	2.47	0.66
1:2:540:G:H4'	26:I:4:LEU:HB2	1.77	0.66
1:2:1346:C:O2'	1:2:1347:U:H5'	1.94	0.66
35:8:56:ARG:NH1	35:8:104:VAL:HA	2.08	0.66
1:2:906:G:C6	1:2:907:C:N3	2.64	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1041:C:O3'	10:X:71:ARG:NH2	2.28	0.66
1:2:642:G:C6	1:2:654:U:C2	2.84	0.66
1:2:884:G:H8	1:2:884:G:O5'	1.79	0.66
1:2:1367:C:H1'	31:1:65:ALA:HB1	0.66	0.66
1:2:1475:C:OP2	29:0:4:LYS:HG2	1.96	0.66
36:9:107:LEU:HB3	36:9:121:ALA:HB1	1.78	0.66
1:2:495:G:N1	1:2:496:C:C4	2.64	0.65
1:2:572:U:H1'	20:V:60:PHE:CZ	2.31	0.65
1:2:2:U:C6	24:F:184:TRP:CZ3	2.85	0.65
1:2:1351:U:C2	1:2:1352:G:N7	2.64	0.65
23:E:192:ASN:HA	23:E:195:ARG:NH2	2.11	0.65
35:8:100:LEU:CA	35:8:104:VAL:HG12	2.27	0.65
36:9:123:GLU:HA	36:9:127:TRP:CD1	2.31	0.65
36:9:175:ARG:NH1	36:9:234:THR:O	2.29	0.65
1:2:199:A:C6	1:2:217:C:H4'	2.32	0.65
34:7:66:GLU:HB3	35:8:13:ARG:HH21	1.58	0.65
36:9:13:GLU:O	36:9:68:VAL:HG23	1.96	0.65
1:2:434:A:C4	20:V:85:TYR:HD1	2.14	0.65
1:2:434:A:C5	20:V:85:TYR:HD1	2.15	0.65
31:1:38:LYS:C	31:1:39:LEU:CD1	2.60	0.65
32:4:46:G:O5'	32:4:46:G:H8	1.80	0.65
34:7:51:TYR:CE2	34:7:294:LEU:HB2	2.32	0.65
30:5:812:G:H3'	30:5:813:A:O4'	1.96	0.65
32:4:12:G:N2	32:4:25:U:C2	2.65	0.65
36:9:109:LEU:O	36:9:113:LYS:HG2	1.96	0.65
36:9:131:ALA:O	36:9:133:TYR:N	2.30	0.65
1:2:6:G:O6	24:F:192:ARG:NH2	2.30	0.65
1:2:121:C:C2	1:2:122:C:C5	2.85	0.65
1:2:439:G:H1'	1:2:440:C:H5	1.61	0.65
1:2:648:A:N6	1:2:741:A:HO2'	1.86	0.65
1:2:16:G:H2'	1:2:17:C:C6	2.31	0.65
1:2:406:U:H2'	1:2:407:G:N7	2.12	0.65
1:2:1371:C:N4	1:2:1372:C:H41	1.95	0.65
1:2:1452:G:H2'	1:2:1453:U:C6	2.32	0.65
34:7:189:ILE:HG21	35:8:14:LEU:O	1.96	0.65
1:2:740:G:N2	1:2:751:C:C2	2.65	0.65
34:7:66:GLU:CB	35:8:13:ARG:NH2	2.59	0.65
1:2:1053:A:C8	19:B:98:PRO:CG	2.74	0.64
1:2:1403:U:N3	1:2:1404:C:C5	2.66	0.64
1:2:1424:G:C6	1:2:1425:C:C4	2.84	0.64
1:2:1448:A:C5	33:6:56:ARG:HG2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1:34:ARG:HB2	31:1:40:MET:CB	2.25	0.64
36:9:95:LEU:CD2	36:9:235:ASN:OD1	2.45	0.64
1:2:1154:G:H2'	1:2:1155:U:C6	2.32	0.64
12:H:43:LEU:HD11	13:K:43:PHE:HB3	1.79	0.64
25:G:78:ILE:CG2	25:G:109:GLY:HA2	2.28	0.64
1:2:151:G:H1'	25:G:120:ASN:ND2	2.11	0.64
1:2:498:C:O2'	1:2:502:U:OP1	2.16	0.64
15:N:103:VAL:HG13	15:N:126:VAL:HG13	1.80	0.64
31:1:26:LYS:C	31:1:27:ILE:HG12	2.17	0.64
36:9:83:LYS:O	36:9:85:VAL:N	2.30	0.64
32:4:23:G:C6	32:4:24:C:N4	2.65	0.64
34:7:20:HIS:O	34:7:149:ASN:ND2	2.28	0.64
35:8:62:MET:O	35:8:66:LEU:HB2	1.96	0.64
24:F:196:ASN:O	24:F:200:ALA:N	2.27	0.64
32:4:77:A:O3'	37:4:101:MET:O	2.15	0.64
1:2:867:A:O2'	1:2:1374:C:O3'	2.14	0.64
25:G:29:LEU:HD11	25:G:63:ILE:HD11	1.79	0.64
35:8:64:TYR:OH	35:8:98:ARG:HD2	1.97	0.64
35:8:109:CYS:C	35:8:110:LYS:HG3	2.17	0.64
1:2:1352:G:N2	1:2:1353:C:C2	2.65	0.64
32:4:43:G:C2	32:4:44:A:N7	2.65	0.64
1:2:1060:G:O3'	1:2:1061:A:P	2.56	0.64
1:2:1401:U:O4	1:2:1402:C:N4	2.31	0.64
1:2:1489:A:C2'	1:2:1490:C:H5'	2.28	0.64
18:A:10:ARG:HD2	36:9:133:TYR:OH	1.97	0.64
19:B:56:GLY:HA3	19:B:174:GLU:CG	2.28	0.64
26:I:46:TYR:HA	26:I:68:ARG:HD3	1.79	0.64
31:1:40:MET:CG	31:1:77:LEU:O	2.46	0.64
1:2:317:A:O2'	25:G:102:ARG:CZ	2.46	0.64
1:2:1131:G:H2'	1:2:1132:C:H6	1.63	0.64
1:2:1299:A:C2	32:4:31:G:N3	2.66	0.64
1:2:1316:U:H3	1:2:1326:G:H1	1.45	0.64
35:8:117:LYS:O	35:8:118:LYS:HG3	1.98	0.64
30:5:812:G:C3'	30:5:813:A:O4'	2.47	0.63
34:7:23:THR:HG23	34:7:34:THR:HG23	1.80	0.63
34:7:189:ILE:CG2	35:8:17:LYS:HB2	2.27	0.63
31:1:35:ARG:HH21	32:4:38:A:C1'	2.10	0.63
32:4:36:A:O5'	32:4:36:A:H8	1.80	0.63
1:2:459:G:H3'	1:2:460:C:O4'	1.98	0.63
1:2:1025:U:C2'	19:B:105:ALA:CB	2.75	0.63
4:L:92:GLU:HB2	4:L:93:ASP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:677:U:C4	1:2:1493:C:H4'	2.33	0.63
1:2:1041:C:C5'	10:X:71:ARG:CZ	2.76	0.63
1:2:1371:C:C4	1:2:1372:C:N4	2.66	0.63
31:1:25:GLN:NE2	31:1:94:PHE:HD1	1.94	0.63
34:7:35:SER:OG	34:7:37:HIS:HB3	1.99	0.63
1:2:127:G:N2	1:2:218:C:C2	2.67	0.63
1:2:901:G:N2	1:2:1302:C:C2	2.66	0.63
1:2:1269:G:H2'	1:2:1270:C:O4'	1.99	0.63
15:N:87:PHE:N	15:N:122:ILE:HG21	2.13	0.63
34:7:187:HIS:HA	35:8:130:CYS:CA	2.27	0.63
36:9:217:ILE:HD13	36:9:246:ILE:HD11	1.80	0.63
1:2:302:A:C2	1:2:303:G:N7	2.67	0.63
24:F:86:LEU:HG	24:F:100:ILE:HG22	1.81	0.63
35:8:7:TYR:O	35:8:10:MET:N	2.32	0.63
36:9:54:ILE:O	36:9:58:LEU:HB2	1.99	0.63
1:2:780:C:H4'	26:I:13:HIS:CG	2.34	0.63
1:2:1462:A:C8	1:2:1486:A:C6	2.87	0.63
15:N:72:ALA:HA	15:N:86:ALA:O	1.99	0.63
16:Q:4:MET:HA	16:Q:7:ARG:HG3	1.81	0.63
24:F:54:LEU:HD13	24:F:61:GLU:HB3	1.81	0.63
1:2:126:G:N2	1:2:219:C:C2	2.67	0.62
34:7:306:THR:O	34:7:306:THR:OG1	2.07	0.62
1:2:996:A:C2	1:2:997:G:C8	2.88	0.62
1:2:1413:G:O3'	25:G:86:VAL:HG21	1.99	0.62
17:R:17:ASP:HB3	17:R:21:CYS:SG	2.39	0.62
24:F:130:SER:HB3	24:F:139:HIS:CE1	2.34	0.62
1:2:1360:C:C6	32:4:35:C:C4	2.87	0.62
23:E:157:ASN:OD1	23:E:162:TYR:CE1	2.52	0.62
34:7:66:GLU:CA	35:8:13:ARG:HH22	2.11	0.62
1:2:332:C:O2	1:2:1424:G:O2'	2.12	0.62
1:2:885:G:O2'	1:2:1487:U:H4'	1.99	0.62
25:G:76:PRO:O	25:G:77:ASP:HB2	1.99	0.62
34:7:187:HIS:ND1	35:8:130:CYS:CB	2.60	0.62
1:2:380:C:H2'	1:2:381:C:C6	2.34	0.62
1:2:1307:G:N2	12:H:48:HIS:CE1	2.68	0.62
36:9:98:LYS:HZ2	36:9:235:ASN:HD22	1.48	0.62
1:2:1424:G:C2	1:2:1425:C:C2	2.88	0.62
1:2:121:C:C2	1:2:122:C:C6	2.87	0.62
16:Q:126:GLU:HA	16:Q:129:ILE:HD12	1.81	0.62
24:F:152:VAL:C	24:F:153:ARG:HD2	2.20	0.62
32:4:25:U:O5'	32:4:25:U:H6	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:472:C:H2'	1:2:473:A:C8	2.35	0.62
1:2:1465:C:OP1	29:0:2:ARG:HB2	2.00	0.62
12:H:46:HIS:O	12:H:48:HIS:N	2.32	0.62
18:A:100:THR:HA	18:A:127:ARG:O	2.00	0.62
27:J:120:VAL:O	27:J:121:ASN:ND2	2.33	0.62
34:7:187:HIS:O	35:8:129:ALA:O	2.18	0.62
36:9:117:SER:OG	36:9:120:ASP:N	2.29	0.62
25:G:53:LYS:HA	25:G:54:GLU:CB	2.28	0.62
34:7:187:HIS:HA	35:8:130:CYS:HA	1.81	0.62
1:2:534:G:O6	1:2:712:G:C8	2.53	0.62
1:2:584:C:H4'	1:2:585:U:OP1	2.00	0.62
1:2:607:U:OP2	16:Q:16:ARG:HD3	2.00	0.62
1:2:1299:A:H2	32:4:31:G:N3	1.98	0.62
34:7:49:LEU:HD12	34:7:218:ILE:HD12	1.80	0.62
1:2:330:U:H4'	25:G:104:LYS:HB2	1.82	0.61
1:2:533:C:C4	1:2:534:G:N1	2.68	0.61
27:J:64:ASN:O	27:J:121:ASN:OD1	2.18	0.61
34:7:38:SER:O	34:7:40:GLU:N	2.27	0.61
1:2:1333:G:N7	12:H:48:HIS:NE2	2.48	0.61
1:2:1339:G:H21	1:2:1341:C:H41	1.48	0.61
31:1:35:ARG:HH21	32:4:38:A:H1'	1.63	0.61
31:1:40:MET:CG	31:1:78:GLN:HA	2.29	0.61
36:9:98:LYS:CD	36:9:175:ARG:NH1	2.49	0.61
1:2:227:C:H2'	1:2:228:G:C8	2.35	0.61
1:2:711:U:H2'	1:2:712:G:O4'	1.99	0.61
34:7:38:SER:C	34:7:40:GLU:H	2.03	0.61
1:2:60:A:C2	1:2:64:G:O6	2.52	0.61
1:2:1360:C:C4	32:4:35:C:N1	2.68	0.61
27:J:10:LYS:HD3	27:J:16:ARG:HA	1.82	0.61
34:7:393:ILE:HB	34:7:413:VAL:HB	1.82	0.61
35:8:57:GLU:HB3	35:8:60:ILE:HG13	1.82	0.61
1:2:867:A:C2'	1:2:1374:C:H4'	2.31	0.61
14:M:97:GLY:HA2	14:M:100:ALA:HB3	1.81	0.61
26:I:7:LEU:HA	26:I:34:ILE:CG1	2.29	0.61
25:G:33:ARG:O	25:G:63:ILE:HD12	2.00	0.61
25:G:55:PHE:N	25:G:56:PRO:HA	2.15	0.61
25:G:78:ILE:CB	25:G:109:GLY:HA2	2.31	0.61
35:8:123:TRP:NE1	35:8:138:PRO:HB3	2.14	0.61
1:2:1013:G:C5	1:2:1014:C:C4	2.89	0.61
1:2:1028:C:C2	1:2:1034:G:C2	2.88	0.61
1:2:533:C:N3	1:2:534:G:C2	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:930:G:C4	1:2:1325:C:H4'	2.36	0.61
1:2:1026:A:C5'	19:B:102:THR:O	2.40	0.61
16:Q:132:LEU:O	16:Q:136:TYR:CD2	2.53	0.61
1:2:822:A:C2'	1:2:823:A:C8	2.78	0.61
1:2:975:A:H2'	1:2:976:A:C5'	2.28	0.61
1:2:1026:A:C5'	19:B:104:PRO:HD2	2.28	0.61
12:H:73:ARG:NH1	12:H:166:ALA:O	2.34	0.61
18:A:71:TYR:CE1	18:A:81:LYS:HB2	2.36	0.61
31:1:34:ARG:CG	31:1:35:ARG:H	2.04	0.61
1:2:380:C:H2'	1:2:381:C:H6	1.65	0.61
1:2:746:A:O2'	1:2:747:U:OP2	2.19	0.61
1:2:876:A:H2'	1:2:877:A:C8	2.36	0.61
32:4:17:C:H5"	32:4:18:U:C6	2.35	0.61
12:H:13:HIS:CE1	13:K:50:ILE:HD11	2.36	0.60
26:I:76:LYS:HB3	26:I:77:PRO:HD3	1.81	0.60
1:2:641:A:H2	1:2:642:G:C4	2.18	0.60
1:2:1348:C:H2'	1:2:1349:C:H6	1.63	0.60
1:2:909:U:OP2	5:O:130:ARG:CD	2.50	0.60
1:2:1360:C:C4	32:4:35:C:C2	2.90	0.60
23:E:45:LEU:HD12	23:E:83:PHE:HB3	1.82	0.60
24:F:148:LYS:HB3	24:F:153:ARG:NH2	2.17	0.60
1:2:540:G:C6	1:2:709:G:C6	2.89	0.60
36:9:111:SER:O	36:9:115:LYS:N	2.35	0.60
1:2:985:C:H3'	1:2:986:G:C2	2.36	0.60
36:9:94:ASN:CG	36:9:236:PRO:CG	2.67	0.60
1:2:1053:A:P	19:B:95:ARG:CD	2.76	0.60
34:7:324:PRO:HD2	34:7:388:VAL:O	2.01	0.60
1:2:260:C:H2'	1:2:261:G:O4'	2.02	0.60
1:2:1298:G:H1'	32:4:43:G:C5'	2.31	0.60
34:7:155:SER:O	34:7:158:GLU:N	2.35	0.60
35:8:118:LYS:HG2	35:8:123:TRP:CD1	2.36	0.60
1:2:229:G:N2	1:2:230:C:N3	2.50	0.60
1:2:1367:C:HO2'	31:1:65:ALA:HB2	1.60	0.60
9:U:62:VAL:HG22	9:U:68:VAL:HG11	1.83	0.60
24:F:191:THR:HG23	24:F:197:PHE:CD1	2.37	0.60
27:J:64:ASN:ND2	27:J:75:VAL:HG12	2.16	0.60
1:2:921:G:H1'	1:2:1161:A:N6	2.17	0.59
1:2:1348:C:H2'	1:2:1349:C:C5	2.37	0.59
34:7:17:HIS:HB2	34:7:129:THR:OG1	2.02	0.59
34:7:313:GLY:O	34:7:364:SER:HB3	2.02	0.59
36:9:69:ILE:HD11	36:9:81:SER:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:607:U:H4'	26:I:57:ARG:HE	1.67	0.59
32:4:42:C:H2'	32:4:43:G:H8	1.67	0.59
1:2:151:G:O2'	25:G:64:ARG:CZ	2.50	0.59
1:2:742:U:C4	1:2:743:U:C4	2.90	0.59
12:H:21:TRP:CH2	12:H:108:PHE:HB3	2.37	0.59
31:1:40:MET:SD	31:1:76:GLU:HB3	2.41	0.59
1:2:229:G:N1	1:2:230:C:N4	2.50	0.59
1:2:461:A:O3'	1:2:462:A:H3'	2.02	0.59
1:2:1275:U:O4	1:2:1276:G:N1	2.35	0.59
1:2:1350:U:C4	1:2:1351:U:C4	2.90	0.59
9:U:80:ARG:HE	12:H:81:VAL:HG11	1.66	0.59
32:4:75:C:O2'	32:4:76:C:OP2	2.21	0.59
35:8:56:ARG:NH1	35:8:103:TYR:O	2.35	0.59
1:2:774:U:H4'	1:2:775:G:OP2	2.02	0.59
34:7:37:HIS:N	34:7:41:LEU:HB2	2.18	0.59
36:9:114:LEU:HD12	36:9:160:TRP:CE3	2.37	0.59
1:2:315:A:H4'	1:2:1423:A:C4'	2.33	0.59
35:8:3:SER:OG	35:8:3:SER:O	2.21	0.59
1:2:537:G:H2'	1:2:538:C:C6	2.38	0.59
1:2:868:C:H4'	1:2:1373:A:C2'	2.32	0.59
1:2:82:G:C6	1:2:83:C:C4	2.91	0.59
1:2:1190:C:C5'	32:4:31:G:H5"	2.33	0.59
1:2:1350:U:O2	1:2:1351:U:C6	2.55	0.59
1:2:1401:U:C4	1:2:1402:C:N4	2.71	0.59
31:1:25:GLN:O	31:1:98:SER:HB2	2.03	0.59
34:7:66:GLU:CA	35:8:13:ARG:NH2	2.66	0.59
36:9:163:PRO:O	36:9:167:GLU:HB2	2.03	0.59
1:2:122:C:C2	1:2:223:G:N2	2.71	0.59
1:2:615:G:O6	1:2:698:A:C6	2.56	0.59
1:2:649:A:H2	1:2:740:G:O2'	1.85	0.59
1:2:1370:U:C2	1:2:1446:G:C2	2.90	0.59
1:2:1401:U:H3	1:2:1414:G:H1	1.50	0.59
23:E:193:VAL:O	23:E:195:ARG:NH1	2.36	0.59
33:6:60:TRP:CE3	33:6:60:TRP:HA	2.37	0.59
1:2:442:C:O5'	1:2:442:C:H6	1.85	0.59
24:F:197:PHE:O	24:F:200:ALA:HB3	2.03	0.59
32:4:27:G:H2'	32:4:28:U:H5'	1.84	0.59
1:2:1414:G:P	25:G:86:VAL:HG11	2.43	0.58
4:L:51:LYS:HB2	4:L:60:THR:O	2.03	0.58
34:7:19:ASP:O	34:7:150:LYS:NZ	2.28	0.58
35:8:109:CYS:O	35:8:110:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1311:C:OP1	12:H:76:GLY:CA	2.51	0.58
1:2:1423:A:H2'	1:2:1424:G:C8	2.38	0.58
34:7:95:PRO:HG2	34:7:100:LEU:HD22	1.84	0.58
34:7:189:ILE:HG23	35:8:17:LYS:CB	2.33	0.58
1:2:4:C:C2	1:2:5:C:C5	2.91	0.58
1:2:353:G:C2	1:2:354:G:C8	2.91	0.58
1:2:369:A:H4'	1:2:434:A:C5	2.39	0.58
1:2:495:G:C6	1:2:496:C:N4	2.71	0.58
32:4:77:A:C2'	34:7:280:ARG:NH2	2.61	0.58
1:2:495:G:C2	1:2:496:C:C5	2.92	0.58
1:2:585:U:H3'	1:2:586:C:C4'	2.34	0.58
1:2:702:G:H22	1:2:706:G:H1	1.49	0.58
1:2:947:G:O2'	1:2:976:A:N6	2.36	0.58
1:2:1062:G:H1'	7:S:6:GLN:NE2	2.17	0.58
34:7:11:ASN:OD1	34:7:293:GLY:N	2.29	0.58
1:2:1049:U:O2'	1:2:1129:A:C2	2.56	0.58
1:2:1397:C:C2	1:2:1419:G:C2	2.91	0.58
1:2:1451:C:OP1	31:1:37:GLY:HA3	2.03	0.58
1:2:1451:C:C5'	31:1:78:GLN:HB2	2.34	0.58
22:D:118:MET:SD	22:D:118:MET:N	2.73	0.58
1:2:1382:G:N2	1:2:1434:C:C2	2.71	0.58
34:7:332:LYS:HB2	34:7:414:GLU:OE2	2.04	0.58
35:8:137:LYS:CG	35:8:139:LEU:HD13	2.30	0.58
1:2:71:C:C2	1:2:79:G:C2	2.92	0.58
1:2:599:G:C6	1:2:600:C:C4	2.90	0.58
1:2:920:U:C2	1:2:1161:A:N6	2.69	0.58
1:2:1443:G:C6	1:2:1444:G:O6	2.56	0.58
1:2:1448:A:H4'	1:2:1449:G:OP1	2.04	0.58
32:4:44:A:H2'	32:4:45:A:H5'	1.86	0.58
35:8:76:ASP:CB	35:8:80:GLU:HB2	2.33	0.58
1:2:459:G:N1	1:2:460:C:C2	2.72	0.58
1:2:1312:C:C2	1:2:1331:G:C2	2.91	0.58
34:7:269:TYR:CE2	34:7:384:ARG:HG3	2.39	0.58
1:2:271:G:C6	1:2:272:C:C4	2.92	0.57
1:2:1298:G:N3	32:4:43:G:C5'	2.67	0.57
1:2:1311:C:H4'	12:H:95:SER:HA	1.86	0.57
1:2:441:U:C4	1:2:442:C:N4	2.72	0.57
1:2:661:C:H4'	14:M:18:HIS:CD2	2.39	0.57
1:2:1059:C:C4	1:2:1060:G:N7	2.71	0.57
1:2:1414:G:H1'	25:G:78:ILE:HA	1.85	0.57
19:B:56:GLY:HA3	19:B:174:GLU:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:165:LEU:HD21	24:F:180:VAL:O	2.05	0.57
32:4:17:C:H5"	32:4:18:U:C5	2.39	0.57
34:7:125:PRO:HB2	34:7:130:ARG:HH11	1.70	0.57
34:7:332:LYS:HG3	34:7:376:ASP:O	2.04	0.57
1:2:360:A:OP1	15:N:131:ARG:NH2	2.37	0.57
1:2:434:A:C5	20:V:85:TYR:CD1	2.92	0.57
1:2:509:C:OP2	15:N:33:ARG:NH2	2.37	0.57
35:8:125:ILE:O	35:8:133:GLN:HA	2.03	0.57
1:2:12:U:H2'	1:2:13:C:C6	2.40	0.57
1:2:110:C:H4'	1:2:588:C:O2	2.04	0.57
1:2:872:A:C6	1:2:873:A:C6	2.92	0.57
1:2:1448:A:C8	33:6:56:ARG:NH2	2.70	0.57
1:2:531:G:C4	1:2:718:G:N2	2.73	0.57
1:2:553:C:C2	1:2:593:G:C2	2.93	0.57
1:2:616:G:C2	1:2:698:A:C6	2.93	0.57
1:2:975:A:C2'	1:2:976:A:H5'	2.33	0.57
1:2:1451:C:C4'	31:1:78:GLN:HB2	2.33	0.57
9:U:62:VAL:HG22	9:U:68:VAL:CG1	2.34	0.57
34:7:188:LYS:CD	35:8:131:GLY:HA3	2.34	0.57
34:7:260:ARG:HA	34:7:268:SER:O	2.05	0.57
1:2:142:G:H4'	25:G:5:LYS:HG2	1.87	0.57
1:2:199:A:N6	1:2:217:C:H4'	2.19	0.57
1:2:297:G:C2	1:2:298:C:C2	2.92	0.57
1:2:1050:G:O4'	1:2:1127:A:N1	2.37	0.57
12:H:21:TRP:CD1	12:H:119:PRO:HD2	2.40	0.57
32:4:53:G:O2'	32:4:54:G:H8	1.77	0.57
37:4:101:MET:CG	34:7:51:TYR:CD1	2.88	0.57
36:9:95:LEU:HD22	36:9:235:ASN:OD1	2.04	0.57
1:2:229:G:C4	1:2:230:C:C5	2.93	0.57
1:2:1195:U:OP2	12:H:78:HIS:HA	2.05	0.57
1:2:1360:C:C4'	30:5:821:G:C6	2.88	0.57
1:2:1399:G:C6	1:2:1417:A:N6	2.72	0.57
1:2:1403:U:C3'	1:2:1404:C:H5'	2.34	0.57
18:A:43:VAL:HG23	18:A:46:ARG:HB2	1.86	0.57
32:4:23:G:O2'	32:4:24:C:H5'	2.04	0.57
34:7:187:HIS:C	35:8:130:CYS:O	2.42	0.57
1:2:462:A:O2'	1:2:463:G:O4'	2.20	0.57
1:2:1142:G:O5'	1:2:1142:G:C8	2.57	0.57
20:V:33:ARG:O	20:V:53:ILE:HG21	2.05	0.57
1:2:586:C:O2'	1:2:587:G:C2	2.58	0.57
1:2:1027:C:O5'	19:B:102:THR:OG1	1.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1347:U:O5'	1:2:1347:U:H6	1.88	0.57
1:2:1414:G:H4'	25:G:84:VAL:HG11	1.86	0.57
12:H:87:ARG:HG3	12:H:90:HIS:CA	2.34	0.57
34:7:74:CYS:C	34:7:76:SER:H	2.09	0.57
34:7:358:MET:H	34:7:405:TRP:HZ3	1.51	0.57
36:9:15:LEU:HD11	36:9:31:LEU:HD22	1.86	0.57
36:9:90:ARG:O	36:9:94:ASN:HB2	2.05	0.57
36:9:179:MET:HG3	36:9:239:ALA:CB	2.34	0.57
1:2:99:C:O2'	1:2:100:A:OP2	2.19	0.57
1:2:394:C:C2	1:2:395:C:C5	2.93	0.57
1:2:607:U:H4'	26:I:57:ARG:NE	2.19	0.57
31:1:35:ARG:NH2	32:4:38:A:C4	2.68	0.57
37:4:101:MET:HG3	34:7:51:TYR:CD1	2.40	0.57
1:2:150:G:H2'	1:2:151:G:C8	2.40	0.56
1:2:879:U:O3'	24:F:73:ARG:NH2	2.38	0.56
1:2:1332:C:O2	12:H:96:LYS:HG3	2.05	0.56
12:H:87:ARG:CA	12:H:88:ARG:HD3	2.35	0.56
34:7:249:VAL:HG12	34:7:250:ASP:OD2	2.06	0.56
1:2:10:G:N7	1:2:1356:A:C6	2.73	0.56
1:2:441:U:O4	1:2:442:C:N4	2.38	0.56
1:2:555:U:H3	1:2:590:G:H1	1.53	0.56
1:2:607:U:C4'	26:I:57:ARG:HE	2.18	0.56
1:2:1055:C:H4'	19:B:97:LEU:HD11	1.86	0.56
1:2:1269:G:C6	1:2:1270:C:C4	2.93	0.56
1:2:1329:C:H2'	1:2:1330:G:C8	2.40	0.56
1:2:1424:G:O5'	1:2:1424:G:H8	1.88	0.56
1:2:1486:A:H5'	1:2:1487:U:OP2	2.06	0.56
18:A:18:TRP:CZ2	18:A:36:PRO:HB3	2.40	0.56
22:D:59:LEU:HD11	24:F:132:GLU:CG	2.34	0.56
32:4:43:G:C4	32:4:44:A:C8	2.93	0.56
37:4:101:MET:HE2	34:7:219:ARG:NH1	2.18	0.56
34:7:190:ASN:CG	35:8:14:LEU:HB2	2.26	0.56
34:7:194:LEU:O	34:7:198:ILE:HG23	2.06	0.56
34:7:324:PRO:O	34:7:387:ALA:HA	2.04	0.56
34:7:331:ILE:HG22	34:7:332:LYS:O	2.05	0.56
1:2:29:G:H1'	15:N:135:LYS:HZ3	1.70	0.56
1:2:93:A:O2'	23:E:5:GLY:HA3	2.05	0.56
1:2:1040:A:C2'	1:2:1041:C:H5'	2.35	0.56
1:2:1299:A:C1'	32:4:42:C:O4'	2.53	0.56
4:L:54:ASP:HB3	4:L:56:GLU:HB2	1.87	0.56
1:2:297:G:C6	1:2:298:C:C4	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:303:G:C8	1:2:304:C:C5	2.92	0.56
1:2:439:G:H4'	1:2:440:C:O5'	2.05	0.56
1:2:885:G:C2	1:2:1351:U:C2	2.93	0.56
1:2:1265:G:HO2'	1:2:1266:A:H8	1.52	0.56
1:2:1360:C:C4	32:4:35:C:C6	2.94	0.56
1:2:1451:C:C5'	31:1:78:GLN:CB	2.83	0.56
24:F:5:TRP:HB3	24:F:57:VAL:CG2	2.35	0.56
1:2:41:C:C2	1:2:392:G:C2	2.94	0.56
1:2:151:G:HO2'	25:G:64:ARG:HB3	1.71	0.56
1:2:236:C:H2'	1:2:237:C:H6	1.71	0.56
1:2:615:G:C6	1:2:698:A:N1	2.73	0.56
1:2:1264:G:C6	1:2:1265:G:C2	2.94	0.56
1:2:1424:G:C5	1:2:1425:C:C5	2.93	0.56
23:E:45:LEU:CD1	23:E:83:PHE:HB3	2.36	0.56
34:7:55:ASN:HD21	34:7:88:ARG:HH21	1.53	0.56
35:8:6:GLU:O	35:8:9:GLU:HB3	2.04	0.56
1:2:38:G:C6	1:2:39:U:C5	2.93	0.56
1:2:732:G:C6	1:2:733:C:C4	2.94	0.56
1:2:1385:U:H2'	1:2:1386:C:C6	2.41	0.56
26:I:32:LYS:O	26:I:36:GLU:N	2.30	0.56
32:4:42:C:C2'	32:4:43:G:C5'	2.84	0.56
35:8:76:ASP:HB2	35:8:80:GLU:H	1.69	0.56
1:2:6:G:C6	1:2:7:G:C5	2.94	0.56
1:2:60:A:N6	1:2:85:A:N6	2.54	0.56
1:2:583:G:C6	1:2:584:C:C4	2.94	0.56
1:2:1013:G:C6	1:2:1014:C:N3	2.74	0.56
1:2:1382:G:C2	1:2:1434:C:N3	2.74	0.56
1:2:1412:A:HO2'	25:G:92:PRO:HG3	1.70	0.56
27:J:34:ASN:C	27:J:34:ASN:HD22	2.09	0.56
32:4:15:G:N2	32:4:49:C:H42	1.99	0.56
1:2:460:C:C5'	1:2:461:A:H5"	2.34	0.56
1:2:884:G:C2	1:2:1460:G:C5	2.93	0.56
34:7:33:TRP:NE1	34:7:36:LYS:HD2	2.20	0.56
1:2:372:G:C6	1:2:373:C:C4	2.94	0.56
1:2:610:G:N2	1:2:705:C:C2	2.74	0.56
1:2:1053:A:C8	19:B:125:GLN:NE2	2.40	0.56
1:2:1352:G:C2	1:2:1353:C:C4	2.94	0.56
1:2:1403:U:N3	25:G:77:ASP:CG	2.59	0.56
18:A:123:ALA:HA	18:A:183:ALA:HA	1.88	0.56
32:4:28:U:O2'	32:4:29:C:H5'	2.06	0.56
35:8:109:CYS:C	35:8:110:LYS:CG	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:452:G:H2'	1:2:453:G:C8	2.40	0.55
32:4:38:A:H3'	32:4:39:A:H8	1.70	0.55
36:9:43:TRP:C	36:9:45:GLU:H	2.09	0.55
1:2:236:C:H2'	1:2:237:C:C6	2.42	0.55
1:2:459:G:C5	1:2:460:C:C6	2.94	0.55
1:2:505:U:H5"	15:N:108:ILE:HD12	1.88	0.55
1:2:533:C:N4	1:2:534:G:N1	2.55	0.55
1:2:549:A:C2	1:2:550:G:C8	2.93	0.55
1:2:607:U:OP1	26:I:57:ARG:HG2	2.07	0.55
1:2:642:G:N2	1:2:643:G:H1'	2.21	0.55
1:2:1061:A:OP2	2:Z:154:VAL:HG22	2.06	0.55
1:2:1096:G:N2	9:U:1:MET:HA	2.20	0.55
28:C:38:UNK:HA	28:C:43:UNK:CB	2.36	0.55
34:7:189:ILE:O	35:8:14:LEU:HD11	2.06	0.55
1:2:234:G:H5'	17:R:55:PHE:CZ	2.41	0.55
1:2:537:G:C6	1:2:538:C:C4	2.94	0.55
1:2:1372:C:H2'	1:2:1373:A:C8	2.41	0.55
1:2:1414:G:H21	25:G:79:HIS:HB3	1.71	0.55
12:H:43:LEU:HD11	13:K:43:PHE:CB	2.37	0.55
31:1:40:MET:HG2	31:1:78:GLN:CA	2.32	0.55
36:9:199:VAL:HG12	36:9:253:ILE:HG22	1.87	0.55
1:2:324:C:H4'	1:2:325:A:O5'	2.06	0.55
1:2:647:G:O6	1:2:742:U:H5'	2.06	0.55
1:2:680:C:H2'	1:2:681:G:O4'	2.07	0.55
1:2:839:G:C6	1:2:840:C:C4	2.93	0.55
1:2:1275:U:C4	1:2:1276:G:C6	2.94	0.55
24:F:131:TRP:NE1	26:I:97:PHE:CE2	2.75	0.55
36:9:221:THR:OG1	36:9:223:GLY:O	2.24	0.55
1:2:616:G:N1	1:2:697:A:C2	2.74	0.55
1:2:649:A:C2	1:2:650:A:C4	2.94	0.55
1:2:1070:C:H2'	1:2:1071:C:C6	2.42	0.55
1:2:1317:G:C5	1:2:1318:U:C4	2.95	0.55
1:2:1320:A:H8	1:2:1320:A:OP1	1.88	0.55
1:2:1348:C:C4	1:2:1349:C:N4	2.74	0.55
34:7:274:THR:OG1	34:7:301:LEU:HD23	2.06	0.55
35:8:100:LEU:HA	35:8:104:VAL:CG1	2.37	0.55
1:2:291:G:H2'	1:2:292:U:O4'	2.07	0.55
1:2:1009:G:H5'	2:Z:134:GLY:HA2	1.87	0.55
1:2:1031:G:N2	1:2:1032:A:C2	2.75	0.55
1:2:1395:G:C5'	25:G:87:LEU:HD13	2.37	0.55
34:7:187:HIS:HB3	35:8:129:ALA:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1299:A:O2'	32:4:42:C:O4'	2.21	0.55
24:F:34:ILE:HB	24:F:53:LEU:HG	1.88	0.55
34:7:189:ILE:CB	35:8:14:LEU:HG	2.36	0.55
1:2:26:A:H2'	1:2:27:C:O4'	2.07	0.55
1:2:426:C:C2	1:2:445:G:C2	2.95	0.55
34:7:273:PHE:O	36:9:190:PRO:HA	2.07	0.55
36:9:95:LEU:CG	36:9:237:LYS:HG3	2.37	0.55
36:9:204:LEU:HD23	36:9:207:ILE:HG21	1.89	0.55
1:2:672:G:C8	14:M:123:HIS:HA	2.42	0.55
1:2:1219:C:C2	1:2:1237:G:N2	2.75	0.55
1:2:1443:G:N1	1:2:1444:G:C6	2.75	0.55
12:H:89:GLU:N	12:H:94:ASN:HB3	2.22	0.55
34:7:74:CYS:O	34:7:76:SER:N	2.39	0.55
34:7:215:MET:HG2	34:7:216:LEU:N	2.21	0.55
34:7:296:ALA:O	34:7:297:ILE:HD13	2.07	0.55
1:2:513:A:H2'	24:F:188:PHE:CE1	2.42	0.55
36:9:94:ASN:OD1	36:9:236:PRO:HG3	2.05	0.55
36:9:111:SER:HA	36:9:160:TRP:CZ3	2.40	0.55
1:2:607:U:H4'	26:I:57:ARG:CZ	2.37	0.54
1:2:813:G:C6	1:2:814:C:C4	2.95	0.54
1:2:955:G:H2'	1:2:956:C:O4'	2.07	0.54
1:2:1299:A:O4'	32:4:42:C:C4'	2.54	0.54
1:2:1311:C:H1'	12:H:96:LYS:HG2	1.89	0.54
1:2:1382:G:C2	1:2:1434:C:C2	2.95	0.54
1:2:1424:G:C6	1:2:1425:C:N3	2.75	0.54
26:I:7:LEU:O	26:I:10:ALA:HB3	2.08	0.54
32:4:68:C:O2	32:4:68:C:H2'	2.05	0.54
35:8:28:GLN:O	35:8:28:GLN:HG2	2.07	0.54
1:2:55:G:H5'	1:2:384:G:OP1	2.08	0.54
1:2:87:C:H2'	1:2:88:G:H5'	1.89	0.54
1:2:891:A:H4'	1:2:892:C:OP1	2.06	0.54
1:2:1041:C:OP1	10:X:71:ARG:HD3	2.05	0.54
7:S:44:LYS:O	7:S:48:ASN:ND2	2.40	0.54
16:Q:126:GLU:O	16:Q:129:ILE:HB	2.07	0.54
1:2:1131:G:C6	1:2:1132:C:N4	2.75	0.54
1:2:1249:A:OP1	12:H:82:ALA:HB3	2.08	0.54
1:2:1344:U:C2	1:2:1345:G:N7	2.75	0.54
19:B:169:TRP:CE2	19:B:192:VAL:HG22	2.43	0.54
1:2:1342:C:C3'	1:2:1343:C:P	2.94	0.54
31:1:34:ARG:CB	31:1:40:MET:HG3	2.37	0.54
34:7:8:PRO:HD2	34:7:281:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:8:53:ARG:NE	35:8:53:ARG:HA	2.23	0.54
1:2:607:U:C4’	26:I:57:ARG:HH21	2.19	0.54
1:2:629:U:H2’	1:2:630:A:C8	2.43	0.54
1:2:1053:A:C1’	19:B:98:PRO:HG2	2.21	0.54
1:2:1343:C:C5	1:2:1344:U:C5	2.95	0.54
4:L:61:PHE:HB2	13:K:119:PRO:HB3	1.90	0.54
12:H:78:HIS:HB2	12:H:88:ARG:HG3	1.89	0.54
32:4:8:U:H1’	32:4:49:C:O2	2.07	0.54
34:7:390:SER:N	34:7:393:ILE:HD11	2.21	0.54
35:8:40:ASN:HA	35:8:86:LYS:HB2	1.89	0.54
36:9:2:ILE:HG23	36:9:122:TRP:CH2	2.43	0.54
36:9:252:LYS:O	36:9:256:GLU:N	2.41	0.54
1:2:1048:G:O2’	1:2:1130:A:O2’	2.22	0.54
1:2:1290:U:O4	1:2:1291:G:N2	2.40	0.54
1:2:1347:U:H2’	1:2:1348:C:H5’	1.87	0.54
20:V:56:ILE:HA	20:V:66:LYS:O	2.08	0.54
26:I:86:PHE:O	26:I:90:GLU:N	2.40	0.54
31:1:25:GLN:OE1	31:1:51:ILE:HD13	2.06	0.54
34:7:106:SER:OG	34:7:363:SER:O	2.12	0.54
1:2:8:U:OP1	1:2:9:U:H5	1.91	0.54
19:B:60:ALA:HA	19:B:179:ARG:HE	1.72	0.54
30:5:812:G:C8	30:5:813:A:C8	2.95	0.54
32:4:3:C:H2’	32:4:4:G:H5’	1.90	0.54
1:2:616:G:C2	1:2:698:A:C5	2.96	0.54
1:2:1033:G:OP1	24:F:102:HIS:NE2	2.40	0.54
19:B:33:TYR:HB2	19:B:44:ASP:N	2.23	0.54
24:F:86:LEU:HD21	24:F:195:VAL:HA	1.90	0.54
36:9:64:VAL:HG12	36:9:65:ILE:H	1.72	0.54
36:9:98:LYS:HZ3	36:9:235:ASN:CG	1.96	0.54
1:2:331:C:H4’	1:2:1393:A:O2’	2.07	0.54
1:2:787:U:C2	1:2:788:C:C5	2.96	0.54
12:H:71:ILE:HG23	12:H:180:PHE:CZ	2.43	0.54
35:8:9:GLU:O	35:8:12:ASP:HB2	2.08	0.54
1:2:378:A:H2’	1:2:379:A:C8	2.43	0.54
1:2:1024:G:H2’	1:2:1025:U:C6	2.43	0.54
1:2:1290:U:C4	1:2:1291:G:C2	2.96	0.54
1:2:1341:C:H2’	1:2:1342:C:H6	1.71	0.54
32:4:28:U:H2’	32:4:29:C:C6	2.34	0.54
34:7:21:GLY:O	34:7:117:VAL:HG11	2.08	0.54
35:8:76:ASP:CB	35:8:80:GLU:H	2.21	0.54
36:9:180:SER:HB2	36:9:228:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:262:G:C8	1:2:262:G:H5”	2.44	0.53
1:2:1311:C:C4’	12:H:95:SER:HA	2.37	0.53
1:2:1312:C:H5”	12:H:80:LYS:HB3	1.90	0.53
1:2:1443:G:H2’	1:2:1444:G:H8	1.71	0.53
31:1:38:LYS:HE3	31:1:38:LYS:CA	2.32	0.53
1:2:1307:G:C2	12:H:48:HIS:CE1	2.96	0.53
1:2:1360:C:N4	32:4:35:C:C6	2.76	0.53
1:2:1385:U:H2’	1:2:1386:C:H6	1.73	0.53
24:F:50:ILE:HD12	24:F:118:LYS:HB3	1.89	0.53
1:2:5:C:O2’	1:2:459:G:O3’	2.26	0.53
1:2:650:A:C2	1:2:740:G:H1’	2.44	0.53
1:2:709:G:OP2	16:Q:131:ARG:NE	2.41	0.53
1:2:1053:A:OP1	19:B:95:ARG:CG	2.56	0.53
31:1:40:MET:HG2	31:1:77:LEU:C	2.26	0.53
35:8:105:GLU:HG3	35:8:110:LYS:HA	1.89	0.53
1:2:431:U:C4’	20:V:33:ARG:HH21	2.21	0.53
1:2:539:C:OP1	15:N:10:GLU:N	2.40	0.53
1:2:642:G:O6	1:2:654:U:C4	2.62	0.53
1:2:988:A:O2’	1:2:989:C:H5’	2.08	0.53
1:2:1131:G:N2	1:2:1132:C:C2	2.76	0.53
1:2:1424:G:C4	1:2:1425:C:C6	2.95	0.53
15:N:43:PRO:O	15:N:45:GLU:N	2.40	0.53
17:R:60:TYR:O	17:R:61:GLU:HB2	2.08	0.53
32:4:23:G:C2’	32:4:24:C:H5’	2.38	0.53
1:2:95:G:H5’	23:E:9:HIS:ND1	2.24	0.53
1:2:642:G:C2	1:2:643:G:H1’	2.43	0.53
1:2:872:A:C6	1:2:873:A:C5	2.97	0.53
1:2:1351:U:H2’	1:2:1352:G:H8	1.73	0.53
1:2:1403:U:C2	1:2:1404:C:C6	2.97	0.53
12:H:72:MET:HE2	12:H:97:LYS:N	2.23	0.53
1:2:324:C:HO2’	1:2:325:A:P	2.31	0.53
1:2:607:U:C5’	26:I:57:ARG:HE	2.22	0.53
1:2:754:G:N2	1:2:755:U:O4	2.41	0.53
1:2:1338:C:C2	10:X:23:ASP:HA	2.44	0.53
1:2:1452:G:P	31:1:78:GLN:OE1	2.65	0.53
25:G:75:ARG:O	25:G:78:ILE:HG13	2.08	0.53
34:7:87:ARG:NH1	34:7:199:GLU:OE2	2.42	0.53
1:2:100:A:H2’	1:2:101:G:O4’	2.09	0.53
1:2:193:G:H2’	1:2:194:C:C6	2.44	0.53
1:2:640:U:HO2’	1:2:641:A:H8	1.57	0.53
1:2:868:C:H4’	1:2:1373:A:O2’	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:101:TYR:CD2	12:H:101:TYR:C	2.82	0.53
24:F:166:VAL:O	24:F:185:SER:HB3	2.08	0.53
1:2:462:A:N6	22:D:18:TRP:CE2	2.76	0.53
25:G:103:ARG:HE	25:G:105:LYS:HE2	1.74	0.53
34:7:307:LYS:HG3	34:7:308:ALA:H	1.73	0.53
35:8:119:GLU:O	35:8:120:LYS:C	2.44	0.53
1:2:492:G:C6	1:2:493:C:C4	2.96	0.53
1:2:531:G:C6	1:2:532:C:C4	2.97	0.53
1:2:855:C:O2	1:2:861:G:C2	2.62	0.53
1:2:872:A:C4	1:2:873:A:N7	2.77	0.53
1:2:906:G:C6	1:2:907:C:C4	2.97	0.53
1:2:1193:G:H2'	1:2:1194:C:C6	2.44	0.53
1:2:1206:G:O2'	9:U:9:GLY:O	2.27	0.53
1:2:1402:C:N4	1:2:1413:G:H22	2.05	0.53
36:9:86:THR:HG22	36:9:88:ASP:H	1.74	0.53
1:2:31:U:H2'	1:2:32:A:O4'	2.08	0.53
1:2:459:G:O6	1:2:460:C:C4	2.62	0.53
1:2:462:A:H5"	22:D:20:LYS:HE2	1.91	0.53
1:2:1144:G:C6	1:2:1145:C:C4	2.97	0.53
1:2:1313:G:H5'	12:H:81:VAL:CG2	2.37	0.53
1:2:1448:A:H2'	33:6:56:ARG:NH2	2.24	0.53
1:2:1487:U:H2'	1:2:1488:C:H6	1.65	0.53
34:7:103:THR:O	34:7:106:SER:HB3	2.10	0.53
36:9:184:THR:O	36:9:261:ILE:HA	2.08	0.53
1:2:458:G:C2	1:2:479:C:O2	2.63	0.52
10:X:7:TYR:CE2	10:X:31:ILE:HG12	2.44	0.52
18:A:127:ARG:HG3	18:A:128:ARG:HG3	1.91	0.52
23:E:126:ARG:NH1	23:E:127:ILE:O	2.42	0.52
1:2:48:G:C6	1:2:49:C:C4	2.97	0.52
12:H:94:ASN:O	12:H:95:SER:OG	2.27	0.52
15:N:63:LYS:HB2	15:N:118:ASP:O	2.08	0.52
34:7:277:SER:N	34:7:298:GLY:O	2.42	0.52
1:2:900:G:N2	1:2:1303:C:C2	2.77	0.52
1:2:1298:G:N2	32:4:43:G:C1'	2.72	0.52
1:2:1448:A:C6	33:6:51:ILE:CD1	2.91	0.52
1:2:1475:C:H2'	1:2:1476:C:C6	2.44	0.52
34:7:33:TRP:HZ2	34:7:36:LYS:HZ2	1.57	0.52
36:9:157:PRO:O	36:9:159:ILE:N	2.33	0.52
1:2:725:C:C2	1:2:763:G:C2	2.97	0.52
4:L:90:VAL:HG11	4:L:96:ILE:HD11	1.91	0.52
9:U:8:PRO:HD2	9:U:140:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:179:SER:O	12:H:183:ALA:N	2.37	0.52
13:K:52:ALA:HB2	13:K:95:LEU:HD11	1.91	0.52
1:2:166:A:C2	1:2:197:A:C8	2.98	0.52
1:2:434:A:N1	20:V:83:PRO:HB3	2.24	0.52
1:2:677:U:C2	1:2:1493:C:H1'	2.45	0.52
1:2:821:G:N2	1:2:824:G:OP2	2.34	0.52
4:L:54:ASP:HB3	4:L:56:GLU:CB	2.38	0.52
31:1:33:LYS:CG	32:4:27:G:H5'	2.35	0.52
31:1:33:LYS:N	32:4:27:G:OP1	2.43	0.52
34:7:95:PRO:HG2	34:7:100:LEU:HB3	1.90	0.52
1:2:95:G:H4'	23:E:9:HIS:CD2	2.45	0.52
1:2:573:C:H4'	22:D:142:TYR:CE1	2.44	0.52
1:2:952:A:H2'	1:2:953:C:H5'	1.92	0.52
1:2:1311:C:H4'	12:H:94:ASN:O	2.09	0.52
1:2:1333:G:N7	12:H:48:HIS:CE1	2.78	0.52
1:2:1344:U:N3	1:2:1345:G:C6	2.78	0.52
1:2:1388:G:H2'	1:2:1389:G:O4'	2.10	0.52
12:H:96:LYS:HE3	12:H:96:LYS:HA	1.91	0.52
24:F:13:LEU:O	24:F:13:LEU:HD12	2.09	0.52
24:F:34:ILE:HA	24:F:37:ILE:HD12	1.91	0.52
34:7:24:THR:HA	34:7:33:TRP:HZ3	1.74	0.52
35:8:76:ASP:HB2	35:8:80:GLU:CB	2.38	0.52
1:2:143:G:H4'	25:G:117:VAL:HG11	1.92	0.52
1:2:213:C:C5	1:2:214:C:C5	2.97	0.52
1:2:392:G:O2'	1:2:394:C:OP1	2.20	0.52
1:2:1253:G:C6	1:2:1254:C:C4	2.98	0.52
1:2:1414:G:OP1	25:G:86:VAL:HG11	2.07	0.52
1:2:1415:U:H2'	1:2:1416:C:C6	2.45	0.52
1:2:1463:A:OP2	14:M:133:ARG:NH1	2.42	0.52
24:F:167:ILE:HG21	24:F:175:LEU:HD12	1.91	0.52
32:4:42:C:O2'	32:4:43:G:C5'	2.45	0.52
1:2:182:A:H2'	1:2:183:A:C8	2.44	0.52
1:2:999:G:O2'	1:2:1176:C:OP1	2.27	0.52
32:4:26:C:O5'	32:4:26:C:H6	1.93	0.52
1:2:60:A:H61	1:2:85:A:N6	2.06	0.52
1:2:229:G:C6	1:2:230:C:N4	2.77	0.52
1:2:359:A:H2'	1:2:360:A:C8	2.45	0.52
1:2:1156:A:C8	2:Z:140:ARG:NH1	2.78	0.52
1:2:1479:C:H5"	14:M:127:ARG:HH22	1.75	0.52
12:H:87:ARG:C	12:H:88:ARG:CD	2.78	0.52
34:7:323:VAL:HG13	34:7:389:TRP:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:217:ILE:HG12	36:9:231:VAL:HG22	1.92	0.52
1:2:642:G:N1	1:2:654:U:C2	2.78	0.52
1:2:1131:G:C4	1:2:1132:C:C5	2.98	0.52
1:2:1453:U:H6	1:2:1453:U:O5'	1.93	0.52
19:B:96:PHE:CE2	19:B:100:THR:HB	2.44	0.52
22:D:39:LYS:HA	22:D:42:TRP:CE3	2.45	0.52
31:1:27:ILE:HG23	31:1:44:GLU:O	2.09	0.52
34:7:177:ASN:O	34:7:177:ASN:ND2	2.42	0.52
34:7:188:LYS:HD2	35:8:131:GLY:CA	2.40	0.52
35:8:67:LYS:NZ	35:8:139:LEU:HD23	2.25	0.52
1:2:459:G:N3	1:2:460:C:O4'	2.43	0.51
1:2:920:U:O4	1:2:1161:A:N1	2.43	0.51
1:2:1006:C:O2	1:2:1006:C:O4'	2.28	0.51
1:2:1367:C:C2'	31:1:65:ALA:HB3	2.35	0.51
1:2:1414:G:H5"	25:G:84:VAL:HG11	1.92	0.51
1:2:1486:A:H3'	1:2:1487:U:C5	2.45	0.51
12:H:67:LEU:O	12:H:71:ILE:HG12	2.09	0.51
25:G:52:GLY:CA	25:G:54:GLU:HB2	2.41	0.51
36:9:247:ILE:HA	36:9:250:LEU:HD12	1.92	0.51
1:2:1352:G:N1	1:2:1353:C:C4	2.78	0.51
1:2:1363:C:O5'	1:2:1363:C:H6	1.93	0.51
1:2:1453:U:C6	1:2:1453:U:O5'	2.63	0.51
20:V:60:PHE:N	20:V:60:PHE:CD1	2.78	0.51
32:4:27:G:C2'	32:4:28:U:H5'	2.40	0.51
34:7:124:PHE:CE1	34:7:166:ILE:HG12	2.45	0.51
1:2:740:G:C2	1:2:751:C:C2	2.98	0.51
1:2:1367:C:C1'	31:1:65:ALA:HB3	2.23	0.51
1:2:1390:G:C2	1:2:1426:C:C2	2.98	0.51
1:2:599:G:C5	1:2:600:C:C5	2.99	0.51
12:H:26:VAL:HG21	12:H:120:ILE:HG23	1.92	0.51
12:H:71:ILE:HD12	12:H:180:PHE:CE1	2.46	0.51
32:4:36:A:C2'	32:4:37:U:H5'	2.39	0.51
34:7:148:GLN:HB3	34:7:182:PRO:HA	1.93	0.51
36:9:21:GLN:O	36:9:27:SER:OG	2.19	0.51
1:2:531:G:C2	1:2:532:C:C2	2.99	0.51
1:2:612:C:H2'	1:2:613:C:C6	2.45	0.51
1:2:784:G:OP1	19:B:25:THR:HA	2.09	0.51
1:2:964:A:N6	1:2:989:C:H4'	2.26	0.51
1:2:1120:G:C6	1:2:1121:C:C4	2.98	0.51
1:2:1298:G:H2'	1:2:1299:A:C8	2.45	0.51
1:2:1313:G:P	12:H:81:VAL:HG23	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1483:U:HO2'	1:2:1484:C:H3'	1.76	0.51
1:2:93:A:O2'	1:2:322:G:N2	2.44	0.51
1:2:431:U:C2'	1:2:432:G:OP1	2.59	0.51
1:2:458:G:N2	1:2:479:C:O2	2.43	0.51
1:2:603:G:C6	1:2:604:C:C4	2.99	0.51
1:2:875:G:H2'	1:2:876:A:C8	2.46	0.51
1:2:1131:G:C2	1:2:1132:C:C4	2.98	0.51
30:5:822:C:O2	30:5:822:C:H2'	2.09	0.51
34:7:355:GLU:OE2	34:7:399:ARG:NE	2.43	0.51
1:2:181:G:H2'	1:2:182:A:C8	2.45	0.51
1:2:525:A:C2	1:2:822:A:C6	2.99	0.51
1:2:910:G:C6	1:2:911:C:C4	2.99	0.51
1:2:1013:G:H1	1:2:1155:U:H3	1.58	0.51
1:2:1311:C:H4'	12:H:95:SER:N	2.26	0.51
1:2:1335:A:C6	1:2:1336:U:C2	2.98	0.51
1:2:1349:C:H6	1:2:1349:C:O5'	1.93	0.51
9:U:39:ARG:HA	9:U:39:ARG:HE	1.76	0.51
12:H:93:LEU:C	12:H:95:SER:N	2.64	0.51
12:H:93:LEU:HG	12:H:96:LYS:O	2.11	0.51
24:F:1:MET:CB	24:F:57:VAL:HG22	2.41	0.51
32:4:5:G:O2'	32:4:6:G:H5'	2.10	0.51
1:2:94:C:OP1	23:E:5:GLY:N	2.37	0.51
1:2:621:G:C6	1:2:622:C:C4	2.99	0.51
1:2:874:G:C2	1:2:875:G:C5	2.99	0.51
1:2:879:U:H4'	24:F:73:ARG:NE	2.24	0.51
1:2:1028:C:C2	1:2:1034:G:N2	2.79	0.51
3:3:39:THR:HG23	3:3:100:ALA:HB2	1.93	0.51
8:T:83:VAL:HB	8:T:107:ALA:HB2	1.93	0.51
12:H:71:ILE:HD12	12:H:180:PHE:HE1	1.75	0.51
12:H:89:GLU:HB2	12:H:95:SER:HB2	1.93	0.51
12:H:111:ILE:HD11	12:H:122:VAL:HG11	1.93	0.51
18:A:135:ARG:HA	18:A:138:ARG:HG3	1.93	0.51
34:7:64:LYS:HG2	34:7:67:ALA:HB3	1.92	0.51
35:8:127:CYS:CB	35:8:130:CYS:HG	2.23	0.51
1:2:276:A:H4'	15:N:14:ARG:CZ	2.41	0.51
1:2:526:A:O2'	1:2:527:A:O4'	2.15	0.51
1:2:869:U:O5'	1:2:869:U:H6	1.93	0.51
1:2:1026:A:O5'	19:B:103:ASN:OD1	2.28	0.51
1:2:1360:C:C5	32:4:35:C:C6	2.99	0.51
16:Q:3:ARG:O	16:Q:7:ARG:NH2	2.42	0.51
25:G:78:ILE:HG22	25:G:109:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:269:TYR:CZ	34:7:384:ARG:HG3	2.46	0.51
34:7:406:ARG:HH11	34:7:406:ARG:HG3	1.75	0.51
1:2:142:G:O6	1:2:150:G:C6	2.64	0.51
1:2:203:A:C2	1:2:204:G:C5	2.99	0.51
1:2:256:G:OP1	27:J:56:ARG:NH1	2.42	0.51
1:2:524:U:H5"	1:2:773:A:C5	2.46	0.51
1:2:884:G:N2	1:2:1460:G:C8	2.79	0.51
1:2:1058:G:C6	1:2:1059:C:C4	2.98	0.51
1:2:1118:C:C5	1:2:1120:G:C8	2.99	0.51
1:2:1311:C:H4'	12:H:95:SER:CA	2.41	0.51
12:H:90:HIS:HB3	12:H:92:SER:H	1.76	0.51
32:4:76:C:O2	32:4:76:C:H2'	2.09	0.51
1:2:140:C:C2	1:2:152:G:N2	2.79	0.50
1:2:461:A:OP1	22:D:16:HIS:NE2	2.44	0.50
1:2:742:U:C5	1:2:743:U:C4	2.99	0.50
1:2:845:G:O2'	1:2:1444:G:OP1	2.29	0.50
1:2:898:G:N1	1:2:899:G:C6	2.79	0.50
1:2:1009:G:C5'	2:Z:134:GLY:HA2	2.40	0.50
1:2:1327:C:OP1	13:K:119:PRO:O	2.29	0.50
12:H:44:LEU:HD11	13:K:40:ILE:HG22	1.93	0.50
32:4:23:G:C6	32:4:24:C:C4	2.99	0.50
36:9:2:ILE:HB	36:9:32:ASP:O	2.10	0.50
36:9:95:LEU:HD11	36:9:237:LYS:CB	2.41	0.50
1:2:271:G:C4	1:2:272:C:C5	2.99	0.50
1:2:988:A:C2'	1:2:989:C:H5'	2.41	0.50
30:5:812:G:H2'	30:5:813:A:O4'	2.10	0.50
34:7:160:LEU:O	34:7:164:ARG:HG2	2.11	0.50
34:7:187:HIS:CE1	35:8:130:CYS:HB2	2.45	0.50
34:7:358:MET:N	34:7:405:TRP:HZ3	2.10	0.50
36:9:184:THR:HG23	36:9:225:PRO:HB2	1.93	0.50
36:9:187:THR:HG22	36:9:189:GLU:HG2	1.92	0.50
1:2:61:A:N6	1:2:377:A:C2	2.78	0.50
1:2:553:C:C2	1:2:593:G:N2	2.79	0.50
1:2:649:A:H2'	1:2:650:A:C8	2.47	0.50
1:2:723:G:N2	1:2:724:C:C2	2.80	0.50
1:2:771:G:C4	1:2:773:A:O4'	2.64	0.50
1:2:947:G:HO2'	1:2:976:A:N6	2.08	0.50
1:2:1260:G:O2'	1:2:1263:C:N4	2.45	0.50
9:U:21:LYS:HG2	9:U:52:TYR:CE1	2.47	0.50
12:H:70:LYS:NZ	12:H:159:ASP:OD1	2.27	0.50
20:V:60:PHE:N	20:V:60:PHE:HD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:I:52:PHE:HA	26:I:60:VAL:O	2.10	0.50
34:7:373:VAL:HA	34:7:378:ILE:HG22	1.93	0.50
35:8:96:MET:O	35:8:99:PHE:HB3	2.11	0.50
36:9:140:ILE:O	36:9:144:VAL:HG22	2.11	0.50
36:9:178:LYS:HG3	36:9:232:VAL:HG12	1.93	0.50
36:9:254:GLY:HA3	36:9:261:ILE:HD12	1.93	0.50
1:2:168:G:C2	1:2:195:C:C2	3.00	0.50
1:2:368:C:H4'	1:2:369:A:O5'	2.11	0.50
1:2:551:U:H2'	1:2:552:C:C6	2.46	0.50
1:2:1346:C:O2'	1:2:1347:U:C5'	2.59	0.50
1:2:1403:U:H2'	1:2:1404:C:H5'	1.93	0.50
1:2:1441:G:H2'	1:2:1442:G:O4'	2.10	0.50
12:H:145:ARG:HH21	30:5:816:U:H1'	1.77	0.50
31:1:80:ASP:OD1	31:1:82:ARG:HD3	2.12	0.50
1:2:526:A:H2'	1:2:527:A:C8	2.47	0.50
1:2:725:C:C2	1:2:763:G:N2	2.79	0.50
1:2:1394:G:H5"	25:G:104:LYS:CE	2.42	0.50
1:2:1452:G:P	31:1:78:GLN:NE2	2.84	0.50
1:2:1472:G:OP1	31:1:58:LYS:HD2	2.10	0.50
24:F:96:VAL:O	24:F:122:ILE:N	2.39	0.50
34:7:36:LYS:HE2	34:7:45:MET:HA	1.93	0.50
34:7:189:ILE:HD12	35:8:18:LEU:CD2	2.32	0.50
35:8:44:ILE:HG22	35:8:47:PHE:N	2.26	0.50
1:2:262:G:H5"	1:2:262:G:H8	1.77	0.50
1:2:458:G:H2'	1:2:459:G:H5"	1.92	0.50
1:2:1054:A:H4'	19:B:95:ARG:HH22	1.59	0.50
1:2:1351:U:H2'	1:2:1352:G:C8	2.46	0.50
1:2:1352:G:C6	1:2:1353:C:N4	2.80	0.50
26:I:7:LEU:HA	26:I:34:ILE:HG12	1.93	0.50
32:4:24:C:H2'	32:4:25:U:C5	2.47	0.50
32:4:37:U:H2'	32:4:38:A:O4'	2.11	0.50
1:2:149:U:H4'	25:G:94:PHE:CD1	2.45	0.50
1:2:432:G:H2'	1:2:433:U:O4'	2.11	0.50
1:2:537:G:C6	1:2:538:C:N4	2.80	0.50
1:2:566:C:H4'	22:D:54:ARG:CZ	2.42	0.50
1:2:1025:U:O2'	19:B:105:ALA:HB3	2.10	0.50
1:2:1345:G:H8	1:2:1345:G:O5'	1.94	0.50
1:2:1367:C:C4'	31:1:65:ALA:HB2	2.42	0.50
19:B:33:TYR:HB2	19:B:43:LEU:C	2.32	0.50
31:1:32:THR:HG1	31:1:42:ILE:HD11	1.77	0.50
34:7:41:LEU:HD22	34:7:47:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:189:ILE:C	35:8:14:LEU:HG	2.31	0.50
1:2:540:G:C6	1:2:709:G:O6	2.65	0.50
4:L:64:TRP:CE3	6:P:52:PHE:HB3	2.47	0.50
25:G:29:LEU:CD1	25:G:63:ILE:HD11	2.42	0.50
30:5:817:A:H4'	30:5:818:A:OP2	2.12	0.50
31:1:34:ARG:HD3	31:1:40:MET:SD	2.51	0.50
34:7:65:PRO:HB3	34:7:193:SER:HA	1.94	0.50
1:2:459:G:N3	1:2:459:G:H5'	2.27	0.50
1:2:556:G:H4'	23:E:224:ASP:HB2	1.94	0.50
1:2:900:G:H5"	12:H:74:SER:HA	1.93	0.50
1:2:985:C:H1'	11:Y:41:GLY:CA	2.42	0.50
1:2:1048:G:HO2'	1:2:1130:A:HO2'	1.54	0.50
20:V:21:PHE:CE1	20:V:69:ALA:HB3	2.47	0.50
23:E:37:HIS:CG	23:E:38:ASN:N	2.80	0.50
24:F:5:TRP:HB3	24:F:57:VAL:HG21	1.94	0.50
1:2:130:G:N2	1:2:163:C:C2	2.79	0.49
1:2:372:G:C2	1:2:373:C:C2	2.99	0.49
1:2:372:G:H2'	1:2:373:C:C6	2.47	0.49
1:2:516:A:N1	1:2:842:U:C4	2.78	0.49
23:E:37:HIS:CD2	23:E:38:ASN:H	2.30	0.49
32:4:53:G:N3	32:4:54:G:C8	2.80	0.49
34:7:41:LEU:HD13	34:7:47:ILE:H	1.77	0.49
34:7:97:HIS:CE1	34:7:99:VAL:HG23	2.46	0.49
1:2:20:G:H4'	1:2:477:G:C2	2.48	0.49
1:2:229:G:H2'	1:2:230:C:H6	1.76	0.49
1:2:866:A:H2'	1:2:867:A:C8	2.47	0.49
1:2:883:G:C6	1:2:885:G:C5	3.00	0.49
1:2:1336:U:H2'	1:2:1337:A:O4'	2.11	0.49
1:2:1395:G:H5"	25:G:87:LEU:HD13	1.94	0.49
34:7:280:ARG:HH11	34:7:283:ASP:HA	1.76	0.49
1:2:29:G:H1'	15:N:135:LYS:NZ	2.27	0.49
1:2:184:G:HO2'	1:2:185:G:H8	1.42	0.49
1:2:244:G:C5	1:2:245:U:C5	3.00	0.49
1:2:250:G:OP1	17:R:97:THR:OG1	2.20	0.49
1:2:369:A:H2'	1:2:370:A:C8	2.46	0.49
1:2:431:U:H3'	1:2:432:G:C8	2.48	0.49
1:2:607:U:H5'	1:2:702:G:O6	2.11	0.49
1:2:762:G:C6	1:2:763:G:C5	3.01	0.49
1:2:868:C:C5'	1:2:1373:A:O2'	2.58	0.49
1:2:872:A:N3	1:2:873:A:C8	2.81	0.49
1:2:930:G:C6	1:2:1325:C:H5'	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1118:C:O2'	7:S:52:GLY:HA3	2.12	0.49
1:2:1219:C:N3	1:2:1237:G:C2	2.80	0.49
1:2:1276:G:H8	1:2:1276:G:O5'	1.94	0.49
1:2:1311:C:H4'	12:H:94:ASN:C	2.33	0.49
1:2:1454:A:N3	1:2:1455:A:C8	2.80	0.49
2:Z:2:ALA:HB3	2:Z:5:ARG:NH1	2.27	0.49
3:3:43:VAL:HG11	3:3:66:LEU:HD21	1.94	0.49
30:5:813:A:H4'	30:5:814:U:OP1	2.09	0.49
1:2:149:U:H2'	1:2:150:G:O4'	2.12	0.49
1:2:242:A:O3'	1:2:243:G:H4'	2.12	0.49
1:2:1317:G:C4	1:2:1326:G:N2	2.81	0.49
1:2:1332:C:H2'	1:2:1333:G:O4'	2.11	0.49
35:8:35:ILE:HD13	35:8:92:ILE:CD1	2.42	0.49
36:9:119:LYS:O	36:9:123:GLU:HB2	2.12	0.49
1:2:8:U:C4	1:2:874:G:C6	3.00	0.49
1:2:166:A:H61	1:2:196:G:H1'	1.77	0.49
1:2:260:C:H4'	17:R:92:ARG:NH1	2.27	0.49
1:2:419:G:C2	1:2:420:C:C6	3.01	0.49
1:2:452:G:C6	1:2:499:G:C2	3.01	0.49
1:2:861:G:C6	1:2:862:C:C4	3.01	0.49
1:2:1030:U:O2'	24:F:199:LYS:HE2	2.13	0.49
12:H:174:TYR:CG	12:H:174:TYR:O	2.65	0.49
14:M:21:SER:OG	14:M:95:GLY:N	2.41	0.49
15:N:119:ILE:HD12	15:N:122:ILE:HB	1.95	0.49
20:V:56:ILE:HG13	20:V:67:GLY:CA	2.38	0.49
24:F:86:LEU:HD11	24:F:195:VAL:HG22	1.93	0.49
34:7:167:LYS:HA	34:7:170:THR:HG22	1.93	0.49
35:8:49:GLU:O	35:8:52:ASP:HB2	2.12	0.49
36:9:161:VAL:O	36:9:165:LEU:HG	2.12	0.49
1:2:271:G:N3	1:2:272:C:C6	2.81	0.49
1:2:297:G:H2'	1:2:298:C:C6	2.48	0.49
1:2:515:U:O4	15:N:26:SER:HB2	2.12	0.49
1:2:974:G:H2'	1:2:974:G:N3	2.28	0.49
1:2:1309:A:C2	1:2:1334:A:C5	3.01	0.49
15:N:23:PHE:N	15:N:23:PHE:CD1	2.78	0.49
25:G:80:GLY:C	25:G:82:ARG:H	2.16	0.49
25:G:84:VAL:CG1	25:G:85:ARG:N	2.75	0.49
34:7:17:HIS:CE1	34:7:128:GLN:H	2.31	0.49
34:7:41:LEU:HD13	34:7:47:ILE:N	2.27	0.49
34:7:115:ILE:HD11	34:7:198:ILE:HG22	1.95	0.49
34:7:274:THR:CG2	34:7:300:TYR:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:30:C:C4	1:2:31:U:C4	3.01	0.49
1:2:533:C:C4	1:2:534:G:C2	3.00	0.49
1:2:556:G:C2	1:2:590:G:C6	3.00	0.49
1:2:715:C:C2	1:2:716:G:C8	3.00	0.49
1:2:1196:A:OP1	12:H:88:ARG:CZ	2.61	0.49
1:2:1312:C:OP1	12:H:78:HIS:O	2.31	0.49
1:2:1324:U:OP1	9:U:83:ARG:NH1	2.41	0.49
12:H:81:VAL:HG12	12:H:82:ALA:N	2.27	0.49
12:H:124:VAL:O	12:H:128:GLU:HG3	2.12	0.49
19:B:59:LEU:HB3	19:B:175:ILE:HG21	1.95	0.49
31:1:33:LYS:HG3	32:4:27:G:P	2.53	0.49
32:4:67:C:H2'	32:4:68:C:H6	1.74	0.49
1:2:81:C:C2	1:2:82:G:C8	3.01	0.49
1:2:314:G:O2'	1:2:1424:G:H5'	2.13	0.49
1:2:541:G:C4	1:2:707:A:C6	3.01	0.49
1:2:541:G:C8	1:2:707:A:C2	3.01	0.49
1:2:881:G:C6	1:2:882:C:C4	3.01	0.49
1:2:1298:G:N3	32:4:43:G:C4'	2.76	0.49
1:2:1409:G:N2	1:2:1410:G:C8	2.80	0.49
1:2:1454:A:C2	1:2:1455:A:C5	3.01	0.49
4:L:92:GLU:HB2	4:L:93:ASP:CB	2.42	0.49
23:E:184:TYR:HA	23:E:197:GLY:O	2.13	0.49
34:7:263:LYS:O	34:7:266:LYS:HG2	2.13	0.49
1:2:2:U:C5	24:F:184:TRP:CZ3	3.00	0.49
1:2:459:G:H3'	1:2:460:C:H4'	1.93	0.49
1:2:649:A:C2	1:2:740:G:O2'	2.66	0.49
1:2:848:G:OP1	29:0:9:ARG:NH2	2.46	0.49
1:2:885:G:N2	1:2:1351:U:C2	2.80	0.49
1:2:898:G:N1	1:2:899:G:O6	2.46	0.49
1:2:1027:C:H5"	19:B:102:THR:HG21	1.33	0.49
1:2:1312:C:H4'	12:H:80:LYS:HG2	1.94	0.49
16:Q:112:HIS:O	16:Q:114:LYS:N	2.45	0.49
18:A:137:ILE:HD13	18:A:180:LEU:HD21	1.95	0.49
34:7:116:LEU:HD21	34:7:129:THR:HG23	1.95	0.49
34:7:124:PHE:O	34:7:126:GLN:N	2.45	0.49
34:7:189:ILE:O	35:8:14:LEU:CD1	2.61	0.49
36:9:98:LYS:HD3	36:9:175:ARG:NH2	2.28	0.49
36:9:162:LYS:HB2	36:9:162:LYS:NZ	2.28	0.49
1:2:297:G:H2'	1:2:298:C:H6	1.78	0.49
1:2:963:A:C8	1:2:987:G:N2	2.81	0.49
1:2:1308:U:C5	1:2:1333:G:N2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1403:U:C2	1:2:1404:C:C5	3.00	0.49
1:2:1450:U:H2'	1:2:1451:C:C6	2.48	0.49
4:L:77:ALA:HB1	4:L:81:ALA:HB3	1.94	0.49
12:H:148:VAL:HG12	12:H:149:ALA:N	2.27	0.49
32:4:42:C:H2'	32:4:43:G:H5'	1.91	0.49
34:7:32:ILE:HG22	34:7:33:TRP:O	2.12	0.49
34:7:188:LYS:CB	35:8:131:GLY:HA3	2.43	0.49
36:9:45:GLU:O	36:9:82:LEU:HD12	2.12	0.49
1:2:318:C:O2'	25:G:102:ARG:HG3	2.13	0.48
1:2:556:G:N2	1:2:590:G:C5	2.80	0.48
1:2:629:U:O4	1:2:669:A:N1	2.46	0.48
23:E:37:HIS:CD2	23:E:38:ASN:N	2.81	0.48
24:F:38:PHE:CE2	24:F:95:TYR:CE1	3.01	0.48
25:G:28:LYS:HE2	25:G:38:ILE:HG23	1.94	0.48
34:7:150:LYS:O	34:7:153:VAL:HG22	2.12	0.48
34:7:236:GLY:O	34:7:299:THR:OG1	2.27	0.48
35:8:48:ALA:HB2	35:8:79:GLY:HA3	1.94	0.48
35:8:137:LYS:HE2	35:8:139:LEU:CD2	2.42	0.48
1:2:6:G:C5	1:2:7:G:N7	2.81	0.48
1:2:62:G:C8	1:2:63:G:C8	3.01	0.48
1:2:521:G:C6	1:2:522:C:C4	3.01	0.48
1:2:1040:A:H2'	1:2:1041:C:H5'	1.95	0.48
1:2:1054:A:C5'	19:B:95:ARG:NH1	2.68	0.48
1:2:1079:G:N2	1:2:1106:A:H62	2.10	0.48
1:2:1344:U:C2	1:2:1345:G:C5	3.01	0.48
1:2:1404:C:C4	1:2:1405:C:C5	3.01	0.48
1:2:1412:A:H2'	1:2:1413:G:C8	2.47	0.48
1:2:1451:C:C5'	31:1:78:GLN:HB3	2.43	0.48
15:N:62:ALA:HB3	15:N:67:SER:HA	1.95	0.48
36:9:95:LEU:HD11	36:9:237:LYS:HB2	1.94	0.48
36:9:140:ILE:HA	36:9:143:ALA:HB3	1.94	0.48
1:2:75:C:O2	1:2:75:C:O4'	2.31	0.48
1:2:93:A:C6	1:2:322:G:C6	3.01	0.48
1:2:152:G:H1'	25:G:64:ARG:NH1	2.28	0.48
1:2:175:G:N2	1:2:188:C:C2	2.81	0.48
1:2:244:G:C6	1:2:245:U:C4	3.01	0.48
1:2:786:G:H2'	1:2:787:U:O4'	2.13	0.48
1:2:1053:A:C8	19:B:98:PRO:HG3	2.47	0.48
12:H:72:MET:CE	12:H:97:LYS:HB2	2.44	0.48
20:V:60:PHE:CD1	20:V:60:PHE:O	2.66	0.48
30:5:819:A:C2	31:1:35:ARG:NH2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:93:A:H2'	1:2:322:G:N2	2.28	0.48
1:2:338:C:C2	1:2:344:G:C2	3.01	0.48
1:2:355:C:H2'	1:2:356:G:C8	2.48	0.48
1:2:492:G:C2	1:2:493:C:C2	3.01	0.48
1:2:541:G:C5	1:2:707:A:C5	3.01	0.48
1:2:677:U:C2	1:2:1493:C:O2'	2.58	0.48
1:2:944:C:C2	1:2:1181:G:C2	3.01	0.48
1:2:1139:A:H2'	1:2:1140:A:O4'	2.13	0.48
1:2:1239:A:H2'	1:2:1239:A:N3	2.29	0.48
1:2:1414:G:O4'	25:G:78:ILE:HG23	2.13	0.48
4:L:59:ALA:HB3	4:L:61:PHE:CE1	2.49	0.48
19:B:63:GLU:HA	19:B:179:ARG:NH2	2.28	0.48
26:I:2:THR:OG1	26:I:3:LEU:N	2.45	0.48
37:4:101:MET:HE1	34:7:219:ARG:HH21	1.73	0.48
34:7:59:CYS:CB	34:7:74:CYS:HG	2.27	0.48
34:7:187:HIS:CA	35:8:130:CYS:C	2.77	0.48
34:7:307:LYS:HD2	36:9:224:ALA:HB3	1.95	0.48
1:2:4:C:H2'	1:2:5:C:H6	1.78	0.48
1:2:53:G:C5	1:2:54:C:C4	3.01	0.48
1:2:193:G:H2'	1:2:194:C:H6	1.78	0.48
1:2:836:G:P	26:I:76:LYS:HG3	2.53	0.48
1:2:1377:G:O2'	1:2:1438:A:N6	2.46	0.48
1:2:1424:G:C4	1:2:1425:C:C5	3.02	0.48
24:F:129:GLY:O	24:F:130:SER:CB	2.61	0.48
36:9:123:GLU:O	36:9:127:TRP:HB2	2.13	0.48
1:2:50:C:O2	1:2:354:G:C2	2.67	0.48
1:2:843:G:C2	1:2:844:G:C8	3.01	0.48
1:2:1206:G:H4'	9:U:13:VAL:HG21	1.96	0.48
1:2:1273:G:C6	1:2:1274:C:C4	3.02	0.48
1:2:1312:C:O2	1:2:1331:G:C2	2.67	0.48
12:H:140:MET:HB3	12:H:145:ARG:HA	1.95	0.48
35:8:28:GLN:C	35:8:29:SER:O	2.50	0.48
36:9:7:LYS:HG3	36:9:8:LEU:H	1.79	0.48
1:2:262:G:O2'	1:2:263:C:OP2	2.25	0.48
1:2:1031:G:H8	1:2:1031:G:O5'	1.96	0.48
1:2:1323:A:N3	1:2:1323:A:O2'	2.36	0.48
1:2:1389:G:N2	1:2:1427:C:C2	2.82	0.48
12:H:212:GLU:O	12:H:215:ARG:HG2	2.14	0.48
19:B:56:GLY:CA	19:B:174:GLU:HG2	2.44	0.48
32:4:42:C:C2	32:4:43:G:C8	3.02	0.48
32:4:48:U:H3'	32:4:49:C:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:41:LEU:HD13	34:7:47:ILE:HB	1.95	0.48
34:7:280:ARG:NH1	34:7:283:ASP:HA	2.28	0.48
34:7:303:PRO:HD3	36:9:193:VAL:HG22	1.95	0.48
36:9:247:ILE:O	36:9:250:LEU:HB2	2.13	0.48
1:2:29:G:C6	1:2:30:C:C4	3.01	0.48
1:2:106:A:HO2'	1:2:308:G:HO2'	1.57	0.48
1:2:1414:G:C4'	25:G:84:VAL:HG11	2.44	0.48
12:H:118:ASN:OD1	12:H:120:ILE:HG22	2.14	0.48
19:B:133:ILE:HA	24:F:43:GLN:OE1	2.14	0.48
24:F:148:LYS:N	24:F:148:LYS:HD2	2.29	0.48
36:9:146:GLU:HB2	36:9:150:ILE:HD11	1.96	0.48
1:2:151:G:O2'	25:G:64:ARG:HB3	2.14	0.48
1:2:646:U:O4	14:M:51:ASP:HB3	2.14	0.48
1:2:692:G:C6	1:2:693:C:C4	3.02	0.48
1:2:991:C:C5	1:2:992:G:N7	2.82	0.48
1:2:1193:G:C2	1:2:1194:C:C2	3.01	0.48
1:2:1344:U:C4	1:2:1345:G:O6	2.66	0.48
1:2:1390:G:N2	1:2:1426:C:C2	2.82	0.48
17:R:1:MET:O	17:R:23:TRP:HB3	2.14	0.48
20:V:9:LYS:HE2	23:E:55:TYR:HA	1.96	0.48
23:E:127:ILE:HG22	23:E:141:ASN:O	2.14	0.48
32:4:14:A:C6	32:4:23:G:C5	3.02	0.48
34:7:45:MET:N	34:7:45:MET:SD	2.87	0.48
34:7:205:PRO:HB2	34:7:207:ARG:HH11	1.79	0.48
35:8:35:ILE:HG12	35:8:44:ILE:HG12	1.95	0.48
1:2:402:G:C6	1:2:403:C:C4	3.02	0.48
1:2:438:A:C3'	1:2:439:G:H5"	2.41	0.48
1:2:518:U:H2'	1:2:519:G:C8	2.48	0.48
1:2:762:G:C6	1:2:763:G:N7	2.82	0.48
1:2:1186:C:H4'	1:2:1187:A:OP1	2.14	0.48
8:T:16:LEU:HB3	8:T:74:PRO:HG2	1.96	0.48
10:X:18:THR:HG22	10:X:19:GLY:H	1.78	0.48
20:V:27:GLY:HA2	22:D:156:ARG:NH2	2.28	0.48
22:D:102:GLU:HA	22:D:107:THR:HG21	1.96	0.48
34:7:110:LEU:CD2	34:7:218:ILE:HD13	2.44	0.48
34:7:152:ASP:OD1	34:7:153:VAL:HG13	2.13	0.48
1:2:157:A:C8	1:2:159:C:C6	3.02	0.47
1:2:453:G:H2'	1:2:454:G:C8	2.48	0.47
1:2:921:G:C6	1:2:933:G:O6	2.67	0.47
4:L:10:SER:HB3	4:L:16:LEU:HB2	1.95	0.47
24:F:5:TRP:HB2	24:F:55:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:125:LYS:O	24:F:208:THR:HG21	2.13	0.47
34:7:23:THR:HG22	34:7:33:TRP:CZ3	2.48	0.47
34:7:57:GLY:C	34:7:69:VAL:HG22	2.35	0.47
34:7:188:LYS:CD	35:8:131:GLY:C	2.82	0.47
1:2:229:G:N2	1:2:230:C:N1	2.62	0.47
1:2:296:A:C2	1:2:519:G:O6	2.68	0.47
1:2:318:C:O2	25:G:100:GLY:HA2	2.14	0.47
1:2:669:A:H2'	1:2:670:C:O4'	2.14	0.47
1:2:723:G:N1	1:2:724:C:C4	2.82	0.47
1:2:1411:G:H2'	1:2:1412:A:C8	2.49	0.47
1:2:1443:G:C2	1:2:1444:G:C5	3.03	0.47
12:H:58:LYS:O	12:H:66:ARG:CZ	2.61	0.47
23:E:9:HIS:O	23:E:31:ARG:NH1	2.47	0.47
24:F:146:GLU:HA	24:F:154:VAL:O	2.14	0.47
32:4:4:G:O2'	32:4:5:G:OP2	2.32	0.47
1:2:87:C:C4	1:2:88:G:N7	2.83	0.47
1:2:1215:G:C2	1:2:1243:C:C2	3.02	0.47
1:2:1284:C:H2'	1:2:1285:C:C6	2.49	0.47
1:2:1311:C:OP1	12:H:77:SER:N	2.46	0.47
1:2:1352:G:C4	1:2:1353:C:C5	3.02	0.47
2:Z:5:ARG:O	2:Z:8:ILE:HG13	2.14	0.47
10:X:23:ASP:OD1	10:X:46:ARG:NH1	2.46	0.47
32:4:65:G:H2'	32:4:66:C:C6	2.48	0.47
34:7:215:MET:HB2	34:7:242:ILE:HA	1.96	0.47
34:7:388:VAL:CG1	34:7:393:ILE:HG13	2.42	0.47
36:9:10:SER:O	36:9:13:GLU:HB2	2.15	0.47
1:2:839:G:C5	1:2:840:C:C5	3.02	0.47
1:2:1120:G:N2	1:2:1121:C:C2	2.82	0.47
1:2:1144:G:C2	1:2:1145:C:C2	3.02	0.47
1:2:1318:U:O4	1:2:1323:A:N1	2.47	0.47
1:2:1450:U:H2'	1:2:1451:C:H6	1.78	0.47
1:2:1472:G:OP1	31:1:58:LYS:CD	2.62	0.47
1:2:1485:G:N3	1:2:1486:A:N7	2.63	0.47
1:2:1488:C:C2	1:2:1489:A:C8	3.01	0.47
27:J:87:ARG:HD2	27:J:90:ALA:HB3	1.96	0.47
32:4:54:G:C8	32:4:55:5MU:H72	2.49	0.47
34:7:329:ILE:HD13	34:7:382:LEU:HD11	1.97	0.47
1:2:4:C:HO2'	1:2:5:C:C5'	2.27	0.47
1:2:10:G:N7	1:2:1356:A:C5	2.83	0.47
1:2:271:G:C2	1:2:272:C:C2	3.03	0.47
12:H:28:VAL:HG11	12:H:34:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:97:LYS:HA	12:H:100:ALA:HB3	1.97	0.47
22:D:93:LEU:HD13	24:F:160:PRO:HB3	1.96	0.47
34:7:281:PHE:CZ	34:7:295:VAL:HG22	2.50	0.47
36:9:64:VAL:HG12	36:9:65:ILE:N	2.30	0.47
1:2:87:C:OP1	25:G:97:LYS:HG2	2.15	0.47
1:2:184:G:O2'	1:2:185:G:H8	1.91	0.47
1:2:572:U:O4	22:D:138:ARG:CZ	2.63	0.47
1:2:1120:G:C2	1:2:1121:C:C6	3.03	0.47
10:X:7:TYR:CG	10:X:60:THR:HG22	2.49	0.47
12:H:68:ILE:HG21	12:H:97:LYS:HG3	1.97	0.47
12:H:89:GLU:CB	12:H:95:SER:HB2	2.45	0.47
15:N:136:GLU:OE2	15:N:143:GLU:N	2.47	0.47
18:A:10:ARG:CD	36:9:133:TYR:OH	2.62	0.47
24:F:48:GLU:O	24:F:52:VAL:HG23	2.15	0.47
29:0:14:LYS:O	29:0:18:LYS:N	2.37	0.47
31:1:26:LYS:O	31:1:27:ILE:HG12	2.14	0.47
32:4:77:A:HO2'	37:4:101:MET:N	2.13	0.47
34:7:295:VAL:HG12	34:7:296:ALA:H	1.80	0.47
1:2:315:A:H1'	1:2:1423:A:C1'	2.27	0.47
1:2:419:G:N2	1:2:420:C:C2	2.82	0.47
1:2:495:G:C4	1:2:496:C:C5	3.03	0.47
1:2:779:G:H2'	1:2:780:C:C6	2.50	0.47
1:2:839:G:C2	1:2:840:C:C2	3.03	0.47
1:2:884:G:N1	1:2:1460:G:C5	2.83	0.47
1:2:898:G:C6	1:2:899:G:O6	2.67	0.47
1:2:992:G:C6	1:2:993:C:N3	2.82	0.47
1:2:1346:C:H2'	1:2:1347:U:H6	1.69	0.47
1:2:1390:G:C6	1:2:1391:U:C4	3.02	0.47
2:Z:89:TYR:HB2	2:Z:123:ASN:CG	2.35	0.47
3:3:43:VAL:HG21	3:3:70:CYS:SG	2.55	0.47
18:A:24:PRO:HA	18:A:27:PHE:O	2.15	0.47
22:D:40:GLU:O	22:D:44:HIS:ND1	2.47	0.47
24:F:86:LEU:CD2	24:F:195:VAL:HA	2.45	0.47
25:G:52:GLY:HA3	25:G:54:GLU:HB2	1.95	0.47
26:I:73:GLY:O	26:I:128:TYR:N	2.41	0.47
30:5:809:G:C4	30:5:810:G:N7	2.83	0.47
34:7:339:VAL:HG23	34:7:339:VAL:O	2.15	0.47
35:8:35:ILE:HD13	35:8:92:ILE:HD13	1.97	0.47
35:8:100:LEU:C	35:8:104:VAL:HG12	2.34	0.47
1:2:82:G:C2	1:2:83:C:C2	3.03	0.47
1:2:459:G:C6	1:2:460:C:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:480:G:C6	1:2:481:C:C4	3.03	0.47
18:A:43:VAL:HA	18:A:46:ARG:HG2	1.97	0.47
18:A:59:PHE:CE2	18:A:162:VAL:HG12	2.49	0.47
22:D:65:GLN:O	22:D:66:ALA:C	2.52	0.47
24:F:146:GLU:HG2	24:F:147:GLY:N	2.29	0.47
37:4:101:MET:HG2	34:7:51:TYR:CD1	2.50	0.47
34:7:221:PHE:O	34:7:237:VAL:HB	2.14	0.47
1:2:329:G:H4'	25:G:103:ARG:NH1	2.29	0.47
1:2:424:U:C4	1:2:425:C:C2	3.03	0.47
1:2:583:G:C2	1:2:584:C:C2	3.02	0.47
1:2:720:A:H2'	1:2:721:A:O4'	2.15	0.47
1:2:893:U:OP1	1:2:893:U:H3'	2.14	0.47
1:2:1414:G:C1'	25:G:78:ILE:HA	2.44	0.47
1:2:1421:C:H4'	27:J:1:MET:O	2.15	0.47
5:O:78:ALA:HB2	9:U:35:VAL:HG21	1.96	0.47
12:H:132:PRO:HB3	12:H:204:LYS:O	2.15	0.47
24:F:82:ARG:HD3	24:F:102:HIS:NE2	2.29	0.47
27:J:103:THR:OG1	27:J:106:GLY:O	2.32	0.47
30:5:812:G:C2'	30:5:813:A:O4'	2.63	0.47
34:7:192:ASP:CG	35:8:13:ARG:HH22	2.16	0.47
34:7:214:VAL:HB	34:7:244:GLN:HG2	1.97	0.47
34:7:332:LYS:O	34:7:411:GLY:HA3	2.15	0.47
36:9:8:LEU:CD1	36:9:73:ARG:HA	2.45	0.47
1:2:459:G:C6	1:2:460:C:C2	3.02	0.47
1:2:685:G:C6	1:2:686:C:C4	3.02	0.47
1:2:757:G:H2'	1:2:758:U:O4'	2.15	0.47
1:2:916:U:O2	1:2:918:A:C8	2.68	0.47
1:2:1344:U:N3	1:2:1345:G:C5	2.83	0.47
1:2:1483:U:O2'	1:2:1484:C:P	2.72	0.47
10:X:46:ARG:HH21	12:H:135:ASP:HB3	1.80	0.47
19:B:56:GLY:HA3	19:B:174:GLU:HG2	1.96	0.47
24:F:36:GLU:O	24:F:40:ARG:NH1	2.48	0.47
25:G:84:VAL:O	25:G:106:THR:OG1	2.12	0.47
34:7:195:ILE:HA	34:7:198:ILE:HG12	1.96	0.47
1:2:434:A:N3	20:V:85:TYR:N	2.63	0.46
1:2:909:U:O4	5:O:130:ARG:NH2	2.48	0.46
1:2:1249:A:H5'	12:H:81:VAL:HA	1.96	0.46
16:Q:95:LEU:HD13	16:Q:132:LEU:HB3	1.97	0.46
36:9:43:TRP:O	36:9:45:GLU:N	2.48	0.46
1:2:521:G:C2	1:2:522:C:C2	3.04	0.46
1:2:1404:C:C4'	25:G:76:PRO:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1414:G:H21	25:G:79:HIS:CB	2.28	0.46
1:2:1463:A:H61	1:2:1482:C:H42	1.63	0.46
2:Z:100:ALA:HA	2:Z:169:ALA:HB2	1.96	0.46
23:E:73:VAL:HG11	23:E:83:PHE:HE2	1.80	0.46
23:E:89:ASP:OD2	23:E:90:VAL:N	2.49	0.46
23:E:168:VAL:N	23:E:169:PRO:HD2	2.30	0.46
24:F:175:LEU:HD23	24:F:205:LEU:HD21	1.96	0.46
34:7:57:GLY:O	34:7:69:VAL:HG22	2.15	0.46
34:7:307:LYS:HB2	34:7:307:LYS:HE3	1.49	0.46
1:2:962:G:H1'	1:2:988:A:N6	2.29	0.46
1:2:1053:A:C2	19:B:98:PRO:CA	2.58	0.46
1:2:1489:A:C6	1:2:1490:C:N4	2.84	0.46
12:H:33:LEU:HD22	12:H:128:GLU:HG2	1.96	0.46
23:E:190:GLY:O	23:E:193:VAL:HG13	2.15	0.46
34:7:22:LYS:O	34:7:26:VAL:HG23	2.15	0.46
1:2:106:A:H62	1:2:235:G:H21	1.64	0.46
1:2:612:C:C2	1:2:613:C:C5	3.03	0.46
1:2:780:C:OP1	26:I:28:LYS:HE2	2.15	0.46
1:2:901:G:C2	1:2:1302:C:N3	2.84	0.46
1:2:1323:A:N3	1:2:1323:A:C2'	2.78	0.46
16:Q:67:LYS:HD3	16:Q:76:LEU:HB3	1.96	0.46
20:V:24:TYR:HA	20:V:63:TYR:O	2.15	0.46
24:F:16:TRP:CE2	24:F:48:GLU:HB2	2.51	0.46
24:F:46:GLU:OE1	24:F:46:GLU:HA	2.16	0.46
34:7:188:LYS:CD	35:8:131:GLY:CA	2.93	0.46
34:7:213:PRO:HB2	34:7:318:LEU:HG	1.96	0.46
36:9:183:ILE:O	36:9:226:ARG:HA	2.16	0.46
1:2:62:G:C8	1:2:63:G:N7	2.83	0.46
1:2:358:G:C5'	15:N:79:LYS:HB2	2.46	0.46
1:2:537:G:C2	1:2:538:C:C2	3.03	0.46
1:2:672:G:N7	14:M:123:HIS:HA	2.31	0.46
1:2:677:U:O2	1:2:1493:C:H1'	2.16	0.46
1:2:694:U:O2'	16:Q:118:SER:OG	2.32	0.46
1:2:910:G:C2	1:2:911:C:C2	3.03	0.46
1:2:1131:G:N1	1:2:1132:C:C4	2.83	0.46
1:2:1264:G:C6	1:2:1265:G:N1	2.83	0.46
4:L:40:LEU:HB3	4:L:41:PRO:CD	2.45	0.46
10:X:8:PRO:HD2	10:X:33:GLU:HG3	1.97	0.46
34:7:274:THR:HG22	34:7:275:LYS:N	2.30	0.46
34:7:310:ASN:C	34:7:312:LEU:H	2.19	0.46
36:9:41:LEU:HD12	36:9:80:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:42:G:H4'	1:2:43:A:OP2	2.16	0.46
1:2:106:A:H62	1:2:235:G:N2	2.12	0.46
1:2:1073:C:O5'	1:2:1073:C:H6	1.99	0.46
1:2:1124:G:C2	1:2:1133:C:C2	3.03	0.46
1:2:1300:A:O2'	32:4:32:G:O2'	2.13	0.46
1:2:1341:C:H1'	10:X:20:THR:HG23	1.98	0.46
1:2:1430:G:C6	1:2:1431:C:C4	3.03	0.46
19:B:59:LEU:O	19:B:179:ARG:NH2	2.49	0.46
32:4:50:G:H1	32:4:66:C:H42	1.63	0.46
1:2:43:A:O2'	1:2:302:A:H4'	2.16	0.46
1:2:474:G:C6	1:2:475:C:C4	3.04	0.46
1:2:537:G:C4	1:2:538:C:C5	3.03	0.46
1:2:768:A:N7	1:2:770:A:C4	2.84	0.46
1:2:779:G:C6	1:2:780:C:C4	3.03	0.46
1:2:788:C:C2	1:2:811:G:C2	3.04	0.46
1:2:1022:U:OP1	24:F:80:ARG:CD	2.64	0.46
1:2:1302:C:H2'	1:2:1303:C:C6	2.50	0.46
1:2:1307:G:HO2'	1:2:1333:G:H1	1.60	0.46
1:2:1451:C:H5"	31:1:78:GLN:CB	2.43	0.46
15:N:108:ILE:HD13	15:N:125:LYS:HD2	1.96	0.46
15:N:128:LYS:HA	15:N:133:SER:HA	1.96	0.46
17:R:1:MET:O	17:R:23:TRP:CD1	2.69	0.46
34:7:134:VAL:HG11	34:7:340:VAL:HG21	1.97	0.46
34:7:169:PHE:C	34:7:171:LYS:H	2.17	0.46
34:7:271:PRO:CA	34:7:272:ILE:N	2.74	0.46
1:2:127:G:C2	1:2:218:C:N3	2.84	0.46
1:2:323:A:C2	1:2:325:A:C4	3.03	0.46
1:2:453:G:H2'	1:2:454:G:H8	1.80	0.46
1:2:568:C:C2	1:2:569:G:C8	3.04	0.46
1:2:632:C:H2'	1:2:633:C:O4'	2.15	0.46
1:2:682:A:C8	16:Q:120:ARG:NH2	2.84	0.46
1:2:1054:A:C4'	19:B:95:ARG:NH2	2.64	0.46
1:2:1200:U:O4'	12:H:103:VAL:HG22	2.15	0.46
1:2:1364:C:H2'	1:2:1365:G:C8	2.50	0.46
1:2:1370:U:C2	1:2:1446:G:N2	2.84	0.46
1:2:1383:A:C2	1:2:1433:C:C2	3.03	0.46
1:2:1402:C:H2'	1:2:1403:U:C1'	2.44	0.46
1:2:1452:G:P	31:1:78:GLN:CD	2.93	0.46
9:U:12:LEU:HA	9:U:136:LEU:HD13	1.97	0.46
21:W:4:PRO:HB3	26:I:28:LYS:CG	2.45	0.46
24:F:94:GLY:O	24:F:95:TYR:CD2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:0:6:ILE:HG22	29:0:10:ILE:HD12	1.98	0.46
32:4:4:G:O2'	32:4:5:G:P	2.74	0.46
32:4:9:G:C6	32:4:46:G:N1	2.83	0.46
34:7:137:GLY:HA3	34:7:174:TRP:CZ3	2.50	0.46
34:7:155:SER:OG	34:7:158:GLU:HG3	2.16	0.46
1:2:137:A:C8	1:2:138:C:C5	3.03	0.46
1:2:193:G:C6	1:2:194:C:C4	3.04	0.46
1:2:462:A:N6	22:D:18:TRP:CZ2	2.84	0.46
1:2:629:U:H2'	1:2:630:A:O4'	2.16	0.46
1:2:742:U:H3'	1:2:743:U:C6	2.51	0.46
1:2:1363:C:O5'	1:2:1363:C:C6	2.69	0.46
1:2:1489:A:O2'	1:2:1490:C:H5'	2.16	0.46
12:H:86:MET:C	12:H:88:ARG:HB2	2.37	0.46
14:M:61:MET:HA	14:M:104:ALA:HB2	1.98	0.46
19:B:83:PHE:HB2	19:B:168:TYR:HB3	1.97	0.46
31:1:25:GLN:O	31:1:98:SER:CB	2.64	0.46
32:4:42:C:C2	32:4:43:G:N7	2.84	0.46
33:6:75:GLN:HG3	33:6:79:ARG:NH2	2.31	0.46
34:7:188:LYS:HG3	35:8:130:CYS:O	2.16	0.46
34:7:333:TYR:CD1	34:7:376:ASP:HA	2.51	0.46
36:9:158:GLU:HA	36:9:161:VAL:HG23	1.98	0.46
36:9:162:LYS:HB2	36:9:163:PRO:HD3	1.98	0.46
1:2:4:C:N3	1:2:5:C:C5	2.84	0.46
1:2:147:A:C5	1:2:148:C:H1'	2.51	0.46
1:2:164:A:H2'	1:2:165:U:C6	2.50	0.46
1:2:971:G:H1	1:2:979:U:H3	1.62	0.46
1:2:1403:U:C2'	1:2:1404:C:H5'	2.45	0.46
1:2:1412:A:C2	25:G:77:ASP:OD2	2.69	0.46
5:O:87:THR:HG21	8:T:6:PHE:CD1	2.51	0.46
24:F:35:HIS:CE1	24:F:95:TYR:HH	2.34	0.46
24:F:53:LEU:O	24:F:55:PRO:HD3	2.16	0.46
31:1:26:LYS:HA	31:1:98:SER:HB2	1.97	0.46
35:8:137:LYS:HE2	35:8:139:LEU:HD22	1.97	0.46
36:9:204:LEU:CD2	36:9:207:ILE:HG21	2.46	0.46
1:2:788:C:C2	1:2:811:G:N2	2.85	0.45
1:2:889:G:N1	1:2:890:C:C4	2.84	0.45
1:2:945:G:H2'	1:2:946:G:O4'	2.17	0.45
1:2:1402:C:O3'	25:G:33:ARG:CZ	2.65	0.45
26:I:87:GLU:O	26:I:90:GLU:HB3	2.15	0.45
31:1:34:ARG:HB2	31:1:40:MET:HG3	1.98	0.45
32:4:71:G:C6	32:4:72:C:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:74:CYS:HB3	34:7:79:SER:O	2.16	0.45
36:9:219:ILE:HG23	36:9:229:VAL:HG12	1.98	0.45
1:2:150:G:H5'	25:G:73:PRO:HB3	1.98	0.45
1:2:157:A:H8	1:2:159:C:C5	2.34	0.45
1:2:321:A:OP2	27:J:47:ARG:NH2	2.49	0.45
1:2:354:G:C2	1:2:355:C:C2	3.04	0.45
1:2:434:A:C4	20:V:85:TYR:CD1	3.01	0.45
1:2:685:G:N1	1:2:686:C:C4	2.84	0.45
1:2:906:G:C2	1:2:907:C:C2	3.04	0.45
1:2:1467:U:O4	29:0:3:TRP:CH2	2.69	0.45
1:2:1472:G:C6	1:2:1473:A:C5	3.04	0.45
12:H:63:ILE:HD13	12:H:124:VAL:HG22	1.98	0.45
12:H:93:LEU:O	12:H:95:SER:N	2.48	0.45
20:V:28:GLU:HB3	20:V:29:PRO:HD2	1.97	0.45
32:4:40:C:O2'	32:4:41:C:H5'	2.16	0.45
1:2:103:A:O2'	1:2:104:A:OP2	2.25	0.45
1:2:113:U:P	17:R:30:HIS:CE1	3.09	0.45
1:2:495:G:N3	1:2:496:C:C5	2.85	0.45
1:2:934:G:O2'	1:2:935:G:OP2	2.24	0.45
1:2:955:G:C2	1:2:956:C:C2	3.05	0.45
1:2:998:A:H2'	1:2:999:G:H5'	1.97	0.45
1:2:1260:G:C2'	1:2:1261:U:OP2	2.64	0.45
1:2:1318:U:C2	1:2:1323:A:N6	2.80	0.45
1:2:1334:A:OP2	12:H:48:HIS:HA	2.16	0.45
1:2:1352:G:H2'	1:2:1353:C:H6	1.80	0.45
1:2:1395:G:H5'	25:G:87:LEU:HD13	1.97	0.45
12:H:132:PRO:N	12:H:204:LYS:HG2	2.32	0.45
32:4:26:C:H2'	32:4:27:G:C8	2.52	0.45
34:7:183:VAL:HA	35:8:14:LEU:CD1	2.47	0.45
1:2:48:G:C2	1:2:49:C:C2	3.04	0.45
1:2:53:G:C6	1:2:54:C:C4	3.04	0.45
1:2:431:U:H2'	1:2:432:G:OP1	2.16	0.45
1:2:605:C:O2'	1:2:606:U:O5'	2.28	0.45
1:2:929:C:P	13:K:130:ARG:HH12	2.40	0.45
1:2:949:G:H2'	1:2:950:C:OP2	2.16	0.45
1:2:973:U:H3'	1:2:974:G:H5"	1.98	0.45
6:P:20:ARG:HA	6:P:26:GLN:O	2.15	0.45
12:H:75:GLY:HA2	12:H:94:ASN:CG	2.36	0.45
19:B:60:ALA:HB2	19:B:178:ASN:HB2	1.97	0.45
26:I:74:ALA:HA	26:I:127:ALA:HA	1.99	0.45
28:C:6:UNK:O	28:C:10:UNK:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:144:LEU:O	34:7:178:VAL:HG13	2.17	0.45
34:7:145:ILE:HD12	34:7:198:ILE:HG22	1.98	0.45
35:8:46:ASN:OD1	35:8:46:ASN:N	2.50	0.45
1:2:53:G:C2	1:2:54:C:C2	3.04	0.45
1:2:385:A:H2'	1:2:386:C:C5'	2.46	0.45
1:2:454:G:H2'	1:2:455:C:C6	2.51	0.45
1:2:507:G:OP1	15:N:111:PRO:CG	2.51	0.45
1:2:648:A:C2	1:2:649:A:H1'	2.52	0.45
1:2:710:G:OP1	16:Q:3:ARG:NH1	2.49	0.45
1:2:1025:U:O2'	19:B:105:ALA:CA	2.64	0.45
1:2:1044:A:C2	1:2:1045:A:C5	3.05	0.45
1:2:1132:C:H2'	1:2:1133:C:H6	1.81	0.45
1:2:1277:C:H2'	1:2:1278:A:O4'	2.16	0.45
1:2:1409:G:C2	1:2:1410:G:C8	3.04	0.45
16:Q:33:ILE:HA	16:Q:36:LEU:HD12	1.97	0.45
18:A:124:ILE:O	18:A:181:ARG:O	2.33	0.45
20:V:55:TYR:O	20:V:67:GLY:CA	2.64	0.45
23:E:204:ARG:HA	23:E:212:VAL:HG12	1.97	0.45
30:5:809:G:N3	30:5:810:G:C8	2.85	0.45
31:1:32:THR:HG23	31:1:40:MET:CB	2.39	0.45
32:4:40:C:H2'	32:4:41:C:H6	1.82	0.45
36:9:151:LEU:HD13	36:9:161:VAL:HA	1.99	0.45
1:2:256:G:H2'	1:2:257:U:O4'	2.16	0.45
1:2:271:G:C5	1:2:272:C:C5	3.04	0.45
1:2:540:G:C4'	26:I:4:LEU:HB2	2.44	0.45
1:2:1320:A:C8	6:P:14:PHE:CD2	3.05	0.45
16:Q:78:ILE:O	16:Q:81:ILE:HB	2.17	0.45
23:E:37:HIS:NE2	23:E:41:THR:HB	2.31	0.45
24:F:67:ASP:HB3	24:F:86:LEU:HD13	1.98	0.45
31:1:61:LYS:HD3	31:1:68:GLY:N	2.32	0.45
32:4:42:C:H2'	32:4:43:G:C5'	2.45	0.45
36:9:182:LEU:HA	36:9:227:TYR:O	2.17	0.45
1:2:722:G:C5	1:2:723:G:N7	2.85	0.45
1:2:836:G:OP2	26:I:76:LYS:HG3	2.16	0.45
1:2:1236:G:H2'	1:2:1237:G:O4'	2.17	0.45
12:H:13:HIS:ND1	13:K:46:LEU:HG	2.32	0.45
16:Q:128:LYS:O	16:Q:132:LEU:HD23	2.16	0.45
18:A:130:GLN:NE2	18:A:178:TYR:OH	2.50	0.45
24:F:26:VAL:HG21	24:F:49:ILE:HG23	1.99	0.45
34:7:7:GLN:OE1	34:7:289:ALA:HA	2.17	0.45
34:7:161:SER:O	34:7:165:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:163:TYR:HE1	34:7:180:ILE:HB	1.81	0.45
1:2:8:U:C2	1:2:873:A:C6	3.01	0.45
1:2:106:A:OP2	27:J:7:ARG:NH1	2.50	0.45
1:2:168:G:C6	1:2:169:C:C4	3.05	0.45
1:2:299:G:OP1	15:N:30:TYR:OH	2.35	0.45
1:2:457:G:H2'	1:2:458:G:H8	1.81	0.45
1:2:459:G:N3	1:2:459:G:C5'	2.80	0.45
1:2:820:G:C5	1:2:821:G:N7	2.85	0.45
1:2:837:C:OP1	15:N:8:ASN:N	2.48	0.45
1:2:878:U:C2	1:2:879:U:C6	3.04	0.45
1:2:992:G:C6	1:2:993:C:C4	3.04	0.45
1:2:1464:C:C2	1:2:1465:C:C6	3.04	0.45
34:7:188:LYS:HD2	35:8:131:GLY:C	2.37	0.45
36:9:132:LYS:O	36:9:133:TYR:C	2.55	0.45
1:2:53:G:C6	1:2:54:C:N3	2.84	0.45
1:2:126:G:C2	1:2:219:C:N3	2.85	0.45
1:2:643:G:C2	1:2:653:C:C4	3.05	0.45
1:2:839:G:H2'	1:2:840:C:O4'	2.17	0.45
1:2:884:G:C2	1:2:1460:G:C4	3.05	0.45
1:2:932:C:H6	1:2:932:C:O5'	1.99	0.45
1:2:1283:G:H2'	1:2:1284:C:C6	2.52	0.45
4:L:44:ARG:HG2	4:L:67:ARG:HG2	1.98	0.45
18:A:68:PHE:HB3	18:A:80:THR:HG22	1.98	0.45
25:G:6:LEU:HD13	25:G:21:ILE:HD12	1.97	0.45
32:4:42:C:H2'	32:4:43:G:C8	2.49	0.45
34:7:37:HIS:H	34:7:41:LEU:HG	1.82	0.45
35:8:81:LEU:HD23	35:8:83:ILE:HG13	1.99	0.45
36:9:176:LYS:HE3	36:9:215:LEU:HG	1.98	0.45
1:2:20:G:H4'	1:2:477:G:N2	2.32	0.45
1:2:603:G:H2'	1:2:604:C:O4'	2.17	0.45
1:2:619:A:O2'	1:2:686:C:O2'	2.24	0.45
1:2:955:G:C6	1:2:956:C:C4	3.04	0.45
1:2:1379:G:C6	1:2:1380:C:C4	3.04	0.45
1:2:1454:A:C2	1:2:1455:A:C4	3.05	0.45
24:F:131:TRP:H	24:F:139:HIS:HE1	1.65	0.45
29:0:1:MET:O	29:0:4:LYS:N	2.49	0.45
31:1:26:LYS:O	31:1:27:ILE:HD13	2.17	0.45
31:1:32:THR:O	31:1:40:MET:HB2	2.17	0.45
35:8:69:LEU:O	35:8:70:ALA:HB3	2.17	0.45
1:2:57:G:N7	1:2:58:U:C4	2.85	0.44
1:2:458:G:C2'	1:2:459:G:H5"	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:603:G:C2	1:2:604:C:C2	3.06	0.44
1:2:768:A:H4'	1:2:1466:G:H5'	1.98	0.44
1:2:813:G:C2	1:2:814:C:C2	3.05	0.44
1:2:1143:G:H3'	1:2:1144:G:H5"	1.98	0.44
1:2:1197:C:P	12:H:88:ARG:NH1	2.90	0.44
19:B:78:LYS:HE2	19:B:194:GLU:O	2.17	0.44
25:G:6:LEU:HD23	25:G:121:VAL:HG21	1.98	0.44
26:I:28:LYS:HB2	26:I:29:PRO:HD3	1.99	0.44
32:4:15:G:H22	32:4:49:C:N4	2.03	0.44
34:7:192:ASP:CG	35:8:13:ARG:NH2	2.60	0.44
34:7:323:VAL:HA	34:7:324:PRO:HD3	1.74	0.44
1:2:2:U:C5	24:F:184:TRP:CE3	3.06	0.44
1:2:94:C:H2'	1:2:95:G:O4'	2.17	0.44
1:2:1468:A:H2'	1:2:1469:G:H8	1.82	0.44
1:2:1489:A:H2'	1:2:1490:C:H5'	1.98	0.44
15:N:93:ALA:O	15:N:95:LYS:N	2.51	0.44
17:R:50:GLU:HA	17:R:69:LYS:HA	1.98	0.44
24:F:5:TRP:HA	24:F:55:PRO:HB2	1.99	0.44
32:4:30:G:O2'	32:4:31:G:H5'	2.17	0.44
34:7:150:LYS:HG2	39:7:502:GNP:C6	2.47	0.44
34:7:187:HIS:ND1	35:8:130:CYS:HA	2.31	0.44
34:7:331:ILE:O	34:7:377:GLU:HA	2.18	0.44
35:8:53:ARG:NE	35:8:53:ARG:CA	2.81	0.44
1:2:90:C:O2'	1:2:375:G:OP1	2.36	0.44
1:2:542:G:C2	1:2:543:C:C2	3.05	0.44
1:2:615:G:C6	1:2:698:A:C6	3.04	0.44
1:2:643:G:C2	1:2:644:G:C4	3.05	0.44
1:2:797:U:H2'	1:2:799:C:C5	2.52	0.44
1:2:878:U:C2	1:2:879:U:C5	3.05	0.44
1:2:878:U:N3	1:2:879:U:C5	2.86	0.44
1:2:1169:C:O2'	1:2:1174:A:N6	2.51	0.44
1:2:1264:G:N1	1:2:1265:G:N2	2.66	0.44
1:2:1341:C:H1'	10:X:20:THR:CG2	2.48	0.44
1:2:1414:G:C2'	1:2:1415:U:H5'	2.47	0.44
1:2:1467:U:O4	29:0:3:TRP:CZ3	2.70	0.44
12:H:26:VAL:HG22	12:H:121:GLN:HB2	1.98	0.44
24:F:196:ASN:O	24:F:199:LYS:N	2.51	0.44
30:5:820:U:H2'	30:5:821:G:C8	2.53	0.44
1:2:4:C:C2	1:2:5:C:C6	3.06	0.44
1:2:57:G:N7	1:2:58:U:C5	2.86	0.44
1:2:419:G:N1	1:2:420:C:C4	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:740:G:C2	1:2:751:C:N3	2.85	0.44
1:2:895:C:C2	1:2:896:A:C8	3.06	0.44
1:2:935:G:OP2	1:2:1318:U:O2'	2.33	0.44
1:2:1360:C:N4	32:4:35:C:C1'	2.81	0.44
1:2:1483:U:O2'	1:2:1484:C:H3'	2.17	0.44
1:2:1493:C:O2'	1:2:1494:C:O5'	2.36	0.44
5:O:134:ASN:O	5:O:135:PHE:CG	2.70	0.44
32:4:11:A:O2'	32:4:12:G:H5'	2.16	0.44
34:7:19:ASP:C	34:7:21:GLY:H	2.21	0.44
36:9:237:LYS:HE3	36:9:237:LYS:HB3	1.58	0.44
1:2:264:C:H2'	1:2:265:C:H6	1.82	0.44
1:2:677:U:O4	1:2:1493:C:H4'	2.16	0.44
1:2:813:G:C5	1:2:814:C:C5	3.06	0.44
1:2:895:C:H2'	1:2:896:A:H8	1.82	0.44
1:2:898:G:H2'	1:2:899:G:C8	2.53	0.44
1:2:978:G:H2'	1:2:979:U:C6	2.52	0.44
1:2:1026:A:C5'	19:B:104:PRO:CD	2.83	0.44
1:2:1333:G:H5"	12:H:97:LYS:HD2	1.98	0.44
1:2:1413:G:N2	25:G:77:ASP:OD1	2.51	0.44
18:A:18:TRP:CH2	18:A:36:PRO:HB3	2.52	0.44
18:A:135:ARG:O	18:A:138:ARG:HB2	2.18	0.44
32:4:9:G:N1	32:4:46:G:C6	2.85	0.44
32:4:54:G:C5	32:4:55:5MU:H72	2.53	0.44
34:7:189:ILE:HG22	35:8:14:LEU:HA	1.98	0.44
36:9:85:VAL:HG21	36:9:90:ARG:HH21	1.83	0.44
1:2:296:A:H1'	1:2:518:U:O2	2.17	0.44
1:2:323:A:N1	1:2:325:A:C2	2.85	0.44
1:2:533:C:N4	1:2:534:G:H1	2.14	0.44
1:2:707:A:C4'	1:2:708:C:C2	3.01	0.44
1:2:905:A:H2'	1:2:906:G:C8	2.53	0.44
1:2:1000:G:H2'	1:2:1002:G:C8	2.52	0.44
1:2:1036:G:C5	1:2:1037:U:C4	3.06	0.44
1:2:1360:C:C4'	30:5:821:G:O6	2.65	0.44
1:2:1462:A:N7	1:2:1486:A:N6	2.65	0.44
8:T:24:LEU:HB3	8:T:28:PHE:CZ	2.52	0.44
14:M:15:GLY:O	14:M:79:VAL:HG13	2.18	0.44
24:F:165:LEU:HD22	24:F:175:LEU:HD13	2.00	0.44
24:F:178:ALA:HB2	24:F:205:LEU:HD23	2.00	0.44
36:9:200:ILE:O	36:9:204:LEU:HB2	2.17	0.44
1:2:10:G:C5	1:2:1356:A:N1	2.86	0.44
1:2:194:C:H4'	27:J:43:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:414:G:C6	1:2:415:C:C4	3.05	0.44
1:2:640:U:O2	1:2:641:A:N7	2.51	0.44
1:2:685:G:N2	1:2:686:C:C2	2.86	0.44
1:2:782:A:H2'	1:2:783:G:O5'	2.18	0.44
1:2:1013:G:H4'	4:L:58:SER:O	2.18	0.44
1:2:1089:C:C4	1:2:1090:C:C5	3.05	0.44
1:2:1260:G:O2'	1:2:1261:U:OP2	2.35	0.44
1:2:1299:A:H4'	32:4:42:C:C5'	2.47	0.44
1:2:1403:U:H2'	1:2:1403:U:O2	2.18	0.44
1:2:1413:G:H5'	25:G:92:PRO:HG3	2.00	0.44
4:L:64:TRP:HE3	6:P:52:PHE:HB3	1.81	0.44
12:H:131:ALA:HB2	12:H:161:ALA:HB2	2.00	0.44
13:K:81:ALA:O	13:K:85:ALA:N	2.46	0.44
19:B:104:PRO:HB3	19:B:109:PHE:CE2	2.52	0.44
32:4:36:A:O5'	32:4:36:A:C8	2.67	0.44
35:8:64:TYR:CD2	35:8:99:PHE:HB2	2.53	0.44
1:2:40:C:C2	1:2:41:C:C5	3.06	0.44
1:2:405:G:OP1	22:D:116:ARG:NH1	2.51	0.44
1:2:853:G:H2'	1:2:854:C:C6	2.53	0.44
1:2:910:G:N7	5:O:132:ARG:NH1	2.66	0.44
1:2:935:G:N1	1:2:1323:A:C6	2.86	0.44
1:2:977:G:O2'	1:2:978:G:OP2	2.34	0.44
1:2:1298:G:N3	32:4:43:G:O4'	2.49	0.44
1:2:1313:G:C6	1:2:1314:C:C4	3.05	0.44
1:2:1372:C:H42	1:2:1443:G:H1	1.66	0.44
9:U:12:LEU:HA	9:U:136:LEU:CD1	2.48	0.44
26:I:102:LEU:HB3	26:I:113:HIS:HB2	2.00	0.44
34:7:20:HIS:CG	34:7:119:ALA:HB2	2.53	0.44
34:7:99:VAL:C	34:7:101:MET:H	2.21	0.44
36:9:98:LYS:HB2	36:9:98:LYS:HE3	1.76	0.44
1:2:87:C:C4	1:2:88:G:C8	3.06	0.44
1:2:168:G:C2	1:2:195:C:O2	2.71	0.44
1:2:641:A:H4'	1:2:642:G:O5'	2.18	0.44
1:2:677:U:N3	1:2:1493:C:C1'	2.81	0.44
1:2:880:G:C6	1:2:881:G:C6	3.06	0.44
1:2:888:A:C2'	1:2:889:G:H5'	2.48	0.44
1:2:908:G:H2'	1:2:909:U:O4'	2.17	0.44
1:2:1350:U:O2'	1:2:1351:U:H5'	2.17	0.44
1:2:1404:C:O4'	25:G:76:PRO:HB2	2.17	0.44
12:H:26:VAL:HG13	12:H:121:GLN:HG3	2.00	0.44
23:E:215:ILE:HG23	23:E:223:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:143:PHE:CE1	24:F:213:ILE:HD11	2.53	0.44
25:G:34:ILE:HG22	25:G:110:ASN:ND2	2.33	0.44
26:I:81:VAL:HG21	26:I:125:LEU:HD23	2.00	0.44
34:7:354:LYS:HE3	34:7:354:LYS:HB2	1.63	0.44
35:8:64:TYR:CE2	35:8:99:PHE:HB2	2.52	0.44
1:2:4:C:N3	1:2:5:C:C4	2.86	0.43
1:2:454:G:H2'	1:2:455:C:H6	1.82	0.43
1:2:531:G:C2'	1:2:532:C:O5'	2.65	0.43
1:2:885:G:H1	1:2:1350:U:H3	1.65	0.43
1:2:1240:A:H5"	4:L:41:PRO:HD3	2.00	0.43
1:2:1454:A:N1	1:2:1455:A:C5	2.86	0.43
12:H:173:CYS:HA	12:H:178:MET:O	2.18	0.43
19:B:104:PRO:HB3	19:B:109:PHE:CZ	2.53	0.43
19:B:104:PRO:CG	24:F:19:LYS:HE2	2.47	0.43
34:7:271:PRO:C	34:7:272:ILE:CA	2.79	0.43
1:2:108:G:C6	1:2:109:U:C4	3.07	0.43
1:2:122:C:N3	1:2:223:G:C2	2.86	0.43
1:2:246:A:O2'	1:2:247:G:OP2	2.33	0.43
1:2:723:G:C6	1:2:724:C:C4	3.06	0.43
1:2:882:C:O2'	1:2:883:G:H5'	2.18	0.43
1:2:1058:G:C2	1:2:1059:C:C2	3.06	0.43
1:2:1075:A:H2'	1:2:1076:G:O4'	2.18	0.43
1:2:1178:C:C4	1:2:1179:C:N4	2.86	0.43
1:2:1283:G:C6	1:2:1284:C:N4	2.87	0.43
1:2:1352:G:H2'	1:2:1353:C:C6	2.53	0.43
1:2:1391:U:H2'	1:2:1392:G:O4'	2.18	0.43
16:Q:115:ASP:O	16:Q:119:MET:HB2	2.18	0.43
18:A:45:ASN:HB3	18:A:46:ARG:NH1	2.33	0.43
19:B:75:TYR:HA	19:B:197:MET:SD	2.58	0.43
22:D:14:PRO:HD3	22:D:22:ARG:NH2	2.33	0.43
25:G:84:VAL:HG12	25:G:85:ARG:N	2.32	0.43
25:G:113:SER:HB3	25:G:114:PRO:CD	2.48	0.43
30:5:819:A:N3	31:1:35:ARG:NH1	2.65	0.43
31:1:39:LEU:O	31:1:79:GLY:C	2.56	0.43
1:2:613:C:H2'	1:2:614:G:C8	2.54	0.43
1:2:745:G:H2'	1:2:746:A:H5'	1.99	0.43
1:2:798:U:O2	1:2:798:U:O4'	2.37	0.43
1:2:921:G:H2'	1:2:922:G:O4'	2.18	0.43
1:2:1248:A:HO2'	1:2:1312:C:HO2'	1.66	0.43
1:2:1405:C:C4	1:2:1406:U:C5	3.06	0.43
35:8:44:ILE:HG22	35:8:44:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:4:SER:HB2	36:9:34:TYR:HA	1.98	0.43
1:2:229:G:N2	1:2:230:C:C4	2.85	0.43
1:2:531:G:C5	1:2:532:C:C5	3.07	0.43
1:2:766:G:O2'	1:2:767:U:OP2	2.30	0.43
1:2:806:G:H2'	1:2:807:C:C6	2.54	0.43
1:2:868:C:C4'	1:2:1373:A:O2'	2.66	0.43
1:2:881:G:C2	1:2:882:C:C2	3.06	0.43
1:2:1024:G:C5	1:2:1025:U:C4	3.06	0.43
1:2:1053:A:N6	19:B:99:GLY:N	2.58	0.43
1:2:1193:G:C6	1:2:1194:C:C4	3.06	0.43
1:2:1269:G:C5	1:2:1270:C:C5	3.06	0.43
1:2:1350:U:O4	1:2:1351:U:O4	2.36	0.43
1:2:1414:G:C5	1:2:1415:U:C4	3.06	0.43
1:2:1472:G:C6	1:2:1473:A:C6	3.06	0.43
1:2:1475:C:H2'	1:2:1476:C:H6	1.83	0.43
24:F:34:ILE:HD11	24:F:121:ILE:HD13	2.01	0.43
32:4:43:G:C2	32:4:44:A:C5	3.06	0.43
34:7:189:ILE:CB	35:8:14:LEU:CG	2.93	0.43
34:7:203:LYS:HB3	34:7:203:LYS:HE3	1.74	0.43
36:9:45:GLU:HB3	36:9:81:SER:CB	2.49	0.43
36:9:94:ASN:OD1	36:9:236:PRO:CD	2.67	0.43
1:2:4:C:O2'	1:2:5:C:O5'	2.37	0.43
1:2:13:C:C4	1:2:14:C:C5	3.06	0.43
1:2:37:G:C2	1:2:397:C:C2	3.07	0.43
1:2:94:C:O2'	23:E:9:HIS:CE1	2.72	0.43
1:2:366:C:C2	1:2:388:G:N2	2.87	0.43
1:2:441:U:N3	1:2:442:C:C4	2.86	0.43
1:2:647:G:O6	1:2:742:U:C5'	2.65	0.43
1:2:649:A:H2	1:2:740:G:HO2'	1.62	0.43
1:2:733:C:H2'	1:2:734:G:O4'	2.18	0.43
1:2:772:G:O2'	1:2:774:U:OP2	2.25	0.43
1:2:836:G:H5'	26:I:4:LEU:HD11	2.00	0.43
1:2:901:G:C2	1:2:1302:C:C2	3.07	0.43
1:2:1179:C:H2'	1:2:1180:G:C8	2.54	0.43
1:2:1325:C:N4	1:2:1326:G:O6	2.50	0.43
1:2:1404:C:C2	1:2:1405:C:C6	3.06	0.43
1:2:1481:G:C6	1:2:1482:C:C4	3.06	0.43
36:9:209:GLN:CA	36:9:212:GLU:HG3	2.44	0.43
1:2:72:C:H3'	1:2:73:U:H6	1.83	0.43
1:2:185:G:H2'	1:2:186:U:O4'	2.19	0.43
1:2:263:C:H2'	1:2:264:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:354:G:C6	1:2:355:C:C4	3.07	0.43
1:2:540:G:H4'	26:I:4:LEU:CB	2.47	0.43
1:2:566:C:H4'	22:D:54:ARG:NH1	2.34	0.43
1:2:901:G:N1	1:2:1302:C:C4	2.86	0.43
1:2:906:G:H2'	1:2:907:C:O4'	2.18	0.43
1:2:1031:G:C2	1:2:1032:A:N1	2.87	0.43
1:2:1249:A:OP1	12:H:82:ALA:CB	2.67	0.43
1:2:1394:G:H5"	25:G:104:LYS:HE3	2.00	0.43
1:2:1487:U:H3'	1:2:1487:U:H6	1.84	0.43
1:2:1489:A:N1	1:2:1490:C:C4	2.87	0.43
15:N:11:PHE:CZ	17:R:54:TYR:CZ	3.06	0.43
19:B:167:ILE:HA	19:B:170:ILE:HG22	2.00	0.43
29:0:9:ARG:O	29:0:13:LEU:HG	2.19	0.43
30:5:815:U:H1'	30:5:816:U:H5	1.84	0.43
31:1:34:ARG:CD	31:1:40:MET:HG3	2.49	0.43
32:4:43:G:N1	32:4:44:A:N7	2.66	0.43
33:6:96:ARG:HD3	33:6:96:ARG:HA	1.70	0.43
34:7:41:LEU:HB3	34:7:45:MET:O	2.17	0.43
34:7:182:PRO:HG3	35:8:7:TYR:OH	2.19	0.43
34:7:330:ARG:HB3	34:7:414:GLU:HB2	2.01	0.43
34:7:342:ALA:HB3	34:7:344:GLU:O	2.18	0.43
1:2:82:G:C5	1:2:83:C:C5	3.06	0.43
1:2:528:G:HO2'	1:2:529:C:P	2.42	0.43
1:2:605:C:H2'	1:2:606:U:C6	2.54	0.43
1:2:642:G:C4	1:2:643:G:C8	3.07	0.43
1:2:1134:G:OP1	12:H:55:HIS:NE2	2.50	0.43
4:L:45:ILE:HD12	4:L:66:LEU:HB3	2.01	0.43
10:X:18:THR:C	10:X:24:VAL:HG13	2.39	0.43
17:R:74:ASN:ND2	17:R:78:ILE:O	2.45	0.43
25:G:94:PHE:HD2	25:G:105:LYS:HG2	1.84	0.43
34:7:58:VAL:HG12	34:7:84:LYS:HG3	2.00	0.43
34:7:358:MET:HA	34:7:367:LEU:HD23	2.00	0.43
35:8:56:ARG:NH2	35:8:115:ILE:O	2.52	0.43
1:2:1:A:P	24:F:166:VAL:CG1	3.07	0.43
1:2:106:A:C6	1:2:107:C:C2	3.07	0.43
1:2:121:C:O2	1:2:122:C:C6	2.71	0.43
1:2:457:G:C4	1:2:488:A:C2	3.07	0.43
1:2:495:G:N3	1:2:496:C:C6	2.87	0.43
1:2:786:G:H1	1:2:812:U:H3	1.67	0.43
1:2:1193:G:H2'	1:2:1194:C:H6	1.82	0.43
1:2:1385:U:C2	1:2:1386:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:31:THR:HG22	14:M:38:THR:HA	2.01	0.43
32:4:77:A:H2'	34:7:280:ARG:CZ	2.44	0.43
34:7:404:ARG:HD3	34:7:406:ARG:NH2	2.34	0.43
35:8:125:ILE:HD11	35:8:136:VAL:HG11	2.00	0.43
36:9:184:THR:HA	36:9:225:PRO:O	2.18	0.43
36:9:195:LYS:HD2	36:9:257:GLU:OE1	2.18	0.43
1:2:248:U:H2'	1:2:249:U:C5	2.54	0.43
1:2:458:G:H3'	1:2:459:G:H5"	2.01	0.43
1:2:830:A:N7	1:2:832:G:C8	2.86	0.43
1:2:1312:C:P	12:H:78:HIS:O	2.76	0.43
1:2:1414:G:C8	1:2:1414:G:O5'	2.72	0.43
9:U:136:LEU:O	9:U:140:LEU:HG	2.18	0.43
24:F:153:ARG:HD2	24:F:153:ARG:N	2.34	0.43
30:5:819:A:N6	32:4:38:A:N6	2.67	0.43
31:1:31:VAL:HG13	31:1:82:ARG:HD2	2.00	0.43
31:1:35:ARG:HH11	31:1:36:PHE:HB2	1.76	0.43
36:9:183:ILE:HG12	36:9:227:TYR:HB2	2.00	0.43
1:2:174:G:C2	1:2:189:C:C2	3.07	0.43
1:2:180:G:C2	1:2:184:G:C6	3.07	0.43
1:2:257:U:C5	27:J:116:GLN:NE2	2.85	0.43
1:2:426:C:C2	1:2:445:G:N2	2.87	0.43
1:2:1334:A:H1'	12:H:69:ASN:ND2	2.34	0.43
1:2:1414:G:C4'	25:G:78:ILE:HG23	2.49	0.43
10:X:46:ARG:HH11	10:X:46:ARG:HB2	1.83	0.43
23:E:195:ARG:HD3	23:E:195:ARG:N	2.34	0.43
27:J:11:LYS:C	27:J:13:SER:H	2.22	0.43
34:7:318:LEU:HD23	34:7:318:LEU:HA	1.60	0.43
34:7:358:MET:N	34:7:405:TRP:CZ3	2.87	0.43
36:9:21:GLN:HB3	36:9:23:PHE:CE1	2.54	0.43
36:9:161:VAL:O	36:9:164:LEU:HB2	2.19	0.43
36:9:183:ILE:CG1	36:9:227:TYR:HB2	2.48	0.43
36:9:217:ILE:HG12	36:9:231:VAL:HA	1.99	0.43
36:9:228:ARG:HD3	36:9:230:ASP:OD1	2.19	0.43
36:9:240:SER:O	36:9:244:ASN:N	2.48	0.43
1:2:6:G:C6	24:F:192:ARG:NH2	2.87	0.42
1:2:157:A:OP2	1:2:159:C:N4	2.51	0.42
1:2:412:U:C5	1:2:413:G:H1'	2.54	0.42
1:2:486:A:C6	1:2:489:C:C4	3.07	0.42
1:2:811:G:C6	1:2:812:U:C4	3.06	0.42
1:2:1142:G:H5"	1:2:1143:G:OP1	2.19	0.42
1:2:1309:A:C2	1:2:1334:A:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1327:C:O2'	4:L:48:THR:HB	2.18	0.42
4:L:16:LEU:CD2	4:L:69:HIS:HB2	2.49	0.42
9:U:88:GLU:HG3	12:H:85:PHE:CE2	2.54	0.42
16:Q:149:ASP:H	16:Q:152:THR:HG22	1.83	0.42
17:R:43:PRO:HB2	17:R:46:THR:HB	2.00	0.42
18:A:11:ASP:HA	18:A:15:LEU:HD13	2.00	0.42
31:1:34:ARG:HB2	31:1:40:MET:CG	2.49	0.42
35:8:69:LEU:HD22	35:8:87:PHE:CD2	2.54	0.42
35:8:76:ASP:HB2	35:8:80:GLU:N	2.33	0.42
36:9:60:GLU:O	36:9:61:ASN:ND2	2.51	0.42
1:2:314:G:H1'	1:2:1424:G:H5'	2.01	0.42
1:2:318:C:H4'	25:G:102:ARG:CD	2.47	0.42
1:2:457:G:H1'	1:2:488:A:C6	2.54	0.42
1:2:472:C:H2'	1:2:473:A:O4'	2.19	0.42
1:2:535:U:C2	1:2:536:A:C8	3.07	0.42
1:2:707:A:O4'	1:2:708:C:N3	2.52	0.42
1:2:787:U:H2'	1:2:788:C:C6	2.54	0.42
1:2:1112:G:H5"	4:L:13:VAL:HG13	2.01	0.42
1:2:1317:G:OP1	1:2:1319:C:N4	2.52	0.42
1:2:1395:G:H5'	25:G:87:LEU:CD1	2.49	0.42
1:2:1401:U:N3	1:2:1402:C:C4	2.87	0.42
15:N:24:ARG:NE	15:N:30:TYR:CZ	2.87	0.42
18:A:57:GLY:O	18:A:61:LYS:HG2	2.19	0.42
24:F:46:GLU:HB2	24:F:49:ILE:CD1	2.49	0.42
34:7:189:ILE:HB	35:8:14:LEU:CG	2.49	0.42
1:2:229:G:H2'	1:2:230:C:C6	2.54	0.42
1:2:234:G:C5'	17:R:55:PHE:CZ	3.02	0.42
1:2:643:G:N1	1:2:653:C:C4	2.87	0.42
1:2:974:G:C8	1:2:974:G:O5'	2.73	0.42
1:2:1033:G:P	24:F:102:HIS:NE2	2.93	0.42
1:2:1124:G:C6	1:2:1125:C:C4	3.07	0.42
1:2:1184:U:H4'	1:2:1185:A:OP1	2.19	0.42
1:2:1197:C:P	12:H:88:ARG:HH12	2.42	0.42
10:X:7:TYR:CD2	10:X:60:THR:HG22	2.54	0.42
15:N:51:ARG:HA	15:N:104:ILE:HA	2.01	0.42
16:Q:4:MET:HA	16:Q:7:ARG:CG	2.49	0.42
22:D:105:LEU:HA	22:D:144:VAL:HG21	2.00	0.42
24:F:165:LEU:HG	24:F:181:GLN:O	2.19	0.42
36:9:235:ASN:HB3	36:9:238:GLU:CD	2.40	0.42
1:2:372:G:H2'	1:2:373:C:H6	1.82	0.42
1:2:498:C:C2	1:2:499:G:C8	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:531:G:N2	1:2:532:C:C2	2.88	0.42
1:2:839:G:C4	1:2:840:C:C6	3.07	0.42
1:2:885:G:H2'	1:2:886:G:H8	1.84	0.42
1:2:932:C:H3'	1:2:933:G:H5"	2.01	0.42
1:2:1053:A:O4'	19:B:98:PRO:HG2	2.20	0.42
1:2:1267:U:H5"	5:O:125:PRO:HG3	2.01	0.42
1:2:1384:G:C2	1:2:1432:U:O2	2.72	0.42
1:2:1395:G:H8	1:2:1395:G:O5'	2.02	0.42
7:S:8:PHE:O	7:S:12:VAL:HG23	2.18	0.42
12:H:79:TYR:O	12:H:88:ARG:HG2	2.19	0.42
16:Q:108:HIS:CE1	16:Q:112:HIS:CD2	3.07	0.42
17:R:91:THR:OG1	17:R:92:ARG:N	2.52	0.42
23:E:192:ASN:HA	23:E:195:ARG:HH21	1.81	0.42
25:G:40:ALA:HB3	25:G:59:VAL:CG1	2.42	0.42
34:7:203:LYS:O	34:7:205:PRO:HD3	2.19	0.42
36:9:83:LYS:C	36:9:85:VAL:H	2.19	0.42
36:9:141:GLU:O	36:9:141:GLU:HG3	2.19	0.42
36:9:142:LYS:HB3	36:9:150:ILE:HD13	2.01	0.42
1:2:22:G:H5'	22:D:15:PRO:O	2.20	0.42
1:2:323:A:C2	1:2:325:A:N3	2.87	0.42
1:2:486:A:H2'	1:2:488:A:OP2	2.18	0.42
1:2:524:U:C5'	1:2:773:A:C5	3.02	0.42
1:2:597:C:C4	1:2:598:U:C5	3.08	0.42
1:2:649:A:C2	1:2:741:A:O4'	2.72	0.42
1:2:832:G:C6	1:2:833:C:C4	3.08	0.42
1:2:1120:G:N1	1:2:1121:C:C4	2.87	0.42
1:2:1249:A:O2'	12:H:80:LYS:NZ	2.40	0.42
1:2:1352:G:C2	1:2:1353:C:C2	3.07	0.42
1:2:1470:G:N2	1:2:1476:C:C2	2.88	0.42
4:L:45:ILE:HG23	4:L:66:LEU:O	2.20	0.42
24:F:175:LEU:O	24:F:178:ALA:HB3	2.19	0.42
25:G:52:GLY:HA2	25:G:53:LYS:HA	1.85	0.42
30:5:809:G:H2'	30:5:810:G:H8	1.85	0.42
34:7:160:LEU:O	34:7:163:TYR:HB3	2.19	0.42
34:7:274:THR:HG23	36:9:190:PRO:O	2.19	0.42
34:7:301:LEU:O	34:7:301:LEU:HD12	2.20	0.42
36:9:7:LYS:HG3	36:9:8:LEU:N	2.34	0.42
1:2:105:C:H4'	1:2:106:A:OP1	2.19	0.42
1:2:354:G:H2'	1:2:355:C:C6	2.54	0.42
1:2:480:G:C2	1:2:481:C:C2	3.08	0.42
1:2:898:G:C2	1:2:899:G:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1200:U:H5	12:H:92:SER:N	2.17	0.42
12:H:61:VAL:CG1	12:H:66:ARG:HG2	2.49	0.42
19:B:57:LYS:HB3	28:C:26:UNK:CB	2.50	0.42
20:V:28:GLU:CB	20:V:29:PRO:HD2	2.49	0.42
20:V:54:GLN:O	20:V:55:TYR:C	2.58	0.42
26:I:89:TRP:CZ3	26:I:93:PHE:CE1	3.08	0.42
27:J:113:ARG:O	27:J:117:ASP:OD2	2.38	0.42
30:5:812:G:C5	30:5:813:A:C4	3.08	0.42
34:7:187:HIS:CA	35:8:130:CYS:CA	2.92	0.42
34:7:249:VAL:HG12	34:7:250:ASP:CG	2.40	0.42
36:9:40:PHE:O	36:9:79:ASP:HA	2.19	0.42
1:2:10:G:C8	1:2:1356:A:C4	3.08	0.42
1:2:22:G:H2'	1:2:23:G:O5'	2.19	0.42
1:2:152:G:C1'	25:G:64:ARG:NH1	2.83	0.42
1:2:253:G:C6	1:2:254:G:C5	3.08	0.42
1:2:265:C:H2'	1:2:266:A:C8	2.55	0.42
1:2:297:G:C5	1:2:298:C:C5	3.08	0.42
1:2:523:C:O4'	1:2:774:U:C2	2.73	0.42
1:2:566:C:C4'	22:D:54:ARG:CZ	2.97	0.42
1:2:984:C:H1'	11:Y:32:ALA:HB2	2.01	0.42
1:2:1027:C:H4'	1:2:1053:A:N6	2.34	0.42
1:2:1483:U:O2'	1:2:1484:C:O5'	2.31	0.42
3:3:58:ASP:HA	3:3:59:PRO:C	2.40	0.42
8:T:30:ALA:HA	8:T:33:ARG:HD3	2.02	0.42
18:A:70:VAL:O	18:A:70:VAL:HG23	2.19	0.42
32:4:62:C:O2'	32:4:63:C:H5'	2.20	0.42
34:7:190:ASN:N	35:8:14:LEU:HG	2.35	0.42
1:2:112:G:O5'	1:2:112:G:C8	2.66	0.42
1:2:422:U:H5"	1:2:423:U:OP1	2.19	0.42
1:2:505:U:C5'	15:N:108:ILE:HD12	2.50	0.42
1:2:574:A:H2'	1:2:575:A:C8	2.55	0.42
1:2:599:G:C4	1:2:600:C:C6	3.08	0.42
1:2:749:C:OP2	1:2:750:C:N4	2.51	0.42
1:2:853:G:C2	1:2:854:C:C2	3.08	0.42
1:2:853:G:C6	1:2:854:C:C4	3.08	0.42
1:2:889:G:C6	1:2:890:C:C4	3.08	0.42
1:2:1307:G:HO2'	1:2:1308:U:P	2.41	0.42
1:2:1307:G:C2'	1:2:1308:U:OP2	2.68	0.42
5:O:78:ALA:CB	9:U:35:VAL:HG21	2.50	0.42
9:U:5:TYR:O	13:K:32:PRO:HD2	2.20	0.42
12:H:108:PHE:HA	12:H:111:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:85:ALA:HB1	14:M:86:PRO:HD2	2.00	0.42
24:F:123:GLU:O	24:F:209:ASN:ND2	2.53	0.42
36:9:31:LEU:HG	36:9:37:LEU:O	2.20	0.42
1:2:234:G:O2'	1:2:235:G:H5'	2.20	0.42
1:2:419:G:C6	1:2:420:C:C4	3.07	0.42
1:2:803:C:P	18:A:128:ARG:HH11	2.42	0.42
1:2:985:C:H1'	11:Y:41:GLY:HA3	2.01	0.42
1:2:1275:U:O4	1:2:1276:G:C6	2.73	0.42
1:2:1275:U:C2	1:2:1279:A:N6	2.87	0.42
1:2:1312:C:H5'	12:H:80:LYS:HE3	2.01	0.42
1:2:1414:G:H5"	25:G:86:VAL:CG2	2.50	0.42
1:2:1451:C:H4'	31:1:78:GLN:CB	2.43	0.42
7:S:3:LYS:C	7:S:3:LYS:HD3	2.40	0.42
8:T:44:GLN:HE22	8:T:47:LEU:HD23	1.84	0.42
33:6:92:ASP:O	33:6:96:ARG:HG2	2.19	0.42
34:7:38:SER:C	34:7:40:GLU:N	2.69	0.42
36:9:247:ILE:O	36:9:251:ILE:HG13	2.19	0.42
36:9:250:LEU:HB3	36:9:261:ILE:HG21	2.01	0.42
1:2:4:C:H2'	1:2:5:C:C6	2.54	0.42
1:2:81:C:N3	1:2:82:G:N7	2.68	0.42
1:2:97:C:H2'	1:2:98:U:C6	2.55	0.42
1:2:387:G:C2	1:2:388:G:C4	3.08	0.42
1:2:432:G:C6	1:2:433:U:C5	3.08	0.42
1:2:459:G:C2	1:2:460:C:C2	3.08	0.42
1:2:531:G:C4	1:2:532:C:C6	3.07	0.42
1:2:616:G:N2	1:2:697:A:C2	2.88	0.42
1:2:887:G:N2	1:2:1348:C:O2	2.51	0.42
1:2:1128:U:O2	1:2:1128:U:O4'	2.38	0.42
1:2:1200:U:OP1	12:H:179:SER:HA	2.19	0.42
1:2:1284:C:H2'	1:2:1285:C:H6	1.83	0.42
4:L:51:LYS:HA	6:P:44:ARG:HD2	2.02	0.42
9:U:80:ARG:HE	12:H:81:VAL:CG1	2.30	0.42
15:N:30:TYR:CE2	15:N:34:VAL:HG21	2.55	0.42
18:A:121:ALA:HB3	18:A:141:MET:CE	2.49	0.42
19:B:77:GLN:NE2	19:B:92:ILE:O	2.51	0.42
32:4:20:G:C2	32:4:58:A:N3	2.88	0.42
32:4:34:U:O5'	32:4:34:U:H6	2.01	0.42
34:7:366:THR:HG21	34:7:384:ARG:O	2.20	0.42
1:2:29:G:C2	1:2:30:C:C2	3.08	0.41
1:2:164:A:H2'	1:2:165:U:H6	1.85	0.41
1:2:276:A:C5	17:R:67:ARG:HD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:350:G:C6	1:2:351:C:C4	3.07	0.41
1:2:552:C:H4'	26:I:122:GLY:C	2.41	0.41
1:2:649:A:C6	1:2:650:A:C6	3.08	0.41
1:2:732:G:H2'	1:2:733:C:O4'	2.20	0.41
1:2:782:A:C2'	1:2:783:G:O5'	2.68	0.41
1:2:858:A:H2'	1:2:859:A:C8	2.55	0.41
1:2:1379:G:C6	1:2:1380:C:N3	2.88	0.41
1:2:1390:G:H2'	1:2:1391:U:O4'	2.20	0.41
12:H:21:TRP:CD1	12:H:119:PRO:CD	3.01	0.41
15:N:72:ALA:CA	15:N:86:ALA:O	2.65	0.41
19:B:173:ARG:HG2	19:B:184:SER:HA	2.01	0.41
24:F:214:SER:O	24:F:217:MET:HB2	2.19	0.41
34:7:51:TYR:CD2	34:7:294:LEU:HD13	2.54	0.41
35:8:137:LYS:HA	35:8:138:PRO:HD2	1.91	0.41
36:9:143:ALA:HA	36:9:150:ILE:HD12	2.00	0.41
36:9:177:VAL:HG21	36:9:236:PRO:HG3	2.02	0.41
1:2:298:C:H4'	15:N:24:ARG:HH22	1.86	0.41
1:2:846:G:H3'	1:2:847:A:H2'	2.01	0.41
1:2:955:G:C5	1:2:956:C:C4	3.08	0.41
1:2:1031:G:C6	1:2:1032:A:N6	2.88	0.41
1:2:1117:A:O4'	1:2:1118:C:C2	2.73	0.41
1:2:1175:C:O2	1:2:1175:C:H2'	2.20	0.41
1:2:1479:C:C4	1:2:1480:G:N7	2.88	0.41
10:X:11:VAL:HA	10:X:29:VAL:HA	2.02	0.41
12:H:111:ILE:HG23	12:H:119:PRO:HB3	2.01	0.41
15:N:24:ARG:HG2	15:N:30:TYR:CD2	2.54	0.41
25:G:10:ASP:HA	25:G:123:LEU:HB2	2.02	0.41
25:G:103:ARG:HG2	25:G:105:LYS:HD3	2.02	0.41
27:J:67:ASP:HB3	27:J:68:LYS:H	1.70	0.41
31:1:33:LYS:CG	32:4:27:G:C5'	2.81	0.41
1:2:66:G:H2'	1:2:67:C:O4'	2.21	0.41
1:2:130:G:C2	1:2:163:C:C2	3.08	0.41
1:2:647:G:C6	1:2:648:A:C5	3.08	0.41
1:2:861:G:C2	1:2:862:C:C2	3.08	0.41
1:2:867:A:H2'	1:2:1374:C:H4'	2.01	0.41
1:2:879:U:C4'	24:F:73:ARG:CZ	2.94	0.41
1:2:889:G:N2	1:2:890:C:C2	2.88	0.41
1:2:944:C:C2	1:2:1181:G:N2	2.89	0.41
1:2:1189:G:OP1	5:O:137:ARG:HA	2.20	0.41
1:2:1193:G:C4	1:2:1194:C:C5	3.09	0.41
1:2:1260:G:HO2'	1:2:1261:U:H6	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1275:U:C4	1:2:1276:G:N1	2.88	0.41
1:2:1372:C:O2'	15:N:121:GLY:HA2	2.21	0.41
1:2:1466:G:H2'	1:2:1467:U:O4'	2.21	0.41
20:V:57:ARG:HH21	20:V:58:SER:C	2.23	0.41
22:D:111:LYS:HA	22:D:177:GLY:CA	2.51	0.41
24:F:40:ARG:HB3	24:F:42:TYR:CD1	2.56	0.41
24:F:163:LEU:HD11	24:F:184:TRP:CZ2	2.56	0.41
24:F:173:LYS:O	24:F:177:LEU:HG	2.20	0.41
31:1:33:LYS:CA	32:4:27:G:OP1	2.60	0.41
34:7:189:ILE:CG2	35:8:14:LEU:O	2.65	0.41
34:7:231:ASN:OD1	34:7:231:ASN:N	2.53	0.41
36:9:240:SER:HB2	36:9:244:ASN:OD1	2.19	0.41
1:2:239:A:H4'	1:2:240:U:H5'	2.02	0.41
1:2:372:G:H2'	1:2:373:C:O4'	2.19	0.41
1:2:521:G:N2	1:2:522:C:C2	2.88	0.41
1:2:641:A:C2	1:2:642:G:C4	3.05	0.41
1:2:779:G:C2	1:2:780:C:C2	3.09	0.41
1:2:874:G:N2	1:2:875:G:C4	2.89	0.41
1:2:888:A:H2'	1:2:889:G:H5'	2.01	0.41
1:2:1115:G:C6	1:2:1116:G:C5	3.08	0.41
1:2:1120:G:N3	1:2:1121:C:C6	2.88	0.41
1:2:1370:U:O2	1:2:1370:U:H2'	2.20	0.41
17:R:89:ALA:HB2	17:R:103:VAL:HG11	2.03	0.41
19:B:52:LEU:O	19:B:52:LEU:HD13	2.20	0.41
24:F:119:LEU:H	24:F:119:LEU:HD22	1.84	0.41
32:4:23:G:H2'	32:4:24:C:H5'	2.01	0.41
34:7:188:LYS:CE	35:8:131:GLY:C	2.73	0.41
35:8:44:ILE:HG22	35:8:47:PHE:H	1.85	0.41
36:9:28:TYR:HE1	36:9:40:PHE:HD2	1.69	0.41
36:9:29:VAL:O	36:9:38:GLN:HA	2.20	0.41
36:9:55:ARG:H	36:9:55:ARG:HG3	1.55	0.41
36:9:114:LEU:HD21	36:9:163:PRO:CG	2.51	0.41
36:9:136:PRO:O	36:9:140:ILE:HG13	2.20	0.41
1:2:368:C:N4	1:2:384:G:OP2	2.53	0.41
1:2:563:U:C4	1:2:564:C:C5	3.08	0.41
1:2:895:C:H2'	1:2:896:A:C8	2.56	0.41
1:2:1026:A:C6	1:2:1027:C:C4	3.07	0.41
1:2:1341:C:C1'	10:X:20:THR:HG1	2.33	0.41
18:A:12:LYS:N	18:A:13:TRP:HA	2.35	0.41
20:V:32:SER:O	20:V:35:ASP:N	2.51	0.41
22:D:158:SER:HB2	22:D:159:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:139:HIS:NE2	24:F:159:GLY:O	2.45	0.41
24:F:143:PHE:CE2	26:I:96:ALA:HB3	2.54	0.41
25:G:67:THR:HG23	25:G:118:GLN:HE22	1.85	0.41
27:J:4:TRP:HB2	27:J:5:GLN:HA	2.03	0.41
31:1:36:PHE:CD1	31:1:37:GLY:N	2.89	0.41
32:4:6:G:H1	32:4:68:C:H42	1.69	0.41
32:4:43:G:N2	32:4:44:A:C4	2.89	0.41
32:4:45:A:H2'	32:4:46:G:O4'	2.20	0.41
34:7:33:TRP:HZ2	34:7:36:LYS:NZ	2.18	0.41
34:7:95:PRO:HG2	34:7:100:LEU:CB	2.51	0.41
35:8:53:ARG:O	35:8:54:ILE:CG2	2.68	0.41
1:2:166:A:N6	1:2:196:G:O2'	2.51	0.41
1:2:355:C:H2'	1:2:356:G:H8	1.85	0.41
1:2:457:G:C2	1:2:458:G:C4	3.09	0.41
1:2:1041:C:C4'	10:X:71:ARG:NH2	2.84	0.41
1:2:1291:G:C2'	1:2:1292:A:OP2	2.68	0.41
2:Z:8:ILE:O	2:Z:12:VAL:HG23	2.21	0.41
12:H:48:HIS:HB3	13:K:10:ARG:NH2	2.34	0.41
13:K:19:ILE:HG23	13:K:19:ILE:O	2.20	0.41
19:B:104:PRO:HG2	24:F:19:LYS:CE	2.49	0.41
23:E:179:PHE:HB3	23:E:232:VAL:HG21	2.03	0.41
26:I:95:PRO:HD3	26:I:130:TYR:CG	2.55	0.41
34:7:37:HIS:O	34:7:39:GLU:N	2.54	0.41
34:7:151:VAL:HG22	34:7:183:VAL:O	2.21	0.41
34:7:261:VAL:HG12	34:7:262:GLU:N	2.36	0.41
36:9:20:LYS:HG2	36:9:21:GLN:HG3	2.02	0.41
1:2:199:A:C6	1:2:217:C:C4'	3.03	0.41
1:2:239:A:C2	1:2:241:U:H2'	2.55	0.41
1:2:330:U:O4	1:2:331:C:N4	2.53	0.41
1:2:451:A:C6	1:2:500:A:C8	3.09	0.41
1:2:883:G:H1	1:2:1351:U:H3	1.66	0.41
1:2:1053:A:H2	19:B:98:PRO:O	1.97	0.41
1:2:1161:A:H1'	1:2:1162:G:OP2	2.20	0.41
1:2:1169:C:HO2'	1:2:1174:A:N6	2.18	0.41
1:2:1253:G:C2	1:2:1254:C:C2	3.08	0.41
1:2:1468:A:H2'	1:2:1469:G:C8	2.55	0.41
34:7:51:TYR:OH	34:7:90:SER:HB2	2.20	0.41
34:7:140:GLY:O	34:7:142:LYS:HG2	2.20	0.41
36:9:64:VAL:HG11	36:9:82:LEU:CD2	2.51	0.41
1:2:14:C:H2'	1:2:15:U:C6	2.55	0.41
1:2:132:G:N2	1:2:161:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:152:G:C4'	25:G:64:ARG:HD2	2.45	0.41
1:2:238:G:H8	1:2:238:G:O5'	2.03	0.41
1:2:314:G:N2	1:2:332:C:C2	2.89	0.41
1:2:318:C:H2'	1:2:319:U:C6	2.55	0.41
1:2:375:G:O2'	1:2:376:G:H5'	2.21	0.41
1:2:387:G:C6	1:2:388:G:C5	3.08	0.41
1:2:695:G:H2'	1:2:696:G:O4'	2.20	0.41
1:2:732:G:C2	1:2:733:C:C2	3.09	0.41
1:2:1026:A:C3'	19:B:102:THR:OG1	2.67	0.41
1:2:1072:C:N3	1:2:1114:G:C2	2.89	0.41
1:2:1317:G:C6	1:2:1318:U:N3	2.89	0.41
1:2:1428:G:C6	1:2:1429:G:C5	3.09	0.41
3:3:26:ALA:HB2	3:3:101:ILE:HD12	2.02	0.41
13:K:13:ALA:HA	13:K:68:GLY:HA3	2.01	0.41
14:M:124:ASP:CG	14:M:125:GLY:N	2.74	0.41
24:F:128:CYS:SG	24:F:138:PRO:HG3	2.60	0.41
24:F:164:GLY:HA2	24:F:182:ASP:HA	2.03	0.41
34:7:132:HIS:O	34:7:135:ALA:N	2.54	0.41
1:2:151:G:C1'	25:G:120:ASN:ND2	2.84	0.41
1:2:430:G:C6	1:2:431:U:H1'	2.56	0.41
1:2:486:A:C2	1:2:489:C:C5	3.09	0.41
1:2:608:G:C2	1:2:707:A:C4	3.09	0.41
1:2:621:G:C2	1:2:622:C:C2	3.08	0.41
1:2:681:G:N2	1:2:684:G:OP2	2.47	0.41
1:2:690:C:C2	1:2:691:G:C8	3.09	0.41
1:2:732:G:C5	1:2:733:C:C5	3.09	0.41
1:2:837:C:P	15:N:7:PRO:HA	2.61	0.41
1:2:841:C:O2'	1:2:842:U:H5'	2.20	0.41
1:2:869:U:O5'	1:2:869:U:C6	2.74	0.41
1:2:1203:G:C2	1:2:1255:C:C2	3.07	0.41
1:2:1313:G:N2	1:2:1314:C:C2	2.88	0.41
12:H:50:ARG:NH1	13:K:110:ASP:HA	2.36	0.41
12:H:80:LYS:HZ1	12:H:95:SER:HB3	1.85	0.41
15:N:128:LYS:HE2	15:N:131:ARG:HA	2.02	0.41
21:W:33:THR:HA	21:W:47:PRO:HG3	2.03	0.41
22:D:108:ILE:HD12	22:D:144:VAL:HB	2.03	0.41
22:D:136:ILE:HG22	22:D:137:ILE:N	2.35	0.41
24:F:191:THR:HG23	24:F:197:PHE:CG	2.55	0.41
32:4:4:G:O2'	32:4:5:G:C8	2.69	0.41
34:7:330:ARG:CZ	34:7:379:GLU:OE2	2.69	0.41
35:8:35:ILE:C	35:8:36:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:58:LEU:HD23	36:9:58:LEU:HA	1.96	0.41
36:9:212:GLU:HB3	36:9:213:SER:H	1.66	0.41
1:2:57:G:C8	1:2:58:U:C5	3.09	0.41
1:2:171:U:O2	1:2:192:G:N2	2.54	0.41
1:2:262:G:O2'	1:2:264:C:OP2	2.38	0.41
1:2:271:G:C4	1:2:272:C:C6	3.09	0.41
1:2:610:G:C4	1:2:611:A:C8	3.09	0.41
1:2:1269:G:C2	1:2:1270:C:C2	3.09	0.41
1:2:1345:G:H2'	1:2:1346:C:C6	2.56	0.41
1:2:1360:C:C6	32:4:35:C:N3	2.89	0.41
1:2:1360:C:N4	32:4:35:C:N1	2.68	0.41
1:2:1403:U:N1	25:G:77:ASP:OD1	2.54	0.41
4:L:50:ARG:HB2	6:P:40:ARG:HD2	2.03	0.41
12:H:174:TYR:CD2	12:H:175:ARG:HD2	2.56	0.41
15:N:10:GLU:O	17:R:63:TYR:N	2.49	0.41
15:N:19:LYS:O	15:N:23:PHE:CD2	2.74	0.41
24:F:20:THR:HG1	24:F:23:GLY:H	1.65	0.41
32:4:28:U:H6	32:4:28:U:O5'	2.03	0.41
34:7:37:HIS:H	34:7:41:LEU:CG	2.33	0.41
34:7:333:TYR:HB2	34:7:410:TRP:O	2.21	0.41
35:8:30:LEU:HD23	35:8:30:LEU:HA	1.71	0.41
1:2:140:C:O2'	25:G:16:ALA:O	2.38	0.40
1:2:534:G:N7	1:2:712:G:N7	2.70	0.40
1:2:885:G:H2'	1:2:886:G:C8	2.56	0.40
1:2:1205:G:OP1	9:U:54:ARG:NH2	2.54	0.40
1:2:1394:G:H5"	25:G:104:LYS:HE2	2.03	0.40
1:2:1413:G:N2	1:2:1414:G:C6	2.89	0.40
1:2:1413:G:N2	25:G:77:ASP:OD2	2.54	0.40
1:2:1414:G:H5"	25:G:86:VAL:HG22	2.02	0.40
1:2:1490:C:H2'	1:2:1491:C:C6	2.57	0.40
12:H:67:LEU:O	12:H:71:ILE:CG1	2.69	0.40
15:N:106:GLU:O	15:N:124:TYR:HB3	2.21	0.40
23:E:19:TRP:CD1	23:E:19:TRP:N	2.87	0.40
26:I:30:ALA:HB3	26:I:59:GLY:C	2.42	0.40
34:7:41:LEU:CD1	34:7:47:ILE:HB	2.50	0.40
36:9:39:ALA:HB1	36:9:78:VAL:O	2.21	0.40
36:9:87:ASP:OD1	36:9:87:ASP:N	2.54	0.40
1:2:492:G:C5	1:2:493:C:C5	3.09	0.40
1:2:599:G:C2	1:2:600:C:C2	3.10	0.40
1:2:643:G:N1	1:2:644:G:C4	2.89	0.40
1:2:811:G:C5	1:2:812:U:C5	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1312:C:C5’	12:H:80:LYS:HB3	2.51	0.40
1:2:1350:U:H2’	1:2:1351:U:O5’	2.21	0.40
12:H:88:ARG:O	12:H:95:SER:OG	2.39	0.40
14:M:20:TYR:CD1	14:M:84:ARG:HG3	2.56	0.40
14:M:54:GLU:HB3	14:M:55:PRO:HD3	2.03	0.40
15:N:42:ASP:HB3	15:N:123:ARG:NH2	2.36	0.40
24:F:127:GLY:O	24:F:138:PRO:HA	2.22	0.40
25:G:40:ALA:O	25:G:44:ASN:HB2	2.21	0.40
32:4:76:C:O2’	32:4:77:A:OP2	2.37	0.40
34:7:14:VAL:O	34:7:22:LYS:HD2	2.22	0.40
34:7:20:HIS:O	34:7:150:LYS:HE3	2.22	0.40
1:2:8:U:C2	1:2:874:G:N7	2.90	0.40
1:2:62:G:N7	1:2:63:G:C8	2.89	0.40
1:2:119:A:H1’	1:2:321:A:C8	2.56	0.40
1:2:330:U:C4	1:2:331:C:C4	3.09	0.40
1:2:389:G:C6	1:2:390:G:N7	2.90	0.40
1:2:474:G:C6	1:2:475:C:C5	3.09	0.40
1:2:502:U:C2	1:2:503:G:C8	3.09	0.40
1:2:556:G:N2	1:2:590:G:C4	2.89	0.40
1:2:649:A:N3	1:2:741:A:H4’	2.36	0.40
1:2:830:A:C8	1:2:832:G:H8	2.35	0.40
1:2:832:G:C2	1:2:833:C:C2	3.09	0.40
1:2:992:G:H2’	1:2:993:C:O4’	2.21	0.40
1:2:1300:A:C4’	32:4:32:G:O2’	2.64	0.40
1:2:1457:A:N3	1:2:1457:A:C2’	2.84	0.40
24:F:152:VAL:O	24:F:153:ARG:NH1	2.54	0.40
1:2:419:G:C6	1:2:420:C:C5	3.09	0.40
1:2:537:G:H2’	1:2:538:C:H6	1.84	0.40
1:2:742:U:H2’	1:2:743:U:O4’	2.21	0.40
1:2:1276:G:C8	1:2:1278:A:OP2	2.75	0.40
1:2:1386:C:C2	1:2:1387:C:C5	3.09	0.40
5:O:87:THR:HG21	8:T:6:PHE:CG	2.56	0.40
20:V:1:MET:SD	20:V:31:PRO:HB3	2.62	0.40
22:D:14:PRO:HD3	22:D:22:ARG:CZ	2.51	0.40
24:F:196:ASN:O	24:F:197:PHE:C	2.59	0.40
31:1:32:THR:O	31:1:40:MET:N	2.54	0.40
34:7:95:PRO:CB	34:7:100:LEU:HD13	2.51	0.40
34:7:195:ILE:O	34:7:199:GLU:HB2	2.21	0.40
34:7:305:LEU:HD11	36:9:188:ASN:HA	2.04	0.40
36:9:5:ARG:HD2	36:9:127:TRP:CG	2.57	0.40
36:9:151:LEU:HD12	36:9:161:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:8:U:O2	1:2:873:A:C5	2.73	0.40
1:2:93:A:C2'	1:2:322:G:N2	2.84	0.40
1:2:225:U:C2	1:2:226:G:C8	3.09	0.40
1:2:258:A:H2'	1:2:259:A:C8	2.56	0.40
1:2:266:A:C6	1:2:267:C:C4	3.10	0.40
1:2:276:A:C4'	15:N:14:ARG:NH2	2.80	0.40
1:2:509:C:OP2	15:N:33:ARG:NH1	2.54	0.40
1:2:540:G:H5'	26:I:4:LEU:HB2	2.02	0.40
1:2:692:G:C2	1:2:693:C:C2	3.10	0.40
1:2:703:U:O2'	16:Q:51:GLY:HA3	2.22	0.40
1:2:804:U:C2	1:2:805:C:C5	3.09	0.40
1:2:1307:G:O2'	1:2:1333:G:N1	2.47	0.40
1:2:1383:A:C2	1:2:1384:G:C4	3.09	0.40
1:2:1392:G:HO2'	1:2:1423:A:H61	1.64	0.40
2:Z:25:LEU:HD12	2:Z:30:TYR:CE1	2.56	0.40
12:H:122:VAL:O	12:H:192:ALA:HB2	2.22	0.40
18:A:11:ASP:C	18:A:13:TRP:HA	2.42	0.40
32:4:53:G:C2	32:4:54:G:C8	3.09	0.40
35:8:43:ILE:HA	35:8:81:LEU:O	2.21	0.40
36:9:14:ILE:HA	36:9:66:VAL:O	2.22	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
2	Z	184/210 (88%)	167 (91%)	15 (8%)	2 (1%)	14 52
3	3	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	3 25
4	L	100/102 (98%)	90 (90%)	3 (3%)	7 (7%)	1 16
5	O	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	P	54/56 (96%)	43 (80%)	10 (18%)	1 (2%)	8 40
7	S	65/67 (97%)	63 (97%)	2 (3%)	0	100 100
8	T	109/132 (83%)	97 (89%)	9 (8%)	3 (3%)	5 32
9	U	142/150 (95%)	129 (91%)	10 (7%)	3 (2%)	7 38
10	X	69/71 (97%)	56 (81%)	11 (16%)	2 (3%)	4 31
11	Y	48/50 (96%)	40 (83%)	8 (17%)	0	100 100
12	H	212/215 (99%)	161 (76%)	32 (15%)	19 (9%)	1 12
13	K	133/135 (98%)	117 (88%)	13 (10%)	3 (2%)	6 36
14	M	131/137 (96%)	116 (88%)	12 (9%)	3 (2%)	6 36
15	N	143/147 (97%)	119 (83%)	12 (8%)	12 (8%)	1 12
16	Q	156/158 (99%)	140 (90%)	12 (8%)	4 (3%)	5 33
17	R	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	17 56
18	A	188/198 (95%)	163 (87%)	15 (8%)	10 (5%)	2 21
19	B	200/202 (99%)	170 (85%)	28 (14%)	2 (1%)	15 54
20	V	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2 21
21	W	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	9 44
22	D	170/180 (94%)	148 (87%)	15 (9%)	7 (4%)	3 25
23	E	239/243 (98%)	209 (87%)	21 (9%)	9 (4%)	3 26
24	F	215/236 (91%)	176 (82%)	32 (15%)	7 (3%)	4 29
25	G	123/125 (98%)	97 (79%)	15 (12%)	11 (9%)	1 12
26	I	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	9 44
27	J	125/127 (98%)	106 (85%)	13 (10%)	6 (5%)	2 23
29	0	20/22 (91%)	20 (100%)	0	0	100 100
31	1	78/102 (76%)	70 (90%)	6 (8%)	2 (3%)	5 33
33	6	95/113 (84%)	95 (100%)	0	0	100 100
34	7	407/415 (98%)	317 (78%)	68 (17%)	22 (5%)	2 21
35	8	125/139 (90%)	95 (76%)	27 (22%)	3 (2%)	6 35
36	9	247/266 (93%)	184 (74%)	46 (19%)	17 (7%)	1 16
All	All	4441/4674 (95%)	3760 (85%)	506 (11%)	175 (4%)	5 25

All (175) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	158	ALA
4	L	30	THR
4	L	92	GLU
10	X	4	ASP
12	H	13	HIS
12	H	47	THR
12	H	50	ARG
12	H	78	HIS
12	H	81	VAL
12	H	89	GLU
12	H	92	SER
12	H	94	ASN
12	H	95	SER
15	N	36	ARG
15	N	42	ASP
15	N	43	PRO
15	N	44	LEU
15	N	63	LYS
15	N	93	ALA
15	N	112	LYS
16	Q	71	ASN
16	Q	78	ILE
18	A	45	ASN
18	A	194	PRO
20	V	61	GLY
20	V	84	GLU
20	V	95	LYS
22	D	84	PRO
22	D	163	PRO
23	E	153	ALA
24	F	92	ARG
24	F	130	SER
25	G	48	ASN
25	G	50	LEU
25	G	56	PRO
25	G	77	ASP
31	1	24	GLU
34	7	39	GLU
34	7	75	LYS
34	7	124	PHE
34	7	176	GLU
34	7	307	LYS
34	7	309	ASP

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Mol	Chain	Res	Type
36	9	74	ARG
36	9	84	LYS
36	9	132	LYS
36	9	158	GLU
36	9	239	ALA
36	9	251	ILE
3	3	95	ALA
4	L	40	LEU
4	L	88	ILE
5	O	129	GLN
9	U	35	VAL
12	H	60	ASN
12	H	77	SER
12	H	179	SER
13	K	89	TRP
13	K	133	SER
14	M	55	PRO
15	N	114	GLY
16	Q	4	MET
18	A	65	LYS
18	A	193	GLU
19	B	29	LYS
20	V	55	TYR
23	E	150	VAL
23	E	160	THR
23	E	161	SER
24	F	61	GLU
25	G	43	LEU
25	G	54	GLU
25	G	60	LYS
25	G	99	LYS
26	I	22	LYS
27	J	3	ILE
27	J	4	TRP
27	J	64	ASN
27	J	105	ILE
34	7	36	LYS
34	7	170	THR
35	8	54	ILE
36	9	44	SER
36	9	133	TYR
36	9	146	GLU

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Mol	Chain	Res	Type
36	9	210	ASP
3	3	122	MET
4	L	90	VAL
5	O	83	LYS
5	O	85	TYR
5	O	143	VAL
8	T	41	THR
9	U	67	PRO
12	H	20	ARG
12	H	158	LEU
13	K	11	LYS
15	N	120	PRO
18	A	100	THR
19	B	23	GLN
22	D	155	ALA
23	E	237	LYS
24	F	32	THR
24	F	49	ILE
24	F	132	GLU
31	1	38	LYS
34	7	72	PRO
34	7	81	ASP
34	7	98	GLU
34	7	250	ASP
36	9	212	GLU
36	9	225	PRO
36	9	250	LEU
3	3	103	GLU
8	T	8	TYR
8	T	20	SER
9	U	117	LYS
10	X	37	LYS
12	H	49	GLY
12	H	82	ALA
12	H	91	ARG
14	M	123	HIS
17	R	16	CYS
18	A	29	GLY
18	A	127	ARG
18	A	129	ILE
21	W	6	ILE
22	D	10	LYS

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Mol	Chain	Res	Type
22	D	66	ALA
24	F	39	ARG
27	J	23	LYS
34	7	61	SER
34	7	127	PRO
36	9	131	ALA
3	3	96	ALA
4	L	93	ASP
5	O	74	ILE
6	P	8	LYS
12	H	90	HIS
15	N	95	LYS
15	N	110	GLY
20	V	28	GLU
22	D	174	ALA
23	E	152	ILE
23	E	175	GLU
25	G	27	GLU
25	G	96	PRO
26	I	57	ARG
27	J	82	GLU
34	7	123	PRO
34	7	311	LEU
35	8	138	PRO
36	9	157	PRO
4	L	91	PRO
14	M	7	ASN
23	E	79	LYS
23	E	157	ASN
36	9	37	LEU
36	9	161	VAL
25	G	55	PHE
34	7	276	ILE
3	3	58	ASP
16	Q	112	HIS
34	7	141	VAL
34	7	292	GLY
5	O	123	GLY
15	N	108	ILE
18	A	39	ASP
22	D	15	PRO
34	7	226	PRO

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Mol	Chain	Res	Type
35	8	137	LYS
2	Z	58	GLY
12	H	83	GLY
18	A	57	GLY
34	7	341	GLY
34	7	393	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	145/167 (87%)	142 (98%)	3 (2%)	53	72
3	3	99/99 (100%)	93 (94%)	6 (6%)	18	45
4	L	91/91 (100%)	85 (93%)	6 (7%)	16	43
5	O	122/122 (100%)	118 (97%)	4 (3%)	38	61
6	P	46/46 (100%)	41 (89%)	5 (11%)	6	24
7	S	61/61 (100%)	58 (95%)	3 (5%)	25	51
8	T	99/114 (87%)	95 (96%)	4 (4%)	31	55
9	U	121/127 (95%)	113 (93%)	8 (7%)	16	43
10	X	60/60 (100%)	53 (88%)	7 (12%)	5	22
11	Y	41/41 (100%)	38 (93%)	3 (7%)	14	40
12	H	183/184 (100%)	167 (91%)	16 (9%)	10	33
13	K	111/111 (100%)	102 (92%)	9 (8%)	11	37
14	M	100/104 (96%)	91 (91%)	9 (9%)	9	32
15	N	118/121 (98%)	105 (89%)	13 (11%)	6	24
16	Q	143/143 (100%)	131 (92%)	12 (8%)	11	36
17	R	102/102 (100%)	99 (97%)	3 (3%)	42	64
18	A	166/171 (97%)	160 (96%)	6 (4%)	35	59
19	B	173/173 (100%)	161 (93%)	12 (7%)	15	42
20	V	89/89 (100%)	81 (91%)	8 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	W	54/54 (100%)	52 (96%)	2 (4%)	34 58
22	D	153/160 (96%)	145 (95%)	8 (5%)	23 49
23	E	212/213 (100%)	194 (92%)	18 (8%)	10 35
24	F	181/197 (92%)	173 (96%)	8 (4%)	28 53
25	G	108/108 (100%)	93 (86%)	15 (14%)	3 18
26	I	107/108 (99%)	96 (90%)	11 (10%)	7 26
27	J	103/103 (100%)	99 (96%)	4 (4%)	32 56
29	0	21/21 (100%)	21 (100%)	0	100 100
31	1	69/91 (76%)	64 (93%)	5 (7%)	14 40
33	6	85/99 (86%)	81 (95%)	4 (5%)	26 52
34	7	352/357 (99%)	299 (85%)	53 (15%)	3 15
35	8	118/126 (94%)	104 (88%)	14 (12%)	5 21
36	9	226/239 (95%)	198 (88%)	28 (12%)	4 20
All	All	3859/4002 (96%)	3552 (92%)	307 (8%)	16 37

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	133	SER
2	Z	172	LYS
2	Z	175	VAL
3	3	1	MET
3	3	51	VAL
3	3	62	ILE
3	3	66	LEU
3	3	82	SER
3	3	84	LYS
4	L	5	ARG
4	L	45	ILE
4	L	46	ARG
4	L	68	VAL
4	L	69	HIS
4	L	84	GLN
5	O	4	PHE
5	O	7	ILE
5	O	139	GLN
5	O	144	SER

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Mol	Chain	Res	Type
6	P	3	LYS
6	P	7	ASN
6	P	14	PHE
6	P	36	LEU
6	P	55	TYR
7	S	6	GLN
7	S	27	ASP
7	S	43	SER
8	T	9	ARG
8	T	34	ARG
8	T	35	SER
8	T	71	ILE
9	U	10	ASP
9	U	15	ARG
9	U	37	THR
9	U	76	TYR
9	U	77	TYR
9	U	81	LYS
9	U	103	GLN
9	U	121	ILE
10	X	17	ARG
10	X	20	THR
10	X	24	VAL
10	X	29	VAL
10	X	36	ASP
10	X	46	ARG
10	X	65	ARG
11	Y	5	TRP
11	Y	15	VAL
11	Y	22	CYS
12	H	9	PHE
12	H	32	SER
12	H	44	LEU
12	H	48	HIS
12	H	50	ARG
12	H	72	MET
12	H	73	ARG
12	H	78	HIS
12	H	86	MET
12	H	87	ARG
12	H	88	ARG
12	H	97	LYS

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Mol	Chain	Res	Type
12	H	98	VAL
12	H	102	GLU
12	H	174	TYR
12	H	175	ARG
13	K	3	ILE
13	K	10	ARG
13	K	16	ARG
13	K	23	LYS
13	K	31	LYS
13	K	55	GLU
13	K	71	PHE
13	K	112	ARG
13	K	119	PRO
14	M	13	LYS
14	M	20	TYR
14	M	22	SER
14	M	31	THR
14	M	41	ARG
14	M	56	SER
14	M	89	SER
14	M	92	LYS
14	M	124	ASP
15	N	16	LEU
15	N	20	ARG
15	N	57	LYS
15	N	61	GLU
15	N	64	GLN
15	N	66	ASN
15	N	69	MET
15	N	80	ASN
15	N	97	ILE
15	N	132	VAL
15	N	135	LYS
15	N	136	GLU
15	N	144	LYS
16	Q	1	MET
16	Q	9	ARG
16	Q	15	LYS
16	Q	46	SER
16	Q	70	ASP
16	Q	97	PHE
16	Q	115	ASP

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Mol	Chain	Res	Type
16	Q	117	HIS
16	Q	118	SER
16	Q	127	SER
16	Q	132	LEU
16	Q	152	THR
17	R	62	ARG
17	R	65	LEU
17	R	84	ASP
18	A	31	GLU
18	A	44	LEU
18	A	72	ASP
18	A	85	MET
18	A	101	THR
18	A	113	ASP
19	B	13	LEU
19	B	26	LYS
19	B	27	ASP
19	B	33	TYR
19	B	38	ASP
19	B	52	LEU
19	B	59	LEU
19	B	66	SER
19	B	114	VAL
19	B	128	ARG
19	B	174	GLU
19	B	188	PHE
20	V	12	LYS
20	V	14	ILE
20	V	50	THR
20	V	57	ARG
20	V	60	PHE
20	V	65	SER
20	V	85	TYR
20	V	88	ILE
21	W	11	SER
21	W	14	LEU
22	D	34	GLU
22	D	46	THR
22	D	94	SER
22	D	118	MET
22	D	125	ILE
22	D	137	ILE

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Mol	Chain	Res	Type
22	D	141	SER
22	D	151	THR
23	E	4	LYS
23	E	17	THR
23	E	42	SER
23	E	98	GLU
23	E	122	ILE
23	E	137	ARG
23	E	141	ASN
23	E	143	HIS
23	E	151	SER
23	E	160	THR
23	E	179	PHE
23	E	195	ARG
23	E	198	ARG
23	E	211	ASP
23	E	212	VAL
23	E	217	ASP
23	E	237	LYS
23	E	242	LEU
24	F	5	TRP
24	F	13	LEU
24	F	45	LYS
24	F	64	GLU
24	F	112	LYS
24	F	128	CYS
24	F	153	ARG
24	F	185	SER
25	G	8	ILE
25	G	13	SER
25	G	15	ILE
25	G	44	ASN
25	G	51	PHE
25	G	57	GLU
25	G	64	ARG
25	G	70	ASP
25	G	86	VAL
25	G	87	LEU
25	G	89	SER
25	G	99	LYS
25	G	102	ARG
25	G	104	LYS

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Mol	Chain	Res	Type
25	G	118	GLN
26	I	3	LEU
26	I	12	SER
26	I	17	SER
26	I	18	GLU
26	I	22	LYS
26	I	24	GLU
26	I	27	ILE
26	I	36	GLU
26	I	77	PRO
26	I	98	GLU
26	I	125	LEU
27	J	34	ASN
27	J	65	VAL
27	J	67	ASP
27	J	112	SER
31	1	35	ARG
31	1	38	LYS
31	1	40	MET
31	1	71	LYS
31	1	84	LYS
33	6	60	TRP
33	6	62	ARG
33	6	85	ARG
33	6	96	ARG
34	7	39	GLU
34	7	41	LEU
34	7	45	MET
34	7	46	THR
34	7	47	ILE
34	7	61	SER
34	7	62	CYS
34	7	73	SER
34	7	75	LYS
34	7	79	SER
34	7	81	ASP
34	7	87	ARG
34	7	90	SER
34	7	100	LEU
34	7	104	MET
34	7	105	LEU
34	7	111	MET

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Mol	Chain	Res	Type
34	7	116	LEU
34	7	155	SER
34	7	156	LYS
34	7	160	LEU
34	7	171	LYS
34	7	176	GLU
34	7	192	ASP
34	7	207	ARG
34	7	212	LYS
34	7	215	MET
34	7	221	PHE
34	7	223	VAL
34	7	229	GLN
34	7	231	ASN
34	7	232	GLU
34	7	246	LEU
34	7	260	ARG
34	7	266	LYS
34	7	277	SER
34	7	294	LEU
34	7	295	VAL
34	7	301	LEU
34	7	306	THR
34	7	307	LYS
34	7	315	ILE
34	7	326	LEU
34	7	343	LYS
34	7	345	MET
34	7	346	LEU
34	7	347	LYS
34	7	354	LYS
34	7	360	SER
34	7	366	THR
34	7	398	SER
34	7	404	ARG
34	7	415	ILE
35	8	11	LEU
35	8	19	PRO
35	8	36	LEU
35	8	45	ARG
35	8	53	ARG
35	8	58	ASP

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Mol	Chain	Res	Type
35	8	61	CYS
35	8	66	LEU
35	8	74	ASN
35	8	76	ASP
35	8	107	SER
35	8	110	LYS
35	8	111	SER
35	8	113	ASP
36	9	18	THR
36	9	30	SER
36	9	54	ILE
36	9	55	ARG
36	9	56	ASP
36	9	59	LYS
36	9	65	ILE
36	9	70	ARG
36	9	74	ARG
36	9	82	LEU
36	9	103	LEU
36	9	117	SER
36	9	127	TRP
36	9	135	ASP
36	9	158	GLU
36	9	166	GLU
36	9	175	ARG
36	9	187	THR
36	9	204	LEU
36	9	208	GLU
36	9	209	GLN
36	9	214	LEU
36	9	215	LEU
36	9	222	ILE
36	9	230	ASP
36	9	255	LYS
36	9	256	GLU
36	9	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
7	S	48	ASN
8	T	44	GLN

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Mol	Chain	Res	Type
9	U	103	GLN
11	Y	19	ASN
12	H	129	ASN
12	H	193	ASN
13	K	117	HIS
14	M	29	HIS
15	N	66	ASN
16	Q	85	HIS
16	Q	104	ASN
16	Q	112	HIS
18	A	130	GLN
19	B	11	GLN
19	B	22	GLN
19	B	23	GLN
19	B	125	GLN
22	D	72	GLN
23	E	37	HIS
23	E	38	ASN
23	E	113	HIS
23	E	139	GLN
23	E	143	HIS
23	E	147	ASN
23	E	157	ASN
24	F	30	GLN
24	F	196	ASN
24	F	207	ASN
25	G	44	ASN
25	G	48	ASN
25	G	110	ASN
25	G	118	GLN
25	G	120	ASN
26	I	13	HIS
26	I	16	ASN
27	J	34	ASN
27	J	52	ASN
27	J	121	ASN
34	7	177	ASN
34	7	400	GLN
35	8	93	ASN
36	9	61	ASN
36	9	235	ASN
36	9	245	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1493/1518 (98%)	338 (22%)	112 (7%)
30	5	17/26 (65%)	12 (70%)	2 (11%)
32	4	75/76 (98%)	25 (33%)	0
All	All	1585/1620 (97%)	375 (23%)	114 (7%)

All (375) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	C
1	2	14	C
1	2	25	C
1	2	38	G
1	2	39	U
1	2	42	G
1	2	43	A
1	2	44	C
1	2	45	U
1	2	46	A
1	2	47	A
1	2	48	G
1	2	49	C
1	2	57	G
1	2	64	G
1	2	71	C
1	2	72	C
1	2	73	U
1	2	74	U
1	2	75	C
1	2	85	A
1	2	100	A
1	2	102	U
1	2	104	A
1	2	105	C
1	2	106	A
1	2	112	G
1	2	114	A
1	2	115	A
1	2	116	C
1	2	131	G
1	2	151	G

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Mol	Chain	Res	Type
1	2	158	U
1	2	177	A
1	2	184	G
1	2	197	A
1	2	199	A
1	2	200	G
1	2	211	G
1	2	236	C
1	2	240	U
1	2	241	U
1	2	243	G
1	2	247	G
1	2	248	U
1	2	249	U
1	2	262	G
1	2	263	C
1	2	268	C
1	2	275	A
1	2	276	A
1	2	277	G
1	2	278	A
1	2	285	C
1	2	286	G
1	2	297	G
1	2	301	G
1	2	308	G
1	2	315	A
1	2	317	A
1	2	318	C
1	2	323	A
1	2	324	C
1	2	325	A
1	2	326	C
1	2	328	G
1	2	340	A
1	2	341	C
1	2	343	G
1	2	348	C
1	2	349	A
1	2	350	G
1	2	363	C
1	2	369	A

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Mol	Chain	Res	Type
1	2	370	A
1	2	380	C
1	2	389	G
1	2	393	A
1	2	394	C
1	2	402	G
1	2	409	C
1	2	410	U
1	2	411	C
1	2	412	U
1	2	413	G
1	2	423	U
1	2	425	C
1	2	430	G
1	2	431	U
1	2	432	G
1	2	434	A
1	2	435	A
1	2	436	A
1	2	438	A
1	2	439	G
1	2	440	C
1	2	449	U
1	2	450	A
1	2	459	G
1	2	460	C
1	2	461	A
1	2	462	A
1	2	463	G
1	2	464	G
1	2	466	C
1	2	471	G
1	2	472	C
1	2	480	G
1	2	485	A
1	2	486	A
1	2	487	U
1	2	494	G
1	2	500	A
1	2	503	G
1	2	509	C
1	2	512	U

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Mol	Chain	Res	Type
1	2	513	A
1	2	514	U
1	2	520	G
1	2	523	C
1	2	525	A
1	2	526	A
1	2	528	G
1	2	529	C
1	2	530	G
1	2	531	G
1	2	532	C
1	2	540	G
1	2	541	G
1	2	574	A
1	2	580	G
1	2	581	G
1	2	585	U
1	2	586	C
1	2	587	G
1	2	588	C
1	2	598	U
1	2	607	U
1	2	619	A
1	2	640	U
1	2	641	A
1	2	642	G
1	2	647	G
1	2	649	A
1	2	652	C
1	2	655	A
1	2	656	U
1	2	657	A
1	2	670	C
1	2	672	G
1	2	673	C
1	2	677	U
1	2	678	G
1	2	685	G
1	2	687	G
1	2	702	G
1	2	703	U
1	2	709	G

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Mol	Chain	Res	Type
1	2	718	G
1	2	729	G
1	2	731	A
1	2	735	A
1	2	736	A
1	2	746	A
1	2	747	U
1	2	748	A
1	2	766	G
1	2	767	U
1	2	769	A
1	2	771	G
1	2	772	G
1	2	775	G
1	2	782	A
1	2	801	A
1	2	816	G
1	2	832	G
1	2	847	A
1	2	860	G
1	2	863	U
1	2	872	A
1	2	884	G
1	2	892	C
1	2	893	U
1	2	904	G
1	2	905	A
1	2	919	U
1	2	920	U
1	2	925	U
1	2	928	A
1	2	931	C
1	2	933	G
1	2	934	G
1	2	935	G
1	2	936	A
1	2	937	A
1	2	948	G
1	2	949	G
1	2	950	C
1	2	951	G
1	2	953	C

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Mol	Chain	Res	Type
1	2	960	A
1	2	961	U
1	2	962	G
1	2	964	A
1	2	965	G
1	2	970	G
1	2	973	U
1	2	974	G
1	2	975	A
1	2	976	A
1	2	977	G
1	2	978	G
1	2	985	C
1	2	986	G
1	2	988	A
1	2	989	C
1	2	993	C
1	2	1001	A
1	2	1002	G
1	2	1005	G
1	2	1006	C
1	2	1017	U
1	2	1018	C
1	2	1020	G
1	2	1032	A
1	2	1037	U
1	2	1038	C
1	2	1041	C
1	2	1043	U
1	2	1046	G
1	2	1047	U
1	2	1048	G
1	2	1053	A
1	2	1054	A
1	2	1064	C
1	2	1077	U
1	2	1078	U
1	2	1079	G
1	2	1081	C
1	2	1082	A
1	2	1083	G
1	2	1096	G

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Mol	Chain	Res	Type
1	2	1102	A
1	2	1105	C
1	2	1112	G
1	2	1115	G
1	2	1119	U
1	2	1128	U
1	2	1143	G
1	2	1144	G
1	2	1151	A
1	2	1156	A
1	2	1157	G
1	2	1161	A
1	2	1162	G
1	2	1171	G
1	2	1172	A
1	2	1175	C
1	2	1184	U
1	2	1185	A
1	2	1186	C
1	2	1187	A
1	2	1198	A
1	2	1200	U
1	2	1201	G
1	2	1209	C
1	2	1216	A
1	2	1218	C
1	2	1221	A
1	2	1227	A
1	2	1239	A
1	2	1240	A
1	2	1242	C
1	2	1245	C
1	2	1246	U
1	2	1247	A
1	2	1258	C
1	2	1260	G
1	2	1261	U
1	2	1262	U
1	2	1263	C
1	2	1265	G
1	2	1268	C
1	2	1279	A

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Mol	Chain	Res	Type
1	2	1280	C
1	2	1292	A
1	2	1307	G
1	2	1308	U
1	2	1313	G
1	2	1321	U
1	2	1323	A
1	2	1324	U
1	2	1325	C
1	2	1330	G
1	2	1332	C
1	2	1336	U
1	2	1338	C
1	2	1339	G
1	2	1340	U
1	2	1341	C
1	2	1346	C
1	2	1348	C
1	2	1354	A
1	2	1358	A
1	2	1361	G
1	2	1375	C
1	2	1389	G
1	2	1402	C
1	2	1403	U
1	2	1404	C
1	2	1409	G
1	2	1410	G
1	2	1413	G
1	2	1414	G
1	2	1415	U
1	2	1424	G
1	2	1434	C
1	2	1436	U
1	2	1437	G
1	2	1445	A
1	2	1447	A
1	2	1448	A
1	2	1454	A
1	2	1457	A
1	2	1458	A
1	2	1459	G

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Mol	Chain	Res	Type
1	2	1460	G
1	2	1461	U
1	2	1472	G
1	2	1475	C
1	2	1484	C
1	2	1485	G
1	2	1486	A
1	2	1487	U
1	2	1488	C
1	2	1490	C
1	2	1494	C
30	5	806	G
30	5	808	A
30	5	812	G
30	5	813	A
30	5	814	U
30	5	815	U
30	5	816	U
30	5	817	A
30	5	818	A
30	5	819	A
30	5	820	U
30	5	822	C
32	4	4	G
32	4	5	G
32	4	8	U
32	4	17	C
32	4	18	U
32	4	19	G
32	4	20	G
32	4	21	H2U
32	4	22	A
32	4	24	C
32	4	25	U
32	4	27	G
32	4	37	U
32	4	43	G
32	4	45	A
32	4	48	U
32	4	49	C
32	4	50	G
32	4	54	G

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Mol	Chain	Res	Type
32	4	68	C
32	4	72	C
32	4	73	U
32	4	75	C
32	4	76	C
32	4	77	A

All (114) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	A
1	2	3	U
1	2	8	U
1	2	42	G
1	2	45	U
1	2	47	A
1	2	56	A
1	2	99	C
1	2	103	A
1	2	111	G
1	2	114	A
1	2	115	A
1	2	176	U
1	2	199	A
1	2	239	A
1	2	246	A
1	2	247	G
1	2	262	G
1	2	270	A
1	2	275	A
1	2	277	G
1	2	323	A
1	2	324	C
1	2	325	A
1	2	347	G
1	2	362	C
1	2	368	C
1	2	399	A
1	2	408	C
1	2	422	U
1	2	434	A
1	2	439	G

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Mol	Chain	Res	Type
1	2	448	A
1	2	462	A
1	2	471	G
1	2	486	A
1	2	512	U
1	2	513	A
1	2	528	G
1	2	529	C
1	2	540	G
1	2	584	C
1	2	598	U
1	2	641	A
1	2	655	A
1	2	687	G
1	2	746	A
1	2	747	U
1	2	766	G
1	2	790	G
1	2	847	A
1	2	856	G
1	2	871	A
1	2	891	A
1	2	892	C
1	2	904	G
1	2	919	U
1	2	924	U
1	2	934	G
1	2	941	C
1	2	959	G
1	2	960	A
1	2	961	U
1	2	963	A
1	2	964	A
1	2	974	G
1	2	975	A
1	2	977	G
1	2	985	C
1	2	1001	A
1	2	1017	U
1	2	1037	U
1	2	1053	A
1	2	1081	C

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Mol	Chain	Res	Type
1	2	1089	C
1	2	1098	G
1	2	1142	G
1	2	1150	G
1	2	1156	A
1	2	1161	A
1	2	1171	G
1	2	1174	A
1	2	1184	U
1	2	1186	C
1	2	1200	U
1	2	1217	C
1	2	1241	U
1	2	1245	C
1	2	1260	G
1	2	1261	U
1	2	1262	U
1	2	1289	G
1	2	1291	G
1	2	1306	A
1	2	1307	G
1	2	1323	A
1	2	1324	U
1	2	1337	A
1	2	1340	U
1	2	1367	C
1	2	1368	A
1	2	1370	U
1	2	1423	A
1	2	1436	U
1	2	1448	A
1	2	1453	U
1	2	1457	A
1	2	1458	A
1	2	1459	G
1	2	1460	G
1	2	1483	U
1	2	1486	A
30	5	811	U
30	5	813	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	H2U	4	21	32	18,21,22	2.21	4 (22%)	21,30,33	1.12	1 (4%)
32	5MU	4	55	32	19,22,23	0.25	0	28,32,35	0.38	0
32	OMC	4	33	32	18,21,23	0.52	0	26,30,34	0.35	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
32	H2U	4	21	32	-	0/7/38/39	0/2/2/2
32	5MU	4	55	32	-	0/7/25/26	0/2/2/2
32	OMC	4	33	32	-	0/7/25/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	21	H2U	C6-C5	-6.88	1.34	1.52
32	4	21	H2U	C6-N1	-4.88	1.38	1.47
32	4	21	H2U	C5-C4	-2.78	1.43	1.50
32	4	21	H2U	C2-N1	2.65	1.39	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	4	21	H2U	C5-C6-N1	3.39	122.80	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	4	21	H2U	1	0
32	4	55	5MU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GNP	7	502	38	29,34,34	2.09	9 (31%)	33,54,54	2.43	8 (24%)
37	MET	4	101	-	6,7,8	0.47	0	2,7,9	0.16	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	GNP	7	502	38	-	7/14/38/38	0/3/3/3
37	MET	4	101	-	-	3/5/6/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PB-O3A	-7.37	1.49	1.59
39	7	502	GNP	C6-N1	3.84	1.39	1.33
39	7	502	GNP	PB-O2B	-3.20	1.48	1.56
39	7	502	GNP	PG-O1G	3.00	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PG-O2G	-2.96	1.48	1.56
39	7	502	GNP	PG-O3G	-2.36	1.50	1.56
39	7	502	GNP	C8-N7	-2.31	1.30	1.34
39	7	502	GNP	PG-N3B	-2.23	1.57	1.63
39	7	502	GNP	PB-N3B	-2.10	1.57	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	7	502	GNP	C5-C6-N1	-8.61	111.66	123.43
39	7	502	GNP	C2-N1-C6	5.57	124.79	115.93
39	7	502	GNP	O1G-PG-N3B	-4.25	105.51	111.77
39	7	502	GNP	C3'-C2'-C1'	3.44	106.16	100.98
39	7	502	GNP	PB-O3A-PA	-3.43	120.55	132.62
39	7	502	GNP	C2-N3-C4	-2.90	112.04	115.36
39	7	502	GNP	O2B-PB-O1B	2.81	115.81	109.92
39	7	502	GNP	N3-C2-N1	-2.35	124.08	127.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	4	101	MET	O-C-CA-CB
39	7	502	GNP	PB-N3B-PG-O1G
39	7	502	GNP	PG-N3B-PB-O1B
39	7	502	GNP	PG-N3B-PB-O3A
39	7	502	GNP	C5'-O5'-PA-O3A
37	4	101	MET	CA-CB-CG-SD
37	4	101	MET	CB-CG-SD-CE
39	7	502	GNP	O4'-C4'-C5'-O5'
39	7	502	GNP	C3'-C4'-C5'-O5'
39	7	502	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

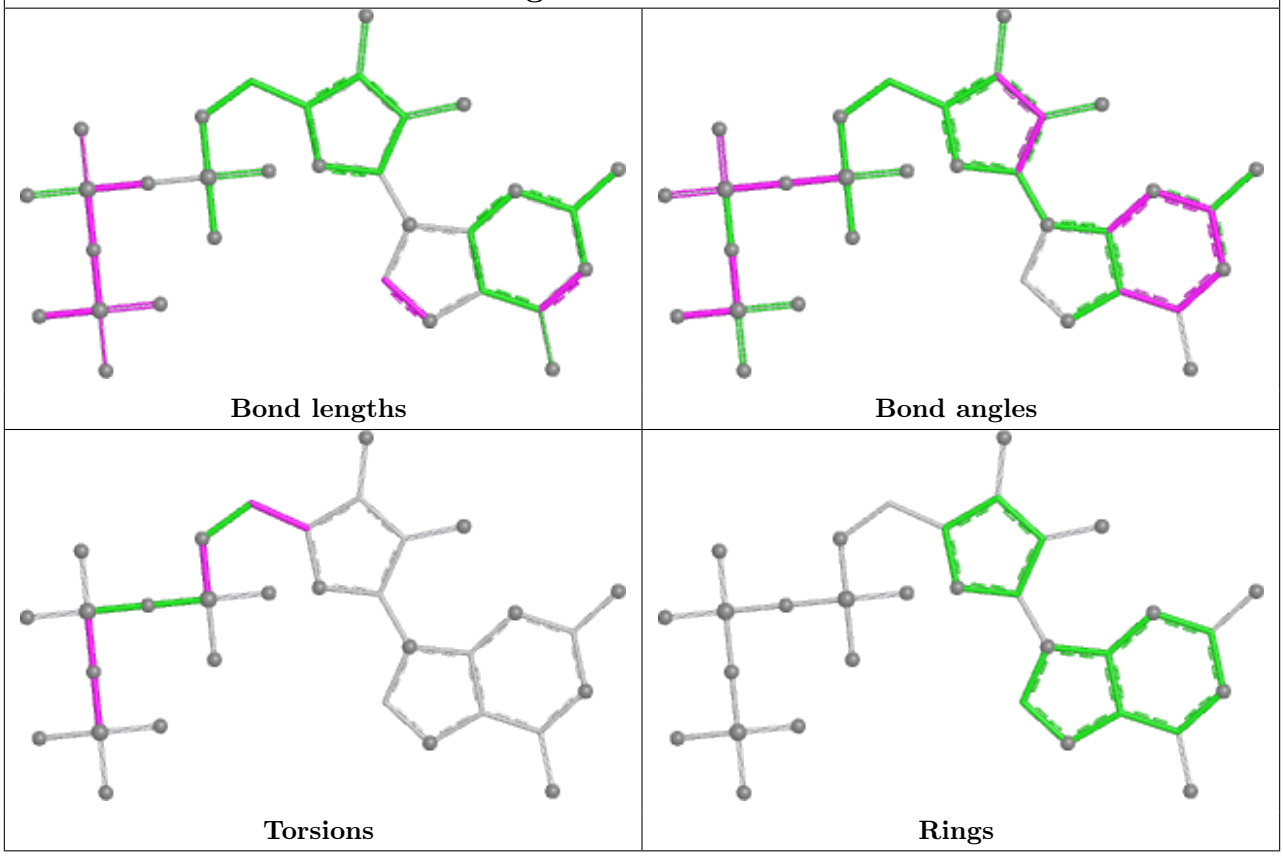
2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	7	502	GNP	1	0
37	4	101	MET	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP 7 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	4
34	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1342:C	O3'	1343:C	P	3.20
1	2	1060:G	O3'	1061:A	P	2.56
1	2	1019:A	O3'	1020:G	P	2.00
1	7	271:PRO	C	272:ILE	N	1.83
1	2	1351:U	O3'	1352:G	P	1.29

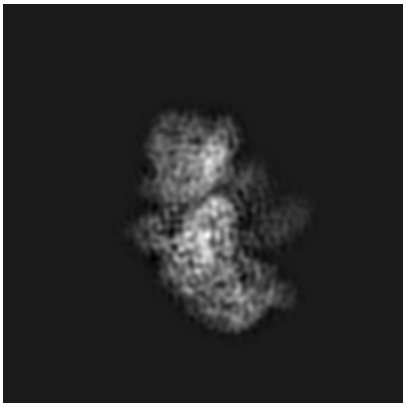
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8149. These allow visual inspection of the internal detail of the map and identification of artifacts.

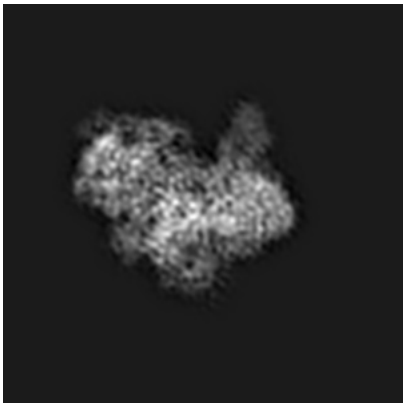
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

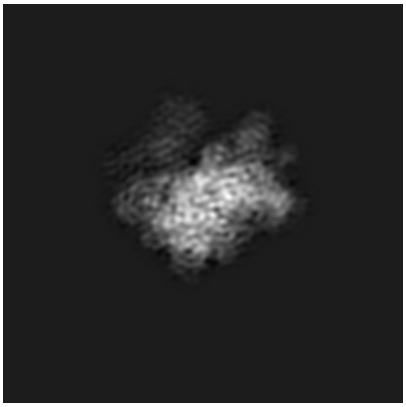
6.1.1 Primary map



X



Y



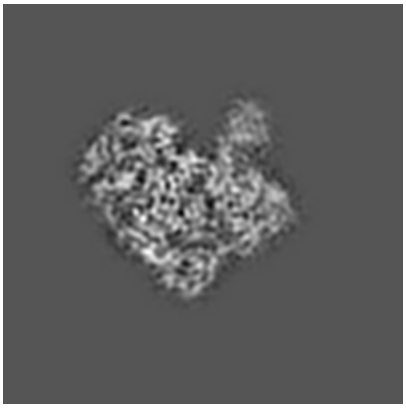
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 174



Y Index: 174

Z Index: 174

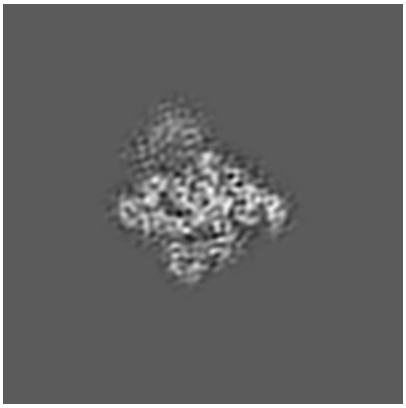
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 174

Y Index: 179

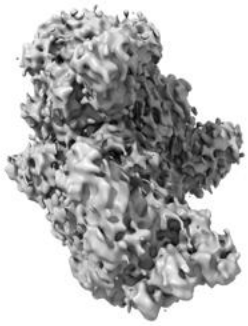


Z Index: 146

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

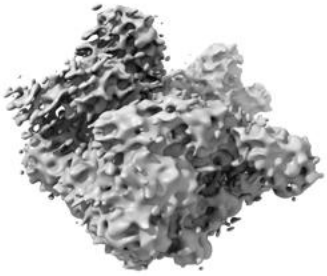
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

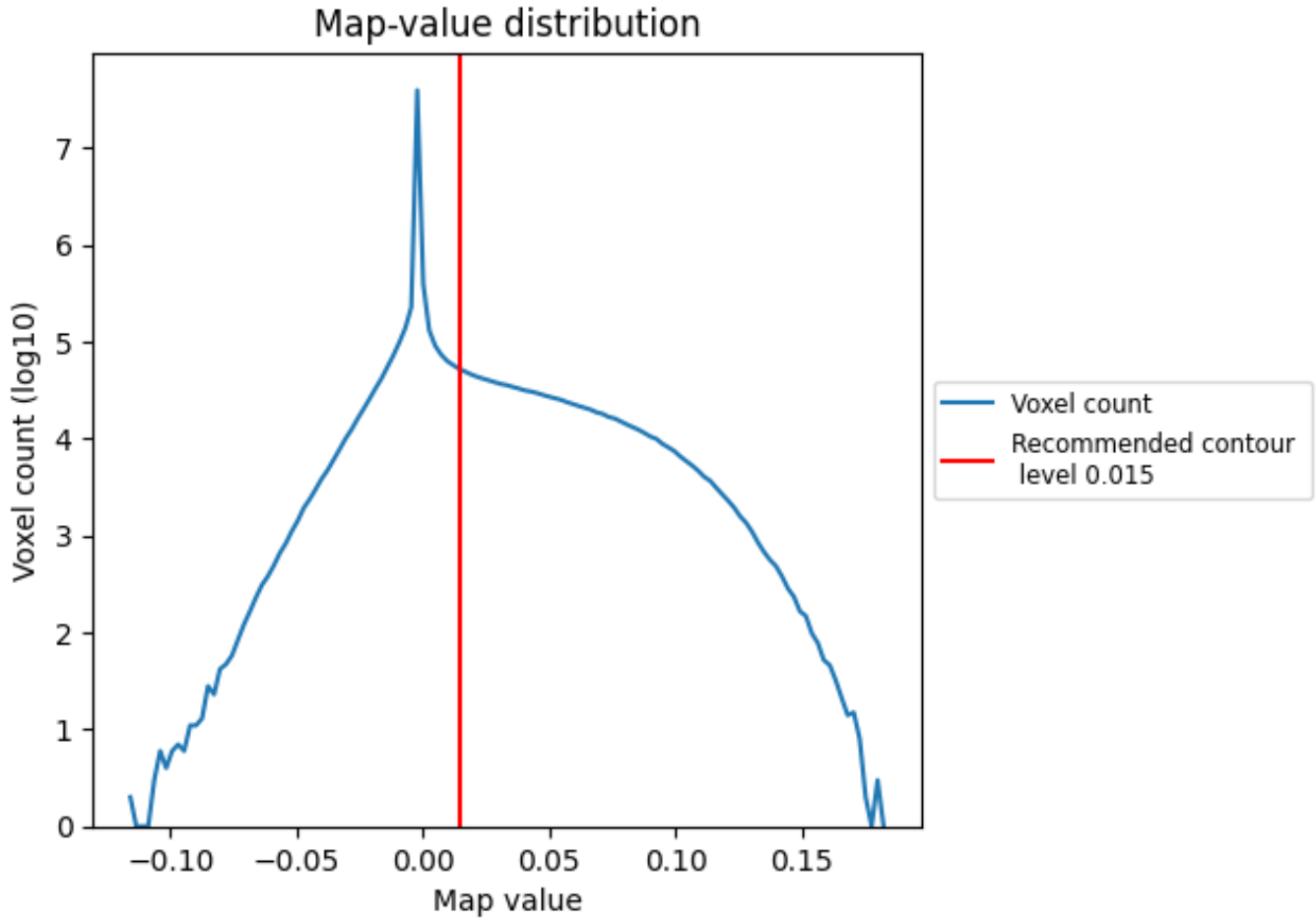
6.5 Mask visualisation (i)

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

7 Map analysis

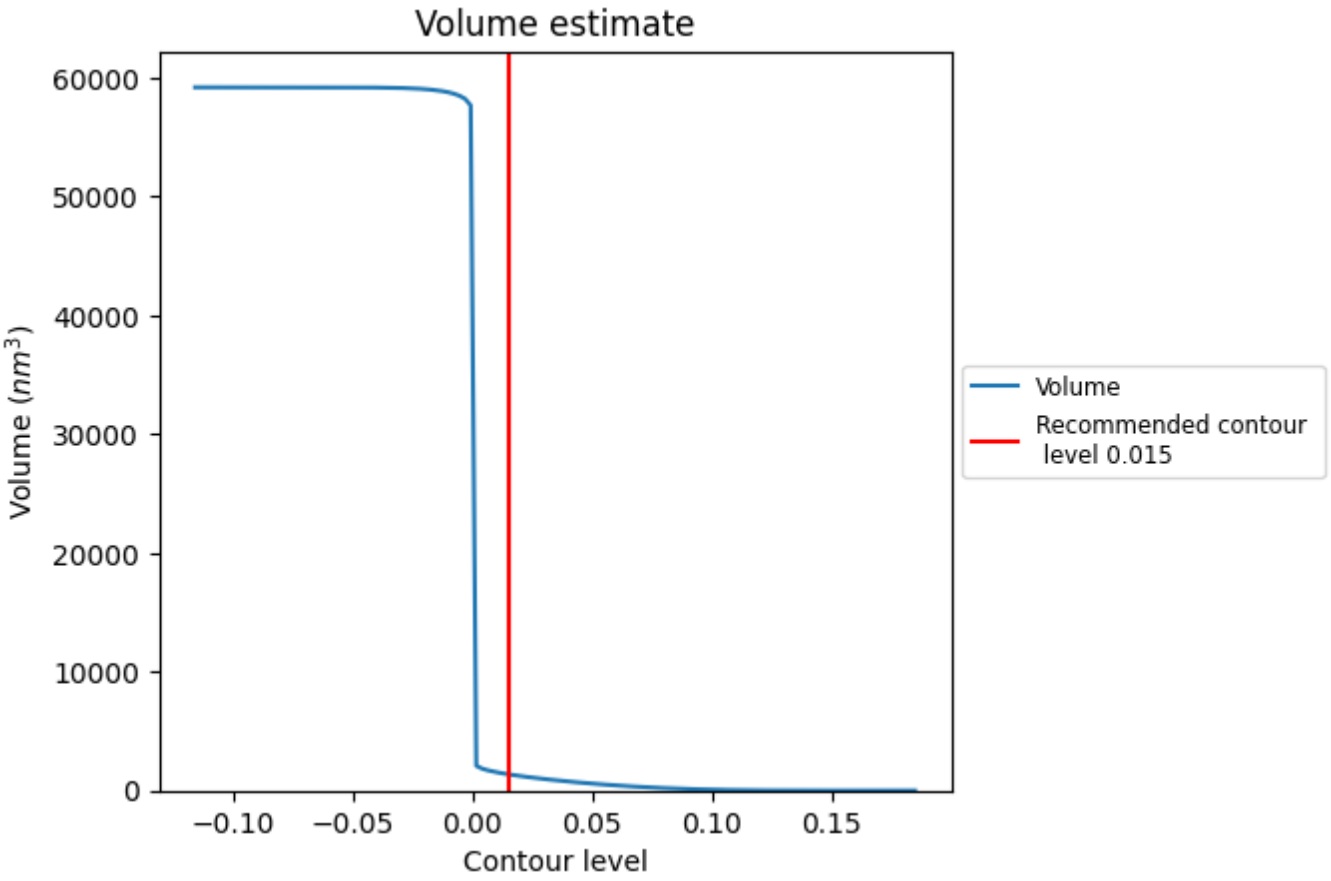
This section contains the results of statistical analysis of the map.

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.

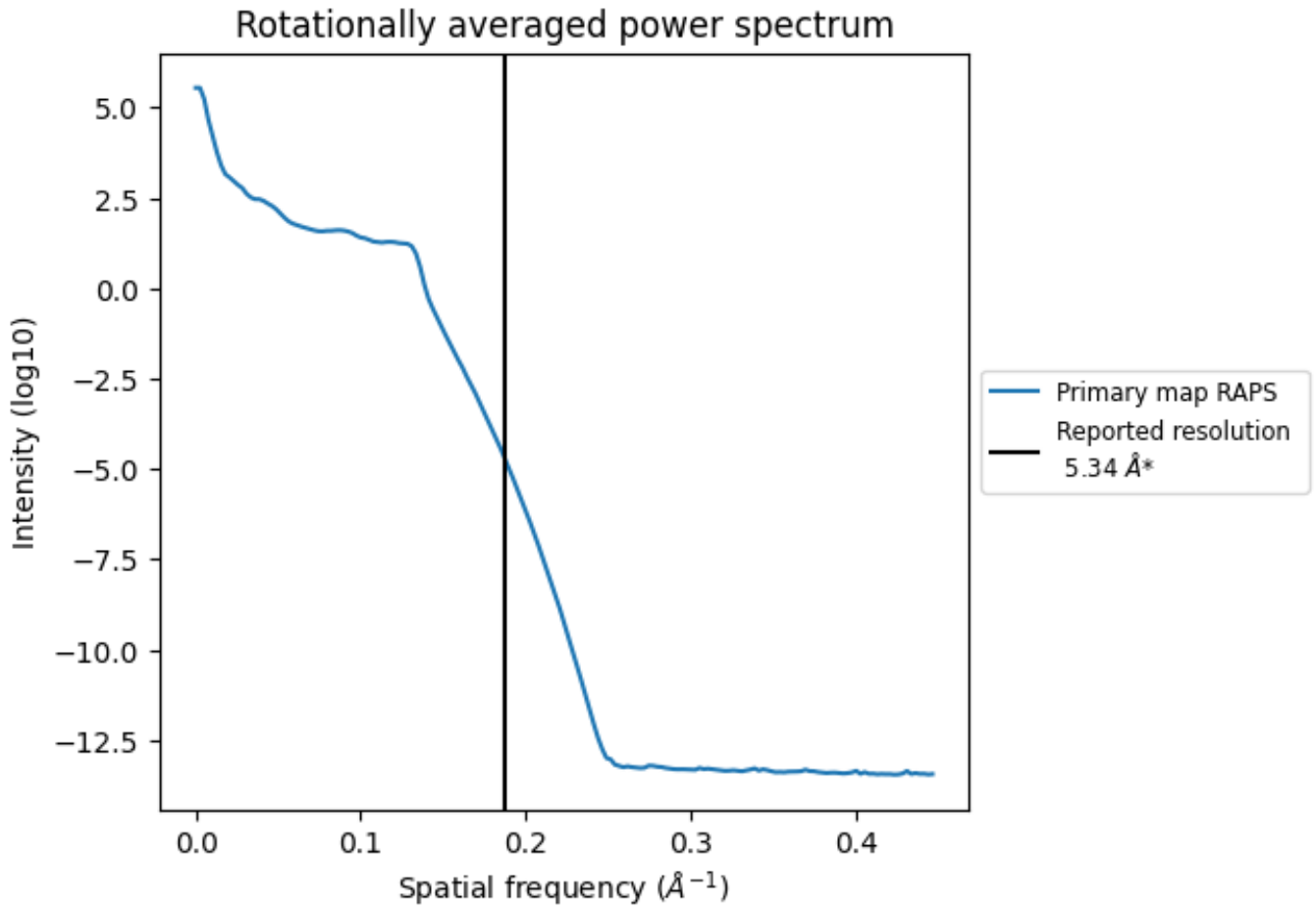
7.2 Volume estimate



The volume at the recommended contour level is 1368 nm^3; this corresponds to an approximate mass of 1236 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)

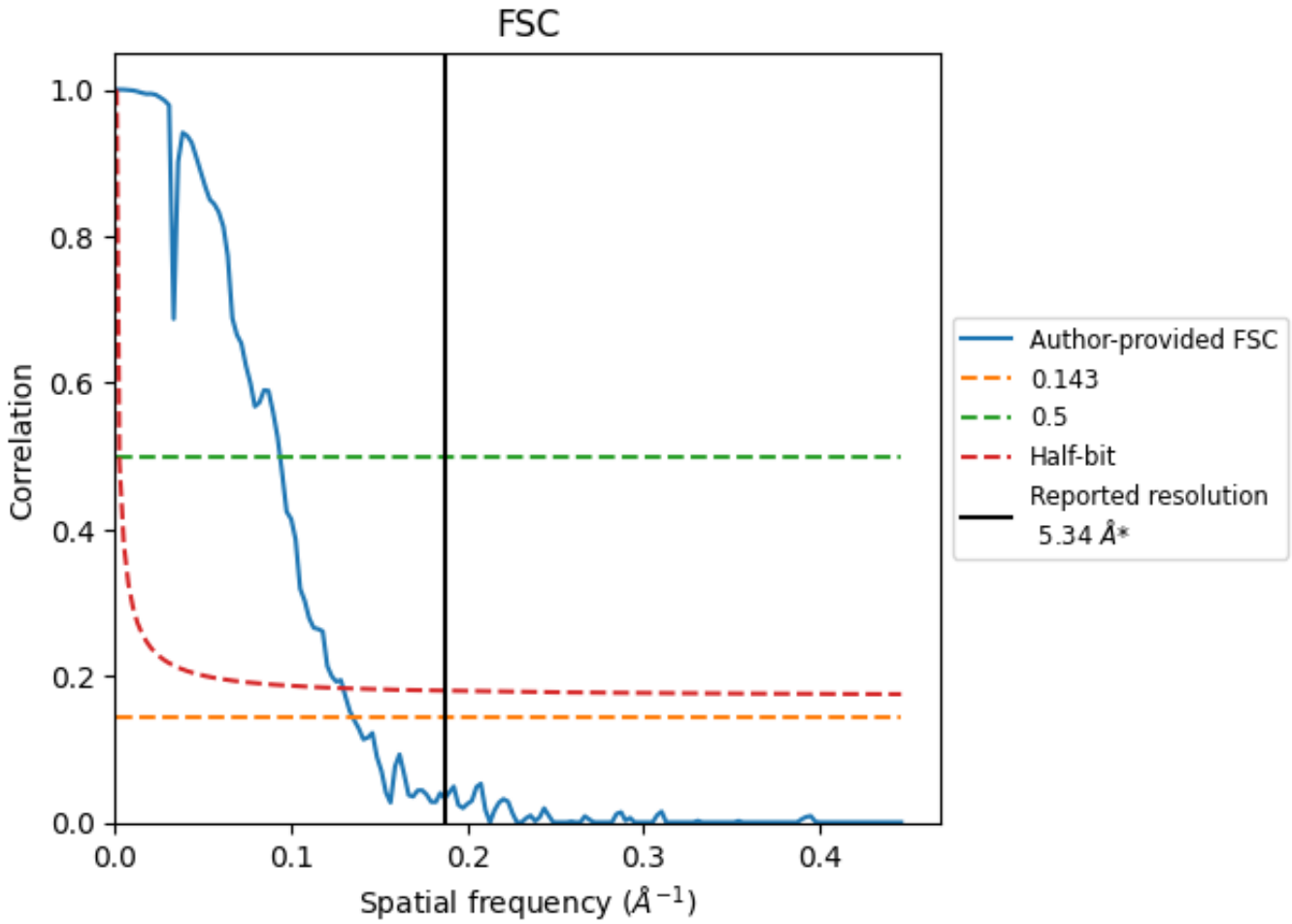


*Reported resolution corresponds to spatial frequency of 0.187 $Å^{-1}$

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 0.187 Å^{-1}

8.2 Resolution estimates (i)

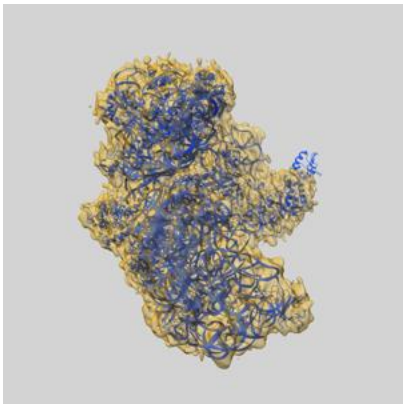
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.34	-	-
Author-provided FSC curve	7.40	10.67	7.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.40 differs from the reported value 5.34 by more than 10 %

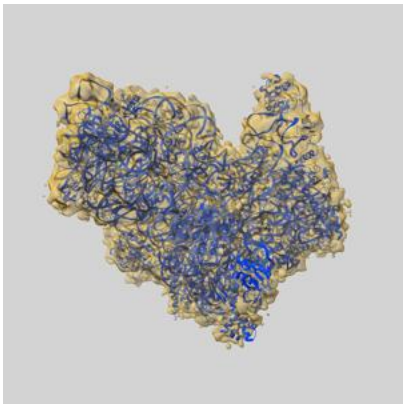
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8149 and PDB model 5JBH. Per-residue inclusion information can be found in section 3 on page 12.

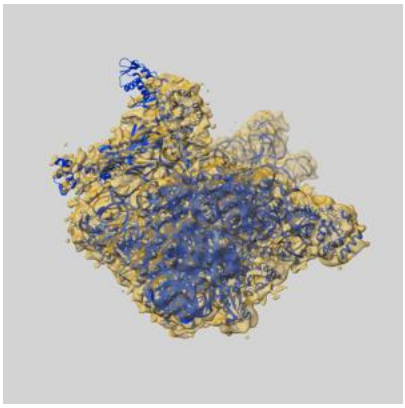
9.1 Map-model overlay



X



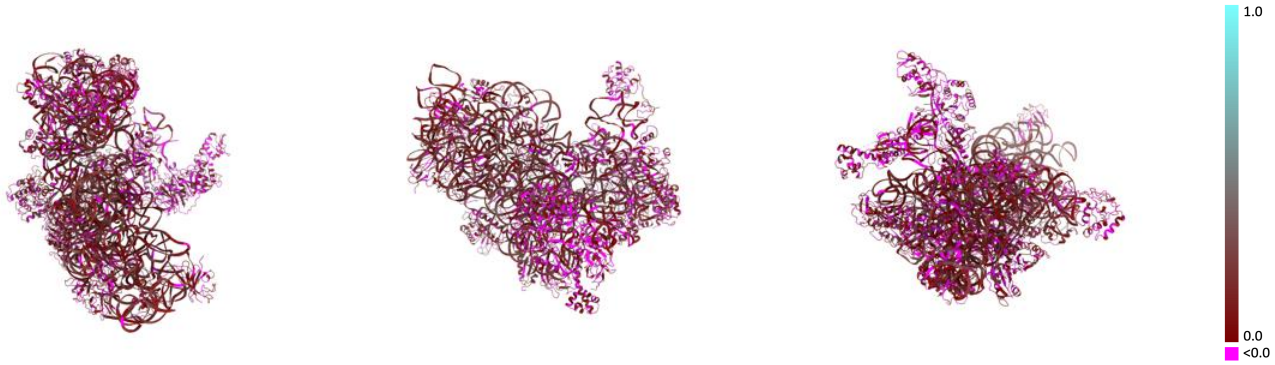
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

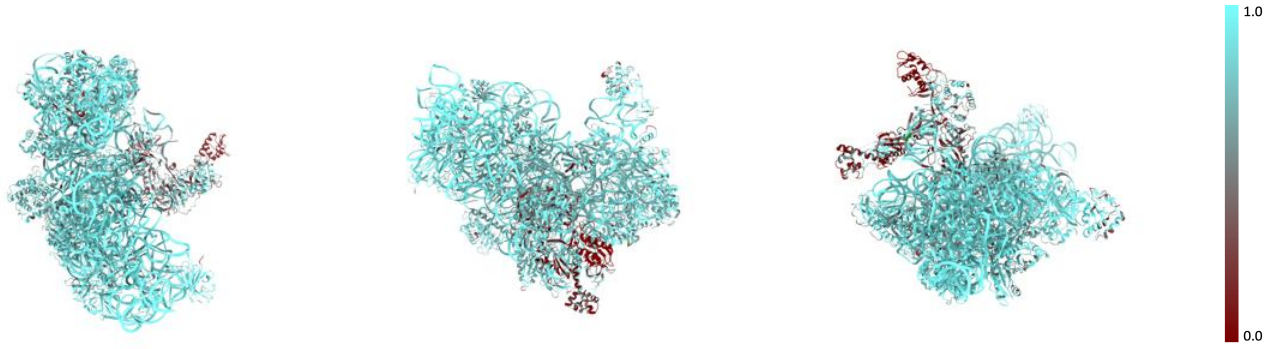
9.2 Q-score mapped to coordinate model



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.

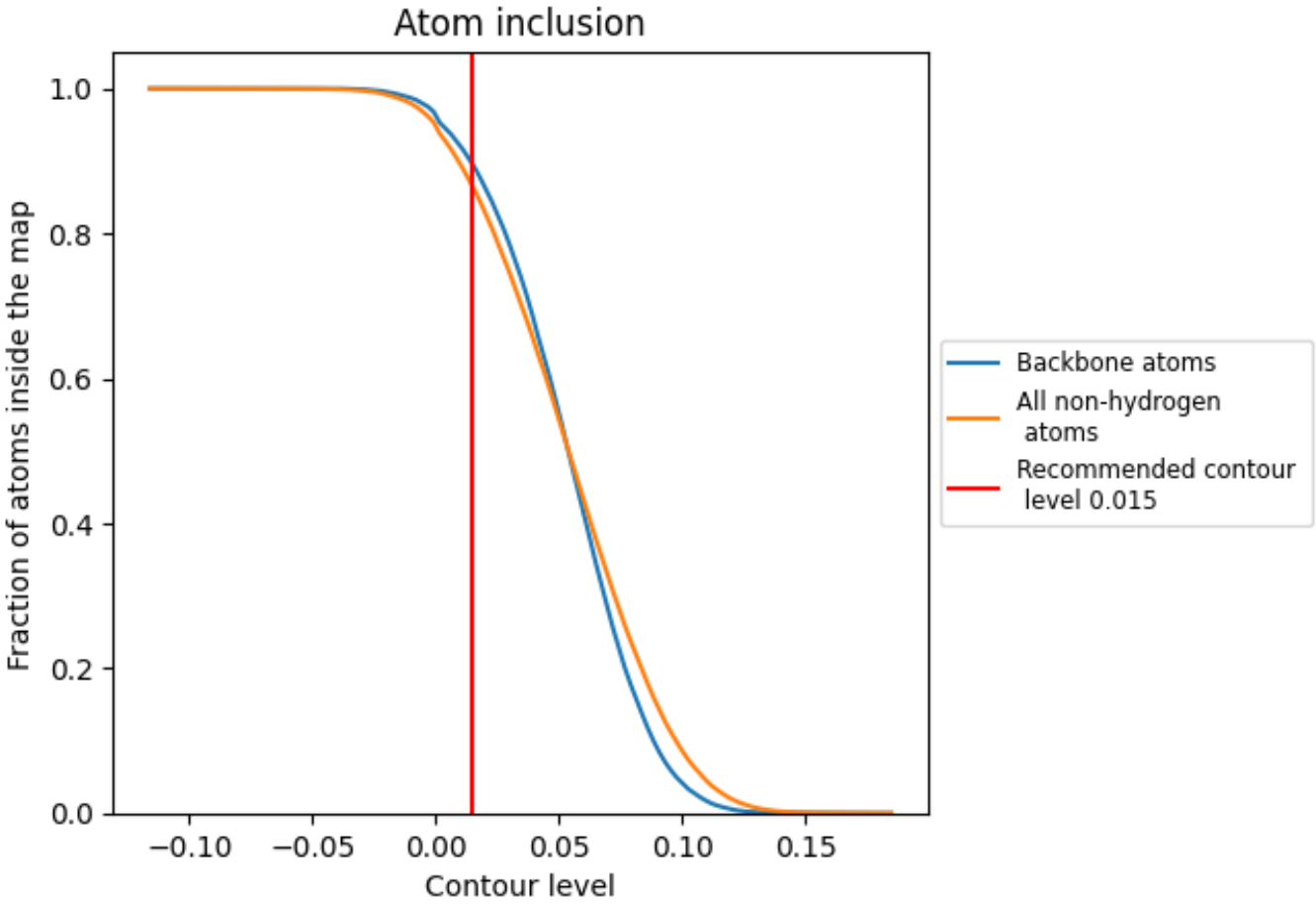
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8651	0.1170
0	0.7056	0.0620
1	0.5942	0.0610
2	0.9764	0.1650
3	0.7435	0.0280
4	0.8072	0.0650
5	0.8737	0.1320
6	0.7242	0.0720
7	0.5999	0.0210
8	0.1537	0.0020
9	0.3686	0.0220
A	0.8566	0.0980
B	0.8504	0.0960
C	0.9056	0.1780
D	0.8399	0.1300
E	0.8525	0.0930
F	0.8108	0.1130
G	0.8827	0.0790
H	0.8287	0.0640
I	0.8205	0.1240
J	0.8601	0.0990
K	0.8745	0.0750
L	0.8499	0.0700
M	0.8426	0.1020
N	0.7958	0.1100
O	0.8156	0.0600
P	0.9138	0.0780
Q	0.8397	0.1080
R	0.8352	0.0950
S	0.8708	0.0760
T	0.8244	0.0580
U	0.8760	0.0560
V	0.8566	0.0960
W	0.8617	0.0840
X	0.8336	0.0990

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Chain	Atom inclusion	Q-score
Y	0.8417	0.0250
Z	0.8648	0.0890