Full wwPDB EM Validation Report ⓘ

Nov 7, 2026 – 01:27 pm GMT

PDB ID	:	9T7X / pdb_00009t7x
EMDB ID	:	EMD-55661
Title	:	Structural characterization of hibernating ribosomes in the Gram-negative pathogen Enterobacter cloacae complex without E-site tRNA
Authors	:	Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on	:	2025-11-12
Resolution	:	3.08 Å(reported)
Based on initial model	:	8B0X

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:

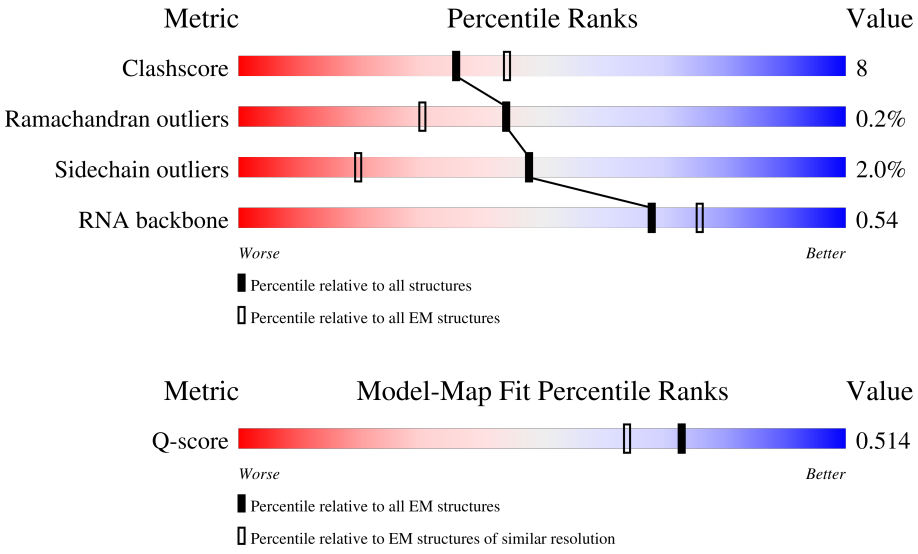
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.08 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.



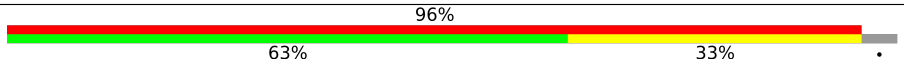
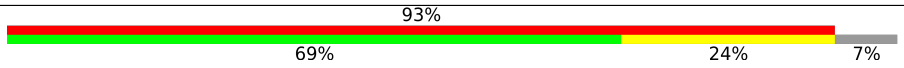
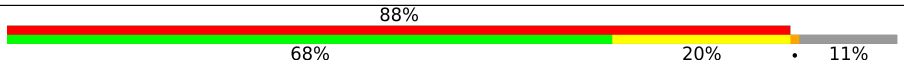
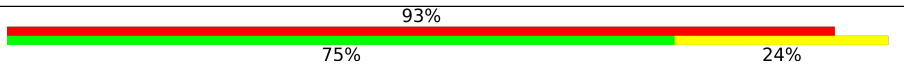
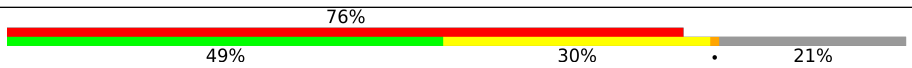
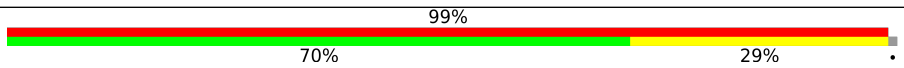
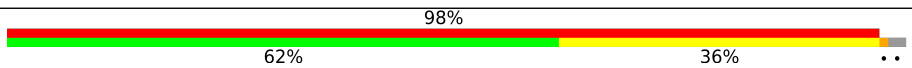
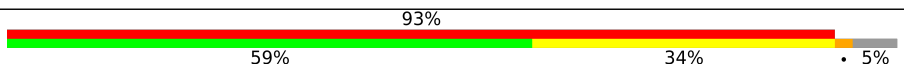
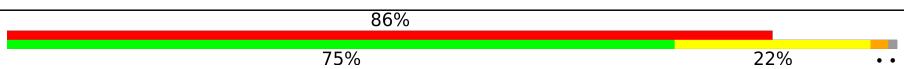
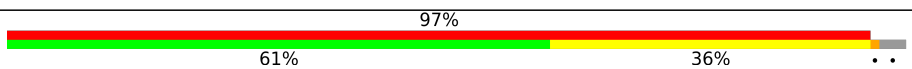
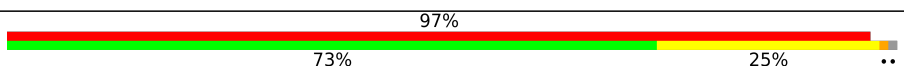
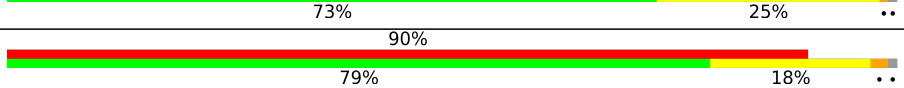
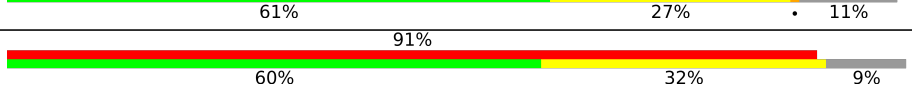
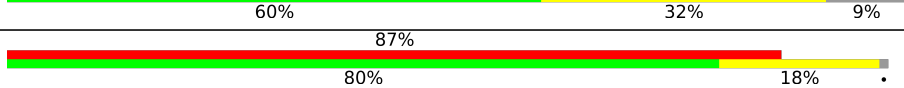
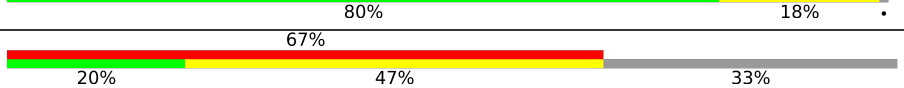
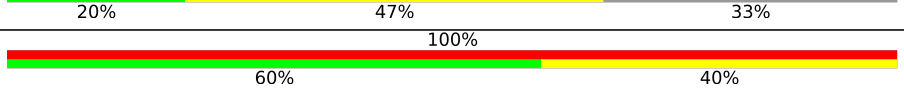
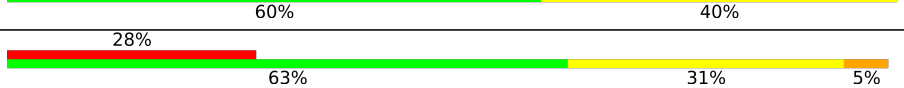
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	0	55	95% 73% 22% 5%
2	1	46	28% 89% 11%
3	2	65	63% 75% 22%

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1541	
7	B	241	
8	C	233	
9	D	206	
10	E	166	
11	F	131	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	W	15	
27	X	95	
28	a	2904	

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Mol	Chain	Length	Quality of chain
29	b	116	62% 62% 28% 9%
30	c	273	49% 84% 15%
31	d	209	54% 86% 14%
32	e	201	69% 81% 18%
33	f	179	98% 63% 35%
34	g	177	98% 74% 24%
35	h	149	100% 61% 36%
36	i	142	58% 78% 22%
37	j	123	67% 76% 24%
38	k	144	65% 79% 21%
39	l	136	78% 79% 20%
40	m	127	45% 76% 19% 6%
41	n	117	88% 82% 16%
42	o	115	64% 83% 16%
43	p	118	38% 82% 16%
44	q	103	68% 85% 15%
45	r	110	59% 76% 23%
46	s	100	66% 69% 24% 7%
47	t	104	87% 81% 15%
48	u	94	85% 76% 22%
49	v	85	45% 80% 12% 8%
50	w	78	62% 85% 13%
51	x	63	90% 73% 25%
52	y	59	63% 86% 12%
53	z	57	56% 86% 11%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 143494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	67	Total	C	N	O	S	0	0
			526	325	100	95	6		

- Molecule 6 is a RNA chain called 16S rRNA (1539-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1539	Total	C	N	O	P	0	0
			33035	14741	6061	10694	1539		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	225	Total	C	N	O	S	0	0
			1761	1110	317	326	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	207	Total	C	N	O	S	0	0
			1632	1034	306	289	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1645	1026	316	299	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	104	Total	C	N	O	S	0	0
			845	533	152	153	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	155	Total	C	N	O	S	0	0
			1228	767	238	219	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			978	618	171	183	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	128	Total	C	N	O	S	0	0
			1028	638	206	181	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			788	493	151	143	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			876	540	173	160	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A837F5X1

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			895	554	178	160	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			796	493	161	139	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			709	438	144	126	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	82	Total	C	N	O	S	0	0
			640	400	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	81	Total	C	N	O	S	0	0
			658	416	123	116	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			668	411	138	116	3		

- Molecule 26 is a RNA chain called non-STOP mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	10	Total	C	N	O	P	0	0
			219	97	41	71	10		

- Molecule 27 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	95	Total	C	N	O	S	0	0
			764	481	137	144	2		

- Molecule 28 is a RNA chain called 23S rRNA (2904-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2904	Total	C	N	O	P	0	0
			62357	27823	11472	20158	2904		

- Molecule 29 is a RNA chain called 5S rRNA (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	116	Total	C	N	O	P	0	0
			2481	1105	449	811	116		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	271	Total	C	N	O	S	0	0
			2079	1285	423	364	7		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	209	Total	C	N	O	S	0	0
			1568	982	288	295	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	178	Total	C	N	O	S	0	0
			1417	901	251	259	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	176	Total	C	N	O	S	0	0
			1317	833	241	241	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	149	Total	C	N	O	S	0	0
			1102	693	197	211	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1130	713	211	201	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	123	Total	C	N	O	S	0	0
			947	594	181	166	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1051	651	207	191	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1074	685	204	179	6		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	n	116	Total 890	C 550	N 178	O 162	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total 815	C 515	N 153	O 145	S 2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total 855	C 530	N 166	O 156	S 3	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	93	Total 739	C 467	N 139	O 131	S 2	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	t	103	Total 788	C 498	N 148	O 142	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	94	Total	C	N	O	S	0	0
			746	476	135	133	2		

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	78	Total	C	N	O	S	0	0
			592	364	119	108	1		

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	77	Total	C	N	O	S	0	0
			626	388	129	107	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	62	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	58	Total	C	N	O	S	0	0
			453	285	87	79	2		

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	55	Total	C	N	O	S	0	0
			435	264	92	78	1		

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
54	1	1	Total	K	0
			1	1	
54	A	44	Total	K	0
			44	44	
54	M	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
54	a	108	Total K 108 108	0
54	b	1	Total K 1 1	0
54	c	4	Total K 4 4	0
54	d	1	Total K 1 1	0
54	e	1	Total K 1 1	0
54	f	1	Total K 1 1	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	3	1	Total Zn 1 1	0
55	4	1	Total Zn 1 1	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

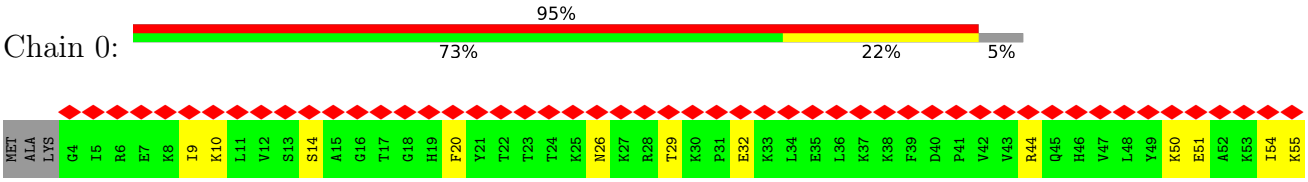
Mol	Chain	Residues	Atoms	AltConf
56	A	95	Total Mg 95 95	0
56	a	252	Total Mg 252 252	0
56	b	5	Total Mg 5 5	0
56	c	2	Total Mg 2 2	0
56	d	1	Total Mg 1 1	0
56	p	1	Total Mg 1 1	0
56	z	1	Total Mg 1 1	0

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.

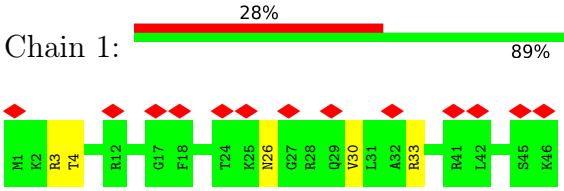
• Molecule 1: Large ribosomal subunit protein bL33

Chain 0:



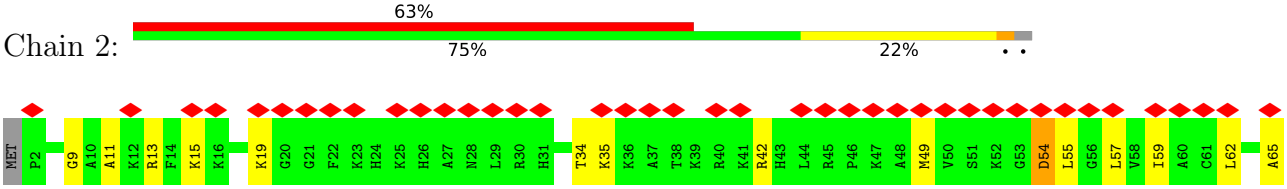
• Molecule 2: Large ribosomal subunit protein bL34

Chain 1:



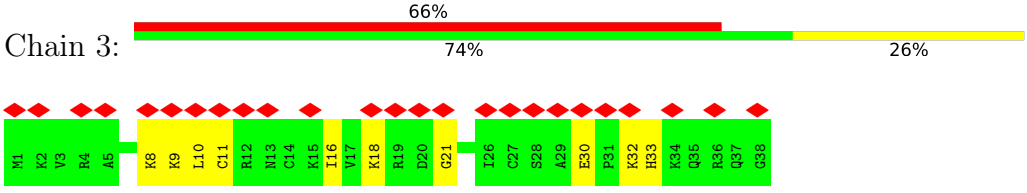
• Molecule 3: Large ribosomal subunit protein bL35

Chain 2:



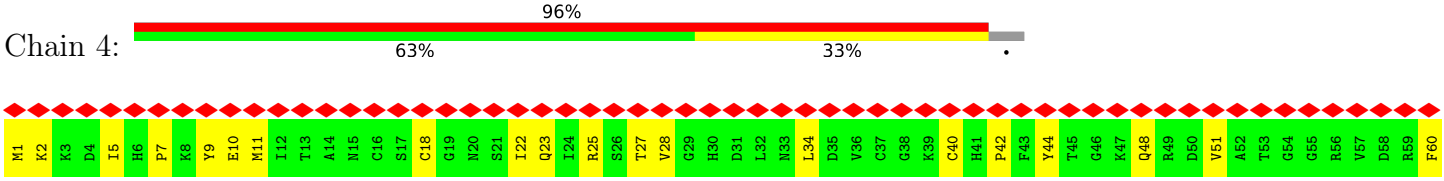
• Molecule 4: Large ribosomal subunit protein bL36

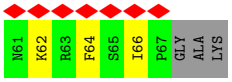
Chain 3:



• Molecule 5: Large ribosomal subunit protein bL31

Chain 4:

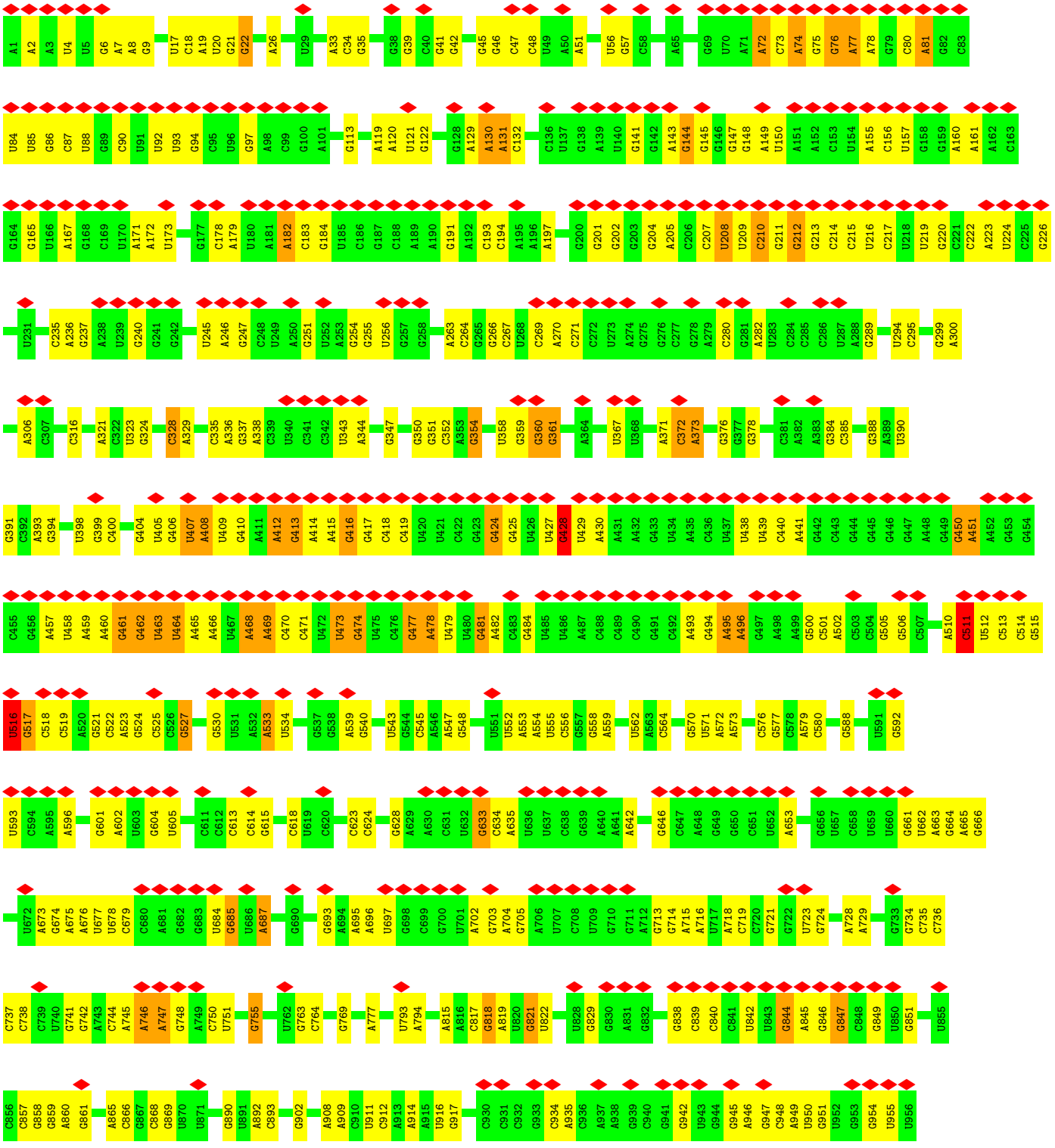


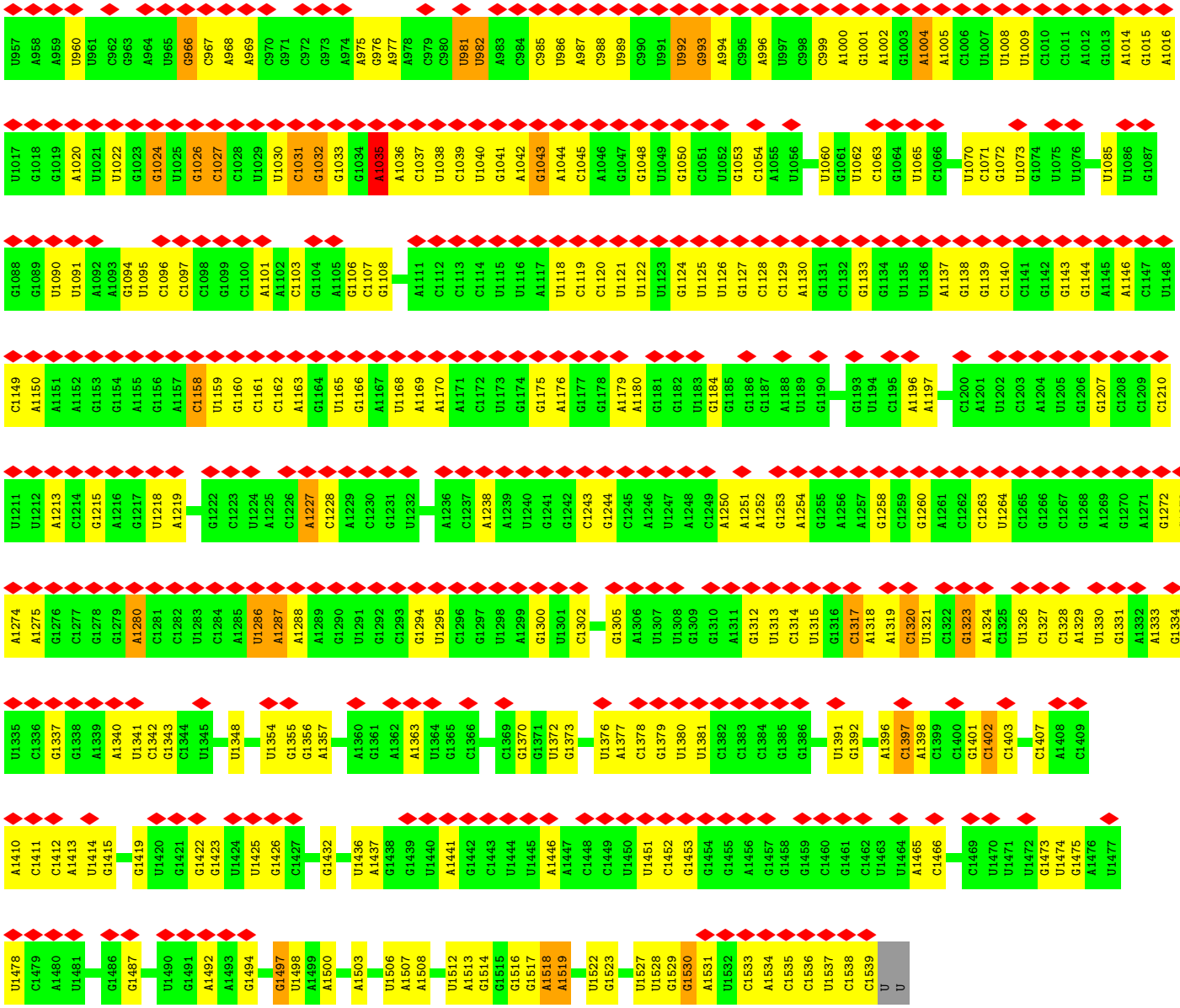


• Molecule 6: 16S rRNA (1539-MER)

Chain A:

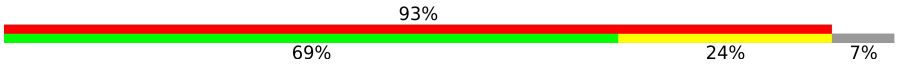


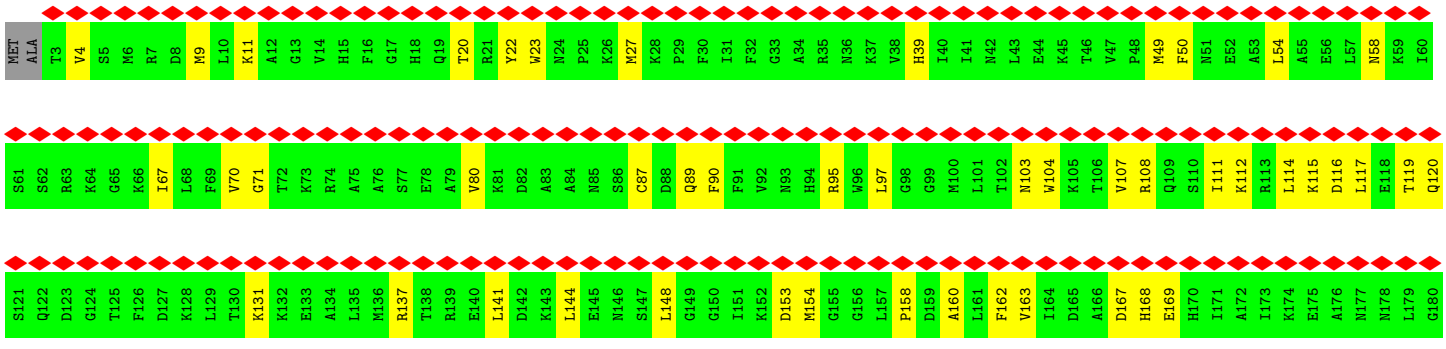


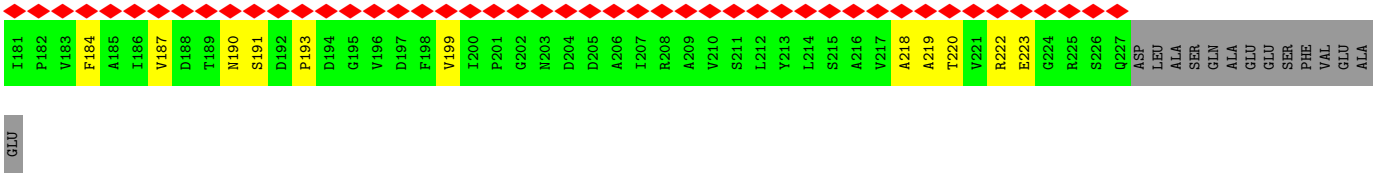


• Molecule 7: Small ribosomal subunit protein uS2

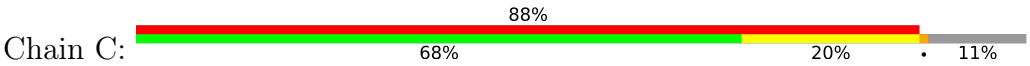
Chain B:

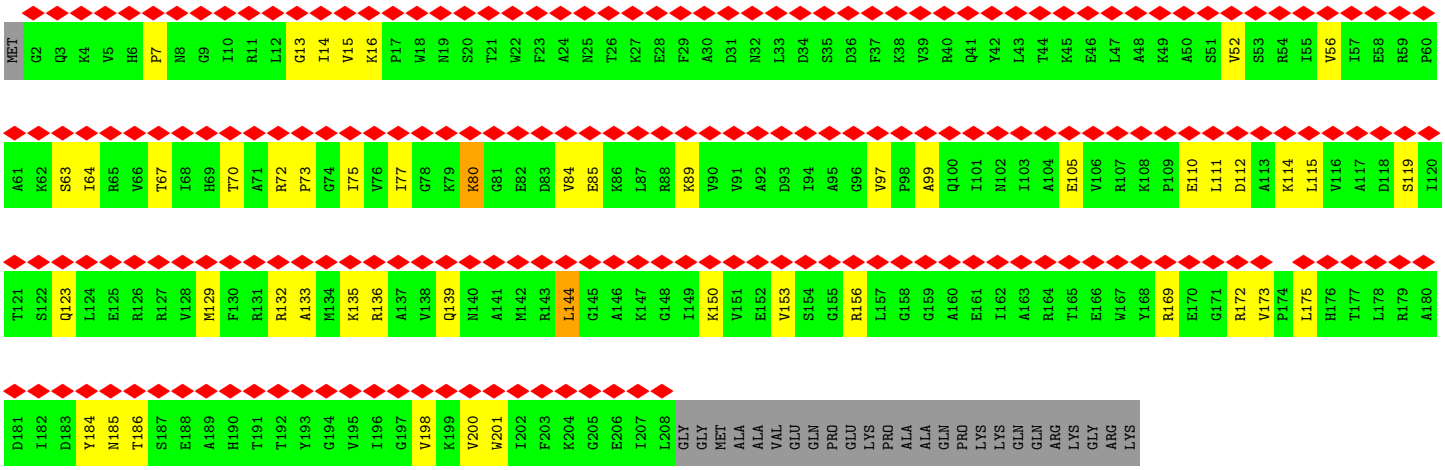




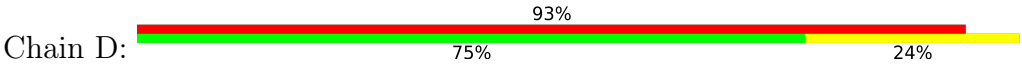


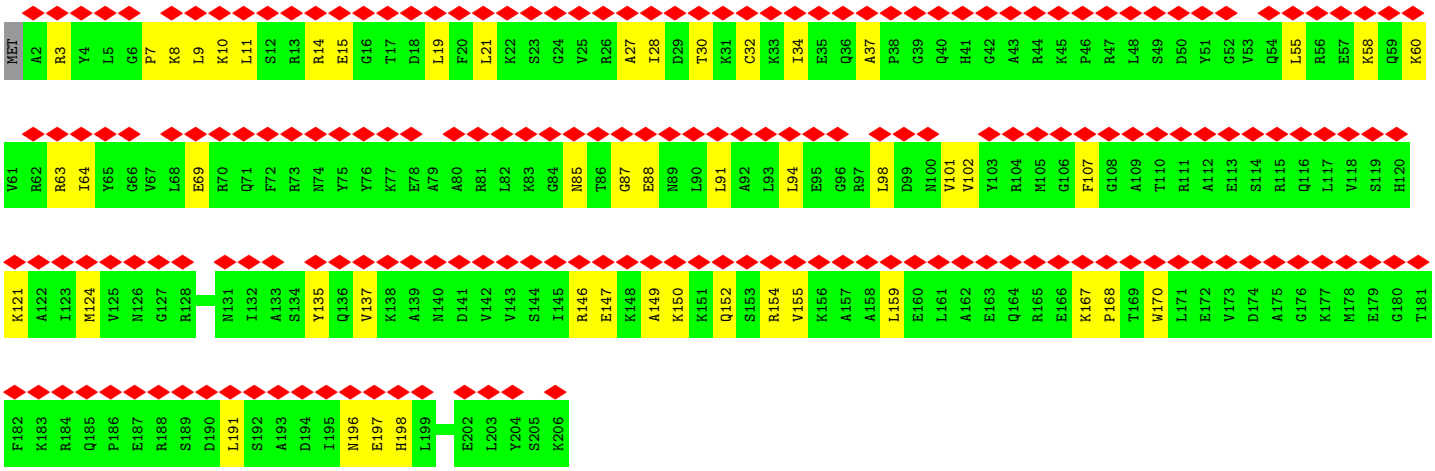
• Molecule 8: Small ribosomal subunit protein uS3



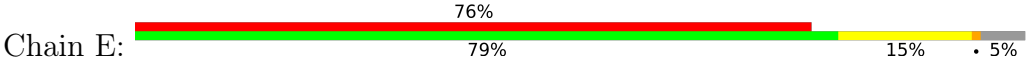


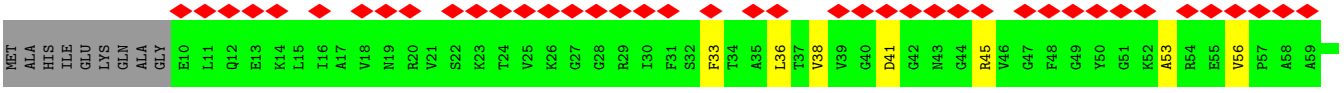
• Molecule 9: Small ribosomal subunit protein uS4

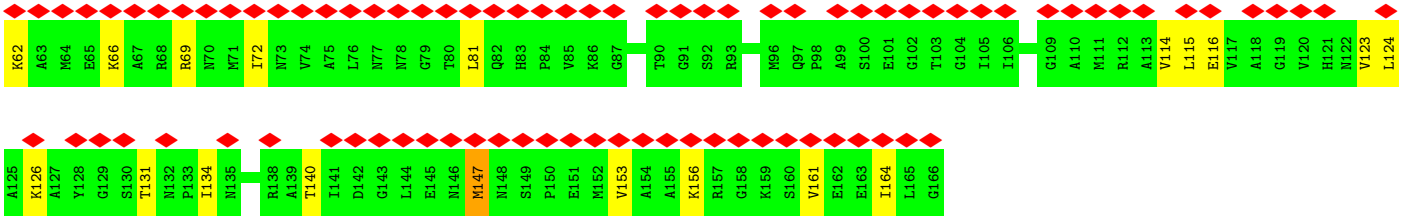




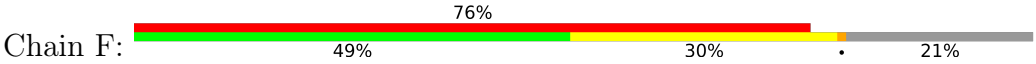
• Molecule 10: Small ribosomal subunit protein uS5

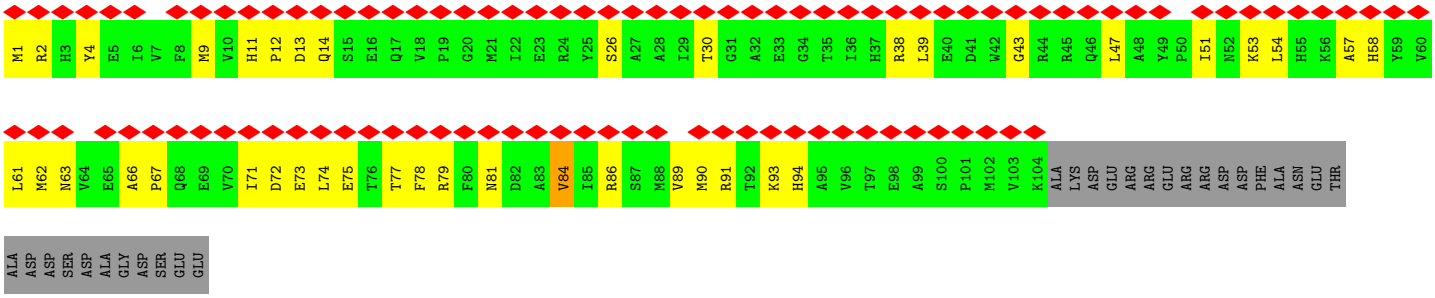






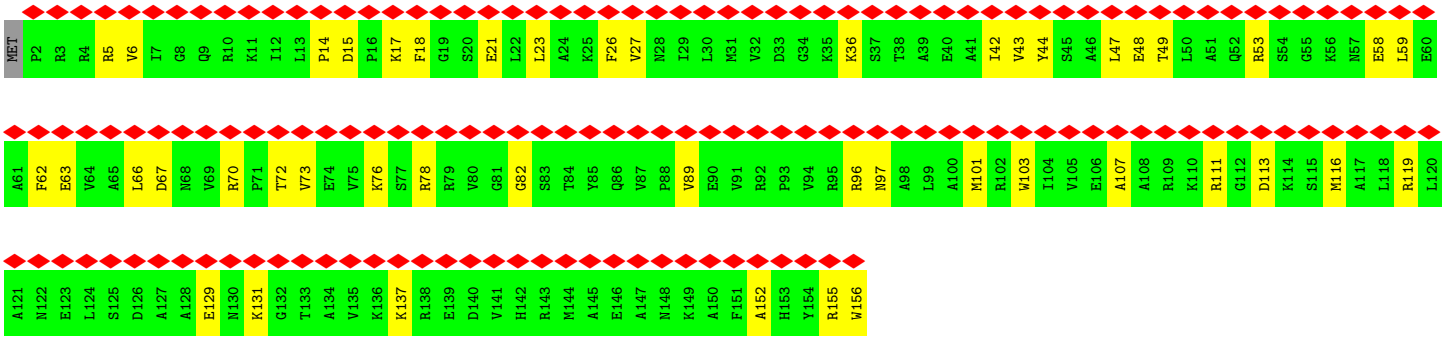
• Molecule 11: Small ribosomal subunit protein bS6



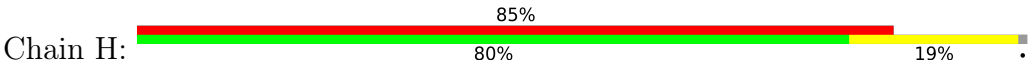


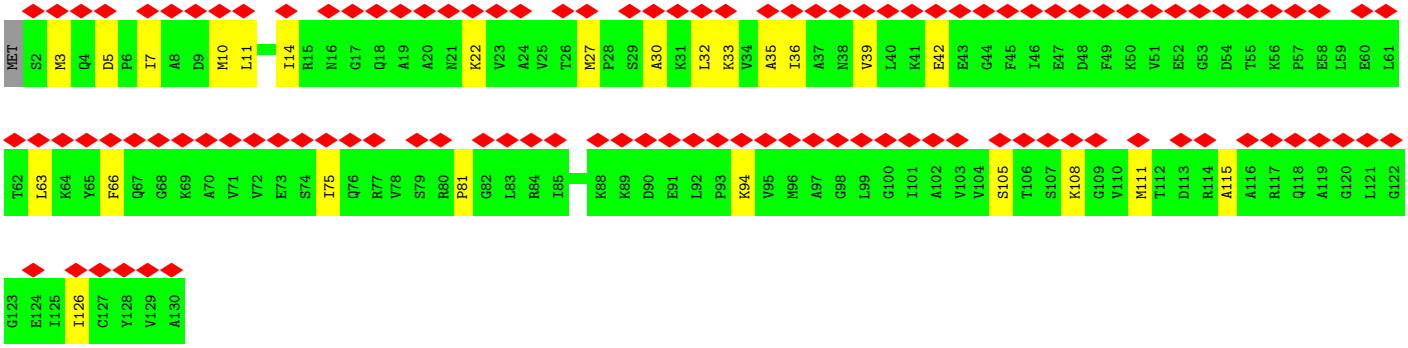
• Molecule 12: Small ribosomal subunit protein uS7





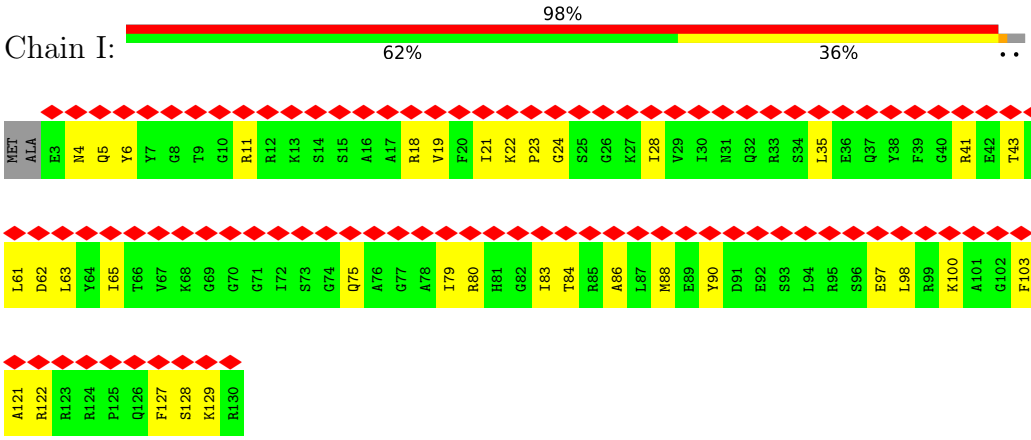
• Molecule 13: Small ribosomal subunit protein uS8





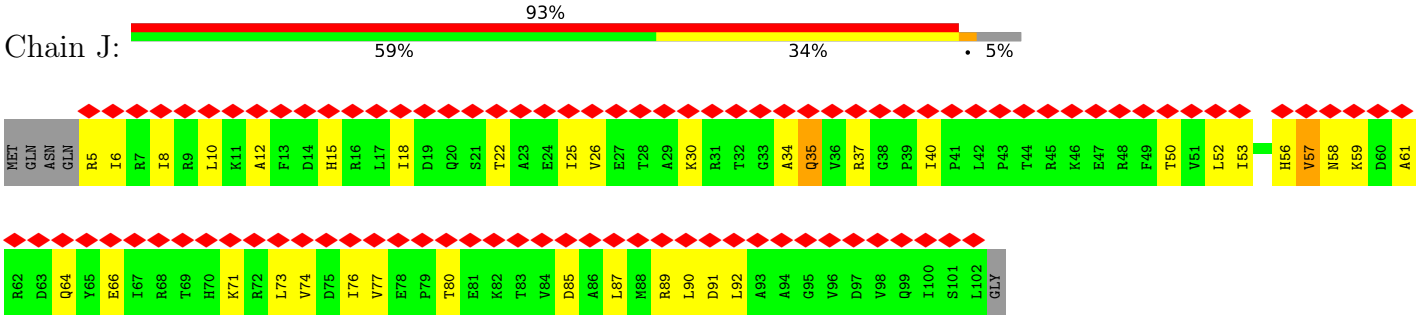
• Molecule 14: Small ribosomal subunit protein uS9

Chain I:



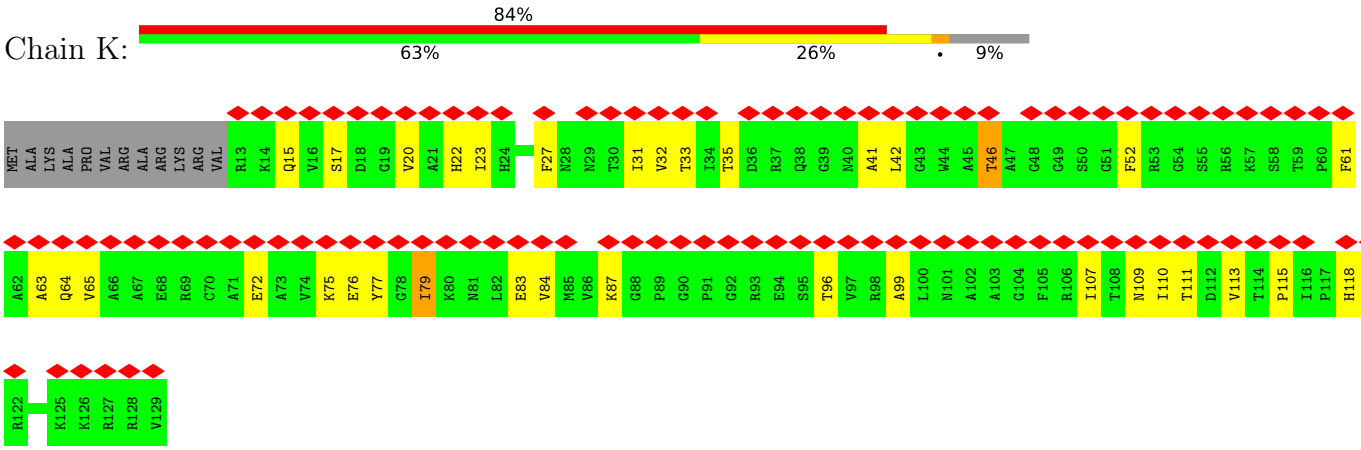
• Molecule 15: Small ribosomal subunit protein uS10

Chain J:



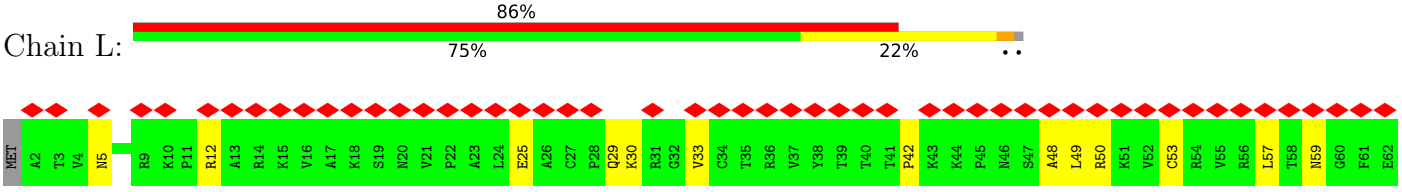
• Molecule 16: Small ribosomal subunit protein uS11

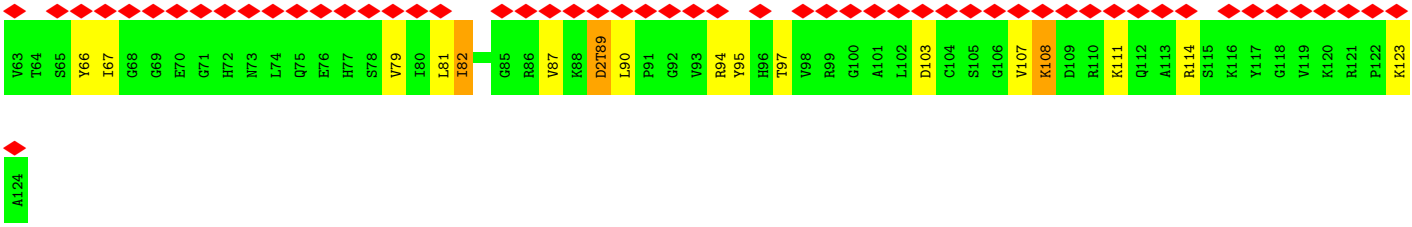
Chain K:



• Molecule 17: Small ribosomal subunit protein uS12

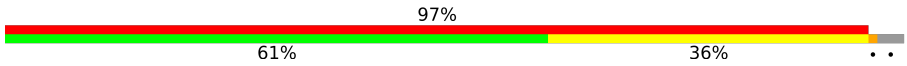
Chain L:

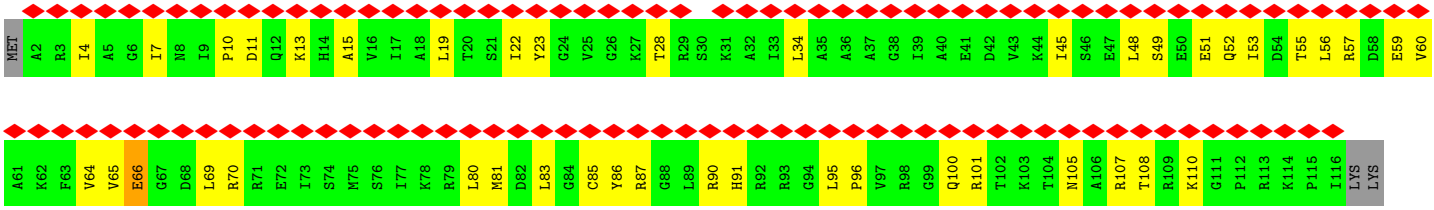




• Molecule 18: Small ribosomal subunit protein uS13

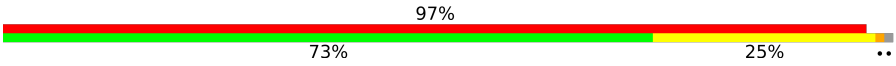
Chain M:

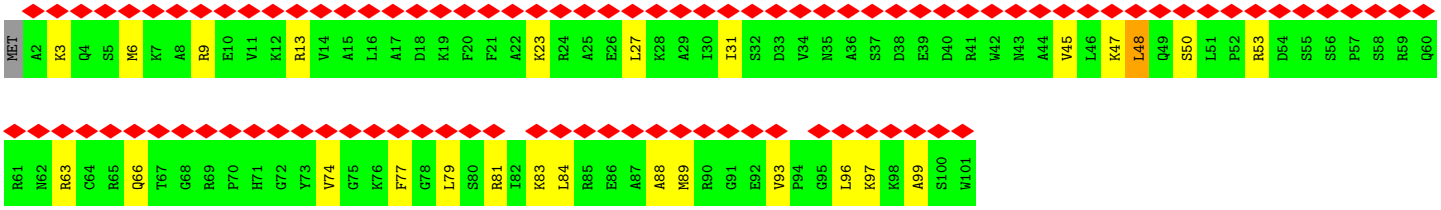




• Molecule 19: Small ribosomal subunit protein uS14

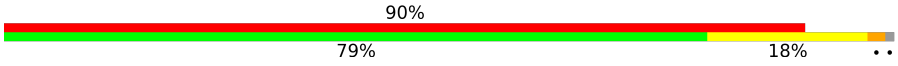
Chain N:

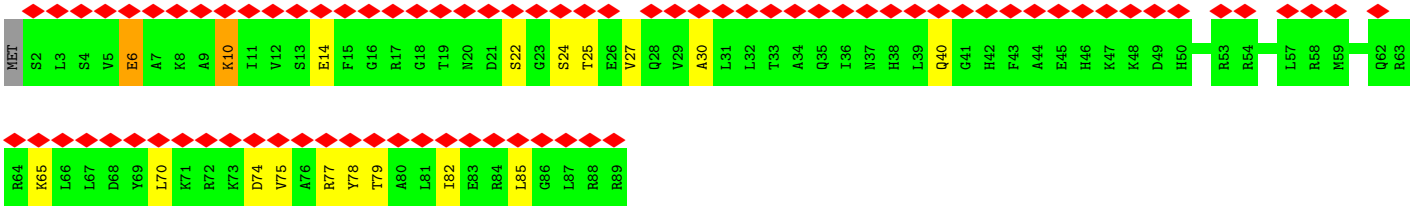




• Molecule 20: Small ribosomal subunit protein uS15

Chain O:

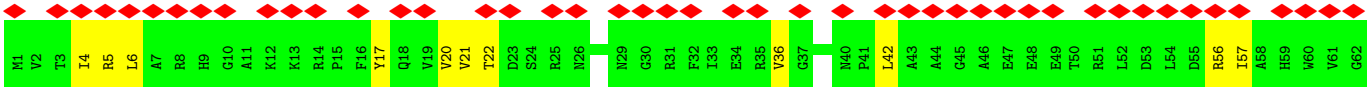




• Molecule 21: Small ribosomal subunit protein bS16

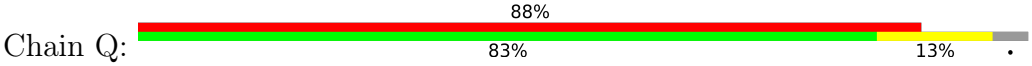
Chain P:

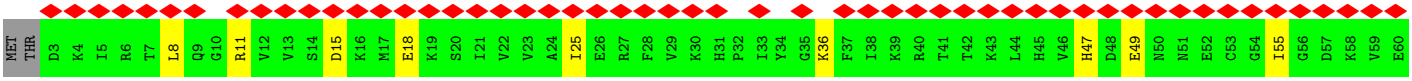


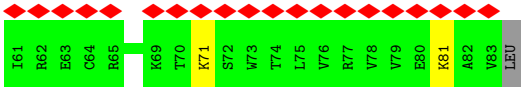




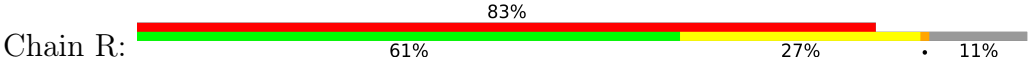
• Molecule 22: Small ribosomal subunit protein uS17

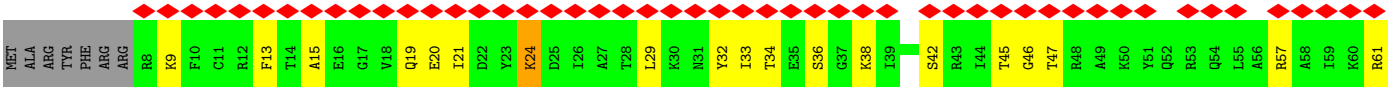


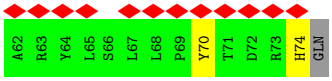




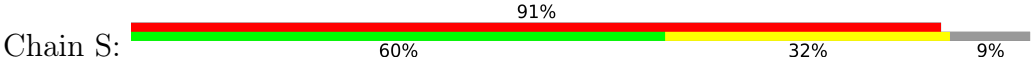
• Molecule 23: Small ribosomal subunit protein bS18



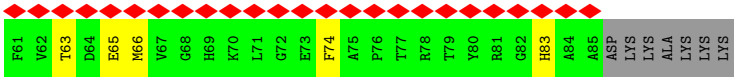




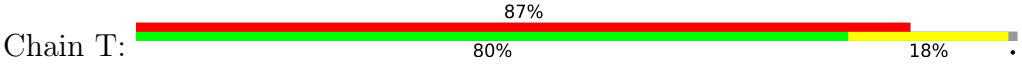
• Molecule 24: Small ribosomal subunit protein uS19

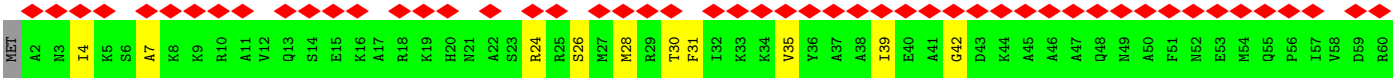


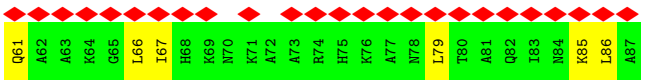




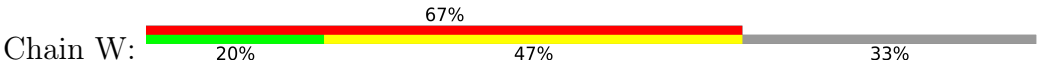
• Molecule 25: Small ribosomal subunit protein bS20

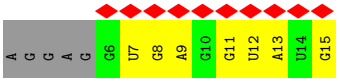






• Molecule 26: non-STOP mRNA

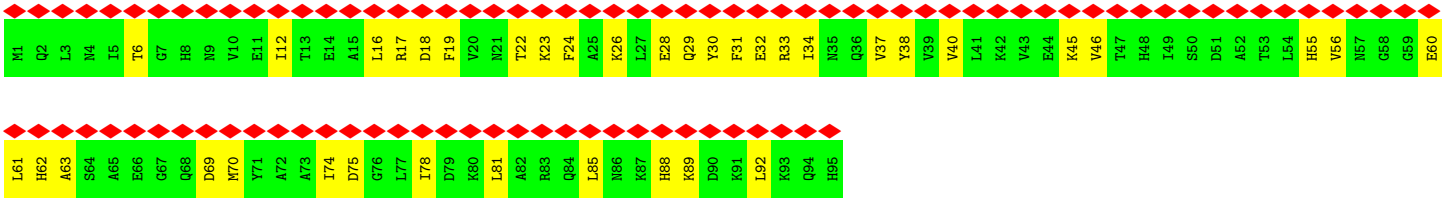




• Molecule 27: Ribosome hibernation promoting factor

Chain X:

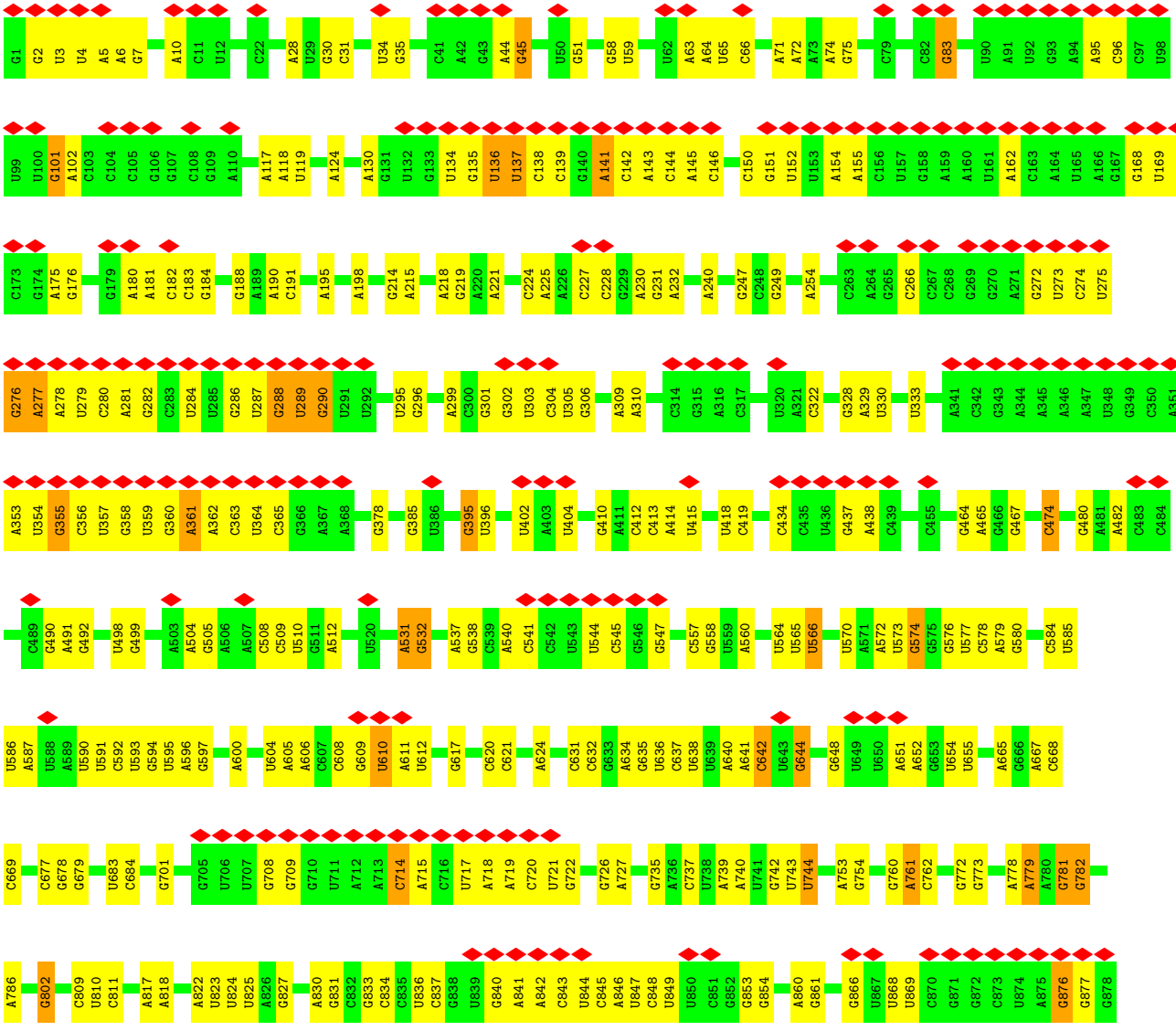


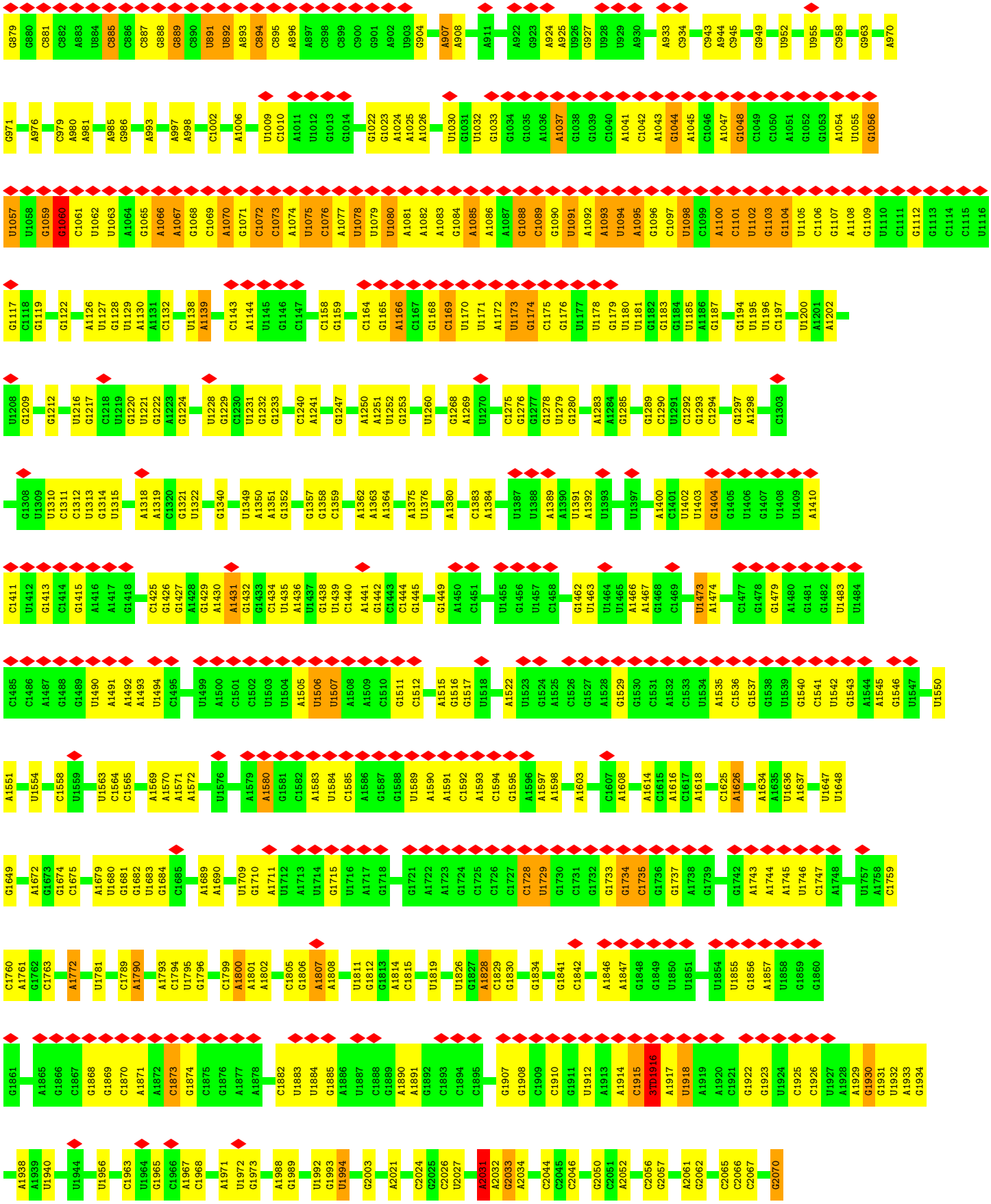


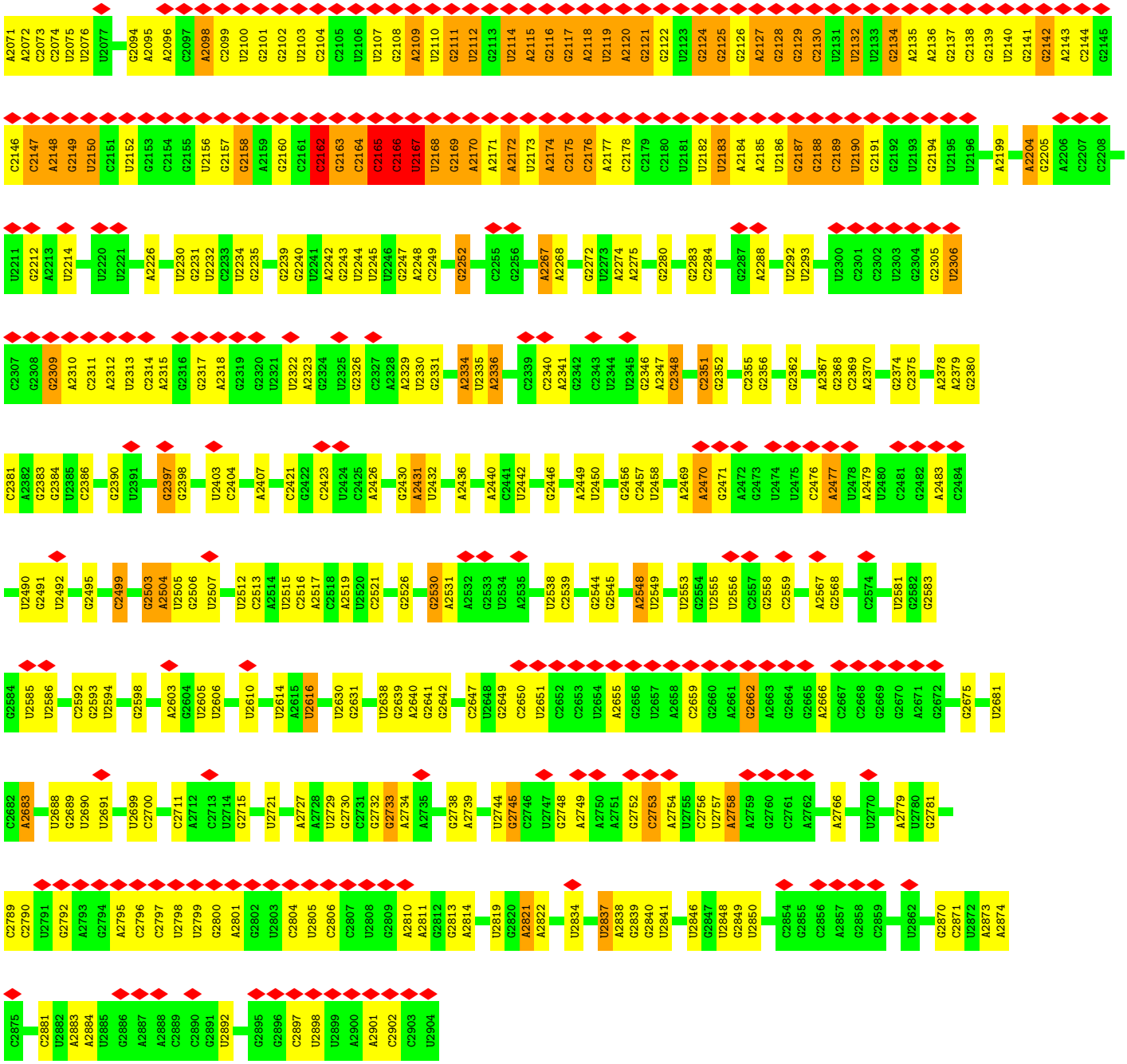
• Molecule 28: 23S rRNA (2904-MER)

Chain a:





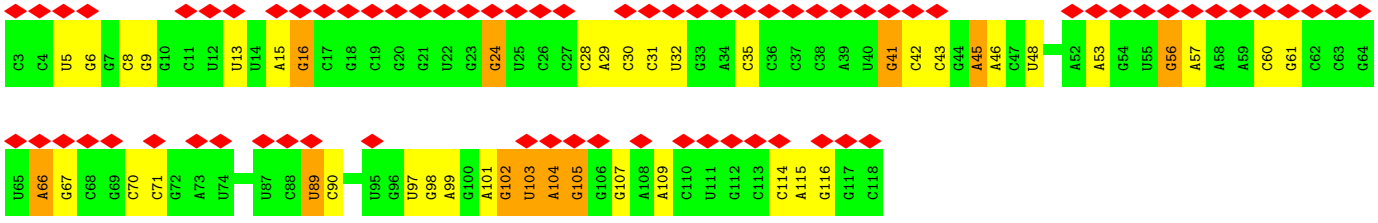

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G971 A976 C979 A980 A981 A985 G986 A993 A997 A998 C1002 A1006 U1009 C1010 A1011 U1012 G1013 G1014 G1022 G1023 A1024 A1025 A1026 U1030 G1031 U1032 G1033 G1034 G1035 A1036 A1037 G1038 G1039 C1040 A1041 C1042 A1043 G1044 A1045 C1046 A1047 G1048 C1049 C1050 A1051 G1052 G1053 A1054 U1055 G1056
U1057 U1058 G1059 G1060 C1061 U1062 U1063 A1064 G1065 A1066 A1067 G1068 C1069 A1070 G1071 C1072 C1073 A1074 U1075 C1076 A1077 U1078 U1079 U1080 A1081 A1082 A1083 G1084 A1085 A1086 A1087 G1088 C1089 G1090 U1091 A1092 A1093 U1094 A1095 G1096 C1097 U1098 C1099 A1100 C1101 U1102 G1103 G1104 U1105 C1106 G1107 A1108 G1109 U1110 C1111 G1112 G1113 C1114 C1115 U1116
G1117 C1118 G1119 G1122 A1126 U1127 G1128 U1129 A1130 A1131 C1132 U1138 A1139 C1143 A1144 U1145 G1146 C1147 C1158 G1159 C1164 G1165 A1166 C1167 G1168 C1169 U1170 U1171 A1172 U1173 G1174 C1175 G1176 U1177 U1178 G1179 U1180 U1181 G1182 G1183 G1184 U1185 A1186 G1187 G1194 U1195 U1196 C1197 U1200 A1201 A1202
U1208 G1209 G1212 U1216 G1217 C1218 U1219 G1220 U1221 G1222 A1223 G1224 U1228 G1229 C1230 U1231 G1232 G1233 C1240 A1241 G1247 A1250 A1251 U1252 G1253 U1260 G1268 A1269 U1270 C1275 G1276 G1277 G1278 U1279 G1280 A1283 A1284 G1285 G1289 C1290 U1291 C1292 G1293 C1294 G1297 A1298 C1303
G1308 U1309 U1310 C1311 C1312 U1313 G1314 U1315 A1318 A1319 C1320 G1321 U1322 G1340 U1349 A1350 A1351 G1352 G1357 G1358 C1359 A1362 A1363 A1364 A1375 U1376 A1380 C1383 A1384 U1387 U1388 A1389 A1390 U1391 A1392 U1393 U1397 A1400 C1401 U1402 U1403 G1404 G1405 U1406 G1407 U1408 U1409 A1410
C1411 U1412 G1413 C1414 G1415 A1416 A1417 G1418 C1425 G1426 G1427 A1428 G1429 A1430 A1431 G1432 G1433 C1434 U1435 A1436 U1437 G1438 U1439 C1440 A1441 G1442 C1443 C1444 G1445 G1449 A1450 C1451 U1455 G1456 U1457 C1458 G1462 U1463 U1464 U1465 A1466 A1467 G1468 C1469 U1473 A1474 C1477 G1478 G1479 A1480 G1481 G1482 U1483 U1484
C1485 C1486 A1487 G1488 G1489 U1490 A1491 A1492 A1493 U1494 C1495 U1499 A1500 C1501 C1502 U1503 U1504 A1505 U1506 U1507 A1508 A1509 C1510 G1511 C1512 A1515 G1516 U1517 U1518 A1522 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 G1546 U1547 U1550
A1551 U1554 C1558 U1559 U1563 C1564 C1565 A1569 A1570 A1571 A1572 U1576 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 C1594 G1595 A1596 A1597 A1598 A1603 C1607 A1608 A1614 C1615 A1616 C1617 A1618 C1625 A1626 A1634 A1635 U1636 A1637 U1647 U1648
G1649 A1672 G1673 G1674 C1675 A1679 U1680 G1681 G1682 U1683 G1684 C1685 A1689 A1690 U1709 G1710 A1711 U1712 A1713 U1714 G1715 U1716 A1717 G1718 G1721 A1722 A1723 G1724 C1725 C1726 C1727 C1728 U1729 G1730 C1731 G1732 G1733 G1734 C1735 G1736 G1737 A1738 G1739 G1742 A1743 A1744 A1745 U1746 C1747 A1748 U1757 A1758 C1759
C1760 A1761 G1762 C1763 A1772 U1781 C1789 A1790 A1793 C1794 U1795 G1796 C1799 A1800 A1801 A1802 C1805 G1806 A1807 A1808 U1811 G1812 G1813 A1814 C1815 U1819 U1826 G1827 A1828 C1829 G1830 G1834 G1841 C1842 A1846 A1847 G1848 G1849 U1850 U1851 U1854 U1855 G1856 A1857 U1858 G1859 G1860
G1861 A1865 G1866 C1867 G1868 G1869 C1870 A1871 A1872 C1873 G1874 C1875 G1876 A1877 A1878 C1882 U1883 U1884 G1885 A1886 U1887 C1888 G1889 A1890 A1891 C1892 C1893 C1894 C1895 G1907 G1908 C1909 C1910 G1911 U1912 A1913 A1914 C1915 3TD1916 A1917 U1918 A1919 A1920 C1921 G1922 G1923 U1924 C1925 C1926 U1927 A1928 A1929 G1930 G1931 U1932 U1933 G1934
A1938 A1939 U1940 U1944 U1956 C1963 U1964 G1965 C1966 A1967 C1968 A1971 U1972 G1973 A1988 G1989 U1992 G1993 U1994 G2003 A2021 C2024 G2025 C2026 U2027 A2031 A2032 G2033 A2034 C2044 C2045 C2046 G2050 C2051 A2052 C2056 G2057 A2061 G2062 C2065 C2066 C2067 G2070



• Molecule 29: 5S rRNA (120-MER)

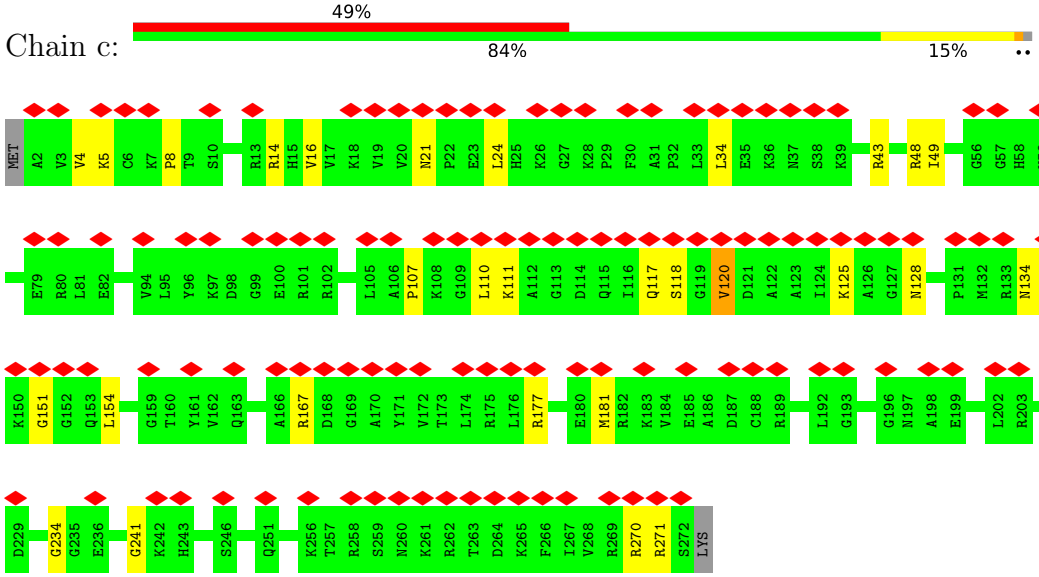
Chain b:





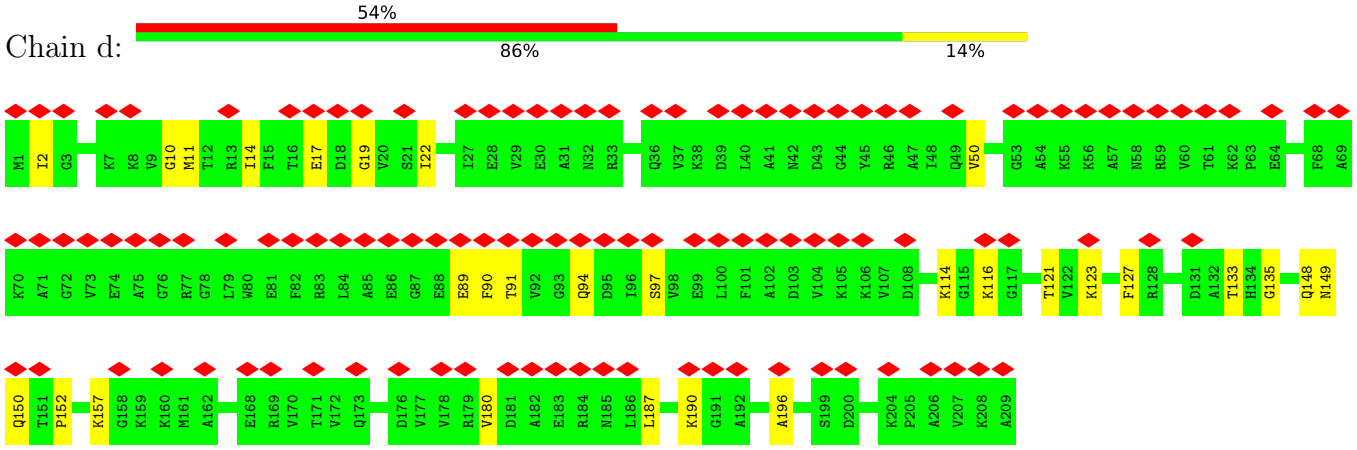
• Molecule 30: Large ribosomal subunit protein uL2

Chain c:



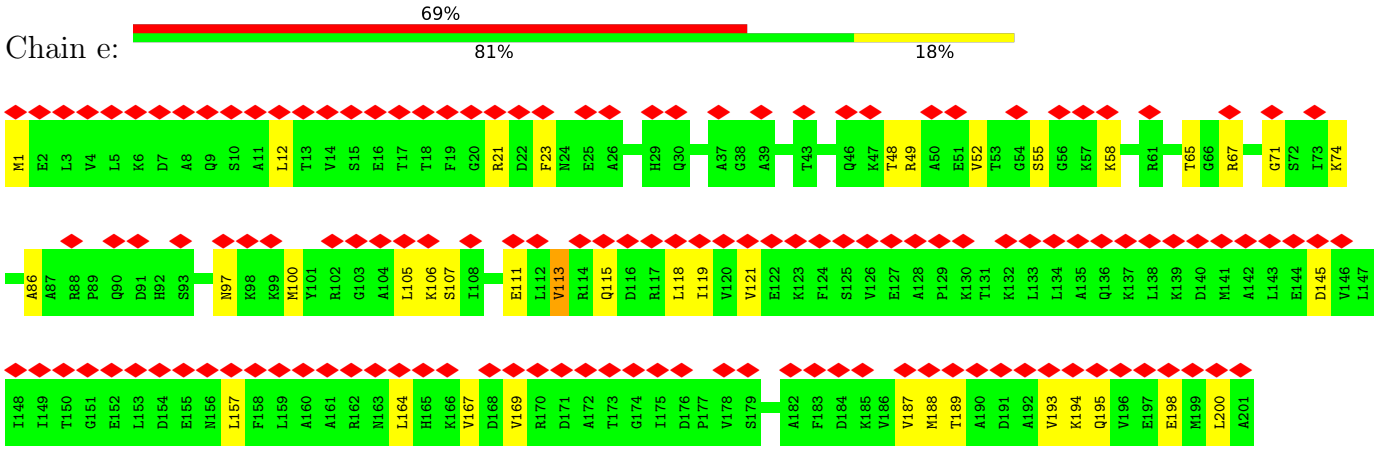
• Molecule 31: Large ribosomal subunit protein uL3

Chain d:



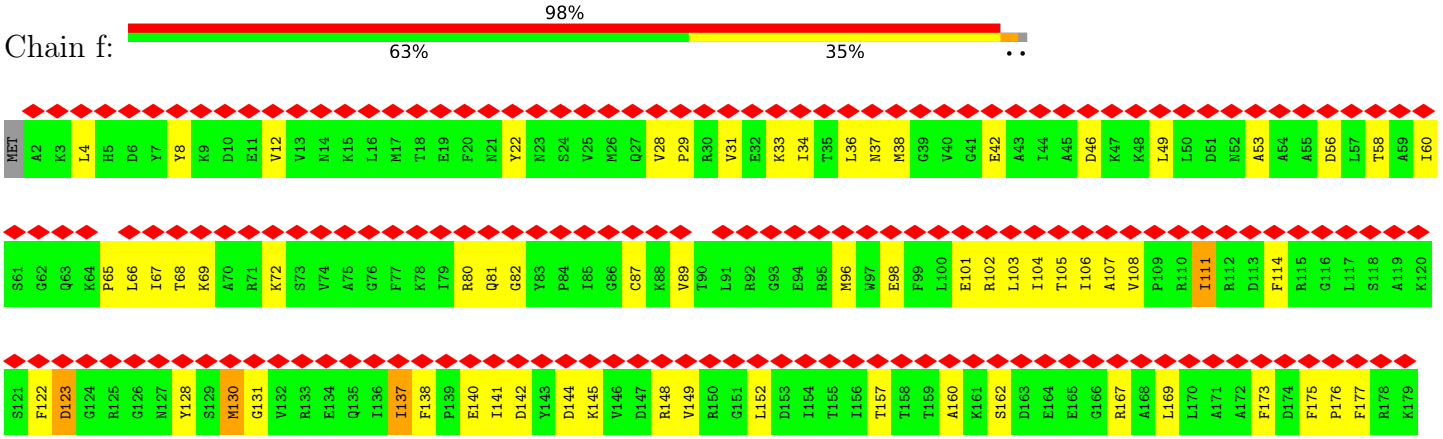
• Molecule 32: Large ribosomal subunit protein uL4

Chain e:



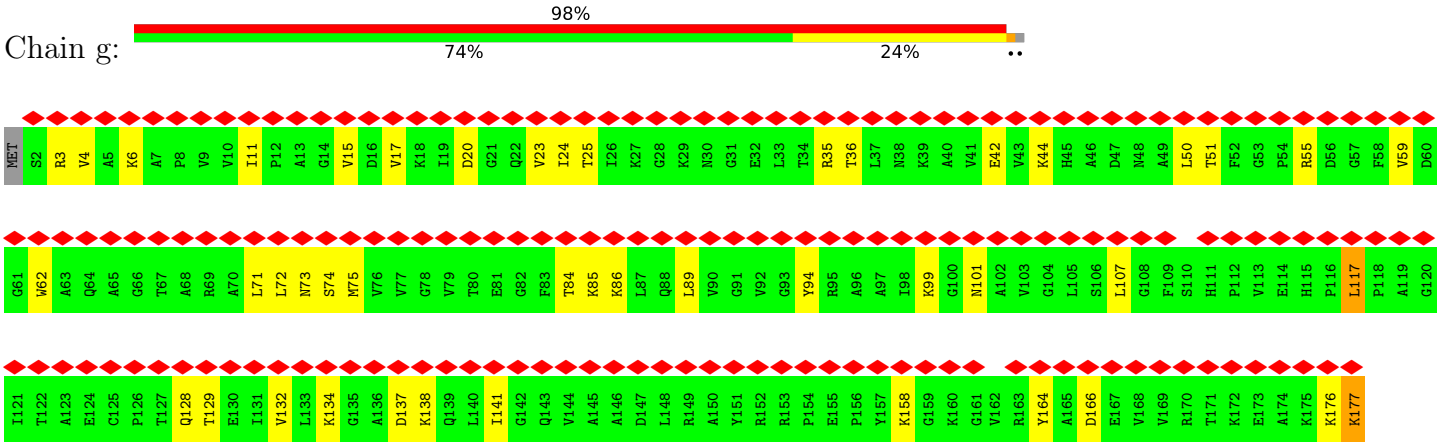
• Molecule 33: Large ribosomal subunit protein uL5

Chain f:



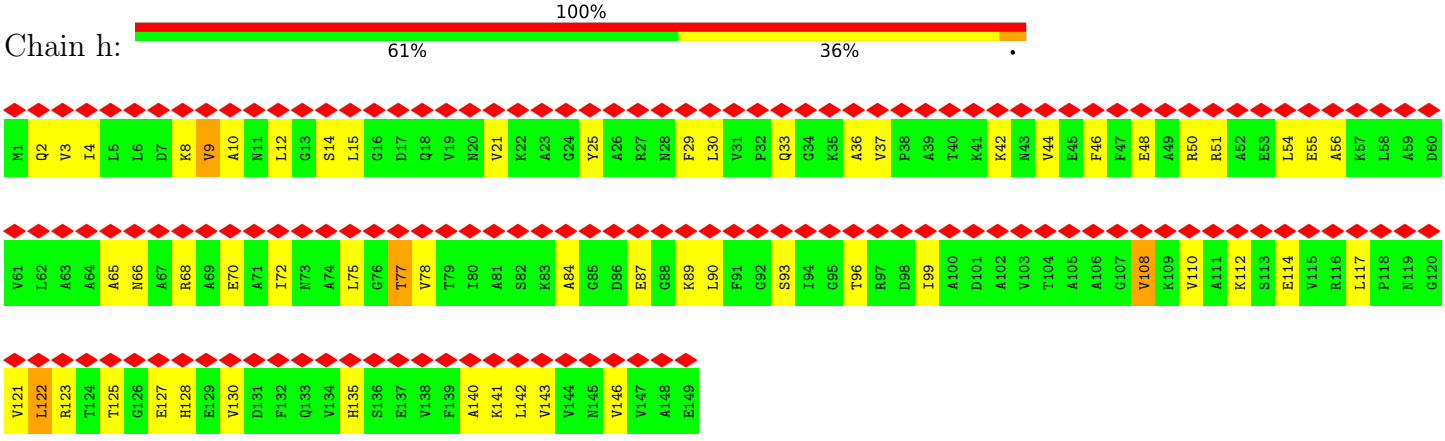
• Molecule 34: Large ribosomal subunit protein uL6

Chain g:



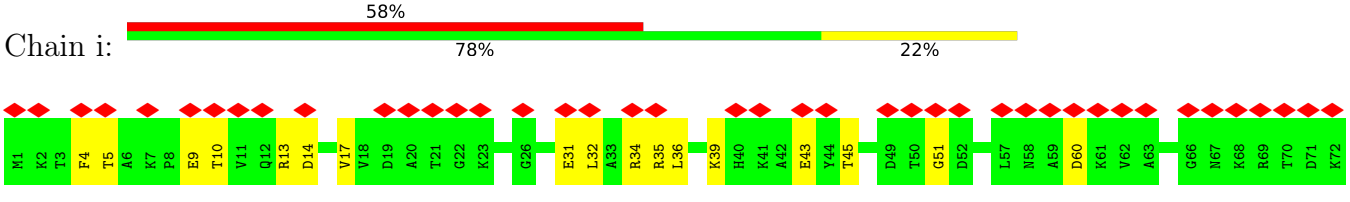
• Molecule 35: Large ribosomal subunit protein bL9

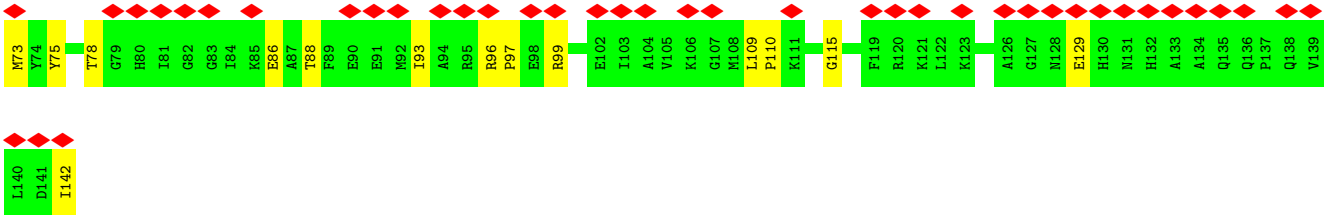
Chain h:



• Molecule 36: Large ribosomal subunit protein uL13

Chain i:

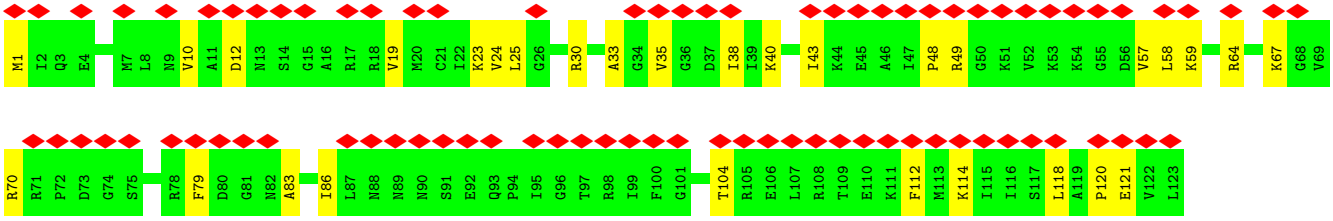




• Molecule 37: Large ribosomal subunit protein uL14

Chain j:

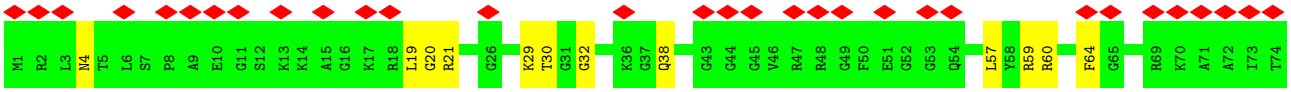




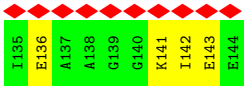
• Molecule 38: Large ribosomal subunit protein uL15

Chain k:





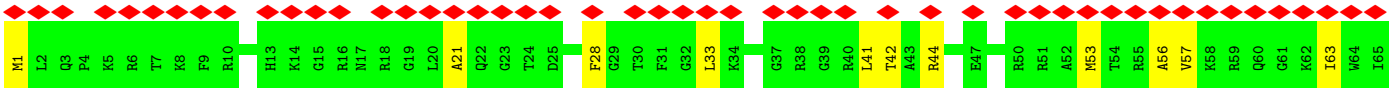


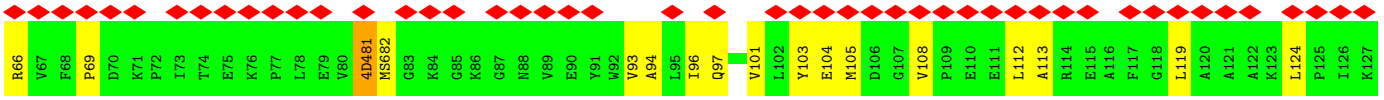


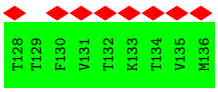
• Molecule 39: Large ribosomal subunit protein uL16

Chain l:



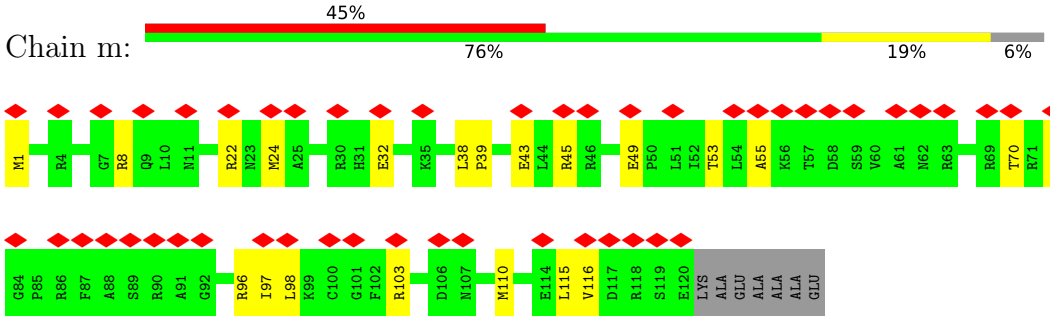






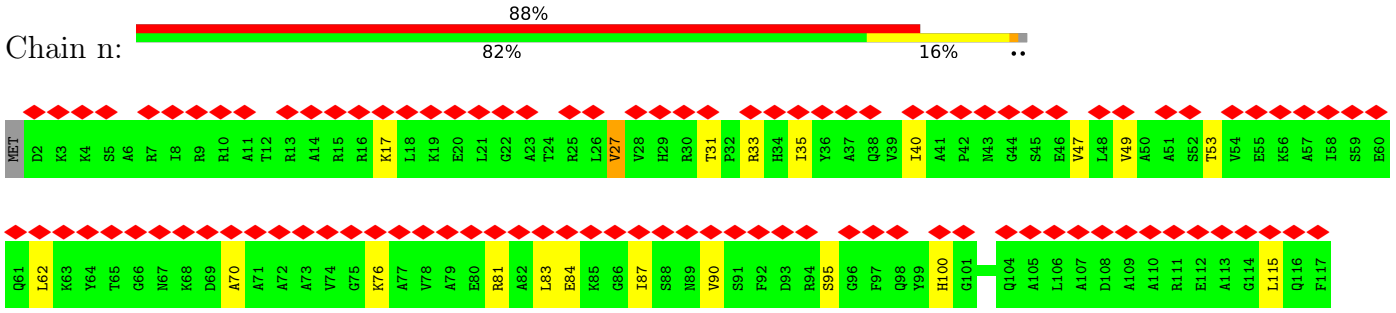
• Molecule 40: Large ribosomal subunit protein bL17

Chain m:



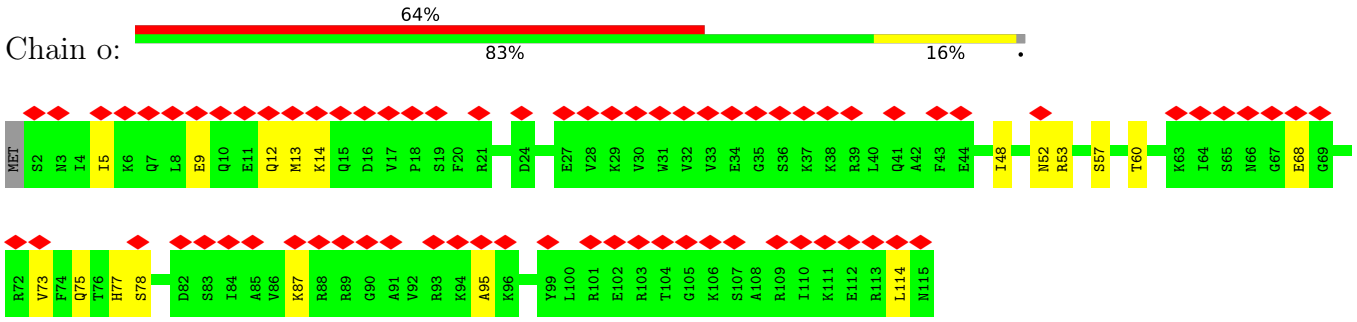
• Molecule 41: Large ribosomal subunit protein uL18

Chain n:



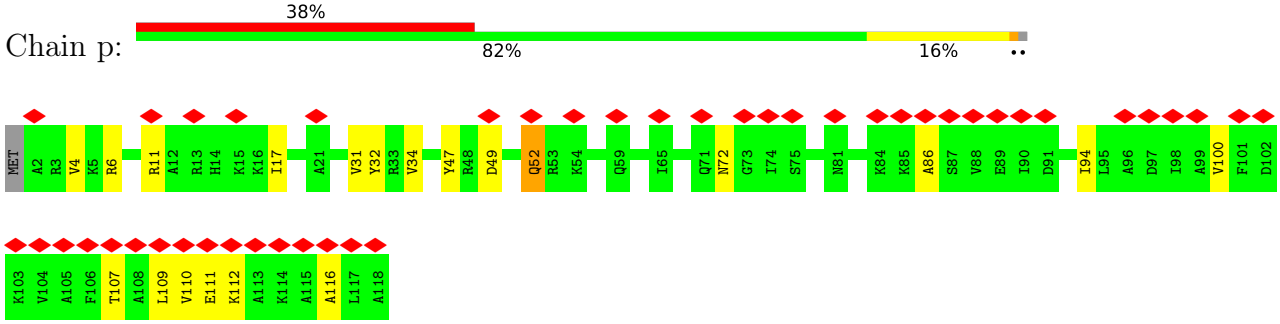
• Molecule 42: Large ribosomal subunit protein bL19

Chain o:



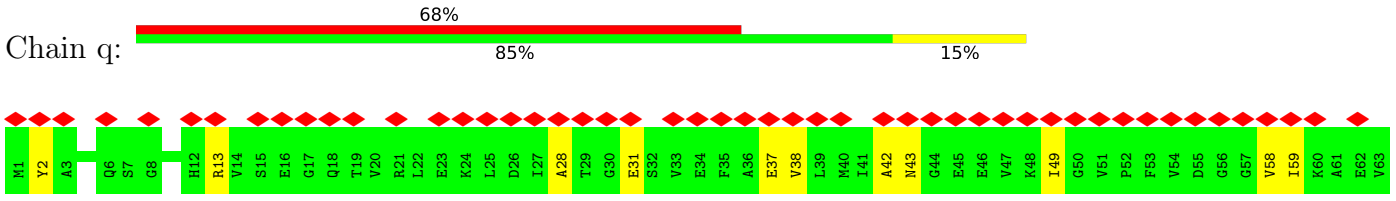
• Molecule 43: Large ribosomal subunit protein bL20

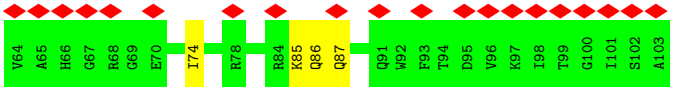
Chain p:



• Molecule 44: Large ribosomal subunit protein bL21

Chain q:

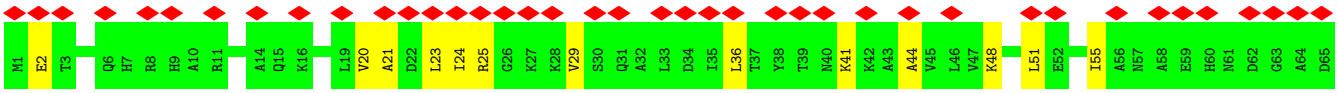


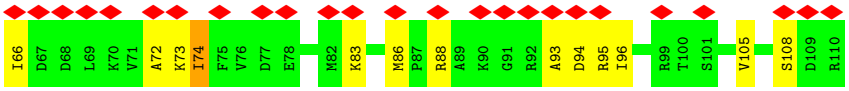


• Molecule 45: Large ribosomal subunit protein uL22

Chain r:



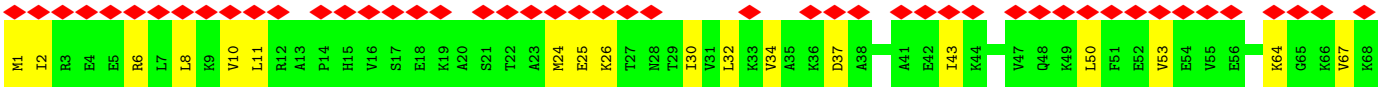


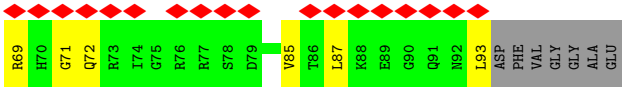


• Molecule 46: Large ribosomal subunit protein uL23

Chain s:



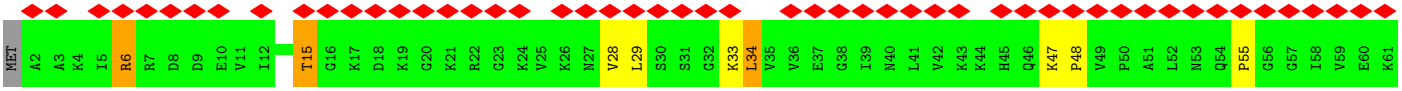


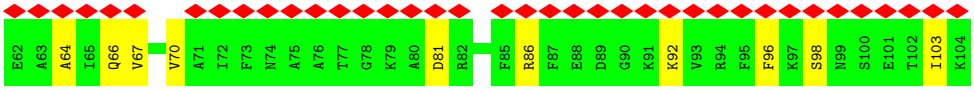


• Molecule 47: Large ribosomal subunit protein uL24

Chain t:



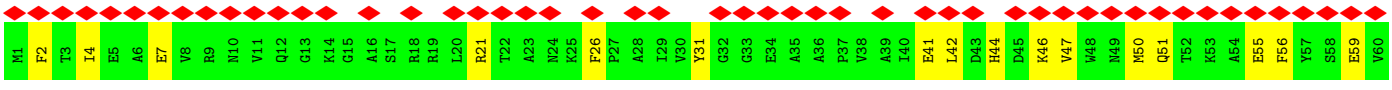


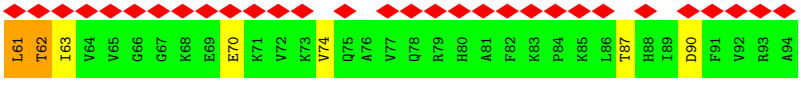


• Molecule 48: Large ribosomal subunit protein bL25

Chain u:

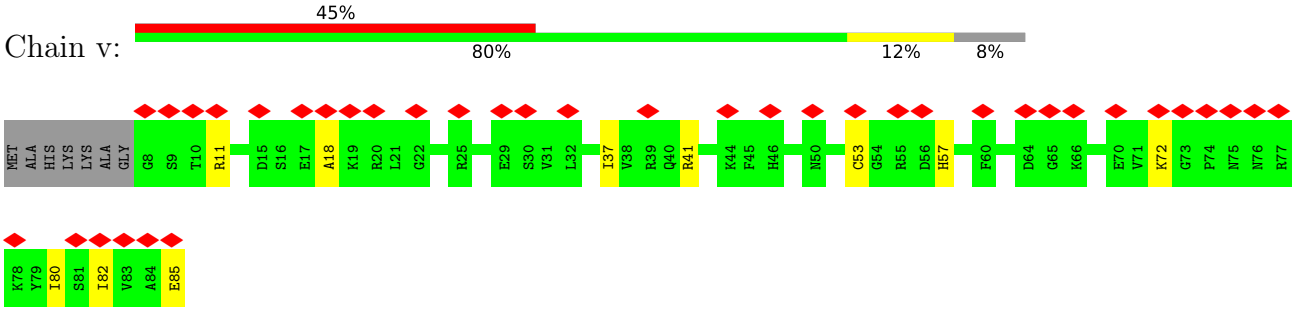






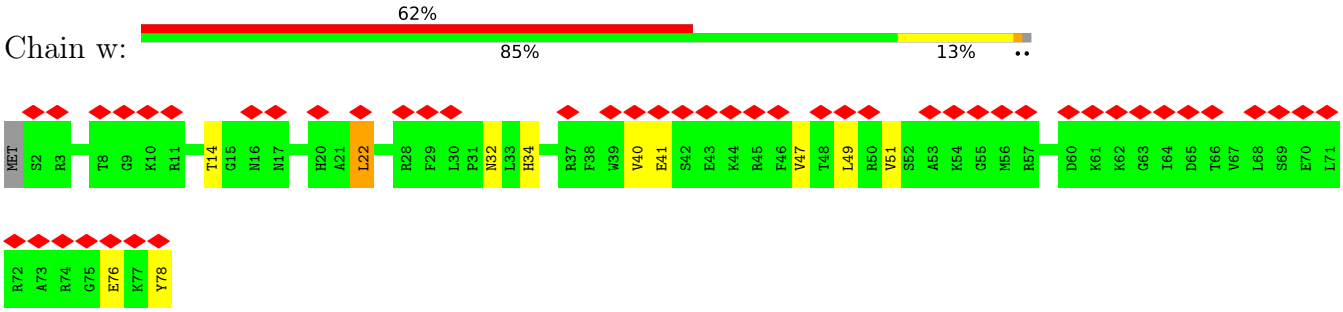
• Molecule 49: Large ribosomal subunit protein bL27

Chain v:



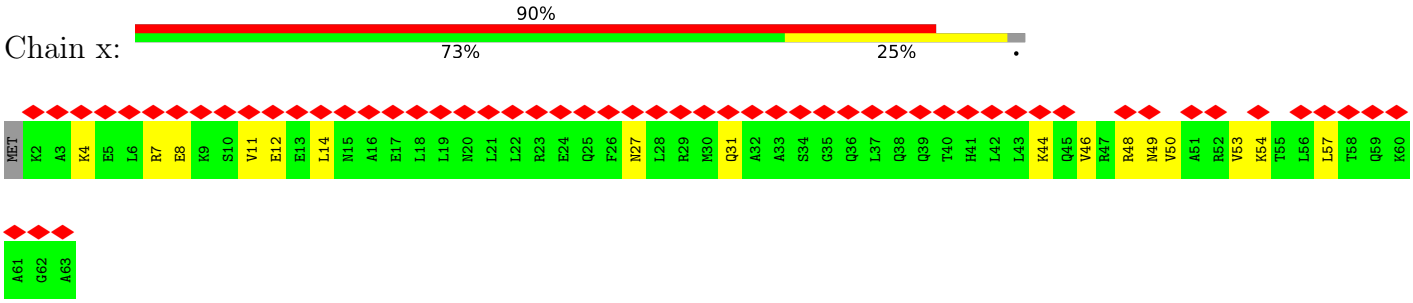
• Molecule 50: Large ribosomal subunit protein bL28

Chain w:



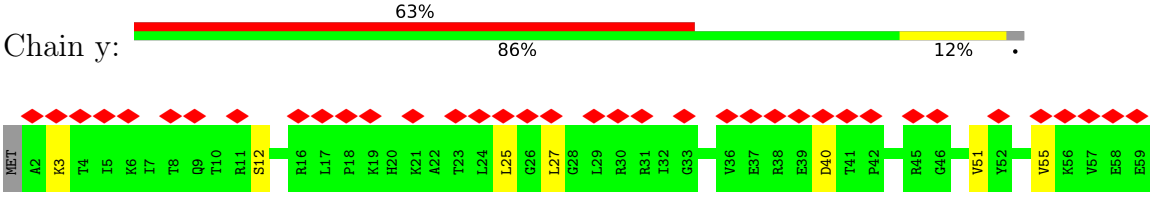
• Molecule 51: Large ribosomal subunit protein uL29

Chain x:



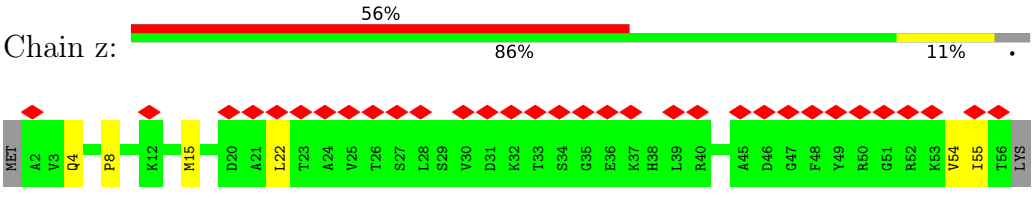
• Molecule 52: Large ribosomal subunit protein uL30

Chain y:



• Molecule 53: Large ribosomal subunit protein bL32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.371	Depositor
Minimum map value	-0.483	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, G7M, H2U, PSU, 4OC, MG, MEQ, UR3, D2T, 2MG, 5MC, MA6, 5MU, ZN, 2MA, K, OMC, OMG, MS6, 6MZ, IAS, 1MG, OMU, 4D4

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	0	0.22	0/433	0.33	0/576
2	1	0.29	0/380	0.34	0/498
3	2	0.26	0/513	0.31	0/676
4	3	0.26	0/303	0.31	0/397
5	4	0.16	0/536	0.46	0/718
6	A	0.56	0/36710	0.74	8/57263 (0.0%)
7	B	0.17	0/1792	0.33	0/2414
8	C	0.21	0/1659	0.35	0/2236
9	D	0.22	0/1666	0.32	0/2227
10	E	0.26	0/1169	0.36	0/1573
11	F	0.22	0/864	0.40	0/1168
12	G	0.19	0/1246	0.33	0/1673
13	H	0.25	0/988	0.36	0/1325
14	I	0.21	0/1040	0.46	0/1384
15	J	0.20	0/798	0.36	0/1078
16	K	0.22	0/884	0.40	0/1191
17	L	0.24	0/960	0.39	0/1286
18	M	0.20	0/903	0.41	1/1208 (0.1%)
19	N	0.21	0/808	0.35	0/1076
20	O	0.22	0/717	0.29	0/955
21	P	0.24	0/650	0.36	0/876
22	Q	0.22	0/667	0.33	0/893
23	R	0.24	0/564	0.40	0/756
24	S	0.20	0/685	0.39	0/922
25	T	0.24	0/674	0.43	0/894
26	W	0.32	0/245	0.69	0/381
27	X	0.23	0/775	0.47	0/1041
28	a	0.64	0/69263	0.77	23/108053 (0.0%)
29	b	0.55	0/2773	0.73	0/4323
30	c	0.28	0/2117	0.35	1/2845 (0.0%)
31	d	0.28	0/1576	0.34	0/2117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.26	0/1571	0.31	0/2113
33	f	0.21	0/1440	0.36	0/1935
34	g	0.22	0/1336	0.40	0/1801
35	h	0.19	0/1113	0.43	0/1504
36	i	0.29	0/1153	0.39	0/1552
37	j	0.29	0/956	0.37	0/1281
38	k	0.28	0/1060	0.38	0/1411
39	l	0.24	0/1072	0.30	0/1434
40	m	0.29	0/973	0.39	0/1301
41	n	0.22	0/900	0.31	0/1206
42	o	0.27	0/929	0.28	0/1242
43	p	0.33	0/960	0.39	0/1278
44	q	0.26	0/828	0.40	0/1105
45	r	0.27	0/862	0.36	0/1154
46	s	0.25	0/745	0.41	0/996
47	t	0.24	0/796	0.43	0/1062
48	u	0.26	0/760	0.46	0/1022
49	v	0.27	0/599	0.34	0/795
50	w	0.27	0/636	0.40	0/849
51	x	0.21	0/500	0.39	0/665
52	y	0.26	0/458	0.37	0/613
53	z	0.26	0/441	0.32	0/589
All	All	0.53	0/154446	0.68	33/230931 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	a	1	0
39	l	0	1
All	All	1	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2167	U	O4'-C1'-N1	11.44	116.51	108.50
28	a	2166	C	N1-C2-O2	10.20	125.02	118.90
28	a	2166	C	C2-N1-C1'	9.63	129.39	118.80
28	a	2119	U	OP1-P-O3'	-9.40	79.78	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	218	PRO	CA-N-CD	-9.32	98.95	112.00
28	a	2119	U	OP2-P-O3'	-7.94	84.19	108.00
28	a	2162	C	N3-C2-O2	-7.80	116.44	121.90
28	a	2166	C	N3-C2-O2	-7.79	116.44	121.90
28	a	1311	C	C2-N1-C1'	6.77	126.25	118.80
28	a	2166	C	C6-N1-C2	-6.63	117.65	120.30
28	a	2166	C	C6-N1-C1'	-6.53	112.96	120.80
28	a	1310	U	C2-N1-C1'	6.43	125.41	117.70
28	a	2125	G	C6-C5-N7	-5.91	126.86	130.40
28	a	1625	C	N3-C2-O2	-5.87	117.79	121.90
18	M	66	GLU	CB-CA-C	-5.71	110.01	116.63
28	a	2165	C	C2-N1-C1'	5.70	125.07	118.80
6	A	1210	C	N1-C2-O2	5.63	122.28	118.90
6	A	1210	C	N3-C2-O2	-5.62	117.97	121.90
6	A	511	C	C2-N1-C1'	5.58	124.94	118.80
28	a	2166	C	C5-C6-N1	5.54	123.77	121.00
6	A	511	C	N1-C2-O2	5.53	122.22	118.90
28	a	834	C	N3-C2-O2	-5.37	118.14	121.90
6	A	428	G	P-O3'-C3'	5.37	126.14	119.70
28	a	2125	G	C4-N9-C1'	5.30	133.39	126.50
28	a	1060	G	C4-N9-C1'	5.18	133.24	126.50
6	A	1158	C	C2-N1-C1'	5.13	124.44	118.80
6	A	1027	C	O5'-C5'-C4'	5.13	113.50	109.40
28	a	1625	C	N1-C2-O2	5.09	121.95	118.90
28	a	1310	U	N3-C2-O2	-5.09	118.64	122.20
28	a	1311	C	C6-N1-C1'	-5.05	114.74	120.80
28	a	2165	C	N1-C2-O2	5.04	121.92	118.90
28	a	1506	U	P-O3'-C3'	5.04	125.74	119.70
6	A	1035	A	P-O3'-C3'	5.01	125.71	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	a	2167	U	C1'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	l	81	4D4	Mainchain

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	0	426	0	464	10	0
2	1	377	0	417	4	0
3	2	504	0	572	11	0
4	3	302	0	340	7	0
5	4	526	0	521	17	0
6	A	33035	0	16640	397	0
7	B	1761	0	1780	37	0
8	C	1632	0	1707	31	0
9	D	1645	0	1708	32	0
10	E	1156	0	1199	16	0
11	F	845	0	838	33	0
12	G	1228	0	1276	31	0
13	H	978	0	1035	17	0
14	I	1028	0	1075	41	0
15	J	788	0	830	28	0
16	K	876	0	885	27	0
17	L	957	0	1018	19	0
18	M	895	0	956	33	0
19	N	796	0	830	24	0
20	O	709	0	738	11	0
21	P	640	0	655	11	0
22	Q	658	0	699	7	0
23	R	555	0	578	15	0
24	S	668	0	693	25	0
25	T	668	0	710	12	0
26	W	219	0	108	2	0
27	X	764	0	770	23	0
28	a	62357	0	31370	628	0
29	b	2481	0	1256	30	0
30	c	2079	0	2149	39	0
31	d	1568	0	1617	17	0
32	e	1552	0	1619	21	0
33	f	1417	0	1454	52	0
34	g	1317	0	1374	26	0
35	h	1102	0	1139	38	0
36	i	1130	0	1155	22	0
37	j	947	0	1025	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	k	1051	0	1120	20	0
39	l	1074	0	1138	15	0
40	m	960	0	1000	19	0
41	n	890	0	922	14	0
42	o	917	0	962	14	0
43	p	947	0	1019	13	0
44	q	815	0	837	10	0
45	r	855	0	915	20	0
46	s	739	0	809	13	0
47	t	788	0	843	12	0
48	u	746	0	765	14	0
49	v	592	0	605	7	0
50	w	626	0	652	8	0
51	x	499	0	536	11	0
52	y	453	0	488	6	0
53	z	435	0	447	5	0
54	1	1	0	0	0	0
54	A	44	0	0	0	0
54	M	1	0	0	0	0
54	a	108	0	0	0	0
54	b	1	0	0	0	0
54	c	4	0	0	0	0
54	d	1	0	0	0	0
54	e	1	0	0	0	0
54	f	1	0	0	0	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
56	A	95	0	0	0	0
56	a	252	0	0	0	0
56	b	5	0	0	0	0
56	c	2	0	0	0	0
56	d	1	0	0	0	0
56	p	1	0	0	0	0
56	z	1	0	0	0	0
All	All	143494	0	96258	1869	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 8.

All (1869) 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)
28:a:2840:G:H4’	40:m:49:GLU:OE1	1.44	1.16
28:a:2074:C:H5”	30:c:228:VAL:HG22	1.19	1.10
28:a:2103:U:H3	28:a:2188:G:H1	1.08	0.99
28:a:2135:A:H62	28:a:2158:G:H4’	1.28	0.97
28:a:2841:U:H5”	40:m:53:THR:HG21	1.48	0.94
6:A:842:U:H2’	6:A:844:G:H1	1.31	0.93
28:a:2305:G:H22	28:a:2313:U:H3	1.17	0.93
28:a:2136:A:H62	28:a:2157:G:H21	1.17	0.92
28:a:2074:C:H5”	30:c:228:VAL:CG2	1.98	0.92
28:a:2074:C:C5’	30:c:228:VAL:HG22	2.01	0.91
28:a:2840:G:C4’	40:m:49:GLU:OE1	2.20	0.89
28:a:2792:G:N2	28:a:2806:C:O2	2.07	0.88
28:a:1090:G:H21	28:a:1095:A:H62	1.21	0.87
10:E:66:LYS:HA	10:E:69:ARG:HE	1.39	0.85
6:A:450:G:H5”	6:A:451:A:H5’	1.58	0.85
28:a:2074:C:C5’	30:c:228:VAL:CG2	2.55	0.84
28:a:2176:C:H2’	28:a:2177:A:H8	1.45	0.81
4:3:11:CYS:SG	4:3:33:HIS:CE1	2.74	0.80
5:4:18:CYS:HB3	5:4:40:CYS:SG	2.21	0.80
32:e:97:ASN:HB2	32:e:100:MET:HG3	1.65	0.79
28:a:2136:A:H62	28:a:2157:G:N2	1.81	0.78
28:a:1073:C:N4	28:a:1074:A:N6	2.31	0.78
48:u:2:PHE:CD1	48:u:50:MET:HE3	2.18	0.78
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.64	0.78
6:A:511:C:H5	6:A:540:G:H1	1.32	0.78
14:I:35:LEU:HD21	14:I:45:ARG:HG3	1.66	0.76
28:a:1073:C:C4	28:a:1074:A:N6	2.52	0.76
41:n:31:THR:HG22	41:n:33:ARG:H	1.48	0.76
14:I:88:MET:HE3	14:I:98:LEU:HD12	1.67	0.76
42:o:60:THR:HG22	42:o:73:VAL:HG22	1.68	0.76
6:A:1373:G:H5”	12:G:36:LYS:HD2	1.67	0.75
36:i:73:MET:HE1	36:i:88:THR:HG22	1.68	0.75
28:a:1915:C:H3’	28:a:1916:3TD:H6	1.69	0.75
28:a:565:U:H1’	28:a:2031:6MZ:H9C1	1.70	0.73
8:C:14:ILE:HG22	8:C:15:VAL:HG13	1.68	0.73
28:a:1404:G:H1	28:a:1595:G:H22	1.36	0.73
28:a:1090:G:N2	28:a:1095:A:H62	1.87	0.72
6:A:673:A:H2’	6:A:674:G:C8	2.24	0.72
19:N:66:GLN:HG3	19:N:79:LEU:HD22	1.72	0.72
28:a:142:C:H2’	28:a:143:A:H8	1.54	0.72
7:B:89:GLN:HG3	7:B:90:PHE:H	1.55	0.72
30:c:107:PRO:HD2	30:c:110:LEU:HD22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:113:ASP:HB3	12:G:119:ARG:HG2	1.72	0.71
18:M:81:MET:HE2	18:M:91:HIS:HB3	1.72	0.71
25:T:4:ILE:HG22	25:T:7:ALA:H	1.56	0.70
35:h:66:ASN:HB3	35:h:135:HIS:HA	1.70	0.70
33:f:56:ASP:O	33:f:60:ILE:HD12	1.91	0.70
36:i:13:ARG:HG3	36:i:13:ARG:HH11	1.57	0.70
45:r:83:LYS:HB3	45:r:95:ARG:HD2	1.74	0.70
28:a:1597:A:H5"	28:a:1598:A:H5'	1.74	0.69
12:G:47:LEU:HD12	12:G:58:GLU:HB3	1.73	0.69
28:a:2127:A:N1	28:a:2166:C:N3	2.40	0.69
35:h:84:ALA:HB2	35:h:90:LEU:HD12	1.73	0.69
6:A:664:G:H22	6:A:741:G:H1	1.39	0.69
34:g:20:ASP:HB3	34:g:23:VAL:HB	1.75	0.69
6:A:1356:G:H2'	6:A:1357:A:C8	2.28	0.69
28:a:1054:A:H1'	28:a:1083:A:H62	1.58	0.69
41:n:62:LEU:HD13	41:n:70:ALA:HA	1.76	0.68
28:a:1042:C:H4'	28:a:1044:G:H1'	1.74	0.68
42:o:5:ILE:O	42:o:9:GLU:HG3	1.94	0.68
6:A:946:A:H2'	6:A:947:G:C8	2.29	0.68
9:D:14:ARG:HH21	9:D:37:ALA:HB1	1.59	0.68
28:a:845:C:H2'	28:a:846:A:H8	1.59	0.68
6:A:458:U:H2'	6:A:459:A:C8	2.29	0.67
32:e:118:LEU:HD11	32:e:188:MET:HE2	1.75	0.67
43:p:86:ALA:HB2	43:p:116:ALA:HB2	1.77	0.67
27:X:24:PHE:HE2	27:X:37:VAL:HG21	1.60	0.67
28:a:1059:G:H2'	28:a:1060:G:H21	1.59	0.67
25:T:24:ARG:HD2	25:T:61:GLN:HE22	1.59	0.67
8:C:77:ILE:HD13	8:C:84:VAL:HG11	1.77	0.67
28:a:853:G:H2'	28:a:854:G:C8	2.30	0.67
28:a:2135:A:N6	28:a:2158:G:H4'	2.08	0.67
43:p:107:THR:O	43:p:111:GLU:HG2	1.95	0.67
28:a:2174:A:H5"	28:a:2175:C:H5	1.60	0.66
13:H:30:ALA:HB3	13:H:33:LYS:HG3	1.78	0.66
28:a:636:U:H2'	28:a:637:C:C6	2.30	0.66
17:L:33:VAL:HG12	17:L:79:VAL:HG12	1.76	0.66
6:A:235:C:H2'	6:A:236:A:H8	1.61	0.66
6:A:407:U:H2'	6:A:408:A:H8	1.59	0.66
6:A:674:G:H2'	6:A:675:A:H8	1.60	0.66
28:a:2107:U:H2'	28:a:2108:G:C8	2.30	0.66
28:a:2114:U:H4'	28:a:2170:A:H4'	1.78	0.66
28:a:2120:A:H61	28:a:2170:A:H5"	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:714:G:H2'	6:A:715:A:C8	2.30	0.66
28:a:2115:A:H2	28:a:2169:G:H5"	1.61	0.66
24:S:3:ARG:HE	24:S:10:PHE:HB2	1.59	0.66
28:a:2156:U:H3'	28:a:2157:G:H8	1.61	0.66
28:a:739:A:H2'	28:a:740:A:C8	2.31	0.66
28:a:1403:U:H2'	28:a:1404:G:C8	2.31	0.66
28:a:2103:U:O4	28:a:2188:G:O6	2.14	0.66
13:H:11:LEU:HD22	13:H:75:ILE:HD11	1.78	0.66
7:B:187:VAL:HG13	7:B:191:SER:HB2	1.78	0.65
6:A:337:G:H2'	6:A:338:A:C8	2.31	0.65
15:J:34:ALA:HB2	15:J:80:THR:HG23	1.78	0.65
8:C:72:ARG:HD2	8:C:75:ILE:HG13	1.78	0.65
48:u:47:VAL:O	48:u:51:GLN:HB3	1.96	0.65
34:g:24:ILE:HG12	34:g:72:LEU:HD11	1.78	0.65
6:A:946:A:H2'	6:A:947:G:H8	1.60	0.65
6:A:1323:G:H2'	6:A:1324:A:C8	2.32	0.65
45:r:74:ILE:HD12	45:r:105:VAL:HG22	1.78	0.65
6:A:407:U:H2'	6:A:408:A:C8	2.32	0.65
17:L:5:ASN:HD21	22:Q:36:LYS:HE3	1.61	0.65
14:I:21:ILE:HG22	14:I:63:LEU:HD22	1.78	0.64
6:A:501:C:H2'	6:A:502:A:H8	1.62	0.64
24:S:11:ILE:HG13	24:S:38:SER:HB3	1.79	0.64
45:r:55:ILE:HD11	45:r:66:ILE:HG23	1.79	0.64
28:a:1059:G:H2'	28:a:1060:G:N2	2.12	0.64
28:a:1795:U:H2'	28:a:1796:G:H8	1.61	0.64
28:a:2804:C:H2'	28:a:2805:U:H6	1.62	0.64
6:A:1535:C:H2'	6:A:1536:C:C6	2.32	0.64
28:a:249:G:H4'	38:k:59:ARG:HD2	1.79	0.64
18:M:4:ILE:HD13	18:M:57:ARG:HG3	1.80	0.64
27:X:45:LYS:HG2	27:X:46:VAL:HG23	1.80	0.64
32:e:12:LEU:HD11	32:e:194:LYS:HE2	1.78	0.64
6:A:1218:U:H2'	6:A:1219:A:C8	2.32	0.64
28:a:1429:G:H2'	28:a:1430:A:C8	2.32	0.64
14:I:88:MET:HE2	14:I:88:MET:HA	1.79	0.64
27:X:12:ILE:HG21	27:X:17:ARG:HH21	1.63	0.64
32:e:48:THR:HG22	32:e:86:ALA:HB3	1.79	0.64
25:T:26:SER:O	25:T:30:THR:HG23	1.97	0.63
6:A:1129:C:H4'	14:I:18:ARG:HH22	1.62	0.63
13:H:7:ILE:HD11	13:H:32:LEU:HB3	1.80	0.63
38:k:101:ILE:HD12	38:k:105:ILE:HB	1.80	0.63
15:J:85:ASP:O	15:J:89:ARG:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:34:THR:HG23	23:R:36:SER:H	1.62	0.63
30:c:144:VAL:HB	30:c:154:LEU:HB2	1.79	0.63
28:a:1037:A:H61	28:a:1112:G:H1	1.45	0.63
6:A:1348:U:H4'	14:I:122:ARG:HD3	1.80	0.63
53:z:54:VAL:HG23	53:z:55:ILE:HG12	1.81	0.63
6:A:562:U:H1'	17:L:12:ARG:HD2	1.79	0.63
6:A:1071:C:H2'	6:A:1072:G:H8	1.63	0.63
28:a:280:C:H2'	28:a:281:A:H8	1.63	0.63
30:c:117:GLN:H	30:c:128:ASN:HD22	1.46	0.63
33:f:29:PRO:HB3	33:f:160:ALA:HB2	1.80	0.63
6:A:948:C:H2'	6:A:949:A:H8	1.63	0.63
13:H:32:LEU:O	13:H:36:ILE:HG13	1.99	0.63
14:I:59:GLU:C	14:I:60:LYS:HD3	2.24	0.63
18:M:49:SER:HB2	18:M:52:GLN:NE2	2.13	0.63
28:a:2095:A:H5'	35:h:25:TYR:HD2	1.64	0.63
33:f:29:PRO:HB2	33:f:169:LEU:HD22	1.81	0.63
35:h:4:ILE:HD11	35:h:44:VAL:HG22	1.81	0.63
31:d:114:LYS:HE3	31:d:196:ALA:HB2	1.79	0.63
14:I:52:LEU:HD12	14:I:58:VAL:HA	1.81	0.62
28:a:2142:G:H2'	28:a:2143:A:C8	2.34	0.62
6:A:461:G:HO2'	6:A:462:G:H8	1.47	0.62
6:A:495:A:H4'	6:A:496:A:H5'	1.81	0.62
8:C:129:MET:HG2	8:C:132:ARG:H	1.63	0.62
28:a:2127:A:N1	28:a:2166:C:C4	2.67	0.62
28:a:2134:G:C2	28:a:2158:G:H2'	2.34	0.62
18:M:10:PRO:HB2	18:M:13:LYS:HG3	1.82	0.62
5:4:11:MET:SD	5:4:23:GLN:HB3	2.39	0.62
11:F:1:MET:HA	11:F:1:MET:HE2	1.81	0.62
28:a:142:C:H2'	28:a:143:A:C8	2.34	0.62
34:g:71:LEU:O	34:g:75:MET:HG2	1.99	0.62
28:a:141:A:H2'	28:a:142:C:C6	2.34	0.62
30:c:228:VAL:O	30:c:228:VAL:HG12	1.98	0.62
6:A:715:A:H2'	6:A:716:A:C8	2.34	0.62
28:a:2101:G:H2'	28:a:2102:G:H8	1.64	0.62
6:A:746:A:H2'	6:A:747:A:C8	2.35	0.62
28:a:1733:G:H2'	28:a:1734:G:H8	1.65	0.62
28:a:1795:U:H2'	28:a:1796:G:C8	2.35	0.62
28:a:2124:G:H2'	28:a:2125:G:C8	2.35	0.62
6:A:21:G:H2'	6:A:22:G:C8	2.34	0.62
5:4:42:PRO:HB3	5:4:48:GLN:HB3	1.82	0.62
16:K:87:LYS:HD3	16:K:115:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1102:U:H2'	28:a:1103:G:C8	2.35	0.62
8:C:73:PRO:HG3	8:C:105:GLU:HG3	1.82	0.61
28:a:2:G:H2'	28:a:3:U:C6	2.35	0.61
28:a:1090:G:H21	28:a:1095:A:N6	1.95	0.61
36:i:73:MET:HA	36:i:73:MET:HE3	1.82	0.61
48:u:2:PHE:HD1	48:u:50:MET:HE3	1.65	0.61
18:M:19:LEU:HD11	18:M:56:LEU:HD11	1.82	0.61
28:a:2548:A:H2'	28:a:2549:U:C6	2.36	0.61
3:2:62:LEU:HB3	3:2:65:ALA:HB2	1.82	0.61
6:A:634:C:H2'	6:A:635:A:H8	1.66	0.61
15:J:40:ILE:HD13	15:J:73:LEU:HD23	1.82	0.61
41:n:87:ILE:H	41:n:87:ILE:HD12	1.64	0.61
12:G:5:ARG:HD2	12:G:6:VAL:H	1.65	0.61
12:G:113:ASP:H	12:G:119:ARG:HE	1.46	0.61
28:a:1873:C:H2'	28:a:1874:G:C8	2.36	0.61
32:e:119:ILE:HB	32:e:187:VAL:HG22	1.83	0.61
18:M:11:ASP:HA	18:M:45:ILE:HB	1.82	0.61
6:A:337:G:H2'	6:A:338:A:H8	1.65	0.61
16:K:61:PHE:HA	16:K:64:GLN:HG2	1.82	0.61
16:K:35:THR:HB	16:K:41:ALA:HA	1.81	0.60
6:A:1175:G:H2'	6:A:1176:A:H8	1.65	0.60
28:a:2095:A:H5'	35:h:25:TYR:CD2	2.36	0.60
28:a:2136:A:N6	28:a:2157:G:H21	1.94	0.60
28:a:2837:U:H2'	28:a:2838:A:H8	1.65	0.60
30:c:218:PRO:HD2	30:c:218:PRO:O	2.00	0.60
6:A:844:G:H2'	6:A:845:A:O4'	2.01	0.60
6:A:1219:A:H5"	19:N:53:ARG:HH21	1.65	0.60
28:a:579:A:H5"	43:p:11:ARG:HH22	1.67	0.60
6:A:113:G:H1'	6:A:354:G:H5'	1.83	0.60
6:A:1060:U:H5"	15:J:53:ILE:HD12	1.82	0.60
25:T:35:VAL:O	25:T:39:ILE:HG13	2.01	0.60
6:A:552:U:H2'	6:A:553:A:H8	1.66	0.60
7:B:71:GLY:HA3	7:B:80:VAL:HG11	1.82	0.60
28:a:1444:C:H2'	28:a:1445:G:H8	1.67	0.60
8:C:114:LYS:HB2	8:C:185:ASN:HD22	1.67	0.60
28:a:2247:G:H2'	28:a:2248:A:H8	1.66	0.60
18:M:90:ARG:HH21	18:M:95:LEU:HD12	1.66	0.60
24:S:19:VAL:HG11	24:S:44:MET:HG2	1.84	0.60
28:a:287:U:H2'	28:a:288:G:C8	2.37	0.60
23:R:70:TYR:HB2	23:R:74:HIS:HE1	1.67	0.60
33:f:38:MET:HG2	33:f:53:ALA:HB1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:745:A:H2'	6:A:746:A:H8	1.65	0.60
40:m:96:ARG:HH22	40:m:116:VAL:HG23	1.67	0.60
28:a:1025:A:H2'	28:a:1026:A:C8	2.37	0.60
28:a:1592:C:H2'	28:a:1593:A:C8	2.36	0.60
28:a:2247:G:H2'	28:a:2248:A:C8	2.36	0.60
6:A:842:U:H2'	6:A:844:G:N1	2.11	0.59
28:a:830:A:H2'	28:a:831:G:H8	1.67	0.59
28:a:1683:U:H2'	28:a:1684:G:H8	1.67	0.59
28:a:2065:C:H2'	28:a:2066:C:C6	2.37	0.59
6:A:1323:G:H2'	6:A:1324:A:H8	1.67	0.59
12:G:76:LYS:HE2	12:G:89:VAL:HG11	1.84	0.59
28:a:1466:A:H2'	28:a:1467:A:C8	2.37	0.59
30:c:137:VAL:HG23	30:c:167:ARG:HH21	1.66	0.59
35:h:75:LEU:HD12	35:h:77:THR:H	1.67	0.59
6:A:211:G:C5	6:A:212:G:H1'	2.37	0.59
7:B:27:MET:HE1	7:B:193:PRO:HD3	1.83	0.59
14:I:79:ILE:O	14:I:83:ILE:HG12	2.02	0.59
27:X:70:MET:O	27:X:74:ILE:HG13	2.03	0.59
28:a:2121:G:H2'	28:a:2122:G:H8	1.66	0.59
27:X:33:ARG:NH1	27:X:33:ARG:HA	2.17	0.59
39:l:108:VAL:HB	39:l:112:LEU:HD23	1.85	0.59
6:A:501:C:H2'	6:A:502:A:C8	2.38	0.59
19:N:89:MET:HA	19:N:89:MET:HE2	1.85	0.59
24:S:15:LEU:O	24:S:19:VAL:HG22	2.03	0.59
28:a:510:U:H4'	28:a:1232:G:H4'	1.84	0.59
28:a:1592:C:H2'	28:a:1593:A:H8	1.67	0.59
6:A:1391:U:H2'	6:A:1392:G:C8	2.38	0.59
9:D:11:LEU:HB3	9:D:63:ARG:HD3	1.84	0.59
16:K:52:PHE:HE1	16:K:65:VAL:HG11	1.67	0.59
28:a:1466:A:H2'	28:a:1467:A:H8	1.68	0.59
6:A:207:C:H2'	6:A:208:U:C6	2.38	0.59
8:C:150:LYS:HB2	8:C:169:ARG:HG3	1.84	0.59
28:a:141:A:H2'	28:a:142:C:H6	1.67	0.59
28:a:739:A:H2'	28:a:740:A:H8	1.67	0.59
28:a:2503:G:H5"	28:a:2504:2MA:H5"	1.84	0.59
33:f:36:LEU:HB2	33:f:89:VAL:HG22	1.84	0.59
45:r:20:VAL:HG11	45:r:44:ALA:HA	1.84	0.59
1:0:32:GLU:H	1:0:32:GLU:CD	2.10	0.59
14:I:75:GLN:O	14:I:79:ILE:HG12	2.03	0.59
43:p:94:ILE:HD12	44:q:13:ARG:HB2	1.85	0.59
46:s:25:GLU:HG3	46:s:26:LYS:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:204:G:H2'	6:A:205:A:H8	1.68	0.58
28:a:802:G:H5"	38:k:38:GLN:HG3	1.84	0.58
38:k:108:ALA:HB3	38:k:125:LEU:HG	1.84	0.58
6:A:1218:U:H2'	6:A:1219:A:H8	1.68	0.58
18:M:19:LEU:HD21	18:M:56:LEU:HD21	1.86	0.58
28:a:2292:U:H2'	28:a:2293:U:C6	2.38	0.58
6:A:713:G:H2'	6:A:714:G:C8	2.38	0.58
14:I:57:MET:HE1	14:I:90:TYR:CE1	2.37	0.58
28:a:879:G:H1	28:a:891:U:H3	1.51	0.58
29:b:41:G:H5"	33:f:66:LEU:HD13	1.85	0.58
14:I:80:ARG:O	14:I:84:THR:HG23	2.02	0.58
6:A:1144:G:H21	6:A:1146:A:H62	1.51	0.58
14:I:55:VAL:HG23	14:I:57:MET:HB3	1.86	0.58
28:a:1590:A:H2'	28:a:1591:A:C8	2.38	0.58
28:a:2675:G:H4'	37:j:30:ARG:HG3	1.86	0.58
6:A:1326:U:H2'	6:A:1327:C:H6	1.66	0.58
6:A:1381:U:H1'	12:G:78:ARG:HH11	1.69	0.58
6:A:216:U:H2'	6:A:217:C:H6	1.69	0.58
6:A:539:A:H2'	6:A:540:G:C8	2.39	0.58
7:B:95:ARG:HH12	7:B:97:LEU:HA	1.69	0.58
5:4:11:MET:HE2	5:4:11:MET:HA	1.86	0.58
6:A:235:C:H2'	6:A:236:A:C8	2.38	0.58
8:C:119:SER:O	8:C:123:GLN:HG2	2.03	0.58
37:j:38:ILE:HD11	37:j:112:PHE:HZ	1.69	0.58
39:l:28:PHE:HB2	39:l:104:GLU:OE1	2.04	0.58
6:A:1015:G:H2'	6:A:1016:A:C8	2.39	0.57
51:x:4:LYS:NZ	51:x:7:ARG:HH12	2.02	0.57
6:A:1169:A:H2'	6:A:1170:A:C8	2.39	0.57
29:b:41:G:H8	33:f:66:LEU:HD11	1.68	0.57
32:e:58:LYS:HG2	32:e:71:GLY:HA2	1.85	0.57
40:m:22:ARG:HG3	40:m:70:THR:HA	1.85	0.57
15:J:90:LEU:HG	15:J:92:LEU:HG	1.87	0.57
6:A:1423:G:H5'	37:j:49:ARG:HH22	1.69	0.57
32:e:188:MET:HE3	32:e:193:VAL:HG22	1.86	0.57
33:f:8:TYR:HD1	33:f:12:VAL:HB	1.69	0.57
1:0:9:ILE:HD12	1:0:51:GLU:HG3	1.85	0.57
4:3:32:LYS:HE2	28:a:2479:A:H5'	1.87	0.57
28:a:846:A:H2'	28:a:847:U:C6	2.39	0.57
28:a:1032:U:H2'	28:a:1033:G:H8	1.70	0.57
48:u:46:LYS:O	48:u:50:MET:HB3	2.04	0.57
9:D:147:GLU:HA	9:D:150:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2659:C:H5”	34:g:158:LYS:HE2	1.85	0.57
28:a:1076:C:H5	28:a:1085:A:C4	2.22	0.57
46:s:30:ILE:HG21	46:s:93:LEU:HG	1.86	0.57
6:A:1314:C:H2’	6:A:1315:U:C6	2.39	0.57
21:P:4:ILE:HG12	21:P:21:VAL:HG22	1.86	0.57
28:a:171:A:H2’	28:a:172:A:C8	2.39	0.57
28:a:280:C:H2’	28:a:281:A:C8	2.39	0.57
28:a:830:A:H2’	28:a:831:G:C8	2.39	0.57
28:a:1743:A:H3’	28:a:1744:A:H8	1.68	0.57
35:h:65:ALA:O	35:h:68:ARG:HG3	2.04	0.57
3:2:34:THR:HG23	28:a:2421:C:OP1	2.04	0.57
23:R:42:SER:HA	23:R:45:THR:HG22	1.86	0.57
28:a:1506:U:H4’	28:a:1507:U:H5”	1.87	0.57
6:A:17:U:H2’	6:A:18:C:C6	2.39	0.56
10:E:115:LEU:HD13	10:E:123:VAL:HG11	1.86	0.56
28:a:287:U:H2’	28:a:288:G:H8	1.70	0.56
28:a:1439:U:H2’	28:a:1440:C:C6	2.40	0.56
12:G:78:ARG:HB2	12:G:156:TRP:CZ3	2.40	0.56
28:a:190:A:H2’	28:a:191:C:C6	2.40	0.56
28:a:2143:A:H2’	28:a:2144:C:O4’	2.05	0.56
28:a:2837:U:H2’	28:a:2838:A:C8	2.40	0.56
40:m:72:ASP:HB3	40:m:75:ILE:HB	1.86	0.56
6:A:131:A:H2’	6:A:132:C:C6	2.41	0.56
6:A:1497:G:H1’	6:A:1518:MA6:H2	1.87	0.56
7:B:167:ASP:HB2	7:B:191:SER:HA	1.86	0.56
10:E:131:THR:HG22	10:E:131:THR:O	2.06	0.56
24:S:40:ILE:HA	24:S:44:MET:HE1	1.88	0.56
28:a:150:C:H2’	28:a:151:G:H8	1.70	0.56
28:a:278:A:N6	28:a:360:G:H1’	2.20	0.56
28:a:817:A:H4’	28:a:833:G:H22	1.70	0.56
28:a:1383:C:H2’	28:a:1384:A:H8	1.70	0.56
28:a:2167:U:H4’	28:a:2168:U:C5’	2.34	0.56
28:a:2804:C:H2’	28:a:2805:U:C6	2.39	0.56
6:A:56:U:H2’	6:A:57:G:C8	2.41	0.56
9:D:27:ALA:HB3	9:D:30:THR:HG22	1.87	0.56
28:a:846:A:H2’	28:a:847:U:H6	1.69	0.56
28:a:848:C:H2’	28:a:849:U:C6	2.41	0.56
28:a:2184:A:H2’	28:a:2185:A:C8	2.41	0.56
6:A:77:A:H2’	6:A:78:A:C8	2.39	0.56
6:A:1250:A:H2’	6:A:1251:A:C8	2.40	0.56
28:a:5:A:H2’	28:a:6:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:997:A:H2'	28:a:998:A:C8	2.41	0.56
28:a:2183:U:H2'	28:a:2184:A:C8	2.40	0.56
28:a:2248:A:H2'	28:a:2249:C:H6	1.69	0.56
28:a:2329:A:H2'	28:a:2330:U:C6	2.41	0.56
6:A:270:A:H2'	6:A:271:C:C6	2.41	0.56
28:a:1683:U:H2'	28:a:1684:G:C8	2.41	0.56
6:A:143:A:H2	6:A:220:G:H1	1.54	0.56
28:a:1165:G:H2'	28:a:1166:A:H8	1.69	0.56
28:a:1819:U:H5	30:c:177:ARG:HH21	1.54	0.56
48:u:61:LEU:HD11	48:u:74:VAL:HG23	1.88	0.56
6:A:1040:U:H2'	6:A:1041:G:C8	2.41	0.56
36:i:4:PHE:CD2	43:p:100:VAL:HG11	2.40	0.56
36:i:9:GLU:HG2	36:i:10:THR:HG23	1.87	0.56
49:v:37:ILE:HG21	49:v:80:ILE:HG21	1.88	0.56
11:F:26:SER:O	11:F:30:THR:HG23	2.06	0.56
17:L:94:ARG:HG3	17:L:95:TYR:CE2	2.41	0.56
28:a:1138:U:H4'	28:a:1139:A:O4'	2.06	0.56
28:a:1589:U:H2'	28:a:1590:A:H8	1.71	0.56
28:a:2127:A:C6	28:a:2166:C:N3	2.74	0.56
50:w:47:VAL:HG21	50:w:78:TYR:HD1	1.70	0.56
28:a:1383:C:H2'	28:a:1384:A:C8	2.41	0.56
28:a:1855:U:H2'	28:a:1856:G:O4'	2.06	0.56
29:b:115:A:H2'	29:b:116:G:C8	2.41	0.56
33:f:142:ASP:HB3	33:f:145:LYS:HG2	1.88	0.56
34:g:84:THR:HG22	34:g:134:LYS:HG2	1.87	0.56
6:A:384:G:H2'	6:A:385:C:C6	2.41	0.55
6:A:1414:U:H2'	6:A:1415:G:H8	1.70	0.55
11:F:2:ARG:HD3	11:F:91:ARG:CZ	2.36	0.55
20:O:25:THR:HG21	20:O:70:LEU:HB2	1.88	0.55
20:O:10:LYS:HG3	20:O:14:GLU:OE2	2.06	0.55
47:t:81:ASP:OD1	47:t:98:SER:HB3	2.05	0.55
28:a:1733:G:H2'	28:a:1734:G:C8	2.41	0.55
28:a:2074:C:H5'	30:c:228:VAL:CG2	2.37	0.55
29:b:104:A:H2'	29:b:105:G:O4'	2.06	0.55
33:f:108:VAL:HA	33:f:111:ILE:HD12	1.88	0.55
6:A:1512:U:H2'	6:A:1513:A:C8	2.41	0.55
28:a:1076:C:H2'	28:a:1077:A:C8	2.41	0.55
31:d:148:GLN:HB2	31:d:152:PRO:HG3	1.88	0.55
28:a:2121:G:H2'	28:a:2122:G:C8	2.40	0.55
14:I:28:ILE:HG22	14:I:63:LEU:HG	1.88	0.55
27:X:33:ARG:HA	27:X:33:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:5:A:H2'	28:a:6:A:H8	1.72	0.55
38:k:57:LEU:HA	38:k:60:ARG:HG2	1.87	0.55
6:A:718:A:H2	23:R:38:LYS:HE2	1.72	0.55
7:B:219:ALA:HA	7:B:222:ARG:HE	1.70	0.55
28:a:1801:A:H2'	28:a:1802:A:C8	2.42	0.55
20:O:30:ALA:HA	20:O:85:LEU:HD11	1.88	0.55
21:P:20:VAL:HG23	21:P:22:THR:HG23	1.89	0.55
28:a:717:U:H2'	28:a:718:A:C8	2.41	0.55
28:a:1100:A:H5"	28:a:1101:C:H5	1.72	0.55
28:a:2075:U:H2'	28:a:2076:U:C6	2.42	0.55
41:n:49:VAL:HG21	41:n:81:ARG:HB3	1.88	0.55
28:a:1091:U:C2	28:a:1093:A:H5"	2.42	0.55
6:A:623:C:H2'	6:A:624:C:H6	1.72	0.54
21:P:57:ILE:HG21	21:P:75:ILE:HD11	1.89	0.54
28:a:538:G:H5'	36:i:9:GLU:OE1	2.07	0.54
28:a:2789:C:H2'	28:a:2790:C:C6	2.42	0.54
6:A:202:G:H21	6:A:466:A:H61	1.55	0.54
16:K:63:ALA:HB1	16:K:96:THR:HG23	1.89	0.54
20:O:24:SER:HB2	20:O:27:VAL:HG23	1.88	0.54
28:a:190:A:H2'	28:a:191:C:H6	1.73	0.54
28:a:281:A:H2'	28:a:282:G:C8	2.43	0.54
6:A:745:A:H2'	6:A:746:A:C8	2.41	0.54
6:A:993:G:H1	6:A:1045:C:H42	1.54	0.54
7:B:67:ILE:HD12	7:B:160:ALA:HB3	1.89	0.54
6:A:1180:A:OP1	14:I:105:THR:HG22	2.07	0.54
14:I:6:TYR:CD2	14:I:90:TYR:HA	2.43	0.54
24:S:3:ARG:HD3	24:S:8:GLY:O	2.07	0.54
28:a:642:C:H2'	28:a:644:G:C8	2.42	0.54
28:a:1745:A:H2'	28:a:1746:U:C6	2.42	0.54
28:a:2592:C:H2'	28:a:2593:G:C8	2.43	0.54
39:l:56:ALA:HB2	39:l:119:LEU:HD12	1.89	0.54
6:A:269:C:H2'	6:A:270:A:C8	2.42	0.54
6:A:674:G:H2'	6:A:675:A:C8	2.42	0.54
8:C:153:VAL:HG22	8:C:198:VAL:HG22	1.90	0.54
21:P:6:LEU:HB3	21:P:17:TYR:HB3	1.89	0.54
28:a:2135:A:N3	28:a:2160:G:H1'	2.23	0.54
28:a:2274:A:H2'	28:a:2275:A:C8	2.43	0.54
6:A:216:U:H2'	6:A:217:C:C6	2.42	0.54
6:A:728:A:H2'	6:A:729:A:C8	2.43	0.54
36:i:13:ARG:HG3	36:i:13:ARG:NH1	2.21	0.54
6:A:1355:G:H2'	6:A:1356:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:72:THR:HG23	12:G:73:VAL:HG23	1.89	0.54
28:a:1793:A:H2'	28:a:1794:C:C6	2.43	0.54
28:a:2183:U:H2'	28:a:2184:A:H8	1.71	0.54
29:b:115:A:H2'	29:b:116:G:H8	1.73	0.54
6:A:458:U:H2'	6:A:459:A:H8	1.70	0.54
12:G:70:ARG:HD2	12:G:96:ARG:HB3	1.89	0.54
19:N:53:ARG:NH1	24:S:37:ARG:HH12	2.06	0.54
28:a:584:C:C2	38:k:19:LEU:HD12	2.43	0.54
28:a:1251:A:H5"	28:a:1252:U:H5"	1.90	0.54
6:A:493:A:H2'	6:A:494:G:C8	2.43	0.54
6:A:1251:A:H2'	6:A:1252:A:C8	2.42	0.54
6:A:1391:U:H2'	6:A:1392:G:H8	1.73	0.54
28:a:1682:G:H2'	28:a:1683:U:C6	2.43	0.54
28:a:2114:U:H5'	28:a:2118:A:H2	1.73	0.54
28:a:2163:G:H4'	28:a:2164:C:OP2	2.08	0.54
6:A:80:C:H2'	6:A:81:A:H8	1.73	0.53
9:D:7:PRO:HB2	9:D:10:LYS:HB2	1.90	0.53
9:D:85:ASN:HB3	9:D:88:GLU:HB3	1.89	0.53
11:F:1:MET:HE3	11:F:67:PRO:HG3	1.90	0.53
28:a:362:A:H2'	28:a:363:C:H6	1.72	0.53
28:a:464:G:H2'	28:a:465:A:C8	2.44	0.53
28:a:1614:A:C2	45:r:93:ALA:HB2	2.43	0.53
28:a:1805:C:O3'	30:c:48:ARG:NH1	2.41	0.53
28:a:2072:A:H2'	28:a:2073:C:C6	2.43	0.53
45:r:86:MET:HB2	45:r:96:ILE:HG13	1.90	0.53
6:A:601:G:H2'	6:A:602:A:H8	1.72	0.53
18:M:107:ARG:HA	18:M:110:LYS:HG2	1.90	0.53
28:a:1438:G:H2'	28:a:1439:U:C6	2.43	0.53
28:a:1806:G:OP1	30:c:48:ARG:NH1	2.40	0.53
28:a:2234:U:H2'	28:a:2235:G:C8	2.42	0.53
51:x:4:LYS:O	51:x:8:GLU:HG2	2.09	0.53
28:a:137:U:H3'	28:a:139:C:N4	2.23	0.53
28:a:894:C:H2'	28:a:895:C:C6	2.44	0.53
28:a:2127:A:N7	28:a:2165:C:H1'	2.23	0.53
28:a:2748:G:O6	28:a:2756:C:H5"	2.08	0.53
34:g:17:VAL:HG11	34:g:50:LEU:HD21	1.90	0.53
35:h:9:VAL:HG11	35:h:12:LEU:HB3	1.89	0.53
47:t:48:PRO:HB3	47:t:55:PRO:HB3	1.90	0.53
28:a:64:A:H2'	28:a:65:U:C6	2.42	0.53
33:f:42:GLU:HG3	33:f:49:LEU:HD23	1.91	0.53
6:A:147:G:H2'	6:A:148:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:152:GLN:HB2	9:D:155:VAL:HG23	1.91	0.53
28:a:596:A:H2'	28:a:597:G:H8	1.73	0.53
28:a:2124:G:H2'	28:a:2125:G:N7	2.24	0.53
35:h:55:GLU:CD	35:h:55:GLU:H	2.17	0.53
35:h:110:VAL:HG13	35:h:114:GLU:HB2	1.91	0.53
36:i:96:ARG:HB3	36:i:99:ARG:HG2	1.89	0.53
33:f:148:ARG:HD2	33:f:149:VAL:H	1.73	0.53
6:A:335:C:H2'	6:A:336:A:H8	1.72	0.53
16:K:76:GLU:HG2	16:K:77:TYR:HD1	1.74	0.53
28:a:636:U:H2'	28:a:637:C:H6	1.74	0.53
33:f:67:ILE:HD13	33:f:87:CYS:HB3	1.90	0.53
35:h:141:LYS:HD2	35:h:142:LEU:N	2.23	0.53
1:0:54:ILE:HG23	1:0:55:LYS:HD3	1.90	0.53
5:4:1:MET:HG2	29:b:43:C:H5"	1.91	0.53
6:A:150:U:H3	6:A:171:A:H62	1.57	0.53
14:I:47:VAL:HA	14:I:50:GLN:HG3	1.90	0.53
28:a:188:G:OP2	50:w:14:THR:HG21	2.09	0.53
51:x:12:GLU:CD	51:x:12:GLU:H	2.16	0.53
6:A:1534:A:H2'	6:A:1535:C:C6	2.44	0.53
15:J:22:THR:O	15:J:26:VAL:HG13	2.09	0.53
28:a:413:C:H2'	28:a:414:A:H8	1.74	0.53
28:a:1929:A:H2'	28:a:1930:G:O4'	2.09	0.53
32:e:65:THR:HG23	32:e:67:ARG:H	1.72	0.53
33:f:72:LYS:HA	33:f:81:GLN:HG3	1.90	0.53
6:A:77:A:H2'	6:A:78:A:H8	1.72	0.53
6:A:634:C:H2'	6:A:635:A:C8	2.43	0.53
9:D:101:VAL:HG21	9:D:137:VAL:HG21	1.91	0.53
28:a:1174:G:H2'	28:a:1175:C:C6	2.44	0.53
28:a:1491:A:H2'	28:a:1492:A:C8	2.44	0.53
33:f:128:TYR:HE2	33:f:130:MET:HB3	1.73	0.53
28:a:413:C:H2'	28:a:414:A:C8	2.44	0.52
28:a:1057:U:H1'	28:a:1059:G:OP2	2.09	0.52
28:a:2111:G:O2'	28:a:2121:G:H5'	2.09	0.52
47:t:47:LYS:HE3	47:t:48:PRO:HD2	1.90	0.52
6:A:1053:G:H4'	6:A:1054:C:H3'	1.90	0.52
9:D:152:GLN:HB3	9:D:154:ARG:HG2	1.90	0.52
46:s:30:ILE:HG13	46:s:85:VAL:HB	1.91	0.52
6:A:178:C:H2'	6:A:179:A:H8	1.74	0.52
6:A:769:G:H4'	6:A:1513:A:H4'	1.91	0.52
6:A:1144:G:N2	6:A:1146:A:H62	2.05	0.52
32:e:111:GLU:O	32:e:115:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:677:U:H3	6:A:713:G:H22	1.58	0.52
11:F:11:HIS:CE1	11:F:54:LEU:HD21	2.45	0.52
24:S:63:THR:H	24:S:66:MET:HE3	1.74	0.52
28:a:144:C:H2'	28:a:145:A:C8	2.45	0.52
5:4:64:PHE:CE2	5:4:66:ILE:HG13	2.45	0.52
6:A:604:G:H2'	6:A:605:U:O4'	2.10	0.52
10:E:38:VAL:HG11	10:E:114:VAL:HG22	1.91	0.52
28:a:1067:A:H2'	28:a:1094:U:H4'	1.92	0.52
28:a:1811:U:H2'	28:a:1812:G:H8	1.73	0.52
47:t:28:VAL:HG13	47:t:34:LEU:HD23	1.91	0.52
2:1:4:THR:HG22	28:a:684:C:H1'	1.91	0.52
6:A:545:C:H5'	9:D:69:GLU:HB2	1.92	0.52
12:G:97:ASN:O	12:G:101:MET:HG3	2.09	0.52
14:I:57:MET:HG3	14:I:60:LYS:HG2	1.91	0.52
24:S:32:ARG:HG2	24:S:57:HIS:CE1	2.45	0.52
28:a:1102:U:H2'	28:a:1103:G:H8	1.75	0.52
28:a:2101:G:H2'	28:a:2102:G:C8	2.44	0.52
39:l:63:ILE:HG12	39:l:105:MET:HG2	1.92	0.52
16:K:84:VAL:HB	16:K:110:ILE:HD13	1.91	0.52
28:a:1734:G:H2'	28:a:1735:C:C6	2.45	0.52
6:A:384:G:H2'	6:A:385:C:H6	1.74	0.52
28:a:586:U:H2'	28:a:587:A:H8	1.74	0.52
28:a:891:U:H2'	28:a:892:U:O4'	2.10	0.52
40:m:45:ARG:HD3	40:m:97:ILE:HD11	1.91	0.52
6:A:1031:C:H4'	6:A:1032:G:C6	2.45	0.52
7:B:67:ILE:HB	7:B:89:GLN:HG2	1.92	0.52
15:J:90:LEU:HD23	15:J:91:ASP:H	1.74	0.52
24:S:29:LYS:HE3	24:S:30:PRO:HD2	1.92	0.52
28:a:1745:A:H2'	28:a:1746:U:H6	1.74	0.52
28:a:2516:C:H2'	28:a:2517:A:H8	1.75	0.52
6:A:215:C:H2'	6:A:216:U:C6	2.45	0.52
9:D:98:LEU:HB2	9:D:135:TYR:HB3	1.92	0.52
12:G:42:ILE:HD13	12:G:116:MET:HB3	1.91	0.52
13:H:105:SER:HB2	13:H:126:ILE:HD11	1.92	0.52
19:N:88:ALA:HB2	19:N:96:LEU:HD23	1.91	0.52
28:a:641:A:H2'	28:a:642:C:O4'	2.10	0.52
47:t:33:LYS:HB3	47:t:64:ALA:HB1	1.92	0.52
3:2:54:ASP:HA	3:2:57:LEU:HD12	1.90	0.51
6:A:1124:G:H5"	15:J:37:ARG:HG3	1.92	0.51
14:I:5:GLN:NE2	14:I:22:LYS:HE2	2.25	0.51
15:J:8:ILE:HB	15:J:74:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:474:C:H4'	28:a:509:C:H5'	1.92	0.51
28:a:1402:U:H2'	28:a:1403:U:C6	2.45	0.51
28:a:1682:G:H2'	28:a:1683:U:H6	1.74	0.51
38:k:91:ASP:HB3	38:k:123:ARG:HB3	1.91	0.51
10:E:161:VAL:HA	10:E:164:ILE:HG22	1.92	0.51
25:T:28:MET:HE1	25:T:67:ILE:HD13	1.91	0.51
28:a:1066:A:H2'	28:a:1070:A:H62	1.75	0.51
33:f:105:THR:HG23	33:f:106:ILE:HG13	1.91	0.51
35:h:9:VAL:HG22	35:h:10:ALA:H	1.75	0.51
6:A:1015:G:H2'	6:A:1016:A:H8	1.75	0.51
28:a:2585:U:H2'	28:a:2586:U:H2'	1.91	0.51
28:a:2738:G:H2'	28:a:2739:A:C8	2.46	0.51
3:2:11:ALA:HA	3:2:62:LEU:HD21	1.92	0.51
6:A:515:G:H2'	6:A:516:PSU:H6	1.75	0.51
9:D:87:GLY:HA3	9:D:197:GLU:HG3	1.91	0.51
15:J:56:HIS:ND1	15:J:57:VAL:HG13	2.26	0.51
21:P:69:ASP:O	21:P:73:THR:HG23	2.10	0.51
28:a:1165:G:H2'	28:a:1166:A:C8	2.46	0.51
28:a:1689:A:H2'	28:a:1690:A:C8	2.45	0.51
28:a:1916:3TD:H3'	28:a:1917:A:H8	1.75	0.51
28:a:2234:U:H2'	28:a:2235:G:H8	1.75	0.51
6:A:56:U:H2'	6:A:57:G:H8	1.75	0.51
7:B:95:ARG:NH1	7:B:97:LEU:HA	2.25	0.51
27:X:34:ILE:HB	27:X:56:VAL:HG12	1.92	0.51
28:a:2176:C:N4	28:a:2177:A:H62	2.08	0.51
28:a:2699:U:H2'	28:a:2700:C:C6	2.45	0.51
6:A:413:G:H21	6:A:428:G:H8	1.57	0.51
6:A:522:C:H41	17:L:50:ARG:NH2	2.08	0.51
6:A:675:A:H1'	16:K:118:HIS:HB2	1.92	0.51
9:D:8:LYS:HB3	9:D:21:LEU:HD13	1.93	0.51
14:I:21:ILE:HD13	14:I:86:ALA:HB1	1.93	0.51
28:a:907:A:H2'	28:a:908:A:C8	2.46	0.51
28:a:1564:C:H2'	28:a:1565:C:C6	2.46	0.51
28:a:1570:A:H2'	28:a:1571:A:C8	2.45	0.51
28:a:2125:G:H2'	28:a:2126:G:O4'	2.10	0.51
28:a:2456:G:H2'	28:a:2457:C:C6	2.46	0.51
37:j:40:LYS:HZ2	37:j:57:VAL:HG12	1.76	0.51
28:a:2317:G:H2'	28:a:2318:A:H8	1.76	0.51
41:n:81:ARG:O	41:n:84:GLU:HG2	2.11	0.51
45:r:51:LEU:O	45:r:55:ILE:HG22	2.10	0.51
6:A:916:U:H2'	6:A:917:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:173:VAL:HG12	8:C:175:LEU:HD21	1.93	0.51
35:h:15:LEU:HD11	35:h:56:ALA:HB1	1.91	0.51
6:A:1380:U:H4'	6:A:1381:U:H5'	1.92	0.51
6:A:1513:A:H2'	6:A:1514:G:C8	2.46	0.51
6:A:1534:A:H2'	6:A:1535:C:H6	1.75	0.51
15:J:53:ILE:HD11	15:J:61:ALA:HB1	1.92	0.51
20:O:78:TYR:O	20:O:82:ILE:HG23	2.11	0.51
22:Q:47:HIS:HE2	22:Q:49:GLU:HG2	1.76	0.51
24:S:11:ILE:HD13	24:S:16:LEU:HD13	1.93	0.51
28:a:1410:A:H2'	28:a:1411:C:C6	2.46	0.51
28:a:2186:U:H2'	28:a:2187:G:C8	2.46	0.51
29:b:5:U:H2'	29:b:6:G:H8	1.76	0.51
35:h:87:GLU:HB2	35:h:89:LYS:HG2	1.92	0.51
48:u:62:THR:HA	48:u:70:GLU:O	2.11	0.51
49:v:37:ILE:HD11	49:v:82:ILE:HD11	1.93	0.51
6:A:222:C:H2'	6:A:223:A:H8	1.76	0.51
14:I:57:MET:HE2	14:I:61:LEU:HD21	1.93	0.51
16:K:20:VAL:HG13	16:K:35:THR:HG23	1.92	0.51
28:a:817:A:H4'	28:a:833:G:N2	2.26	0.51
28:a:2107:U:H2'	28:a:2108:G:H8	1.72	0.51
46:s:34:VAL:HG21	46:s:43:ILE:HD11	1.93	0.51
6:A:1048:G:H5"	19:N:3:LYS:HD2	1.93	0.50
28:a:1590:A:H2'	28:a:1591:A:H8	1.76	0.50
30:c:135:ILE:HD13	30:c:141:VAL:HG11	1.93	0.50
6:A:1287:A:H2'	6:A:1288:A:C8	2.47	0.50
24:S:10:PHE:O	24:S:39:THR:HG22	2.12	0.50
25:T:28:MET:HE1	25:T:67:ILE:HG21	1.93	0.50
28:a:482:A:H5"	47:t:47:LYS:HD2	1.93	0.50
36:i:5:THR:HG23	36:i:45:THR:HG21	1.92	0.50
38:k:141:LYS:NZ	38:k:143:GLU:HB3	2.27	0.50
5:4:2:LYS:HD3	5:4:5:ILE:HD11	1.93	0.50
6:A:736:C:H2'	6:A:737:C:H6	1.75	0.50
12:G:15:ASP:OD1	12:G:23:LEU:HB3	2.12	0.50
15:J:26:VAL:O	15:J:30:LYS:HG2	2.11	0.50
17:L:53:CYS:HB3	17:L:67:ILE:HD11	1.92	0.50
28:a:136:U:H3'	28:a:137:U:H5"	1.93	0.50
28:a:2244:U:H2'	28:a:2245:U:C6	2.46	0.50
6:A:470:C:H2'	6:A:471:C:C6	2.47	0.50
9:D:149:ALA:HB1	9:D:152:GLN:HE22	1.75	0.50
28:a:281:A:H2'	28:a:282:G:H8	1.75	0.50
6:A:1130:A:C8	6:A:1146:A:N1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:43:GLY:HA2	11:F:58:HIS:NE2	2.27	0.50
28:a:578:C:H2'	28:a:579:A:H8	1.75	0.50
28:a:778:A:O4'	30:c:218:PRO:HG2	2.11	0.50
28:a:1082:A:H4'	28:a:1102:U:H4'	1.93	0.50
28:a:2174:A:H5"	28:a:2175:C:C5	2.44	0.50
6:A:514:C:H2'	6:A:515:G:H8	1.76	0.50
6:A:1149:C:H2'	6:A:1150:A:C8	2.46	0.50
8:C:85:GLU:O	8:C:89:LYS:HG2	2.12	0.50
9:D:8:LYS:HB3	9:D:21:LEU:HB3	1.93	0.50
28:a:357:U:H2'	28:a:358:G:C8	2.47	0.50
28:a:2103:U:H2'	28:a:2104:C:C6	2.47	0.50
24:S:11:ILE:HA	24:S:38:SER:HB3	1.94	0.50
28:a:810:U:H2'	28:a:811:C:C6	2.47	0.50
28:a:1438:G:H2'	28:a:1439:U:H6	1.77	0.50
28:a:2149:G:H2'	28:a:2150:U:C6	2.47	0.50
35:h:78:VAL:HG21	35:h:142:LEU:HD21	1.93	0.50
6:A:1330:U:H4'	18:M:23:TYR:CE1	2.47	0.50
6:A:1533:C:H2'	6:A:1534:A:H8	1.76	0.50
16:K:23:ILE:HG13	16:K:32:VAL:HG13	1.93	0.50
28:a:631:C:H2'	28:a:632:C:C6	2.47	0.50
40:m:55:ALA:HA	40:m:80:PHE:CZ	2.47	0.50
9:D:28:ILE:HD11	9:D:34:ILE:HD13	1.93	0.50
24:S:31:LEU:H	24:S:31:LEU:HD12	1.76	0.50
28:a:1391:U:H2'	28:a:1392:A:O4'	2.11	0.50
28:a:1890:A:H2'	28:a:1891:A:C8	2.47	0.50
6:A:335:C:H2'	6:A:336:A:C8	2.47	0.49
6:A:981:U:H5"	19:N:63:ARG:HH21	1.77	0.49
28:a:95:A:H2'	28:a:96:C:O4'	2.12	0.49
28:a:2555:U:H2'	28:a:2556:U:C6	2.47	0.49
36:i:34:ARG:HG3	36:i:39:LYS:HB2	1.94	0.49
43:p:112:LYS:HD3	44:q:49:ILE:HG21	1.94	0.49
28:a:1077:A:H2'	28:a:1078:U:C6	2.47	0.49
28:a:2515:U:H2'	28:a:2516:C:C6	2.46	0.49
28:a:2649:G:H2'	28:a:2650:C:C6	2.47	0.49
6:A:358:U:H2'	6:A:359:G:H8	1.77	0.49
6:A:1072:G:H2'	6:A:1073:U:C6	2.48	0.49
6:A:1121:U:H2'	6:A:1122:U:H6	1.77	0.49
6:A:1286:U:H2'	6:A:1287:A:H5'	1.93	0.49
6:A:1401:G:H2'	6:A:1402:4OC:O4'	2.12	0.49
9:D:11:LEU:O	9:D:15:GLU:HG2	2.12	0.49
12:G:66:LEU:HD21	12:G:101:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:30:LYS:HB3	17:L:57:LEU:HD22	1.92	0.49
22:Q:11:ARG:HB2	22:Q:11:ARG:HH11	1.77	0.49
28:a:1626:A:OP2	28:a:1626:A:H8	1.95	0.49
6:A:954:G:H2'	6:A:955:U:C6	2.47	0.49
7:B:70:VAL:HB	7:B:163:VAL:HG22	1.94	0.49
14:I:24:GLY:HA3	14:I:62:ASP:CG	2.38	0.49
27:X:88:HIS:O	27:X:92:LEU:HB2	2.12	0.49
28:a:848:C:H2'	28:a:849:U:H6	1.77	0.49
29:b:60:C:H2'	29:b:61:G:H8	1.78	0.49
29:b:114:C:H2'	29:b:115:A:H8	1.77	0.49
35:h:93:SER:HB3	35:h:123:ARG:CZ	2.42	0.49
6:A:746:A:H2'	6:A:747:A:H8	1.77	0.49
6:A:1005:A:H62	6:A:1024:G:H21	1.59	0.49
6:A:1107:C:C4	6:A:1108:G:C8	3.01	0.49
12:G:26:PHE:CD1	12:G:62:PHE:HZ	2.31	0.49
28:a:1805:C:O2'	30:c:48:ARG:HD2	2.12	0.49
49:v:53:CYS:SG	49:v:57:HIS:HA	2.53	0.49
6:A:323:U:H2'	6:A:324:G:O4'	2.13	0.49
6:A:350:G:H2'	6:A:351:G:C8	2.48	0.49
25:T:42:GLY:HA2	25:T:86:LEU:HD21	1.94	0.49
28:a:2:G:H2'	28:a:3:U:H6	1.75	0.49
28:a:65:U:H2'	28:a:66:C:H6	1.78	0.49
28:a:944:A:H2'	28:a:945:C:C6	2.47	0.49
28:a:1076:C:H2'	28:a:1077:A:H8	1.77	0.49
28:a:2115:A:N3	28:a:2116:G:H4'	2.27	0.49
6:A:413:G:H21	6:A:428:G:H1'	1.77	0.49
7:B:9:MET:HE1	7:B:50:PHE:HD2	1.78	0.49
11:F:9:MET:HE1	11:F:86:ARG:HD2	1.94	0.49
17:L:107:VAL:O	17:L:108:LYS:HB2	2.12	0.49
18:M:86:TYR:CZ	18:M:90:ARG:HD2	2.48	0.49
28:a:305:U:H3	28:a:309:A:H62	1.61	0.49
28:a:781:G:H5'	28:a:782:G:OP1	2.13	0.49
28:a:1884:U:H2'	28:a:1885:G:O4'	2.12	0.49
28:a:2075:U:H2'	28:a:2076:U:H6	1.77	0.49
28:a:2170:A:H3'	28:a:2171:A:H8	1.77	0.49
28:a:2330:U:H2'	28:a:2331:G:C8	2.48	0.49
40:m:96:ARG:NH2	40:m:116:VAL:HG23	2.27	0.49
4:3:30:GLU:HG3	4:3:32:LYS:HG2	1.94	0.49
6:A:1513:A:H2'	6:A:1514:G:H8	1.78	0.49
7:B:49:MET:HG2	7:B:199:VAL:O	2.13	0.49
17:L:48:ALA:O	17:L:49:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:595:U:H2'	28:a:596:A:H8	1.78	0.49
28:a:1811:U:H2'	28:a:1812:G:C8	2.48	0.49
28:a:2732:G:O2'	28:a:2733:G:H5'	2.13	0.49
31:d:10:GLY:HA3	42:o:5:ILE:HD11	1.94	0.49
37:j:114:LYS:O	37:j:118:LEU:HD12	2.12	0.49
6:A:463:U:H2'	6:A:464:U:C6	2.48	0.49
6:A:981:U:H2'	6:A:982:U:C5	2.48	0.49
11:F:9:MET:HB3	11:F:57:ALA:HB1	1.94	0.49
28:a:2125:G:H8	28:a:2125:G:O5'	1.95	0.49
33:f:104:ILE:HD11	33:f:175:PHE:HA	1.93	0.49
1:0:55:LYS:HD3	1:0:55:LYS:N	2.28	0.49
9:D:102:VAL:HG13	9:D:107:PHE:HB2	1.95	0.49
14:I:41:ARG:HG2	14:I:43:THR:HG22	1.95	0.49
28:a:1079:U:H2'	28:a:1080:U:C2	2.48	0.49
6:A:524:G:H2'	6:A:525:C:C6	2.48	0.48
6:A:693:G:H1'	12:G:82:GLY:HA3	1.95	0.48
6:A:696:A:H2'	6:A:697:U:H6	1.78	0.48
6:A:750:C:H2'	6:A:751:U:H6	1.77	0.48
6:A:1294:G:H2'	6:A:1295:U:C6	2.48	0.48
7:B:90:PHE:HE1	7:B:153:ASP:HB3	1.78	0.48
28:a:860:A:H2'	28:a:861:G:H8	1.78	0.48
28:a:2810:A:H2'	28:a:2811:A:C8	2.48	0.48
35:h:46:PHE:HA	35:h:50:ARG:HH11	1.76	0.48
48:u:26:PHE:CE1	48:u:42:LEU:HD12	2.48	0.48
5:4:9:TYR:HD2	5:4:25:ARG:NH2	2.11	0.48
6:A:555:U:H2'	6:A:556:C:C6	2.48	0.48
6:A:719:C:O2'	23:R:38:LYS:HB3	2.13	0.48
6:A:1314:C:H2'	6:A:1315:U:H6	1.78	0.48
6:A:1412:C:H2'	6:A:1413:A:C8	2.48	0.48
10:E:114:VAL:HG11	10:E:140:THR:HG23	1.95	0.48
28:a:2838:A:H2'	28:a:2839:G:H8	1.79	0.48
32:e:195:GLN:O	32:e:198:GLU:HG3	2.13	0.48
34:g:89:LEU:HD23	34:g:94:TYR:HB3	1.94	0.48
6:A:144:G:H2'	6:A:145:G:C8	2.47	0.48
6:A:399:G:H2'	6:A:400:C:C6	2.49	0.48
6:A:950:U:H2'	6:A:951:G:H8	1.78	0.48
17:L:29:GLN:HB3	17:L:81:LEU:HG	1.95	0.48
28:a:860:A:H2'	28:a:861:G:C8	2.49	0.48
28:a:1829:C:H2'	28:a:1830:G:H8	1.78	0.48
45:r:41:LYS:HD2	53:z:22:LEU:HD11	1.96	0.48
3:2:42:ARG:NH2	28:a:2383:G:H21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:33:A:H2'	6:A:34:C:C6	2.48	0.48
6:A:461:G:O2'	6:A:462:G:H8	1.96	0.48
12:G:103:TRP:NE1	12:G:137:LYS:HE3	2.29	0.48
13:H:35:ALA:O	13:H:39:VAL:HG23	2.14	0.48
28:a:578:C:H2'	28:a:579:A:C8	2.48	0.48
28:a:1260:U:O2'	53:z:8:PRO:HD2	2.14	0.48
28:a:2095:A:H4'	35:h:25:TYR:HE2	1.77	0.48
28:a:2272:G:OP1	49:v:18:ALA:HB1	2.13	0.48
40:m:8:ARG:HD2	40:m:43:GLU:HG2	1.95	0.48
11:F:47:LEU:HD13	11:F:51:ILE:HD12	1.96	0.48
12:G:18:PHE:HB3	12:G:59:LEU:HD11	1.94	0.48
16:K:31:ILE:HG13	16:K:46:THR:HG23	1.94	0.48
18:M:81:MET:HB3	28:a:885:C:N4	2.27	0.48
28:a:876:G:H2'	28:a:877:G:C8	2.48	0.48
28:a:955:U:H2'	29:b:89:U:C2	2.48	0.48
34:g:42:GLU:HB2	34:g:55:ARG:HE	1.78	0.48
38:k:78:ARG:NH1	38:k:113:ALA:HB1	2.28	0.48
10:E:36:LEU:HD11	10:E:134:ILE:HA	1.96	0.48
28:a:594:G:H2'	28:a:595:U:C6	2.48	0.48
28:a:1550:U:H2'	28:a:1551:A:C8	2.48	0.48
6:A:736:C:H2'	6:A:737:C:C6	2.48	0.48
14:I:60:LYS:HD3	14:I:60:LYS:N	2.29	0.48
28:a:537:A:H2'	28:a:538:G:O4'	2.14	0.48
28:a:1637:A:H5'	28:a:1759:C:O2'	2.14	0.48
28:a:2128:G:C6	28:a:2129:G:O6	2.67	0.48
30:c:145:GLU:HG2	30:c:151:GLY:C	2.39	0.48
47:t:34:LEU:HD21	47:t:67:VAL:HG23	1.96	0.48
52:y:3:LYS:O	52:y:40:ASP:HB2	2.14	0.48
4:3:8:LYS:HB2	4:3:8:LYS:HE2	1.43	0.48
6:A:451:A:N6	6:A:481:G:H5'	2.28	0.48
6:A:908:A:H2'	6:A:909:A:H8	1.78	0.48
6:A:1014:A:H2'	6:A:1015:G:C8	2.49	0.48
13:H:5:ASP:OD2	13:H:81:PRO:HD3	2.13	0.48
27:X:18:ASP:O	27:X:22:THR:HG23	2.14	0.48
6:A:715:A:H2'	6:A:716:A:H8	1.77	0.48
6:A:1162:C:H2'	6:A:1163:A:C8	2.48	0.48
7:B:58:ASN:OD1	7:B:220:THR:HG22	2.13	0.48
8:C:64:ILE:HG22	8:C:99:ALA:HA	1.94	0.48
13:H:3:MET:HE2	13:H:3:MET:HA	1.94	0.48
28:a:579:A:H2'	28:a:580:G:H8	1.79	0.48
28:a:1104:G:H2'	28:a:1104:G:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2026:C:H2'	28:a:2027:U:C6	2.49	0.48
28:a:2314:C:H2'	28:a:2315:A:C8	2.48	0.48
34:g:73:ASN:C	34:g:73:ASN:HD22	2.22	0.48
44:q:38:VAL:HG22	44:q:59:ILE:HD12	1.96	0.48
6:A:75:G:N3	6:A:76:G:H1'	2.29	0.48
26:W:11:G:H2'	26:W:12:U:C6	2.49	0.48
28:a:144:C:H2'	28:a:145:A:H8	1.79	0.48
33:f:137:ILE:HG13	33:f:138:PHE:N	2.28	0.48
35:h:46:PHE:O	35:h:51:ARG:HG2	2.14	0.48
36:i:60:ASP:HB3	36:i:97:PRO:HB3	1.95	0.48
6:A:468:A:H2'	6:A:469:A:C8	2.49	0.47
6:A:676:A:H5"	16:K:115:PRO:HB3	1.94	0.47
6:A:1032:G:H3'	6:A:1032:G:N3	2.29	0.47
6:A:1125:U:OP1	15:J:37:ARG:HG2	2.14	0.47
6:A:1436:U:H2'	6:A:1437:A:C8	2.49	0.47
7:B:117:LEU:HD11	7:B:137:ARG:HD2	1.95	0.47
28:a:1196:U:H2'	28:a:1197:C:H6	1.79	0.47
32:e:157:LEU:HG	32:e:169:VAL:HG21	1.95	0.47
33:f:65:PRO:HB2	33:f:87:CYS:HB2	1.95	0.47
33:f:101:GLU:O	33:f:105:THR:HG22	2.13	0.47
6:A:41:G:H2'	6:A:42:G:H8	1.78	0.47
6:A:160:A:H2'	6:A:161:A:O4'	2.14	0.47
6:A:468:A:H2'	6:A:469:A:H8	1.79	0.47
6:A:916:U:H2'	6:A:917:G:C8	2.49	0.47
6:A:1118:U:H2'	6:A:1119:C:H6	1.80	0.47
18:M:65:VAL:HG12	18:M:66:GLU:HG2	1.95	0.47
28:a:44:A:H2'	28:a:45:G:O4'	2.15	0.47
28:a:1318:A:C4	28:a:1319:A:C8	3.02	0.47
28:a:1636:U:H2'	28:a:1637:A:C8	2.49	0.47
35:h:96:THR:HA	35:h:99:ILE:HD12	1.96	0.47
37:j:24:VAL:HG13	37:j:33:ALA:HB2	1.96	0.47
6:A:148:G:H2'	6:A:149:A:O4'	2.14	0.47
6:A:219:U:C2	6:A:220:G:C8	3.03	0.47
28:a:1351:A:H2'	28:a:1352:G:O4'	2.14	0.47
32:e:21:ARG:HD3	32:e:106:LYS:HB3	1.95	0.47
41:n:90:VAL:HG21	41:n:115:LEU:HD13	1.95	0.47
6:A:1124:G:H1'	6:A:1125:U:H5	1.79	0.47
7:B:116:ASP:O	7:B:120:GLN:HG2	2.13	0.47
11:F:66:ALA:HB3	11:F:71:ILE:HD11	1.95	0.47
14:I:6:TYR:HB2	14:I:21:ILE:CG1	2.44	0.47
18:M:4:ILE:HD11	18:M:53:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:564:U:H2'	28:a:565:U:O4'	2.15	0.47
28:a:1173:U:H2'	28:a:1174:G:O4'	2.15	0.47
28:a:1890:A:H2'	28:a:1891:A:H8	1.80	0.47
28:a:2314:C:H2'	28:a:2315:A:H8	1.78	0.47
29:b:66:A:H61	29:b:107:G:H2'	1.80	0.47
30:c:227:PRO:HG3	30:c:234:GLY:HA3	1.97	0.47
31:d:22:ILE:HG23	31:d:190:LYS:HG3	1.97	0.47
43:p:72:ASN:HB3	43:p:110:VAL:HG11	1.97	0.47
6:A:155:A:H2'	6:A:156:C:C6	2.50	0.47
6:A:215:C:H2'	6:A:216:U:H6	1.79	0.47
8:C:112:ASP:OD2	8:C:115:LEU:HB2	2.15	0.47
28:a:305:U:H2'	28:a:306:G:O4'	2.14	0.47
28:a:576:G:H2'	28:a:577:U:C6	2.50	0.47
28:a:2752:G:C4	34:g:3:ARG:HD2	2.49	0.47
28:a:2848:U:H2'	28:a:2849:G:O4'	2.13	0.47
37:j:10:VAL:HG12	37:j:12:ASP:H	1.80	0.47
6:A:6:G:H2'	10:E:124:LEU:HD21	1.95	0.47
6:A:360:G:H2'	6:A:361:G:C8	2.50	0.47
6:A:601:G:H2'	6:A:602:A:C8	2.50	0.47
6:A:948:C:H3'	18:M:105:ASN:HD22	1.80	0.47
6:A:1118:U:H2'	6:A:1119:C:C6	2.49	0.47
10:E:53:ALA:HB2	10:E:62:LYS:HD2	1.96	0.47
15:J:66:GLU:HG2	19:N:99:ALA:HB2	1.96	0.47
27:X:31:PHE:CD1	27:X:89:LYS:HB2	2.50	0.47
27:X:55:HIS:HA	27:X:60:GLU:OE2	2.13	0.47
28:a:83:G:H2'	28:a:101:G:H21	1.79	0.47
28:a:531:A:H4'	28:a:532:G:C8	2.49	0.47
28:a:579:A:H2'	28:a:580:G:C8	2.50	0.47
28:a:590:U:H2'	28:a:591:U:C6	2.50	0.47
28:a:2306:U:H5"	33:f:131:GLY:HA3	1.95	0.47
28:a:2744:U:H2'	28:a:2745:G:O4'	2.15	0.47
6:A:34:C:H2'	6:A:35:G:H8	1.78	0.47
6:A:246:A:C2	6:A:282:A:C5	3.03	0.47
6:A:440:C:C2	6:A:441:A:C8	3.03	0.47
6:A:821:G:H2'	6:A:822:U:C6	2.49	0.47
6:A:1103:C:H5"	7:B:97:LEU:HD22	1.96	0.47
8:C:56:VAL:HB	8:C:67:THR:HB	1.95	0.47
11:F:74:LEU:O	11:F:78:PHE:HD1	1.98	0.47
22:Q:81:LYS:HA	22:Q:81:LYS:HD2	1.76	0.47
23:R:45:THR:HG23	23:R:47:THR:H	1.79	0.47
28:a:181:A:H2'	28:a:182:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:586:U:H2'	28:a:587:A:C8	2.50	0.47
28:a:894:C:H2'	28:a:895:C:H6	1.80	0.47
28:a:1180:U:H2'	28:a:1181:U:C6	2.50	0.47
28:a:2115:A:OP1	28:a:2118:A:H1'	2.14	0.47
31:d:91:THR:HG23	31:d:94:GLN:HB2	1.96	0.47
35:h:44:VAL:O	35:h:48:GLU:HB3	2.14	0.47
50:w:40:VAL:O	50:w:41:GLU:HB3	2.13	0.47
6:A:376:G:H5"	21:P:5:ARG:HB2	1.97	0.47
6:A:838:G:C6	6:A:849:G:C6	3.03	0.47
6:A:1175:G:H2'	6:A:1176:A:C8	2.49	0.47
28:a:840:G:H2'	28:a:841:A:C8	2.49	0.47
28:a:868:U:H2'	28:a:869:U:C6	2.49	0.47
28:a:981:A:H2'	28:a:981:A:N3	2.30	0.47
28:a:985:A:P	52:y:12:SER:HB3	2.55	0.47
28:a:2167:U:H4'	28:a:2168:U:H5"	1.96	0.47
28:a:2174:A:H3'	28:a:2175:C:C6	2.49	0.47
28:a:2846:U:H5"	42:o:52:ASN:O	2.15	0.47
30:c:228:VAL:O	30:c:228:VAL:CG1	2.61	0.47
32:e:23:PHE:HA	32:e:107:SER:OG	2.15	0.47
49:v:72:LYS:HB3	49:v:72:LYS:HE2	1.79	0.47
6:A:41:G:H2'	6:A:42:G:C8	2.50	0.47
6:A:75:G:H5'	6:A:76:G:OP2	2.15	0.47
6:A:254:G:H5"	22:Q:71:LYS:HD3	1.96	0.47
10:E:41:ASP:OD1	10:E:45:ARG:HB2	2.15	0.47
23:R:19:GLN:HG3	23:R:20:GLU:N	2.30	0.47
24:S:3:ARG:HH12	24:S:7:LYS:HE2	1.79	0.47
28:a:1037:A:N6	28:a:1112:G:H1	2.10	0.47
28:a:1073:C:N4	28:a:1074:A:H61	2.11	0.47
28:a:1350:A:H2'	28:a:1351:A:C8	2.50	0.47
28:a:1589:U:H2'	28:a:1590:A:C8	2.50	0.47
28:a:1925:C:H2'	28:a:1926:C:C6	2.49	0.47
28:a:2351:C:H2'	28:a:2352:G:O4'	2.15	0.47
6:A:269:C:H2'	6:A:270:A:H8	1.79	0.47
6:A:393:A:C2	6:A:394:G:C8	3.03	0.47
6:A:945:G:C2	6:A:946:A:C8	3.03	0.47
6:A:1425:U:H2'	6:A:1426:G:H8	1.78	0.47
11:F:73:GLU:O	11:F:77:THR:HG23	2.15	0.47
28:a:168:G:H2'	28:a:169:U:C6	2.49	0.47
28:a:1391:U:H4'	28:a:1603:A:H4'	1.97	0.47
28:a:1511:G:H2'	28:a:1512:C:C6	2.49	0.47
28:a:2189:C:H2'	28:a:2190:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2729:U:O2'	28:a:2730:G:H8	1.98	0.47
30:c:8:PRO:HB3	30:c:14:ARG:HG3	1.97	0.47
33:f:102:ARG:O	33:f:106:ILE:HB	2.15	0.47
37:j:120:PRO:HB2	37:j:121:GLU:OE1	2.15	0.47
38:k:122:VAL:HB	38:k:142:ILE:HG23	1.96	0.47
39:l:21:ALA:HB2	39:l:97:GLN:HB2	1.96	0.47
40:m:96:ARG:HD2	40:m:98:LEU:HD21	1.97	0.47
6:A:92:U:H2'	6:A:93:U:O4'	2.16	0.46
6:A:371:A:H2'	6:A:372:C:O4'	2.15	0.46
6:A:1041:G:H2'	6:A:1042:A:C8	2.50	0.46
6:A:1253:G:H2'	6:A:1254:A:C8	2.49	0.46
16:K:17:SER:HA	16:K:79:ILE:HA	1.96	0.46
16:K:75:LYS:HZ3	16:K:76:GLU:HA	1.80	0.46
27:X:28:GLU:O	27:X:32:GLU:HG3	2.15	0.46
28:a:836:U:H2'	28:a:837:C:C6	2.50	0.46
28:a:1426:G:H2'	28:a:1427:G:H8	1.80	0.46
28:a:2334:A:H5'	28:a:2336:A:H1'	1.97	0.46
29:b:42:C:C6	33:f:66:LEU:HB2	2.50	0.46
29:b:60:C:H2'	29:b:61:G:C8	2.50	0.46
42:o:14:LYS:HE3	42:o:77:HIS:HA	1.97	0.46
45:r:23:LEU:HD23	45:r:23:LEU:HA	1.77	0.46
46:s:11:LEU:HD22	46:s:32:LEU:HD13	1.97	0.46
3:2:15:LYS:HG2	38:k:64:PHE:HZ	1.80	0.46
5:4:44:TYR:OH	33:f:176:PRO:HG3	2.14	0.46
6:A:570:G:H2'	6:A:571:U:C6	2.50	0.46
7:B:104:TRP:CD1	7:B:108:ARG:HH21	2.33	0.46
7:B:112:LYS:O	7:B:115:LYS:HG3	2.15	0.46
11:F:75:GLU:O	11:F:79:ARG:HG3	2.15	0.46
19:N:23:LYS:O	19:N:27:LEU:HD13	2.15	0.46
19:N:77:PHE:CD2	19:N:84:LEU:HD11	2.50	0.46
28:a:585:U:H2'	28:a:586:U:C6	2.50	0.46
28:a:1078:U:H2'	28:a:1079:U:C6	2.50	0.46
28:a:1174:G:H2'	28:a:1175:C:H6	1.79	0.46
28:a:2033:G:C5	31:d:150:MEQ:HE3	2.50	0.46
33:f:46:ASP:HB2	33:f:49:LEU:HD22	1.97	0.46
33:f:65:PRO:HA	33:f:89:VAL:HG12	1.97	0.46
46:s:8:LEU:HD13	46:s:50:LEU:HD21	1.97	0.46
6:A:1328:C:C2	6:A:1329:A:C8	3.04	0.46
8:C:77:ILE:HA	8:C:84:VAL:HG13	1.97	0.46
12:G:129:GLU:HB3	12:G:131:LYS:HE2	1.98	0.46
14:I:11:ARG:HB3	14:I:106:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:9:ARG:HB3	19:N:13:ARG:NH1	2.30	0.46
24:S:44:MET:O	24:S:47:LEU:HB2	2.15	0.46
28:a:708:G:H1	28:a:717:U:H3	1.63	0.46
28:a:1933:A:H2'	28:a:1934:G:O4'	2.15	0.46
30:c:120:VAL:HG12	30:c:134:ASN:HD21	1.80	0.46
39:l:69:PRO:HA	39:l:94:ALA:HB2	1.97	0.46
46:s:53:VAL:HG21	46:s:87:LEU:HD22	1.97	0.46
6:A:865:A:H2'	6:A:866:C:C6	2.51	0.46
6:A:1318:A:O2'	24:S:37:ARG:HD2	2.14	0.46
15:J:6:ILE:HB	15:J:76:ILE:HB	1.97	0.46
17:L:57:LEU:HD21	17:L:82:ILE:HD13	1.98	0.46
23:R:9:LYS:HB2	23:R:46:GLY:HA3	1.97	0.46
36:i:60:ASP:HA	36:i:93:ILE:HD11	1.96	0.46
6:A:144:G:H2'	6:A:145:G:H8	1.81	0.46
6:A:299:G:H2'	6:A:300:A:C8	2.50	0.46
6:A:821:G:H2'	6:A:822:U:H6	1.80	0.46
8:C:13:GLY:HA3	19:N:97:LYS:HE2	1.98	0.46
11:F:78:PHE:HD2	11:F:84:VAL:HG21	1.81	0.46
20:O:85:LEU:HD23	20:O:85:LEU:HA	1.79	0.46
28:a:1194:G:H2'	28:a:1195:U:H6	1.80	0.46
28:a:2248:A:H2'	28:a:2249:C:C6	2.48	0.46
30:c:125:LYS:HB3	30:c:125:LYS:HE2	1.52	0.46
33:f:34:ILE:HG13	33:f:96:MET:HG3	1.97	0.46
33:f:38:MET:SD	33:f:152:LEU:HB3	2.55	0.46
1:0:10:LYS:HG3	1:0:20:PHE:CD2	2.51	0.46
6:A:1071:C:H2'	6:A:1072:G:C8	2.48	0.46
6:A:1354:U:H2'	6:A:1355:G:H8	1.79	0.46
6:A:1372:U:H2'	6:A:1373:G:O4'	2.16	0.46
7:B:54:LEU:HD23	7:B:54:LEU:HA	1.76	0.46
19:N:83:LYS:HD3	19:N:83:LYS:HA	1.56	0.46
27:X:74:ILE:O	27:X:78:ILE:HG23	2.16	0.46
28:a:665:A:H2'	28:a:667:A:H62	1.80	0.46
28:a:718:A:H2'	28:a:719:A:C8	2.51	0.46
28:a:1023:G:H2'	28:a:1024:A:H8	1.80	0.46
28:a:2640:A:H2'	28:a:2641:G:O4'	2.16	0.46
28:a:2752:G:H4'	34:g:4:VAL:HG23	1.96	0.46
6:A:210:C:H4'	6:A:211:G:C8	2.51	0.46
6:A:1313:U:H2'	6:A:1314:C:C6	2.50	0.46
8:C:63:SER:HA	8:C:97:VAL:HB	1.98	0.46
8:C:135:LYS:O	8:C:139:GLN:HG2	2.16	0.46
9:D:168:PRO:HB3	9:D:170:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:418:U:H2'	28:a:419:C:C6	2.50	0.46
28:a:1075:U:H1'	28:a:1085:A:C2	2.51	0.46
28:a:2125:G:H3'	28:a:2126:G:H8	1.80	0.46
28:a:2592:C:H2'	28:a:2593:G:H8	1.78	0.46
31:d:116:LYS:HA	40:m:1:MET:SD	2.56	0.46
33:f:31:VAL:O	33:f:96:MET:HE1	2.16	0.46
39:l:103:TYR:HE2	39:l:124:LEU:HD11	1.81	0.46
2:1:26:ASN:CG	28:a:679:G:H5'	2.41	0.46
6:A:129:A:H1'	6:A:130:A:C8	2.51	0.46
6:A:208:U:H2'	6:A:210:C:C4	2.51	0.46
6:A:427:U:H2'	6:A:428:G:H21	1.80	0.46
6:A:543:U:OP1	9:D:14:ARG:HD2	2.16	0.46
11:F:43:GLY:HA2	11:F:58:HIS:CE1	2.50	0.46
12:G:152:ALA:HB1	12:G:155:ARG:NH1	2.31	0.46
14:I:54:LEU:HD11	14:I:97:GLU:HG3	1.97	0.46
18:M:80:LEU:HD13	18:M:85:CYS:SG	2.56	0.46
18:M:83:LEU:HD11	24:S:65:GLU:HG3	1.98	0.46
28:a:272:G:H2'	28:a:273:U:C6	2.50	0.46
28:a:358:G:H2'	28:a:359:U:H6	1.79	0.46
28:a:577:U:H2'	28:a:578:C:C6	2.50	0.46
28:a:1089:C:H3'	28:a:1090:G:C8	2.50	0.46
28:a:1196:U:H2'	28:a:1197:C:C6	2.51	0.46
28:a:1439:U:H2'	28:a:1440:C:H6	1.79	0.46
28:a:1793:A:H2'	28:a:1794:C:H6	1.77	0.46
35:h:72:ILE:HD11	35:h:108:VAL:HG13	1.98	0.46
37:j:48:PRO:HB2	37:j:49:ARG:HD2	1.97	0.46
44:q:2:TYR:CE1	44:q:42:ALA:HB3	2.51	0.46
6:A:328:C:H4'	6:A:329:A:H5'	1.98	0.46
6:A:404:G:H2'	6:A:405:U:O4'	2.16	0.46
6:A:1319:A:C8	6:A:1323:G:C6	3.04	0.46
6:A:1410:A:H2'	6:A:1411:C:C6	2.50	0.46
6:A:1410:A:H2'	6:A:1411:C:H6	1.80	0.46
16:K:15:GLN:OE1	16:K:15:GLN:N	2.49	0.46
28:a:714:C:H3'	28:a:715:A:H8	1.81	0.46
28:a:1095:A:H3'	28:a:1096:G:H8	1.81	0.46
35:h:30:LEU:HB3	35:h:36:ALA:HB3	1.98	0.46
6:A:236:A:H2'	6:A:237:G:H8	1.81	0.46
6:A:985:C:H2'	6:A:986:U:C6	2.51	0.46
14:I:11:ARG:HB3	14:I:106:ARG:NH2	2.31	0.46
23:R:32:TYR:HE1	23:R:45:THR:HG1	1.62	0.46
28:a:354:U:H2'	28:a:355:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1179:G:H2'	28:a:1180:U:O4'	2.16	0.46
28:a:1511:G:H2'	28:a:1512:C:H6	1.81	0.46
28:a:2544:G:H2'	28:a:2545:G:C8	2.51	0.46
28:a:2821:A:H2'	28:a:2821:A:N3	2.32	0.46
28:a:2883:A:OP1	40:m:96:ARG:HD3	2.16	0.46
6:A:1253:G:H2'	6:A:1254:A:H8	1.81	0.45
19:N:3:LYS:HB2	19:N:6:MET:HG2	1.98	0.45
27:X:63:ALA:HB3	27:X:81:LEU:HD12	1.97	0.45
28:a:230:A:H2'	28:a:231:G:O4'	2.15	0.45
28:a:362:A:H2'	28:a:363:C:C6	2.51	0.45
28:a:1169:C:H2'	28:a:1170:U:O4'	2.16	0.45
28:a:1441:A:H2'	28:a:1442:G:H8	1.81	0.45
28:a:2167:U:C4	28:a:2172:A:H4'	2.51	0.45
28:a:2681:U:OP1	31:d:114:LYS:HG3	2.16	0.45
32:e:1:MET:HE1	32:e:113:VAL:HG11	1.99	0.45
34:g:35:ARG:HG3	34:g:36:THR:N	2.31	0.45
1:0:14:SER:HB2	1:0:50:LYS:NZ	2.31	0.45
6:A:687:A:C2	6:A:704:A:C5	3.05	0.45
9:D:58:LYS:HB3	9:D:58:LYS:HE3	1.55	0.45
15:J:15:HIS:O	15:J:18:ILE:HG22	2.16	0.45
18:M:51:GLU:O	18:M:55:THR:HG23	2.16	0.45
19:N:31:ILE:HD12	19:N:45:VAL:HG23	1.97	0.45
27:X:29:GLN:HG3	27:X:30:TYR:N	2.30	0.45
28:a:605:A:H2'	28:a:606:A:C8	2.50	0.45
28:a:1228:U:H2'	28:a:1229:G:H8	1.81	0.45
35:h:12:LEU:HD21	35:h:21:VAL:HG11	1.98	0.45
6:A:505:G:H2'	6:A:506:G:H8	1.82	0.45
6:A:1313:U:H2'	6:A:1314:C:H6	1.81	0.45
14:I:65:ILE:HG21	14:I:79:ILE:HD12	1.98	0.45
28:a:1289:G:H2'	28:a:1290:C:C6	2.51	0.45
28:a:1435:U:H2'	28:a:1436:A:H8	1.81	0.45
28:a:1571:A:H2'	28:a:1572:A:C8	2.52	0.45
5:4:60:PHE:CE2	24:S:42:PRO:HD3	2.52	0.45
6:A:398:U:H2'	6:A:399:G:H8	1.82	0.45
8:C:150:LYS:HG2	8:C:201:TRP:CE3	2.51	0.45
11:F:4:TYR:CE2	11:F:71:ILE:HG13	2.52	0.45
11:F:61:LEU:HD11	23:R:24:LYS:HE3	1.98	0.45
12:G:48:GLU:HG3	12:G:49:THR:N	2.31	0.45
28:a:151:G:H2'	28:a:152:U:C6	2.52	0.45
28:a:1563:U:H2'	28:a:1564:C:C6	2.52	0.45
28:a:2176:C:H2'	28:a:2177:A:C8	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:125:THR:HG23	35:h:146:VAL:O	2.16	0.45
6:A:204:G:H2'	6:A:205:A:C8	2.49	0.45
6:A:845:A:P	23:R:15:ALA:HA	2.56	0.45
6:A:1070:U:H2'	6:A:1071:C:C6	2.51	0.45
6:A:1317:C:H42	19:N:53:ARG:HH11	1.65	0.45
14:I:84:THR:HG21	14:I:103:PHE:HB3	1.97	0.45
14:I:127:PHE:HD2	14:I:129:LYS:NZ	2.15	0.45
25:T:85:LYS:HE3	25:T:85:LYS:HB3	1.57	0.45
28:a:1194:G:H2'	28:a:1195:U:C6	2.51	0.45
28:a:1195:U:H2'	28:a:1196:U:C6	2.52	0.45
28:a:1571:A:H2'	28:a:1572:A:H8	1.82	0.45
28:a:2112:U:H2'	28:a:2146:C:C2	2.52	0.45
28:a:2515:U:H2'	28:a:2516:C:H6	1.81	0.45
34:g:74:SER:OG	34:g:138:LYS:HD2	2.17	0.45
3:2:19:LYS:HG3	28:a:648:G:H5'	1.98	0.45
4:3:9:LYS:HE3	4:3:16:ILE:HD12	1.97	0.45
5:4:25:ARG:HD3	33:f:98:GLU:OE2	2.17	0.45
6:A:171:A:H2'	6:A:172:A:C8	2.51	0.45
6:A:424:G:H2'	6:A:425:G:H8	1.80	0.45
6:A:845:A:H2'	6:A:846:G:O4'	2.17	0.45
11:F:90:MET:HE3	11:F:90:MET:HB2	1.87	0.45
15:J:12:ALA:CB	15:J:18:ILE:HD13	2.46	0.45
23:R:29:LEU:O	23:R:33:ILE:HG23	2.16	0.45
28:a:596:A:H2'	28:a:597:G:C8	2.50	0.45
6:A:593:U:H3	6:A:646:G:H1	1.65	0.45
6:A:966:2MG:C6	27:X:62:HIS:ND1	2.85	0.45
15:J:25:ILE:HD11	15:J:90:LEU:HD12	1.99	0.45
28:a:303:U:H2'	28:a:304:C:C6	2.52	0.45
28:a:573:U:H2'	28:a:574:G:C8	2.51	0.45
28:a:1444:C:H2'	28:a:1445:G:C8	2.48	0.45
36:i:39:LYS:HE2	36:i:39:LYS:HB3	1.79	0.45
45:r:83:LYS:HD3	45:r:95:ARG:NH1	2.32	0.45
6:A:182:A:C4	6:A:184:G:C8	3.05	0.45
6:A:860:A:H2'	6:A:861:G:O4'	2.16	0.45
6:A:1121:U:H2'	6:A:1122:U:C6	2.52	0.45
6:A:1355:G:H2'	6:A:1356:G:C8	2.51	0.45
28:a:2870:G:H2'	28:a:2871:C:C6	2.52	0.45
32:e:105:LEU:HD23	32:e:200:LEU:HD11	1.98	0.45
34:g:6:LYS:HE3	34:g:62:TRP:CH2	2.51	0.45
35:h:3:VAL:CG2	35:h:36:ALA:HB1	2.47	0.45
35:h:70:GLU:HG3	35:h:140:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:1:MET:HG3	37:j:67:LYS:HG2	1.98	0.45
43:p:49:ASP:HA	43:p:52:GLN:HB2	1.99	0.45
48:u:21:ARG:HE	48:u:87:THR:HG23	1.81	0.45
6:A:695:A:H2'	6:A:696:A:C8	2.52	0.45
6:A:911:U:H2'	6:A:912:C:C6	2.52	0.45
6:A:948:C:H2'	6:A:949:A:C8	2.47	0.45
6:A:1106:G:H5"	8:C:172:ARG:HG2	1.99	0.45
6:A:1273:C:H2'	6:A:1274:A:O4'	2.17	0.45
6:A:1312:G:H5'	24:S:5:LEU:HD11	1.98	0.45
8:C:80:LYS:HA	8:C:80:LYS:HD2	1.59	0.45
8:C:133:ALA:O	8:C:136:ARG:HG2	2.17	0.45
10:E:126:LYS:HD2	10:E:126:LYS:HA	1.75	0.45
28:a:150:C:H2'	28:a:151:G:C8	2.49	0.45
28:a:641:A:C2	28:a:2370:A:H1'	2.51	0.45
28:a:927:G:H1'	52:y:25:LEU:HD11	1.99	0.45
28:a:1178:U:H2'	28:a:1179:G:C8	2.51	0.45
28:a:1221:U:H2'	28:a:1222:G:C8	2.51	0.45
28:a:1545:A:H2'	28:a:1546:G:O4'	2.17	0.45
28:a:2757:U:H1'	28:a:2758:A:H5"	1.98	0.45
45:r:2:GLU:N	45:r:2:GLU:OE2	2.50	0.45
6:A:839:C:H2'	6:A:840:C:C6	2.52	0.45
6:A:1062:U:H2'	6:A:1063:C:C6	2.52	0.45
6:A:1118:U:H1'	6:A:1179:A:C5	2.52	0.45
6:A:1129:C:H5'	14:I:18:ARG:HH12	1.82	0.45
6:A:1354:U:H2'	6:A:1355:G:C8	2.52	0.45
7:B:111:ILE:HD11	7:B:148:LEU:HB3	1.99	0.45
13:H:22:LYS:O	13:H:63:LEU:HD12	2.17	0.45
16:K:107:ILE:HG21	16:K:110:ILE:HD11	1.99	0.45
20:O:74:ASP:OD1	20:O:77:ARG:HB2	2.17	0.45
28:a:1088:G:H2'	28:a:1089:C:C6	2.52	0.45
33:f:80:ARG:HA	33:f:80:ARG:HD2	1.74	0.45
33:f:103:LEU:O	33:f:108:VAL:HG23	2.16	0.45
36:i:31:GLU:O	36:i:35:ARG:HG3	2.17	0.45
50:w:49:LEU:HB3	50:w:51:VAL:HG13	1.98	0.45
6:A:390:U:H2'	6:A:391:G:C8	2.51	0.44
6:A:857:C:H2'	6:A:858:G:O4'	2.17	0.44
6:A:1143:G:H2'	6:A:1144:G:C8	2.52	0.44
6:A:1527:U:H2'	6:A:1528:U:C6	2.52	0.44
11:F:81:ASN:OD1	11:F:84:VAL:HG12	2.17	0.44
24:S:17:LYS:O	24:S:21:LYS:HG2	2.16	0.44
28:a:304:C:H2'	28:a:305:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:566:U:H5”	28:a:818:A:N1	2.32	0.44
28:a:779:A:N7	30:c:220:VAL:HG21	2.32	0.44
28:a:1826:U:OP2	30:c:221:ARG:HD2	2.17	0.44
28:a:1925:C:H2’	28:a:1926:C:H6	1.82	0.44
29:b:28:C:H2’	29:b:29:A:C8	2.52	0.44
31:d:157:LYS:HE3	31:d:157:LYS:HB2	1.77	0.44
33:f:22:TYR:HE2	33:f:29:PRO:HD3	1.82	0.44
35:h:42:LYS:HD2	35:h:42:LYS:HA	1.72	0.44
6:A:459:A:H2’	6:A:460:A:H8	1.81	0.44
6:A:592:G:H2’	6:A:593:U:C6	2.52	0.44
28:a:1025:A:N6	28:a:1122:G:H2’	2.32	0.44
28:a:1542:U:H2’	28:a:1543:G:O4’	2.17	0.44
28:a:1709:U:H2’	28:a:1710:G:C8	2.52	0.44
28:a:2184:A:H2’	28:a:2185:A:H8	1.81	0.44
28:a:2374:G:H2’	28:a:2375:C:C6	2.52	0.44
29:b:114:C:H2’	29:b:115:A:C8	2.52	0.44
46:s:69:ARG:HH11	46:s:72:GLN:H	1.64	0.44
52:y:27:LEU:HD23	52:y:27:LEU:HA	1.87	0.44
6:A:413:G:N2	6:A:428:G:H1’	2.32	0.44
6:A:1001:G:H2’	6:A:1002:A:H8	1.82	0.44
6:A:1356:G:H2’	6:A:1357:A:H8	1.81	0.44
6:A:1512:U:H2’	6:A:1513:A:H8	1.82	0.44
6:A:1530:G:H2’	6:A:1531:A:C8	2.53	0.44
27:X:6:THR:HB	27:X:40:VAL:HG12	2.00	0.44
28:a:591:U:H2’	28:a:592:C:C6	2.52	0.44
28:a:677:C:H2’	28:a:678:G:C8	2.52	0.44
28:a:895:C:H2’	28:a:896:A:C8	2.51	0.44
28:a:1516:G:C4	28:a:1517:G:C8	3.05	0.44
36:i:36:LEU:O	36:i:51:GLY:HA3	2.18	0.44
37:j:40:LYS:NZ	37:j:57:VAL:HG12	2.33	0.44
40:m:103:ARG:HD3	40:m:110:MET:SD	2.58	0.44
3:2:55:LEU:O	3:2:59:ILE:HG13	2.18	0.44
5:4:28:VAL:HG13	33:f:140:GLU:HG3	1.99	0.44
6:A:76:G:N3	6:A:76:G:H2’	2.32	0.44
6:A:1539:C:H1’	26:W:8:G:N2	2.32	0.44
16:K:72:GLU:O	16:K:75:LYS:HG2	2.18	0.44
19:N:93:VAL:HG11	19:N:96:LEU:HD22	2.00	0.44
27:X:19:PHE:CZ	27:X:23:LYS:HE3	2.52	0.44
28:a:169:U:H2’	28:a:170:U:C6	2.53	0.44
28:a:437:G:H2’	28:a:438:A:C8	2.52	0.44
28:a:1988:A:H2’	28:a:1989:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2688:U:H2'	28:a:2689:G:O4'	2.17	0.44
28:a:2813:G:H2'	28:a:2814:A:C8	2.52	0.44
29:b:30:C:H1'	29:b:57:A:H61	1.82	0.44
37:j:19:VAL:HG12	37:j:43:ILE:HA	1.99	0.44
44:q:28:ALA:HB3	44:q:31:GLU:OE1	2.16	0.44
6:A:678:U:H2'	6:A:679:C:H6	1.82	0.44
6:A:1376:U:H2'	6:A:1377:A:C8	2.52	0.44
7:B:111:ILE:HD13	7:B:111:ILE:HA	1.87	0.44
28:a:299:A:H2'	28:a:333:U:H1'	2.00	0.44
28:a:721:U:H2'	28:a:722:G:C8	2.52	0.44
28:a:1540:G:H2'	28:a:1541:C:C6	2.53	0.44
28:a:2431:A:H5"	28:a:2432:U:OP2	2.17	0.44
31:d:17:GLU:C	31:d:19:GLY:H	2.23	0.44
37:j:64:ARG:HB2	37:j:83:ALA:HB3	1.99	0.44
43:p:17:ILE:HG13	43:p:32:TYR:HE1	1.82	0.44
6:A:73:C:O2'	6:A:74:A:H5'	2.18	0.44
6:A:428:G:H5"	6:A:430:A:H1'	2.00	0.44
6:A:755:G:OP2	20:O:65:LYS:HD3	2.17	0.44
6:A:950:U:H2'	6:A:951:G:C8	2.52	0.44
9:D:60:LYS:O	9:D:64:ILE:HG13	2.18	0.44
11:F:11:HIS:ND1	11:F:12:PRO:HD2	2.33	0.44
13:H:7:ILE:O	13:H:11:LEU:HG	2.18	0.44
16:K:76:GLU:HG2	16:K:77:TYR:CD1	2.52	0.44
16:K:77:TYR:CD1	16:K:77:TYR:N	2.85	0.44
17:L:79:VAL:HG22	17:L:103:ASP:OD2	2.17	0.44
25:T:61:GLN:OE1	25:T:61:GLN:HA	2.18	0.44
27:X:61:LEU:HD13	27:X:85:LEU:HD22	1.98	0.44
28:a:708:G:H2'	28:a:709:G:H8	1.82	0.44
28:a:753:A:H2'	28:a:754:G:O4'	2.17	0.44
28:a:2065:C:H2'	28:a:2066:C:H6	1.79	0.44
28:a:2440:A:H61	28:a:2586:U:H5'	1.83	0.44
34:g:44:LYS:HA	34:g:44:LYS:HD3	1.81	0.44
47:t:96:PHE:CZ	47:t:103:ILE:HG23	2.52	0.44
6:A:21:G:H2'	6:A:22:G:H8	1.78	0.44
6:A:415:A:C4	6:A:416:G:C8	3.06	0.44
6:A:678:U:H2'	6:A:679:C:C6	2.52	0.44
6:A:989:U:H1'	6:A:1016:A:H2	1.82	0.44
6:A:1465:A:H2'	6:A:1466:C:H6	1.82	0.44
8:C:110:GLU:HB2	8:C:144:LEU:HD12	2.00	0.44
17:L:111:LYS:HA	17:L:114:ARG:HD3	2.00	0.44
28:a:1143:C:C2	28:a:1144:A:C8	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1278:G:H2'	28:a:1279:U:C6	2.53	0.44
28:a:2470:A:H2'	28:a:2471:G:O4'	2.17	0.44
28:a:2662:G:H8	28:a:2662:G:OP2	2.01	0.44
29:b:15:A:H3'	29:b:16:G:H8	1.83	0.44
37:j:23:LYS:HA	37:j:23:LYS:HD3	1.77	0.44
4:3:10:LEU:HD13	4:3:33:HIS:CD2	2.52	0.44
6:A:737:C:H2'	6:A:738:C:H6	1.83	0.44
6:A:950:U:OP2	18:M:101:ARG:HD2	2.18	0.44
6:A:1317:C:H42	19:N:53:ARG:NH1	2.16	0.44
12:G:107:ALA:O	12:G:111:ARG:HG3	2.18	0.44
18:M:23:TYR:CE2	18:M:70:ARG:HG2	2.53	0.44
18:M:80:LEU:HD12	18:M:87:ARG:HG2	2.00	0.44
28:a:183:C:H2'	28:a:184:G:H8	1.82	0.44
28:a:637:C:H2'	28:a:638:U:C6	2.53	0.44
28:a:1183:G:H8	28:a:1183:G:O5'	2.01	0.44
28:a:1314:G:H2'	28:a:1315:U:C6	2.52	0.44
28:a:2170:A:H3'	28:a:2171:A:C8	2.53	0.44
28:a:2642:G:H5"	36:i:78:THR:HB	1.99	0.44
28:a:2813:G:H2'	28:a:2814:A:H8	1.82	0.44
29:b:103:U:O2'	29:b:104:A:H8	2.01	0.44
31:d:2:ILE:HG21	31:d:90:PHE:HE2	1.82	0.44
6:A:954:G:H2'	6:A:955:U:H6	1.83	0.44
7:B:117:LEU:HD23	7:B:141:LEU:HG	1.99	0.44
7:B:162:PHE:HA	7:B:184:PHE:O	2.18	0.44
10:E:66:LYS:HA	10:E:69:ARG:NE	2.20	0.44
10:E:81:LEU:HD23	10:E:147:MET:HE1	2.00	0.44
14:I:112:GLU:HG2	14:I:121:ALA:HB1	1.99	0.44
19:N:47:LYS:HA	19:N:50:SER:OG	2.18	0.44
27:X:69:ASP:C	27:X:69:ASP:OD1	2.60	0.44
28:a:322:C:H6	28:a:1202:A:C2	2.35	0.44
28:a:1680:U:H2'	28:a:1681:G:O4'	2.18	0.44
28:a:2165:C:H2'	28:a:2168:U:P	2.57	0.44
29:b:70:C:H2'	29:b:71:C:H6	1.83	0.44
30:c:16:VAL:HG22	30:c:206:GLY:HA3	2.00	0.44
33:f:107:ALA:HB1	33:f:137:ILE:HD12	2.00	0.44
34:g:86:LYS:HG2	34:g:132:VAL:HG22	1.99	0.44
45:r:25:ARG:HG3	45:r:74:ILE:HG22	1.99	0.44
1:0:32:GLU:CD	1:0:32:GLU:N	2.76	0.43
6:A:424:G:H2'	6:A:425:G:C8	2.53	0.43
6:A:439:U:H5"	9:D:121:LYS:HD2	2.00	0.43
6:A:1128:C:H2'	6:A:1129:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1330:U:H2'	6:A:1331:G:O4'	2.18	0.43
6:A:1500:A:H5"	6:A:1508:A:H5"	2.00	0.43
13:H:10:MET:HE2	13:H:14:ILE:HD11	1.99	0.43
21:P:4:ILE:HB	21:P:67:VAL:HG12	1.99	0.43
28:a:810:U:H2'	28:a:811:C:H6	1.83	0.43
28:a:1059:G:C6	28:a:1074:A:N1	2.86	0.43
28:a:1358:G:H2'	28:a:1359:C:C6	2.53	0.43
28:a:1550:U:H2'	28:a:1551:A:H8	1.83	0.43
28:a:1807:A:H3'	28:a:1808:A:C8	2.53	0.43
34:g:117:LEU:HA	34:g:117:LEU:HD12	1.72	0.43
35:h:8:LYS:HE2	35:h:14:SER:HB2	1.99	0.43
35:h:117:LEU:HD22	35:h:121:VAL:HA	1.99	0.43
39:l:53:MET:HE1	39:l:103:TYR:CD1	2.53	0.43
44:q:85:LYS:HB2	44:q:85:LYS:HE3	1.68	0.43
7:B:131:LYS:HB3	7:B:131:LYS:HE3	1.68	0.43
28:a:175:A:O2'	28:a:176:G:H5'	2.18	0.43
28:a:1033:G:C6	28:a:1117:G:C6	3.06	0.43
28:a:1158:C:H2'	28:a:1159:G:H8	1.83	0.43
28:a:1384:A:H5'	28:a:1466:A:H1'	1.99	0.43
28:a:2095:A:H4'	35:h:25:TYR:CE2	2.53	0.43
28:a:2182:U:H2'	28:a:2183:U:O4'	2.18	0.43
29:b:28:C:OP1	41:n:31:THR:HG21	2.19	0.43
30:c:125:LYS:HB3	30:c:128:ASN:OD1	2.18	0.43
33:f:33:LYS:HG2	33:f:157:THR:HB	2.00	0.43
33:f:122:PHE:O	33:f:123:ASP:C	2.61	0.43
38:k:77:ILE:HD11	38:k:101:ILE:CG2	2.47	0.43
46:s:24:MET:HE1	46:s:30:ILE:HG22	2.00	0.43
1:0:14:SER:HB2	1:0:50:LYS:HZ3	1.83	0.43
6:A:155:A:H2'	6:A:156:C:H6	1.84	0.43
6:A:513:C:H2'	6:A:514:C:C6	2.54	0.43
7:B:114:LEU:HB2	7:B:144:LEU:HB3	2.01	0.43
12:G:63:GLU:O	12:G:67:ASP:OD1	2.36	0.43
16:K:20:VAL:HA	16:K:83:GLU:O	2.19	0.43
17:L:108:LYS:HA	17:L:108:LYS:HD3	1.65	0.43
18:M:69:LEU:HD12	18:M:69:LEU:HA	1.88	0.43
18:M:86:TYR:OH	18:M:90:ARG:HD2	2.19	0.43
21:P:42:LEU:O	21:P:42:LEU:HD12	2.18	0.43
28:a:1292:C:C2	28:a:1293:G:C8	3.05	0.43
28:a:2071:A:H2'	28:a:2072:A:O4'	2.18	0.43
28:a:2347:A:H3'	28:a:2348:C:H5"	2.00	0.43
28:a:2378:A:H2'	28:a:2379:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:144:ASP:HB2	33:f:145:LYS:HD2	1.99	0.43
35:h:29:PHE:HE1	35:h:33:GLN:HE21	1.66	0.43
5:4:10:GLU:HG2	5:4:11:MET:N	2.34	0.43
6:A:212:G:C4	6:A:213:G:C8	3.05	0.43
6:A:376:G:H5"	21:P:5:ARG:HD2	2.00	0.43
6:A:992:U:H4'	6:A:993:G:H5"	2.00	0.43
6:A:1037:C:H2'	6:A:1038:U:C6	2.54	0.43
12:G:76:LYS:HG3	12:G:156:TRP:CZ3	2.53	0.43
13:H:108:LYS:HA	13:H:108:LYS:HD2	1.70	0.43
25:T:31:PHE:O	25:T:35:VAL:HG23	2.17	0.43
28:a:540:A:H2'	28:a:541:C:C6	2.53	0.43
28:a:2367:A:H2'	28:a:2368:G:O4'	2.18	0.43
28:a:2655:A:N1	28:a:2666:A:H5"	2.33	0.43
28:a:2897:C:H2'	28:a:2898:U:C6	2.54	0.43
33:f:141:ILE:HD13	33:f:141:ILE:HA	1.80	0.43
37:j:35:VAL:HG11	37:j:104:THR:OG1	2.18	0.43
40:m:75:ILE:HD13	40:m:75:ILE:HA	1.82	0.43
41:n:35:ILE:HG22	41:n:53:THR:HG23	1.99	0.43
6:A:684:U:H2'	6:A:685:G:O4'	2.18	0.43
6:A:868:C:H2'	6:A:869:G:O4'	2.19	0.43
6:A:1165:U:H2'	6:A:1166:G:O4'	2.19	0.43
6:A:1326:U:H2'	6:A:1327:C:C6	2.50	0.43
7:B:11:LYS:HA	7:B:11:LYS:HD3	1.81	0.43
8:C:136:ARG:HA	8:C:139:GLN:HG2	2.01	0.43
9:D:91:LEU:HD23	9:D:91:LEU:HA	1.89	0.43
25:T:39:ILE:HD11	25:T:79:LEU:HD22	1.99	0.43
28:a:1710:G:H2'	28:a:1711:A:C8	2.54	0.43
28:a:1746:U:H2'	28:a:1747:C:C6	2.53	0.43
28:a:2132:U:OP1	28:a:2134:G:H5'	2.19	0.43
28:a:2162:C:H1'	28:a:2166:C:H5	1.84	0.43
28:a:2901:A:H2'	28:a:2902:C:C6	2.54	0.43
29:b:8:C:O2'	41:n:40:ILE:HD13	2.18	0.43
29:b:66:A:N6	29:b:107:G:H2'	2.34	0.43
32:e:49:ARG:O	32:e:74:LYS:HE2	2.19	0.43
35:h:51:ARG:HD2	35:h:55:GLU:OE1	2.18	0.43
39:l:42:THR:HG22	39:l:93:VAL:HG12	1.99	0.43
39:l:105:MET:HE1	39:l:113:ALA:HA	2.01	0.43
40:m:22:ARG:HE	40:m:22:ARG:HB2	1.53	0.43
1:0:44:ARG:NH1	28:a:640:A:H1'	2.34	0.43
6:A:26:A:H61	6:A:558:G:H1'	1.84	0.43
6:A:500:G:H2'	6:A:501:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1465:A:H2'	6:A:1466:C:C6	2.53	0.43
8:C:7:PRO:HG2	8:C:201:TRP:HE1	1.83	0.43
13:H:111:MET:HB2	13:H:115:ALA:HB3	2.01	0.43
18:M:23:TYR:HE2	18:M:70:ARG:HG2	1.84	0.43
28:a:642:C:H2'	28:a:644:G:N7	2.33	0.43
28:a:1041:A:H1'	28:a:1045:A:H1'	2.00	0.43
28:a:1056:G:C8	28:a:1057:U:H2'	2.54	0.43
28:a:1187:G:H5"	38:k:32:GLY:HA2	2.00	0.43
32:e:52:VAL:O	32:e:74:LYS:HE3	2.19	0.43
36:i:43:GLU:OE1	36:i:43:GLU:N	2.52	0.43
6:A:661:G:H2'	6:A:662:U:C6	2.53	0.43
6:A:744:C:H2'	6:A:745:A:C8	2.54	0.43
6:A:1263:C:H2'	6:A:1264:U:H6	1.84	0.43
7:B:87:CYS:HB3	7:B:218:ALA:HB1	2.01	0.43
13:H:39:VAL:HA	13:H:42:GLU:OE2	2.18	0.43
15:J:52:LEU:HB2	19:N:81:ARG:HD2	1.99	0.43
28:a:355:G:H2'	28:a:355:G:N3	2.34	0.43
28:a:358:G:H2'	28:a:359:U:C6	2.53	0.43
28:a:2100:U:H2'	28:a:2101:G:H8	1.83	0.43
28:a:2558:G:H2'	28:a:2559:C:C6	2.53	0.43
33:f:4:LEU:HD23	33:f:4:LEU:HA	1.81	0.43
6:A:418:C:H2'	6:A:419:C:C6	2.54	0.43
6:A:662:U:H2'	6:A:663:A:C8	2.54	0.43
6:A:1127:G:H5'	6:A:1280:A:O2'	2.18	0.43
6:A:1317:C:N3	19:N:53:ARG:HD2	2.34	0.43
24:S:66:MET:HB2	24:S:74:PHE:CZ	2.54	0.43
28:a:171:A:H2'	28:a:172:A:H8	1.83	0.43
28:a:414:A:H2'	28:a:415:U:C6	2.54	0.43
28:a:595:U:H2'	28:a:596:A:C8	2.54	0.43
28:a:1212:G:H1	28:a:1231:U:H3	1.66	0.43
33:f:128:TYR:CE2	33:f:130:MET:HB3	2.52	0.43
47:t:6:ARG:HE	47:t:6:ARG:HB3	1.70	0.43
6:A:728:A:H2'	6:A:729:A:H8	1.82	0.43
6:A:1317:C:H4'	19:N:48:LEU:HD12	2.01	0.43
6:A:1422:G:H1	6:A:1478:U:H3	1.66	0.43
12:G:14:PRO:HG3	12:G:21:GLU:HG3	2.01	0.43
20:O:75:VAL:O	20:O:79:THR:HG22	2.19	0.43
28:a:1279:U:H2'	28:a:1280:G:O4'	2.18	0.43
28:a:1410:A:H2'	28:a:1411:C:H6	1.84	0.43
28:a:2593:G:H2'	28:a:2594:U:O4'	2.18	0.43
29:b:97:U:H2'	29:b:98:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:5:LYS:HE3	30:c:5:LYS:HB3	1.79	0.43
45:r:73:LYS:HE2	45:r:73:LYS:HB3	1.67	0.43
6:A:842:U:O2	6:A:845:A:C6	2.72	0.43
6:A:1001:G:H2'	6:A:1002:A:C8	2.52	0.43
6:A:1158:C:C4	6:A:1160:G:C8	3.07	0.43
12:G:129:GLU:O	12:G:131:LYS:HG3	2.18	0.43
14:I:23:PRO:HA	14:I:61:LEU:HD13	2.01	0.43
28:a:301:G:H2'	28:a:302:G:H8	1.84	0.43
28:a:352:C:H2'	28:a:353:A:C8	2.54	0.43
28:a:557:C:H2'	28:a:558:G:O4'	2.18	0.43
28:a:1074:A:C2	28:a:1085:A:C5	3.06	0.43
28:a:1200:U:H1'	38:k:4:ASN:OD1	2.19	0.43
28:a:1841:G:H2'	28:a:1842:C:C6	2.54	0.43
28:a:2120:A:H2	28:a:2170:A:N3	2.16	0.43
28:a:2598:G:H5"	30:c:241:GLY:HA3	2.01	0.43
30:c:21:ASN:HB3	30:c:24:LEU:HG	2.01	0.43
31:d:121:THR:HB	31:d:127:PHE:CD2	2.54	0.43
34:g:24:ILE:HG21	34:g:72:LEU:HD21	2.01	0.43
37:j:43:ILE:HD11	37:j:58:LEU:HD12	2.01	0.43
42:o:75:GLN:HB2	42:o:78:SER:HB2	2.01	0.43
6:A:214:C:H2'	6:A:215:C:H6	1.84	0.42
6:A:1328:C:OP1	18:M:28:THR:HG21	2.18	0.42
6:A:1536:C:C4	6:A:1537:U:C4	3.07	0.42
8:C:7:PRO:HD2	8:C:184:TYR:CD2	2.54	0.42
12:G:66:LEU:HD23	12:G:66:LEU:HA	1.85	0.42
12:G:72:THR:HA	12:G:96:ARG:HE	1.84	0.42
17:L:25:GLU:CD	17:L:59:ASN:HD22	2.27	0.42
28:a:30:G:H2'	28:a:31:C:C6	2.53	0.42
28:a:467:G:H5"	32:e:55:SER:HB3	2.00	0.42
28:a:1090:G:H2'	28:a:1091:U:C6	2.54	0.42
28:a:1614:A:N1	45:r:93:ALA:HB2	2.33	0.42
28:a:2052:A:H8	28:a:2052:A:OP2	2.02	0.42
28:a:2244:U:H2'	28:a:2245:U:H6	1.83	0.42
28:a:2470:A:C6	28:a:2483:A:C8	3.06	0.42
29:b:48:U:H4'	41:n:100:HIS:HD2	1.84	0.42
34:g:128:GLN:HG3	34:g:129:THR:HG23	2.01	0.42
48:u:7:GLU:HG3	48:u:41:GLU:HG2	2.01	0.42
49:v:11:ARG:N	49:v:11:ARG:HD2	2.33	0.42
6:A:255:G:H2'	6:A:256:U:C6	2.54	0.42
6:A:270:A:H2'	6:A:271:C:H6	1.82	0.42
6:A:517:G:H5'	6:A:519:C:C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:533:A:O2'	6:A:534:U:H5'	2.19	0.42
18:M:59:GLU:HA	18:M:59:GLU:OE2	2.19	0.42
20:O:6:GLU:CD	20:O:6:GLU:H	2.26	0.42
28:a:240:A:N1	28:a:254:A:H5"	2.34	0.42
28:a:1047:A:C2	28:a:1048:G:H1'	2.53	0.42
28:a:1100:A:H2'	28:a:1100:A:N3	2.34	0.42
39:l:33:LEU:HD12	39:l:33:LEU:HA	1.91	0.42
6:A:1162:C:H2'	6:A:1163:A:H8	1.83	0.42
6:A:1326:U:C2	6:A:1327:C:C5	3.06	0.42
6:A:1402:4OC:H2'	6:A:1403:C:O4'	2.18	0.42
6:A:1507:A:H2'	6:A:1508:A:C8	2.54	0.42
11:F:74:LEU:HG	11:F:78:PHE:HE1	1.85	0.42
12:G:27:VAL:HG22	12:G:43:VAL:HG21	2.00	0.42
28:a:1594:C:H2'	28:a:1595:G:O4'	2.19	0.42
28:a:2616:U:C2	53:z:4:GLN:HA	2.54	0.42
28:a:2638:U:H2'	28:a:2639:G:O4'	2.19	0.42
35:h:93:SER:HB3	35:h:123:ARG:NE	2.35	0.42
44:q:74:ILE:HB	44:q:87:GLN:HB3	2.00	0.42
45:r:88:ARG:HG3	45:r:94:ASP:OD2	2.20	0.42
47:t:33:LYS:HG2	47:t:66:GLN:HA	2.00	0.42
4:3:18:LYS:NZ	4:3:21:GLY:HA2	2.34	0.42
6:A:1004:A:H2'	6:A:1005:A:C8	2.54	0.42
6:A:1072:G:H2'	6:A:1073:U:H6	1.83	0.42
6:A:1327:C:H2'	6:A:1328:C:H6	1.83	0.42
7:B:22:TYR:O	7:B:190:ASN:HB3	2.19	0.42
8:C:111:LEU:HD23	8:C:111:LEU:HA	1.81	0.42
14:I:129:LYS:HA	27:X:55:HIS:CE1	2.55	0.42
16:K:42:LEU:HB3	16:K:77:TYR:CE2	2.55	0.42
28:a:30:G:H2'	28:a:31:C:H6	1.84	0.42
28:a:364:U:H2'	28:a:365:C:C6	2.54	0.42
28:a:620:C:H2'	28:a:621:C:C6	2.54	0.42
28:a:924:A:H2'	28:a:925:A:C8	2.54	0.42
28:a:933:A:H2'	28:a:934:C:C6	2.54	0.42
28:a:1074:A:H2'	28:a:1075:U:O4'	2.19	0.42
28:a:1175:C:H2'	28:a:1176:G:C8	2.55	0.42
28:a:1431:A:H2'	28:a:1432:G:H8	1.84	0.42
28:a:1473:U:H2'	28:a:1474:A:H8	1.85	0.42
28:a:1505:A:H2'	28:a:1505:A:N3	2.35	0.42
28:a:2103:U:H2'	28:a:2104:C:H6	1.82	0.42
28:a:2230:U:H2'	28:a:2231:G:H8	1.83	0.42
29:b:31:C:C2	29:b:32:U:C5	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:218:PRO:O	30:c:218:PRO:CD	2.66	0.42
31:d:180:VAL:HG22	31:d:187:LEU:HD12	2.01	0.42
45:r:72:ALA:HB2	45:r:108:SER:HB3	2.02	0.42
52:y:51:VAL:HG12	52:y:51:VAL:O	2.19	0.42
2:1:30:VAL:HG22	2:1:33:ARG:NH2	2.35	0.42
6:A:33:A:H2'	6:A:34:C:H6	1.83	0.42
6:A:343:U:O2'	6:A:344:A:H2'	2.19	0.42
6:A:398:U:H2'	6:A:399:G:C8	2.54	0.42
6:A:451:A:H61	6:A:481:G:H5'	1.84	0.42
6:A:908:A:H2'	6:A:909:A:C8	2.54	0.42
7:B:168:HIS:HB3	7:B:169:GLU:OE2	2.19	0.42
8:C:16:LYS:HA	8:C:16:LYS:HD2	1.80	0.42
8:C:156:ARG:HE	8:C:156:ARG:HB3	1.59	0.42
15:J:50:THR:HG23	15:J:64:GLN:HG2	2.02	0.42
23:R:13:PHE:CE2	23:R:21:ILE:HG13	2.54	0.42
28:a:6:A:H2'	28:a:7:G:H8	1.84	0.42
28:a:227:C:H4'	28:a:228:C:H5"	2.01	0.42
28:a:2230:U:O2	50:w:34:HIS:HE1	2.01	0.42
28:a:2650:C:H2'	28:a:2651:U:C6	2.55	0.42
29:b:5:U:H2'	29:b:6:G:C8	2.54	0.42
42:o:87:LYS:HB3	42:o:87:LYS:HE3	1.82	0.42
9:D:9:LEU:HD13	9:D:32:CYS:HB3	2.02	0.42
9:D:94:LEU:HD12	9:D:94:LEU:HA	1.88	0.42
10:E:153:VAL:HA	10:E:156:LYS:HG2	2.01	0.42
11:F:93:LYS:HA	11:F:93:LYS:HD3	1.91	0.42
13:H:94:LYS:HE2	13:H:94:LYS:HB2	1.81	0.42
17:L:66:TYR:CD2	17:L:66:TYR:C	2.98	0.42
17:L:87:VAL:HG23	17:L:90:LEU:HB2	2.02	0.42
18:M:96:PRO:HB2	18:M:100:GLN:HB2	2.00	0.42
21:P:76:LYS:HD2	21:P:76:LYS:HA	1.73	0.42
28:a:276:G:OP2	28:a:276:G:H8	2.02	0.42
28:a:740:A:OP1	31:d:135:GLY:HA2	2.20	0.42
28:a:1672:A:C2	28:a:2583:G:H5'	2.55	0.42
28:a:2310:A:H2'	28:a:2311:C:C6	2.54	0.42
41:n:40:ILE:HG12	41:n:47:VAL:HG22	2.00	0.42
41:n:76:LYS:HB2	41:n:76:LYS:HE2	1.84	0.42
43:p:109:LEU:HD23	44:q:49:ILE:HD11	2.02	0.42
6:A:157:U:H1'	6:A:165:G:N2	2.34	0.42
6:A:193:C:H2'	6:A:194:C:H6	1.85	0.42
6:A:579:A:H2'	6:A:580:C:C6	2.55	0.42
6:A:1120:C:H2'	6:A:1121:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1446:A:H8	6:A:1446:A:OP1	2.02	0.42
9:D:124:MET:HE3	9:D:146:ARG:HG2	2.00	0.42
12:G:49:THR:HG22	12:G:53:ARG:HD3	2.02	0.42
20:O:22:SER:HA	20:O:27:VAL:HG11	2.01	0.42
28:a:726:G:O2'	28:a:760:G:H4'	2.20	0.42
28:a:1070:A:C6	28:a:1071:G:C5	3.07	0.42
28:a:1294:C:OP1	28:a:2711:C:H4'	2.20	0.42
28:a:2187:G:H2'	28:a:2188:G:C8	2.55	0.42
33:f:37:ASN:OD1	33:f:37:ASN:C	2.62	0.42
34:g:85:LYS:HE2	34:g:85:LYS:HB2	1.90	0.42
34:g:94:TYR:CD2	34:g:107:LEU:HD23	2.54	0.42
50:w:22:LEU:HD13	50:w:22:LEU:HA	1.86	0.42
51:x:14:LEU:HD23	51:x:14:LEU:HA	1.93	0.42
2:1:3:ARG:HD3	2:1:3:ARG:HA	1.80	0.42
6:A:45:G:H2'	6:A:46:G:C8	2.54	0.42
6:A:119:A:H4'	6:A:120:A:C4	2.55	0.42
6:A:193:C:H2'	6:A:194:C:C6	2.55	0.42
6:A:294:U:H2'	6:A:295:C:C6	2.55	0.42
6:A:859:G:H2'	6:A:860:A:C8	2.55	0.42
11:F:4:TYR:CD2	11:F:71:ILE:HG13	2.55	0.42
11:F:38:ARG:HB3	11:F:63:ASN:HB2	2.02	0.42
14:I:4:ASN:HB3	14:I:6:TYR:HE1	1.85	0.42
18:M:48:LEU:HD23	18:M:48:LEU:HA	1.86	0.42
28:a:4:U:H2'	28:a:5:A:H8	1.84	0.42
28:a:412:C:H2'	28:a:413:C:C6	2.55	0.42
28:a:605:A:H2'	28:a:606:A:H8	1.84	0.42
28:a:781:G:O2'	28:a:782:G:H5"	2.20	0.42
28:a:1066:A:C4	28:a:1070:A:N7	2.88	0.42
30:c:181:MET:HE2	30:c:181:MET:HB2	1.87	0.42
30:c:270:ARG:HG2	30:c:271:ARG:H	1.85	0.42
35:h:8:LYS:O	35:h:9:VAL:HG12	2.19	0.42
35:h:122:LEU:HD22	35:h:146:VAL:HG21	2.01	0.42
51:x:49:ASN:O	51:x:53:VAL:HG23	2.20	0.42
5:4:44:TYR:HE1	33:f:114:PHE:HE2	1.68	0.42
6:A:358:U:C2	6:A:359:G:C8	3.08	0.42
6:A:704:A:C4	6:A:705:G:C8	3.08	0.42
6:A:1227:A:H5"	24:S:83:HIS:CE1	2.54	0.42
6:A:1342:C:H2'	6:A:1343:G:C8	2.55	0.42
11:F:11:HIS:HD2	11:F:14:GLN:OE1	2.02	0.42
11:F:72:ASP:HA	11:F:75:GLU:OE2	2.19	0.42
15:J:40:ILE:HD12	15:J:73:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:378:G:N1	28:a:395:G:C6	2.88	0.42
28:a:396:U:H5”	50:w:32:ASN:HB2	2.02	0.42
28:a:608:C:H2’	28:a:609:G:O4’	2.20	0.42
28:a:1216:U:H2’	28:a:1217:G:H8	1.84	0.42
28:a:2380:G:H2’	28:a:2381:C:C6	2.54	0.42
34:g:176:LYS:HG2	34:g:177:LYS:H	1.85	0.42
36:i:109:LEU:HD23	36:i:109:LEU:HA	1.85	0.42
42:o:53:ARG:HA	42:o:53:ARG:HD3	1.82	0.42
48:u:4:ILE:HD11	48:u:56:PHE:HE1	1.85	0.42
48:u:4:ILE:O	48:u:63:ILE:HA	2.20	0.42
6:A:223:A:H2’	6:A:224:U:C6	2.55	0.42
6:A:513:C:H2’	6:A:514:C:H6	1.85	0.42
6:A:1014:A:C2	6:A:1219:A:H1’	2.55	0.42
6:A:1040:U:H2’	6:A:1041:G:H8	1.83	0.42
9:D:167:LYS:HB2	9:D:167:LYS:HE2	1.91	0.42
13:H:10:MET:HG3	13:H:27:MET:HE1	2.01	0.42
18:M:56:LEU:O	18:M:60:VAL:HG12	2.20	0.42
28:a:309:A:H5”	47:t:15:THR:HG23	2.01	0.42
28:a:1415:G:H21	28:a:1580:A:H2	1.68	0.42
28:a:1789:C:H2’	28:a:1790:A:C5	2.55	0.42
28:a:2108:G:C6	28:a:2109:A:C6	3.07	0.42
37:j:79:PHE:HB3	42:o:68:GLU:OE2	2.20	0.42
37:j:114:LYS:H	37:j:114:LYS:HG2	1.67	0.42
38:k:112:LEU:HD12	38:k:130:GLY:C	2.44	0.42
6:A:462:G:HO2’	6:A:463:U:H6	1.66	0.41
6:A:981:U:H5”	19:N:63:ARG:NH2	2.34	0.41
6:A:1035:A:O2’	6:A:1037:C:H5	2.02	0.41
6:A:1042:A:O2’	6:A:1043:G:H5’	2.20	0.41
7:B:115:LYS:O	7:B:119:THR:HG23	2.19	0.41
7:B:154:MET:HE3	7:B:154:MET:HB3	1.95	0.41
9:D:159:LEU:HD23	9:D:159:LEU:HA	1.95	0.41
16:K:87:LYS:HB2	16:K:113:VAL:HG13	2.00	0.41
18:M:81:MET:CE	18:M:91:HIS:HB3	2.46	0.41
28:a:58:G:H2’	28:a:59:U:C6	2.55	0.41
28:a:218:A:H2’	28:a:219:G:C8	2.55	0.41
28:a:949:G:C6	28:a:963:G:C6	3.08	0.41
28:a:1275:C:H2’	28:a:1276:G:H8	1.84	0.41
28:a:2283:G:H4’	28:a:2390:G:O2’	2.20	0.41
28:a:2397:G:C2	28:a:2398:G:C8	3.08	0.41
28:a:2753:C:H2’	28:a:2754:A:O4’	2.20	0.41
32:e:164:LEU:HB2	32:e:167:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:17:LYS:O	41:n:17:LYS:HD3	2.20	0.41
46:s:1:MET:HG2	46:s:2:ILE:H	1.84	0.41
5:4:7:PRO:HG3	33:f:58:THR:HG23	2.02	0.41
6:A:294:U:H2'	6:A:295:C:H6	1.85	0.41
6:A:553:A:H2'	6:A:554:A:H8	1.85	0.41
6:A:1039:C:H2'	6:A:1040:U:C6	2.55	0.41
7:B:20:THR:HG22	7:B:39:HIS:CE1	2.55	0.41
28:a:1312:C:H2'	28:a:1313:U:C6	2.55	0.41
28:a:1492:A:H2'	28:a:1493:A:C8	2.55	0.41
28:a:1679:A:H2'	28:a:1680:U:C6	2.55	0.41
28:a:1841:G:H2'	28:a:1842:C:H6	1.84	0.41
28:a:2098:A:H2'	28:a:2099:C:C6	2.55	0.41
28:a:2130:C:OP1	28:a:2176:C:H1'	2.19	0.41
28:a:2162:C:H5"	28:a:2163:G:C2	2.54	0.41
28:a:2369:C:H2'	28:a:2370:A:H8	1.85	0.41
28:a:2683:A:C8	31:d:11:MET:HE2	2.55	0.41
51:x:4:LYS:HZ2	51:x:7:ARG:HH12	1.66	0.41
6:A:19:A:H2'	6:A:20:U:C6	2.55	0.41
6:A:1004:A:C2	6:A:1026:G:C6	3.07	0.41
6:A:1522:U:H2'	6:A:1523:G:H8	1.85	0.41
7:B:89:GLN:HG3	7:B:90:PHE:N	2.31	0.41
8:C:184:TYR:HA	8:C:200:VAL:O	2.20	0.41
16:K:64:GLN:HG3	16:K:65:VAL:N	2.34	0.41
18:M:90:ARG:HD3	18:M:96:PRO:O	2.20	0.41
28:a:83:G:N2	28:a:101:G:H1'	2.34	0.41
28:a:840:G:H2'	28:a:841:A:H8	1.85	0.41
28:a:845:C:H2'	28:a:846:A:C8	2.48	0.41
28:a:1196:U:H1'	43:p:4:VAL:HG22	2.03	0.41
28:a:2120:A:N6	28:a:2170:A:H5"	2.31	0.41
28:a:2252:OMG:HM23	28:a:2252:OMG:H1'	1.72	0.41
33:f:175:PHE:HB3	33:f:177:PHE:HE1	1.85	0.41
35:h:9:VAL:HG13	35:h:10:ALA:N	2.35	0.41
37:j:70:ARG:HE	37:j:70:ARG:HB3	1.61	0.41
38:k:136:GLU:OE1	38:k:136:GLU:HA	2.20	0.41
45:r:95:ARG:HG2	45:r:95:ARG:HH11	1.85	0.41
6:A:1125:U:C2	6:A:1127:G:C8	3.09	0.41
15:J:10:LEU:O	15:J:71:LYS:HA	2.21	0.41
22:Q:15:ASP:OD1	22:Q:55:ILE:HG12	2.21	0.41
27:X:23:LYS:HD3	27:X:26:LYS:CE	2.50	0.41
28:a:1283:A:H1'	28:a:1285:G:OP2	2.20	0.41
28:a:2127:A:H4'	28:a:2128:G:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2368:G:C2	28:a:2369:C:C5	3.08	0.41
30:c:34:LEU:HD23	30:c:34:LEU:HA	1.81	0.41
48:u:31:TYR:CE2	48:u:90:ASP:HB3	2.55	0.41
1:0:26:ASN:OD1	1:0:29:THR:HG23	2.20	0.41
28:a:279:U:H2'	28:a:280:C:C6	2.55	0.41
28:a:1097:C:H2'	28:a:1098:U:C6	2.55	0.41
28:a:1440:C:H2'	28:a:1441:A:H8	1.86	0.41
28:a:1728:C:H2'	28:a:1729:U:O4'	2.20	0.41
28:a:1772:A:N7	28:a:1828:A:H1'	2.36	0.41
28:a:2147:C:H5"	28:a:2148:A:C8	2.56	0.41
28:a:2699:U:H2'	28:a:2700:C:H6	1.84	0.41
28:a:2849:G:N7	42:o:95:ALA:HB2	2.36	0.41
33:f:8:TYR:HB2	33:f:173:PHE:CE1	2.56	0.41
38:k:21:ARG:HD3	38:k:21:ARG:HA	1.89	0.41
39:l:41:LEU:HG	39:l:96:ILE:HG13	2.02	0.41
40:m:32:GLU:HG3	40:m:115:LEU:HD12	2.03	0.41
6:A:735:C:H2'	6:A:736:C:H6	1.86	0.41
6:A:892:A:H2'	6:A:893:C:H6	1.85	0.41
6:A:1160:G:C6	6:A:1161:C:C4	3.09	0.41
11:F:53:LYS:HA	11:F:53:LYS:HD3	1.65	0.41
15:J:12:ALA:HB2	15:J:18:ILE:HD13	2.03	0.41
16:K:20:VAL:CG1	16:K:35:THR:HG23	2.51	0.41
28:a:593:U:H2'	28:a:594:G:H8	1.86	0.41
28:a:970:A:H5'	28:a:1185:U:H1'	2.02	0.41
28:a:976:A:H2'	28:a:979:C:H42	1.85	0.41
28:a:1357:G:N7	28:a:1358:G:C8	2.89	0.41
28:a:2074:C:H5'	30:c:228:VAL:HG21	2.02	0.41
28:a:2330:U:H2'	28:a:2331:G:H8	1.85	0.41
29:b:24:G:N7	29:b:56:G:C4	2.89	0.41
33:f:69:LYS:HB3	33:f:82:GLY:C	2.46	0.41
39:l:1:MET:HE1	39:l:44:ARG:NH1	2.34	0.41
39:l:53:MET:O	39:l:57:VAL:HG23	2.19	0.41
40:m:38:LEU:HB3	40:m:39:PRO:HD3	2.02	0.41
41:n:27:VAL:HG23	41:n:95:SER:OG	2.20	0.41
43:p:31:VAL:HG12	43:p:34:VAL:H	1.85	0.41
5:4:34:LEU:HD21	33:f:106:ILE:HG12	2.02	0.41
5:4:62:LYS:HB3	5:4:62:LYS:HE3	1.74	0.41
6:A:373:A:C2	6:A:482:A:C6	3.08	0.41
6:A:846:G:H2'	6:A:847:G:C8	2.55	0.41
6:A:1272:G:H2'	6:A:1273:C:C6	2.55	0.41
6:A:1327:C:C2	6:A:1328:C:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1340:A:H2'	6:A:1341:U:O4'	2.20	0.41
9:D:19:LEU:HB2	9:D:21:LEU:HG	2.02	0.41
16:K:64:GLN:HB2	16:K:99:ALA:HB2	2.03	0.41
19:N:48:LEU:HA	19:N:48:LEU:HD22	1.82	0.41
28:a:277:A:C6	28:a:361:A:C8	3.08	0.41
28:a:654:U:H2'	28:a:655:U:C6	2.56	0.41
28:a:1070:A:C6	28:a:1071:G:C6	3.09	0.41
28:a:1350:A:H2'	28:a:1351:A:H8	1.86	0.41
28:a:1462:G:H2'	28:a:1463:U:O4'	2.21	0.41
28:a:2127:A:C5	28:a:2165:C:H1'	2.55	0.41
28:a:2169:G:O3'	28:a:2171:A:H5"	2.20	0.41
28:a:2548:A:H2'	28:a:2549:U:H6	1.82	0.41
30:c:111:LYS:HB3	30:c:111:LYS:HE3	1.83	0.41
38:k:29:LYS:HB3	38:k:30:THR:H	1.67	0.41
47:t:86:ARG:O	47:t:92:LYS:HG3	2.20	0.41
6:A:2:A:H1'	6:A:613:C:O2'	2.21	0.41
6:A:263:A:H2'	6:A:264:C:C6	2.55	0.41
6:A:409:U:H2'	6:A:410:G:O4'	2.19	0.41
6:A:412:A:O2'	6:A:414:A:H5'	2.21	0.41
6:A:1096:C:H2'	6:A:1097:C:H6	1.86	0.41
6:A:1169:A:H2'	6:A:1170:A:H8	1.85	0.41
6:A:1320:C:H2'	6:A:1321:U:C6	2.56	0.41
10:E:66:LYS:HE3	10:E:66:LYS:HB3	1.91	0.41
11:F:2:ARG:HD3	11:F:91:ARG:NE	2.36	0.41
11:F:11:HIS:NE2	11:F:13:ASP:HB3	2.36	0.41
12:G:17:LYS:HB2	12:G:44:TYR:CZ	2.55	0.41
14:I:100:LYS:HD3	14:I:100:LYS:HA	1.70	0.41
18:M:7:ILE:HD11	18:M:22:ILE:HA	2.02	0.41
24:S:17:LYS:HG2	24:S:21:LYS:NZ	2.36	0.41
28:a:72:A:C8	51:x:54:LYS:HD3	2.55	0.41
28:a:145:A:H2'	28:a:146:C:C6	2.56	0.41
28:a:822:A:H2'	28:a:823:U:C6	2.56	0.41
28:a:1321:G:H1'	28:a:1616:A:N6	2.35	0.41
28:a:2066:C:H2'	28:a:2067:C:H6	1.85	0.41
29:b:28:C:H2'	29:b:29:A:H8	1.86	0.41
35:h:122:LEU:HD21	35:h:128:HIS:HB2	2.03	0.41
37:j:25:LEU:HD13	37:j:59:LYS:HE3	2.03	0.41
48:u:26:PHE:CE2	48:u:44:HIS:HA	2.56	0.41
51:x:46:VAL:O	51:x:50:VAL:HG23	2.21	0.41
3:2:35:LYS:HB2	3:2:35:LYS:HE2	1.74	0.41
6:A:26:A:N6	6:A:558:G:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:72:A:H2'	6:A:73:C:H6	1.86	0.41
6:A:477:G:H2'	6:A:478:A:C8	2.56	0.41
6:A:999:C:H2'	6:A:1000:A:C8	2.56	0.41
6:A:1333:A:H2'	6:A:1334:G:O4'	2.21	0.41
7:B:103:ASN:O	7:B:107:VAL:HG23	2.19	0.41
9:D:196:ASN:HB3	9:D:198:HIS:CD2	2.56	0.41
11:F:47:LEU:HD21	11:F:57:ALA:HB3	2.03	0.41
14:I:52:LEU:HA	14:I:55:VAL:HG22	2.03	0.41
15:J:57:VAL:HG23	15:J:58:ASN:N	2.36	0.41
17:L:89:D2T:H7	17:L:89:D2T:H4	1.91	0.41
22:Q:8:LEU:HD23	22:Q:25:ILE:HG12	2.03	0.41
25:T:79:LEU:HD23	25:T:79:LEU:HA	1.74	0.41
28:a:6:A:H2'	28:a:7:G:C8	2.56	0.41
28:a:154:A:H2'	28:a:155:A:C8	2.55	0.41
28:a:491:A:H2'	28:a:492:G:O4'	2.20	0.41
28:a:590:U:H2'	28:a:591:U:H6	1.86	0.41
28:a:888:G:C6	28:a:889:G:C5	3.08	0.41
28:a:1220:G:C6	28:a:1224:G:C6	3.09	0.41
28:a:1882:C:H2'	28:a:1883:U:O4'	2.20	0.41
28:a:2127:A:C2	28:a:2166:C:N4	2.89	0.41
28:a:2127:A:N6	28:a:2166:C:O2	2.45	0.41
28:a:2242:A:H2'	28:a:2243:G:C8	2.56	0.41
28:a:2340:C:H2'	28:a:2341:A:C8	2.55	0.41
28:a:2469:A:H2'	28:a:2477:A:C6	2.56	0.41
28:a:2490:U:H2'	28:a:2491:G:O4'	2.21	0.41
28:a:2530:G:H5"	28:a:2531:A:H5"	2.02	0.41
28:a:2839:G:C4	28:a:2840:G:C8	3.08	0.41
30:c:217:ARG:HB3	30:c:218:PRO:HD3	2.02	0.41
31:d:14:ILE:HD13	42:o:12:GLN:OE1	2.21	0.41
33:f:22:TYR:CE2	33:f:28:VAL:HA	2.56	0.41
34:g:137:ASP:O	34:g:141:ILE:HG22	2.21	0.41
42:o:9:GLU:O	42:o:13:MET:HG3	2.21	0.41
45:r:21:ALA:HB1	45:r:74:ILE:HG12	2.02	0.41
45:r:36:LEU:HD13	45:r:48:LYS:HA	2.03	0.41
49:v:41:ARG:HA	49:v:41:ARG:HD3	1.82	0.41
52:y:51:VAL:O	52:y:55:VAL:HG22	2.20	0.41
6:A:236:A:H2'	6:A:237:G:C8	2.56	0.41
6:A:633:G:H2'	6:A:634:C:C6	2.56	0.41
6:A:676:A:H2'	6:A:677:U:H6	1.86	0.41
6:A:1106:G:H2'	6:A:1107:C:H6	1.86	0.41
6:A:1243:C:H2'	6:A:1244:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:154:MET:HE1	7:B:158:PRO:HG3	2.02	0.41
11:F:91:ARG:HG3	11:F:91:ARG:HH11	1.86	0.41
14:I:41:ARG:CG	14:I:43:THR:HG22	2.51	0.41
15:J:5:ARG:C	15:J:6:ILE:HD13	2.45	0.41
18:M:15:ALA:HB3	18:M:34:LEU:HD11	2.02	0.41
23:R:57:ARG:HD2	23:R:61:ARG:HH22	1.86	0.41
28:a:604:U:C5	28:a:617:G:C5	3.09	0.41
28:a:610:U:H3'	28:a:611:A:H8	1.86	0.41
28:a:1363:A:H2'	28:a:1364:A:O4'	2.20	0.41
28:a:1922:G:H2'	28:a:1923:G:H8	1.86	0.41
42:o:48:ILE:HG13	42:o:60:THR:OG1	2.20	0.41
43:p:47:TYR:HD2	44:q:74:ILE:HG23	1.85	0.41
46:s:6:ARG:HE	46:s:10:VAL:HG13	1.85	0.41
51:x:57:LEU:HD23	51:x:57:LEU:HA	1.88	0.41
3:2:49:MET:HE3	3:2:49:MET:HB3	1.87	0.40
6:A:763:G:H2'	6:A:764:C:C6	2.57	0.40
6:A:818:G:O2'	6:A:819:A:H5'	2.22	0.40
6:A:987:A:H2'	6:A:988:C:C6	2.56	0.40
8:C:52:VAL:HA	8:C:70:THR:HG22	2.02	0.40
9:D:3:ARG:CZ	9:D:3:ARG:HB3	2.51	0.40
13:H:5:ASP:HB2	13:H:81:PRO:HG2	2.03	0.40
27:X:75:ASP:O	27:X:78:ILE:HG13	2.21	0.40
28:a:289:U:H5'	28:a:290:G:OP2	2.20	0.40
28:a:635:G:C5	28:a:648:G:C2	3.09	0.40
28:a:1800:A:H5'	28:a:2204:A:O2'	2.20	0.40
28:a:2231:G:H2'	28:a:2232:U:C6	2.56	0.40
30:c:43:ARG:NH2	30:c:49:ILE:HD11	2.35	0.40
32:e:121:VAL:O	32:e:189:THR:HA	2.20	0.40
34:g:99:LYS:HA	34:g:99:LYS:HD2	1.85	0.40
36:i:32:LEU:HD23	36:i:32:LEU:HA	1.88	0.40
39:l:66:ARG:HB2	39:l:101:VAL:O	2.21	0.40
45:r:24:ILE:HD11	45:r:74:ILE:HD13	2.03	0.40
48:u:55:GLU:HB3	48:u:59:GLU:OE2	2.21	0.40
51:x:27:ASN:O	51:x:31:GLN:HG3	2.21	0.40
6:A:473:U:H3'	6:A:474:G:H8	1.86	0.40
6:A:1473:G:H2'	6:A:1474:U:O4'	2.22	0.40
14:I:6:TYR:CE2	14:I:90:TYR:HA	2.56	0.40
17:L:42:PRO:HA	17:L:90:LEU:HD23	2.04	0.40
28:a:1100:A:H5"	28:a:1101:C:C5	2.54	0.40
28:a:1275:C:H5'	40:m:24:MET:HE3	2.03	0.40
28:a:2115:A:C6	28:a:2169:G:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2267:A:H4'	28:a:2268:A:N3	2.36	0.40
28:a:2309:G:H2'	28:a:2309:G:N3	2.37	0.40
28:a:2355:C:H2'	28:a:2356:G:H8	1.86	0.40
28:a:2512:U:H2'	28:a:2513:C:O4'	2.22	0.40
29:b:45:A:C4	29:b:46:A:C8	3.09	0.40
34:g:164:TYR:C	34:g:166:ASP:H	2.29	0.40
36:i:110:PRO:O	36:i:115:GLY:HA3	2.21	0.40
37:j:10:VAL:HG22	37:j:86:ILE:HD11	2.03	0.40
46:s:37:ASP:OD2	46:s:37:ASP:C	2.64	0.40
51:x:44:LYS:O	51:x:48:ARG:HG2	2.21	0.40
6:A:201:G:H21	6:A:469:A:H1'	1.86	0.40
6:A:1396:A:H4'	6:A:1397:C:H5"	2.02	0.40
15:J:30:LYS:NZ	15:J:35:GLN:HA	2.36	0.40
15:J:52:LEU:HD21	15:J:59:LYS:HA	2.02	0.40
15:J:76:ILE:HG13	15:J:87:LEU:HD11	2.03	0.40
21:P:36:VAL:HG23	21:P:56:ARG:HB2	2.03	0.40
28:a:28:A:H1'	28:a:512:A:C2	2.57	0.40
28:a:295:U:H2'	28:a:296:G:C8	2.56	0.40
28:a:498:U:H2'	28:a:499:G:O4'	2.21	0.40
28:a:720:C:H2'	28:a:721:U:O4'	2.21	0.40
28:a:761:A:H5'	30:c:209:GLY:HA2	2.02	0.40
28:a:1096:G:H2'	28:a:1097:C:O4'	2.21	0.40
28:a:1164:C:H2'	28:a:1165:G:H8	1.87	0.40
28:a:1240:C:H2'	28:a:1241:A:O4'	2.22	0.40
29:b:102:G:H2'	29:b:102:G:N3	2.36	0.40
32:e:100:MET:HE2	32:e:100:MET:HB3	2.00	0.40
33:f:122:PHE:CE1	33:f:128:TYR:HD1	2.39	0.40
36:i:99:ARG:HD2	36:i:99:ARG:HA	1.73	0.40
38:k:110:VAL:O	38:k:128:THR:HG23	2.22	0.40
44:q:37:GLU:OE1	44:q:37:GLU:HA	2.21	0.40
6:A:2:A:H2	6:A:614:C:H1'	1.86	0.40
6:A:1090:U:H2'	6:A:1091:U:C6	2.56	0.40
6:A:1106:G:H2'	6:A:1107:C:C6	2.57	0.40
10:E:33:PHE:CD2	10:E:56:VAL:HG22	2.56	0.40
11:F:39:LEU:HD13	11:F:62:MET:HG2	2.02	0.40
11:F:74:LEU:HD12	11:F:74:LEU:HA	1.76	0.40
14:I:52:LEU:HB3	14:I:58:VAL:HG22	2.04	0.40
16:K:20:VAL:HG23	16:K:83:GLU:O	2.21	0.40
16:K:22:HIS:HB2	16:K:33:THR:HG22	2.02	0.40
23:R:70:TYR:HB2	23:R:74:HIS:CE1	2.52	0.40
28:a:1127:U:HO2'	28:a:1128:G:H8	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1689:A:H2'	28:a:1690:A:H8	1.86	0.40
28:a:1994:U:H4'	31:d:133:THR:OG1	2.20	0.40
28:a:2046:C:H5"	53:z:15:MET:SD	2.62	0.40
28:a:2117:G:N3	28:a:2117:G:H2'	2.36	0.40
28:a:2538:U:H2'	28:a:2539:C:C6	2.57	0.40
34:g:137:ASP:OD1	34:g:137:ASP:C	2.64	0.40
42:o:53:ARG:H	42:o:57:SER:HB3	1.86	0.40
46:s:71:GLY:O	46:s:72:GLN:HB3	2.21	0.40
3:2:9:GLY:O	3:2:13:ARG:HD3	2.21	0.40
6:A:155:A:C6	6:A:167:A:N1	2.90	0.40
6:A:522:C:H2'	6:A:523:A:O4'	2.21	0.40
28:a:224:C:H2'	28:a:225:A:O4'	2.21	0.40
28:a:668:C:H2'	28:a:669:C:C6	2.57	0.40
28:a:1071:G:C6	28:a:1072:C:N4	2.89	0.40
28:a:1105:U:H2'	28:a:1106:C:C6	2.55	0.40
28:a:1760:C:H2'	28:a:1761:A:O4'	2.22	0.40
28:a:2142:G:H2'	28:a:2143:A:H8	1.81	0.40
28:a:2650:C:H2'	28:a:2651:U:H6	1.86	0.40
33:f:167:ARG:HD3	33:f:177:PHE:CE2	2.56	0.40
33:f:175:PHE:HB3	33:f:177:PHE:CE1	2.55	0.40
36:i:75:TYR:CD1	36:i:86:GLU:HB2	2.57	0.40
38:k:20:GLY:O	38:k:21:ARG:HD3	2.21	0.40
50:w:76:GLU:OE1	50:w:76:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	65/70 (93%)	60 (92%)	3 (5%)	2 (3%)	3	16
7	B	223/241 (92%)	208 (93%)	15 (7%)	0	100	100
8	C	205/233 (88%)	196 (96%)	9 (4%)	0	100	100
9	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
10	E	155/166 (93%)	147 (95%)	8 (5%)	0	100	100
11	F	102/131 (78%)	95 (93%)	7 (7%)	0	100	100
12	G	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
13	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	I	126/130 (97%)	115 (91%)	10 (8%)	1 (1%)	16	44
15	J	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	12	39
16	K	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14	41
17	L	120/124 (97%)	104 (87%)	14 (12%)	2 (2%)	7	27
18	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
21	P	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
22	Q	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
23	R	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
24	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
27	X	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
30	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
31	d	203/209 (97%)	190 (94%)	12 (6%)	1 (0%)	24	54
32	e	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
33	f	176/179 (98%)	161 (92%)	14 (8%)	1 (1%)	21	49
34	g	171/177 (97%)	156 (91%)	14 (8%)	1 (1%)	21	49
35	h	147/149 (99%)	130 (88%)	14 (10%)	3 (2%)	6	23
36	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
37	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	k	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
39	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
40	m	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
41	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
42	o	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
43	p	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
44	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	91/100 (91%)	79 (87%)	12 (13%)	0	100	100
47	t	101/104 (97%)	88 (87%)	12 (12%)	1 (1%)	12	39
48	u	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
49	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
50	w	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
51	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
52	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
53	z	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
All	All	5631/5909 (95%)	5315 (94%)	302 (5%)	14 (0%)	44	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	22	ILE
15	J	57	VAL
17	L	108	LYS
31	d	149	ASN
33	f	123	ASP
35	h	9	VAL
35	h	112	LYS
47	t	29	LEU
5	4	51	VAL
17	L	123	LYS
16	K	79	ILE
14	I	128	SER
34	g	51	THR
35	h	54	LEU

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	
1	0	47/49 (96%)	47 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	69
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	59/60 (98%)	58 (98%)	1 (2%)	53	71
7	B	189/201 (94%)	186 (98%)	3 (2%)	55	72
8	C	171/190 (90%)	168 (98%)	3 (2%)	51	70
9	D	172/173 (99%)	170 (99%)	2 (1%)	63	75
10	E	119/125 (95%)	116 (98%)	3 (2%)	42	66
11	F	91/113 (80%)	88 (97%)	3 (3%)	33	60
12	G	127/128 (99%)	127 (100%)	0	100	100
13	H	104/105 (99%)	103 (99%)	1 (1%)	68	77
14	I	106/107 (99%)	104 (98%)	2 (2%)	50	70
15	J	87/91 (96%)	85 (98%)	2 (2%)	44	67
16	K	89/98 (91%)	85 (96%)	4 (4%)	24	53
17	L	102/103 (99%)	100 (98%)	2 (2%)	48	69
18	M	94/97 (97%)	92 (98%)	2 (2%)	47	68
19	N	82/83 (99%)	80 (98%)	2 (2%)	43	66
20	O	75/76 (99%)	72 (96%)	3 (4%)	28	56
21	P	63/63 (100%)	63 (100%)	0	100	100
22	Q	75/78 (96%)	74 (99%)	1 (1%)	61	74
23	R	58/65 (89%)	57 (98%)	1 (2%)	53	71
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	64 (98%)	1 (2%)	57	73
27	X	82/82 (100%)	80 (98%)	2 (2%)	43	66
30	c	215/217 (99%)	212 (99%)	3 (1%)	59	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	d	163/163 (100%)	159 (98%)	4 (2%)	42	66
32	e	165/165 (100%)	163 (99%)	2 (1%)	63	75
33	f	150/151 (99%)	145 (97%)	5 (3%)	33	60
34	g	135/136 (99%)	128 (95%)	7 (5%)	21	49
35	h	112/112 (100%)	104 (93%)	8 (7%)	13	39
36	i	116/116 (100%)	112 (97%)	4 (3%)	32	60
37	j	104/104 (100%)	104 (100%)	0	100	100
38	k	103/103 (100%)	103 (100%)	0	100	100
39	l	107/107 (100%)	107 (100%)	0	100	100
40	m	100/103 (97%)	99 (99%)	1 (1%)	68	77
41	n	87/88 (99%)	85 (98%)	2 (2%)	44	67
42	o	99/100 (99%)	98 (99%)	1 (1%)	68	77
43	p	89/90 (99%)	87 (98%)	2 (2%)	45	68
44	q	84/84 (100%)	81 (96%)	3 (4%)	31	58
45	r	92/92 (100%)	90 (98%)	2 (2%)	45	68
46	s	80/84 (95%)	78 (98%)	2 (2%)	42	66
47	t	84/85 (99%)	80 (95%)	4 (5%)	23	51
48	u	77/77 (100%)	75 (97%)	2 (3%)	40	65
49	v	60/64 (94%)	59 (98%)	1 (2%)	53	71
50	w	68/69 (99%)	67 (98%)	1 (2%)	57	73
51	x	53/54 (98%)	52 (98%)	1 (2%)	50	70
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/49 (96%)	47 (100%)	0	100	100
All	All	4690/4818 (97%)	4596 (98%)	94 (2%)	48	69

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	54	ASP
5	4	27	THR
7	B	4	VAL
7	B	23	TRP
7	B	223	GLU
8	C	80	LYS

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Mol	Chain	Res	Type
8	C	144	LEU
8	C	186	THR
9	D	55	LEU
9	D	191	LEU
10	E	72	ILE
10	E	116	GLU
10	E	147	MET
11	F	84	VAL
11	F	89	VAL
11	F	94	HIS
13	H	66	PHE
14	I	19	VAL
14	I	59	GLU
15	J	35	GLN
15	J	77	VAL
16	K	27	PHE
16	K	46	THR
16	K	109	ASN
16	K	111	THR
17	L	82	ILE
17	L	97	THR
18	M	64	VAL
18	M	108	THR
19	N	48	LEU
19	N	74	VAL
20	O	6	GLU
20	O	10	LYS
20	O	40	GLN
22	Q	18	GLU
23	R	24	LYS
25	T	66	LEU
27	X	16	LEU
27	X	38	TYR
30	c	4	VAL
30	c	118	SER
30	c	120	VAL
31	d	50	VAL
31	d	89	GLU
31	d	97	SER
31	d	123	LYS
32	e	113	VAL
32	e	145	ASP

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Mol	Chain	Res	Type
33	f	68	THR
33	f	111	ILE
33	f	130	MET
33	f	137	ILE
33	f	162	SER
34	g	11	ILE
34	g	15	VAL
34	g	25	THR
34	g	59	VAL
34	g	101	ASN
34	g	117	LEU
34	g	177	LYS
35	h	2	GLN
35	h	37	VAL
35	h	77	THR
35	h	108	VAL
35	h	122	LEU
35	h	127	GLU
35	h	130	VAL
35	h	143	VAL
36	i	14	ASP
36	i	17	VAL
36	i	129	GLU
36	i	142	ILE
40	m	83	LEU
41	n	27	VAL
41	n	83	LEU
42	o	114	LEU
43	p	6	ARG
43	p	52	GLN
44	q	43	ASN
44	q	58	VAL
44	q	86	GLN
45	r	29	VAL
45	r	74	ILE
46	s	64	LYS
46	s	67	VAL
47	t	6	ARG
47	t	15	THR
47	t	34	LEU
47	t	70	VAL
48	u	61	LEU

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Mol	Chain	Res	Type
48	u	62	THR
49	v	85	GLU
50	w	22	LEU
51	x	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	35	GLN
7	B	146	ASN
8	C	140	ASN
10	E	132	ASN
11	F	11	HIS
11	F	14	GLN
11	F	37	HIS
11	F	68	GLN
11	F	94	HIS
15	J	58	ASN
16	K	40	ASN
17	L	5	ASN
17	L	72	HIS
23	R	74	HIS
25	T	61	GLN
30	c	53	HIS
30	c	128	ASN
31	d	58	ASN
34	g	22	GLN
35	h	20	ASN
35	h	66	ASN
35	h	73	ASN
36	i	58	ASN
36	i	128	ASN
36	i	136	GLN
37	j	89	ASN
41	n	61	GLN
45	r	6	GLN
45	r	9	HIS
50	w	36	HIS
51	x	15	ASN
52	y	9	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	W	9/15 (60%)	4 (44%)	0
28	a	2903/2904 (99%)	445 (15%)	0
29	b	115/116 (99%)	20 (17%)	0
6	A	1538/1541 (99%)	231 (15%)	10 (0%)
All	All	4565/4576 (99%)	700 (15%)	10 (0%)

All (700) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	7	A
6	A	8	A
6	A	9	G
6	A	22	G
6	A	39	G
6	A	47	C
6	A	48	C
6	A	51	A
6	A	72	A
6	A	74	A
6	A	76	G
6	A	77	A
6	A	81	A
6	A	84	U
6	A	85	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	90	C
6	A	94	G
6	A	97	G
6	A	121	U
6	A	122	G
6	A	130	A
6	A	131	A
6	A	141	G
6	A	144	G
6	A	173	U
6	A	182	A
6	A	183	C
6	A	191	G

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Mol	Chain	Res	Type
6	A	197	A
6	A	208	U
6	A	209	U
6	A	210	C
6	A	212	G
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	280	C
6	A	289	G
6	A	306	A
6	A	316	C
6	A	321	A
6	A	328	C
6	A	347	G
6	A	352	C
6	A	354	G
6	A	361	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	378	G
6	A	388	G
6	A	406	G
6	A	407	U
6	A	408	A
6	A	412	A
6	A	413	G
6	A	417	G
6	A	424	G
6	A	428	G
6	A	429	U
6	A	438	U
6	A	450	G
6	A	451	A
6	A	457	A
6	A	461	G
6	A	462	G

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Mol	Chain	Res	Type
6	A	463	U
6	A	464	U
6	A	465	A
6	A	468	A
6	A	469	A
6	A	473	U
6	A	474	G
6	A	477	G
6	A	478	A
6	A	479	U
6	A	481	G
6	A	484	G
6	A	495	A
6	A	496	A
6	A	510	A
6	A	511	C
6	A	512	U
6	A	517	G
6	A	518	C
6	A	521	G
6	A	527	G7M
6	A	530	G
6	A	533	A
6	A	547	A
6	A	548	G
6	A	559	A
6	A	564	C
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	588	G
6	A	596	A
6	A	615	G
6	A	618	C
6	A	628	G
6	A	633	G
6	A	642	A
6	A	653	A
6	A	665	A
6	A	666	G
6	A	685	G

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Mol	Chain	Res	Type
6	A	687	A
6	A	702	A
6	A	703	G
6	A	721	G
6	A	723	U
6	A	724	G
6	A	734	G
6	A	742	G
6	A	746	A
6	A	747	A
6	A	748	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	815	A
6	A	817	C
6	A	818	G
6	A	821	G
6	A	829	G
6	A	844	G
6	A	847	G
6	A	851	G
6	A	890	G
6	A	902	G
6	A	914	A
6	A	934	C
6	A	935	A
6	A	942	G
6	A	960	U
6	A	968	A
6	A	969	A
6	A	975	A
6	A	976	G
6	A	977	A
6	A	981	U
6	A	982	U
6	A	992	U
6	A	993	G
6	A	994	A
6	A	996	A
6	A	1004	A

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Mol	Chain	Res	Type
6	A	1008	U
6	A	1009	U
6	A	1020	A
6	A	1022	U
6	A	1024	G
6	A	1026	G
6	A	1027	C
6	A	1030	U
6	A	1031	C
6	A	1032	G
6	A	1033	G
6	A	1036	A
6	A	1043	G
6	A	1044	A
6	A	1050	G
6	A	1065	U
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1126	U
6	A	1133	G
6	A	1137	A
6	A	1138	G
6	A	1139	G
6	A	1140	C
6	A	1159	U
6	A	1168	U
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1213	A
6	A	1215	G
6	A	1227	A
6	A	1228	C
6	A	1238	A
6	A	1258	G
6	A	1260	G
6	A	1275	A
6	A	1280	A
6	A	1286	U
6	A	1287	A

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Mol	Chain	Res	Type
6	A	1300	G
6	A	1302	C
6	A	1305	G
6	A	1317	C
6	A	1320	C
6	A	1323	G
6	A	1337	G
6	A	1363	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1397	C
6	A	1398	A
6	A	1419	G
6	A	1432	G
6	A	1441	A
6	A	1451	U
6	A	1452	C
6	A	1453	G
6	A	1475	G
6	A	1487	G
6	A	1492	A
6	A	1494	G
6	A	1497	G
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1519	MA6
6	A	1529	G
6	A	1530	G
6	A	1538	C
26	W	7	U
26	W	9	A
26	W	13	A
26	W	15	G
28	a	10	A
28	a	34	U
28	a	35	G
28	a	45	G
28	a	51	G
28	a	63	A
28	a	71	A

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Mol	Chain	Res	Type
28	a	74	A
28	a	75	G
28	a	83	G
28	a	101	G
28	a	102	A
28	a	117	A
28	a	118	A
28	a	119	U
28	a	124	A
28	a	130	A
28	a	134	U
28	a	135	G
28	a	136	U
28	a	137	U
28	a	138	C
28	a	141	A
28	a	162	A
28	a	180	A
28	a	195	A
28	a	198	A
28	a	214	G
28	a	215	A
28	a	221	A
28	a	232	A
28	a	247	G
28	a	266	C
28	a	274	C
28	a	275	U
28	a	276	G
28	a	277	A
28	a	284	U
28	a	286	G
28	a	288	G
28	a	289	U
28	a	290	G
28	a	310	A
28	a	328	G
28	a	329	A
28	a	330	U
28	a	355	G
28	a	356	C
28	a	361	A

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Mol	Chain	Res	Type
28	a	385	G
28	a	395	G
28	a	402	U
28	a	404	U
28	a	410	G
28	a	434	C
28	a	474	C
28	a	480	G
28	a	490	G
28	a	504	A
28	a	505	G
28	a	508	C
28	a	531	A
28	a	532	G
28	a	544	U
28	a	545	C
28	a	547	G
28	a	560	A
28	a	566	U
28	a	570	U
28	a	572	A
28	a	574	G
28	a	600	A
28	a	610	U
28	a	612	U
28	a	624	A
28	a	634	A
28	a	642	C
28	a	644	G
28	a	651	A
28	a	652	A
28	a	683	U
28	a	701	G
28	a	714	C
28	a	727	A
28	a	735	G
28	a	737	C
28	a	744	5MU
28	a	761	A
28	a	762	C
28	a	772	G
28	a	773	G

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Mol	Chain	Res	Type
28	a	779	A
28	a	781	G
28	a	782	G
28	a	786	A
28	a	802	G
28	a	809	C
28	a	824	U
28	a	825	U
28	a	827	G
28	a	842	A
28	a	843	C
28	a	844	U
28	a	866	G
28	a	876	G
28	a	881	C
28	a	885	C
28	a	887	C
28	a	889	G
28	a	891	U
28	a	892	U
28	a	893	A
28	a	894	C
28	a	904	G
28	a	907	A
28	a	943	C
28	a	958	C
28	a	971	G
28	a	980	A
28	a	986	G
28	a	993	A
28	a	1002	C
28	a	1006	A
28	a	1009	U
28	a	1010	C
28	a	1022	G
28	a	1030	U
28	a	1037	A
28	a	1043	A
28	a	1044	G
28	a	1048	G
28	a	1055	U
28	a	1056	G

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Mol	Chain	Res	Type
28	a	1057	U
28	a	1059	G
28	a	1060	G
28	a	1061	C
28	a	1062	U
28	a	1063	U
28	a	1065	G
28	a	1066	A
28	a	1067	A
28	a	1068	G
28	a	1069	C
28	a	1070	A
28	a	1072	C
28	a	1073	C
28	a	1075	U
28	a	1076	C
28	a	1078	U
28	a	1080	U
28	a	1081	A
28	a	1084	G
28	a	1085	A
28	a	1086	A
28	a	1088	G
28	a	1089	C
28	a	1091	U
28	a	1092	A
28	a	1093	A
28	a	1094	U
28	a	1095	A
28	a	1098	U
28	a	1100	A
28	a	1101	C
28	a	1102	U
28	a	1103	G
28	a	1104	G
28	a	1107	G
28	a	1108	A
28	a	1109	G
28	a	1119	G
28	a	1126	A
28	a	1129	U
28	a	1130	A

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Mol	Chain	Res	Type
28	a	1132	C
28	a	1139	A
28	a	1166	A
28	a	1168	G
28	a	1169	C
28	a	1171	U
28	a	1172	A
28	a	1173	U
28	a	1174	G
28	a	1209	G
28	a	1233	G
28	a	1247	G
28	a	1250	A
28	a	1253	G
28	a	1268	G
28	a	1269	A
28	a	1297	G
28	a	1298	A
28	a	1322	U
28	a	1340	G
28	a	1349	U
28	a	1362	A
28	a	1375	A
28	a	1376	U
28	a	1380	A
28	a	1389	A
28	a	1400	A
28	a	1404	G
28	a	1413	G
28	a	1425	C
28	a	1431	A
28	a	1434	C
28	a	1449	G
28	a	1473	U
28	a	1479	G
28	a	1483	U
28	a	1490	U
28	a	1494	U
28	a	1507	U
28	a	1515	A
28	a	1522	A
28	a	1529	G

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Mol	Chain	Res	Type
28	a	1535	A
28	a	1536	C
28	a	1537	G
28	a	1554	U
28	a	1558	C
28	a	1569	A
28	a	1580	A
28	a	1583	A
28	a	1584	U
28	a	1585	C
28	a	1608	A
28	a	1626	A
28	a	1634	A
28	a	1647	U
28	a	1648	U
28	a	1649	G
28	a	1674	G
28	a	1675	C
28	a	1715	G
28	a	1728	C
28	a	1729	U
28	a	1734	G
28	a	1735	C
28	a	1737	G
28	a	1763	C
28	a	1772	A
28	a	1781	U
28	a	1790	A
28	a	1799	C
28	a	1800	A
28	a	1807	A
28	a	1814	A
28	a	1815	C
28	a	1828	A
28	a	1846	A
28	a	1847	A
28	a	1857	A
28	a	1868	G
28	a	1869	G
28	a	1870	C
28	a	1871	A
28	a	1873	C

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Mol	Chain	Res	Type
28	a	1907	G
28	a	1908	G
28	a	1910	C
28	a	1914	A
28	a	1915	C
28	a	1916	3TD
28	a	1918	PSU
28	a	1930	G
28	a	1931	G
28	a	1932	U
28	a	1938	A
28	a	1956	U
28	a	1965	G
28	a	1967	A
28	a	1968	C
28	a	1971	A
28	a	1972	U
28	a	1973	G
28	a	1992	U
28	a	1993	G
28	a	1994	U
28	a	2003	G
28	a	2021	A
28	a	2024	C
28	a	2031	6MZ
28	a	2032	A
28	a	2033	G
28	a	2034	A
28	a	2044	C
28	a	2050	G
28	a	2056	C
28	a	2057	G
28	a	2061	A
28	a	2062	G
28	a	2070	G7M
28	a	2094	G
28	a	2096	A
28	a	2098	A
28	a	2109	A
28	a	2110	U
28	a	2111	G
28	a	2112	U

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Mol	Chain	Res	Type
28	a	2114	U
28	a	2115	A
28	a	2116	G
28	a	2117	G
28	a	2118	A
28	a	2119	U
28	a	2120	A
28	a	2121	G
28	a	2124	G
28	a	2127	A
28	a	2128	G
28	a	2129	G
28	a	2130	C
28	a	2132	U
28	a	2134	G
28	a	2137	G
28	a	2138	C
28	a	2139	G
28	a	2140	U
28	a	2141	G
28	a	2142	G
28	a	2147	C
28	a	2148	A
28	a	2149	G
28	a	2150	U
28	a	2152	U
28	a	2158	G
28	a	2162	C
28	a	2163	G
28	a	2164	C
28	a	2165	C
28	a	2166	C
28	a	2167	U
28	a	2168	U
28	a	2169	G
28	a	2170	A
28	a	2172	A
28	a	2173	U
28	a	2174	A
28	a	2175	C
28	a	2176	C
28	a	2178	C

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Mol	Chain	Res	Type
28	a	2183	U
28	a	2187	G
28	a	2188	G
28	a	2189	C
28	a	2190	U
28	a	2191	G
28	a	2194	G
28	a	2199	A
28	a	2204	A
28	a	2205	G
28	a	2212	G
28	a	2214	U
28	a	2226	A
28	a	2239	G
28	a	2240	G
28	a	2267	A
28	a	2280	G
28	a	2284	C
28	a	2288	A
28	a	2306	U
28	a	2309	G
28	a	2312	A
28	a	2322	U
28	a	2323	A
28	a	2326	G
28	a	2334	A
28	a	2335	U
28	a	2336	A
28	a	2346	G
28	a	2348	C
28	a	2351	C
28	a	2362	G
28	a	2384	G
28	a	2386	C
28	a	2397	G
28	a	2403	U
28	a	2404	C
28	a	2407	A
28	a	2423	C
28	a	2426	A
28	a	2430	G
28	a	2431	A

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Mol	Chain	Res	Type
28	a	2436	A
28	a	2442	U
28	a	2449	A
28	a	2470	A
28	a	2476	C
28	a	2477	A
28	a	2492	U
28	a	2495	G
28	a	2499	OMC
28	a	2503	G
28	a	2506	G
28	a	2507	U
28	a	2519	A
28	a	2521	C
28	a	2526	G
28	a	2530	G
28	a	2548	A
28	a	2567	A
28	a	2568	G
28	a	2603	A
28	a	2610	U
28	a	2614	U
28	a	2616	U
28	a	2630	U
28	a	2631	G
28	a	2647	C
28	a	2662	G
28	a	2683	A
28	a	2690	U
28	a	2691	U
28	a	2715	G
28	a	2721	U
28	a	2727	A
28	a	2733	G
28	a	2734	A
28	a	2745	G
28	a	2749	A
28	a	2753	C
28	a	2758	A
28	a	2766	A
28	a	2779	A
28	a	2781	G

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Mol	Chain	Res	Type
28	a	2795	A
28	a	2796	C
28	a	2797	C
28	a	2798	U
28	a	2799	U
28	a	2800	G
28	a	2801	A
28	a	2819	U
28	a	2821	A
28	a	2822	A
28	a	2834	U
28	a	2837	U
28	a	2850	U
28	a	2873	A
28	a	2874	A
28	a	2881	C
28	a	2884	A
28	a	2892	U
29	b	9	G
29	b	13	U
29	b	16	G
29	b	24	G
29	b	35	C
29	b	41	G
29	b	45	A
29	b	53	A
29	b	56	G
29	b	66	A
29	b	67	G
29	b	89	U
29	b	90	C
29	b	99	A
29	b	101	A
29	b	102	G
29	b	103	U
29	b	104	A
29	b	105	G
29	b	109	A

All (10) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
6	A	360	G
6	A	406	G
6	A	407	U
6	A	416	G
6	A	428	G
6	A	516	PSU
6	A	547	A
6	A	1026	G
6	A	1035	A
6	A	1506	U

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

40 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	$\#\|Z\| > 2$
6	5MC	A	1407	6	18,22,23	2.01	6 (33%)	26,32,35	1.38	2 (7%)
17	D2T	L	89	17	7,9,10	1.16	0	6,11,13	1.69	1 (16%)
6	2MG	A	1516	6	23,26,27	2.57	6 (26%)	32,38,41	2.08	10 (31%)
28	PSU	a	2458	28	18,21,22	2.12	9 (50%)	22,30,33	1.85	4 (18%)
6	5MC	A	967	6	18,22,23	1.92	6 (33%)	26,32,35	1.36	2 (7%)
6	PSU	A	516	6	18,21,22	1.99	7 (38%)	22,30,33	1.86	5 (22%)
6	MA6	A	1519	6	23,26,27	1.26	3 (13%)	34,38,41	2.28	10 (29%)
6	2MG	A	1207	54,6	23,26,27	2.58	5 (21%)	32,38,41	2.09	11 (34%)
28	PSU	a	1912	28	18,21,22	2.06	7 (38%)	22,30,33	1.86	3 (13%)
28	3TD	a	1916	-	18,22,23	2.77	7 (38%)	22,32,35	1.72	2 (9%)
31	MEQ	d	150	31	8,9,10	0.99	0	5,10,12	0.62	0
6	UR3	A	1498	6	19,22,23	2.59	6 (31%)	26,32,35	1.32	2 (7%)
28	6MZ	a	1618	28	22,25,26	2.35	3 (13%)	30,36,39	2.33	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MA6	A	1518	6	23,26,27	1.21	3 (13%)	34,38,41	2.19	9 (26%)
28	2MG	a	1834	28	23,26,27	2.57	7 (30%)	32,38,41	2.07	10 (31%)
28	5MU	a	1940	54,28	19,22,23	2.59	7 (36%)	28,32,35	3.94	10 (35%)
28	PSU	a	743	56,28	18,21,22	2.04	7 (38%)	22,30,33	1.75	3 (13%)
28	2MG	a	2446	28	23,26,27	2.58	6 (26%)	32,38,41	2.07	11 (34%)
28	2MA	a	2504	56,54,28	22,25,26	1.35	4 (18%)	33,37,40	2.06	8 (24%)
28	PSU	a	2505	54,28	18,21,22	2.09	7 (38%)	22,30,33	1.89	4 (18%)
28	PSU	a	2605	28	18,21,22	2.04	7 (38%)	22,30,33	1.80	3 (13%)
28	6MZ	a	2031	28	22,25,26	2.39	3 (13%)	30,36,39	2.50	10 (33%)
39	MS6	l	82	39	5,7,8	0.49	0	2,7,9	1.82	1 (50%)
28	OMU	a	2553	56,54,28	19,22,23	2.64	7 (36%)	26,31,34	1.81	6 (23%)
28	PSU	a	2581	54,28	18,21,22	2.14	8 (44%)	22,30,33	1.90	5 (22%)
39	4D4	l	81	39	9,11,12	0.78	0	8,13,15	1.55	2 (25%)
28	1MG	a	742	28	22,26,27	2.54	6 (27%)	33,39,42	2.01	7 (21%)
16	IAS	K	119	16	5,6,8	1.86	1 (20%)	3,6,10	3.52	1 (33%)
28	5MU	a	744	28	19,22,23	2.54	7 (36%)	28,32,35	3.89	11 (39%)
28	PSU	a	1918	28	18,21,22	2.09	7 (38%)	22,30,33	1.73	4 (18%)
28	G7M	a	2070	54,28	23,26,27	2.24	5 (21%)	35,39,42	1.83	7 (20%)
6	G7M	A	527	54,6	23,26,27	2.21	5 (21%)	35,39,42	1.84	7 (20%)
28	OMC	a	2499	56,28	19,22,23	1.85	4 (21%)	26,31,34	1.00	2 (7%)
6	4OC	A	1402	6	20,23,24	2.26	3 (15%)	26,32,35	1.00	2 (7%)
28	H2U	a	2450	28	18,21,22	4.10	5 (27%)	21,30,33	5.35	7 (33%)
28	5MC	a	1963	54,28	18,22,23	1.92	6 (33%)	26,32,35	1.35	2 (7%)
28	PSU	a	2606	28	18,21,22	2.08	8 (44%)	22,30,33	1.84	3 (13%)
28	PSU	a	952	28	18,21,22	2.08	7 (38%)	22,30,33	1.77	3 (13%)
6	2MG	A	966	6	23,26,27	2.58	5 (21%)	32,38,41	2.04	9 (28%)
28	OMG	a	2252	54,28	23,26,27	2.35	6 (26%)	33,38,41	1.80	10 (30%)

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
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	3/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
28	PSU	a	2458	28	-	0/7/25/26	0/2/2/2
6	5MC	A	967	6	-	1/7/25/26	0/2/2/2
6	PSU	A	516	6	-	0/7/25/26	0/2/2/2
6	MA6	A	1519	6	-	5/11/29/30	0/3/3/3
6	2MG	A	1207	54,6	-	0/9/27/28	0/3/3/3
28	PSU	a	1912	28	-	0/7/25/26	0/2/2/2
28	3TD	a	1916	-	-	3/7/25/26	0/2/2/2
31	MEQ	d	150	31	-	2/8/9/11	-
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
28	6MZ	a	1618	28	-	0/9/27/28	0/3/3/3
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
28	2MG	a	1834	28	-	2/9/27/28	0/3/3/3
28	5MU	a	1940	54,28	-	0/7/25/26	0/2/2/2
28	PSU	a	743	56,28	-	1/7/25/26	0/2/2/2
28	2MG	a	2446	28	-	0/9/27/28	0/3/3/3
28	2MA	a	2504	56,54,28	-	1/7/25/26	0/3/3/3
28	PSU	a	2505	54,28	-	2/7/25/26	0/2/2/2
28	PSU	a	2605	28	-	0/7/25/26	0/2/2/2
28	6MZ	a	2031	28	-	2/9/27/28	0/3/3/3
39	MS6	l	82	39	-	1/4/6/8	-
28	OMU	a	2553	56,54,28	-	0/9/27/28	0/2/2/2
28	PSU	a	2581	54,28	-	0/7/25/26	0/2/2/2
39	4D4	l	81	39	-	3/11/12/14	-
28	1MG	a	742	28	-	0/7/25/26	0/3/3/3
16	IAS	K	119	16	-	2/3/5/8	-
28	5MU	a	744	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1918	28	-	3/7/25/26	0/2/2/2
28	G7M	a	2070	54,28	-	1/7/25/26	0/3/3/3
6	G7M	A	527	54,6	-	3/7/25/26	0/3/3/3
28	OMC	a	2499	56,28	-	0/9/27/28	0/2/2/2
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
28	H2U	a	2450	28	-	0/7/38/39	0/2/2/2
28	5MC	a	1963	54,28	-	0/7/25/26	0/2/2/2
28	PSU	a	2606	28	-	0/7/25/26	0/2/2/2
28	PSU	a	952	28	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	2/9/27/28	0/3/3/3
28	OMG	a	2252	54,28	-	1/9/27/28	0/3/3/3

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2450	H2U	O4-C4	9.96	1.43	1.23
28	a	1618	6MZ	C6-N6	9.79	1.44	1.34
28	a	2031	6MZ	C6-N6	9.68	1.44	1.34
6	A	966	2MG	O6-C6	9.11	1.40	1.23
6	A	1207	2MG	O6-C6	9.08	1.40	1.23
6	A	1516	2MG	O6-C6	9.00	1.40	1.23
28	a	2446	2MG	O6-C6	8.98	1.40	1.23
28	a	1834	2MG	O6-C6	8.94	1.40	1.23
6	A	1498	UR3	O4-C4	8.68	1.42	1.23
28	a	2252	OMG	O6-C6	8.47	1.39	1.23
28	a	2450	H2U	C2-N1	8.16	1.47	1.35
28	a	1916	3TD	O4-C4	8.15	1.40	1.23
28	a	2450	H2U	O2-C2	8.15	1.37	1.23
28	a	2070	G7M	O6-C6	8.09	1.39	1.23
28	a	2553	OMU	O4-C4	7.99	1.40	1.24
6	A	527	G7M	O6-C6	7.99	1.38	1.23
28	a	742	1MG	O6-C6	7.93	1.39	1.23
28	a	2450	H2U	C2-N3	6.62	1.49	1.38
6	A	1402	4OC	O2-C2	6.62	1.35	1.23
28	a	1940	5MU	C2-N1	-6.50	1.28	1.38
28	a	744	5MU	C2-N1	-6.08	1.28	1.38
28	a	742	1MG	C2-N2	6.06	1.45	1.34
6	A	1207	2MG	C2-N2	5.94	1.46	1.33
6	A	966	2MG	C2-N2	5.93	1.46	1.33
6	A	1516	2MG	C2-N2	5.79	1.46	1.33
28	a	2446	2MG	C2-N2	5.72	1.46	1.33
28	a	1834	2MG	C2-N2	5.57	1.45	1.33
6	A	1402	4OC	C4-N4	5.51	1.47	1.35
28	a	2450	H2U	C4-N3	4.93	1.46	1.37
28	a	1940	5MU	C2-N3	-4.90	1.29	1.38
28	a	744	5MU	C2-N3	-4.80	1.29	1.38
28	a	2499	OMC	C4-N4	4.76	1.45	1.33
28	a	744	5MU	C6-N1	-4.70	1.30	1.38
28	a	1940	5MU	C6-N1	-4.64	1.30	1.38
28	a	2553	OMU	C2-N1	-4.54	1.31	1.38
28	a	2504	2MA	C6-N6	4.34	1.45	1.34
28	a	2499	OMC	C2-N1	-4.27	1.30	1.40
28	a	1916	3TD	C2-N1	-4.22	1.31	1.37
6	A	967	5MC	C4-N4	4.21	1.45	1.34
6	A	1407	5MC	C2-N1	-4.12	1.31	1.40
28	a	742	1MG	C6-N1	-4.10	1.31	1.40
6	A	1407	5MC	C4-N4	4.07	1.44	1.34
28	a	2581	PSU	C2-N1	-4.06	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2252	OMG	C2-N2	4.04	1.43	1.34
28	a	1963	5MC	C4-N4	4.00	1.44	1.34
28	a	1916	3TD	C4-N3	-3.99	1.31	1.40
28	a	2252	OMG	C6-N1	-3.94	1.31	1.38
28	a	743	PSU	C2-N1	-3.92	1.31	1.36
28	a	2505	PSU	C2-N1	-3.91	1.31	1.36
28	a	1963	5MC	C2-N1	-3.91	1.31	1.40
28	a	2458	PSU	C2-N1	-3.91	1.31	1.36
6	A	527	G7M	C5-N7	-3.90	1.34	1.39
28	a	2606	PSU	C4-N3	-3.90	1.31	1.38
28	a	1912	PSU	C2-N1	-3.90	1.31	1.36
28	a	2458	PSU	C4-N3	-3.87	1.31	1.38
28	a	2070	G7M	C5-N7	-3.81	1.34	1.39
28	a	2505	PSU	C4-N3	-3.81	1.31	1.38
6	A	967	5MC	C2-N1	-3.80	1.31	1.40
28	a	952	PSU	C2-N1	-3.80	1.31	1.36
6	A	1498	UR3	C4-N3	-3.77	1.32	1.40
28	a	2581	PSU	C4-N3	-3.77	1.31	1.38
28	a	1918	PSU	C4-N3	-3.77	1.31	1.38
6	A	516	PSU	C2-N1	-3.75	1.31	1.36
28	a	952	PSU	C4-N3	-3.73	1.31	1.38
28	a	2553	OMU	C4-N3	-3.71	1.31	1.38
28	a	2606	PSU	C2-N1	-3.70	1.31	1.36
28	a	2605	PSU	C2-N1	-3.70	1.31	1.36
6	A	1402	4OC	C2-N1	-3.70	1.32	1.40
28	a	2605	PSU	C4-N3	-3.67	1.32	1.38
28	a	1918	PSU	C2-N1	-3.65	1.31	1.36
28	a	1912	PSU	C4-N3	-3.63	1.32	1.38
28	a	743	PSU	C4-N3	-3.62	1.32	1.38
28	a	2458	PSU	C2-N3	-3.62	1.31	1.37
16	K	119	IAS	OD1-CG	3.60	1.40	1.19
28	a	2606	PSU	C2-N3	-3.56	1.31	1.37
6	A	1519	MA6	C8-N9	-3.54	1.31	1.37
28	a	2605	PSU	C2-N3	-3.52	1.31	1.37
28	a	952	PSU	C2-N3	-3.52	1.31	1.37
28	a	1918	PSU	C2-N3	-3.51	1.31	1.37
28	a	2505	PSU	C2-N3	-3.51	1.31	1.37
28	a	2553	OMU	C2-N3	-3.48	1.31	1.38
6	A	516	PSU	C4-N3	-3.47	1.32	1.38
28	a	1963	5MC	C6-N1	-3.44	1.32	1.38
28	a	2581	PSU	C2-N3	-3.43	1.31	1.37
28	a	1940	5MU	C4-N3	-3.42	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1912	PSU	C2-N3	-3.41	1.31	1.37
6	A	1407	5MC	C6-N1	-3.40	1.32	1.38
6	A	516	PSU	C2-N3	-3.38	1.31	1.37
28	a	744	5MU	C4-N3	-3.38	1.32	1.38
28	a	1940	5MU	C6-C5	3.38	1.40	1.34
6	A	1498	UR3	C2-N3	-3.37	1.32	1.39
28	a	743	PSU	C2-N3	-3.37	1.31	1.37
6	A	1518	MA6	C6-N6	3.37	1.46	1.36
28	a	2070	G7M	C6-N1	-3.35	1.32	1.38
6	A	527	G7M	C6-N1	-3.35	1.32	1.38
28	a	2031	6MZ	C8-N9	-3.34	1.31	1.37
28	a	1916	3TD	C6-C5	3.32	1.39	1.35
6	A	1519	MA6	C6-N6	3.30	1.46	1.36
28	a	744	5MU	C6-C5	3.30	1.40	1.34
28	a	1918	PSU	C6-C5	3.25	1.39	1.35
6	A	967	5MC	C6-N1	-3.23	1.32	1.38
6	A	1498	UR3	C2-N1	-3.19	1.34	1.38
28	a	1834	2MG	C6-N1	-3.18	1.32	1.38
28	a	2446	2MG	C6-N1	-3.15	1.33	1.38
28	a	1834	2MG	C5-N7	-3.14	1.33	1.39
6	A	1407	5MC	O2-C2	-3.10	1.18	1.23
6	A	527	G7M	C2-N2	3.10	1.41	1.34
6	A	1518	MA6	C8-N9	-3.08	1.32	1.37
28	a	1618	6MZ	C8-N9	-3.04	1.32	1.37
28	a	1912	PSU	C6-C5	3.03	1.38	1.35
28	a	2070	G7M	C2-N2	3.02	1.41	1.34
6	A	1516	2MG	C6-N1	-3.01	1.33	1.38
28	a	1916	3TD	C2-N3	-3.00	1.31	1.38
6	A	1207	2MG	C6-N1	-3.00	1.33	1.38
6	A	966	2MG	C6-N1	-2.96	1.33	1.38
28	a	2605	PSU	C6-C5	2.94	1.38	1.35
28	a	952	PSU	C6-C5	2.91	1.38	1.35
6	A	1207	2MG	C5-N7	-2.89	1.33	1.39
28	a	2581	PSU	C6-C5	2.87	1.38	1.35
6	A	516	PSU	C6-C5	2.86	1.38	1.35
6	A	1516	2MG	C5-N7	-2.86	1.33	1.39
28	a	2606	PSU	O4-C4	-2.81	1.18	1.23
28	a	744	5MU	O4-C4	-2.80	1.18	1.23
28	a	1918	PSU	O4-C4	-2.80	1.18	1.23
28	a	1963	5MC	O2-C2	-2.78	1.18	1.23
6	A	967	5MC	O2-C2	-2.77	1.18	1.23
6	A	966	2MG	C5-N7	-2.76	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	952	PSU	O4-C4	-2.72	1.18	1.23
28	a	2446	2MG	C5-N7	-2.71	1.33	1.39
28	a	2458	PSU	O4-C4	-2.71	1.18	1.23
28	a	2505	PSU	C6-C5	2.71	1.38	1.35
6	A	967	5MC	C6-C5	2.70	1.39	1.34
28	a	2031	6MZ	C5-N7	-2.69	1.33	1.39
28	a	2458	PSU	C6-N1	-2.68	1.31	1.36
28	a	2605	PSU	O4-C4	-2.68	1.18	1.23
28	a	742	1MG	C5-N7	-2.66	1.33	1.39
6	A	1407	5MC	C6-C5	2.66	1.39	1.34
28	a	2606	PSU	C6-C5	2.65	1.38	1.35
28	a	2252	OMG	C8-N9	-2.65	1.31	1.37
28	a	2581	PSU	O4-C4	-2.64	1.18	1.23
28	a	2505	PSU	O4-C4	-2.63	1.18	1.23
28	a	743	PSU	O4-C4	-2.62	1.18	1.23
6	A	516	PSU	O4-C4	-2.60	1.18	1.23
28	a	2505	PSU	C6-N1	-2.60	1.31	1.36
28	a	1940	5MU	O4-C4	-2.57	1.18	1.23
28	a	743	PSU	C6-N1	-2.57	1.32	1.36
28	a	2581	PSU	C6-N1	-2.57	1.32	1.36
28	a	2458	PSU	C6-C5	2.57	1.38	1.35
28	a	743	PSU	C6-C5	2.55	1.38	1.35
28	a	742	1MG	C8-N9	-2.55	1.31	1.37
28	a	1618	6MZ	C5-N7	-2.54	1.34	1.39
28	a	1912	PSU	C6-N1	-2.54	1.32	1.36
28	a	1912	PSU	O4-C4	-2.53	1.18	1.23
28	a	1940	5MU	O2-C2	-2.53	1.18	1.23
28	a	2070	G7M	C2-N1	-2.53	1.31	1.37
28	a	2553	OMU	O2-C2	-2.52	1.18	1.23
28	a	744	5MU	O2-C2	-2.49	1.18	1.23
28	a	1916	3TD	C6-N1	-2.48	1.32	1.36
28	a	2581	PSU	O2-C2	-2.47	1.18	1.23
28	a	2252	OMG	C5-N7	-2.46	1.34	1.39
28	a	1918	PSU	C6-N1	-2.45	1.32	1.36
28	a	2606	PSU	C6-N1	-2.45	1.32	1.36
28	a	952	PSU	C6-N1	-2.45	1.32	1.36
28	a	2553	OMU	C6-N1	-2.44	1.32	1.38
28	a	2505	PSU	O2-C2	-2.44	1.18	1.23
28	a	1912	PSU	O2-C2	-2.43	1.18	1.23
28	a	1916	3TD	O2-C2	-2.40	1.18	1.23
28	a	2581	PSU	O4'-C1'	-2.40	1.40	1.43
6	A	1519	MA6	C5-N7	-2.38	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2458	PSU	O2-C2	-2.37	1.18	1.23
6	A	527	G7M	C2-N1	-2.37	1.31	1.37
6	A	1498	UR3	C6-N1	-2.36	1.32	1.38
6	A	1518	MA6	C5-N7	-2.36	1.34	1.39
28	a	1963	5MC	C6-C5	2.35	1.38	1.34
28	a	2605	PSU	C6-N1	-2.34	1.32	1.36
28	a	2605	PSU	O2-C2	-2.33	1.18	1.23
28	a	952	PSU	O2-C2	-2.33	1.18	1.23
28	a	2252	OMG	C2-N1	-2.32	1.32	1.37
6	A	516	PSU	C6-N1	-2.29	1.32	1.36
28	a	2499	OMC	C5-C4	-2.28	1.37	1.42
6	A	516	PSU	O2-C2	-2.28	1.18	1.23
28	a	1918	PSU	O2-C2	-2.27	1.18	1.23
28	a	2606	PSU	O2-C2	-2.27	1.18	1.23
28	a	743	PSU	O2-C2	-2.24	1.18	1.23
28	a	2446	2MG	C4-N9	-2.24	1.32	1.38
6	A	1498	UR3	O2-C2	2.23	1.26	1.22
6	A	1516	2MG	C4-N9	-2.22	1.32	1.38
6	A	1407	5MC	C2-N3	-2.22	1.31	1.36
28	a	2553	OMU	C5-C4	-2.19	1.38	1.43
28	a	2504	2MA	C5-N7	-2.14	1.35	1.39
28	a	2499	OMC	C2-N3	-2.14	1.32	1.36
28	a	1963	5MC	C2-N3	-2.13	1.32	1.36
6	A	966	2MG	C4-N9	-2.12	1.32	1.38
28	a	1834	2MG	C8-N9	-2.09	1.32	1.37
28	a	2446	2MG	CM2-N2	-2.09	1.41	1.45
28	a	2504	2MA	C8-N9	-2.09	1.33	1.37
28	a	2458	PSU	O4'-C1'	-2.08	1.41	1.43
6	A	1516	2MG	CM2-N2	-2.07	1.41	1.45
28	a	1834	2MG	C4-N9	-2.06	1.32	1.38
28	a	1834	2MG	CM2-N2	-2.06	1.41	1.45
6	A	967	5MC	C2-N3	-2.05	1.32	1.36
28	a	2606	PSU	C4-C5	-2.04	1.38	1.44
28	a	742	1MG	C5-C6	-2.04	1.40	1.45
28	a	2504	2MA	C4-N9	-2.03	1.33	1.37
6	A	1207	2MG	C4-N9	-2.00	1.32	1.38
28	a	2458	PSU	C4-C5	-2.00	1.38	1.44

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2450	H2U	C4-N3-C2	-16.53	112.08	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2450	H2U	O2-C2-N1	-10.91	109.41	123.11
28	a	1940	5MU	C4-N3-C2	-8.93	115.79	127.35
28	a	744	5MU	C5M-C5-C4	8.82	128.47	118.77
28	a	744	5MU	C4-N3-C2	-8.63	116.17	127.35
28	a	1940	5MU	C5M-C5-C4	8.60	128.24	118.77
28	a	1940	5MU	N3-C2-N1	8.59	126.29	114.89
28	a	744	5MU	N3-C2-N1	8.15	125.71	114.89
28	a	1940	5MU	C5-C6-N1	-7.89	115.23	123.34
28	a	2450	H2U	O4-C4-N3	-7.83	107.86	120.28
28	a	744	5MU	C5-C6-N1	-7.67	115.44	123.34
28	a	2504	2MA	C5-C4-N3	-7.21	119.08	127.19
6	A	1207	2MG	C2-N3-C4	7.17	120.93	112.04
28	a	2450	H2U	N3-C2-N1	-7.17	109.07	116.65
6	A	1516	2MG	C2-N3-C4	7.11	120.85	112.04
28	a	744	5MU	C5M-C5-C6	-7.07	113.41	122.85
28	a	2031	6MZ	C9-N6-C6	-7.05	116.80	122.87
28	a	742	1MG	C5-C4-N3	-6.99	117.12	128.46
28	a	2446	2MG	C2-N3-C4	6.95	120.66	112.04
6	A	966	2MG	C2-N3-C4	6.95	120.66	112.04
28	a	1834	2MG	C2-N3-C4	6.93	120.63	112.04
28	a	1940	5MU	C5M-C5-C6	-6.85	113.70	122.85
28	a	1916	3TD	N1-C2-N3	6.78	121.49	116.14
28	a	2450	H2U	O4-C4-C5	-6.71	107.84	122.17
28	a	1940	5MU	C5-C4-N3	6.38	120.75	115.31
28	a	744	5MU	C5-C4-N3	6.29	120.68	115.31
28	a	2450	H2U	O2-C2-N3	-6.26	109.84	121.50
6	A	1519	MA6	C5-C4-N3	-6.16	118.71	126.75
16	K	119	IAS	OD1-CG-CB	-6.03	107.84	125.43
28	a	2505	PSU	N1-C2-N3	5.83	121.74	115.13
6	A	1518	MA6	C5-C4-N3	-5.77	119.22	126.75
28	a	2581	PSU	N1-C2-N3	5.61	121.48	115.13
28	a	1912	PSU	N1-C2-N3	5.57	121.44	115.13
28	a	2458	PSU	N1-C2-N3	5.56	121.43	115.13
28	a	2504	2MA	N3-C4-N9	5.52	134.65	126.99
28	a	2606	PSU	N1-C2-N3	5.45	121.30	115.13
28	a	2553	OMU	N3-C2-N1	5.43	122.10	114.89
6	A	1407	5MC	C5-C6-N1	-5.41	117.78	123.34
28	a	2252	OMG	C5-C4-N3	-5.37	119.75	128.46
6	A	967	5MC	C5-C6-N1	-5.31	117.87	123.34
28	a	743	PSU	N1-C2-N3	5.30	121.14	115.13
28	a	2605	PSU	N1-C2-N3	5.30	121.13	115.13
28	a	1618	6MZ	C5-C4-N3	-5.27	119.88	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	952	PSU	N1-C2-N3	5.25	121.08	115.13
28	a	1918	PSU	N1-C2-N3	5.24	121.07	115.13
28	a	1834	2MG	C5-C4-N3	-5.23	119.98	128.46
6	A	1207	2MG	C5-C4-N3	-5.22	119.99	128.46
6	A	516	PSU	N1-C2-N3	5.17	120.99	115.13
6	A	527	G7M	C2-N3-C4	5.13	121.44	112.30
28	a	1963	5MC	C5-C6-N1	-5.11	118.08	123.34
28	a	1618	6MZ	C9-N6-C6	-5.07	118.50	122.87
28	a	2031	6MZ	N1-C2-N3	-5.06	120.69	128.60
28	a	2070	G7M	C2-N3-C4	5.03	121.27	112.30
28	a	2446	2MG	C5-C4-N3	-5.02	120.31	128.46
28	a	742	1MG	C2-N3-C4	4.99	123.19	111.98
28	a	1618	6MZ	N1-C2-N3	-4.99	120.80	128.60
6	A	1516	2MG	C5-C4-N3	-4.97	120.40	128.46
6	A	1519	MA6	N3-C4-N9	4.91	135.17	127.08
28	a	2031	6MZ	C5-C4-N3	-4.90	120.36	126.75
28	a	742	1MG	N9-C4-N3	4.86	135.71	125.94
6	A	966	2MG	C5-C4-N3	-4.85	120.58	128.46
6	A	1518	MA6	N1-C2-N3	-4.80	121.09	128.60
6	A	1498	UR3	C4-N3-C2	-4.68	120.16	124.56
6	A	1519	MA6	N1-C2-N3	-4.68	121.28	128.60
6	A	527	G7M	C5-C4-N3	-4.62	119.29	128.15
28	a	2553	OMU	C4-N3-C2	-4.54	120.59	126.58
28	a	2252	OMG	C2-N3-C4	4.45	120.22	112.30
28	a	1940	5MU	O2-C2-N1	-4.37	116.98	122.79
28	a	2070	G7M	C5-C4-N3	-4.25	120.00	128.15
6	A	1518	MA6	N3-C4-N9	4.24	134.07	127.08
6	A	527	G7M	C5-C6-N1	4.23	120.61	111.79
28	a	2070	G7M	C5-C6-N1	4.17	120.49	111.79
6	A	1519	MA6	C2-N3-C4	4.15	121.56	111.75
6	A	1518	MA6	C2-N1-C6	4.14	121.53	111.75
28	a	1940	5MU	O4-C4-N3	-4.09	112.27	120.12
6	A	1518	MA6	C2-N3-C4	4.09	121.40	111.75
6	A	1519	MA6	C2-N1-C6	3.95	121.09	111.75
28	a	744	5MU	O4-C4-N3	-3.93	112.58	120.12
28	a	1618	6MZ	C2-N3-C4	3.92	121.00	111.75
28	a	2252	OMG	N9-C4-N3	3.83	133.64	125.94
28	a	2031	6MZ	C2-N3-C4	3.83	120.79	111.75
28	a	2606	PSU	C4-N3-C2	-3.78	120.89	126.34
28	a	2458	PSU	C4-N3-C2	-3.72	120.98	126.34
28	a	2505	PSU	C4-N3-C2	-3.70	121.01	126.34
28	a	1912	PSU	C4-N3-C2	-3.65	121.08	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	744	5MU	O2-C2-N1	-3.65	117.94	122.79
28	a	2605	PSU	C4-N3-C2	-3.62	121.13	126.34
28	a	2070	G7M	C6-C5-N7	3.61	136.62	132.25
28	a	743	PSU	C4-N3-C2	-3.57	121.19	126.34
28	a	1834	2MG	N9-C4-N3	3.52	133.00	125.94
6	A	1207	2MG	N9-C4-N3	3.51	133.00	125.94
28	a	1618	6MZ	N3-C4-N9	3.50	132.85	127.08
6	A	1518	MA6	C5-N7-C8	3.48	108.46	103.51
6	A	527	G7M	N9-C4-N3	3.48	132.93	125.94
28	a	743	PSU	O2-C2-N1	-3.46	118.98	122.79
28	a	2031	6MZ	N9-C8-N7	-3.45	109.20	113.91
6	A	1518	MA6	N9-C8-N7	-3.44	109.21	113.91
28	a	2031	6MZ	C6-C5-N7	3.43	136.10	132.39
6	A	1519	MA6	N9-C8-N7	-3.43	109.22	113.91
28	a	952	PSU	C4-N3-C2	-3.43	121.40	126.34
6	A	516	PSU	C4-N3-C2	-3.42	121.41	126.34
6	A	527	G7M	O6-C6-C5	-3.42	120.34	128.06
28	a	2070	G7M	O6-C6-C5	-3.42	120.35	128.06
28	a	2581	PSU	C4-N3-C2	-3.39	121.46	126.34
6	A	966	2MG	N9-C4-N3	3.38	132.73	125.94
6	A	1519	MA6	C5-N7-C8	3.38	108.31	103.51
28	a	2553	OMU	O2-C2-N1	-3.35	118.33	122.79
28	a	2031	6MZ	C5-N7-C8	3.33	108.24	103.51
28	a	2581	PSU	O2-C2-N1	-3.33	119.12	122.79
28	a	2070	G7M	N9-C4-N3	3.30	132.56	125.94
28	a	1618	6MZ	C6-C5-N7	3.29	135.95	132.39
28	a	1912	PSU	O2-C2-N1	-3.29	119.17	122.79
28	a	2446	2MG	N9-C4-N3	3.29	132.54	125.94
28	a	1618	6MZ	C5-N7-C8	3.28	108.17	103.51
28	a	2505	PSU	O2-C2-N1	-3.28	119.18	122.79
28	a	2031	6MZ	N3-C4-N9	3.27	132.46	127.08
6	A	1519	MA6	C4-N9-C8	3.26	109.26	105.73
6	A	1516	2MG	N9-C4-N3	3.21	132.38	125.94
6	A	527	G7M	C6-C5-N7	3.15	136.06	132.25
28	a	1618	6MZ	C4-C5-N7	-3.13	106.81	110.62
28	a	2031	6MZ	C4-C5-N7	-3.13	106.81	110.62
28	a	2458	PSU	O2-C2-N1	-3.12	119.36	122.79
6	A	1518	MA6	C4-C5-N7	-3.12	106.82	110.62
6	A	516	PSU	O2-C2-N1	-3.09	119.39	122.79
28	a	1618	6MZ	N9-C8-N7	-3.05	109.74	113.91
39	l	81	4D4	NE-CZ-NH2	3.03	126.02	120.70
28	a	1918	PSU	C4-N3-C2	-3.02	121.98	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2504	2MA	N9-C8-N7	-2.95	109.88	113.91
28	a	2605	PSU	O2-C2-N1	-2.94	119.55	122.79
6	A	1516	2MG	C6-C5-N7	2.93	135.71	130.25
28	a	2499	OMC	O2-C2-N3	-2.91	117.60	122.33
6	A	1519	MA6	C4-C5-N7	-2.90	107.09	110.62
28	a	952	PSU	O2-C2-N1	-2.89	119.61	122.79
6	A	527	G7M	C2-N1-C6	-2.88	119.84	125.10
28	a	2446	2MG	C6-C5-N7	2.88	135.60	130.25
6	A	1518	MA6	C4-N9-C8	2.84	108.81	105.73
6	A	966	2MG	C6-C5-N7	2.81	135.48	130.25
28	a	2606	PSU	O2-C2-N1	-2.80	119.71	122.79
28	a	2450	H2U	C5-C4-N3	-2.79	113.52	116.65
17	L	89	D2T	OD1-CG-CB	-2.78	116.62	122.44
28	a	744	5MU	O2-C2-N3	-2.76	116.35	121.50
28	a	2504	2MA	C5-N7-C8	2.73	107.39	103.51
28	a	2504	2MA	C4-N9-C8	2.69	108.64	105.73
28	a	1918	PSU	O2-C2-N1	-2.68	119.83	122.79
28	a	2553	OMU	C5-C4-N3	2.68	118.84	114.84
6	A	1207	2MG	C6-C5-N7	2.65	135.17	130.25
28	a	2031	6MZ	C4-N9-C8	2.63	108.58	105.73
28	a	2252	OMG	C6-C5-N7	2.61	135.11	130.25
28	a	1834	2MG	CM2-N2-C2	-2.60	118.12	123.86
28	a	2070	G7M	C2-N1-C6	-2.60	120.36	125.10
28	a	1940	5MU	O2-C2-N3	-2.56	116.73	121.50
28	a	1940	5MU	C6-N1-C2	2.55	123.88	121.30
28	a	744	5MU	C6-N1-C2	2.54	123.87	121.30
28	a	1834	2MG	C6-C5-N7	2.52	134.94	130.25
28	a	744	5MU	C1'-N1-C6	-2.52	116.93	121.12
28	a	2553	OMU	O4-C4-C5	-2.51	120.74	125.16
28	a	2446	2MG	CM2-N2-C2	-2.51	118.31	123.86
28	a	1834	2MG	O6-C6-C5	-2.51	119.94	126.60
28	a	2504	2MA	N6-C6-N1	2.50	120.57	117.03
39	l	82	MS6	CE-SD-CG	2.50	108.97	100.40
6	A	967	5MC	C5-C4-N3	-2.49	118.99	121.67
28	a	2446	2MG	C4-C5-N7	-2.47	106.82	110.72
28	a	742	1MG	C5-C6-N1	2.46	119.66	114.91
6	A	966	2MG	O6-C6-C5	-2.42	120.17	126.60
28	a	2581	PSU	C6-N1-C2	-2.36	120.27	122.68
6	A	1407	5MC	C5-C4-N3	-2.35	119.14	121.67
6	A	1402	4OC	O2-C2-N3	-2.35	118.50	122.33
28	a	2252	OMG	C5-C6-N1	2.35	119.15	113.19
28	a	742	1MG	C4-C5-N7	-2.35	107.01	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1516	2MG	C4-C5-N7	-2.34	107.02	110.72
28	a	2581	PSU	O4'-C1'-C2'	2.34	108.44	105.14
28	a	1834	2MG	C2-N1-C6	-2.34	121.79	124.48
6	A	1516	2MG	O6-C6-C5	-2.32	120.46	126.60
6	A	1516	2MG	CM2-N2-C2	-2.31	118.75	123.86
28	a	2446	2MG	C2-N1-C6	-2.31	121.82	124.48
6	A	1207	2MG	C4-C5-N7	-2.31	107.06	110.72
6	A	1498	UR3	C5-C6-N1	-2.31	117.94	121.81
28	a	2499	OMC	N1-C2-N3	2.29	122.98	118.81
28	a	2504	2MA	C4-C5-N7	-2.29	107.83	110.62
6	A	1516	2MG	C2-N1-C6	-2.28	121.85	124.48
28	a	1963	5MC	C5-C4-N3	-2.28	119.21	121.67
28	a	1834	2MG	C4-C5-N7	-2.27	107.12	110.72
28	a	2446	2MG	O6-C6-C5	-2.27	120.58	126.60
28	a	2252	OMG	C4-C5-N7	-2.27	107.13	110.72
28	a	2252	OMG	C8-N7-C5	2.26	108.32	104.24
6	A	1207	2MG	C2-N1-C6	-2.26	121.89	124.48
6	A	1207	2MG	O6-C6-C5	-2.26	120.61	126.60
6	A	1516	2MG	C5-C6-N1	2.25	118.91	113.19
6	A	966	2MG	C5-C6-N1	2.24	118.89	113.19
28	a	1918	PSU	C6-N1-C2	-2.24	120.39	122.68
6	A	516	PSU	O3'-C3'-C2'	2.22	119.01	111.82
6	A	1519	MA6	C4-C5-C6	2.22	118.36	115.88
28	a	2505	PSU	C6-N1-C2	-2.18	120.45	122.68
6	A	516	PSU	C6-C5-C4	-2.18	116.67	118.20
6	A	1207	2MG	C5-C6-N1	2.18	118.72	113.19
28	a	2458	PSU	O4'-C1'-C2'	2.17	108.21	105.14
28	a	2252	OMG	O6-C6-C5	-2.17	120.85	126.60
28	a	742	1MG	C6-C5-N7	2.17	134.25	129.35
6	A	966	2MG	N1-C2-N3	-2.16	120.61	123.95
28	a	2504	2MA	N3-C2-N1	-2.16	121.75	125.72
6	A	966	2MG	C4-C5-N7	-2.15	107.31	110.72
28	a	2446	2MG	C5-C6-N1	2.14	118.62	113.19
28	a	1834	2MG	C5-C6-N1	2.13	118.60	113.19
28	a	2553	OMU	C5-C6-N1	-2.13	118.25	121.81
6	A	1207	2MG	CM2-N2-C2	-2.13	119.16	123.86
6	A	1402	4OC	C5-C4-N3	-2.12	119.18	122.59
6	A	966	2MG	C2-N1-C6	-2.11	122.05	124.48
28	a	2446	2MG	C8-N7-C5	2.11	108.06	104.24
28	a	1618	6MZ	C4-N9-C8	2.11	108.01	105.73
28	a	1916	3TD	C4-N3-C2	-2.10	122.33	124.61
6	A	1207	2MG	N1-C2-N3	-2.10	120.71	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1516	2MG	N1-C2-N3	-2.09	120.72	123.95
28	a	2252	OMG	N9-C8-N7	-2.08	109.47	113.39
28	a	2252	OMG	C2-N1-C6	-2.08	121.31	125.10
28	a	742	1MG	C8-N7-C5	2.08	108.00	104.24
39	l	81	4D4	NH1-CZ-NE	-2.06	114.44	119.19
6	A	1207	2MG	C8-N7-C5	2.05	107.94	104.24
28	a	1834	2MG	C8-N7-C5	2.02	107.89	104.24
28	a	2446	2MG	N9-C8-N7	-2.01	109.61	113.39

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	966	2MG	N1-C2-N2-CM2
6	A	966	2MG	N3-C2-N2-CM2
6	A	1519	MA6	O4'-C4'-C5'-O5'
17	L	89	D2T	O-C-CA-CB
17	L	89	D2T	CA-CB-SB-CB1
39	l	81	4D4	CA-CB-CG-CD
16	K	119	IAS	O-C-CA-CB
16	K	119	IAS	N-CA-CB-CG
28	a	1916	3TD	C2'-C1'-C5-C4
28	a	1918	PSU	C3'-C4'-C5'-O5'
28	a	1918	PSU	O4'-C4'-C5'-O5'
28	a	2252	OMG	C1'-C2'-O2'-CM2
6	A	1519	MA6	C3'-C4'-C5'-O5'
28	a	2031	6MZ	O4'-C4'-C5'-O5'
28	a	2031	6MZ	C3'-C4'-C5'-O5'
28	a	2505	PSU	O4'-C4'-C5'-O5'
6	A	527	G7M	C3'-C4'-C5'-O5'
39	l	82	MS6	CB-CG-SD-CE
6	A	1519	MA6	C5-C6-N6-C10
28	a	1916	3TD	C3'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
6	A	527	G7M	C4'-C5'-O5'-P
31	d	150	MEQ	N-CA-CB-CG
28	a	1834	2MG	O4'-C4'-C5'-O5'
39	l	81	4D4	OB-CB-CG-CD
6	A	527	G7M	O4'-C4'-C5'-O5'
6	A	1519	MA6	C5-C6-N6-C9
28	a	1918	PSU	C4'-C5'-O5'-P
28	a	1834	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
28	a	1916	3TD	O4'-C4'-C5'-O5'
28	a	2505	PSU	C3'-C4'-C5'-O5'
6	A	967	5MC	O4'-C4'-C5'-O5'
28	a	2504	2MA	O4'-C4'-C5'-O5'
6	A	1402	4OC	O4'-C4'-C5'-O5'
28	a	743	PSU	O4'-C1'-C5-C6
28	a	2070	G7M	O4'-C4'-C5'-O5'
39	l	81	4D4	O-C-CA-CB
6	A	1519	MA6	C4'-C5'-O5'-P
31	d	150	MEQ	CA-CB-CG-CD

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	89	D2T	1	0
6	A	516	PSU	1	0
28	a	1916	3TD	2	0
31	d	150	MEQ	1	0
6	A	1518	MA6	1	0
28	a	2504	2MA	1	0
28	a	2031	6MZ	1	0
6	A	1402	4OC	2	0
6	A	966	2MG	1	0
28	a	2252	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 521 ligands modelled in this entry, 521 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	a	2
31	d	2
34	g	2
16	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	118:HIS	C	119:IAS	N	3.42
1	a	1915:C	O3'	1916:3TD	P	3.10
1	a	1916:3TD	O3'	1917:A	P	3.09
1	d	103:ASP	C	104:VAL	N	2.99
1	g	150:ALA	C	151:TYR	N	2.98
1	d	102:ALA	C	103:ASP	N	2.97
1	g	149:ARG	C	150:ALA	N	2.87

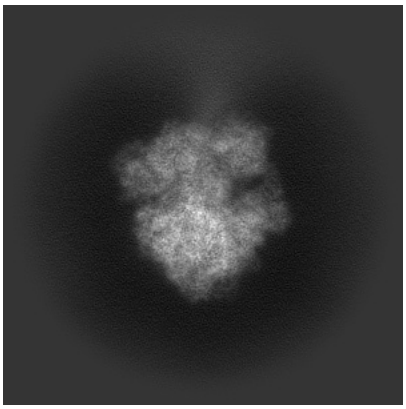
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55661. These allow visual inspection of the internal detail of the map and identification of artifacts.

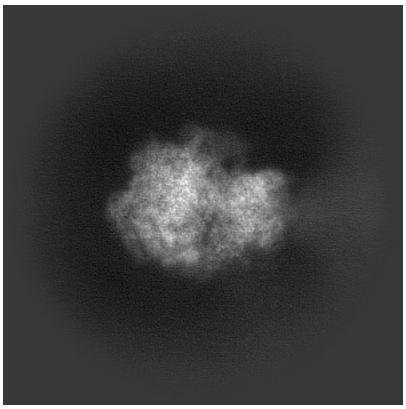
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

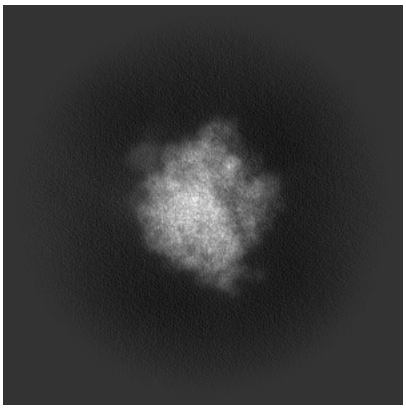
6.1.1 Primary map



X

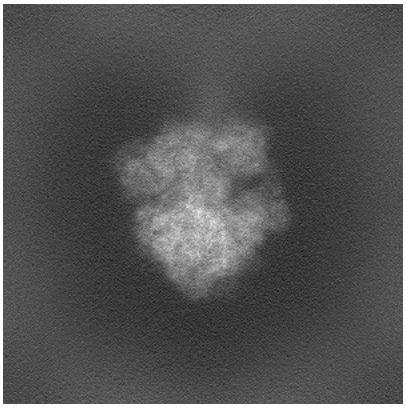


Y

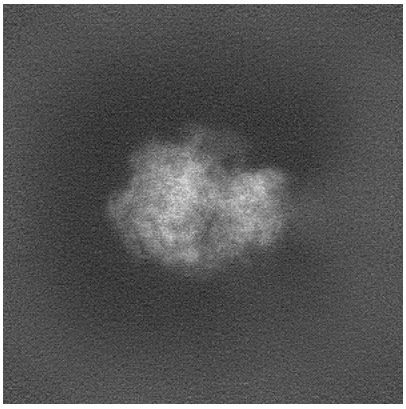


Z

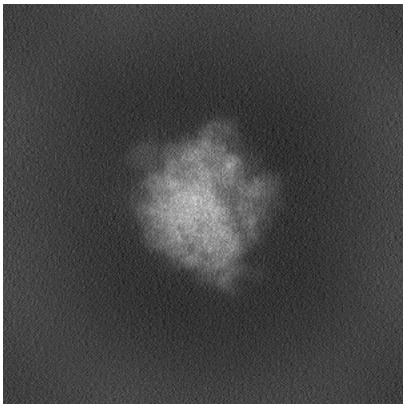
6.1.2 Raw map



X



Y

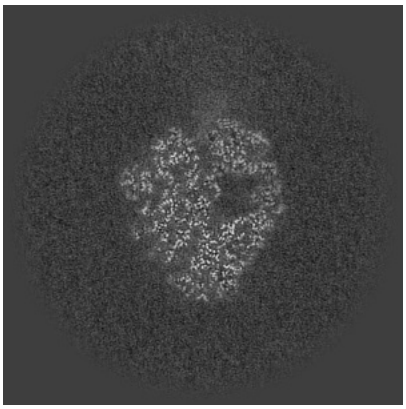


Z

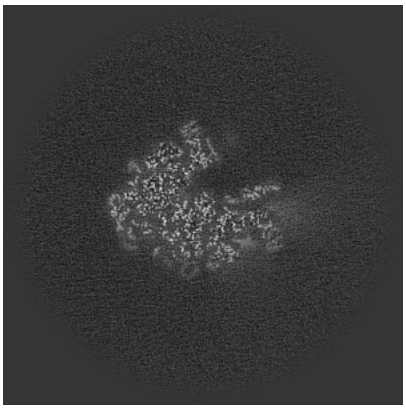
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

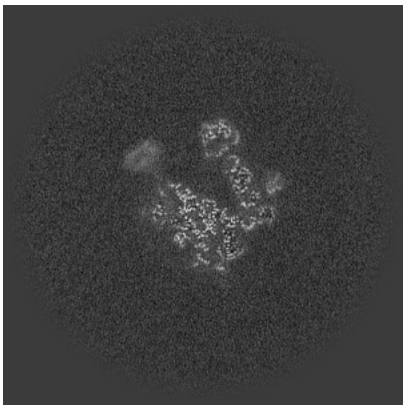
6.2.1 Primary map



X Index: 256

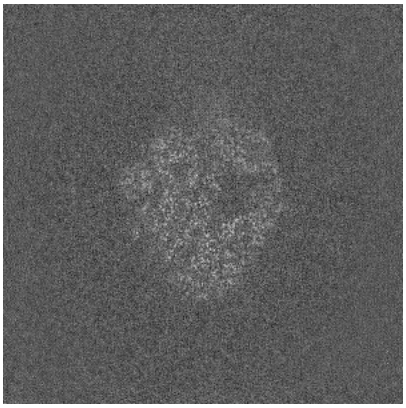


Y Index: 256

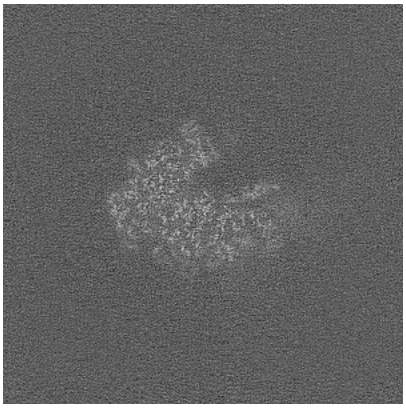


Z Index: 256

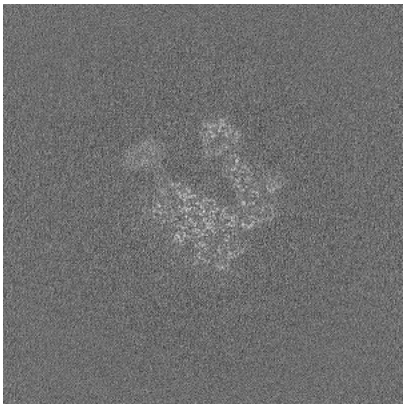
6.2.2 Raw map



X Index: 256



Y Index: 256

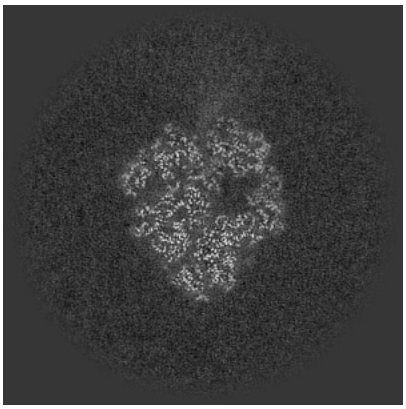


Z Index: 256

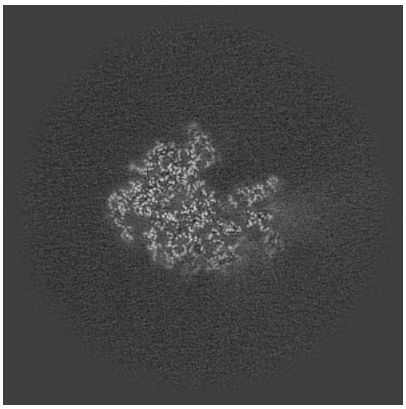
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

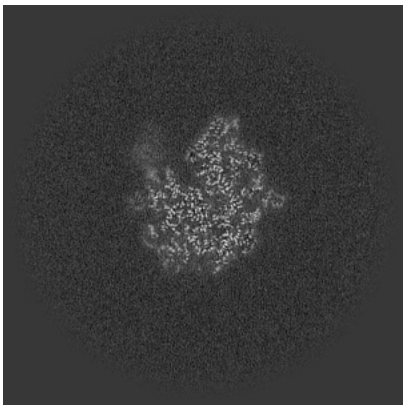
6.3.1 Primary map



X Index: 261

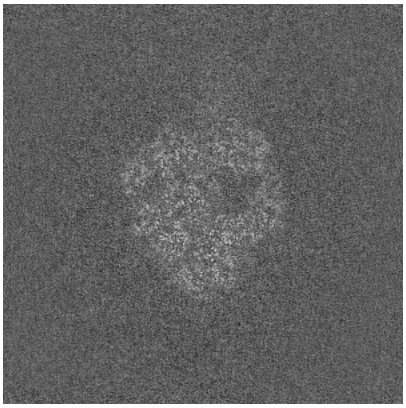


Y Index: 250

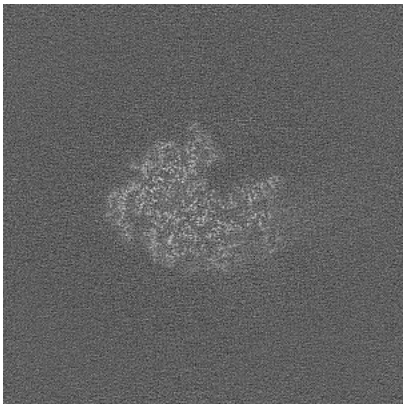


Z Index: 234

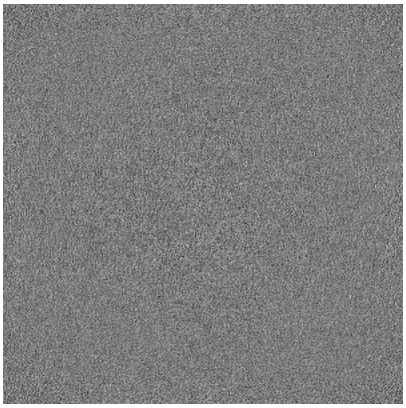
6.3.2 Raw map



X Index: 261



Y Index: 249

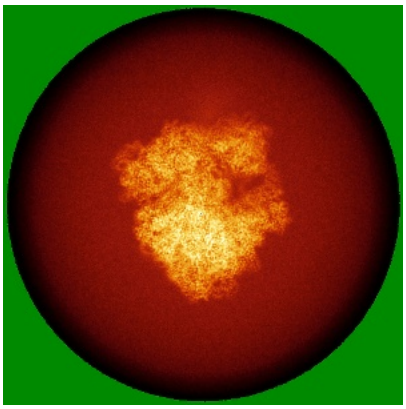


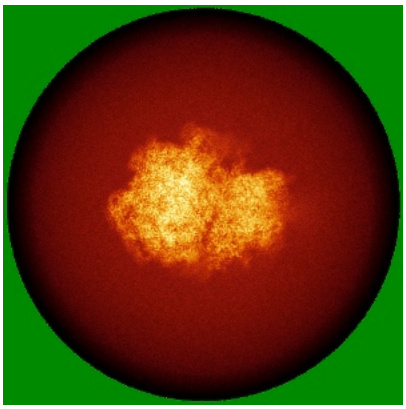
Z Index: 0

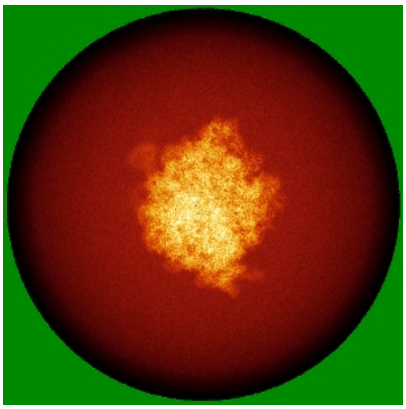
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

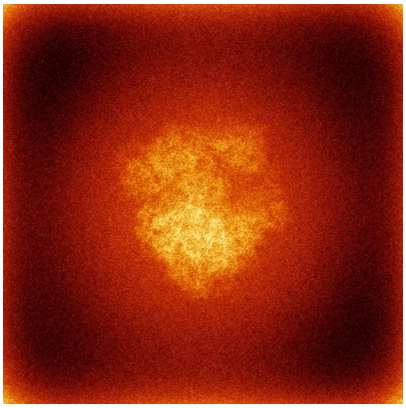
6.4.1 Primary map

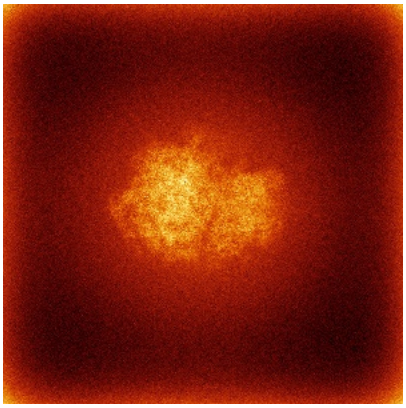

X

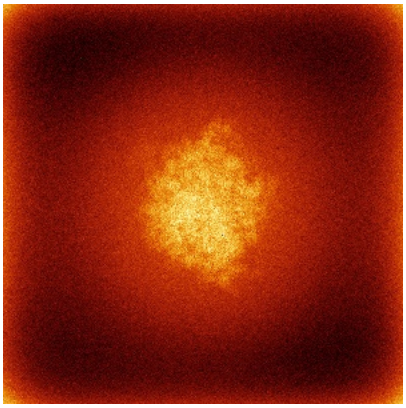

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

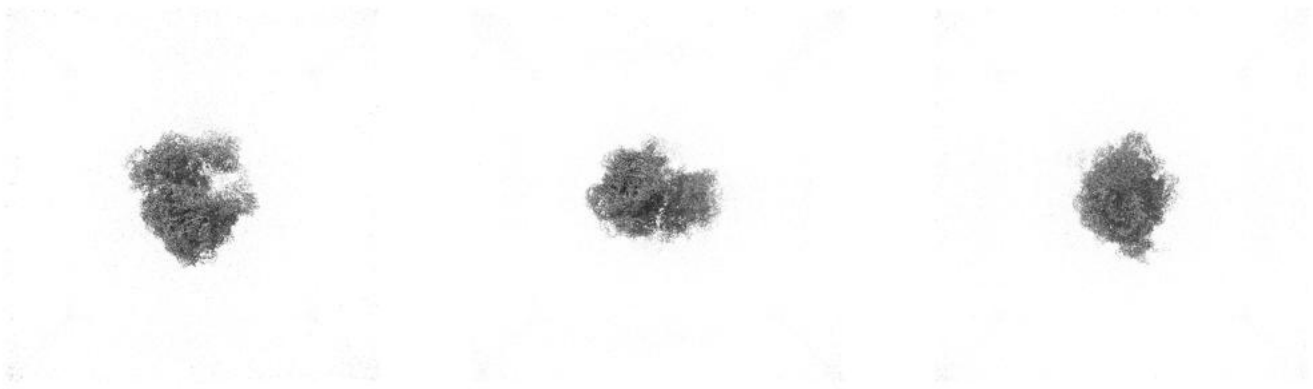
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

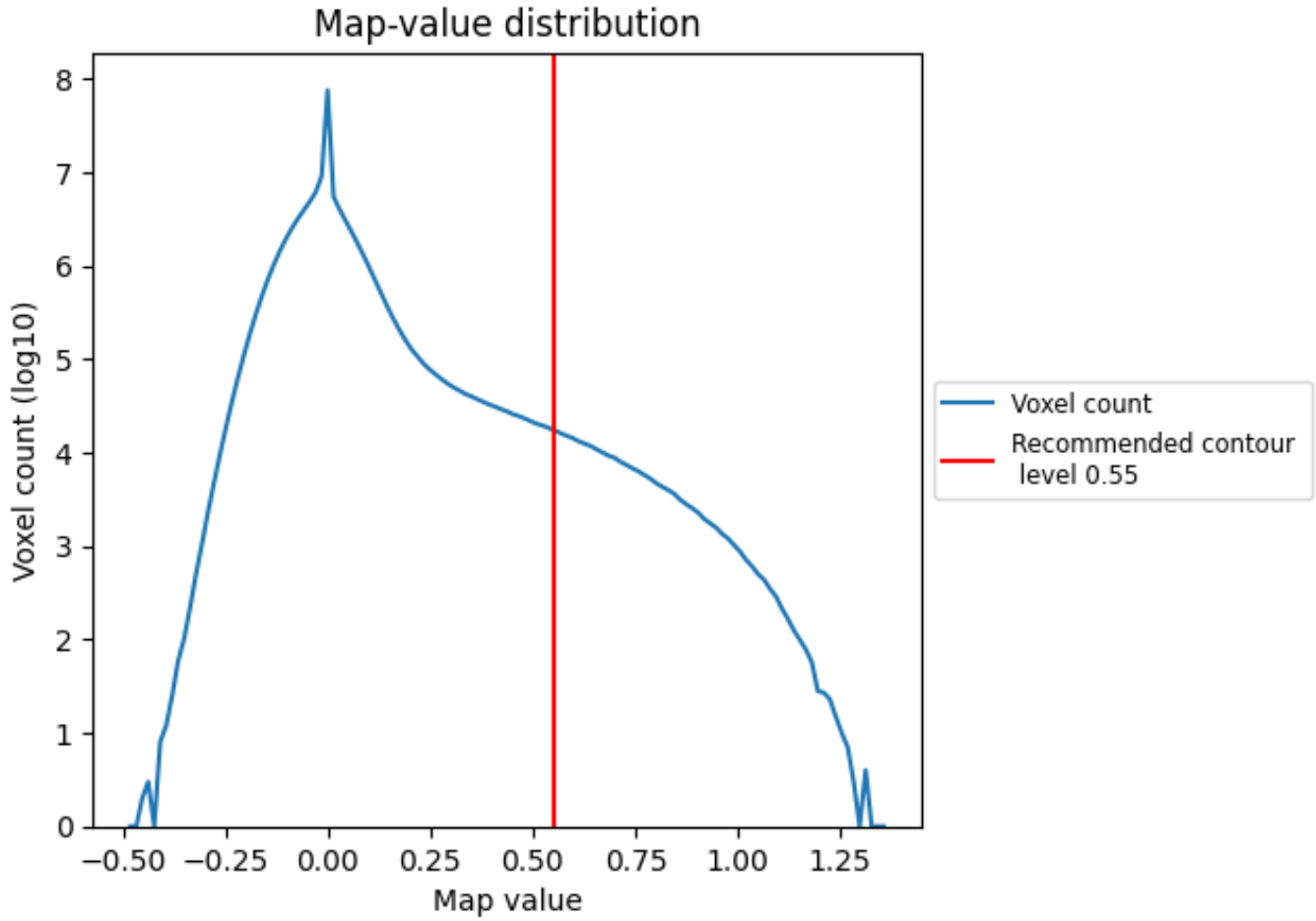
6.6 Mask visualisation (i)

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

7 Map analysis

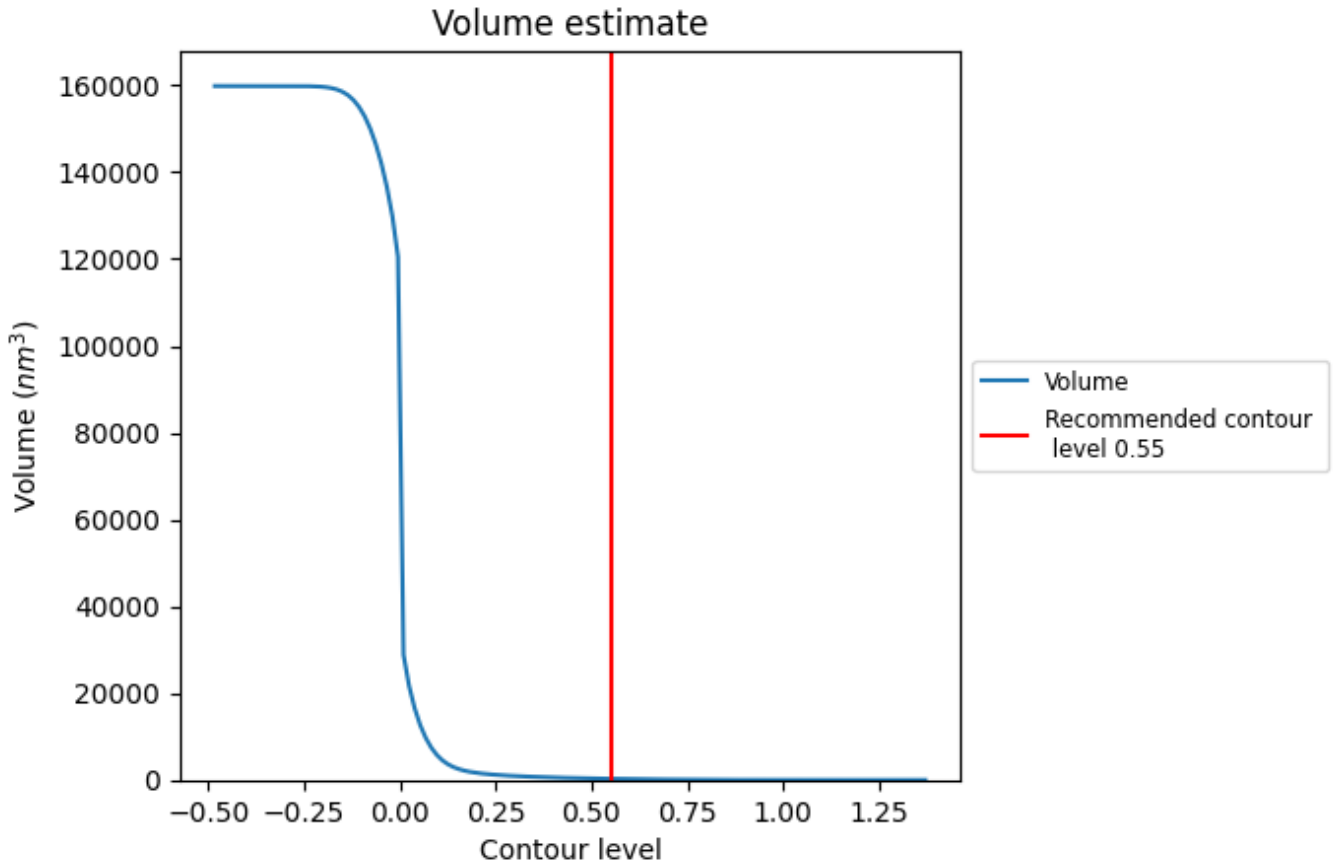
This section contains the results of statistical analysis of the map.

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.

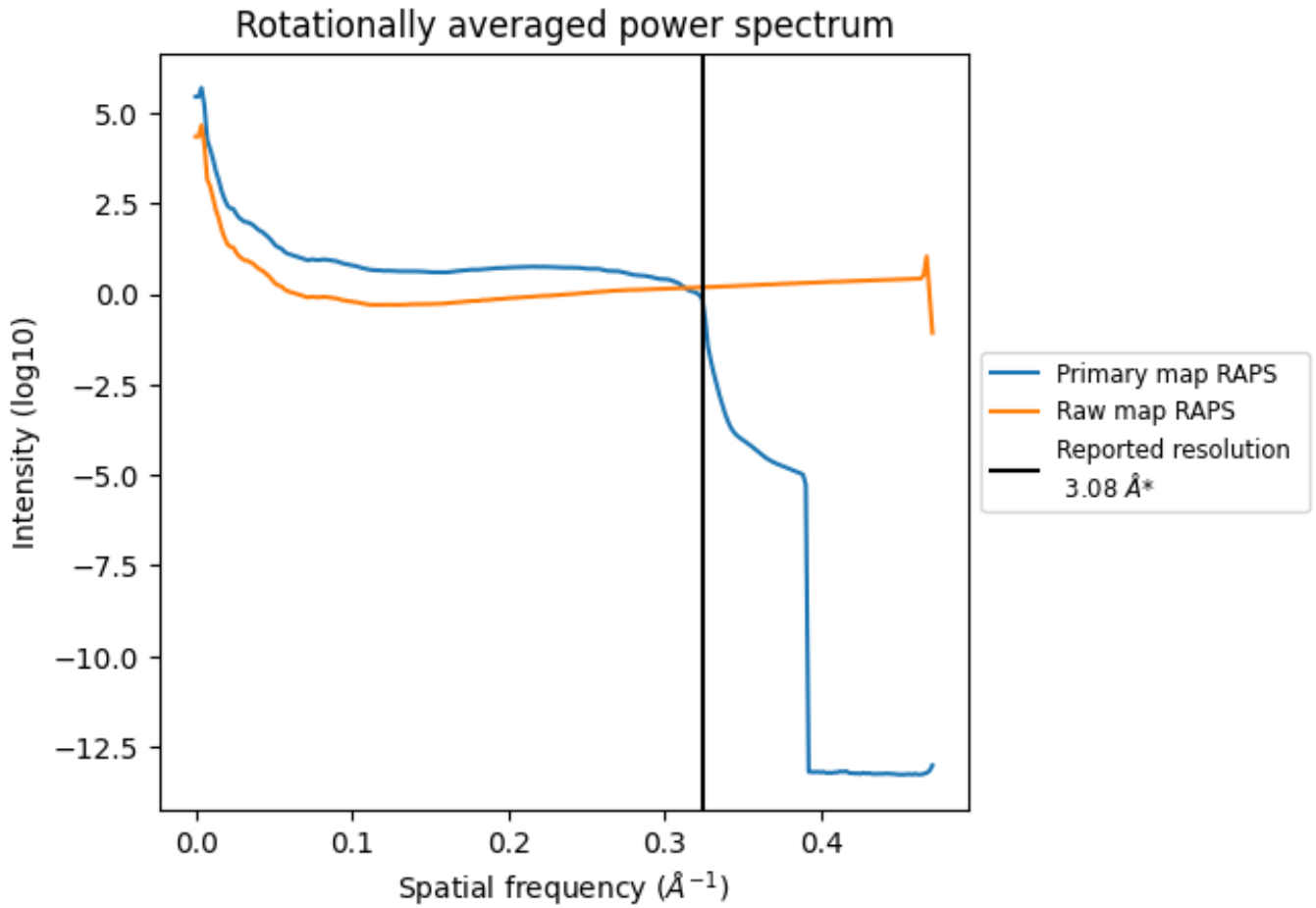
7.2 Volume estimate



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 241 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)

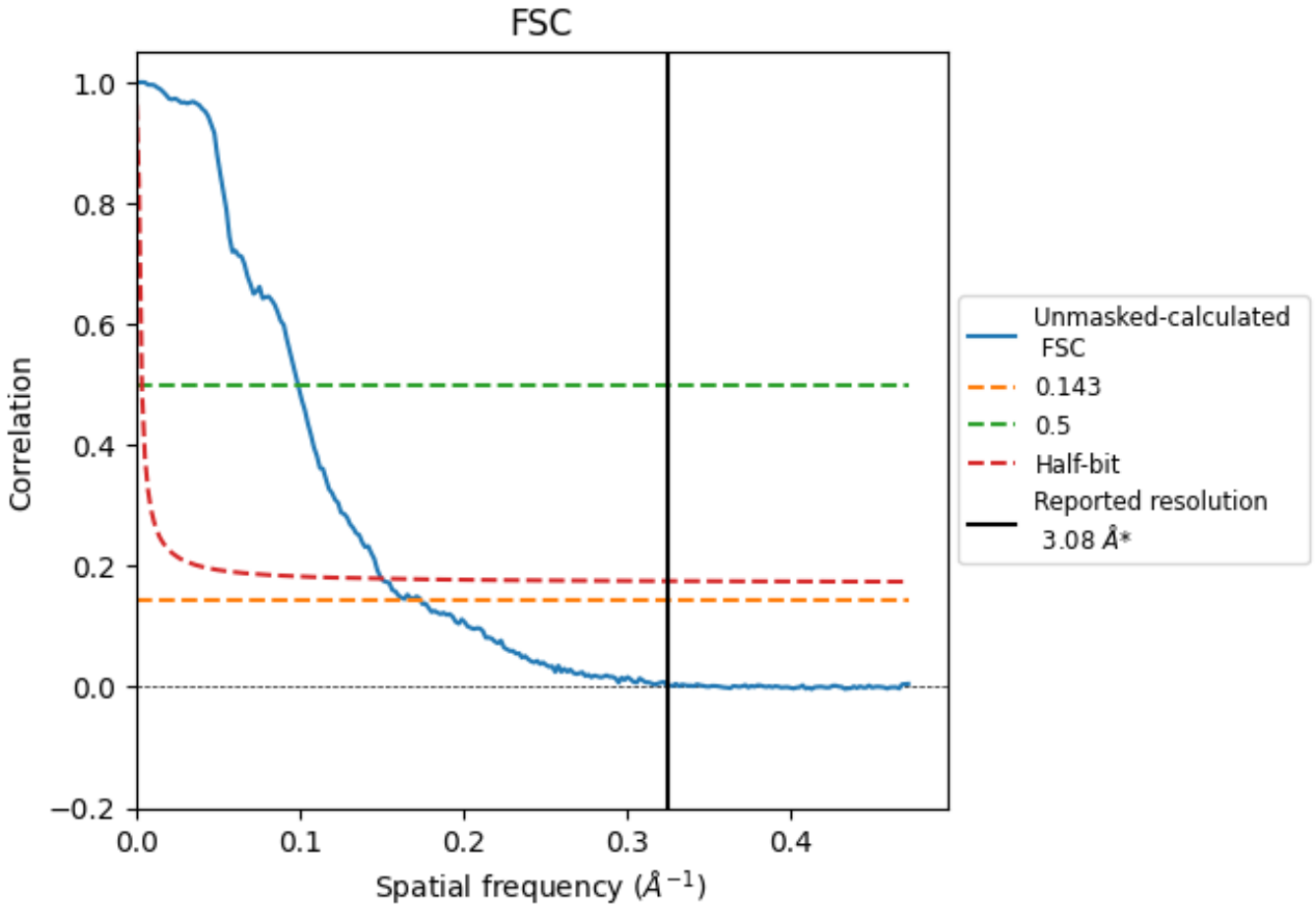


*Reported resolution corresponds to spatial frequency of 0.325 $Å^{-1}$

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 0.325 Å^{-1}

8.2 Resolution estimates (i)

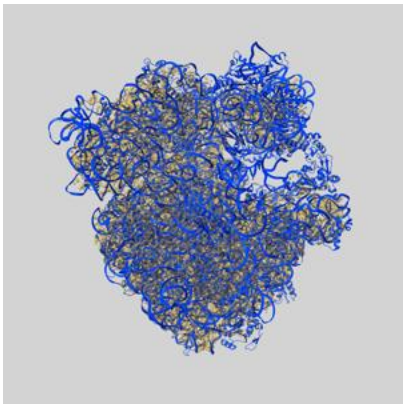
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.75	10.10	6.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.75 differs from the reported value 3.08 by more than 10 %

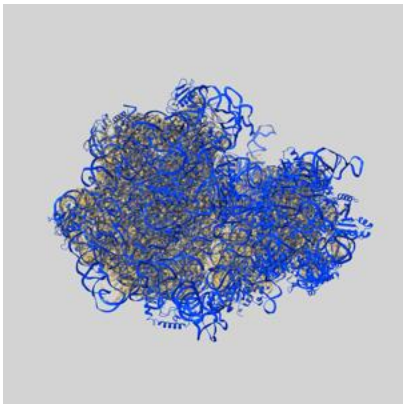
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55661 and PDB model 9T7X. Per-residue inclusion information can be found in section 3 on page 14.

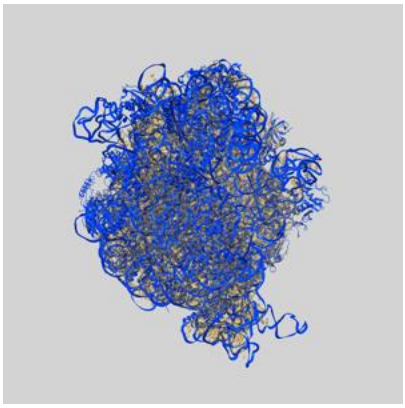
9.1 Map-model overlay



X



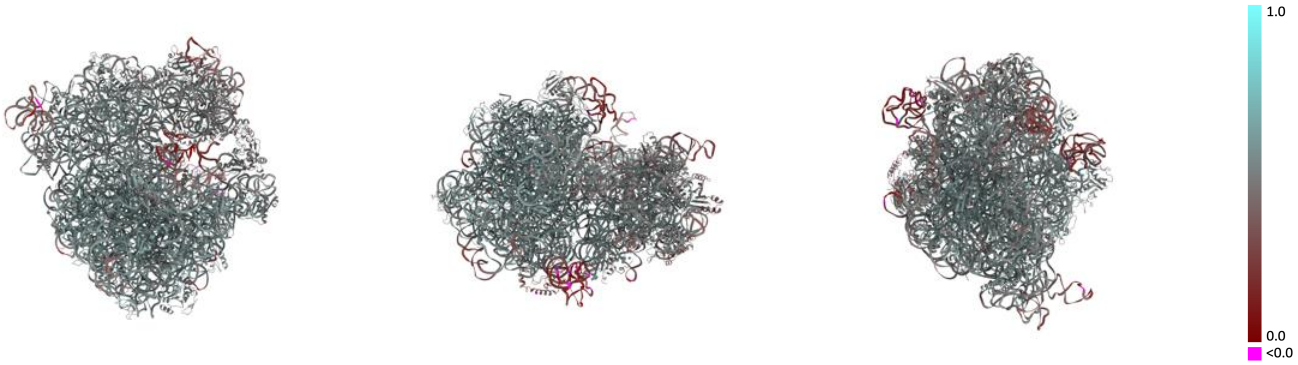
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

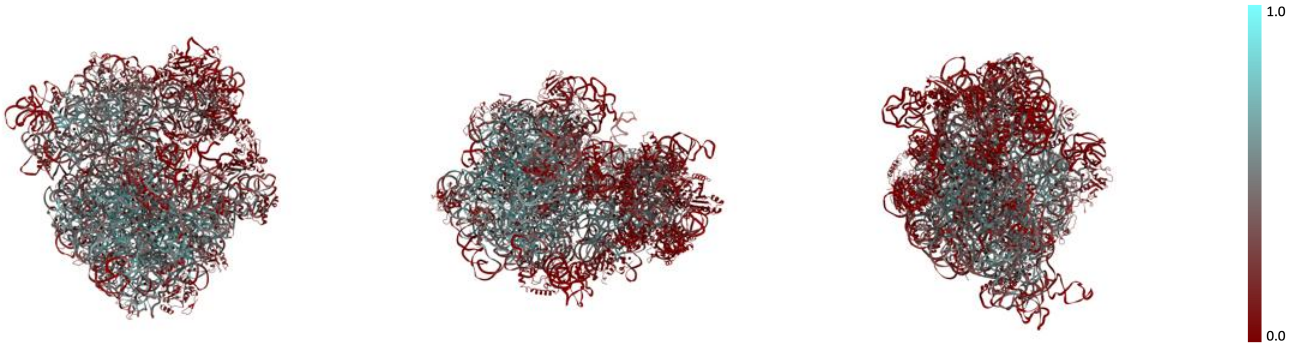
9.2 Q-score mapped to coordinate model (i)



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.

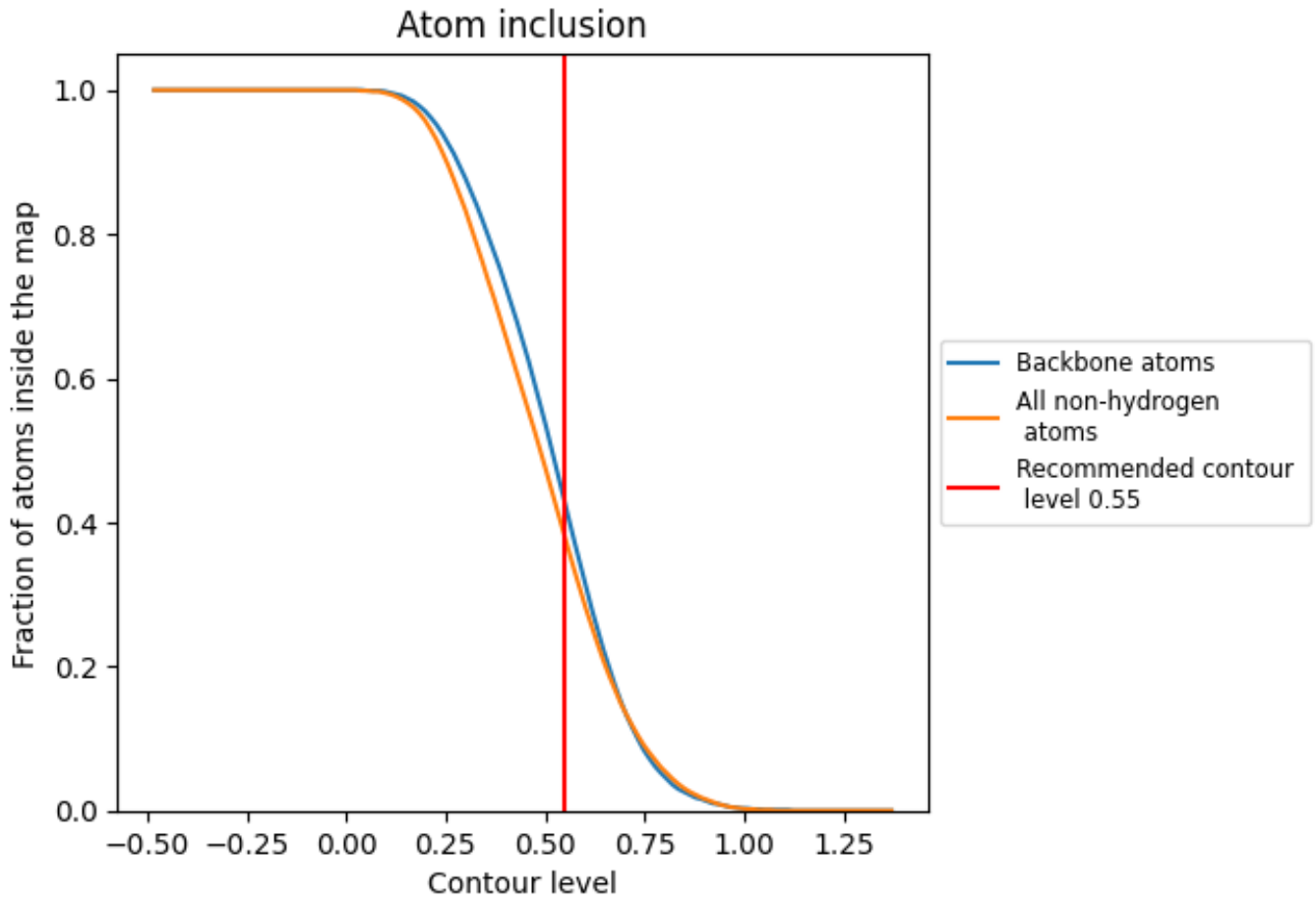
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 43% of all backbone atoms, 38% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3790	0.5140
0	0.1100	0.5430
1	0.4970	0.5670
2	0.3750	0.5720
3	0.3110	0.5500
4	0.0000	0.4260
A	0.3810	0.5010
B	0.0100	0.4480
C	0.0760	0.4950
D	0.1460	0.5130
E	0.2510	0.5410
F	0.1060	0.4950
G	0.0350	0.4590
H	0.2480	0.5380
I	0.0660	0.4860
J	0.0510	0.4700
K	0.1410	0.5070
L	0.2110	0.5360
M	0.0390	0.4870
N	0.0700	0.4910
O	0.1940	0.5280
P	0.2780	0.5380
Q	0.1740	0.5180
R	0.1500	0.4860
S	0.0170	0.4710
T	0.2210	0.5040
W	0.0180	0.2870
X	0.0400	0.4670
a	0.5000	0.5170
b	0.3510	0.5090
c	0.3980	0.5700
d	0.3580	0.5620
e	0.2770	0.5390
f	0.0450	0.4850
g	0.0670	0.4950



Continued on next page...

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Chain	Atom inclusion	Q-score
h	0.0040	0.3770
i	0.3700	0.5550
j	0.3230	0.5600
k	0.3260	0.5560
l	0.2670	0.5560
m	0.4260	0.5670
n	0.1850	0.5230
o	0.3190	0.5550
p	0.4610	0.5580
q	0.2900	0.5550
r	0.3660	0.5530
s	0.2770	0.5450
t	0.1680	0.5190
u	0.1870	0.5330
v	0.3970	0.5630
w	0.3450	0.5520
x	0.1290	0.5030
y	0.3360	0.5370
z	0.3540	0.5610