Full wwPDB EM Validation Report (i)

Sep 17, 2026 – 04:35 AM EDT

PDB ID	:	6V3B / pdb_00006v3b
EMDB ID	:	EMD-21032
Title	:	Cryo-EM structure of the Acinetobacter baumannii Ribosome: 70S in Empty state
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2019-11-25
Resolution	:	2.91 Å(reported)
Based on initial model	:	5AFI

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 (i) 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 (1)) were used in the production of this report:

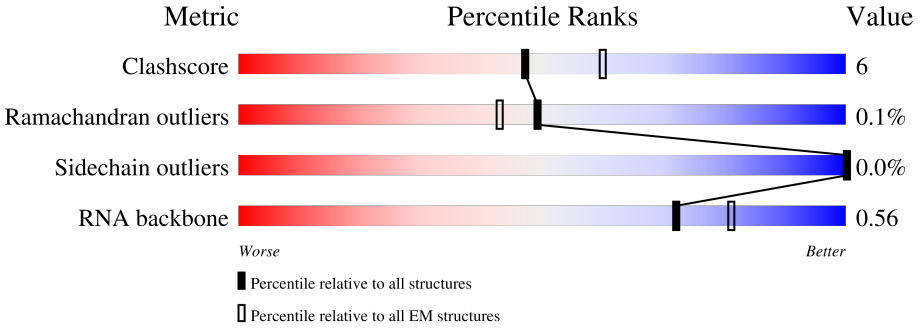
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

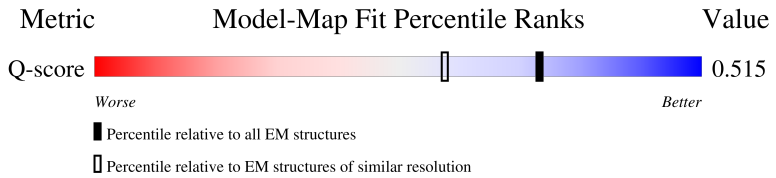
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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	51	8% 92% 8%
2	1	44	86% 14%
3	2	64	77% 17% • • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	92% 8%
5	AN1	2918	7% 64% 30% 5%
6	B	115	54% 37% 10%
7	C	274	88% 11%
8	D	212	92% 8%
9	E	200	5% 84% 9% 7%
10	F	178	20% 58% 40%
11	G	177	7% 81% 17%
12	H	148	19% 28% 13% 59%
13	I	142	82% 18%
14	J	122	93% 7%
15	K	146	80% 20%
16	L	137	7% 92% 8%
17	M	125	90% 5% 5%
18	N	116	7% 84% 14%
19	O	122	84% 12%
20	P	119	6% 90% 8%
21	Q	103	11% 83% 17%
22	R	109	93% 7%
23	S	106	8% 72% 13% 15%
24	T	105	16% 83% 12% 5%
25	U	98	8% 84% 15%
26	V	85	6% 87% 7% 6%
27	W	78	6% 90% 9%
28	X	65	11% 83% 12% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Y	58	10% 90% 10%
30	Z	61	13% 77% 13% 10%
31	sN1	1544	5% 64% 30% 5%
32	b	250	56% 59% 30% 10%
33	c	250	68% 18% 14%
34	d	208	7% 78% 21%
35	e	165	82% 12% 6%
36	f	127	19% 46% 28% 26%
37	g	156	17% 74% 17% 10%
38	h	131	84% 15%
39	i	128	90% 9%
40	j	103	5% 89% 8%
41	k	128	27% 74% 17% 9%
42	l	124	10% 78% 20%
43	m	118	82% 15%
44	n	101	81% 18%
45	o	89	96%
46	p	101	80% 18%
47	q	85	86% 8% 6%
48	r	75	51% 20% 29%
49	s	91	84% 7% 10%
50	t	88	92% 5%
51	u	71	23% 20% 10% 70%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 140290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	51	427	274	77	73	3	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	363	222	85	54	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	319	110	76	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	295	179	64	48	4	0	0

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	AN1	2892	62023	27689	11345	20098	2891	0	0

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	115	2450	1095	440	800	115	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	270	2096	1291	434	363	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	211	1572	972	297	300	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	186	1419	893	265	257	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	175	1381	877	247	249	8	0	0

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	174	1318	832	236	249	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	60	458	287	84	86	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	142	1125	718	200	203	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	122	946	592	180	169	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	146	1089	673	215	200	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	137	1087	687	210	185	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	119	942	590	186	163	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	114	857	528	173	155	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	O	117	919	578	177	164	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	117	934	589	197	146	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	103	807	506	155	143	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	109	826	514	158	150	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	S	90	702	447	127	128	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	T	100	749	465	139	145	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	97	760	477	143	139	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	80	598	370	115	111	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	77	632	395	130	105	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	62	498	308	96	93	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	58	463	286	88	85	4	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	55	456	271	102	82	1	0	0

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	sN1	1528	32782	14631	5994	10630	1527	0	0

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	225	1769	1110	328	325	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	215	1690	1065	318	299	8	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	207	1631	1017	313	299	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	155	1129	700	217	207	5	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	94	793	499	147	143	4	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	141	1111	696	210	199	6	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	130	985	615	177	187	6	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	127	995	621	198	175	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	100	801	500	150	148	3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	117	862	535	167	159	1	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l	122	945	580	193	167	5	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	m	115	903	558	184	158	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	100	792	493	158	137	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	88	705	434	144	126	1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	83	649	406	129	113	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	80	630	396	118	115	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	r	53	438	282	75	81	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	82	646	412	125	107	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t	85	658	406	138	112	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	u	21	182	115	37	30	0	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	3	1	1	1	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	AN1	52	52	52	0
53	sN1	41	41	41	0

- Molecule 54 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
54	AN1	1	1	1	0

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
55	3	1	1	1	0
55	AN1	253	253	253	0

Continued on next page...

Continued from previous page...

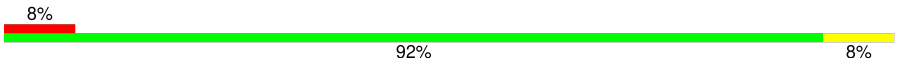
Mol	Chain	Residues	Atoms	AltConf
55	B	5	Total O 5 5	0
55	C	3	Total O 3 3	0
55	D	3	Total O 3 3	0
55	E	2	Total O 2 2	0
55	K	3	Total O 3 3	0
55	M	1	Total O 1 1	0
55	P	1	Total O 1 1	0
55	Q	3	Total O 3 3	0
55	R	1	Total O 1 1	0
55	V	2	Total O 2 2	0
55	Y	1	Total O 1 1	0
55	Z	1	Total O 1 1	0
55	sN1	107	Total O 107 107	0
55	g	1	Total O 1 1	0
55	h	1	Total O 1 1	0
55	i	2	Total O 2 2	0
55	m	2	Total O 2 2	0
55	n	1	Total O 1 1	0
55	s	3	Total O 3 3	0
55	t	1	Total O 1 1	0

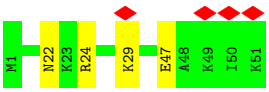
3 Residue-property plots (i)

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: 50S ribosomal protein L33

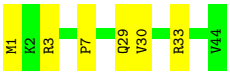
Chain 0:





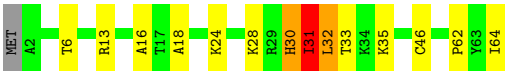
- Molecule 2: 50S ribosomal protein L34

Chain 1:



- Molecule 3: 50S ribosomal protein L35

Chain 2:

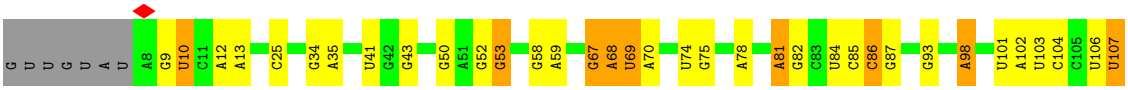


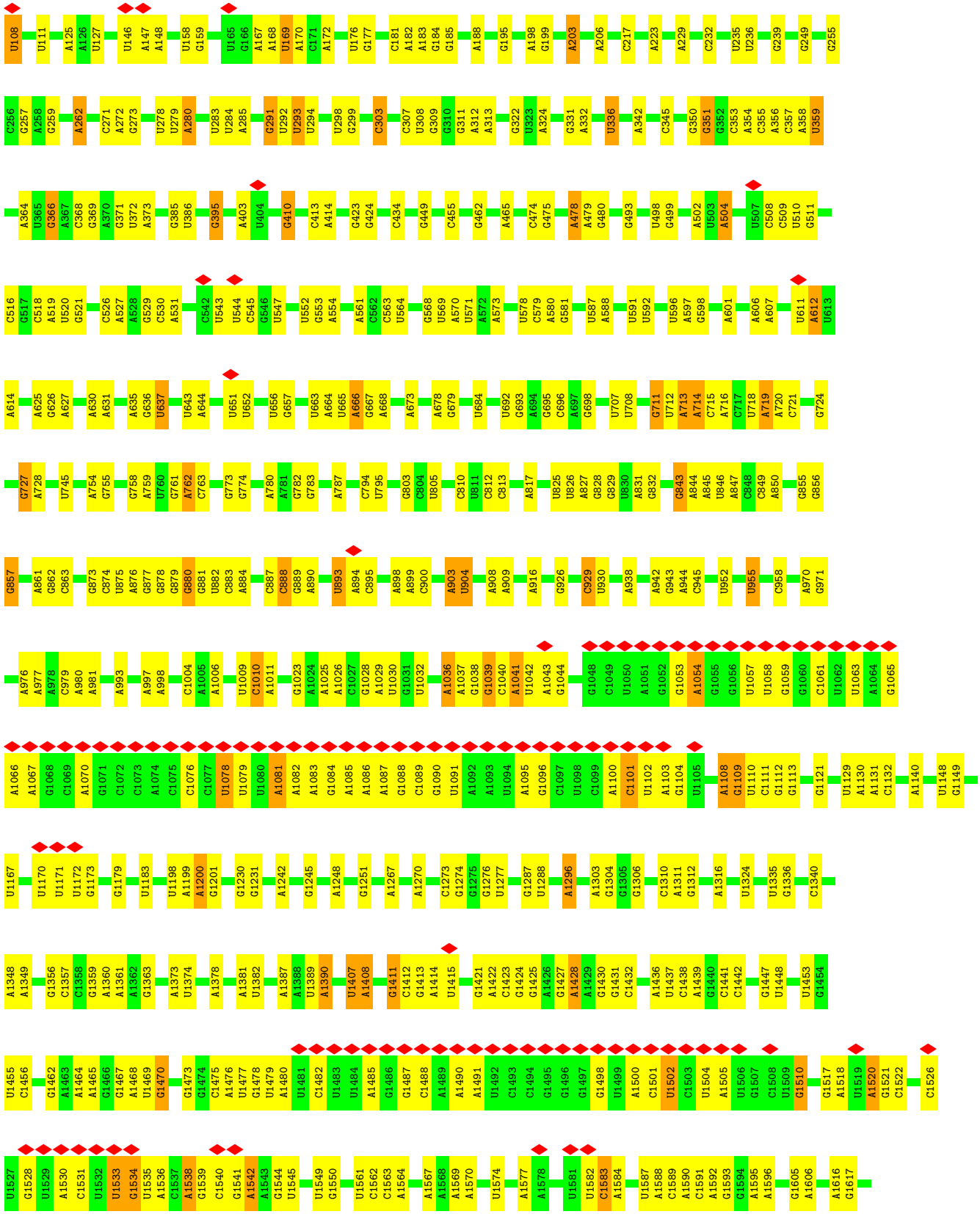
- Molecule 4: 50S ribosomal protein L36

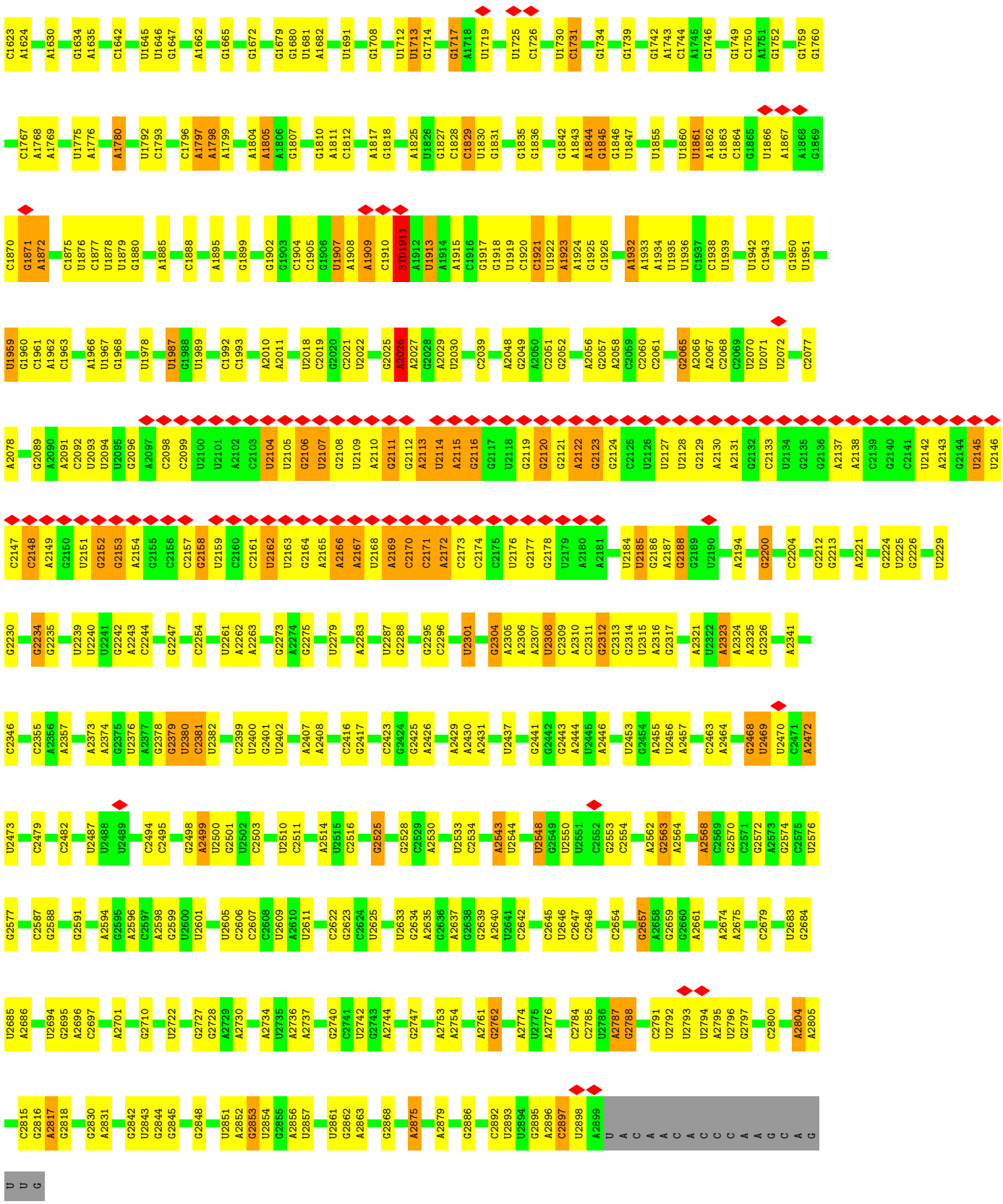
Chain 3:

- Molecule 5: 23s ribosomal RNA

Chain AN1:

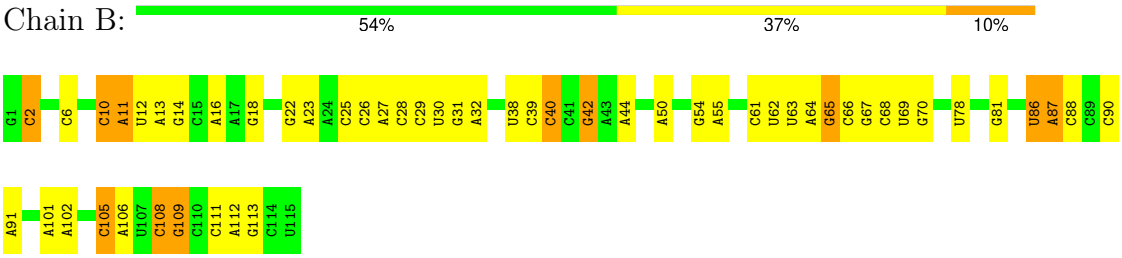



U108 U111 A125 A126 U127 U146 A147 A148 U158 G159 U165 G166 A167 A168 U169 A170 C171 A172 U176 G177 C181 A182 A183 G184 G185 A188 G195 A198 G199 A203 A206 C217 A223 A229 C232 U235 U236 G239 G249 G255
C256 G257 A258 G259 A262 C271 A272 G273 U278 U279 A280 U283 U284 A285 G291 U292 U293 U294 U298 G299 C303 C307 U308 G309 G310 G311 A312 A313 G322 U323 A324 G331 A332 U336 A342 C345 G350 G351 G352 C353 A354 C355 A356 C357 A358 U359
A364 U365 G366 A367 C368 G369 A370 G371 U372 A373 G385 U386 G395 A403 U404 G410 C413 A414 G423 G424 C434 G449 C455 G462 A465 C474 G475 A478 A479 G480 G493 U498 G499 A502 U503 A504 U507 C508 C509 U510 G511
C516 G517 C518 A519 U520 G521 C526 A527 A528 G529 C530 A531 C542 U543 U544 C545 G546 U547 U552 G553 A554 A561 C562 C563 U564 G568 U569 A570 U571 A572 A573 U578 C579 A580 G581 U587 A588 U591 U592 U596 A597 G598 A601 A606 A607 U611 A612 U613
A614 A625 G626 A627 A630 A631 A635 G636 U637 U643 A644 U651 U652 U656 G657 U663 A664 U665 A666 G667 A668 A673 A678 G679 U684 U692 G693 A694 G695 C696 A697 G698 U707 U708 G711 U712 A713 A714 C715 A716 C717 U718 A719 A720 C721 G724
G727 A728 U745 A754 G755 G758 A759 U760 G761 A762 C763 G773 G774 A780 A781 G782 G783 A787 C794 U795 G803 C804 U805 C810 U811 C812 C813 A817 U825 U826 A827 G828 G829 U830 A831 G832 G843 A844 A845 U846 A847 C848 C849 A850 G855 G856
G857 A861 G862 C863 G873 C874 U875 A876 G877 G878 G879 G880 G881 U882 C883 A884 C887 C888 G889 A890 U893 A894 C895 A898 A899 C900 A903 U904 A908 A909 A916 G926 C929 U930 A938 A942 G943 A944 C945 U952 U955 C958 A970 G971
A976 A977 A978 C979 A980 A981 A993 A997 A998 C1004 A1005 A1006 U1009 C1010 A1011 G1023 A1024 A1025 A1026 C1027 G1028 A1029 U1030 G1031 U1032 A1036 A1037 G1038 G1039 C1040 A1041 U1042 A1043 G1044 G1048 C1049 U1050 A1051 G1052 G1053 A1054 G1055 G1056 U1057 U1058 G1059 G1060 C1061 U1062 U1063 A1064 G1065
A1066 A1067 G1068 C1069 A1070 G1071 C1072 C1073 A1074 C1075 C1076 C1077 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 A1103 G1104 U1105 A1108 G1109 U1110 C1111 G1112 G1113 G1121 U1129 A1130 A1131 C1132 A1140 U1148 G1149
U1167 U1170 U1171 U1172 G1173 G1179 U1183 U1198 A1199 A1200 G1201 G1230 G1231 A1242 G1245 A1248 G1251 A1267 A1270 C1273 G1274 G1275 G1276 U1277 G1287 U1288 A1296 A1303 G1304 G1305 G1306 C1310 A1311 G1312 A1316 U1324 U1335 G1336 C1340
A1348 A1349 G1356 C1357 C1358 G1359 A1360 A1361 A1362 G1363 A1373 U1374 A1378 A1381 U1382 A1387 A1388 U1389 A1390 U1407 A1408 G1411 C1412 G1413 A1414 U1415 G1421 A1422 C1423 G1424 G1425 A1426 G1427 A1428 A1429 G1430 G1431 C1432 A1436 U1437 C1438 A1439 G1440 C1441 C1442 G1447 U1448 U1453 G1454
U1455 C1456 G1462 A1463 A1464 A1465 G1466 G1467 A1468 U1469 G1470 G1473 G1474 C1475 A1476 U1477 G1478 U1479 A1480 U1481 C1482 U1483 U1484 A1485 G1486 G1487 C1488 A1489 A1490 A1491 U1492 C1493 C1494 G1495 G1496 G1497 G1498 U1499 A1500 C1501 U1502 C1503 U1504 A1505 U1506 G1507 C1508 U1509 G1510 G1517 A1518 U1519 A1520 G1521 C1522 C1526
U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 A1536 C1537 A1538 G1539 C1540 G1541 A1542 A1543 G1544 U1545 U1549 G1550 U1561 C1562 C1563 A1564 A1567 A1568 A1569 A1570 U1574 A1577 A1578 U1581 U1582 C1583 A1584 U1587 A1588 C1589 A1590 C1591 A1592 G1593 G1594 A1595 A1596 G1605 A1606 A1616 G1617



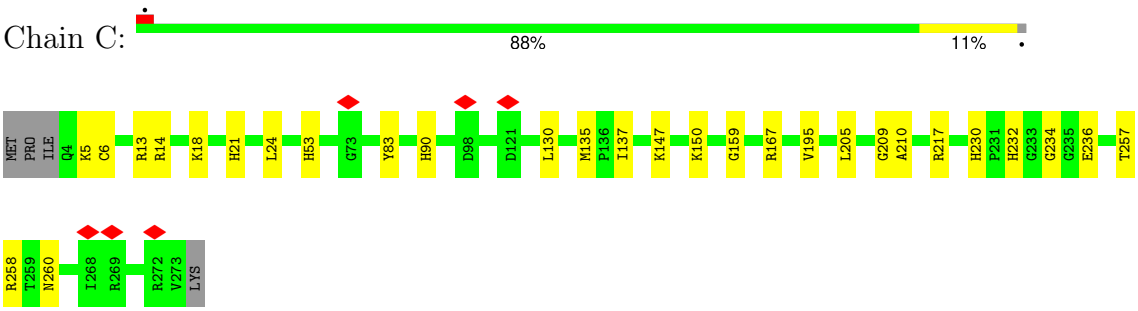
- Molecule 6: 5s ribosomal RNA

Chain B:



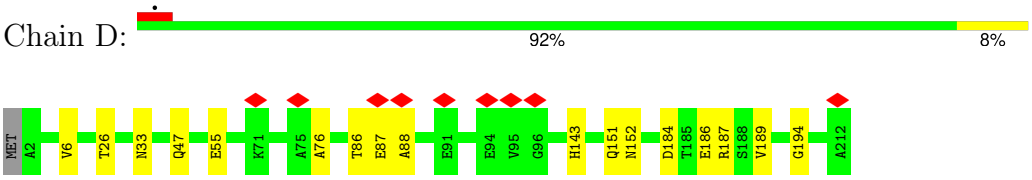
• Molecule 7: 50S ribosomal protein L2

Chain C:



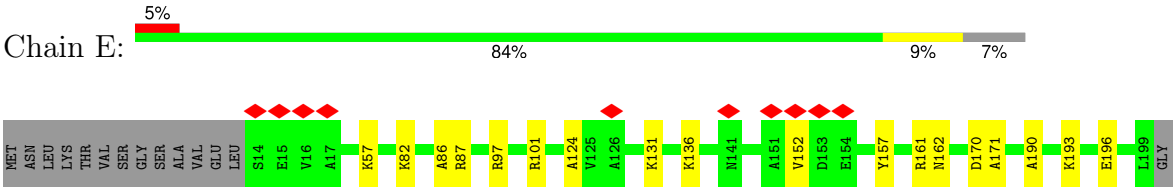
• Molecule 8: 50S ribosomal protein L3

Chain D:



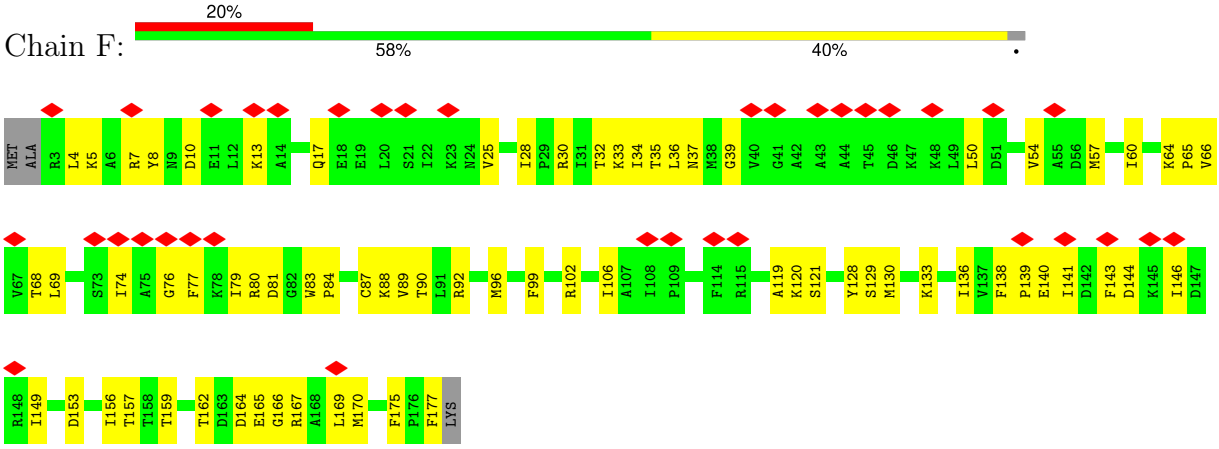
• Molecule 9: 50S ribosomal protein L4

Chain E:



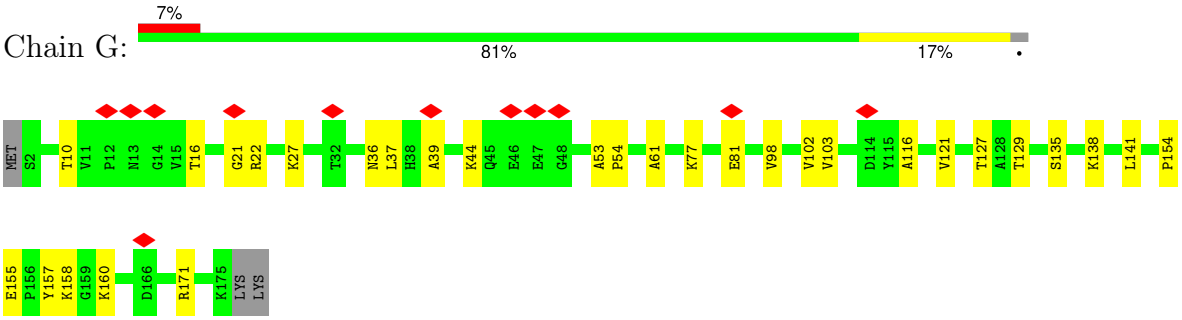
• Molecule 10: 50S ribosomal protein L5

Chain F:



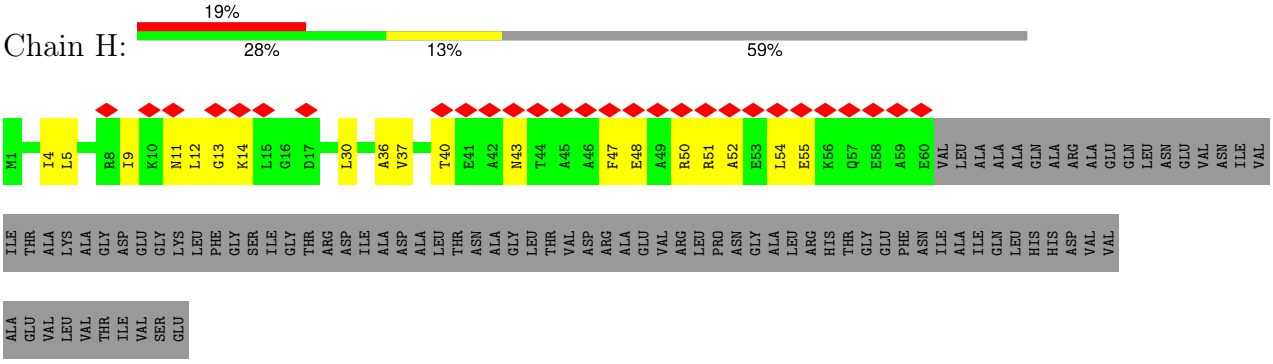
• Molecule 11: 50S ribosomal protein L6

Chain G:



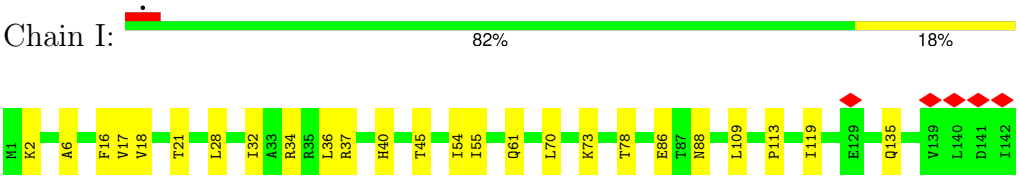
- Molecule 12: 50S ribosomal protein L9

Chain H:



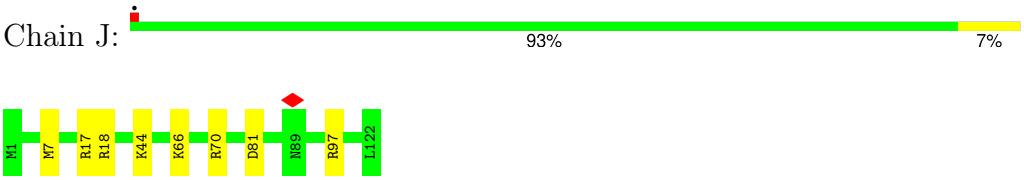
- Molecule 13: 50S ribosomal protein L13

Chain I:



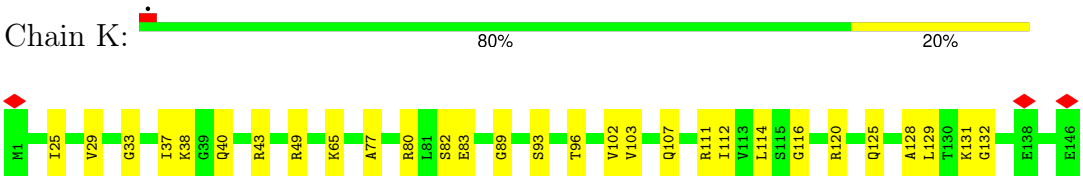
- Molecule 14: 50S ribosomal protein L14

Chain J:



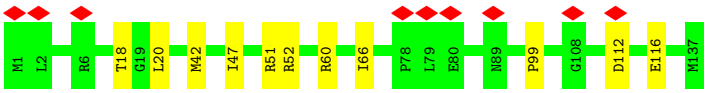
- Molecule 15: 50S ribosomal protein L15

Chain K:



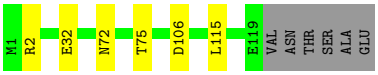
- Molecule 16: 50S ribosomal protein L16

Chain L:



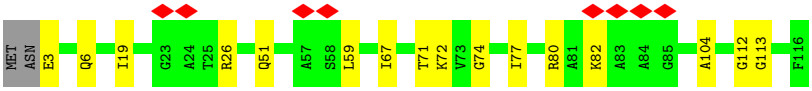
• Molecule 17: 50S ribosomal protein L17

Chain M:



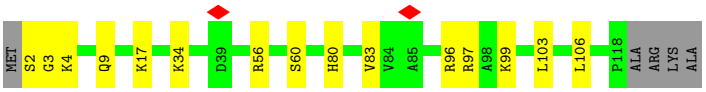
• Molecule 18: 50S ribosomal protein L18

Chain N:



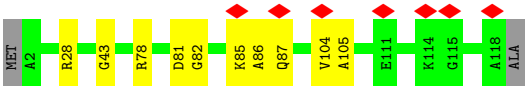
• Molecule 19: 50S ribosomal protein L19

Chain O:



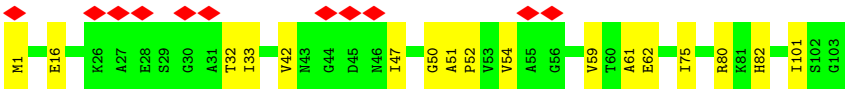
• Molecule 20: 50S ribosomal protein L20

Chain P:



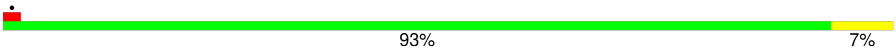
• Molecule 21: 50S ribosomal protein L21

Chain Q:



• Molecule 22: 50S ribosomal protein L22

Chain R:

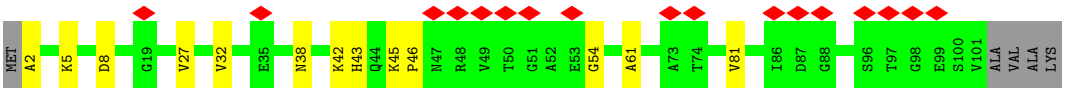


• Molecule 23: 50S ribosomal protein L23

Chain S:

- Molecule 24: 50S ribosomal protein L24

Chain T:

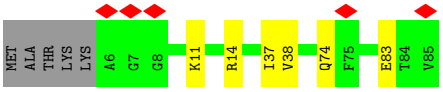


- Molecule 25: 50S ribosomal protein L25

Chain U:

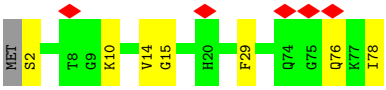
- Molecule 26: 50S ribosomal protein L27

Chain V:



- Molecule 27: 50S ribosomal protein L28

Chain W:

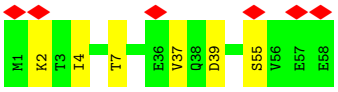


- Molecule 28: 50S ribosomal protein L29

Chain X:

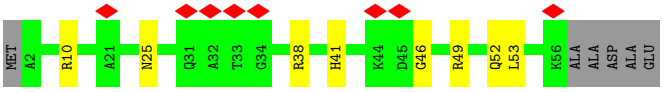
- Molecule 29: 50S ribosomal protein L30

Chain Y:



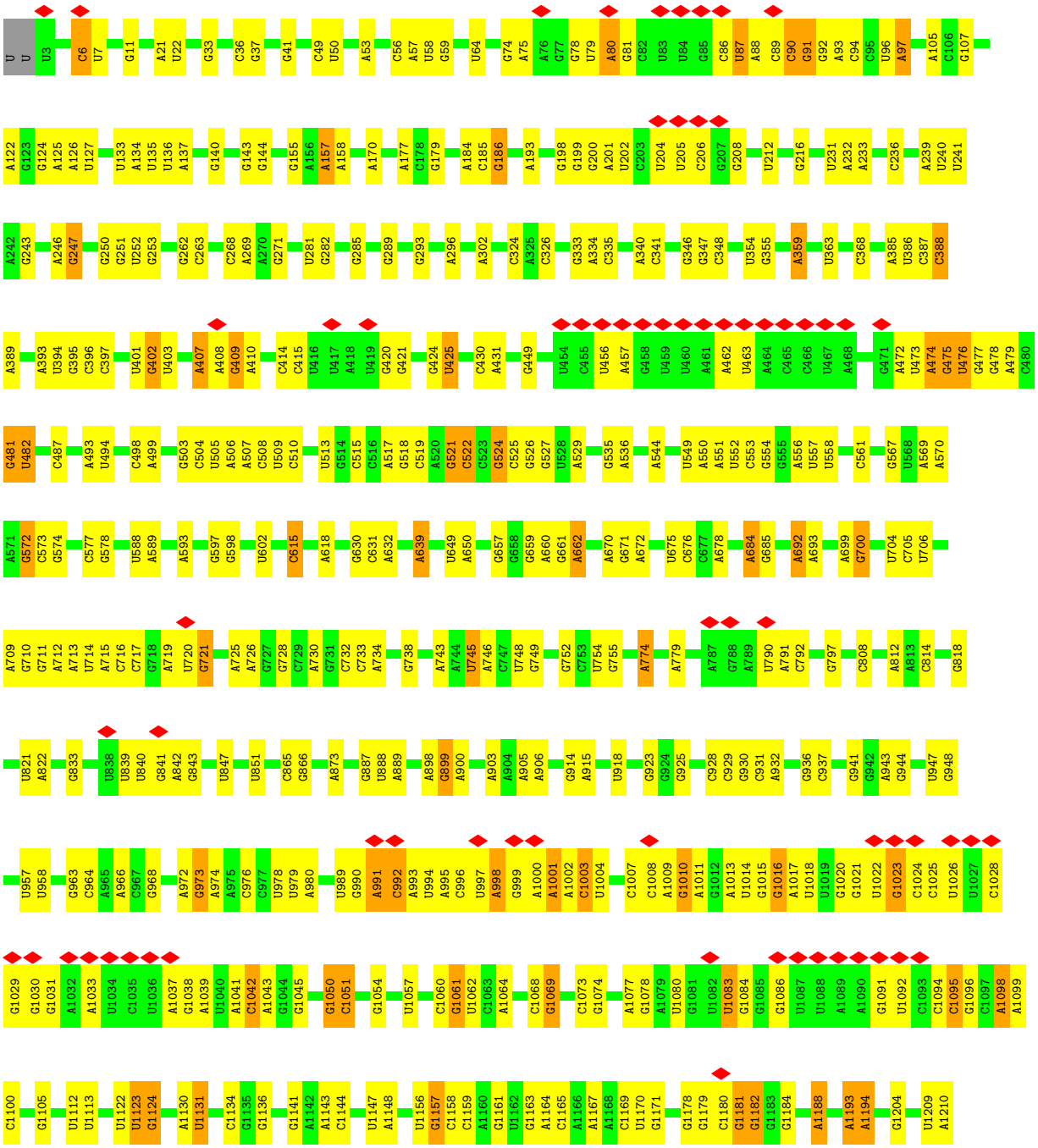
- Molecule 30: 50S ribosomal protein L32

Chain Z:



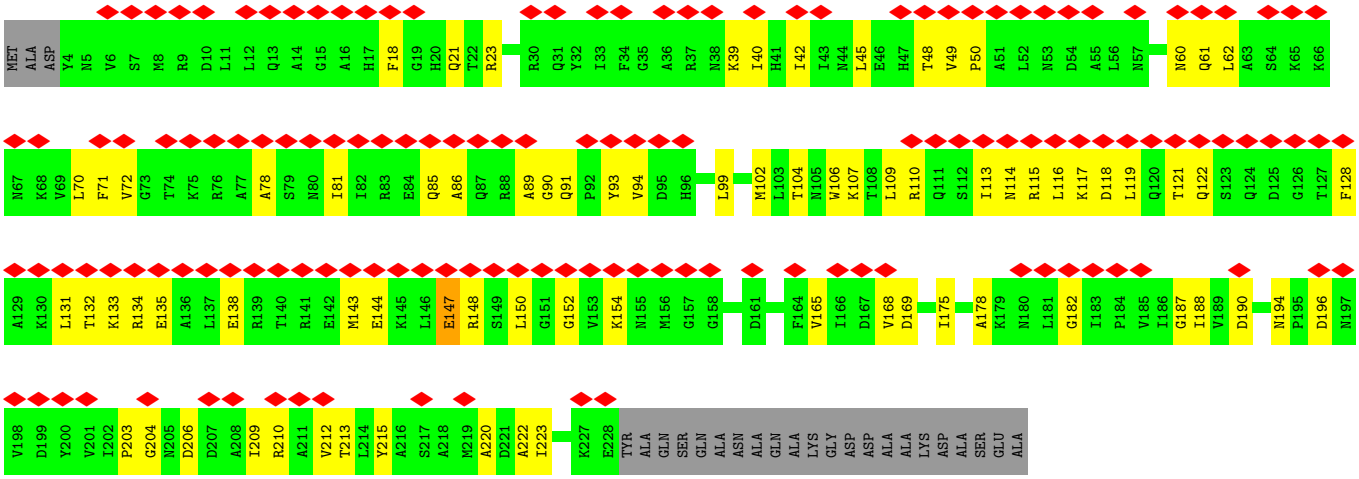
- Molecule 31: 16s Ribosomal RNA

Chain sN1:



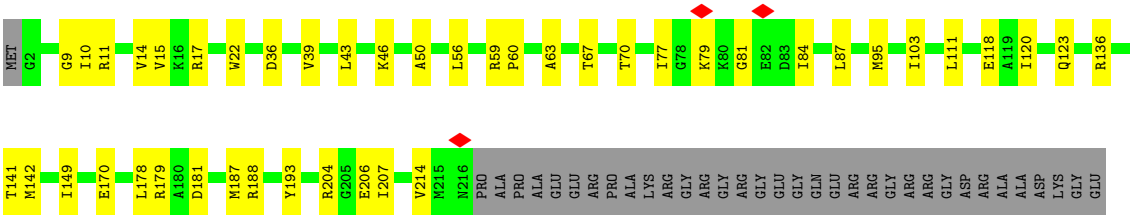
- Molecule 32: 30S ribosomal protein S2

Chain b:



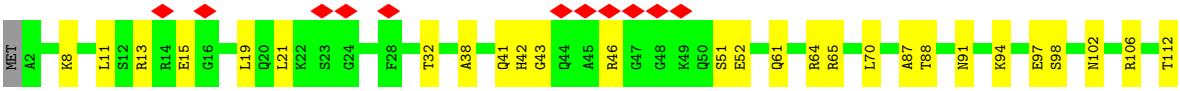
- Molecule 33: 30S ribosomal protein S3

Chain c:



- Molecule 34: 30S ribosomal protein S4

Chain d:

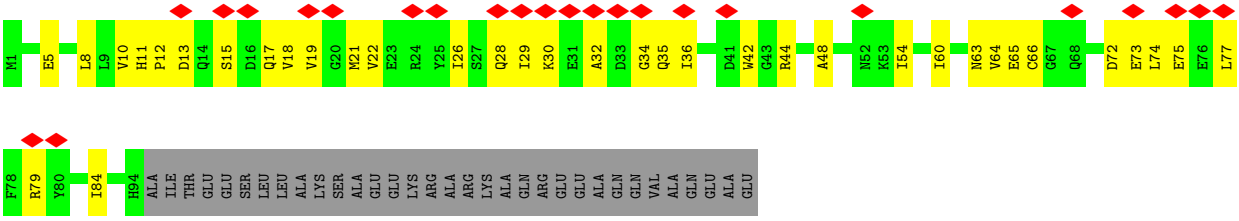


• Molecule 35: 30S ribosomal protein S5

Chain e:

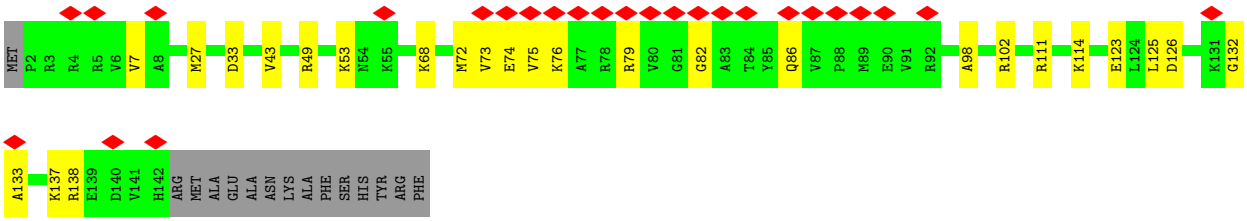
• Molecule 36: 30S ribosomal protein S6

Chain f:



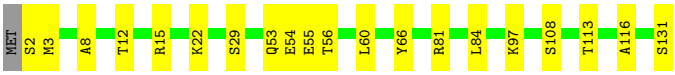
• Molecule 37: 30S ribosomal protein S7

Chain g:



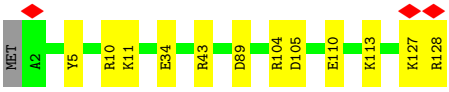
• Molecule 38: 30S ribosomal protein S8

Chain h:



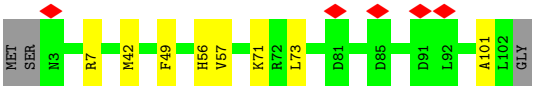
• Molecule 39: 30S ribosomal protein S9

Chain i:



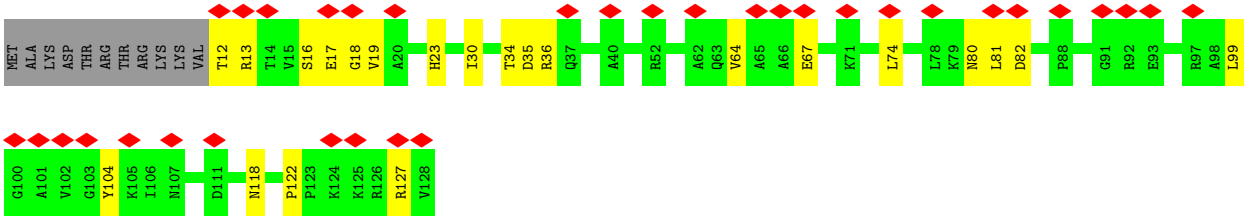
• Molecule 40: 30S ribosomal protein S10

Chain j:



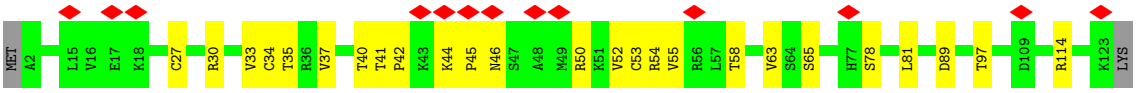
• Molecule 41: 30S ribosomal protein S11

Chain k:



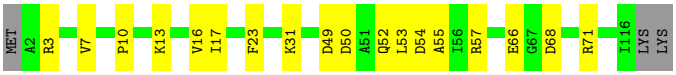
• Molecule 42: 30S ribosomal protein S12

Chain l:



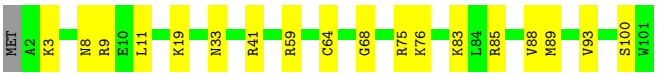
• Molecule 43: 30S ribosomal protein S13

Chain m:



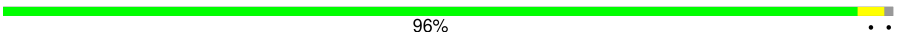
• Molecule 44: 30S ribosomal protein S14

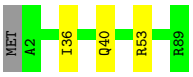
Chain n:



• Molecule 45: 30S ribosomal protein S15

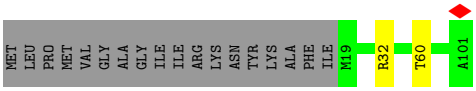
Chain o:





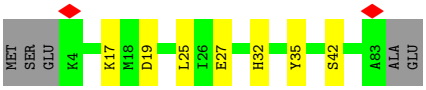
• Molecule 46: 30S ribosomal protein S16

Chain p:



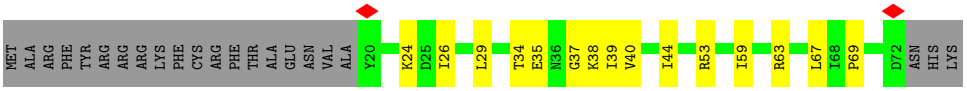
• Molecule 47: 30S ribosomal protein S17

Chain q:



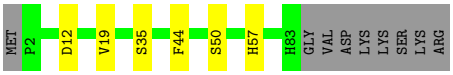
• Molecule 48: 30S ribosomal protein S18

Chain r:



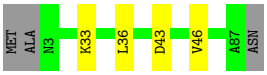
• Molecule 49: 30S ribosomal protein S19

Chain s:



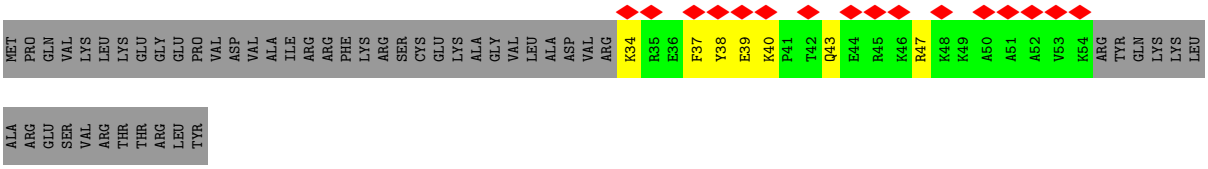
• Molecule 50: 30S ribosomal protein S20

Chain t:



• Molecule 51: 30S ribosomal protein S21

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.794	Depositor
Minimum map value	-2.515	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	544.768, 544.768, 544.768	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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: 2MA, PSU, 3TD, MG, OMG, 6MZ, 4OC, UR3, 5MC, MA6, 7MG, OMU, ZN, 2MG, NA, 5MU

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	0.14	0/434	0.36	0/573
2	1	0.13	0/367	0.36	0/481
3	2	0.17	0/515	0.51	0/678
4	3	0.15	0/296	0.46	0/389
5	AN1	0.10	0/69101	0.24	0/107780
6	B	0.09	0/2739	0.22	0/4266
7	C	0.13	0/2136	0.36	0/2869
8	D	0.13	0/1590	0.33	0/2142
9	E	0.12	0/1440	0.31	0/1944
10	F	0.19	0/1401	0.53	0/1877
11	G	0.15	0/1337	0.41	2/1807 (0.1%)
12	H	0.18	0/461	0.57	0/616
13	I	0.13	0/1151	0.32	0/1551
14	J	0.13	0/956	0.36	0/1286
15	K	0.13	0/1097	0.40	0/1461
16	L	0.13	0/1104	0.32	0/1475
17	M	0.14	0/956	0.37	0/1282
18	N	0.13	0/865	0.37	0/1156
19	O	0.13	0/931	0.34	0/1249
20	P	0.14	0/947	0.33	0/1262
21	Q	0.15	0/818	0.37	0/1094
22	R	0.11	0/831	0.31	0/1113
23	S	0.13	0/708	0.31	0/947
24	T	0.15	0/753	0.47	0/1010
25	U	0.13	0/770	0.35	0/1036
26	V	0.13	0/606	0.34	0/810
27	W	0.12	0/642	0.33	0/856
28	X	0.12	0/499	0.30	0/662
29	Y	0.13	0/468	0.35	0/624
30	Z	0.13	0/462	0.36	0/615
31	sN1	0.09	0/36476	0.21	0/56895
32	b	0.19	0/1799	0.50	0/2429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.13	0/1714	0.35	0/2304
34	d	0.12	0/1653	0.35	0/2213
35	e	0.12	0/1141	0.32	0/1537
36	f	0.16	0/808	0.49	0/1089
37	g	0.14	0/1127	0.36	0/1511
38	h	0.12	0/993	0.30	0/1331
39	i	0.13	0/1006	0.36	0/1346
40	j	0.14	0/811	0.37	0/1096
41	k	0.15	0/878	0.42	0/1189
42	l	0.16	0/958	0.46	0/1284
43	m	0.16	0/913	0.41	0/1226
44	n	0.12	0/803	0.32	0/1071
45	o	0.10	0/715	0.27	0/958
46	p	0.11	0/660	0.31	0/886
47	q	0.13	0/637	0.34	0/858
48	r	0.15	0/445	0.38	0/601
49	s	0.12	0/664	0.33	0/897
50	t	0.14	0/664	0.30	0/885
51	u	0.27	0/184	0.68	0/240
All	All	0.11	0/151430	0.27	2/226757 (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
3	2	0	1
12	H	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	10	THR	CA-C-N	-5.11	118.91	122.59
11	G	10	THR	C-N-CA	-5.11	118.91	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	HIS	Peptide
12	H	47	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	2	0
2	1	363	0	401	5	0
3	2	509	0	566	12	0
4	3	295	0	326	2	0
5	AN1	62023	0	31194	500	0
6	B	2450	0	1241	44	0
7	C	2096	0	2157	20	0
8	D	1572	0	1610	13	0
9	E	1419	0	1464	16	0
10	F	1381	0	1433	56	0
11	G	1318	0	1373	20	0
12	H	458	0	480	13	0
13	I	1125	0	1148	16	0
14	J	946	0	1007	6	0
15	K	1089	0	1159	18	0
16	L	1087	0	1162	7	0
17	M	942	0	987	4	0
18	N	857	0	899	10	0
19	O	919	0	973	9	0
20	P	934	0	997	8	0
21	Q	807	0	842	16	0
22	R	826	0	894	6	0
23	S	702	0	756	11	0
24	T	749	0	797	9	0
25	U	760	0	783	11	0
26	V	598	0	600	4	0
27	W	632	0	667	6	0
28	X	498	0	537	6	0
29	Y	463	0	488	3	0
30	Z	456	0	448	6	0
31	sN1	32782	0	16507	310	0
32	b	1769	0	1787	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	1690	0	1774	28	0
34	d	1631	0	1691	30	0
35	e	1129	0	1174	11	0
36	f	793	0	788	24	0
37	g	1111	0	1163	15	0
38	h	985	0	1047	12	0
39	i	995	0	1053	7	0
40	j	801	0	832	5	0
41	k	862	0	877	15	0
42	l	945	0	996	16	0
43	m	903	0	962	15	0
44	n	792	0	833	15	0
45	o	705	0	712	2	0
46	p	649	0	660	1	0
47	q	630	0	678	5	0
48	r	438	0	456	11	0
49	s	646	0	663	3	0
50	t	658	0	710	2	0
51	u	182	0	198	7	0
52	3	1	0	0	0	0
53	AN1	52	0	0	0	0
53	sN1	41	0	0	0	0
54	AN1	1	0	0	0	0
55	3	1	0	0	0	0
55	AN1	253	0	0	2	0
55	B	5	0	0	1	0
55	C	3	0	0	0	0
55	D	3	0	0	0	0
55	E	2	0	0	0	0
55	K	3	0	0	0	0
55	M	1	0	0	0	0
55	P	1	0	0	1	0
55	Q	3	0	0	0	0
55	R	1	0	0	0	0
55	V	2	0	0	0	0
55	Y	1	0	0	0	0
55	Z	1	0	0	0	0
55	g	1	0	0	0	0
55	h	1	0	0	0	0
55	i	2	0	0	0	0
55	m	2	0	0	0	0
55	n	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	s	3	0	0	0	0
55	sN1	107	0	0	1	0
55	t	1	0	0	0	0
All	All	140290	0	93412	1323	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 6.

All (1323) 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)
5:AN1:1462:G:H1	5:AN1:1520:A:N6	1.43	1.16
31:sN1:1157:G:N7	31:sN1:1179:G:N2	2.18	0.91
5:AN1:2096:G:H1	5:AN1:2185:U:H3	0.91	0.90
6:B:70:G:H21	6:B:101:A:H62	1.11	0.89
6:B:2:C:O2	6:B:113:G:N2	2.08	0.86
31:sN1:74:G:H1	31:sN1:93:A:H61	1.24	0.85
10:F:146:ILE:HD12	10:F:149:ILE:HD11	1.59	0.84
31:sN1:657:G:N1	31:sN1:743:A:N6	2.24	0.84
34:d:11:LEU:HD22	34:d:65:ARG:HE	1.42	0.82
5:AN1:1846:G:N2	5:AN1:1888:C:O2	2.11	0.82
31:sN1:928:C:O2	31:sN1:1383:G:N2	2.10	0.81
31:sN1:1442:U:H3	31:sN1:1454:G:H1	1.29	0.80
5:AN1:873:G:N1	5:AN1:900:C:N3	2.30	0.79
5:AN1:1713:U:H3	5:AN1:1739:G:H1	1.30	0.79
6:B:70:G:N2	6:B:101:A:H62	1.80	0.79
5:AN1:873:G:N2	5:AN1:900:C:O2	2.16	0.79
3:2:30:HIS:O	3:2:32:LEU:N	2.16	0.78
10:F:120:LYS:HG3	10:F:121:SER:H	1.48	0.78
31:sN1:657:G:C6	31:sN1:743:A:N6	2.50	0.78
18:N:82:LYS:NZ	18:N:112:GLY:O	2.15	0.78
31:sN1:503:G:N1	31:sN1:522:C:N3	2.29	0.78
43:m:23:PHE:HB3	43:m:66:GLU:HG2	1.66	0.77
5:AN1:1595:A:H5"	5:AN1:1596:A:H5'	1.66	0.77
1:0:29:LYS:HB3	1:0:47:GLU:HB3	1.67	0.77
6:B:18:G:N1	6:B:61:C:N3	2.29	0.77
32:b:144:GLU:OE2	32:b:148:ARG:NH1	2.15	0.76
7:C:5:LYS:NZ	7:C:14:ARG:O	2.17	0.75
6:B:2:C:N3	6:B:113:G:N1	2.31	0.75
5:AN1:875:U:O2	5:AN1:898:A:N7	2.19	0.75
5:AN1:1862:A:H61	5:AN1:1871:G:H2'	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:34:CYS:HA	42:l:55:VAL:HA	1.68	0.74
5:AN1:879:G:H2'	5:AN1:880:G:H8	1.52	0.74
5:AN1:1036:A:H61	5:AN1:1113:G:H1	1.32	0.74
31:sN1:1157:G:O6	31:sN1:1179:G:N1	2.19	0.74
17:M:32:GLU:HG2	17:M:115:LEU:HD12	1.71	0.73
6:B:18:G:N2	6:B:61:C:O2	2.15	0.73
5:AN1:878:G:H2'	5:AN1:879:G:H8	1.54	0.72
5:AN1:2301:U:H3	10:F:39:GLY:H	1.35	0.72
31:sN1:473:U:H2'	31:sN1:474:A:H8	1.54	0.72
5:AN1:2159:U:OP1	5:AN1:2161:C:N4	2.23	0.71
31:sN1:449:G:H1	31:sN1:476:U:H3	1.38	0.71
6:B:70:G:H21	6:B:101:A:N6	1.86	0.71
5:AN1:474:C:O2	5:AN1:478:A:N6	2.23	0.71
33:c:46:LYS:HZ1	33:c:87:LEU:HD11	1.54	0.71
31:sN1:503:G:N2	31:sN1:522:C:O2	2.20	0.71
5:AN1:1749:G:N2	5:AN1:1752:G:OP2	2.23	0.70
10:F:80:ARG:H	10:F:83:TRP:HD1	1.39	0.70
34:d:15:GLU:O	34:d:46:ARG:NH1	2.24	0.70
33:c:77:ILE:HD11	33:c:103:ILE:HG13	1.72	0.70
3:2:28:LYS:HA	3:2:32:LEU:HD11	1.74	0.70
31:sN1:1074:G:N2	31:sN1:1077:A:OP2	2.22	0.69
5:AN1:829:G:O2'	15:K:40:GLN:NE2	2.25	0.69
34:d:8:LYS:HB3	34:d:21:LEU:HD13	1.74	0.69
31:sN1:75:A:N1	31:sN1:92:G:O6	2.24	0.69
5:AN1:1041:A:O2'	5:AN1:1108:A:N6	2.25	0.69
31:sN1:1159:C:H42	31:sN1:1171:G:H1	1.41	0.69
35:e:103:GLY:H	35:e:121:ASN:HD22	1.41	0.69
5:AN1:342:A:O2'	9:E:161:ARG:NH1	2.26	0.69
31:sN1:420:G:H2'	31:sN1:421:G:C8	2.28	0.69
5:AN1:711:G:H8	5:AN1:716:A:H62	1.41	0.68
48:r:26:ILE:HG22	48:r:67:LEU:HD23	1.73	0.68
12:H:48:GLU:O	12:H:52:ALA:HB3	1.93	0.68
9:E:193:LYS:HA	9:E:196:GLU:HG2	1.74	0.68
31:sN1:1144:C:HO2'	39:i:5:TYR:HH	1.38	0.68
5:AN1:1528:G:O2'	5:AN1:1536:A:N1	2.26	0.67
31:sN1:670:A:H2'	31:sN1:671:G:C8	2.29	0.67
5:AN1:1662:A:H61	5:AN1:1992:C:H42	1.43	0.67
5:AN1:52:G:H5"	5:AN1:53:G:H5'	1.76	0.67
31:sN1:671:G:H2'	31:sN1:672:A:H8	1.59	0.67
5:AN1:293:U:H3	5:AN1:351:G:H1	1.41	0.67
31:sN1:661:G:OP1	48:r:53:ARG:NH2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:37:PHE:HB3	51:u:40:LYS:HB2	1.75	0.67
5:AN1:364:A:OP2	5:AN1:424:G:O2'	2.13	0.67
32:b:60:ASN:ND2	32:b:222:ALA:O	2.28	0.67
5:AN1:2301:U:O2'	10:F:133:LYS:NZ	2.27	0.66
5:AN1:93:G:HO2'	5:AN1:111:U:HO2'	1.40	0.66
5:AN1:879:G:O6	5:AN1:893:U:O2	2.12	0.66
41:k:16:SER:O	41:k:80:ASN:ND2	2.27	0.66
23:S:3:ASN:HD21	23:S:48:LYS:HE2	1.61	0.66
31:sN1:678:A:H61	31:sN1:706:U:H3	1.43	0.66
31:sN1:992:C:O2	44:n:8:ASN:ND2	2.29	0.66
32:b:128:PHE:HA	32:b:131:LEU:HD21	1.78	0.66
21:Q:16:GLU:HG3	21:Q:101:ILE:HG13	1.78	0.66
31:sN1:293:G:N2	31:sN1:296:A:OP2	2.26	0.66
31:sN1:1157:G:OP1	32:b:133:LYS:NZ	2.29	0.66
2:1:7:PRO:HB2	5:AN1:1304:G:H4'	1.77	0.66
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.77	0.65
5:AN1:195:G:H5'	27:W:14:VAL:HG21	1.77	0.65
5:AN1:1413:G:N2	5:AN1:1577:A:OP2	2.30	0.65
5:AN1:1647:G:O2'	17:M:106:ASP:OD2	2.14	0.65
48:r:39:ILE:HD11	48:r:59:ILE:HG21	1.78	0.65
5:AN1:198:A:H3'	5:AN1:199:G:H21	1.61	0.65
5:AN1:1361:A:OP1	27:W:2:SER:OG	2.15	0.65
5:AN1:2804:A:O2'	5:AN1:2886:G:O6	2.14	0.65
31:sN1:670:A:H2'	31:sN1:671:G:H8	1.61	0.65
5:AN1:294:U:H3	5:AN1:350:G:H22	1.44	0.65
31:sN1:74:G:H1	31:sN1:93:A:N6	1.92	0.65
5:AN1:2130:A:OP2	5:AN1:2152:G:N1	2.30	0.65
41:k:17:GLU:HA	41:k:80:ASN:HB2	1.78	0.65
5:AN1:70:A:H61	5:AN1:98:A:H61	1.45	0.65
31:sN1:177:A:O2'	31:sN1:179:G:N1	2.30	0.64
33:c:14:VAL:HG12	33:c:15:VAL:HG13	1.79	0.64
6:B:108:C:H2'	6:B:109:G:H8	1.60	0.64
42:l:35:THR:N	42:l:54:ARG:O	2.30	0.64
37:g:68:LYS:O	37:g:138:ARG:NH2	2.31	0.64
5:AN1:2879:A:OP2	30:Z:49:ARG:NH1	2.31	0.64
5:AN1:2130:A:H62	5:AN1:2153:G:H4'	1.62	0.64
30:Z:25:ASN:OD1	30:Z:38:ARG:NH2	2.31	0.64
31:sN1:1004:U:OP1	44:n:19:LYS:NZ	2.30	0.64
32:b:114:ASN:HA	32:b:117:LYS:HE3	1.79	0.64
34:d:165:ALA:HA	34:d:169:ILE:HD11	1.79	0.64
5:AN1:1750:C:H5	19:O:97:ARG:HH11	1.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:97:ARG:NH1	31:sN1:335:C:OP2	2.31	0.63
21:Q:42:VAL:HG22	21:Q:47:ILE:HG23	1.79	0.63
5:AN1:280:A:H2	5:AN1:364:A:H62	1.47	0.63
10:F:143:PHE:HB2	43:m:71:ARG:HD2	1.79	0.63
31:sN1:684:A:H62	31:sN1:700:G:H21	1.45	0.63
31:sN1:239:A:H4'	31:sN1:240:U:H3'	1.79	0.63
43:m:3:ARG:O	43:m:57:ARG:NH2	2.31	0.63
5:AN1:1775:U:OP2	5:AN1:1780:A:N6	2.27	0.62
48:r:37:GLY:O	48:r:63:ARG:NH1	2.32	0.62
34:d:15:GLU:HG3	34:d:19:LEU:HD11	1.80	0.62
41:k:19:VAL:N	41:k:34:THR:O	2.32	0.62
44:n:33:ASN:O	44:n:41:ARG:NH1	2.32	0.62
31:sN1:1113:U:O2	31:sN1:1181:G:O6	2.17	0.62
31:sN1:1406:C:H2'	31:sN1:1407:A:H8	1.64	0.62
5:AN1:2324:A:H2'	5:AN1:2325:A:C8	2.34	0.62
31:sN1:1078:G:OP2	35:e:51:LYS:NZ	2.32	0.62
5:AN1:1587:U:H2'	5:AN1:1588:A:H8	1.64	0.62
36:f:8:LEU:HD22	36:f:84:ILE:HD11	1.82	0.62
5:AN1:2309:C:O4'	10:F:37:ASN:ND2	2.33	0.62
10:F:32:THR:OG1	10:F:157:THR:O	2.16	0.62
34:d:13:ARG:HH21	34:d:32:THR:HB	1.65	0.62
5:AN1:527:A:H5'	13:I:113:PRO:HG3	1.82	0.62
5:AN1:1310:C:O2'	5:AN1:1387:A:N3	2.33	0.61
10:F:34:ILE:HG12	10:F:156:ILE:HG22	1.82	0.61
10:F:74:ILE:HG22	10:F:76:GLY:H	1.65	0.61
34:d:97:GLU:HA	34:d:102:ASN:HD22	1.64	0.61
36:f:17:GLN:HB3	36:f:21:MET:HE2	1.82	0.61
2:1:30:VAL:HG22	2:1:33:ARG:HH11	1.65	0.61
24:T:38:ASN:HB3	24:T:61:ALA:HB3	1.81	0.61
31:sN1:79:U:O4	31:sN1:80:A:N6	2.32	0.61
5:AN1:2287:U:H2'	5:AN1:2288:G:C8	2.35	0.61
7:C:230:HIS:HD2	7:C:232:HIS:H	1.48	0.61
31:sN1:410:A:OP2	31:sN1:424:G:N2	2.28	0.61
5:AN1:877:G:H2'	5:AN1:878:G:C8	2.36	0.61
12:H:48:GLU:O	12:H:52:ALA:CB	2.49	0.61
31:sN1:1068:C:OP1	35:e:53:ARG:NH1	2.33	0.61
22:R:11:ALA:H	22:R:100:THR:HG23	1.65	0.61
31:sN1:808:C:O2'	31:sN1:898:A:N1	2.34	0.61
31:sN1:1024:C:N4	31:sN1:1031:G:O6	2.34	0.61
9:E:124:ALA:O	9:E:136:LYS:NZ	2.33	0.60
31:sN1:733:C:H2'	31:sN1:734:A:H8	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:49:VAL:HG23	32:b:50:PRO:HD3	1.83	0.60
32:b:114:ASN:OD1	32:b:115:ARG:N	2.34	0.60
41:k:36:ARG:NH2	41:k:82:ASP:OD2	2.34	0.60
5:AN1:843:G:O2'	5:AN1:845:A:N7	2.33	0.60
31:sN1:899:G:H2'	31:sN1:900:A:H8	1.66	0.60
42:l:65:SER:HG	42:l:97:THR:HG1	1.46	0.60
5:AN1:2107:U:O2	5:AN1:2111:G:N2	2.33	0.60
5:AN1:2111:G:O2'	5:AN1:2113:A:N7	2.34	0.60
34:d:98:SER:OG	34:d:138:GLN:NE2	2.34	0.60
11:G:121:VAL:HG22	11:G:135:SER:HB2	1.82	0.60
32:b:131:LEU:HD23	32:b:131:LEU:H	1.66	0.60
5:AN1:570:A:OP2	21:Q:80:ARG:NH2	2.33	0.60
8:D:6:VAL:H	8:D:33:ASN:HD21	1.48	0.60
31:sN1:1299:C:OP1	43:m:13:LYS:NZ	2.34	0.60
39:i:10:ARG:HG3	39:i:11:LYS:HG2	1.83	0.60
5:AN1:846:U:H2'	5:AN1:847:A:H8	1.66	0.60
10:F:136:ILE:HG13	10:F:138:PHE:HD1	1.66	0.60
5:AN1:1111:C:H2'	5:AN1:1112:G:C8	2.36	0.60
31:sN1:657:G:N1	31:sN1:743:A:C6	2.70	0.60
33:c:142:MET:HG3	33:c:170:GLU:HG2	1.84	0.60
5:AN1:673:A:OP1	9:E:57:LYS:NZ	2.35	0.59
34:d:154:GLN:HE21	34:d:157:ILE:HG23	1.67	0.59
10:F:69:LEU:HA	10:F:84:PRO:HA	1.83	0.59
31:sN1:662:A:N7	31:sN1:721:G:O6	2.36	0.59
31:sN1:6:C:H2'	31:sN1:7:U:H2'	1.84	0.59
31:sN1:425:U:OP2	34:d:13:ARG:NH2	2.26	0.59
43:m:16:VAL:HG13	43:m:17:ILE:HD12	1.84	0.59
31:sN1:473:U:H2'	31:sN1:474:A:C8	2.35	0.59
31:sN1:710:G:H2'	31:sN1:711:G:C8	2.38	0.59
19:O:4:LYS:O	19:O:9:GLN:NE2	2.36	0.59
31:sN1:143:G:N3	55:sN1:1707:HOH:O	2.32	0.59
5:AN1:168:A:H3'	5:AN1:169:U:H5"	1.84	0.59
5:AN1:1535:U:H2'	5:AN1:1536:A:H8	1.67	0.59
5:AN1:2401:G:O2'	5:AN1:2407:A:N6	2.36	0.59
5:AN1:955:U:O2'	6:B:86:U:O4	2.19	0.59
31:sN1:715:A:H5'	41:k:118:ASN:HD21	1.68	0.59
33:c:17:ARG:NH2	33:c:214:VAL:O	2.36	0.58
33:c:123:GLN:OE1	33:c:136:ARG:NH1	2.36	0.58
5:AN1:2577:G:OP2	5:AN1:2577:G:N2	2.34	0.58
6:B:18:G:O6	6:B:61:C:N4	2.32	0.58
31:sN1:649:U:O4	31:sN1:749:G:O2'	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2596:A:N6	7:C:236:GLU:OE1	2.36	0.58
31:sN1:711:G:H2'	31:sN1:712:A:C8	2.39	0.58
3:2:30:HIS:O	3:2:32:LEU:HD22	2.04	0.58
5:AN1:1533:U:N3	5:AN1:1534:G:N3	2.47	0.58
3:2:24:LYS:NZ	3:2:46:CYS:SG	2.77	0.58
5:AN1:719:A:H2'	5:AN1:720:A:C8	2.38	0.58
5:AN1:84:U:OP1	28:X:52:ARG:NH2	2.37	0.58
5:AN1:1719:U:O4	5:AN1:1734:G:N2	2.37	0.58
6:B:12:U:OP2	6:B:68:C:O2'	2.22	0.58
14:J:7:MET:HB3	14:J:18:ARG:HH11	1.68	0.58
31:sN1:657:G:C2	31:sN1:743:A:C6	2.92	0.58
5:AN1:879:G:N2	5:AN1:893:U:O2'	2.32	0.58
5:AN1:2301:U:H4'	10:F:133:LYS:HE2	1.85	0.58
8:D:47:GLN:NE2	8:D:87:GLU:OE1	2.36	0.58
23:S:53:GLU:CD	23:S:53:GLU:H	2.11	0.58
5:AN1:410:G:OP2	5:AN1:2402:U:O2'	2.22	0.58
38:h:81:ARG:HG3	38:h:84:LEU:H	1.69	0.57
5:AN1:2166:A:H2'	5:AN1:2167:A:H5"	1.85	0.57
31:sN1:1353:G:H2'	31:sN1:1354:A:C8	2.39	0.57
5:AN1:2077:C:H2'	5:AN1:2078:A:H8	1.68	0.57
33:c:111:LEU:O	33:c:204:ARG:NH2	2.37	0.57
39:i:104:ARG:NH1	39:i:105:ASP:O	2.37	0.57
5:AN1:2309:C:H5"	10:F:88:LYS:HD2	1.86	0.57
10:F:87:CYS:SG	10:F:88:LYS:N	2.76	0.57
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.85	0.57
32:b:70:LEU:HD12	32:b:71:PHE:H	1.69	0.57
5:AN1:518:C:H2'	5:AN1:519:A:H8	1.68	0.57
10:F:138:PHE:O	10:F:140:GLU:N	2.37	0.57
5:AN1:303:C:H5"	5:AN1:336:U:H2'	1.86	0.57
5:AN1:719:A:H2'	5:AN1:720:A:H8	1.70	0.57
31:sN1:487:C:OP2	34:d:123:ARG:NH1	2.36	0.57
34:d:61:GLN:OE1	34:d:65:ARG:NH1	2.35	0.57
10:F:10:ASP:OD1	10:F:13:LYS:NZ	2.38	0.57
31:sN1:997:U:O4	31:sN1:998:A:N6	2.38	0.57
3:2:30:HIS:C	3:2:32:LEU:H	2.09	0.57
5:AN1:1111:C:H2'	5:AN1:1112:G:H8	1.68	0.57
5:AN1:2309:C:H2'	5:AN1:2310:A:H8	1.68	0.57
5:AN1:2784:C:O2'	5:AN1:2805:A:N3	2.37	0.57
11:G:21:GLY:O	11:G:22:ARG:NH2	2.38	0.57
18:N:71:THR:HG22	18:N:104:ALA:HB1	1.87	0.56
31:sN1:231:U:H2'	31:sN1:232:A:H8	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:252:U:H2'	31:sN1:253:G:H8	1.68	0.56
39:i:34:GLU:HA	39:i:43:ARG:HD3	1.87	0.56
3:2:6:THR:HG22	3:2:62:PRO:HD2	1.88	0.56
3:2:31:ILE:O	3:2:33:THR:N	2.39	0.56
5:AN1:516:C:OP2	30:Z:10:ARG:NH2	2.39	0.56
5:AN1:878:G:H2'	5:AN1:879:G:C8	2.37	0.56
5:AN1:1462:G:H1	5:AN1:1520:A:H61	0.66	0.56
5:AN1:2151:U:OP2	5:AN1:2153:G:N2	2.38	0.56
24:T:45:LYS:HD2	24:T:46:PRO:HD2	1.86	0.56
29:Y:2:LYS:O	29:Y:39:ASP:N	2.31	0.56
32:b:210:ARG:HA	32:b:213:THR:HG22	1.87	0.56
5:AN1:2315:U:H2'	5:AN1:2317:G:H1	1.70	0.56
45:o:36:ILE:O	45:o:40:GLN:HG2	2.05	0.56
5:AN1:1713:U:O2	5:AN1:1739:G:N2	2.31	0.56
33:c:14:VAL:HG21	33:c:178:LEU:HD23	1.88	0.56
43:m:68:ASP:OD1	43:m:68:ASP:N	2.38	0.56
23:S:29:GLN:OE1	23:S:90:GLN:NE2	2.31	0.56
6:B:64:A:H61	6:B:105:C:H2'	1.71	0.56
10:F:80:ARG:HG2	10:F:81:ASP:H	1.71	0.56
31:sN1:143:G:H2'	31:sN1:144:G:C8	2.41	0.56
5:AN1:579:C:H2'	5:AN1:580:A:H8	1.71	0.56
5:AN1:2701:A:O2'	5:AN1:2848:G:OP1	2.22	0.56
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.88	0.56
31:sN1:503:G:O6	31:sN1:522:C:N4	2.26	0.56
31:sN1:1016:G:H2'	31:sN1:1017:A:H8	1.71	0.56
5:AN1:1717:G:N2	5:AN1:1734:G:O2'	2.38	0.55
34:d:91:ASN:HA	34:d:94:LYS:HD3	1.87	0.55
37:g:72:MET:HG2	37:g:73:VAL:HG22	1.88	0.55
5:AN1:167:A:N3	5:AN1:2204:C:O2'	2.38	0.55
5:AN1:877:G:H2'	5:AN1:878:G:H8	1.70	0.55
5:AN1:1535:U:H2'	5:AN1:1536:A:C8	2.41	0.55
15:K:102:VAL:HG23	15:K:103:VAL:HG23	1.89	0.55
18:N:51:GLN:O	18:N:80:ARG:NH2	2.39	0.55
31:sN1:1016:G:H2'	31:sN1:1017:A:C8	2.40	0.55
31:sN1:1037:A:H2'	31:sN1:1038:G:C8	2.42	0.55
31:sN1:1147:U:O4	31:sN1:1148:A:N6	2.39	0.55
5:AN1:322:G:N7	9:E:131:LYS:NZ	2.54	0.55
9:E:97:ARG:HD3	9:E:101:ARG:HH21	1.71	0.55
5:AN1:2119:G:N2	5:AN1:2120:G:O6	2.39	0.55
5:AN1:2654:C:H5"	11:G:158:LYS:HE3	1.88	0.55
10:F:17:GLN:HE22	10:F:25:VAL:HA	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:114:LEU:HD22	15:K:132:GLY:HA3	1.87	0.55
31:sN1:873:A:H1'	38:h:12:THR:HG21	1.89	0.55
38:h:2:SER:OG	38:h:3:MET:N	2.39	0.55
5:AN1:718:U:HO2'	5:AN1:719:A:H8	1.55	0.55
5:AN1:1276:G:H2'	5:AN1:1277:U:C6	2.42	0.55
32:b:85:GLN:NE2	32:b:213:THR:OG1	2.40	0.55
5:AN1:2587:C:H2'	5:AN1:2588:G:H8	1.72	0.55
8:D:86:THR:HG22	8:D:88:ALA:H	1.71	0.55
23:S:7:TYR:O	28:X:29:ARG:NH1	2.39	0.55
5:AN1:1842:G:H2'	5:AN1:1843:A:C8	2.42	0.55
5:AN1:2242:G:H2'	5:AN1:2243:A:H8	1.72	0.55
34:d:87:ALA:O	34:d:91:ASN:ND2	2.40	0.55
5:AN1:579:C:H2'	5:AN1:580:A:C8	2.43	0.55
31:sN1:1352:G:H2'	31:sN1:1353:G:H8	1.72	0.55
5:AN1:2254:C:O2'	5:AN1:2423:C:OP2	2.25	0.54
31:sN1:498:C:H2'	31:sN1:499:A:H8	1.72	0.54
31:sN1:1409:C:H2'	31:sN1:1410:A:C8	2.42	0.54
5:AN1:2123:G:H2'	5:AN1:2124:G:C8	2.43	0.54
31:sN1:588:U:H2'	31:sN1:589:A:H8	1.72	0.54
31:sN1:1095:C:H2'	31:sN1:1096:G:H8	1.71	0.54
31:sN1:1513:G:N2	31:sN1:1516:MA6:OP2	2.36	0.54
44:n:88:VAL:HG22	44:n:93:VAL:HG21	1.89	0.54
5:AN1:1870:C:H3'	5:AN1:1871:G:H4'	1.90	0.54
31:sN1:671:G:H2'	31:sN1:672:A:C8	2.40	0.54
32:b:168:VAL:HG23	32:b:175:ILE:HG21	1.88	0.54
5:AN1:1310:C:H2'	5:AN1:1311:A:H8	1.73	0.54
31:sN1:1050:G:H4'	31:sN1:1051:C:H5'	1.89	0.54
34:d:64:ARG:HH11	34:d:70:LEU:HA	1.72	0.54
5:AN1:2568:A:H2'	8:D:152:ASN:HD21	1.71	0.54
30:Z:46:GLY:O	30:Z:53:LEU:N	2.38	0.54
31:sN1:487:C:OP1	34:d:131:ARG:NH1	2.40	0.54
36:f:8:LEU:HB2	36:f:60:ILE:HG23	1.89	0.54
5:AN1:552:U:H2'	5:AN1:553:G:O4'	2.07	0.54
5:AN1:881:G:H2'	5:AN1:882:U:H6	1.73	0.54
5:AN1:1462:G:N2	5:AN1:1520:A:N1	2.41	0.54
18:N:19:ILE:HG21	18:N:26:ARG:HB3	1.89	0.54
31:sN1:1294:G:N2	37:g:114:LYS:O	2.41	0.54
5:AN1:520:U:H2'	5:AN1:521:G:H8	1.72	0.54
5:AN1:1348:A:H2'	5:AN1:1349:A:H8	1.73	0.54
38:h:53:GLN:NE2	38:h:54:GLU:O	2.41	0.54
24:T:27:VAL:HG22	24:T:32:VAL:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:1057:U:OP1	44:n:85:ARG:NH2	2.41	0.54
31:sN1:1347:A:O2'	37:g:33:ASP:OD1	2.24	0.54
31:sN1:549:U:H2'	31:sN1:550:A:H8	1.73	0.54
31:sN1:1054:G:N3	33:c:188:ARG:NH1	2.56	0.54
31:sN1:1461:U:H2'	31:sN1:1462:A:H8	1.72	0.54
5:AN1:1919:U:H2'	5:AN1:1920:C:C6	2.44	0.53
5:AN1:1932:A:H2	5:AN1:1939:U:H3	1.56	0.53
31:sN1:1323:U:H2'	31:sN1:1324:C:H6	1.73	0.53
31:sN1:1100:C:H4'	32:b:99:LEU:HD21	1.90	0.53
32:b:21:GLN:OE1	32:b:23:ARG:HG2	2.08	0.53
5:AN1:805:U:OP2	15:K:43:ARG:NH2	2.39	0.53
31:sN1:588:U:H2'	31:sN1:589:A:C8	2.43	0.53
5:AN1:1526:C:N4	5:AN1:1538:A:N3	2.55	0.53
5:AN1:1962:A:N3	5:AN1:2588:G:O2'	2.38	0.53
5:AN1:2468:G:N2	5:AN1:2469:U:O2'	2.42	0.53
5:AN1:2734:A:N1	5:AN1:2762:G:O6	2.41	0.53
31:sN1:1376:G:N2	31:sN1:1378:U:O4	2.42	0.53
5:AN1:395:G:OP2	27:W:10:LYS:NZ	2.41	0.53
5:AN1:2479:C:H1'	16:L:52:ARG:HH12	1.72	0.53
23:S:55:VAL:HG23	23:S:87:LYS:HG2	1.90	0.53
31:sN1:1042:C:H2'	31:sN1:1043:A:H8	1.74	0.53
5:AN1:2242:G:H2'	5:AN1:2243:A:C8	2.44	0.53
5:AN1:2528:G:N2	5:AN1:2659:G:O2'	2.41	0.53
5:AN1:1911:3TD:N1	5:AN1:1938:C:O2	2.36	0.53
10:F:5:LYS:HG3	10:F:7:ARG:H	1.73	0.53
5:AN1:86:C:H2'	5:AN1:87:G:H8	1.74	0.53
5:AN1:2308:U:H2'	10:F:37:ASN:HD21	1.73	0.53
11:G:44:LYS:HZ2	11:G:53:ALA:HB3	1.73	0.53
31:sN1:1284:A:H2	31:sN1:1350:G:H1'	1.73	0.53
31:sN1:1411:U:H2'	31:sN1:1412:G:H8	1.74	0.53
31:sN1:1320:G:H2'	31:sN1:1321:A:C8	2.44	0.53
31:sN1:1406:C:H2'	31:sN1:1407:A:C8	2.44	0.53
31:sN1:888:U:H2'	31:sN1:889:A:H8	1.74	0.53
31:sN1:1483:G:H2'	31:sN1:1484:G:C8	2.44	0.53
10:F:162:THR:HG22	10:F:164:ASP:H	1.74	0.52
31:sN1:887:G:O2'	31:sN1:903:A:N6	2.41	0.52
31:sN1:973:G:OP2	31:sN1:1355:U:O2'	2.27	0.52
31:sN1:1353:G:H2'	31:sN1:1354:A:H8	1.73	0.52
50:t:43:ASP:HB3	50:t:46:VAL:HG22	1.91	0.52
5:AN1:499:G:N1	5:AN1:502:A:OP2	2.37	0.52
5:AN1:627:A:N3	5:AN1:637:U:O2'	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:862:G:H2'	5:AN1:863:C:C6	2.45	0.52
5:AN1:1311:A:H2'	5:AN1:1312:G:H8	1.74	0.52
20:P:105:ALA:HA	21:Q:47:ILE:HD13	1.91	0.52
31:sN1:359:A:N6	42:l:27:CYS:SG	2.83	0.52
5:AN1:1387:A:N6	23:S:17:GLU:OE1	2.39	0.52
10:F:5:LYS:H	10:F:8:TYR:HB2	1.75	0.52
11:G:22:ARG:HH11	11:G:39:ALA:HA	1.74	0.52
21:Q:32:THR:HA	21:Q:62:GLU:HA	1.91	0.52
31:sN1:89:C:O2'	31:sN1:90:C:OP2	2.27	0.52
31:sN1:1215:C:H2'	31:sN1:1216:A:C8	2.44	0.52
34:d:172:TRP:CD1	34:d:173:ILE:HG23	2.44	0.52
5:AN1:1025:A:H2'	5:AN1:1026:A:C8	2.45	0.52
5:AN1:1083:A:H1'	5:AN1:1100:A:H61	1.74	0.52
5:AN1:1306:G:OP2	5:AN1:1306:G:N2	2.36	0.52
5:AN1:2049:G:H5'	8:D:152:ASN:O	2.10	0.52
5:AN1:2325:A:H2'	5:AN1:2326:G:C8	2.45	0.52
31:sN1:597:G:H2'	31:sN1:598:G:H8	1.75	0.52
5:AN1:35:A:H61	5:AN1:511:G:H1'	1.73	0.52
5:AN1:2067:A:H2'	5:AN1:2068:C:C6	2.44	0.52
15:K:89:GLY:O	15:K:120:ARG:NH2	2.42	0.52
19:O:34:LYS:HE3	19:O:83:VAL:HA	1.91	0.52
31:sN1:91:G:H2'	31:sN1:92:G:H8	1.74	0.52
31:sN1:232:A:H2'	31:sN1:233:A:C8	2.45	0.52
10:F:83:TRP:HE3	10:F:84:PRO:HD2	1.74	0.52
5:AN1:462:G:N2	5:AN1:465:A:OP2	2.32	0.52
5:AN1:1442:C:O2'	5:AN1:1542:A:N3	2.43	0.52
31:sN1:1215:C:H2'	31:sN1:1216:A:H8	1.75	0.52
36:f:15:SER:O	36:f:19:VAL:HG13	2.10	0.52
5:AN1:1430:G:H2'	5:AN1:1431:G:C8	2.45	0.52
5:AN1:2091:A:OP1	12:H:11:ASN:ND2	2.42	0.52
31:sN1:1083:U:H3	31:sN1:1096:G:H1	1.56	0.52
38:h:55:GLU:HG2	38:h:56:THR:HG23	1.92	0.52
5:AN1:1413:G:O2'	5:AN1:1577:A:N6	2.43	0.52
32:b:194:ASN:ND2	32:b:196:ASP:OD2	2.39	0.52
42:l:44:LYS:HD3	42:l:46:ASN:H	1.75	0.52
5:AN1:2229:U:H2'	5:AN1:2230:G:C8	2.45	0.52
7:C:6:CYS:SG	7:C:18:LYS:NZ	2.83	0.52
33:c:60:PRO:HG2	33:c:63:ALA:HB3	1.92	0.52
48:r:29:LEU:HD22	48:r:59:ILE:HG13	1.92	0.52
20:P:28:ARG:NH1	55:P:201:HOH:O	2.40	0.51
31:sN1:200:G:H3'	31:sN1:201:A:H8	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:12:GLU:HG2	35:e:38:VAL:HG12	1.91	0.51
5:AN1:1199:A:H4'	5:AN1:1200:A:H5'	1.92	0.51
5:AN1:1412:C:H3'	5:AN1:1413:G:H8	1.74	0.51
27:W:76:GLN:HB3	27:W:78:ILE:HG23	1.92	0.51
33:c:120:ILE:HA	33:c:123:GLN:HE21	1.76	0.51
39:i:89:ASP:N	39:i:89:ASP:OD1	2.43	0.51
5:AN1:1421:G:OP2	5:AN1:1422:A:O2'	2.28	0.51
6:B:64:A:N6	6:B:105:C:H2'	2.25	0.51
21:Q:50:GLY:H	21:Q:54:VAL:HG22	1.75	0.51
31:sN1:177:A:HO2'	31:sN1:179:G:H1	1.54	0.51
5:AN1:2171:C:H2'	5:AN1:2172:A:N7	2.24	0.51
5:AN1:2852:A:H2'	5:AN1:2853:G:O4'	2.11	0.51
12:H:9:ILE:HD13	12:H:12:LEU:HD11	1.92	0.51
24:T:46:PRO:HB3	24:T:54:GLY:H	1.76	0.51
5:AN1:510:U:H4'	5:AN1:1230:G:H4'	1.93	0.51
5:AN1:1487:G:H5"	5:AN1:1488:C:H5"	1.92	0.51
5:AN1:1528:G:N2	5:AN1:1535:U:O4	2.44	0.51
6:B:108:C:H2'	6:B:109:G:C8	2.44	0.51
15:K:77:ALA:HB2	15:K:107:GLN:HE21	1.76	0.51
31:sN1:1031:G:O6	31:sN1:1033:A:N6	2.43	0.51
5:AN1:714:A:C5	5:AN1:715:C:H1'	2.45	0.51
5:AN1:1025:A:N3	5:AN1:2482:C:O2'	2.40	0.51
5:AN1:1103:A:N6	5:AN1:1104:G:O6	2.44	0.51
5:AN1:2116:G:H5"	5:AN1:2164:G:H22	1.76	0.51
5:AN1:2137:A:H2	5:AN1:2138:A:H62	1.57	0.51
5:AN1:2861:U:OP2	5:AN1:2862:G:O2'	2.23	0.51
31:sN1:36:C:H2'	31:sN1:37:G:H8	1.75	0.51
31:sN1:941:G:N1	31:sN1:1335:G:OP2	2.35	0.51
32:b:132:THR:HB	32:b:135:GLU:HB2	1.92	0.51
34:d:51:SER:OG	34:d:52:GLU:N	2.44	0.51
5:AN1:9:G:H2'	5:AN1:10:U:C6	2.46	0.51
5:AN1:158:U:H2'	5:AN1:159:G:H8	1.75	0.51
5:AN1:2591:G:N2	5:AN1:2594:A:OP2	2.32	0.51
6:B:22:G:O2'	6:B:25:C:N4	2.44	0.51
32:b:188:ILE:HD11	32:b:204:GLY:HA3	1.93	0.51
5:AN1:12:A:H2'	5:AN1:13:A:C8	2.45	0.51
31:sN1:498:C:H2'	31:sN1:499:A:C8	2.45	0.51
31:sN1:754:U:H2'	31:sN1:755:G:O4'	2.11	0.51
38:h:8:ALA:O	38:h:12:THR:HG23	2.11	0.51
39:i:110:GLU:OE2	39:i:113:LYS:NZ	2.43	0.51
41:k:12:THR:HG22	41:k:13:ARG:HE	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:293:U:O4	5:AN1:351:G:O6	2.28	0.51
31:sN1:519:C:H41	42:l:50:ARG:HH12	1.58	0.51
4:3:18:ARG:HE	4:3:21:GLY:HA2	1.75	0.50
5:AN1:1108:A:H8	5:AN1:1109:G:H4'	1.75	0.50
5:AN1:1356:G:H2'	5:AN1:1357:C:C6	2.46	0.50
6:B:108:C:O2'	6:B:109:G:OP1	2.26	0.50
10:F:4:LEU:HD12	10:F:8:TYR:HB3	1.92	0.50
10:F:129:SER:O	10:F:130:MET:HE2	2.10	0.50
25:U:11:ARG:HH21	25:U:31:PRO:HB3	1.76	0.50
31:sN1:929:C:H2'	31:sN1:930:G:C8	2.47	0.50
31:sN1:1010:G:N2	31:sN1:1013:A:OP2	2.42	0.50
31:sN1:1122:U:H2'	31:sN1:1123:U:H2'	1.93	0.50
31:sN1:1357:A:OP2	44:n:75:ARG:NH2	2.44	0.50
40:j:42:MET:HB2	40:j:71:LYS:HB3	1.94	0.50
5:AN1:879:G:H2'	5:AN1:880:G:C8	2.39	0.50
31:sN1:998:A:H2'	31:sN1:999:G:C8	2.45	0.50
31:sN1:1112:U:H3	31:sN1:1182:G:H1	1.58	0.50
36:f:30:LYS:HA	36:f:35:GLN:CD	2.36	0.50
5:AN1:372:U:H2'	5:AN1:373:A:H8	1.75	0.50
5:AN1:1591:C:H2'	5:AN1:1592:A:C8	2.47	0.50
11:G:44:LYS:NZ	11:G:53:ALA:HB3	2.27	0.50
28:X:30:MET:O	28:X:34:THR:HG23	2.10	0.50
31:sN1:998:A:N1	31:sN1:1037:A:N6	2.59	0.50
32:b:178:ALA:O	32:b:182:GLY:N	2.41	0.50
5:AN1:2287:U:H2'	5:AN1:2288:G:H8	1.77	0.50
7:C:159:GLY:H	7:C:195:VAL:HB	1.77	0.50
18:N:67:ILE:O	18:N:71:THR:HG23	2.12	0.50
31:sN1:661:G:H22	31:sN1:738:G:H1	1.58	0.50
32:b:220:ALA:HA	32:b:223:ILE:HG12	1.93	0.50
36:f:28:GLN:HG3	36:f:77:LEU:HD21	1.94	0.50
5:AN1:1680:G:H2'	5:AN1:1681:U:C6	2.46	0.50
5:AN1:2311:C:O2'	5:AN1:2312:G:H8	1.94	0.50
5:AN1:2853:G:N1	5:AN1:2856:A:OP2	2.42	0.50
10:F:166:GLY:O	10:F:169:LEU:HG	2.12	0.50
19:O:2:SER:OG	19:O:3:GLY:N	2.43	0.50
31:sN1:792:C:H4'	41:k:127:ARG:HH21	1.75	0.50
31:sN1:1447:G:N2	31:sN1:1449:A:O2'	2.44	0.50
5:AN1:887:C:H3'	5:AN1:888:C:H5"	1.93	0.50
5:AN1:1095:A:H2'	5:AN1:1096:G:H8	1.75	0.50
5:AN1:1844:A:H5"	5:AN1:1845:G:OP1	2.12	0.50
13:I:6:ALA:H	13:I:45:THR:HG21	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:472:A:H2'	31:sN1:473:U:C6	2.46	0.50
31:sN1:1020:G:H2'	31:sN1:1021:G:C8	2.47	0.50
43:m:10:PRO:HB2	43:m:13:LYS:HG3	1.92	0.50
5:AN1:1767:C:H2'	5:AN1:1768:A:H8	1.77	0.50
5:AN1:2639:G:H2'	5:AN1:2640:A:H8	1.76	0.50
7:C:24:LEU:HD13	7:C:83:TYR:HB2	1.93	0.50
31:sN1:779:A:H62	31:sN1:797:G:H21	1.60	0.50
31:sN1:1247:A:H2'	31:sN1:1248:A:C8	2.46	0.50
32:b:119:LEU:HA	32:b:122:GLN:HG3	1.94	0.50
43:m:23:PHE:HD2	43:m:66:GLU:HA	1.76	0.50
5:AN1:34:G:H22	5:AN1:511:G:H2'	1.77	0.50
13:I:18:VAL:HG11	13:I:28:LEU:HD11	1.94	0.50
33:c:179:ARG:NE	33:c:206:GLU:OE2	2.42	0.50
35:e:71:ILE:HD12	35:e:144:ARG:HB3	1.94	0.50
5:AN1:727:G:OP1	7:C:13:ARG:HG2	2.12	0.50
5:AN1:1798:A:H2'	5:AN1:1799:A:C8	2.46	0.50
31:sN1:692:A:H2'	31:sN1:693:A:C8	2.47	0.50
31:sN1:978:U:OP1	44:n:9:ARG:NH2	2.45	0.50
5:AN1:1827:G:H2'	5:AN1:1828:C:C6	2.47	0.49
5:AN1:2105:U:OP1	5:AN1:2145:U:N3	2.29	0.49
5:AN1:2212:G:H2'	5:AN1:2213:G:H8	1.77	0.49
10:F:66:VAL:HG13	10:F:68:THR:OG1	2.12	0.49
31:sN1:991:A:H8	31:sN1:994:U:H3	1.58	0.49
34:d:38:ALA:HB3	34:d:43:GLY:HA3	1.93	0.49
38:h:12:THR:HG22	38:h:15:ARG:HH12	1.77	0.49
5:AN1:70:A:H61	5:AN1:98:A:N6	2.09	0.49
5:AN1:148:A:H61	5:AN1:1593:G:HO2'	1.54	0.49
5:AN1:580:A:H2'	5:AN1:581:G:C8	2.47	0.49
5:AN1:2115:A:H2'	5:AN1:2165:A:H2	1.76	0.49
6:B:16:A:H1'	6:B:65:G:N2	2.27	0.49
7:C:137:ILE:HD11	7:C:167:ARG:HG2	1.93	0.49
31:sN1:333:G:H2'	31:sN1:334:A:C8	2.48	0.49
31:sN1:1376:G:H2'	31:sN1:1377:U:C6	2.47	0.49
31:sN1:1523:G:OP2	51:u:39:GLU:HG3	2.12	0.49
49:s:12:ASP:OD2	49:s:35:SER:OG	2.30	0.49
5:AN1:413:C:H2'	5:AN1:414:A:C8	2.47	0.49
5:AN1:2172:A:H2'	5:AN1:2173:C:C6	2.47	0.49
6:B:26:C:H2'	6:B:27:A:C8	2.47	0.49
21:Q:59:VAL:HG22	21:Q:101:ILE:HG23	1.93	0.49
32:b:48:THR:HA	32:b:203:PRO:HD2	1.94	0.49
37:g:27:MET:HG2	37:g:43:VAL:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:184:G:H3'	5:AN1:185:G:H8	1.77	0.49
5:AN1:678:A:H2'	5:AN1:679:G:C8	2.47	0.49
5:AN1:1010:C:H2'	5:AN1:1011:A:H8	1.78	0.49
5:AN1:1438:C:H2'	5:AN1:1439:A:H8	1.77	0.49
5:AN1:1767:C:H2'	5:AN1:1768:A:C8	2.48	0.49
5:AN1:2225:U:H2'	5:AN1:2226:G:H8	1.77	0.49
9:E:86:ALA:O	9:E:87:ARG:NH1	2.44	0.49
31:sN1:1475:C:H2'	31:sN1:1476:G:H8	1.77	0.49
5:AN1:413:C:H2'	5:AN1:414:A:H8	1.78	0.49
31:sN1:1017:A:H2'	31:sN1:1018:U:C6	2.48	0.49
33:c:22:TRP:HB3	33:c:59:ARG:HB2	1.95	0.49
5:AN1:879:G:C6	5:AN1:893:U:O2	2.65	0.49
31:sN1:475:G:O2'	31:sN1:476:U:OP1	2.23	0.49
31:sN1:918:U:O2'	35:e:23:VAL:O	2.27	0.49
31:sN1:1327:U:H4'	43:m:23:PHE:CE1	2.48	0.49
33:c:39:VAL:HG11	33:c:95:MET:HE3	1.94	0.49
5:AN1:1053:G:H21	5:AN1:1101:C:H41	1.60	0.49
5:AN1:1411:G:H2'	5:AN1:1412:C:C6	2.47	0.49
5:AN1:1500:A:O2'	5:AN1:1502:U:O4'	2.30	0.49
5:AN1:1591:C:H2'	5:AN1:1592:A:H8	1.76	0.49
9:E:190:ALA:O	9:E:193:LYS:HG3	2.11	0.49
16:L:112:ASP:O	16:L:116:GLU:HG3	2.12	0.49
31:sN1:1094:C:H2'	31:sN1:1095:C:C6	2.48	0.49
31:sN1:1313:G:N1	31:sN1:1316:A:OP2	2.41	0.49
5:AN1:1273:C:H2'	5:AN1:1274:G:H8	1.78	0.49
31:sN1:475:G:HO2'	31:sN1:476:U:P	2.34	0.49
31:sN1:943:A:H2'	31:sN1:944:G:C8	2.48	0.49
31:sN1:999:G:H2'	31:sN1:1000:A:C8	2.48	0.49
32:b:144:GLU:CD	32:b:148:ARG:HH11	2.15	0.49
33:c:36:ASP:OD1	33:c:59:ARG:NH1	2.46	0.49
42:l:42:PRO:HB3	42:l:89:ASP:HB2	1.94	0.49
5:AN1:35:A:N6	5:AN1:511:G:O2'	2.46	0.49
5:AN1:2637:A:H5"	13:I:78:THR:HG21	1.95	0.49
16:L:20:LEU:HD23	16:L:99:PRO:HG2	1.94	0.49
41:k:18:GLY:HA2	41:k:35:ASP:HA	1.95	0.49
15:K:111:ARG:HG2	15:K:128:ALA:HB3	1.94	0.49
31:sN1:397:C:O2'	31:sN1:618:A:N3	2.41	0.49
31:sN1:402:G:H21	34:d:118:GLN:HE22	1.61	0.49
32:b:45:LEU:O	32:b:48:THR:HG22	2.13	0.49
5:AN1:85:C:HO2'	5:AN1:86:C:H6	1.62	0.48
5:AN1:1588:A:H2'	5:AN1:1589:C:H6	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2309:C:H2'	5:AN1:2310:A:C8	2.47	0.48
5:AN1:2787:A:O2'	5:AN1:2788:G:H8	1.96	0.48
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.95	0.48
31:sN1:271:G:H5'	47:q:17:LYS:HE3	1.94	0.48
31:sN1:712:A:H2'	31:sN1:713:A:C8	2.48	0.48
31:sN1:715:A:OP2	31:sN1:717:C:N4	2.46	0.48
31:sN1:1311:C:H2'	31:sN1:1312:U:C6	2.48	0.48
31:sN1:1446:U:H3	31:sN1:1451:A:H61	1.60	0.48
5:AN1:322:G:N3	9:E:162:ASN:ND2	2.61	0.48
5:AN1:520:U:H2'	5:AN1:521:G:C8	2.48	0.48
5:AN1:873:G:O6	5:AN1:900:C:N4	2.34	0.48
30:Z:52:GLN:NE2	30:Z:53:LEU:O	2.46	0.48
31:sN1:976:C:O2	44:n:59:ARG:HG2	2.14	0.48
9:E:170:ASP:OD1	9:E:171:ALA:N	2.45	0.48
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.95	0.48
31:sN1:246:A:H4'	31:sN1:247:G:H5'	1.95	0.48
31:sN1:721:G:OP1	31:sN1:851:U:O2'	2.24	0.48
31:sN1:928:C:N3	31:sN1:1383:G:N1	2.45	0.48
31:sN1:1381:C:H2'	31:sN1:1382:G:C8	2.48	0.48
32:b:86:ALA:O	32:b:90:GLY:N	2.45	0.48
5:AN1:844:A:H61	5:AN1:929:C:H1'	1.79	0.48
5:AN1:1348:A:H2'	5:AN1:1349:A:C8	2.47	0.48
5:AN1:1792:U:H2'	5:AN1:1793:C:C6	2.48	0.48
31:sN1:333:G:H2'	31:sN1:334:A:H8	1.77	0.48
31:sN1:925:G:O2'	31:sN1:1530:C:OP1	2.31	0.48
31:sN1:1267:U:H2'	31:sN1:1268:G:H8	1.79	0.48
5:AN1:1589:C:H2'	5:AN1:1590:A:H8	1.78	0.48
5:AN1:2694:U:H2'	5:AN1:2695:G:C8	2.48	0.48
10:F:140:GLU:HG2	10:F:141:ILE:H	1.78	0.48
31:sN1:80:A:H2'	31:sN1:81:G:C8	2.49	0.48
48:r:40:VAL:HB	48:r:44:ILE:HD11	1.95	0.48
5:AN1:308:U:H2'	5:AN1:309:G:O4'	2.14	0.48
5:AN1:1517:G:OP2	5:AN1:1518:A:O2'	2.24	0.48
5:AN1:1797:A:OP2	7:C:150:LYS:NZ	2.46	0.48
5:AN1:2060:C:H2'	5:AN1:2061:C:C6	2.49	0.48
20:P:82:GLY:O	20:P:86:ALA:N	2.45	0.48
31:sN1:476:U:H2'	31:sN1:477:G:C8	2.48	0.48
31:sN1:1045:G:H4'	44:n:3:LYS:HE2	1.94	0.48
5:AN1:2161:C:N4	5:AN1:2162:U:O4	2.47	0.48
5:AN1:2229:U:H2'	5:AN1:2230:G:H8	1.78	0.48
5:AN1:2563:G:H2'	5:AN1:2564:A:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2818:G:O6	17:M:2:ARG:NH1	2.44	0.48
7:C:230:HIS:CD2	7:C:232:HIS:H	2.31	0.48
10:F:140:GLU:HG2	10:F:141:ILE:N	2.28	0.48
5:AN1:1879:U:H2'	5:AN1:1880:G:O4'	2.14	0.48
5:AN1:1938:C:OP2	5:AN1:1939:U:O2'	2.23	0.48
5:AN1:2123:G:N2	5:AN1:2158:G:O6	2.46	0.48
5:AN1:2147:C:O2	5:AN1:2148:C:N4	2.47	0.48
5:AN1:2674:A:H2'	5:AN1:2675:A:C8	2.48	0.48
11:G:158:LYS:HD2	11:G:160:LYS:HD2	1.96	0.48
13:I:17:VAL:HG22	13:I:55:ILE:HB	1.96	0.48
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.94	0.48
31:sN1:1388:U:H2'	31:sN1:1389:G:H8	1.79	0.48
5:AN1:1081:A:O3'	5:AN1:1102:U:O2'	2.31	0.48
5:AN1:1427:G:H2'	5:AN1:1428:A:C8	2.48	0.48
6:B:28:C:H2'	6:B:29:C:O4'	2.14	0.48
10:F:17:GLN:NE2	10:F:28:ILE:HD11	2.29	0.48
12:H:4:ILE:N	12:H:37:VAL:O	2.42	0.48
31:sN1:407:A:N3	31:sN1:409:G:O2'	2.40	0.48
5:AN1:1054:A:N6	5:AN1:1084:G:OP2	2.46	0.48
5:AN1:1087:A:H2'	5:AN1:1088:G:C8	2.48	0.48
5:AN1:2324:A:H2'	5:AN1:2325:A:H8	1.75	0.48
31:sN1:232:A:H2'	31:sN1:233:A:H8	1.79	0.48
31:sN1:1002:A:H5"	31:sN1:1003:C:H5	1.78	0.48
34:d:119:LEU:O	34:d:124:SER:OG	2.32	0.48
40:j:56:HIS:CD2	40:j:57:VAL:HG13	2.48	0.48
47:q:32:HIS:HD2	47:q:35:TYR:H	1.62	0.48
5:AN1:1521:G:H2'	5:AN1:1522:C:C6	2.49	0.47
5:AN1:2166:A:H2'	5:AN1:2166:A:N3	2.28	0.47
10:F:33:LYS:HE2	10:F:92:ARG:HH12	1.79	0.47
10:F:119:ALA:O	10:F:167:ARG:NH1	2.45	0.47
16:L:42:MET:HE2	16:L:47:ILE:HG12	1.96	0.47
21:Q:1:MET:HE3	21:Q:101:ILE:HB	1.96	0.47
5:AN1:2727:G:H2'	5:AN1:2728:G:C8	2.50	0.47
5:AN1:2843:U:H2'	5:AN1:2844:G:O4'	2.14	0.47
6:B:29:C:H2'	6:B:30:U:C5	2.49	0.47
10:F:57:MET:HA	10:F:60:ILE:HB	1.95	0.47
19:O:17:LYS:HD3	19:O:80:HIS:HA	1.96	0.47
32:b:116:LEU:HD11	32:b:143:MET:HA	1.97	0.47
5:AN1:1921:C:H2'	5:AN1:1922:U:C6	2.49	0.47
5:AN1:2048:A:O3'	8:D:152:ASN:HA	2.14	0.47
5:AN1:2570:G:H1'	8:D:151:GLN:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:61:C:H2'	6:B:62:U:C6	2.48	0.47
6:B:68:C:H2'	6:B:69:U:H6	1.79	0.47
11:G:155:GLU:HG2	11:G:157:TYR:H	1.79	0.47
18:N:59:LEU:HD21	18:N:72:LYS:HB3	1.96	0.47
31:sN1:21:A:H2'	31:sN1:22:U:C6	2.49	0.47
31:sN1:202:U:O2	31:sN1:208:G:O6	2.31	0.47
31:sN1:1098:A:H61	32:b:104:THR:HG21	1.78	0.47
5:AN1:107:U:OP1	5:AN1:108:U:O2'	2.27	0.47
7:C:53:HIS:HA	7:C:217:ARG:HB2	1.96	0.47
36:f:18:VAL:O	36:f:22:VAL:HG23	2.15	0.47
36:f:32:ALA:HB3	36:f:35:GLN:NE2	2.29	0.47
5:AN1:665:U:H2'	5:AN1:666:A:O4'	2.13	0.47
5:AN1:1108:A:H2'	5:AN1:1109:G:H4'	1.95	0.47
5:AN1:1730:U:H2'	5:AN1:1731:C:C6	2.49	0.47
10:F:87:CYS:SG	10:F:89:VAL:HG23	2.55	0.47
18:N:3:GLU:HB2	18:N:6:GLN:HG2	1.95	0.47
31:sN1:1410:A:H2	31:sN1:1484:G:H22	1.62	0.47
32:b:78:ALA:HA	32:b:81:ILE:HG12	1.95	0.47
5:AN1:2070:U:H2'	5:AN1:2071:U:C6	2.49	0.47
31:sN1:1002:A:H5"	31:sN1:1003:C:C5	2.48	0.47
31:sN1:1352:G:H2'	31:sN1:1353:G:C8	2.49	0.47
33:c:46:LYS:HZ1	33:c:87:LEU:HD21	1.79	0.47
51:u:37:PHE:O	51:u:40:LYS:N	2.44	0.47
2:1:29:GLN:NE2	5:AN1:217:C:OP1	2.47	0.47
5:AN1:663:U:H2'	5:AN1:664:A:H8	1.78	0.47
5:AN1:970:A:H5'	5:AN1:1183:U:H1'	1.97	0.47
5:AN1:1430:G:H2'	5:AN1:1431:G:H8	1.80	0.47
5:AN1:1662:A:H61	5:AN1:1992:C:N4	2.09	0.47
5:AN1:2200:G:OP2	7:C:147:LYS:NZ	2.45	0.47
5:AN1:2622:C:H2'	5:AN1:2623:G:C8	2.50	0.47
6:B:11:A:O2'	6:B:13:A:OP2	2.27	0.47
18:N:82:LYS:NZ	18:N:113:GLY:HA3	2.30	0.47
31:sN1:498:C:OP1	42:l:114:ARG:NH2	2.45	0.47
31:sN1:518:G:O6	31:sN1:526:G:N1	2.48	0.47
31:sN1:1510:A:H2'	31:sN1:1511:G:C8	2.50	0.47
35:e:102:THR:HG21	35:e:123:LEU:HD11	1.95	0.47
46:p:32:ARG:NH1	46:p:60:THR:OG1	2.46	0.47
5:AN1:12:A:H2'	5:AN1:13:A:H8	1.80	0.47
5:AN1:43:G:N3	5:AN1:449:G:O2'	2.47	0.47
5:AN1:1475:C:H2'	5:AN1:1476:A:C8	2.50	0.47
20:P:104:VAL:HG12	21:Q:47:ILE:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:631:C:H2'	31:sN1:632:A:H8	1.80	0.47
31:sN1:659:G:H2'	31:sN1:660:A:C8	2.50	0.47
31:sN1:1068:C:H2'	31:sN1:1069:G:H8	1.80	0.47
44:n:64:CYS:HB3	44:n:68:GLY:H	1.80	0.47
3:2:16:ALA:HB2	3:2:64:ILE:HG13	1.97	0.47
5:AN1:591:U:H2'	5:AN1:592:U:C6	2.50	0.47
5:AN1:2072:U:OP2	5:AN1:2234:G:N2	2.40	0.47
10:F:128:TYR:CE2	10:F:170:MET:HE1	2.49	0.47
15:K:37:ILE:HG22	15:K:38:LYS:H	1.80	0.47
19:O:56:ARG:O	19:O:60:SER:OG	2.32	0.47
24:T:2:ALA:HA	24:T:81:VAL:HB	1.95	0.47
26:V:83:GLU:N	26:V:83:GLU:OE1	2.48	0.47
31:sN1:1080:U:O2'	31:sN1:1099:A:OP2	2.33	0.47
31:sN1:1141:G:N2	31:sN1:1143:A:H62	2.13	0.47
33:c:81:GLY:HA2	33:c:84:ILE:HD13	1.97	0.47
34:d:106:ARG:HB3	34:d:170:PRO:HG2	1.96	0.47
5:AN1:498:U:H2'	5:AN1:499:G:O4'	2.15	0.47
7:C:130:LEU:HB2	7:C:135:MET:HE2	1.97	0.47
23:S:49:LEU:HD13	28:X:26:PHE:CZ	2.50	0.47
37:g:53:LYS:HD3	37:g:125:LEU:HD11	1.97	0.47
51:u:43:GLN:HG2	51:u:47:ARG:HD2	1.97	0.47
5:AN1:309:G:N1	5:AN1:312:A:OP2	2.43	0.46
14:J:66:LYS:HE2	14:J:81:ASP:HA	1.97	0.46
25:U:40:GLU:O	25:U:97:ARG:NH2	2.35	0.46
31:sN1:1325:C:C2	31:sN1:1326:A:C8	3.03	0.46
5:AN1:199:G:N2	5:AN1:199:G:OP2	2.48	0.46
5:AN1:762:A:H5'	7:C:209:GLY:HA2	1.97	0.46
5:AN1:2543:A:H2'	5:AN1:2544:U:C6	2.49	0.46
5:AN1:2645:C:H2'	5:AN1:2646:U:H6	1.80	0.46
31:sN1:1402:G:O2'	31:sN1:1515:MA6:O2'	2.32	0.46
32:b:61:GLN:NE2	32:b:62:LEU:HD12	2.30	0.46
49:s:50:SER:HB3	49:s:57:HIS:HB3	1.98	0.46
5:AN1:13:A:O2'	13:I:135:GLN:NE2	2.48	0.46
5:AN1:587:U:H2'	5:AN1:588:A:H8	1.80	0.46
5:AN1:1004:C:OP1	13:I:37:ARG:NH1	2.48	0.46
5:AN1:2306:A:H2'	5:AN1:2307:A:H5"	1.96	0.46
6:B:90:C:OP1	25:U:26:ARG:NH2	2.49	0.46
7:C:21:HIS:ND1	7:C:90:HIS:HE1	2.14	0.46
25:U:47:GLU:HB3	25:U:50:GLU:HG2	1.97	0.46
32:b:89:ALA:HB1	32:b:223:ILE:HD11	1.97	0.46
42:l:44:LYS:HG2	42:l:45:PRO:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:102:VAL:HG12	11:G:116:ALA:HA	1.96	0.46
31:sN1:386:U:H2'	31:sN1:387:C:C6	2.51	0.46
31:sN1:1095:C:H2'	31:sN1:1096:G:C8	2.49	0.46
5:AN1:578:U:H2'	5:AN1:579:C:C6	2.50	0.46
5:AN1:1078:U:H2'	5:AN1:1079:U:C5	2.49	0.46
5:AN1:1878:U:H2'	5:AN1:1879:U:C6	2.50	0.46
5:AN1:2106:G:O5'	5:AN1:2114:U:H2'	2.14	0.46
13:I:34:ARG:HH22	13:I:40:HIS:HB3	1.80	0.46
31:sN1:991:A:N7	31:sN1:995:A:N6	2.64	0.46
33:c:141:THR:HG21	33:c:149:ILE:HD12	1.98	0.46
40:j:7:ARG:HB3	40:j:101:ALA:HB3	1.97	0.46
41:k:122:PRO:HB3	51:u:34:LYS:HB3	1.98	0.46
43:m:54:ASP:OD1	43:m:55:ALA:N	2.49	0.46
3:2:18:ALA:HB2	5:AN1:626:G:H5'	1.97	0.46
5:AN1:1437:U:H2'	5:AN1:1438:C:H6	1.80	0.46
5:AN1:1479:U:O4	5:AN1:1480:A:N6	2.44	0.46
5:AN1:2119:G:H1'	5:AN1:2172:A:C2	2.51	0.46
11:G:22:ARG:NH1	11:G:39:ALA:HA	2.30	0.46
16:L:60:ARG:HD2	16:L:60:ARG:HA	1.84	0.46
32:b:106:TRP:NE1	32:b:110:ARG:HD3	2.31	0.46
34:d:112:THR:OG1	34:d:113:ARG:N	2.48	0.46
5:AN1:1490:A:H2'	5:AN1:1491:A:H8	1.79	0.46
5:AN1:2287:U:OP1	5:AN1:2376:U:O2'	2.32	0.46
5:AN1:2683:U:H2'	5:AN1:2684:G:O4'	2.16	0.46
6:B:27:A:H2'	6:B:28:C:C6	2.51	0.46
25:U:84:HIS:HD2	25:U:87:LYS:H	1.63	0.46
27:W:15:GLY:HA3	27:W:29:PHE:HE1	1.80	0.46
31:sN1:517:A:H62	31:sN1:526:G:N2	2.13	0.46
32:b:93:TYR:O	32:b:152:GLY:HA3	2.16	0.46
32:b:116:LEU:HD21	32:b:143:MET:HG3	1.97	0.46
5:AN1:844:A:N6	5:AN1:929:C:O2'	2.49	0.46
5:AN1:909:A:H8	5:AN1:2273:G:H21	1.62	0.46
5:AN1:1437:U:H2'	5:AN1:1438:C:C6	2.51	0.46
5:AN1:2111:G:H4'	5:AN1:2113:A:H62	1.81	0.46
31:sN1:928:C:H2'	31:sN1:929:C:C6	2.50	0.46
36:f:12:PRO:O	36:f:44:ARG:NH2	2.49	0.46
10:F:30:ARG:H	10:F:159:THR:HB	1.81	0.46
34:d:11:LEU:O	34:d:15:GLU:HG2	2.16	0.46
5:AN1:203:A:OP2	15:K:49:ARG:NH2	2.49	0.46
5:AN1:493:G:H21	22:R:57:ASN:HD21	1.64	0.46
5:AN1:916:A:N3	6:B:78:U:O2'	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1490:A:H2'	5:AN1:1491:A:C8	2.51	0.46
5:AN1:1828:C:H2'	5:AN1:1829:C:O4'	2.16	0.46
5:AN1:2104:U:O2	5:AN1:2177:G:N2	2.47	0.46
5:AN1:2533:U:H2'	5:AN1:2534:C:H6	1.81	0.46
11:G:16:THR:HB	11:G:27:LYS:HE3	1.98	0.46
22:R:22:ASP:OD1	22:R:25:ARG:NH2	2.30	0.46
5:AN1:1588:A:H2'	5:AN1:1589:C:C6	2.51	0.45
5:AN1:2830:G:H2'	5:AN1:2875:A:H61	1.81	0.45
6:B:38:U:N3	6:B:42:G:OP2	2.37	0.45
19:O:103:LEU:HD23	19:O:106:LEU:HD12	1.98	0.45
31:sN1:481:G:H4'	31:sN1:482:U:H3'	1.97	0.45
31:sN1:1464:C:H2'	31:sN1:1465:A:H8	1.81	0.45
37:g:75:VAL:HG11	37:g:86:GLN:HB2	1.98	0.45
5:AN1:1356:G:H2'	5:AN1:1357:C:H6	1.79	0.45
15:K:93:SER:HB2	15:K:125:GLN:HE21	1.82	0.45
31:sN1:401:U:H3'	31:sN1:402:G:H5'	1.98	0.45
36:f:26:ILE:HD12	36:f:30:LYS:HE2	1.97	0.45
5:AN1:1862:A:H2'	5:AN1:1863:G:C8	2.51	0.45
5:AN1:2096:G:O6	5:AN1:2185:U:O4	2.35	0.45
31:sN1:78:G:H21	31:sN1:90:C:H41	1.63	0.45
36:f:29:ILE:HD13	36:f:74:LEU:HD12	1.99	0.45
41:k:64:VAL:HA	41:k:67:GLU:HG2	1.99	0.45
42:l:40:THR:HG22	42:l:41:THR:H	1.82	0.45
3:2:13:ARG:HD2	15:K:65:LYS:HG2	1.97	0.45
5:AN1:1381:A:H2'	5:AN1:1382:U:C6	2.51	0.45
5:AN1:1681:U:H2'	5:AN1:1682:A:C8	2.52	0.45
5:AN1:1681:U:H2'	5:AN1:1682:A:H8	1.82	0.45
5:AN1:1923:A:H2'	5:AN1:1924:A:C8	2.52	0.45
13:I:73:LYS:HD3	13:I:86:GLU:OE2	2.16	0.45
25:U:94:ASP:OD1	25:U:94:ASP:N	2.47	0.45
26:V:11:LYS:O	26:V:14:ARG:NH1	2.41	0.45
47:q:25:LEU:HD11	47:q:42:SER:HB2	1.98	0.45
5:AN1:86:C:H2'	5:AN1:87:G:C8	2.52	0.45
5:AN1:1793:C:O2'	7:C:257:THR:OG1	2.35	0.45
11:G:77:LYS:O	11:G:81:GLU:HG3	2.17	0.45
26:V:37:ILE:HG22	26:V:38:VAL:HG23	1.97	0.45
31:sN1:250:G:O2'	47:q:19:ASP:O	2.35	0.45
31:sN1:733:C:H2'	31:sN1:734:A:C8	2.49	0.45
31:sN1:1379:C:C2	31:sN1:1380:C:H5	2.34	0.45
36:f:48:ALA:HB1	48:r:69:PRO:HG3	1.98	0.45
37:g:111:ARG:HD3	37:g:123:GLU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:34:THR:HG22	48:r:35:GLU:N	2.32	0.45
50:t:33:LYS:HA	50:t:36:LEU:HG	1.97	0.45
5:AN1:475:G:N1	5:AN1:478:A:OP2	2.44	0.45
5:AN1:1311:A:H2'	5:AN1:1312:G:C8	2.52	0.45
5:AN1:1478:G:H2'	5:AN1:1479:U:C6	2.52	0.45
31:sN1:80:A:N1	31:sN1:88:A:H1'	2.31	0.45
31:sN1:133:U:H2'	31:sN1:134:A:H8	1.80	0.45
31:sN1:535:G:H2'	31:sN1:536:A:H8	1.81	0.45
31:sN1:821:U:H2'	31:sN1:822:A:C8	2.52	0.45
5:AN1:1846:G:H2'	5:AN1:1847:U:C6	2.52	0.45
5:AN1:2622:C:H2'	5:AN1:2623:G:H8	1.82	0.45
14:J:17:ARG:HD3	14:J:17:ARG:HA	1.76	0.45
31:sN1:521:G:OP1	31:sN1:521:G:N2	2.41	0.45
37:g:133:ALA:O	37:g:137:LYS:HG2	2.17	0.45
5:AN1:291:G:O2'	5:AN1:292:U:H5"	2.17	0.45
5:AN1:1467:G:O6	5:AN1:1468:A:N6	2.50	0.45
5:AN1:2021:C:H2'	5:AN1:2022:U:C6	2.52	0.45
5:AN1:2026:6MZ:H2	5:AN1:2495:C:H5"	1.99	0.45
5:AN1:2373:A:H2'	5:AN1:2374:A:C8	2.51	0.45
10:F:77:PHE:CE2	10:F:79:ILE:HG12	2.52	0.45
12:H:9:ILE:HB	12:H:12:LEU:HG	1.98	0.45
32:b:18:PHE:HA	32:b:42:ILE:HG22	1.99	0.45
5:AN1:636:G:H2'	5:AN1:637:U:C6	2.52	0.45
5:AN1:1680:G:H2'	5:AN1:1681:U:H6	1.81	0.45
31:sN1:1407:A:H2'	31:sN1:1408:C:C6	2.52	0.45
5:AN1:2169:A:H2'	5:AN1:2170:C:C5	2.52	0.45
29:Y:4:ILE:HB	29:Y:37:VAL:HG23	1.99	0.45
31:sN1:198:G:H2'	31:sN1:199:G:C8	2.52	0.45
31:sN1:709:A:H2'	31:sN1:710:G:C8	2.51	0.45
31:sN1:1269:U:H2'	31:sN1:1270:G:C8	2.52	0.45
36:f:15:SER:HA	36:f:18:VAL:HG22	1.99	0.45
37:g:74:GLU:OE1	37:g:76:LYS:HG2	2.16	0.45
48:r:34:THR:HG22	48:r:35:GLU:H	1.82	0.45
5:AN1:713:A:H2'	5:AN1:714:A:O4'	2.17	0.44
5:AN1:1470:G:H5"	5:AN1:1510:G:O6	2.17	0.44
10:F:120:LYS:HG3	10:F:121:SER:N	2.24	0.44
31:sN1:552:U:H2'	31:sN1:553:C:C6	2.51	0.44
32:b:48:THR:HB	32:b:203:PRO:HG2	1.98	0.44
32:b:113:ILE:HD12	32:b:150:LEU:HB3	1.99	0.44
5:AN1:2312:G:H2'	5:AN1:2313:C:C6	2.52	0.44
5:AN1:2674:A:H2'	5:AN1:2675:A:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:144:ASP:O	10:F:146:ILE:HG23	2.17	0.44
23:S:67:LYS:NZ	23:S:76:ARG:HE	2.15	0.44
25:U:9:GLN:O	25:U:45:THR:N	2.43	0.44
31:sN1:134:A:H2'	31:sN1:135:U:H6	1.83	0.44
31:sN1:716:C:H1'	48:r:38:LYS:HB3	1.99	0.44
32:b:107:LYS:HA	32:b:110:ARG:HE	1.82	0.44
37:g:49:ARG:HD2	37:g:49:ARG:HA	1.81	0.44
5:AN1:664:A:H2'	5:AN1:665:U:C6	2.52	0.44
5:AN1:2048:A:O2'	8:D:151:GLN:O	2.34	0.44
31:sN1:78:G:N2	31:sN1:90:C:H41	2.15	0.44
31:sN1:639:A:N7	38:h:108:SER:HA	2.32	0.44
32:b:86:ALA:HB1	32:b:91:GLN:O	2.17	0.44
38:h:97:LYS:HE2	38:h:131:SER:HB2	1.98	0.44
41:k:23:HIS:N	41:k:30:ILE:O	2.51	0.44
42:l:33:VAL:HA	42:l:78:SER:O	2.17	0.44
51:u:37:PHE:CD1	51:u:40:LYS:HD3	2.52	0.44
5:AN1:307:C:H2'	5:AN1:308:U:C6	2.52	0.44
5:AN1:342:A:HO2'	9:E:161:ARG:HH12	1.64	0.44
5:AN1:372:U:H2'	5:AN1:373:A:C8	2.51	0.44
5:AN1:1089:C:H3'	5:AN1:1090:G:H8	1.83	0.44
5:AN1:1303:A:N7	55:AN1:3135:HOH:O	2.36	0.44
5:AN1:1562:C:H2'	5:AN1:1563:C:C6	2.53	0.44
5:AN1:1583:C:H3'	5:AN1:1584:A:H8	1.82	0.44
7:C:205:LEU:HB3	7:C:210:ALA:HB3	1.99	0.44
31:sN1:136:U:H2'	31:sN1:137:A:H8	1.82	0.44
31:sN1:928:C:H2'	31:sN1:929:C:H6	1.82	0.44
31:sN1:1060:C:OP2	31:sN1:1061:G:O2'	2.23	0.44
32:b:115:ARG:O	32:b:118:ASP:HB3	2.16	0.44
5:AN1:849:C:H2'	5:AN1:850:A:H8	1.82	0.44
5:AN1:1475:C:H2'	5:AN1:1476:A:H8	1.83	0.44
5:AN1:1961:C:H5"	5:AN1:1962:A:H2'	2.00	0.44
5:AN1:2295:G:H2'	5:AN1:2296:C:C6	2.53	0.44
5:AN1:2323:A:H2'	5:AN1:2324:A:C8	2.52	0.44
5:AN1:2815:C:H2'	5:AN1:2817:A:N7	2.33	0.44
6:B:68:C:H2'	6:B:69:U:C6	2.53	0.44
32:b:102:MET:HA	32:b:109:LEU:HD11	2.00	0.44
40:j:7:ARG:HD2	40:j:73:LEU:HD11	2.00	0.44
41:k:81:LEU:HG	41:k:99:LEU:HD21	1.98	0.44
47:q:27:GLU:HG2	47:q:42:SER:HB3	2.00	0.44
5:AN1:606:A:H2'	5:AN1:607:A:C8	2.53	0.44
5:AN1:861:A:H2'	5:AN1:862:G:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:997:A:H2'	5:AN1:998:A:C8	2.52	0.44
5:AN1:1412:C:H3'	5:AN1:1413:G:C8	2.53	0.44
5:AN1:1561:U:H2'	5:AN1:1562:C:C6	2.52	0.44
5:AN1:2107:U:O4'	5:AN1:2114:U:O2'	2.35	0.44
5:AN1:2176:U:H2'	5:AN1:2177:G:C8	2.52	0.44
5:AN1:2185:U:H2'	5:AN1:2186:G:H8	1.83	0.44
10:F:99:PHE:HD1	10:F:102:ARG:HH11	1.66	0.44
12:H:40:THR:OG1	12:H:43:ASN:ND2	2.50	0.44
22:R:65:ASP:OD1	22:R:65:ASP:N	2.51	0.44
42:l:55:VAL:HG22	42:l:63:VAL:O	2.18	0.44
5:AN1:67:G:C6	5:AN1:81:A:C6	3.05	0.44
5:AN1:873:G:H2'	5:AN1:874:C:C6	2.53	0.44
6:B:87:A:H2'	16:L:18:THR:HG22	1.99	0.44
31:sN1:124:G:H2'	31:sN1:125:A:C8	2.52	0.44
31:sN1:1011:A:C2	31:sN1:1216:A:H1'	2.53	0.44
32:b:116:LEU:HD22	32:b:147:GLU:OE2	2.18	0.44
5:AN1:1634:G:H2'	5:AN1:1635:A:C8	2.53	0.44
5:AN1:2587:C:H2'	5:AN1:2588:G:C8	2.53	0.44
5:AN1:2594:A:H5"	7:C:234:GLY:HA3	1.99	0.44
31:sN1:96:U:O2'	31:sN1:97:A:N7	2.50	0.44
31:sN1:615:C:N4	31:sN1:618:A:OP2	2.45	0.44
31:sN1:684:A:H62	31:sN1:700:G:N2	2.14	0.44
33:c:181:ASP:HB2	33:c:207:ILE:HG12	1.99	0.44
5:AN1:580:A:H2'	5:AN1:581:G:H8	1.82	0.44
5:AN1:720:A:H2'	5:AN1:721:C:C6	2.53	0.44
5:AN1:1743:A:H2'	5:AN1:1744:C:C6	2.53	0.44
5:AN1:1876:U:H2'	5:AN1:1877:C:C6	2.53	0.44
5:AN1:2169:A:H2'	5:AN1:2170:C:C6	2.53	0.44
5:AN1:2301:U:C5	10:F:153:ASP:HB2	2.53	0.44
5:AN1:2304:G:O2'	5:AN1:2306:A:OP2	2.30	0.44
5:AN1:2747:G:OP1	5:AN1:2747:G:N2	2.47	0.44
8:D:55:GLU:HA	8:D:76:ALA:O	2.18	0.44
10:F:162:THR:HB	10:F:165:GLU:HG3	2.00	0.44
12:H:5:LEU:CD1	12:H:13:GLY:HA3	2.48	0.44
12:H:50:ARG:NH1	12:H:54:LEU:HD22	2.33	0.44
13:I:109:LEU:HD12	13:I:119:ILE:HD13	2.00	0.44
20:P:78:ARG:HD3	20:P:78:ARG:HA	1.77	0.44
31:sN1:81:G:N2	31:sN1:87:U:O2'	2.51	0.44
31:sN1:251:G:H2'	31:sN1:252:U:C6	2.52	0.44
31:sN1:346:G:H2'	31:sN1:347:G:C8	2.53	0.44
31:sN1:414:C:H2'	31:sN1:415:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:1488:G:H2'	31:sN1:1489:A:C8	2.52	0.44
32:b:209:ILE:HG13	32:b:210:ARG:N	2.32	0.44
5:AN1:181:C:H2'	5:AN1:182:A:H8	1.83	0.43
5:AN1:596:U:H2'	5:AN1:597:A:C8	2.53	0.43
5:AN1:2262:A:H4'	5:AN1:2263:A:N3	2.33	0.43
5:AN1:2896:A:H2'	5:AN1:2897:C:C6	2.53	0.43
6:B:26:C:H2'	6:B:27:A:H8	1.83	0.43
31:sN1:991:A:H4'	31:sN1:992:C:C5'	2.48	0.43
33:c:118:GLU:HA	33:c:187:MET:HG2	2.00	0.43
40:j:49:PHE:HZ	44:n:76:LYS:HD3	1.83	0.43
5:AN1:2734:A:H2	5:AN1:2762:G:H1	1.66	0.43
10:F:34:ILE:HD12	10:F:96:MET:HB2	2.00	0.43
31:sN1:1015:G:C2	31:sN1:1016:G:C6	3.06	0.43
33:c:56:LEU:HB3	33:c:67:THR:HB	2.00	0.43
41:k:81:LEU:HD21	41:k:104:TYR:CD1	2.52	0.43
5:AN1:720:A:H2'	5:AN1:721:C:H6	1.82	0.43
5:AN1:1310:C:H2'	5:AN1:1311:A:C8	2.52	0.43
5:AN1:2170:C:H2'	5:AN1:2171:C:O4'	2.18	0.43
5:AN1:2510:U:H2'	5:AN1:2511:C:C6	2.53	0.43
6:B:22:G:O6	6:B:54:G:O2'	2.35	0.43
14:J:44:LYS:HA	14:J:44:LYS:HD3	1.82	0.43
15:K:80:ARG:HB2	15:K:83:GLU:HG3	2.00	0.43
24:T:5:LYS:N	24:T:8:ASP:OD2	2.36	0.43
31:sN1:250:G:O6	31:sN1:269:A:N6	2.52	0.43
31:sN1:354:U:H2'	31:sN1:355:G:H8	1.83	0.43
31:sN1:704:U:H2'	31:sN1:705:C:C6	2.52	0.43
42:l:30:ARG:NH2	42:l:58:THR:OG1	2.51	0.43
5:AN1:278:U:H3	5:AN1:366:G:H22	1.66	0.43
5:AN1:695:G:H2'	5:AN1:696:C:C6	2.54	0.43
5:AN1:2172:A:O2'	5:AN1:2173:C:O4'	2.32	0.43
5:AN1:2187:A:H2'	5:AN1:2188:G:C8	2.53	0.43
6:B:6:C:O3'	18:N:26:ARG:NH2	2.45	0.43
20:P:81:ASP:OD1	20:P:85:LYS:NZ	2.51	0.43
36:f:11:HIS:HD2	36:f:13:ASP:HB2	1.84	0.43
36:f:35:GLN:O	36:f:36:ILE:HD13	2.17	0.43
5:AN1:158:U:H2'	5:AN1:159:G:C8	2.54	0.43
5:AN1:563:C:P	21:Q:80:ARG:H	2.41	0.43
5:AN1:758:G:H2'	5:AN1:759:A:O4'	2.17	0.43
5:AN1:1038:G:N1	5:AN1:1039:G:O6	2.52	0.43
5:AN1:2239:U:H2'	5:AN1:2240:U:C6	2.54	0.43
5:AN1:2463:C:H2'	5:AN1:2464:A:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2639:G:H2'	5:AN1:2640:A:C8	2.53	0.43
6:B:28:C:H1'	6:B:55:A:H61	1.82	0.43
15:K:29:VAL:HG12	15:K:33:GLY:HA2	2.01	0.43
25:U:84:HIS:CD2	25:U:86:ALA:H	2.36	0.43
31:sN1:1022:U:H4'	31:sN1:1023:G:O4'	2.18	0.43
31:sN1:1113:U:C2	31:sN1:1181:G:O6	2.72	0.43
31:sN1:1263:G:N2	31:sN1:1266:A:OP2	2.32	0.43
31:sN1:1509:U:H2'	31:sN1:1510:A:C8	2.53	0.43
38:h:22:LYS:O	38:h:66:TYR:OH	2.28	0.43
5:AN1:611:U:H5"	5:AN1:612:A:C8	2.54	0.43
5:AN1:2010:A:H2'	5:AN1:2011:A:C8	2.53	0.43
5:AN1:2066:A:H2'	5:AN1:2067:A:H8	1.84	0.43
5:AN1:2679:C:O2	14:J:70:ARG:NH2	2.51	0.43
6:B:54:G:H4'	6:B:55:A:H8	1.84	0.43
8:D:184:ASP:HB3	8:D:189:VAL:HG22	2.00	0.43
13:I:16:PHE:HB2	13:I:54:ILE:HD13	2.01	0.43
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	2.00	0.43
31:sN1:550:A:H2'	31:sN1:551:A:H8	1.84	0.43
31:sN1:1464:C:H2'	31:sN1:1465:A:C8	2.54	0.43
31:sN1:1527:G:H2'	31:sN1:1528:A:C8	2.54	0.43
32:b:116:LEU:HD23	32:b:116:LEU:O	2.19	0.43
36:f:72:ASP:OD2	36:f:73:GLU:N	2.51	0.43
5:AN1:2379:G:O2'	5:AN1:2380:U:OP1	2.33	0.43
5:AN1:2533:U:H2'	5:AN1:2534:C:C6	2.53	0.43
6:B:10:C:C5	26:V:74:GLN:HB3	2.54	0.43
31:sN1:936:G:H2'	31:sN1:937:C:C6	2.54	0.43
33:c:46:LYS:NZ	33:c:87:LEU:HD11	2.30	0.43
36:f:54:ILE:O	36:f:54:ILE:HG22	2.19	0.43
37:g:98:ALA:O	37:g:102:ARG:HG3	2.19	0.43
41:k:74:LEU:HG	41:k:104:TYR:OH	2.19	0.43
5:AN1:358:A:HO2'	5:AN1:359:U:H6	1.66	0.43
5:AN1:568:G:H2'	5:AN1:2026:6MZ:N7	2.34	0.43
5:AN1:587:U:H2'	5:AN1:588:A:C8	2.54	0.43
5:AN1:1382:U:H5'	5:AN1:1464:A:H1'	2.00	0.43
10:F:35:THR:HA	10:F:90:THR:HA	2.01	0.43
12:H:51:ARG:HE	12:H:55:GLU:HG2	1.84	0.43
31:sN1:675:U:H2'	31:sN1:676:C:H6	1.83	0.43
31:sN1:1369:U:H2'	31:sN1:1370:G:O4'	2.18	0.43
35:e:81:GLN:H	35:e:146:MET:HE3	1.83	0.43
5:AN1:413:C:H1'	5:AN1:1860:U:H1'	2.00	0.43
5:AN1:631:A:O2'	5:AN1:2400:U:OP1	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:713:A:N1	45:o:53:ARG:NH1	2.66	0.43
5:AN1:1679:G:N2	5:AN1:1759:G:OP2	2.41	0.43
10:F:120:LYS:CG	10:F:121:SER:H	2.22	0.43
13:I:21:THR:HA	13:I:61:GLN:HB3	2.01	0.43
20:P:87:GLN:C	21:Q:51:ALA:HB1	2.44	0.43
24:T:46:PRO:HD3	24:T:54:GLY:HA3	2.00	0.43
5:AN1:67:G:C2	5:AN1:68:A:N6	2.87	0.43
5:AN1:569:U:H3'	21:Q:80:ARG:NH2	2.34	0.43
5:AN1:1078:U:H2'	5:AN1:1079:U:H5	1.83	0.43
5:AN1:1590:A:H2'	5:AN1:1591:C:H6	1.84	0.43
5:AN1:2309:C:O3'	10:F:88:LYS:NZ	2.38	0.43
5:AN1:2795:A:H2'	5:AN1:2797:G:OP2	2.18	0.43
25:U:76:VAL:HG12	25:U:97:ARG:HA	2.01	0.43
31:sN1:198:G:H21	31:sN1:462:A:H61	1.67	0.43
31:sN1:552:U:H2'	31:sN1:553:C:H6	1.84	0.43
2:1:1:MET:N	5:AN1:1617:G:H21	2.16	0.42
5:AN1:298:U:H2'	5:AN1:299:G:C8	2.54	0.42
5:AN1:502:A:H4'	5:AN1:504:A:H5"	2.01	0.42
9:E:152:VAL:HG11	9:E:157:TYR:CZ	2.53	0.42
11:G:154:PRO:HA	11:G:160:LYS:O	2.19	0.42
31:sN1:675:U:H2'	31:sN1:676:C:C6	2.54	0.42
32:b:190:ASP:HB2	32:b:206:ASP:OD2	2.19	0.42
35:e:108:GLY:HA2	35:e:111:ARG:HG2	2.00	0.42
36:f:75:GLU:O	36:f:79:ARG:HG2	2.19	0.42
38:h:113:THR:HG23	38:h:116:ALA:H	1.84	0.42
5:AN1:1287:G:H2'	5:AN1:1288:U:C6	2.55	0.42
5:AN1:2093:U:H2'	5:AN1:2094:U:C6	2.54	0.42
5:AN1:2416:C:H2'	5:AN1:2417:G:H8	1.84	0.42
5:AN1:2456:U:C2	5:AN1:2457:A:C8	3.07	0.42
6:B:40:C:OP1	10:F:64:LYS:NZ	2.53	0.42
6:B:81:G:O6	6:B:91:A:N6	2.52	0.42
6:B:111:C:H2'	6:B:112:A:H8	1.84	0.42
29:Y:7:THR:HG23	29:Y:55:SER:HB3	2.01	0.42
32:b:21:GLN:HE21	32:b:39:LYS:HD2	1.84	0.42
36:f:5:GLU:HA	36:f:63:ASN:HA	2.01	0.42
41:k:64:VAL:O	41:k:67:GLU:HG2	2.19	0.42
43:m:50:ASP:HA	43:m:53:LEU:HB3	2.01	0.42
5:AN1:1810:G:OP2	5:AN1:1811:A:O2'	2.33	0.42
5:AN1:2109:U:O4	5:AN1:2163:U:O2'	2.38	0.42
12:H:13:GLY:C	12:H:14:LYS:HD3	2.45	0.42
31:sN1:281:U:H2'	31:sN1:282:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:388:C:C2	31:sN1:389:A:C8	3.07	0.42
31:sN1:1064:A:N1	31:sN1:1105:G:O2'	2.44	0.42
31:sN1:1184:G:N3	44:n:100:SER:OG	2.52	0.42
5:AN1:69:U:H2'	5:AN1:70:A:H8	1.84	0.42
5:AN1:831:A:H2'	5:AN1:832:G:C8	2.54	0.42
5:AN1:1587:U:H2'	5:AN1:1588:A:C8	2.50	0.42
5:AN1:1861:U:H2'	5:AN1:1862:A:C8	2.54	0.42
5:AN1:2110:A:H3'	5:AN1:2111:G:H8	1.84	0.42
5:AN1:2553:G:H2'	5:AN1:2554:C:C6	2.54	0.42
5:AN1:2696:A:H2'	5:AN1:2697:C:C6	2.54	0.42
6:B:13:A:H5"	6:B:105:C:C2	2.54	0.42
6:B:88:C:OP2	55:B:201:HOH:O	2.22	0.42
31:sN1:58:U:H2'	31:sN1:59:G:C8	2.54	0.42
31:sN1:657:G:C2	31:sN1:743:A:N1	2.88	0.42
31:sN1:865:C:H2'	31:sN1:866:G:O4'	2.19	0.42
31:sN1:947:U:H2'	31:sN1:948:G:C8	2.54	0.42
34:d:170:PRO:HB2	34:d:173:ILE:HG12	2.00	0.42
35:e:33:THR:OG1	35:e:49:ARG:NH1	2.52	0.42
39:i:127:LYS:HE2	39:i:128:ARG:NH1	2.34	0.42
5:AN1:9:G:H2'	5:AN1:10:U:H6	1.82	0.42
5:AN1:1908:A:H2	5:AN1:1913:PSU:HN3	1.66	0.42
5:AN1:2098:C:H2'	5:AN1:2099:C:O4'	2.19	0.42
7:C:258:ARG:NH2	7:C:260:ASN:O	2.53	0.42
10:F:36:LEU:N	10:F:89:VAL:O	2.37	0.42
23:S:53:GLU:HG2	23:S:87:LYS:H	1.85	0.42
25:U:40:GLU:HG2	25:U:41:PRO:O	2.20	0.42
31:sN1:252:U:H2'	31:sN1:253:G:C8	2.52	0.42
31:sN1:732:C:H2'	31:sN1:733:C:H6	1.84	0.42
31:sN1:1100:C:H5'	32:b:99:LEU:HD11	2.01	0.42
31:sN1:1159:C:H42	31:sN1:1171:G:H22	1.67	0.42
42:l:37:VAL:HG12	42:l:53:CYS:SG	2.59	0.42
7:C:6:CYS:SG	7:C:13:ARG:NH2	2.90	0.42
9:E:152:VAL:HG11	9:E:157:TYR:CE1	2.54	0.42
31:sN1:719:A:H61	31:sN1:730:A:H61	1.67	0.42
32:b:165:VAL:O	32:b:187:GLY:HA2	2.20	0.42
33:c:77:ILE:HG22	33:c:79:LYS:H	1.84	0.42
37:g:79:ARG:HD2	37:g:82:GLY:HA2	2.02	0.42
5:AN1:826:U:H2'	5:AN1:827:A:C8	2.55	0.42
5:AN1:2110:A:H3'	5:AN1:2111:G:C8	2.54	0.42
5:AN1:2381:C:H2'	5:AN1:2382:U:C6	2.55	0.42
5:AN1:2633:U:H2'	5:AN1:2634:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2657:G:OP2	5:AN1:2657:G:H8	2.02	0.42
5:AN1:2784:C:H2'	5:AN1:2785:C:C6	2.54	0.42
24:T:5:LYS:HE2	24:T:5:LYS:HB3	1.84	0.42
24:T:42:LYS:NZ	24:T:43:HIS:O	2.50	0.42
43:m:7:VAL:HG21	43:m:66:GLU:OE2	2.20	0.42
43:m:49:ASP:OD2	43:m:52:GLN:NE2	2.53	0.42
5:AN1:353:C:H2'	5:AN1:354:A:H8	1.85	0.42
5:AN1:754:A:H2'	5:AN1:755:G:O4'	2.19	0.42
5:AN1:856:G:H3'	5:AN1:857:G:C8	2.55	0.42
5:AN1:1835:G:C2	5:AN1:1836:G:C8	3.07	0.42
5:AN1:1909:A:O2'	5:AN1:1959:U:O4	2.36	0.42
5:AN1:2472:A:H61	5:AN1:2525:G:H2'	1.85	0.42
5:AN1:2647:C:H2'	5:AN1:2648:C:C6	2.55	0.42
11:G:127:THR:HG22	11:G:129:THR:H	1.84	0.42
15:K:82:SER:OG	15:K:116:GLY:HA3	2.20	0.42
31:sN1:268:C:H2'	31:sN1:269:A:H8	1.84	0.42
31:sN1:386:U:H2'	31:sN1:387:C:H6	1.85	0.42
31:sN1:1002:A:H3'	31:sN1:1003:C:H6	1.85	0.42
31:sN1:1448:C:N3	31:sN1:1450:A:N6	2.68	0.42
49:s:19:VAL:HG11	49:s:44:PHE:CE1	2.54	0.42
1:0:22:ASN:HD21	1:0:24:ARG:CZ	2.33	0.42
5:AN1:1482:C:N4	5:AN1:1498:G:H1	2.18	0.42
31:sN1:557:U:H4'	31:sN1:558:U:H5"	2.01	0.42
31:sN1:572:G:O2'	31:sN1:818:G:H5'	2.20	0.42
31:sN1:979:U:H4'	31:sN1:980:A:O4'	2.20	0.42
31:sN1:1449:A:H5"	31:sN1:1450:A:C2	2.54	0.42
42:l:52:VAL:HG23	42:l:65:SER:O	2.19	0.42
3:2:32:LEU:HD12	3:2:35:LYS:HD2	2.01	0.42
5:AN1:292:U:H2'	5:AN1:293:U:C6	2.55	0.42
5:AN1:612:A:H5'	5:AN1:614:A:C6	2.55	0.42
5:AN1:976:A:H2'	5:AN1:979:C:H41	1.85	0.42
5:AN1:1296:A:H2	5:AN1:1624:A:H2	1.68	0.42
5:AN1:1359:G:N7	27:W:2:SER:N	2.68	0.42
10:F:128:TYR:CD2	10:F:170:MET:HE1	2.55	0.42
31:sN1:509:U:H2'	31:sN1:510:C:C6	2.54	0.42
31:sN1:631:C:H2'	31:sN1:632:A:C8	2.55	0.42
5:AN1:309:G:N2	5:AN1:311:G:H3'	2.35	0.41
5:AN1:1441:C:H2'	5:AN1:1442:C:H6	1.85	0.41
5:AN1:1862:A:H2	5:AN1:1872:A:C8	2.38	0.41
5:AN1:1942:U:H2'	5:AN1:1943:C:H6	1.85	0.41
5:AN1:2736:A:H2'	5:AN1:2737:A:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:101:A:H2'	6:B:102:A:O4'	2.20	0.41
23:S:2:ASN:ND2	28:X:19:ASP:OD1	2.52	0.41
31:sN1:1001:A:N6	31:sN1:1021:G:O2'	2.53	0.41
31:sN1:1193:A:O2'	31:sN1:1194:A:OP1	2.33	0.41
31:sN1:1483:G:H2'	31:sN1:1484:G:H8	1.83	0.41
32:b:18:PHE:HB2	32:b:40:ILE:HG21	2.02	0.41
37:g:126:ASP:O	37:g:132:GLY:N	2.53	0.41
4:3:2:LYS:HE3	4:3:2:LYS:HB2	1.92	0.41
5:AN1:103:U:H2'	5:AN1:104:C:O4'	2.20	0.41
5:AN1:1590:A:H2'	5:AN1:1591:C:C6	2.55	0.41
5:AN1:2243:A:H2'	5:AN1:2244:C:H6	1.86	0.41
5:AN1:2572:G:H5'	5:AN1:2574:G:N7	2.35	0.41
11:G:98:VAL:HG22	11:G:103:VAL:HG23	2.00	0.41
31:sN1:1009:A:H2'	31:sN1:1009:A:N3	2.35	0.41
31:sN1:1014:U:N3	31:sN1:1015:G:N7	2.68	0.41
31:sN1:1522:G:H5"	51:u:38:TYR:CE2	2.55	0.41
33:c:9:GLY:HA3	44:n:89:MET:HE3	2.02	0.41
5:AN1:34:G:N2	5:AN1:511:G:H2'	2.35	0.41
5:AN1:67:G:O6	5:AN1:81:A:N6	2.52	0.41
5:AN1:86:C:C2	5:AN1:87:G:C8	3.08	0.41
5:AN1:880:G:C6	5:AN1:893:U:H1'	2.55	0.41
5:AN1:1749:G:H5"	19:O:96:ARG:HD3	2.02	0.41
5:AN1:1804:A:H2'	5:AN1:1805:A:C8	2.55	0.41
10:F:50:LEU:O	10:F:54:VAL:HG13	2.21	0.41
11:G:36:ASN:OD1	11:G:37:LEU:N	2.50	0.41
31:sN1:430:C:H2'	31:sN1:431:A:C8	2.55	0.41
31:sN1:529:A:N7	33:c:193:TYR:OH	2.43	0.41
31:sN1:725:A:H2'	31:sN1:726:A:C8	2.55	0.41
31:sN1:1188:A:H8	31:sN1:1188:A:OP2	2.03	0.41
31:sN1:1374:A:C6	37:g:7:VAL:HG21	2.55	0.41
32:b:70:LEU:HD11	32:b:94:VAL:HG23	2.03	0.41
5:AN1:707:U:H2'	5:AN1:708:U:C6	2.56	0.41
5:AN1:881:G:H2'	5:AN1:882:U:C6	2.55	0.41
5:AN1:903:A:H3'	5:AN1:904:U:H5"	2.01	0.41
5:AN1:1041:A:H1'	5:AN1:1108:A:H62	1.85	0.41
5:AN1:1665:G:O2'	5:AN1:1987:U:O4	2.28	0.41
5:AN1:2892:C:H2'	5:AN1:2893:U:C6	2.55	0.41
9:E:97:ARG:HG2	9:E:101:ARG:HE	1.84	0.41
11:G:135:SER:HB3	11:G:141:LEU:HB2	2.03	0.41
12:H:30:LEU:HB3	12:H:36:ALA:HB3	2.02	0.41
13:I:32:ILE:O	13:I:36:LEU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:155:G:N2	31:sN1:158:A:OP2	2.53	0.41
31:sN1:456:U:H2'	31:sN1:457:A:C8	2.55	0.41
31:sN1:519:C:H42	31:sN1:525:C:N4	2.18	0.41
31:sN1:577:C:H2'	31:sN1:578:G:O4'	2.21	0.41
32:b:135:GLU:O	32:b:138:GLU:HB3	2.20	0.41
35:e:131:ASN:HB3	35:e:134:ASN:HB2	2.02	0.41
36:f:10:VAL:HG21	36:f:18:VAL:HG11	2.02	0.41
5:AN1:25:C:O2'	5:AN1:552:U:OP1	2.37	0.41
5:AN1:597:A:H2'	5:AN1:598:G:H8	1.85	0.41
5:AN1:630:A:H2'	5:AN1:631:A:C8	2.56	0.41
5:AN1:1464:A:H2'	5:AN1:1465:A:C8	2.55	0.41
5:AN1:2122:A:H2	5:AN1:2159:U:H3	1.68	0.41
31:sN1:136:U:H2'	31:sN1:137:A:C8	2.56	0.41
32:b:49:VAL:CG2	32:b:50:PRO:HD3	2.48	0.41
33:c:50:ALA:O	33:c:70:THR:OG1	2.38	0.41
5:AN1:298:U:H2'	5:AN1:299:G:H8	1.86	0.41
5:AN1:981:A:N3	5:AN1:981:A:H2'	2.36	0.41
5:AN1:1335:U:OP1	23:S:18:LYS:NZ	2.52	0.41
5:AN1:1569:A:H2'	5:AN1:1570:A:C8	2.56	0.41
5:AN1:1708:G:H4'	5:AN1:2854:U:O2	2.20	0.41
6:B:66:C:H2'	6:B:67:G:O4'	2.21	0.41
31:sN1:943:A:H2'	31:sN1:944:G:H8	1.86	0.41
31:sN1:996:C:H2'	31:sN1:997:U:C6	2.55	0.41
43:m:23:PHE:CD2	43:m:66:GLU:HA	2.55	0.41
44:n:8:ASN:O	44:n:11:LEU:HG	2.19	0.41
44:n:83:LYS:HD3	44:n:83:LYS:HA	1.87	0.41
5:AN1:2645:C:H2'	5:AN1:2646:U:C6	2.55	0.41
5:AN1:2842:G:H2'	5:AN1:2843:U:C6	2.56	0.41
10:F:102:ARG:O	10:F:106:ILE:HG12	2.21	0.41
18:N:74:GLY:O	18:N:77:ILE:HG22	2.21	0.41
31:sN1:402:G:H2'	31:sN1:403:U:H6	1.85	0.41
31:sN1:1427:C:H42	31:sN1:1467:G:H1	1.68	0.41
32:b:72:VAL:HG13	32:b:165:VAL:HG23	2.03	0.41
33:c:43:LEU:HD23	33:c:43:LEU:HA	1.93	0.41
36:f:64:VAL:HG12	36:f:66:CYS:H	1.85	0.41
3:2:31:ILE:H	3:2:31:ILE:HG13	1.40	0.41
5:AN1:176:U:H2'	5:AN1:177:G:H8	1.85	0.41
5:AN1:239:G:H8	5:AN1:239:G:OP2	2.04	0.41
5:AN1:249:G:N2	5:AN1:262:A:OP2	2.48	0.41
5:AN1:1065:G:O6	5:AN1:1066:A:N6	2.53	0.41
5:AN1:1407:U:O4	5:AN1:1408:A:N6	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1911:3TD:OP1	5:AN1:1911:3TD:O3'	2.38	0.41
10:F:36:LEU:HB2	10:F:89:VAL:HB	2.03	0.41
13:I:70:LEU:HA	13:I:88:ASN:HD21	1.86	0.41
15:K:93:SER:H	15:K:96:THR:HG1	1.68	0.41
31:sN1:122:A:OP1	31:sN1:602:U:O2'	2.37	0.41
31:sN1:359:A:H5'	42:l:81:LEU:HD11	2.03	0.41
31:sN1:553:C:H2'	31:sN1:554:G:H8	1.85	0.41
31:sN1:1170:U:H2'	31:sN1:1171:G:C8	2.56	0.41
36:f:34:GLY:H	36:f:35:GLN:NE2	2.18	0.41
38:h:29:SER:HB2	38:h:60:LEU:HB2	2.03	0.41
5:AN1:324:A:OP2	9:E:162:ASN:HB2	2.20	0.41
5:AN1:518:C:H2'	5:AN1:519:A:C8	2.53	0.41
5:AN1:794:C:H2'	5:AN1:795:U:C6	2.56	0.41
5:AN1:876:A:H3'	5:AN1:877:G:C8	2.56	0.41
5:AN1:1389:U:H2'	5:AN1:1390:A:O4'	2.21	0.41
5:AN1:1589:C:H2'	5:AN1:1590:A:C8	2.55	0.41
5:AN1:1817:A:H2'	5:AN1:1818:G:H8	1.85	0.41
5:AN1:1844:A:H4'	5:AN1:1845:G:H8	1.85	0.41
5:AN1:2895:G:C6	5:AN1:2896:A:N6	2.89	0.41
55:AN1:3126:HOH:O	8:D:143:HIS:NE2	2.36	0.41
6:B:40:C:H1'	10:F:64:LYS:O	2.21	0.41
8:D:186:GLU:OE2	8:D:187:ARG:HG3	2.20	0.41
19:O:99:LYS:HA	19:O:99:LYS:HD3	1.87	0.41
21:Q:33:ILE:N	21:Q:61:ALA:O	2.34	0.41
31:sN1:385:A:H3'	31:sN1:386:U:H6	1.86	0.41
31:sN1:395:G:H2'	31:sN1:396:C:C6	2.56	0.41
31:sN1:711:G:H1'	31:sN1:774:A:C8	2.56	0.41
31:sN1:745:U:H2'	31:sN1:746:A:C8	2.56	0.41
31:sN1:748:U:H2'	31:sN1:749:G:O4'	2.21	0.41
31:sN1:821:U:H2'	31:sN1:822:A:H8	1.85	0.41
31:sN1:1073:C:H2'	31:sN1:1074:G:C8	2.56	0.41
31:sN1:1123:U:O2'	31:sN1:1124:G:H8	2.04	0.41
31:sN1:1157:G:N2	31:sN1:1158:C:H1'	2.36	0.41
31:sN1:1163:G:O2'	31:sN1:1167:A:N6	2.41	0.41
31:sN1:1269:U:H2'	31:sN1:1270:G:H8	1.84	0.41
31:sN1:1407:A:H2'	31:sN1:1408:C:H6	1.84	0.41
32:b:113:ILE:HD11	32:b:154:LYS:HA	2.03	0.41
32:b:117:LYS:O	32:b:121:THR:HG23	2.21	0.41
34:d:41:GLN:HG3	34:d:42:HIS:CD2	2.56	0.41
34:d:88:THR:HA	34:d:91:ASN:HD21	1.86	0.41
5:AN1:74:U:C2	5:AN1:75:G:C8	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1876:U:H2'	5:AN1:1877:C:H6	1.85	0.41
10:F:175:PHE:HB3	10:F:177:PHE:HD1	1.85	0.41
13:I:119:ILE:HD12	13:I:119:ILE:HA	1.93	0.41
25:U:84:HIS:CD2	25:U:87:LYS:H	2.39	0.41
31:sN1:905:A:H2'	31:sN1:906:A:C8	2.56	0.41
5:AN1:698:G:O2'	5:AN1:1630:A:N3	2.52	0.40
5:AN1:944:A:H2'	5:AN1:945:C:C6	2.56	0.40
5:AN1:1029:A:H2'	5:AN1:1030:U:C6	2.56	0.40
5:AN1:1296:A:H2	5:AN1:1624:A:C2	2.40	0.40
5:AN1:1424:G:H2'	5:AN1:1425:G:H8	1.85	0.40
5:AN1:1549:U:H2'	5:AN1:1550:G:O4'	2.20	0.40
5:AN1:2224:G:H2'	5:AN1:2225:U:C6	2.56	0.40
15:K:25:ILE:HG12	21:Q:82:HIS:CE1	2.56	0.40
31:sN1:58:U:H2'	31:sN1:59:G:H8	1.86	0.40
31:sN1:157:A:H2'	31:sN1:158:A:C8	2.56	0.40
31:sN1:394:U:H2'	31:sN1:395:G:H8	1.85	0.40
31:sN1:503:G:H2'	31:sN1:504:C:C6	2.56	0.40
31:sN1:553:C:H2'	31:sN1:554:G:C8	2.56	0.40
34:d:172:TRP:CD2	34:d:188:PRO:HB3	2.56	0.40
5:AN1:493:G:N2	22:R:57:ASN:HD21	2.19	0.40
5:AN1:727:G:O2'	5:AN1:761:G:H4'	2.22	0.40
8:D:26:THR:OG1	8:D:194:GLY:O	2.39	0.40
13:I:2:LYS:HE2	13:I:2:LYS:HB3	1.79	0.40
15:K:131:LYS:HG3	15:K:132:GLY:H	1.86	0.40
31:sN1:657:G:H1	31:sN1:743:A:N6	2.14	0.40
31:sN1:1003:C:H2'	31:sN1:1004:U:H6	1.86	0.40
31:sN1:1038:G:H2'	31:sN1:1039:A:C8	2.56	0.40
31:sN1:1178:G:H1'	31:sN1:1179:G:C4	2.57	0.40
32:b:133:LYS:HD2	32:b:134:ARG:HG3	2.02	0.40
32:b:212:VAL:HA	32:b:215:TYR:HD1	1.85	0.40
33:c:10:ILE:HG23	33:c:11:ARG:HG3	2.03	0.40
34:d:170:PRO:HB3	34:d:172:TRP:CH2	2.56	0.40
43:m:31:LYS:HB3	43:m:31:LYS:HE2	1.88	0.40
5:AN1:181:C:H2'	5:AN1:182:A:C8	2.57	0.40
5:AN1:182:A:H2'	5:AN1:183:A:C8	2.57	0.40
5:AN1:1198:U:OP2	5:AN1:1199:A:O2'	2.34	0.40
5:AN1:1381:A:H2'	5:AN1:1382:U:H6	1.86	0.40
12:H:50:ARG:HH12	12:H:54:LEU:HD22	1.86	0.40
17:M:72:ASN:HB3	17:M:75:THR:HB	2.03	0.40
31:sN1:185:C:H4'	31:sN1:186:G:O5'	2.20	0.40
31:sN1:1002:A:H3'	31:sN1:1003:C:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:sN1:1130:A:H2'	31:sN1:1131:U:C6	2.57	0.40
32:b:168:VAL:HG13	32:b:169:ASP:OD1	2.20	0.40
36:f:36:ILE:HB	36:f:65:GLU:HB2	2.03	0.40
36:f:42:TRP:HZ2	48:r:24:LYS:HD2	1.86	0.40
2:1:3:ARG:HD3	2:1:3:ARG:HA	1.90	0.40
5:AN1:1623:C:H2'	5:AN1:1624:A:O4'	2.21	0.40
5:AN1:2096:G:N2	5:AN1:2185:U:O2	2.32	0.40
5:AN1:2742:U:H5"	11:G:138:LYS:HD2	2.04	0.40
5:AN1:2791:C:H2'	5:AN1:2792:U:C6	2.56	0.40
9:E:82:LYS:HE2	9:E:82:LYS:HB3	1.85	0.40
11:G:157:TYR:O	11:G:171:ARG:NH1	2.50	0.40
31:sN1:914:G:H2'	31:sN1:915:A:C8	2.57	0.40
34:d:158:LYS:O	34:d:161:ILE:HG22	2.21	0.40
5:AN1:812:C:H2'	5:AN1:813:C:H6	1.86	0.40
5:AN1:976:A:H2'	5:AN1:979:C:N4	2.35	0.40
5:AN1:1436:A:H2'	5:AN1:1437:U:C6	2.57	0.40
6:B:62:U:H2'	6:B:63:U:C5	2.57	0.40
10:F:65:PRO:HA	10:F:89:VAL:HG22	2.02	0.40
30:Z:38:ARG:HB3	30:Z:41:HIS:HB2	2.02	0.40
31:sN1:21:A:H2'	31:sN1:22:U:H6	1.86	0.40
31:sN1:201:A:H2'	31:sN1:202:U:C6	2.56	0.40
31:sN1:833:G:H1	31:sN1:847:U:H3	1.70	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	49/51 (96%)	47 (96%)	2 (4%)	0	100 100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
3	2	61/64 (95%)	58 (95%)	1 (2%)	2 (3%)	3 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	C	268/274 (98%)	260 (97%)	8 (3%)	0	100	100
8	D	209/212 (99%)	203 (97%)	6 (3%)	0	100	100
9	E	184/200 (92%)	184 (100%)	0	0	100	100
10	F	173/178 (97%)	151 (87%)	21 (12%)	1 (1%)	21	50
11	G	172/177 (97%)	166 (96%)	6 (4%)	0	100	100
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
15	K	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
16	L	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
17	M	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	111 (96%)	4 (4%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
22	R	107/109 (98%)	107 (100%)	0	0	100	100
23	S	88/106 (83%)	85 (97%)	3 (3%)	0	100	100
24	T	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
26	V	78/85 (92%)	78 (100%)	0	0	100	100
27	W	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
28	X	60/65 (92%)	58 (97%)	2 (3%)	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	211 (95%)	12 (5%)	0	100	100
33	c	213/250 (85%)	204 (96%)	9 (4%)	0	100	100
34	d	205/208 (99%)	204 (100%)	1 (0%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	92/127 (72%)	88 (96%)	4 (4%)	0	100	100
37	g	139/156 (89%)	137 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
40	j	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
41	k	115/128 (90%)	109 (95%)	6 (5%)	0	100	100
42	l	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	81/101 (80%)	80 (99%)	1 (1%)	0	100	100
47	q	78/85 (92%)	77 (99%)	1 (1%)	0	100	100
48	r	51/75 (68%)	51 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	83/88 (94%)	83 (100%)	0	0	100	100
51	u	19/71 (27%)	16 (84%)	3 (16%)	0	100	100
All	All	5361/5872 (91%)	5203 (97%)	155 (3%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	PRO

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	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	51 (98%)	1 (2%)	50	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	216/220 (98%)	216 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	144/155 (93%)	144 (100%)	0	100	100
10	F	145/147 (99%)	145 (100%)	0	100	100
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	108/108 (100%)	108 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	99/102 (97%)	99 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	54/56 (96%)	54 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	184 (100%)	1 (0%)	81	93
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	86/111 (78%)	86 (100%)	0	100	100
37	g	116/128 (91%)	116 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	99 (100%)	0	100	100
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	72/76 (95%)	72 (100%)	0	100	100
48	r	47/66 (71%)	47 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	18/62 (29%)	18 (100%)	0	100	100
All	All	4436/4756 (93%)	4434 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
32	b	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	16	HIS
3	2	19	ASN
3	2	50	HIS
7	C	25	HIS
7	C	48	HIS
7	C	58	HIS
7	C	60	GLN
7	C	90	HIS
7	C	117	GLN
7	C	153	GLN
7	C	230	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	C	243	GLN
7	C	250	GLN
8	D	50	GLN
9	E	61	GLN
9	E	96	ASN
9	E	114	GLN
10	F	17	GLN
10	F	95	GLN
11	G	19	GLN
11	G	20	ASN
11	G	106	ASN
12	H	43	ASN
13	I	13	HIS
13	I	40	HIS
13	I	77	HIS
13	I	95	HIS
13	I	135	GLN
14	J	59	ASN
15	K	18	HIS
15	K	40	GLN
15	K	107	GLN
15	K	125	GLN
16	L	22	HIS
17	M	5	ASN
19	O	13	ASN
19	O	78	GLN
20	P	11	HIS
20	P	44	GLN
21	Q	48	GLN
21	Q	82	HIS
21	Q	87	GLN
22	R	37	ASN
22	R	57	ASN
22	R	60	HIS
22	R	62	ASN
22	R	102	HIS
24	T	72	ASN
25	U	16	GLN
25	U	75	ASN
25	U	84	HIS
27	W	6	GLN
27	W	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	X	21	GLN
28	X	61	GLN
30	Z	6	ASN
30	Z	41	HIS
32	b	60	ASN
32	b	80	ASN
32	b	85	GLN
32	b	105	ASN
33	c	3	GLN
33	c	6	HIS
33	c	19	ASN
33	c	176	HIS
34	d	102	ASN
34	d	118	GLN
34	d	138	GLN
34	d	154	GLN
35	e	121	ASN
35	e	131	ASN
36	f	11	HIS
36	f	35	GLN
36	f	55	HIS
36	f	94	HIS
37	g	32	GLN
38	h	86	GLN
39	i	30	ASN
39	i	73	GLN
39	i	79	HIS
39	i	98	GLN
40	j	15	HIS
40	j	56	HIS
41	k	49	GLN
41	k	117	HIS
43	m	105	ASN
45	o	37	ASN
45	o	42	HIS
45	o	48	HIS
46	p	44	ASN
47	q	32	HIS
48	r	36	ASN
49	s	52	HIS
50	t	6	GLN
50	t	13	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	t	75	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	sN1	1527/1544 (98%)	211 (13%)	0
5	AN1	2891/2918 (99%)	495 (17%)	10 (0%)
6	B	114/115 (99%)	18 (15%)	1 (0%)
All	All	4532/4577 (99%)	724 (15%)	11 (0%)

All (724) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	10	U
5	AN1	41	U
5	AN1	50	G
5	AN1	53	G
5	AN1	58	G
5	AN1	59	A
5	AN1	67	G
5	AN1	68	A
5	AN1	69	U
5	AN1	78	A
5	AN1	81	A
5	AN1	82	G
5	AN1	86	C
5	AN1	98	A
5	AN1	101	U
5	AN1	102	A
5	AN1	106	U
5	AN1	107	U
5	AN1	108	U
5	AN1	125	A
5	AN1	127	U
5	AN1	146	U
5	AN1	147	A
5	AN1	169	U
5	AN1	170	A
5	AN1	172	A
5	AN1	188	A
5	AN1	203	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	206	A
5	AN1	223	A
5	AN1	229	A
5	AN1	232	C
5	AN1	235	U
5	AN1	236	U
5	AN1	255	G
5	AN1	257	G
5	AN1	259	G
5	AN1	262	A
5	AN1	271	C
5	AN1	272	A
5	AN1	273	G
5	AN1	279	U
5	AN1	280	A
5	AN1	283	U
5	AN1	284	U
5	AN1	285	A
5	AN1	291	G
5	AN1	293	U
5	AN1	303	C
5	AN1	313	A
5	AN1	331	G
5	AN1	332	A
5	AN1	336	U
5	AN1	345	C
5	AN1	351	G
5	AN1	356	A
5	AN1	357	C
5	AN1	359	U
5	AN1	366	G
5	AN1	368	C
5	AN1	369	G
5	AN1	371	G
5	AN1	385	G
5	AN1	386	U
5	AN1	395	G
5	AN1	403	A
5	AN1	410	G
5	AN1	423	G
5	AN1	434	C
5	AN1	455	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	479	A
5	AN1	480	G
5	AN1	504	A
5	AN1	508	C
5	AN1	509	C
5	AN1	526	C
5	AN1	529	G
5	AN1	530	C
5	AN1	531	A
5	AN1	543	U
5	AN1	544	U
5	AN1	545	C
5	AN1	547	U
5	AN1	554	A
5	AN1	561	A
5	AN1	564	U
5	AN1	571	U
5	AN1	573	A
5	AN1	601	A
5	AN1	612	A
5	AN1	625	A
5	AN1	635	A
5	AN1	637	U
5	AN1	643	U
5	AN1	644	A
5	AN1	651	U
5	AN1	652	U
5	AN1	656	U
5	AN1	657	G
5	AN1	666	A
5	AN1	667	G
5	AN1	668	A
5	AN1	684	U
5	AN1	692	U
5	AN1	693	G
5	AN1	711	G
5	AN1	712	U
5	AN1	713	A
5	AN1	714	A
5	AN1	719	A
5	AN1	724	G
5	AN1	727	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	728	A
5	AN1	745	U
5	AN1	762	A
5	AN1	763	C
5	AN1	773	G
5	AN1	774	G
5	AN1	780	A
5	AN1	782	G
5	AN1	783	G
5	AN1	787	A
5	AN1	803	G
5	AN1	810	C
5	AN1	817	A
5	AN1	825	U
5	AN1	828	G
5	AN1	843	G
5	AN1	855	G
5	AN1	857	G
5	AN1	880	G
5	AN1	883	C
5	AN1	884	A
5	AN1	888	C
5	AN1	889	G
5	AN1	890	A
5	AN1	894	A
5	AN1	895	C
5	AN1	899	A
5	AN1	903	A
5	AN1	904	U
5	AN1	908	A
5	AN1	926	G
5	AN1	929	C
5	AN1	930	U
5	AN1	938	A
5	AN1	942	A
5	AN1	943	G
5	AN1	955	U
5	AN1	958	C
5	AN1	971	G
5	AN1	977	A
5	AN1	980	A
5	AN1	993	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	1006	A
5	AN1	1009	U
5	AN1	1010	C
5	AN1	1023	G
5	AN1	1028	G
5	AN1	1032	U
5	AN1	1036	A
5	AN1	1037	A
5	AN1	1039	G
5	AN1	1040	C
5	AN1	1041	A
5	AN1	1042	U
5	AN1	1043	A
5	AN1	1044	G
5	AN1	1054	A
5	AN1	1057	U
5	AN1	1058	U
5	AN1	1059	G
5	AN1	1061	C
5	AN1	1063	U
5	AN1	1067	A
5	AN1	1070	A
5	AN1	1076	C
5	AN1	1078	U
5	AN1	1081	A
5	AN1	1082	A
5	AN1	1085	A
5	AN1	1086	A
5	AN1	1091	U
5	AN1	1101	C
5	AN1	1108	A
5	AN1	1109	G
5	AN1	1110	U
5	AN1	1121	G
5	AN1	1129	U
5	AN1	1130	A
5	AN1	1131	A
5	AN1	1132	C
5	AN1	1140	A
5	AN1	1148	U
5	AN1	1149	G
5	AN1	1167	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	1170	U
5	AN1	1171	U
5	AN1	1172	U
5	AN1	1173	G
5	AN1	1179	G
5	AN1	1200	A
5	AN1	1201	G
5	AN1	1231	G
5	AN1	1242	A
5	AN1	1245	G
5	AN1	1248	A
5	AN1	1251	G
5	AN1	1267	A
5	AN1	1270	A
5	AN1	1296	A
5	AN1	1316	A
5	AN1	1324	U
5	AN1	1336	G
5	AN1	1340	C
5	AN1	1360	A
5	AN1	1363	G
5	AN1	1373	A
5	AN1	1374	U
5	AN1	1378	A
5	AN1	1390	A
5	AN1	1407	U
5	AN1	1408	A
5	AN1	1411	G
5	AN1	1414	A
5	AN1	1415	U
5	AN1	1423	C
5	AN1	1428	A
5	AN1	1432	C
5	AN1	1447	G
5	AN1	1448	U
5	AN1	1453	U
5	AN1	1455	U
5	AN1	1456	C
5	AN1	1469	U
5	AN1	1470	G
5	AN1	1473	G
5	AN1	1477	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	1485	A
5	AN1	1501	C
5	AN1	1502	U
5	AN1	1504	U
5	AN1	1505	A
5	AN1	1510	G
5	AN1	1520	A
5	AN1	1530	A
5	AN1	1531	C
5	AN1	1533	U
5	AN1	1534	G
5	AN1	1539	G
5	AN1	1540	C
5	AN1	1541	G
5	AN1	1542	A
5	AN1	1544	G
5	AN1	1545	U
5	AN1	1564	A
5	AN1	1567	A
5	AN1	1574	U
5	AN1	1582	U
5	AN1	1583	C
5	AN1	1605	G
5	AN1	1606	A
5	AN1	1616	A
5	AN1	1642	C
5	AN1	1645	U
5	AN1	1646	U
5	AN1	1672	G
5	AN1	1691	U
5	AN1	1712	U
5	AN1	1713	U
5	AN1	1714	G
5	AN1	1717	G
5	AN1	1725	U
5	AN1	1726	C
5	AN1	1731	C
5	AN1	1742	G
5	AN1	1746	G
5	AN1	1760	G
5	AN1	1769	A
5	AN1	1776	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	1780	A
5	AN1	1796	C
5	AN1	1797	A
5	AN1	1798	A
5	AN1	1805	A
5	AN1	1807	G
5	AN1	1812	C
5	AN1	1825	A
5	AN1	1829	C
5	AN1	1830	U
5	AN1	1831	G
5	AN1	1844	A
5	AN1	1845	G
5	AN1	1855	U
5	AN1	1861	U
5	AN1	1864	C
5	AN1	1866	U
5	AN1	1867	A
5	AN1	1871	G
5	AN1	1872	A
5	AN1	1875	C
5	AN1	1885	A
5	AN1	1895	A
5	AN1	1899	G
5	AN1	1902	G
5	AN1	1904	C
5	AN1	1905	C
5	AN1	1907	PSU
5	AN1	1909	A
5	AN1	1910	C
5	AN1	1911	3TD
5	AN1	1915	A
5	AN1	1917	G
5	AN1	1918	G
5	AN1	1921	C
5	AN1	1923	A
5	AN1	1925	G
5	AN1	1926	G
5	AN1	1932	A
5	AN1	1933	A
5	AN1	1934	A
5	AN1	1936	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	1950	G
5	AN1	1951	U
5	AN1	1959	U
5	AN1	1960	G
5	AN1	1963	C
5	AN1	1966	A
5	AN1	1967	U
5	AN1	1968	G
5	AN1	1978	U
5	AN1	1987	U
5	AN1	1989	U
5	AN1	1993	C
5	AN1	2018	U
5	AN1	2019	C
5	AN1	2025	G
5	AN1	2026	6MZ
5	AN1	2027	A
5	AN1	2029	A
5	AN1	2030	U
5	AN1	2039	C
5	AN1	2051	C
5	AN1	2052	G
5	AN1	2056	A
5	AN1	2057	G
5	AN1	2058	A
5	AN1	2065	7MG
5	AN1	2089	G
5	AN1	2092	C
5	AN1	2104	U
5	AN1	2106	G
5	AN1	2107	U
5	AN1	2108	G
5	AN1	2111	G
5	AN1	2112	G
5	AN1	2113	A
5	AN1	2114	U
5	AN1	2115	A
5	AN1	2116	G
5	AN1	2120	G
5	AN1	2121	G
5	AN1	2122	A
5	AN1	2123	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	2127	U
5	AN1	2128	U
5	AN1	2129	G
5	AN1	2131	A
5	AN1	2133	C
5	AN1	2142	U
5	AN1	2143	A
5	AN1	2145	U
5	AN1	2146	U
5	AN1	2148	C
5	AN1	2149	A
5	AN1	2152	G
5	AN1	2153	G
5	AN1	2154	A
5	AN1	2157	C
5	AN1	2158	G
5	AN1	2162	U
5	AN1	2166	A
5	AN1	2167	A
5	AN1	2168	U
5	AN1	2169	A
5	AN1	2171	C
5	AN1	2172	A
5	AN1	2174	C
5	AN1	2178	G
5	AN1	2184	U
5	AN1	2185	U
5	AN1	2188	G
5	AN1	2194	A
5	AN1	2200	G
5	AN1	2221	A
5	AN1	2234	G
5	AN1	2235	G
5	AN1	2261	U
5	AN1	2275	G
5	AN1	2279	U
5	AN1	2283	A
5	AN1	2301	U
5	AN1	2304	G
5	AN1	2305	A
5	AN1	2308	U
5	AN1	2312	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	2314	G
5	AN1	2316	A
5	AN1	2321	A
5	AN1	2323	A
5	AN1	2341	A
5	AN1	2346	C
5	AN1	2355	C
5	AN1	2357	A
5	AN1	2378	G
5	AN1	2379	G
5	AN1	2380	U
5	AN1	2381	C
5	AN1	2399	C
5	AN1	2408	A
5	AN1	2425	G
5	AN1	2426	A
5	AN1	2429	A
5	AN1	2430	A
5	AN1	2431	A
5	AN1	2437	U
5	AN1	2443	G
5	AN1	2444	A
5	AN1	2446	A
5	AN1	2455	A
5	AN1	2468	G
5	AN1	2469	U
5	AN1	2470	U
5	AN1	2472	A
5	AN1	2473	U
5	AN1	2487	U
5	AN1	2494	C
5	AN1	2498	G
5	AN1	2499	2MA
5	AN1	2501	G
5	AN1	2503	C
5	AN1	2514	A
5	AN1	2516	C
5	AN1	2525	G
5	AN1	2530	A
5	AN1	2543	A
5	AN1	2548	OMU
5	AN1	2550	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	2562	A
5	AN1	2563	G
5	AN1	2568	A
5	AN1	2598	A
5	AN1	2599	G
5	AN1	2605	U
5	AN1	2606	C
5	AN1	2607	C
5	AN1	2609	U
5	AN1	2611	U
5	AN1	2625	U
5	AN1	2635	A
5	AN1	2642	C
5	AN1	2657	G
5	AN1	2661	A
5	AN1	2685	U
5	AN1	2686	A
5	AN1	2710	G
5	AN1	2722	U
5	AN1	2730	A
5	AN1	2740	G
5	AN1	2744	A
5	AN1	2753	A
5	AN1	2754	A
5	AN1	2761	A
5	AN1	2762	G
5	AN1	2774	A
5	AN1	2776	A
5	AN1	2787	A
5	AN1	2788	G
5	AN1	2793	U
5	AN1	2794	U
5	AN1	2796	U
5	AN1	2800	C
5	AN1	2804	A
5	AN1	2816	G
5	AN1	2817	A
5	AN1	2831	A
5	AN1	2845	G
5	AN1	2851	U
5	AN1	2853	G
5	AN1	2857	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AN1	2863	A
5	AN1	2868	G
5	AN1	2875	A
5	AN1	2897	C
5	AN1	2898	U
6	B	2	C
6	B	10	C
6	B	11	A
6	B	14	G
6	B	23	A
6	B	31	G
6	B	32	A
6	B	39	C
6	B	40	C
6	B	42	G
6	B	44	A
6	B	50	A
6	B	65	G
6	B	86	U
6	B	87	A
6	B	105	C
6	B	106	A
6	B	109	G
31	sN1	6	C
31	sN1	11	G
31	sN1	33	G
31	sN1	41	G
31	sN1	49	C
31	sN1	50	U
31	sN1	53	A
31	sN1	56	C
31	sN1	57	A
31	sN1	64	U
31	sN1	80	A
31	sN1	86	C
31	sN1	87	U
31	sN1	90	C
31	sN1	91	G
31	sN1	94	C
31	sN1	97	A
31	sN1	105	A
31	sN1	107	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	sN1	126	A
31	sN1	127	U
31	sN1	140	G
31	sN1	157	A
31	sN1	170	A
31	sN1	184	A
31	sN1	186	G
31	sN1	193	A
31	sN1	204	U
31	sN1	205	U
31	sN1	206	C
31	sN1	212	U
31	sN1	216	G
31	sN1	236	C
31	sN1	241	U
31	sN1	243	G
31	sN1	247	G
31	sN1	262	G
31	sN1	263	C
31	sN1	285	G
31	sN1	289	G
31	sN1	302	A
31	sN1	324	C
31	sN1	326	C
31	sN1	340	A
31	sN1	341	C
31	sN1	348	C
31	sN1	359	A
31	sN1	363	U
31	sN1	368	C
31	sN1	388	C
31	sN1	393	A
31	sN1	402	G
31	sN1	407	A
31	sN1	408	A
31	sN1	409	G
31	sN1	425	U
31	sN1	463	U
31	sN1	474	A
31	sN1	475	G
31	sN1	476	U
31	sN1	478	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	sN1	479	A
31	sN1	481	G
31	sN1	482	U
31	sN1	493	A
31	sN1	494	U
31	sN1	505	U
31	sN1	506	A
31	sN1	507	A
31	sN1	508	C
31	sN1	515	C
31	sN1	521	G
31	sN1	522	C
31	sN1	524	7MG
31	sN1	527	G
31	sN1	544	A
31	sN1	556	A
31	sN1	561	C
31	sN1	567	G
31	sN1	569	A
31	sN1	570	A
31	sN1	572	G
31	sN1	573	C
31	sN1	574	G
31	sN1	593	A
31	sN1	615	C
31	sN1	630	G
31	sN1	639	A
31	sN1	650	A
31	sN1	662	A
31	sN1	684	A
31	sN1	685	G
31	sN1	692	A
31	sN1	699	A
31	sN1	700	G
31	sN1	714	U
31	sN1	720	U
31	sN1	721	G
31	sN1	728	G
31	sN1	745	U
31	sN1	752	G
31	sN1	774	A
31	sN1	790	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	sN1	791	A
31	sN1	812	A
31	sN1	814	C
31	sN1	839	U
31	sN1	840	U
31	sN1	841	G
31	sN1	842	A
31	sN1	843	G
31	sN1	899	G
31	sN1	923	G
31	sN1	931	C
31	sN1	932	A
31	sN1	957	U
31	sN1	958	U
31	sN1	966	A
31	sN1	968	G
31	sN1	972	A
31	sN1	973	G
31	sN1	974	A
31	sN1	989	U
31	sN1	990	G
31	sN1	991	A
31	sN1	992	C
31	sN1	993	A
31	sN1	998	A
31	sN1	1001	A
31	sN1	1003	C
31	sN1	1007	C
31	sN1	1008	C
31	sN1	1010	G
31	sN1	1016	G
31	sN1	1023	G
31	sN1	1025	C
31	sN1	1026	U
31	sN1	1028	C
31	sN1	1029	G
31	sN1	1030	G
31	sN1	1041	A
31	sN1	1042	C
31	sN1	1050	G
31	sN1	1051	C
31	sN1	1061	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	sN1	1062	U
31	sN1	1069	G
31	sN1	1083	U
31	sN1	1084	G
31	sN1	1086	G
31	sN1	1091	G
31	sN1	1092	U
31	sN1	1095	C
31	sN1	1098	A
31	sN1	1123	U
31	sN1	1124	G
31	sN1	1131	U
31	sN1	1134	C
31	sN1	1136	G
31	sN1	1156	U
31	sN1	1157	G
31	sN1	1161	G
31	sN1	1164	A
31	sN1	1165	C
31	sN1	1169	C
31	sN1	1180	C
31	sN1	1181	G
31	sN1	1182	G
31	sN1	1188	A
31	sN1	1193	A
31	sN1	1194	A
31	sN1	1209	U
31	sN1	1210	A
31	sN1	1217	G
31	sN1	1224	A
31	sN1	1235	A
31	sN1	1247	A
31	sN1	1255	G
31	sN1	1257	U
31	sN1	1259	C
31	sN1	1277	A
31	sN1	1284	A
31	sN1	1295	U
31	sN1	1297	G
31	sN1	1299	C
31	sN1	1302	G
31	sN1	1317	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	sN1	1360	A
31	sN1	1378	U
31	sN1	1380	C
31	sN1	1385	C
31	sN1	1394	C
31	sN1	1395	A
31	sN1	1398	G
31	sN1	1402	G
31	sN1	1404	C
31	sN1	1425	A
31	sN1	1427	C
31	sN1	1444	A
31	sN1	1448	C
31	sN1	1449	A
31	sN1	1450	A
31	sN1	1488	G
31	sN1	1490	A
31	sN1	1491	G
31	sN1	1496	A
31	sN1	1499	A
31	sN1	1503	U
31	sN1	1517	C
31	sN1	1526	G
31	sN1	1527	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AN1	355	C
5	AN1	356	A
5	AN1	368	C
5	AN1	478	A
5	AN1	782	G
5	AN1	893	U
5	AN1	1171	U
5	AN1	1538	A
5	AN1	2170	C
5	AN1	2379	G
6	B	108	C

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

24 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	$\#\|Z\| > 2$
5	2MG	AN1	2441	5	23,26,27	2.89	8 (34%)	33,38,41	2.22	11 (33%)
5	6MZ	AN1	2026	5	22,25,26	2.47	4 (18%)	29,36,39	3.40	10 (34%)
5	PSU	AN1	2601	5	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
5	OMU	AN1	2548	5	19,22,23	3.12	8 (42%)	25,31,34	1.80	5 (20%)
31	MA6	sN1	1515	31	23,26,27	1.37	4 (17%)	33,38,41	3.26	12 (36%)
5	PSU	AN1	2500	5	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
31	2MG	sN1	1204	31	23,26,27	2.91	8 (34%)	33,38,41	2.21	12 (36%)
31	MA6	sN1	1516	31	23,26,27	1.37	4 (17%)	33,38,41	3.32	12 (36%)
5	PSU	AN1	1907	5	18,21,22	1.15	1 (5%)	21,30,33	1.90	4 (19%)
5	7MG	AN1	2065	5	23,26,27	3.53	10 (43%)	27,39,42	2.17	9 (33%)
31	7MG	sN1	524	31	23,26,27	3.63	11 (47%)	27,39,42	2.16	9 (33%)
5	PSU	AN1	1913	5	18,21,22	1.13	1 (5%)	21,30,33	1.81	5 (23%)
31	PSU	sN1	513	31	18,21,22	1.20	1 (5%)	21,30,33	1.62	4 (19%)
5	PSU	AN1	952	5	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
31	4OC	sN1	1399	31	20,23,24	3.23	8 (40%)	25,32,35	0.92	1 (4%)
31	UR3	sN1	1495	31	19,22,23	2.96	6 (31%)	26,32,35	1.59	3 (11%)
31	2MG	sN1	963	31	23,26,27	2.93	8 (34%)	33,38,41	2.21	12 (36%)
5	PSU	AN1	2576	5	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
31	5MC	sN1	964	31	19,22,23	3.94	8 (42%)	26,32,35	0.99	2 (7%)
5	3TD	AN1	1911	5	19,22,23	4.30	7 (36%)	23,32,35	1.82	3 (13%)
5	PSU	AN1	2453	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	6 (28%)
5	2MA	AN1	2499	53,5	22,25,26	3.99	9 (40%)	32,37,40	2.78	11 (34%)
5	5MU	AN1	1935	5	19,22,23	4.98	7 (36%)	27,32,35	3.62	9 (33%)
5	OMG	AN1	2247	5	23,26,27	2.38	8 (34%)	32,38,41	1.90	8 (25%)

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
5	2MG	AN1	2441	5	-	1/9/27/28	0/3/3/3
5	6MZ	AN1	2026	5	-	2/9/27/28	0/3/3/3
5	PSU	AN1	2601	5	-	0/7/25/26	0/2/2/2
5	OMU	AN1	2548	5	-	2/9/27/28	0/2/2/2
31	MA6	sN1	1515	31	-	0/11/29/30	0/3/3/3
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2
31	2MG	sN1	1204	31	-	0/9/27/28	0/3/3/3
31	MA6	sN1	1516	31	-	4/11/29/30	0/3/3/3
5	PSU	AN1	1907	5	-	1/7/25/26	0/2/2/2
5	7MG	AN1	2065	5	-	2/7/37/38	0/3/3/3
31	7MG	sN1	524	31	-	3/7/37/38	0/3/3/3
5	PSU	AN1	1913	5	-	3/7/25/26	0/2/2/2
31	PSU	sN1	513	31	-	0/7/25/26	0/2/2/2
5	PSU	AN1	952	5	-	0/7/25/26	0/2/2/2
31	4OC	sN1	1399	31	-	2/9/29/30	0/2/2/2
31	UR3	sN1	1495	31	-	2/7/25/26	0/2/2/2
31	2MG	sN1	963	31	-	0/9/27/28	0/3/3/3
5	PSU	AN1	2576	5	-	0/7/25/26	0/2/2/2
31	5MC	sN1	964	31	-	0/7/25/26	0/2/2/2
5	3TD	AN1	1911	5	-	4/7/25/26	0/2/2/2
5	PSU	AN1	2453	5	-	0/7/25/26	0/2/2/2
5	2MA	AN1	2499	53,5	-	3/7/25/26	0/3/3/3
5	5MU	AN1	1935	5	-	0/7/25/26	0/2/2/2
5	OMG	AN1	2247	5	-	0/9/27/28	0/3/3/3

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	1911	3TD	C6-C5	12.81	1.49	1.35
5	AN1	2499	2MA	C4-N3	12.26	1.50	1.34
5	AN1	1935	5MU	C2-N1	11.53	1.56	1.38
5	AN1	1935	5MU	C6-N1	10.89	1.56	1.38
5	AN1	1935	5MU	C4-C5	10.19	1.61	1.44
5	AN1	2026	6MZ	C6-N6	10.06	1.45	1.34
5	AN1	1911	3TD	C2-N1	10.04	1.49	1.37
31	sN1	964	5MC	C6-C5	9.27	1.49	1.34
31	sN1	524	7MG	C8-N9	8.56	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2065	7MG	C8-N9	8.22	1.51	1.45
31	sN1	963	2MG	C2-N3	7.73	1.46	1.32
31	sN1	1204	2MG	C2-N3	7.68	1.46	1.32
5	AN1	2441	2MG	C2-N3	7.60	1.46	1.32
5	AN1	2499	2MA	C2-N3	7.52	1.46	1.34
5	AN1	2548	OMU	C2-N1	7.42	1.50	1.38
31	sN1	1495	UR3	C2-N1	7.34	1.48	1.38
31	sN1	524	7MG	C5-N7	7.28	1.44	1.35
5	AN1	1935	5MU	C4-N3	-7.25	1.25	1.38
31	sN1	1399	4OC	C4-N3	7.19	1.44	1.32
31	sN1	964	5MC	C5-C4	7.07	1.49	1.44
5	AN1	2065	7MG	C5-N7	6.99	1.44	1.35
5	AN1	2499	2MA	C6-N1	6.97	1.44	1.35
31	sN1	964	5MC	C4-N3	6.95	1.45	1.34
5	AN1	2548	OMU	C2-N3	6.88	1.49	1.38
31	sN1	1495	UR3	C6-C5	6.85	1.50	1.35
5	AN1	1935	5MU	C6-C5	6.74	1.45	1.34
31	sN1	963	2MG	C4-N3	6.71	1.49	1.34
5	AN1	2441	2MG	C4-N3	6.65	1.49	1.34
31	sN1	1204	2MG	C4-N3	6.65	1.49	1.34
5	AN1	2247	OMG	C4-N3	6.48	1.49	1.34
31	sN1	1399	4OC	C2-N3	6.34	1.48	1.36
31	sN1	1399	4OC	C6-C5	6.33	1.49	1.35
31	sN1	964	5MC	C2-N3	6.32	1.48	1.36
5	AN1	2499	2MA	C2-N1	6.10	1.44	1.34
5	AN1	1911	3TD	C6-N1	6.01	1.46	1.36
31	sN1	524	7MG	C2-N3	5.90	1.47	1.33
31	sN1	963	2MG	C2-N2	5.89	1.45	1.33
5	AN1	2065	7MG	C2-N3	5.87	1.47	1.33
31	sN1	524	7MG	C4-N3	5.85	1.47	1.34
31	sN1	1204	2MG	C2-N2	5.78	1.45	1.33
31	sN1	1495	UR3	C2-N3	5.78	1.50	1.39
5	AN1	2065	7MG	C4-N3	5.76	1.47	1.34
5	AN1	2441	2MG	C2-N2	5.75	1.45	1.33
5	AN1	2548	OMU	C6-C5	5.74	1.48	1.35
5	AN1	2247	OMG	C2-N3	5.60	1.46	1.33
31	sN1	524	7MG	C4-N9	5.33	1.44	1.37
5	AN1	1911	3TD	C2-N3	5.17	1.49	1.38
31	sN1	524	7MG	C2-N2	5.04	1.46	1.34
5	AN1	2065	7MG	C4-N9	5.02	1.44	1.37
5	AN1	2065	7MG	C2-N2	4.97	1.45	1.34
31	sN1	1204	2MG	C2-N1	4.94	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	sN1	963	2MG	C2-N1	4.93	1.44	1.36
31	sN1	1399	4OC	C4-N4	4.86	1.46	1.36
5	AN1	2441	2MG	C2-N1	4.86	1.44	1.36
5	AN1	2499	2MA	C5-C6	4.71	1.54	1.41
31	sN1	964	5MC	C6-N1	4.64	1.45	1.38
31	sN1	964	5MC	C4-N4	4.47	1.45	1.34
31	sN1	1399	4OC	C2-N1	4.46	1.49	1.40
31	sN1	964	5MC	C2-N1	4.43	1.49	1.40
5	AN1	2548	OMU	C4-N3	4.37	1.46	1.38
5	AN1	2247	OMG	C2-N2	4.08	1.43	1.34
31	sN1	513	PSU	C6-C5	4.04	1.39	1.35
31	sN1	1515	MA6	C6-N6	4.00	1.47	1.36
31	sN1	1516	MA6	C6-N6	3.93	1.47	1.36
5	AN1	1907	PSU	C6-C5	3.90	1.39	1.35
5	AN1	2065	7MG	C2-N1	3.88	1.47	1.37
31	sN1	524	7MG	C2-N1	3.87	1.47	1.37
5	AN1	1913	PSU	C6-C5	3.84	1.39	1.35
31	sN1	1399	4OC	C5-C4	3.74	1.49	1.41
31	sN1	524	7MG	C5-C6	3.71	1.52	1.43
5	AN1	2500	PSU	C6-C5	3.65	1.39	1.35
5	AN1	2576	PSU	C6-C5	3.63	1.39	1.35
5	AN1	2601	PSU	C6-C5	3.61	1.39	1.35
5	AN1	952	PSU	C6-C5	3.56	1.39	1.35
5	AN1	2065	7MG	C5-C6	3.51	1.52	1.43
5	AN1	2453	PSU	C6-C5	3.49	1.39	1.35
31	sN1	1495	UR3	C6-N1	3.42	1.46	1.38
5	AN1	2499	2MA	C6-N6	-3.37	1.25	1.34
31	sN1	1399	4OC	C6-N1	3.34	1.46	1.38
31	sN1	524	7MG	C6-N1	3.24	1.44	1.38
5	AN1	2065	7MG	C6-N1	3.20	1.44	1.38
5	AN1	2441	2MG	C5-N7	-2.94	1.33	1.39
5	AN1	2548	OMU	O4-C4	-2.93	1.18	1.24
5	AN1	2548	OMU	C6-N1	2.90	1.45	1.38
5	AN1	1935	5MU	O4-C4	-2.89	1.18	1.23
5	AN1	1911	3TD	C4-N3	2.87	1.46	1.40
31	sN1	1204	2MG	C5-N7	-2.87	1.33	1.39
5	AN1	2026	6MZ	C5-N7	-2.87	1.33	1.39
5	AN1	2026	6MZ	C5-C4	-2.86	1.34	1.39
31	sN1	963	2MG	C5-N7	-2.83	1.33	1.39
31	sN1	1515	MA6	C5-C4	-2.81	1.34	1.39
31	sN1	964	5MC	O2-C2	-2.79	1.18	1.23
5	AN1	2247	OMG	O6-C6	-2.77	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2247	OMG	C5-N7	-2.76	1.33	1.39
31	sN1	1516	MA6	C5-C4	-2.76	1.34	1.39
31	sN1	1495	UR3	C4-N3	2.69	1.46	1.40
31	sN1	1399	4OC	O2-C2	-2.58	1.18	1.23
5	AN1	2065	7MG	O6-C6	-2.57	1.18	1.23
5	AN1	2247	OMG	C2-N1	2.56	1.43	1.37
5	AN1	1935	5MU	O2-C2	-2.55	1.18	1.23
5	AN1	2247	OMG	C6-N1	2.53	1.43	1.38
31	sN1	963	2MG	C5-C6	2.52	1.53	1.44
31	sN1	963	2MG	C6-N1	2.51	1.43	1.38
31	sN1	1204	2MG	O6-C6	-2.51	1.18	1.23
5	AN1	2441	2MG	C5-C6	2.51	1.53	1.44
5	AN1	2441	2MG	O6-C6	-2.51	1.18	1.23
5	AN1	2548	OMU	C5-C4	2.51	1.49	1.43
31	sN1	1204	2MG	C5-C6	2.50	1.53	1.44
31	sN1	963	2MG	O6-C6	-2.48	1.18	1.23
5	AN1	2499	2MA	C5-N7	-2.45	1.34	1.39
31	sN1	1204	2MG	C6-N1	2.45	1.43	1.38
5	AN1	2548	OMU	O2-C2	-2.42	1.18	1.23
5	AN1	1911	3TD	O2-C2	-2.41	1.18	1.23
31	sN1	524	7MG	O6-C6	-2.41	1.19	1.23
5	AN1	2247	OMG	C5-C6	2.41	1.53	1.44
31	sN1	1495	UR3	C5-C4	2.37	1.49	1.43
5	AN1	2026	6MZ	C8-N9	-2.33	1.33	1.37
5	AN1	2441	2MG	C6-N1	2.28	1.43	1.38
31	sN1	1515	MA6	C5-N7	-2.26	1.35	1.39
31	sN1	1516	MA6	C5-N7	-2.22	1.35	1.39
5	AN1	2499	2MA	C4-N9	-2.18	1.33	1.37
5	AN1	2499	2MA	C8-N7	2.17	1.35	1.31
31	sN1	524	7MG	C5-C4	2.07	1.44	1.37
31	sN1	1516	MA6	C8-N9	-2.07	1.34	1.37
5	AN1	1911	3TD	O4-C4	-2.05	1.18	1.23
31	sN1	1515	MA6	C8-N9	-2.01	1.34	1.37

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	sN1	1516	MA6	N1-C6-N6	-12.18	102.02	116.86
5	AN1	1935	5MU	C5-C4-N3	11.93	125.69	115.32
31	sN1	1515	MA6	N1-C6-N6	-11.82	102.46	116.86
5	AN1	2026	6MZ	C4-N9-C1'	-9.78	103.75	126.63
5	AN1	1935	5MU	C5-C6-N1	-9.63	112.85	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AN1	2026	6MZ	C1'-N9-C8	9.61	148.43	127.09
31	sN1	1516	MA6	C5-C6-N6	8.11	138.17	125.33
31	sN1	1515	MA6	C5-C6-N6	7.96	137.93	125.33
5	AN1	2499	2MA	C1'-N9-C8	-7.60	110.22	127.09
5	AN1	2441	2MG	C2-N3-C4	6.66	120.33	112.00
31	sN1	963	2MG	C2-N3-C4	6.54	120.18	112.00
31	sN1	1204	2MG	C2-N3-C4	6.46	120.08	112.00
5	AN1	2499	2MA	N9-C8-N7	-5.81	105.69	113.94
5	AN1	2499	2MA	C5-C4-N3	-5.75	121.13	127.18
31	sN1	1515	MA6	N1-C2-N3	-5.64	120.05	128.58
31	sN1	1516	MA6	N1-C2-N3	-5.62	120.07	128.58
5	AN1	2548	OMU	C4-N3-C2	-5.61	119.65	126.61
31	sN1	1495	UR3	C4-N3-C2	-5.56	120.11	124.58
5	AN1	1911	3TD	N1-C2-N3	5.53	120.15	116.13
5	AN1	2441	2MG	C5-C4-N3	-5.47	119.68	128.39
5	AN1	2026	6MZ	C5-C4-N3	-5.46	119.20	126.72
5	AN1	2026	6MZ	N1-C2-N3	-5.34	120.49	128.58
31	sN1	963	2MG	C5-C4-N3	-5.20	120.11	128.39
5	AN1	2499	2MA	C4-N9-C1'	5.19	138.76	126.63
5	AN1	2247	OMG	C5-C4-N3	-5.13	120.23	128.39
31	sN1	1204	2MG	C5-C4-N3	-5.12	120.24	128.39
5	AN1	2065	7MG	C5-C6-N1	5.05	119.82	110.94
5	AN1	2499	2MA	C4-N9-C8	5.03	111.02	105.74
31	sN1	524	7MG	C5-C6-N1	5.03	119.79	110.94
5	AN1	1935	5MU	O4-C4-C5	-4.97	119.24	124.92
5	AN1	2453	PSU	C4-N3-C2	-4.93	119.58	126.37
5	AN1	952	PSU	C4-N3-C2	-4.91	119.61	126.37
5	AN1	952	PSU	N1-C2-N3	4.88	120.31	115.17
5	AN1	2576	PSU	N1-C2-N3	4.85	120.28	115.17
31	sN1	1516	MA6	C5-C4-N3	-4.82	120.07	126.72
5	AN1	2601	PSU	C4-N3-C2	-4.81	119.74	126.37
5	AN1	1935	5MU	C4-N3-C2	-4.81	121.03	127.34
5	AN1	2453	PSU	N1-C2-N3	4.79	120.22	115.17
31	sN1	1515	MA6	C5-C4-N3	-4.78	120.14	126.72
5	AN1	2500	PSU	N1-C2-N3	4.78	120.21	115.17
5	AN1	1907	PSU	N1-C2-N3	4.77	120.20	115.17
5	AN1	2576	PSU	C4-N3-C2	-4.77	119.81	126.37
5	AN1	2500	PSU	C4-N3-C2	-4.75	119.83	126.37
5	AN1	1907	PSU	C4-N3-C2	-4.72	119.88	126.37
5	AN1	2601	PSU	N1-C2-N3	4.70	120.13	115.17
31	sN1	524	7MG	C2-N3-C4	4.60	120.22	112.30
5	AN1	1913	PSU	N1-C2-N3	4.57	119.99	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AN1	2065	7MG	C2-N3-C4	4.56	120.16	112.30
5	AN1	2247	OMG	C2-N3-C4	4.54	120.12	112.30
5	AN1	1913	PSU	C4-N3-C2	-4.50	120.17	126.37
5	AN1	1935	5MU	N3-C2-N1	4.46	120.70	114.89
5	AN1	1911	3TD	C4-N3-C2	-4.44	119.92	124.61
5	AN1	2499	2MA	N3-C4-N9	4.36	132.53	126.99
31	sN1	1516	MA6	N9-C8-N7	-4.35	107.77	113.94
31	sN1	1515	MA6	N9-C8-N7	-4.32	107.80	113.94
5	AN1	2441	2MG	C2-N1-C6	-4.22	119.45	124.55
31	sN1	524	7MG	C5-C4-N3	-4.15	120.34	128.13
31	sN1	1204	2MG	C2-N1-C6	-4.13	119.56	124.55
31	sN1	513	PSU	C4-N3-C2	-4.12	120.69	126.37
5	AN1	2065	7MG	C5-C4-N3	-4.11	120.42	128.13
5	AN1	2026	6MZ	C4-C5-C6	4.06	120.16	116.78
31	sN1	963	2MG	C2-N1-C6	-4.04	119.67	124.55
31	sN1	513	PSU	N1-C2-N3	3.99	119.38	115.17
31	sN1	1515	MA6	C4-C5-C6	3.98	120.02	115.91
5	AN1	2548	OMU	N3-C2-N1	3.87	119.93	114.89
31	sN1	1516	MA6	C4-C5-C6	3.86	119.90	115.91
5	AN1	2026	6MZ	N9-C8-N7	-3.85	108.47	113.94
5	AN1	2065	7MG	C4-C5-N7	3.83	109.91	105.38
5	AN1	1935	5MU	C5M-C5-C6	-3.80	117.70	122.85
5	AN1	1935	5MU	C5M-C5-C4	3.74	122.78	118.78
31	sN1	524	7MG	C4-C5-N7	3.70	109.75	105.38
31	sN1	1495	UR3	C5-C4-N3	3.64	119.83	115.04
5	AN1	2548	OMU	C5-C4-N3	3.61	119.86	114.80
5	AN1	2026	6MZ	N3-C4-N9	3.55	133.21	127.17
31	sN1	1204	2MG	N1-C2-N2	3.50	120.13	116.56
31	sN1	1515	MA6	C2-N1-C6	3.47	120.31	111.83
5	AN1	2026	6MZ	C2-N3-C4	3.47	120.30	111.83
31	sN1	963	2MG	N1-C2-N2	3.44	120.07	116.56
5	AN1	2499	2MA	C5-N7-C8	3.43	108.83	103.45
31	sN1	1516	MA6	C2-N1-C6	3.42	120.18	111.83
5	AN1	2499	2MA	N3-C2-N1	-3.36	119.83	125.77
31	sN1	1516	MA6	C2-N3-C4	3.33	119.97	111.83
5	AN1	2441	2MG	N9-C4-N3	3.33	132.61	125.95
5	AN1	2441	2MG	N1-C2-N2	3.31	119.94	116.56
31	sN1	1515	MA6	C2-N3-C4	3.30	119.88	111.83
31	sN1	524	7MG	C5-C4-N9	3.18	110.40	106.33
5	AN1	2247	OMG	N9-C8-N7	-3.15	107.55	113.40
31	sN1	964	5MC	C5-C6-N1	-3.13	119.92	123.31
5	AN1	2247	OMG	N9-C4-N3	3.08	132.11	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	sN1	963	2MG	N9-C4-N3	3.05	132.05	125.95
5	AN1	2247	OMG	C2-N1-C6	-3.04	119.59	125.11
31	sN1	1204	2MG	N9-C4-N3	3.03	132.01	125.95
5	AN1	2065	7MG	C5-C4-N9	3.03	110.21	106.33
31	sN1	1204	2MG	N9-C8-N7	-2.96	107.90	113.40
5	AN1	952	PSU	O2-C2-N1	-2.96	119.73	122.79
31	sN1	1515	MA6	C5-N7-C8	2.94	108.07	103.45
31	sN1	1516	MA6	C5-N7-C8	2.93	108.06	103.45
31	sN1	1516	MA6	N3-C4-N9	2.93	132.14	127.17
31	sN1	963	2MG	N9-C8-N7	-2.91	108.00	113.40
31	sN1	1515	MA6	N3-C4-N9	2.89	132.08	127.17
5	AN1	2441	2MG	N9-C8-N7	-2.86	108.10	113.40
5	AN1	2065	7MG	O6-C6-C5	-2.85	120.61	127.62
5	AN1	2548	OMU	O4-C4-C5	-2.84	120.26	125.16
5	AN1	2500	PSU	O2-C2-N1	-2.80	119.90	122.79
5	AN1	2065	7MG	C2-N1-C6	-2.78	120.07	125.11
5	AN1	1907	PSU	O2-C2-N1	-2.77	119.94	122.79
31	sN1	524	7MG	C2-N1-C6	-2.75	120.12	125.11
5	AN1	2026	6MZ	C5-N7-C8	2.74	107.75	103.45
5	AN1	2453	PSU	O2-C2-N1	-2.73	119.97	122.79
5	AN1	2576	PSU	O2-C2-N1	-2.72	119.98	122.79
31	sN1	524	7MG	O6-C6-C5	-2.70	121.00	127.62
5	AN1	1913	PSU	O2-C2-N1	-2.69	120.01	122.79
31	sN1	1204	2MG	C5-C6-N1	2.69	120.10	113.25
5	AN1	1935	5MU	O4-C4-N3	-2.68	115.08	120.11
5	AN1	2247	OMG	C5-C6-N1	2.67	120.06	113.25
5	AN1	2065	7MG	N9-C4-N3	2.67	129.38	125.46
5	AN1	2441	2MG	C5-C6-N1	2.67	120.05	113.25
31	sN1	963	2MG	C5-C6-N1	2.66	120.02	113.25
31	sN1	524	7MG	N9-C4-N3	2.59	129.26	125.46
5	AN1	1913	PSU	C6-N1-C2	-2.58	120.30	122.69
5	AN1	1911	3TD	C6-C5-C4	2.57	119.91	118.19
5	AN1	2601	PSU	O2-C2-N1	-2.57	120.14	122.79
31	sN1	1204	2MG	O6-C6-C5	-2.55	119.81	126.53
31	sN1	1516	MA6	C4-N9-C8	2.55	108.41	105.74
31	sN1	1204	2MG	C1'-N9-C4	-2.53	119.01	126.49
5	AN1	2441	2MG	O6-C6-C5	-2.51	119.91	126.53
31	sN1	963	2MG	O6-C6-C5	-2.49	119.96	126.53
31	sN1	963	2MG	C1'-N9-C4	-2.48	119.16	126.49
5	AN1	2247	OMG	O6-C6-C5	-2.47	120.01	126.53
5	AN1	2500	PSU	C6-N1-C2	-2.46	120.40	122.69
5	AN1	1907	PSU	C6-N1-C2	-2.45	120.41	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	sN1	1515	MA6	C4-N9-C8	2.44	108.31	105.74
5	AN1	2576	PSU	C6-N1-C2	-2.44	120.42	122.69
5	AN1	1935	5MU	O2-C2-N1	-2.44	119.62	122.80
5	AN1	952	PSU	C6-N1-C2	-2.39	120.47	122.69
5	AN1	2026	6MZ	C5-C6-N1	2.39	120.72	118.15
31	sN1	524	7MG	N9-C8-N7	2.38	106.74	103.37
5	AN1	2453	PSU	C6-N1-C2	-2.34	120.52	122.69
31	sN1	1399	4OC	C6-C5-C4	2.32	119.79	117.00
5	AN1	2601	PSU	C6-N1-C2	-2.31	120.55	122.69
31	sN1	1516	MA6	C4-C5-N7	-2.28	107.98	110.58
31	sN1	513	PSU	C6-N1-C2	-2.27	120.58	122.69
31	sN1	1495	UR3	C6-N1-C2	-2.23	119.98	121.80
5	AN1	2065	7MG	N9-C8-N7	2.23	106.53	103.37
31	sN1	1515	MA6	C4-C5-N7	-2.22	108.04	110.58
5	AN1	2499	2MA	CM2-C2-N1	2.21	120.44	117.13
31	sN1	963	2MG	N1-C2-N3	-2.21	119.96	123.68
5	AN1	2247	OMG	C8-N7-C5	2.20	108.19	104.26
5	AN1	2499	2MA	N6-C6-N1	2.20	120.00	117.03
5	AN1	2499	2MA	C4-C5-N7	-2.17	108.10	110.58
31	sN1	1204	2MG	N1-C2-N3	-2.15	120.06	123.68
5	AN1	2576	PSU	C6-C5-C4	2.12	119.61	118.17
31	sN1	1204	2MG	C8-N7-C5	2.12	108.03	104.26
31	sN1	963	2MG	C8-N7-C5	2.11	108.02	104.26
31	sN1	1204	2MG	C1'-N9-C8	2.11	132.72	126.73
5	AN1	2441	2MG	C8-N7-C5	2.10	108.01	104.26
31	sN1	513	PSU	O4'-C1'-C2'	2.10	108.06	105.15
31	sN1	963	2MG	C1'-N9-C8	2.09	132.67	126.73
5	AN1	2441	2MG	N1-C2-N3	-2.09	120.16	123.68
5	AN1	2441	2MG	C1'-N9-C4	-2.06	120.40	126.49
31	sN1	964	5MC	CM5-C5-C6	-2.05	120.07	122.85
5	AN1	2453	PSU	C6-C5-C4	2.05	119.56	118.17
5	AN1	952	PSU	C6-C5-C4	2.05	119.55	118.17
5	AN1	1913	PSU	O4'-C1'-C2'	2.02	107.94	105.15
5	AN1	2548	OMU	O2-C2-N1	-2.01	120.18	122.80
5	AN1	2453	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AN1	1913	PSU	O4'-C1'-C5-C4
5	AN1	1913	PSU	O4'-C1'-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	AN1	2548	OMU	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	C5-C6-N6-C9
5	AN1	2548	OMU	C3'-C4'-C5'-O5'
31	sN1	524	7MG	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	O4'-C4'-C5'-O5'
5	AN1	2499	2MA	O4'-C4'-C5'-O5'
5	AN1	2499	2MA	C3'-C4'-C5'-O5'
31	sN1	1399	4OC	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	C3'-C4'-C5'-O5'
31	sN1	524	7MG	O4'-C4'-C5'-O5'
31	sN1	1495	UR3	O4'-C4'-C5'-O5'
5	AN1	1913	PSU	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	N1-C6-N6-C9
5	AN1	1911	3TD	C4'-C5'-O5'-P
5	AN1	1911	3TD	O4'-C1'-C5-C4
31	sN1	1399	4OC	C3'-C4'-C5'-O5'
5	AN1	2441	2MG	C3'-C4'-C5'-O5'
5	AN1	1907	PSU	C4'-C5'-O5'-P
31	sN1	1495	UR3	C3'-C4'-C5'-O5'
31	sN1	524	7MG	C4'-C5'-O5'-P
5	AN1	2065	7MG	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	C5-C6-N6-C10
5	AN1	2065	7MG	C4'-C5'-O5'-P
5	AN1	2499	2MA	O4'-C1'-N9-C8
31	sN1	1516	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AN1	2026	6MZ	2	0
31	sN1	1515	MA6	1	0
31	sN1	1516	MA6	1	0
5	AN1	1913	PSU	1	0
5	AN1	1911	3TD	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 95 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

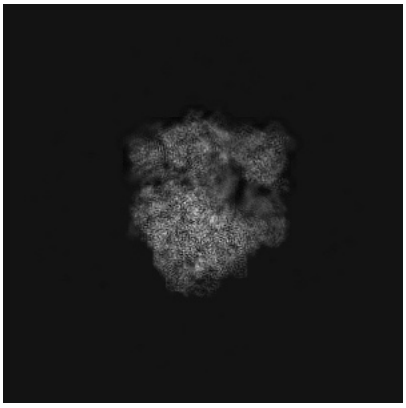
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21032. These allow visual inspection of the internal detail of the map and identification of artifacts.

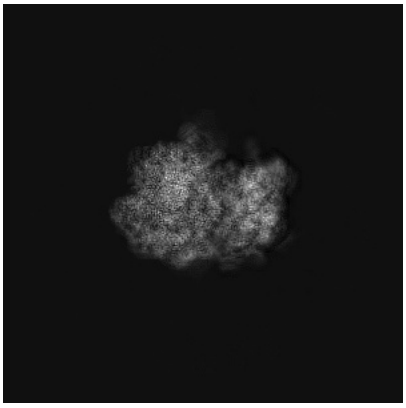
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

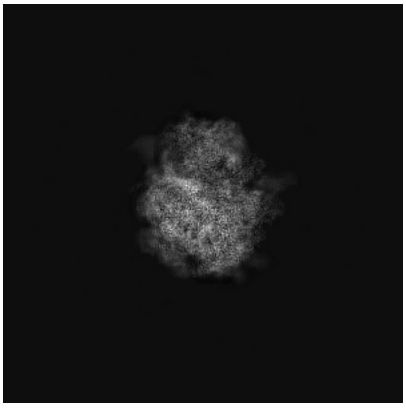
6.1.1 Primary map



X



Y



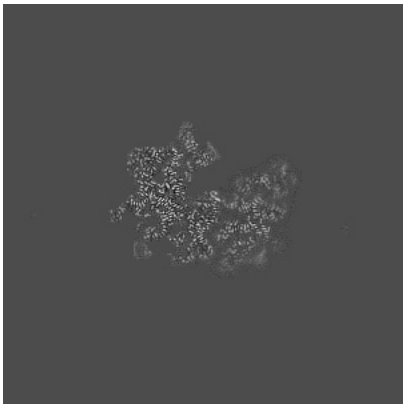
Z

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

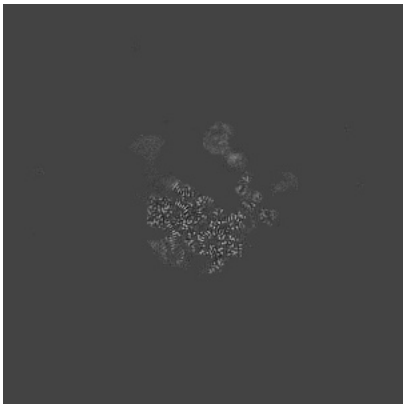
6.2 Central slices (i)

6.2.1 Primary map

X Index: 256



Y Index: 256

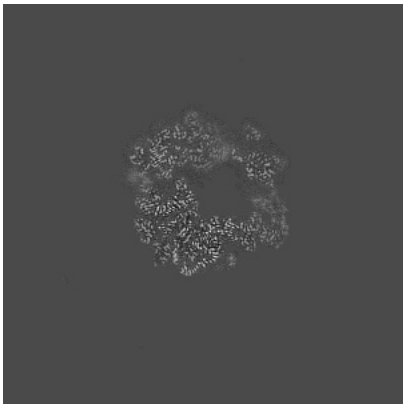


Z Index: 256

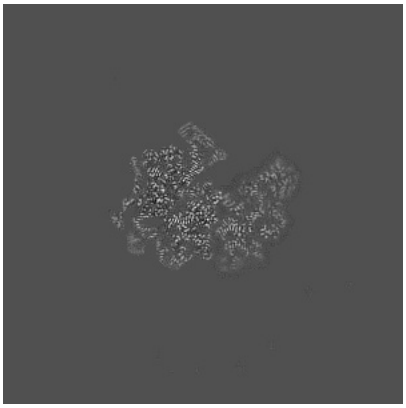
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

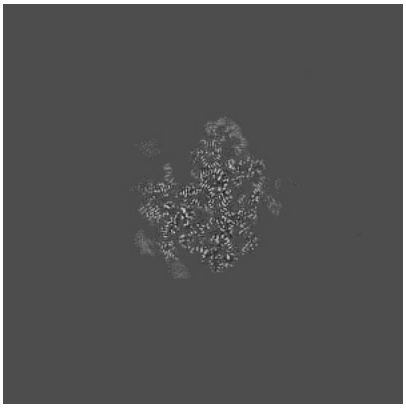
6.3.1 Primary map



X Index: 277



Y Index: 245

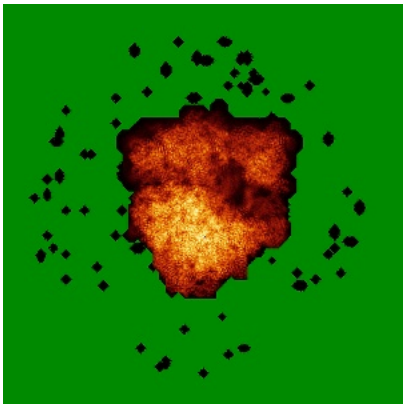


Z Index: 227

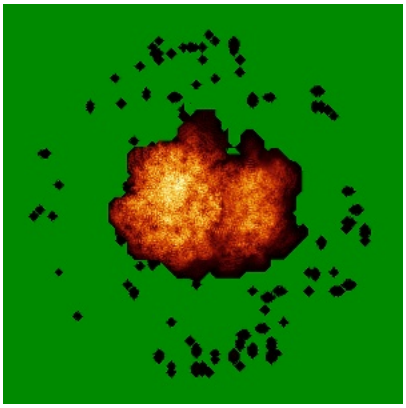
The images above show the largest variance slices of the map in three orthogonal directions.

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

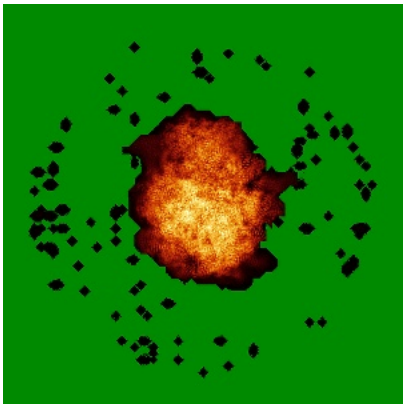
6.4.1 Primary map



X



Y

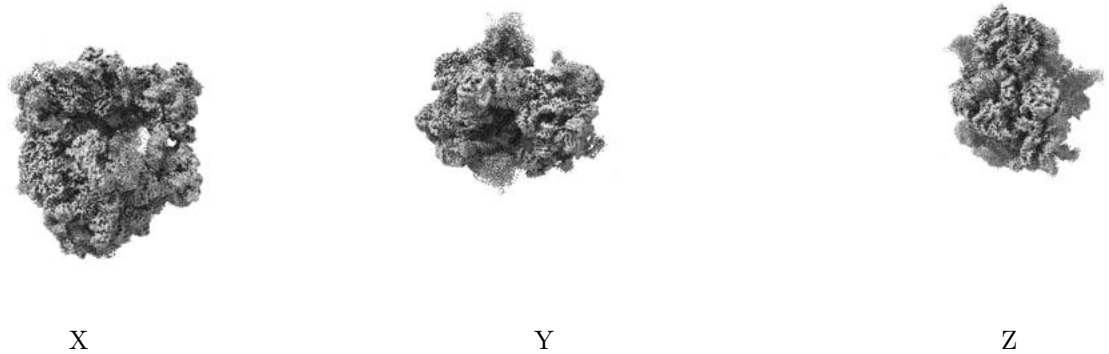


Z

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

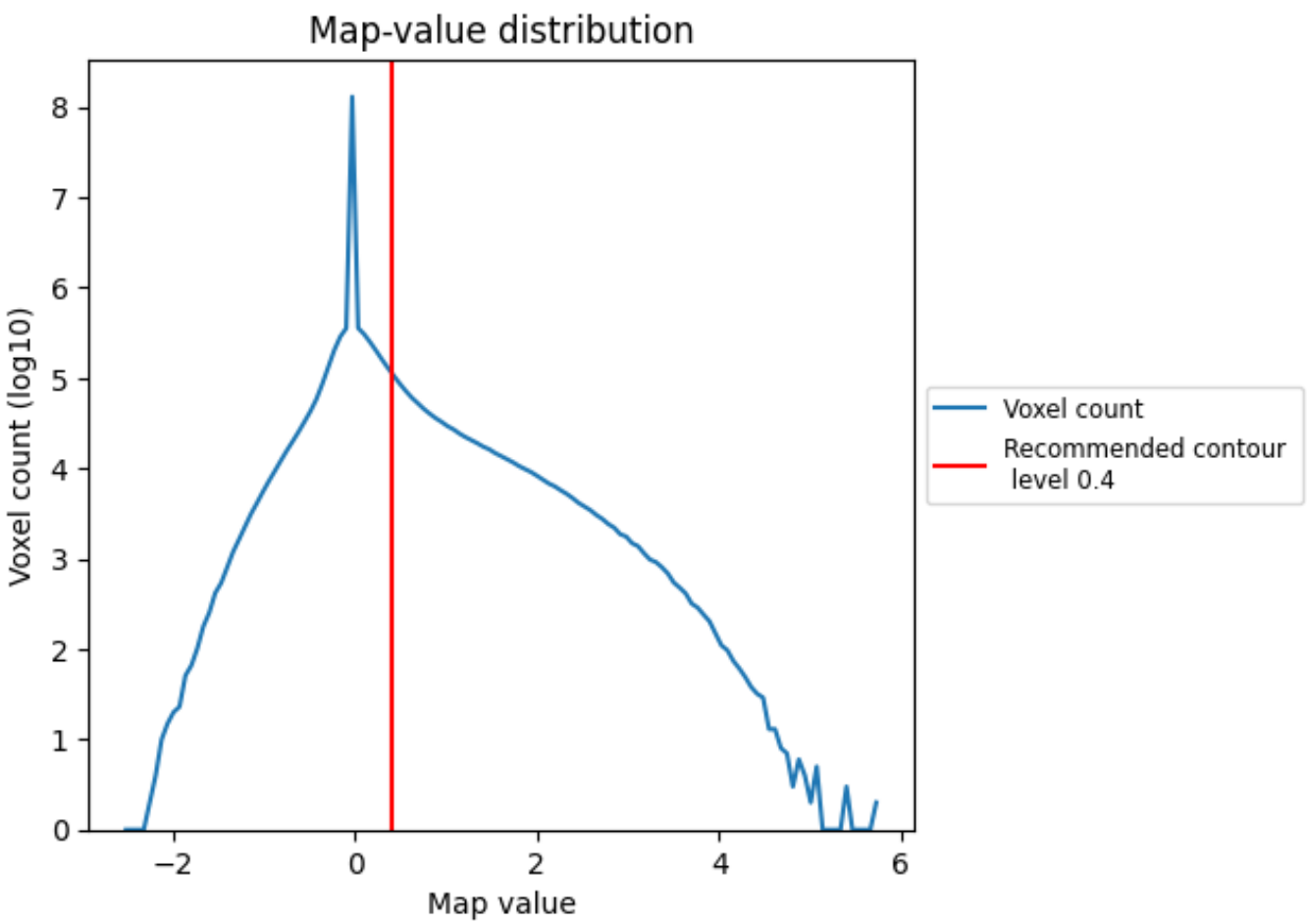
6.6 Mask visualisation (i)

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

7 Map analysis (i)

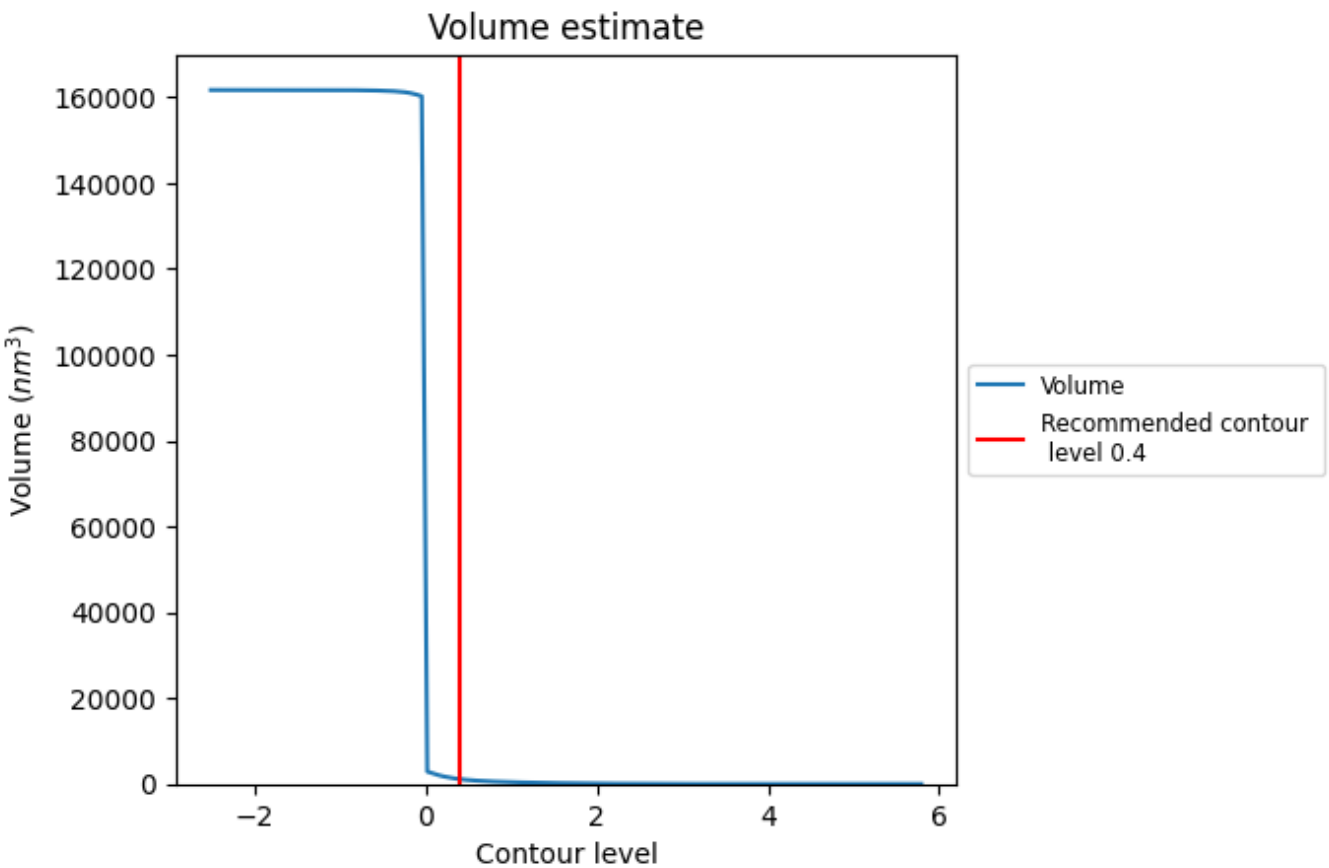
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

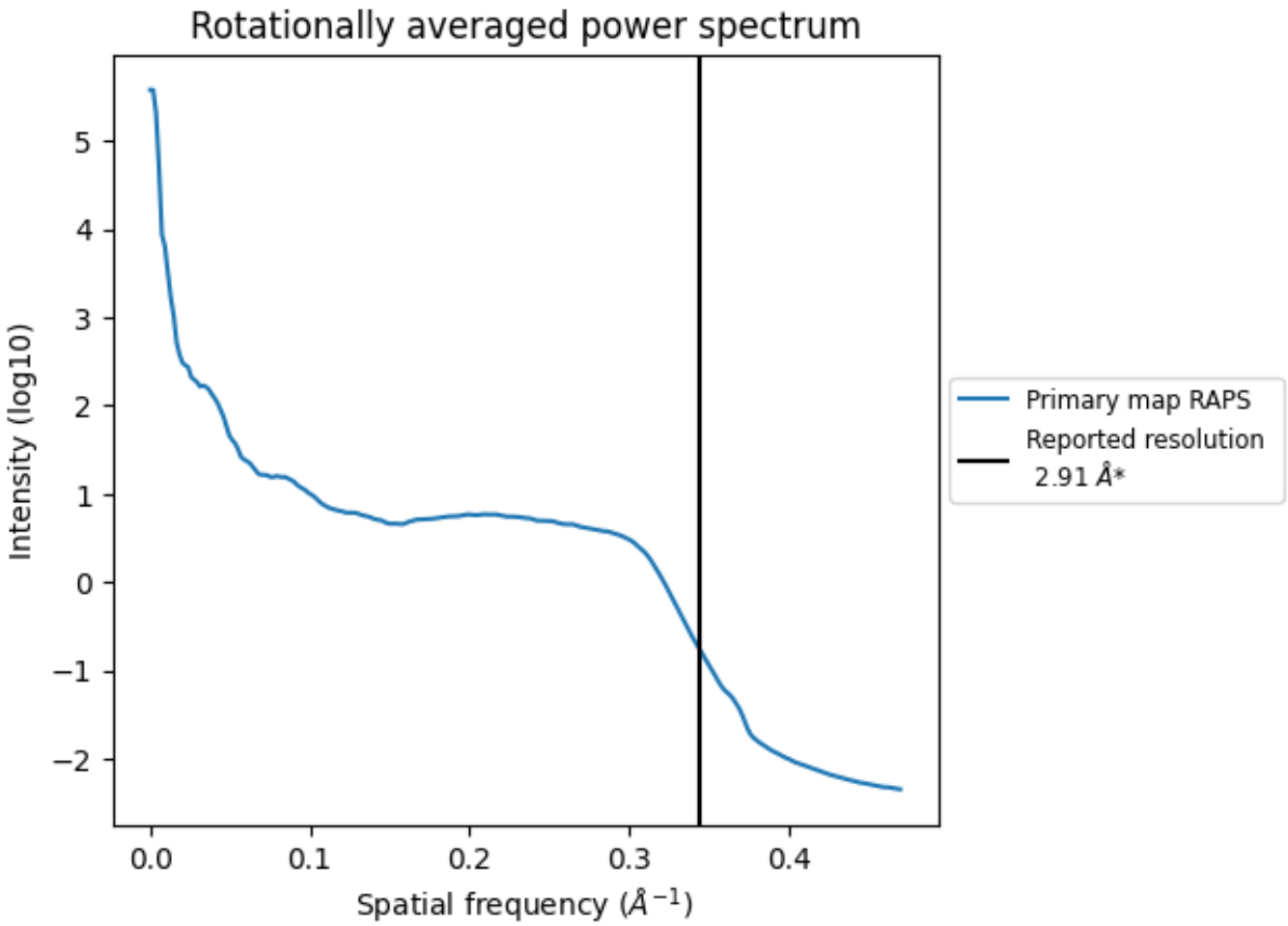
7.2 Volume estimate (i)



The volume at the recommended contour level is 1118 nm^3; this corresponds to an approximate mass of 1010 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 0.344 Å^{-1}

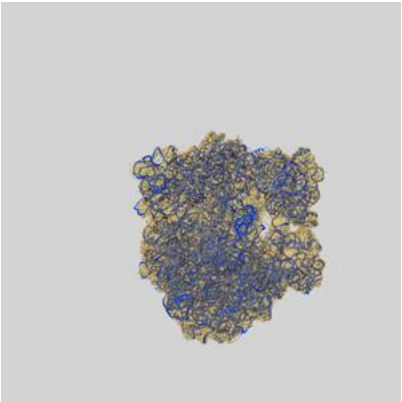
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

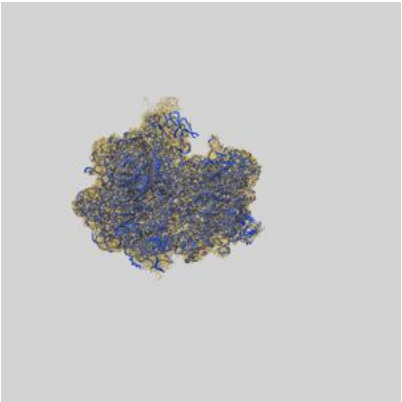
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21032 and PDB model 6V3B. Per-residue inclusion information can be found in section 3 on page 14.

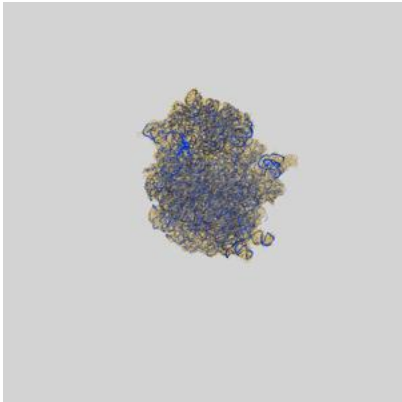
9.1 Map-model overlay (i)



X



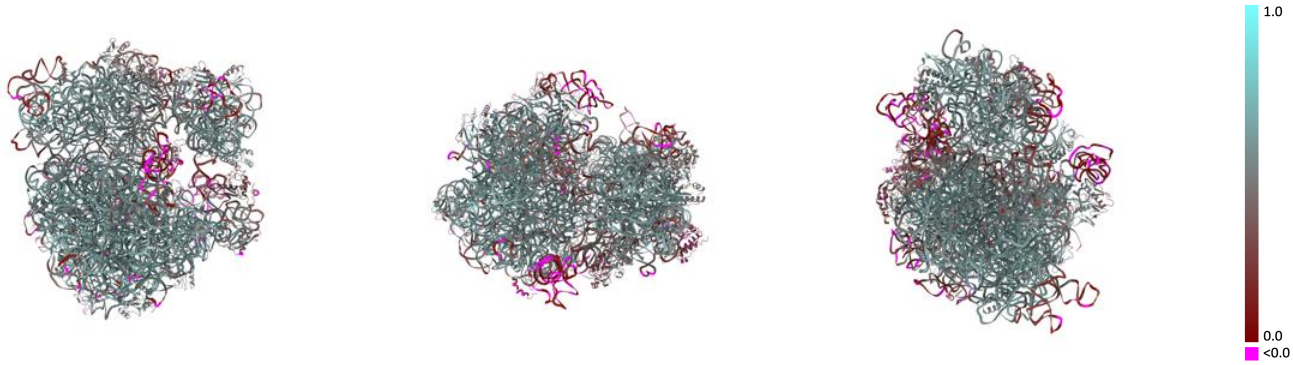
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

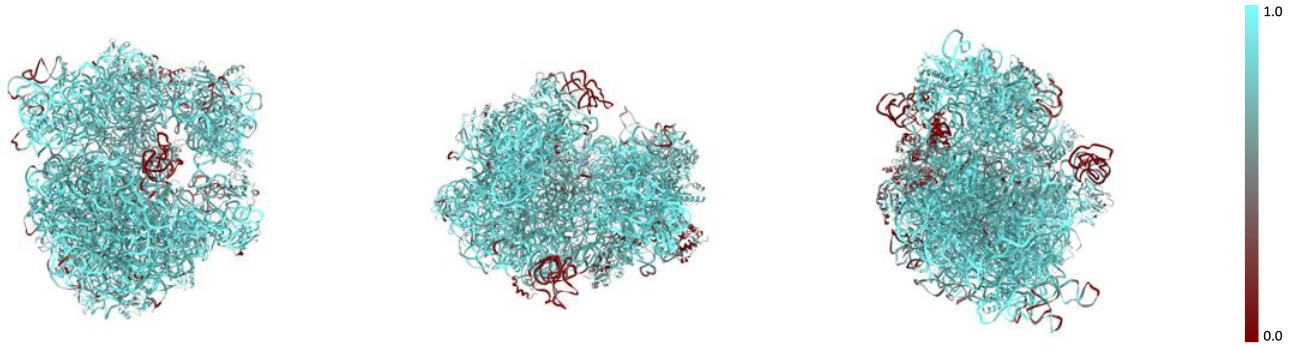
9.2 Q-score mapped to coordinate model (i)



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.

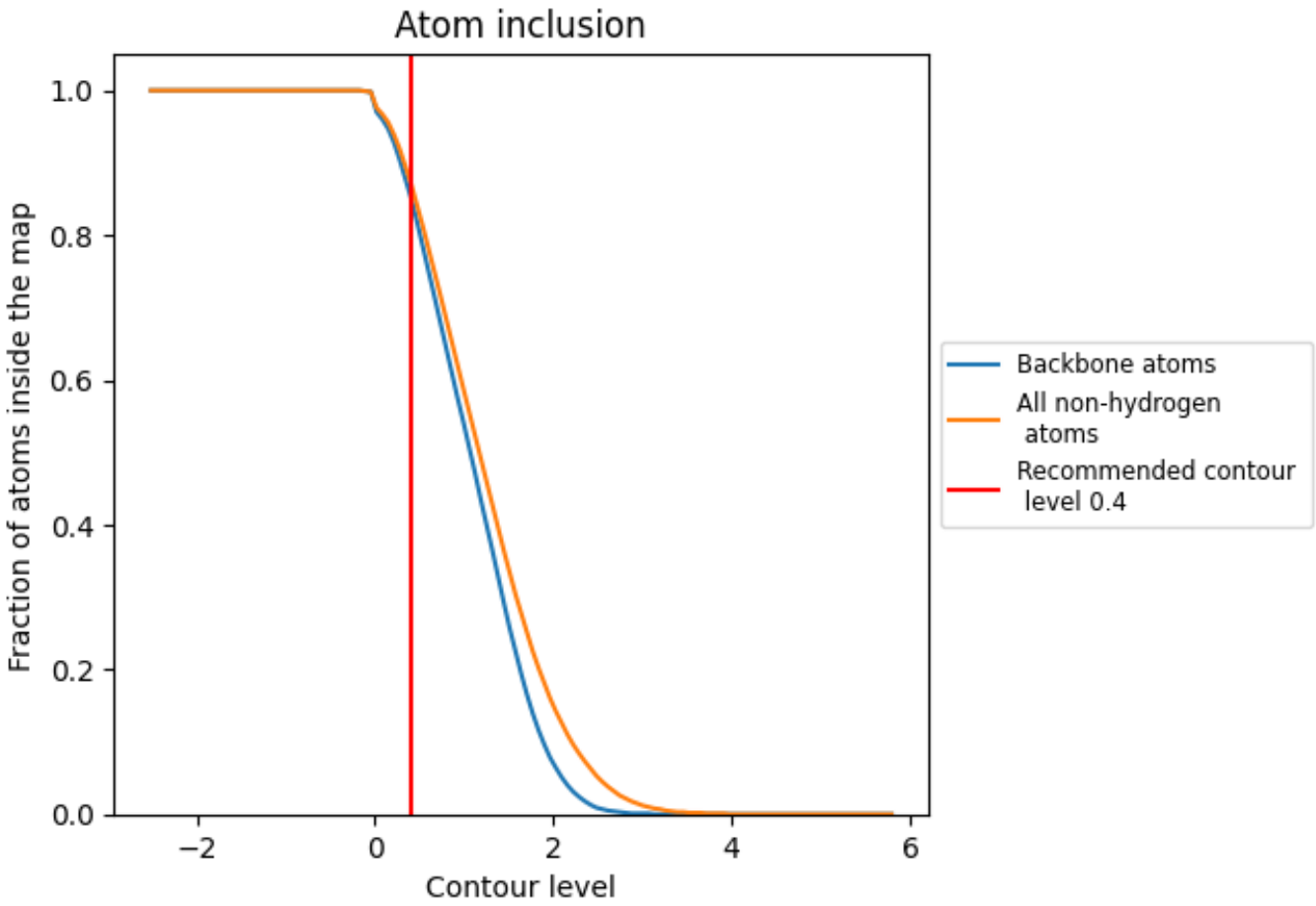
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.5150
0	0.8230	0.5200
1	0.9500	0.6270
2	0.9390	0.5900
3	0.9480	0.5550
AN1	0.8900	0.5260
B	0.9240	0.4750
C	0.9200	0.5830
D	0.9220	0.5850
E	0.8830	0.5540
F	0.6360	0.2780
G	0.7610	0.4330
H	0.4830	0.3220
I	0.9000	0.5640
J	0.9260	0.5850
K	0.9090	0.5680
L	0.8670	0.5480
M	0.9620	0.6090
N	0.8530	0.4870
O	0.9090	0.5670
P	0.9150	0.5830
Q	0.8550	0.5360
R	0.9100	0.5820
S	0.8450	0.5230
T	0.7270	0.4330
U	0.8260	0.5200
V	0.8900	0.5820
W	0.8710	0.5560
X	0.7560	0.4410
Y	0.8410	0.5200
Z	0.8250	0.5230
b	0.3130	0.2870
c	0.8500	0.5230
d	0.7580	0.4480
e	0.8950	0.5240

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.5740	0.3610
g	0.6900	0.4250
h	0.9140	0.5670
i	0.9080	0.5650
j	0.8150	0.5210
k	0.5720	0.3400
l	0.7370	0.5040
m	0.8790	0.5340
n	0.8810	0.5580
o	0.9020	0.5320
p	0.9150	0.5720
q	0.8640	0.5420
r	0.7620	0.4600
s	0.9360	0.5700
sN1	0.9110	0.5080
t	0.9150	0.5560
u	0.2740	0.3110