Full wwPDB EM Validation Report

Nov 12, 2022 – 04:19 PM EST

PDB ID	:	6V3A
EMDB ID	:	EMD-21031
Title	:	Cryo-EM structure of the Acinetobacter baumannii Ribosome: 70S with E-site tRNA
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2019-11-25
Resolution	:	2.82 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 (i)) were used in the production of this report:

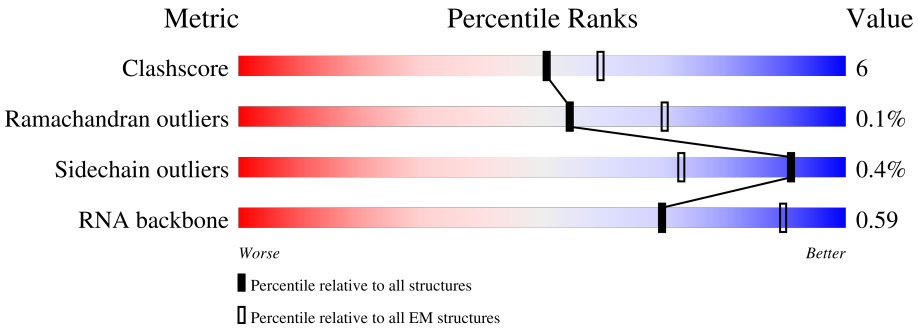
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.82 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	51	16% 88% 12%
2	1	44	84% 16%
3	2	64	81% 12%
4	3	38	11% 82% 18%
5	AN1	2918	5% 65% 29% 5%
6	B	115	61% 32% 7%
7	C	274	5% 82% 17%

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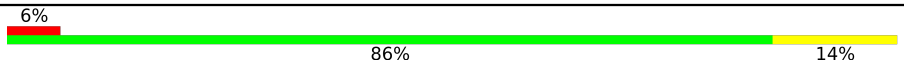
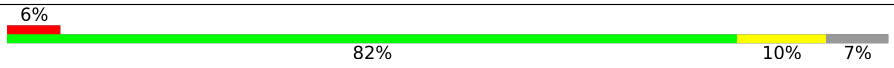
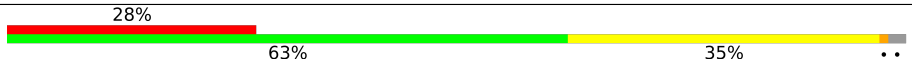
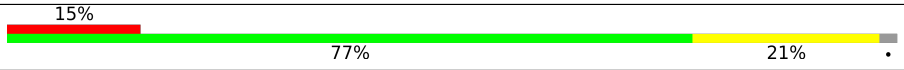
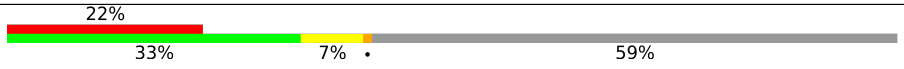
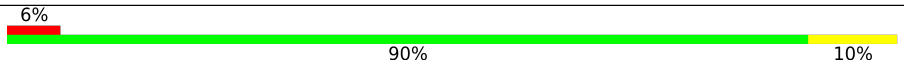
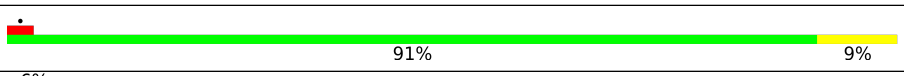
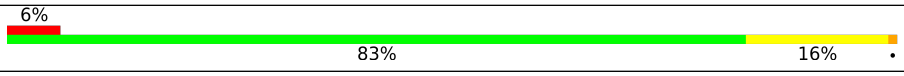
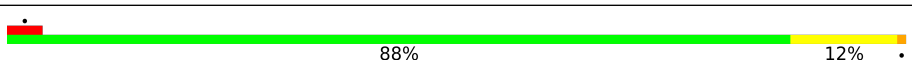
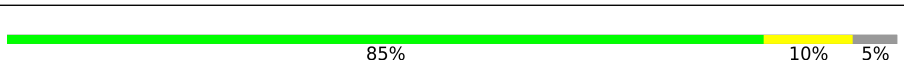
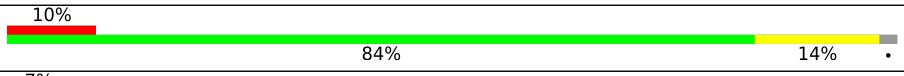
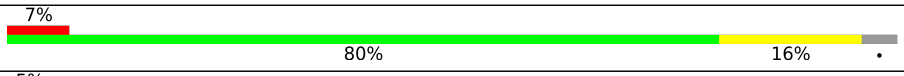
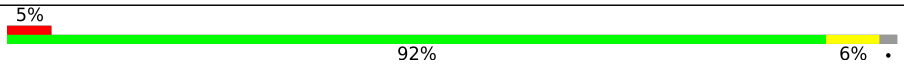
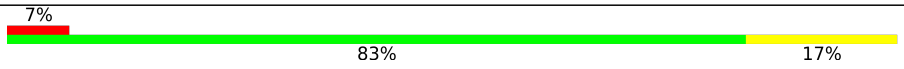
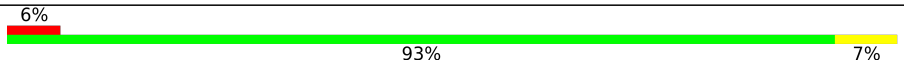
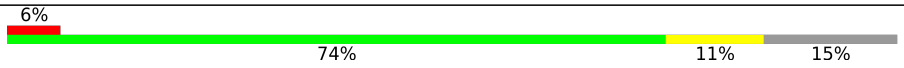
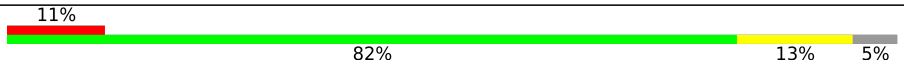
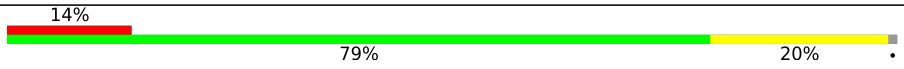
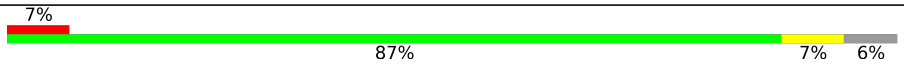
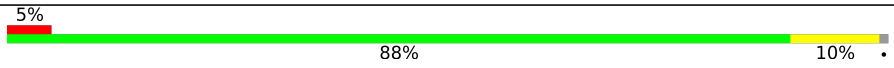
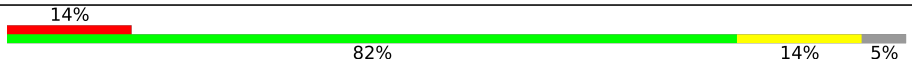
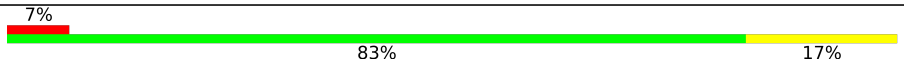
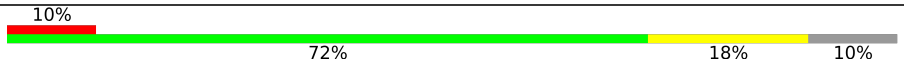
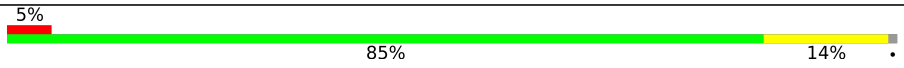
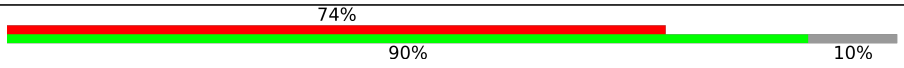
Mol	Chain	Length	Quality of chain
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	
31	sN1	1544	
32	b	250	

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Mol	Chain	Length	Quality of chain
33	c	250	86% 14%
34	d	208	12% 99%
35	e	165	94% 6%
36	f	127	29% 74% 26%
37	g	156	15% 90% 10%
38	h	131	99%
39	i	128	98%
40	j	103	5% 97%
41	k	128	38% 91% 9%
42	l	124	13% 97%
43	m	118	97%
44	n	101	98%
45	o	89	99%
46	p	101	82% 18%
47	q	85	94% 6%
48	r	75	71% 29%
49	s	91	90% 10%
50	t	88	97%
51	u	71	30% 28% 70%
52	v	77	62% 35%
53	w	3	67% 33%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 142113 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
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total 1636	C 733	N 291	O 535	P 76	S 1	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	3	Total 65	C 29	N 12	O 21	P 3	0	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total 1	Zn 1	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	AN1	49	Total 49	Mg 49	0
55	sN1	44	Total 44	Mg 44	0

- Molecule 56 is SODIUM ION (three-letter code: NA) (formula: Na).

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

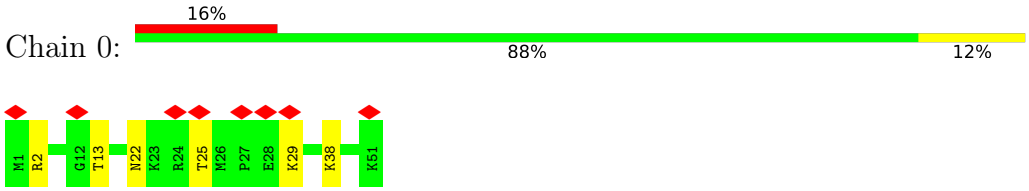
- Molecule 57 is water.

Mol	Chain	Residues	Atoms	AltConf
57	AN1	319	Total O 319 319	0
57	B	4	Total O 4 4	0
57	C	5	Total O 5 5	0
57	D	3	Total O 3 3	0
57	E	3	Total O 3 3	0
57	K	3	Total O 3 3	0
57	O	1	Total O 1 1	0
57	P	3	Total O 3 3	0
57	Q	1	Total O 1 1	0
57	U	1	Total O 1 1	0
57	sN1	163	Total O 163 163	0
57	i	5	Total O 5 5	0
57	j	2	Total O 2 2	0
57	m	1	Total O 1 1	0
57	o	1	Total O 1 1	0
57	p	1	Total O 1 1	0
57	q	2	Total O 2 2	0
57	t	2	Total O 2 2	0

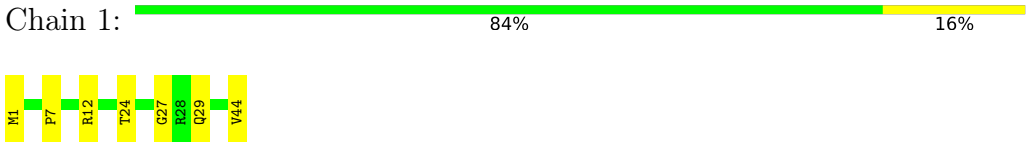
3 Residue-property plots (i)

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.

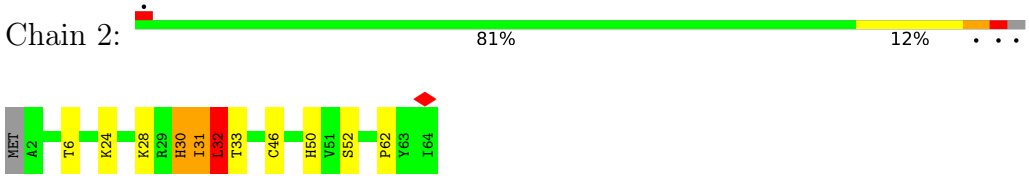
• Molecule 1: 50S ribosomal protein L33



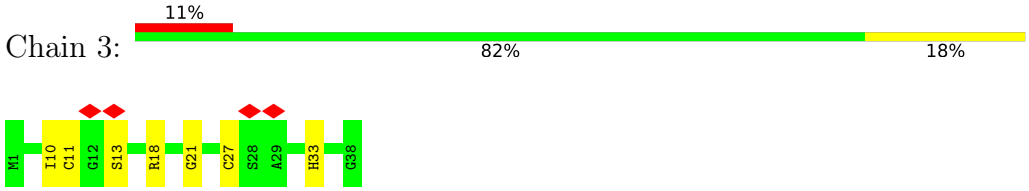
• Molecule 2: 50S ribosomal protein L34



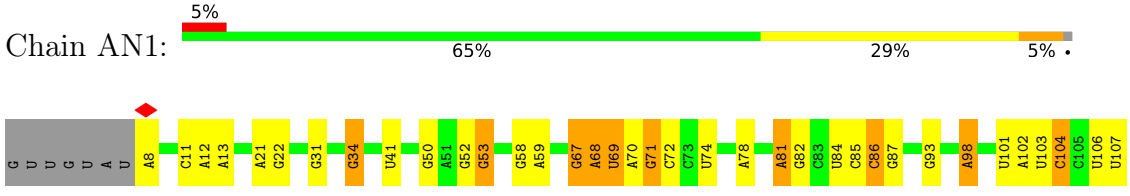
• Molecule 3: 50S ribosomal protein L35

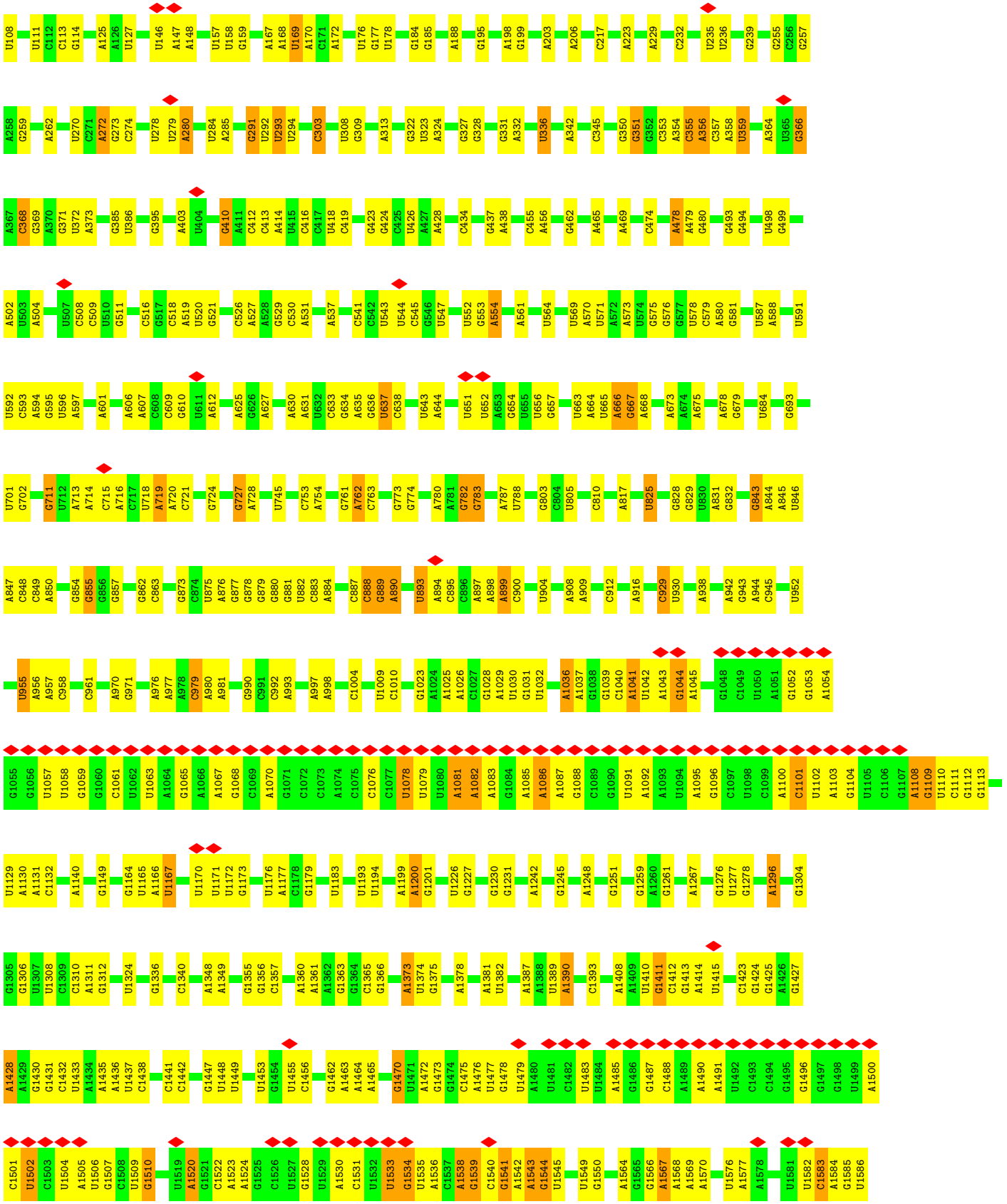


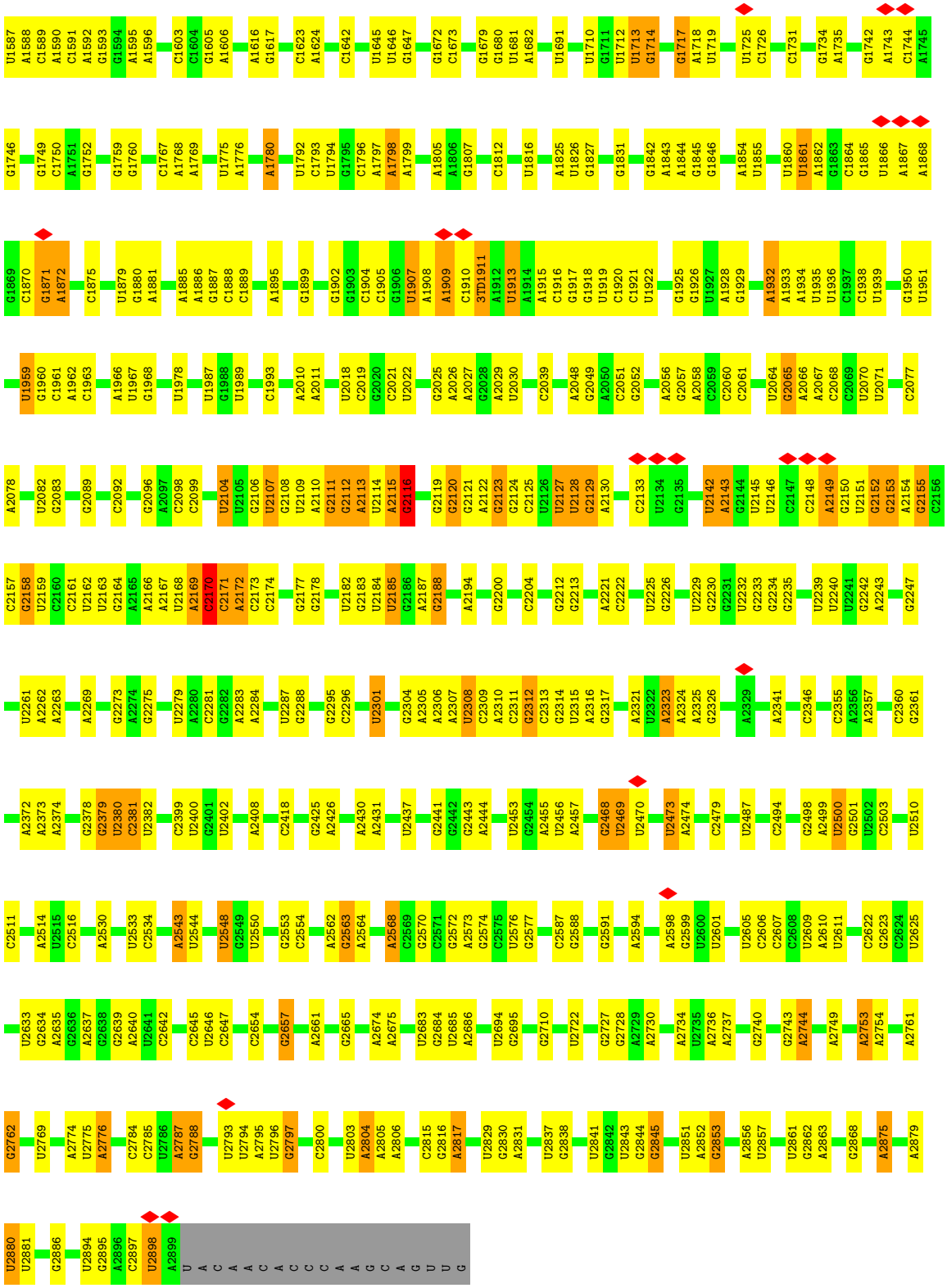
• Molecule 4: 50S ribosomal protein L36



• Molecule 5: 23s ribosomal RNA

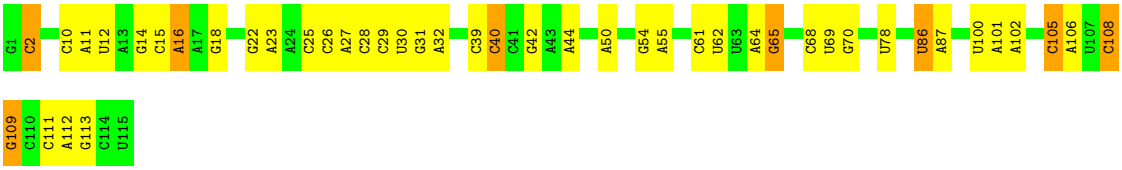



U108 U111 C112 C113 G114 A125 A126 U127 U146 A147 A148 U157 U158 G159 A167 A168 U169 A170 C171 A172 U176 G177 U178 G184 G185 A188 G195 A198 G199 A203 A206 C217 A223 A229 C232 U235 U236 G239 G255 C256 G257
A258 G259 A262 U270 C271 A272 G273 C274 U278 U279 A280 U284 A285 G291 U292 U293 U294 C303 U308 G309 A313 G322 U323 A324 G327 G328 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 A411 C412 C413 A414 U415 C416 C417 U418 C419 G423 G424 C425 U426 A427 A428 C434 G437 A438 C455 A456 G462 A465 A469 C474 A478 A479 G480 G493 G494 U498 G499
A502 U503 A504 U507 C508 C509 U510 G511 C516 G517 C518 A519 U520 G521 C526 A527 A528 G529 C530 A531 A537 C541 C542 U543 U544 C545 G546 U547 U552 G553 A554 A561 U564 U569 A570 U571 A572 A573 U574 G575 G576 G577 U578 C579 A580 G581 U587 A588 U591
U592 C593 A594 G595 U596 A597 A601 A606 A607 C608 C609 G610 U611 A612 A625 G626 A627 A630 A631 U632 C633 G634 A635 G636 U637 C638 U643 A644 U651 U652 A653 G654 U655 U656 G657 U663 A664 U665 A666 G667 A668 A673 A674 A675 A678 G679 U684 G693
U701 G702 G711 U712 A713 A714 C715 A716 C717 U718 A719 A720 C721 G724 G727 A728 U745 C753 A754 G761 A762 C763 G773 G774 A780 A781 G782 G783 A787 U788 G803 C804 U805 C810 A817 U825 G828 G829 U830 A831 G832 G843 A844 A845 U846
A847 C848 C849 A850 C854 G855 G856 C857 G862 C863 G873 C874 U875 A876 C877 G878 G879 G880 G881 U882 C883 A884 C887 G888 G889 A890 U893 A894 C895 G896 A897 A898 A899 C900 U904 A908 A909 C912 A916 G929 U930 A938 A942 G943 A944 C945 U952
U955 A956 A957 C958 C961 A970 G971 A976 A977 A978 C979 A980 A981 G990 C991 C992 A993 A997 A998 C1004 U1009 C1010 G1023 A1024 A1025 A1026 C1027 G1028 A1029 U1030 G1031 U1032 A1036 A1037 G1038 G1039 C1040 A1041 U1042 A1043 G1044 A1045 C1048 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 C1106 G1107 A1108 G1109 U1110 C1111 G1112 G1113
U1129 A1130 A1131 C1132 A1140 G1149 G1164 U1165 A1166 U1167 U1170 U1171 U1172 G1173 U1176 A1177 C1178 G1179 U1183 U1193 U1194 A1199 A1200 G1201 U1226 G1227 G1230 G1231 A1242 G1245 A1248 G1251 G1259 A1260 G1261 A1267 G1276 U1277 G1278 A1296 G1304
G1305 G1306 U1307 U1308 C1309 C1310 A1311 G1312 U1324 G1336 C1340 A1348 A1349 G1355 G1356 C1357 A1360 A1361 A1362 G1363 G1364 C1365 G1366 A1373 U1374 G1375 A1378 A1381 U1382 A1387 A1388 U1389 A1390 C1393 A1408 A1409 U1410 G1411 C1412 G1413 A1414 U1415 C1423 G1424 G1425 A1426 G1427
A1428 A1429 G1430 G1431 C1432 U1433 A1434 A1435 A1436 U1437 C1438 C1441 C1442 G1447 U1448 U1449 U1453 G1454 U1455 C1456 G1462 A1463 A1464 A1465 G1470 U1471 A1472 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 U1519 A1520 C1521 C1522 A1523 A1524 G1525 C1526 U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 A1536 C1537 A1538 G1539 C1540 G1541 A1542 A1543 G1544 U1545 U1549 G1550 A1564 G1565 G1566 A1567 A1568 A1569 A1570 U1576 A1577 A1578 U1581 U1582 C1583 A1584 G1585 U1586

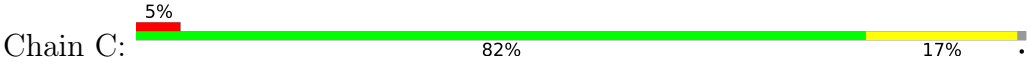


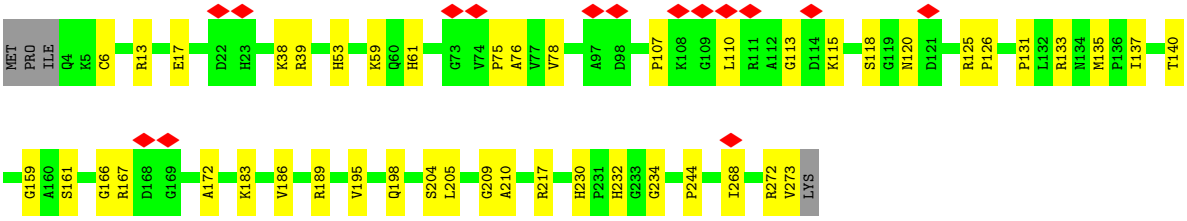
• Molecule 6: 5s ribosomal RNA

Chain B:

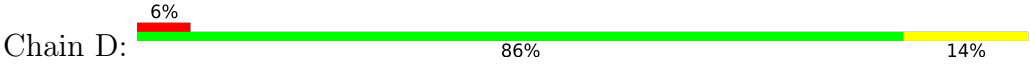


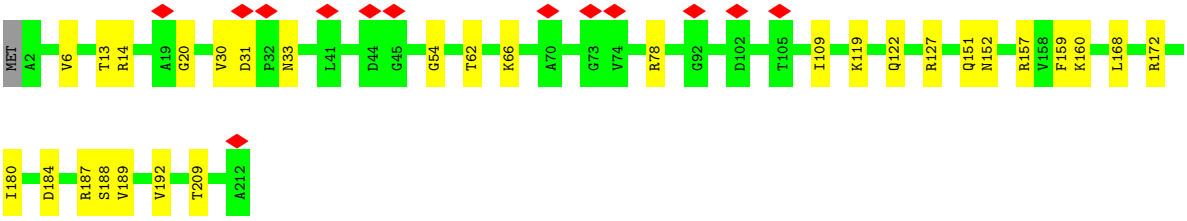
• Molecule 7: 50S ribosomal protein L2



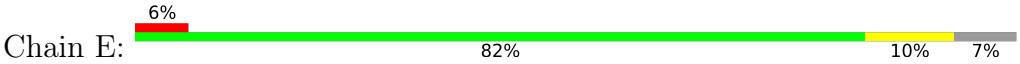


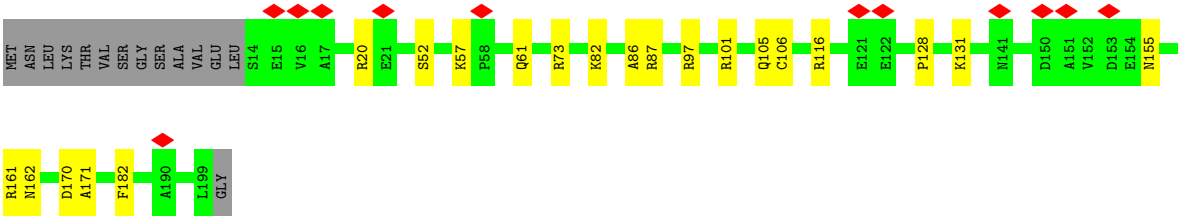
• Molecule 8: 50S ribosomal protein L3



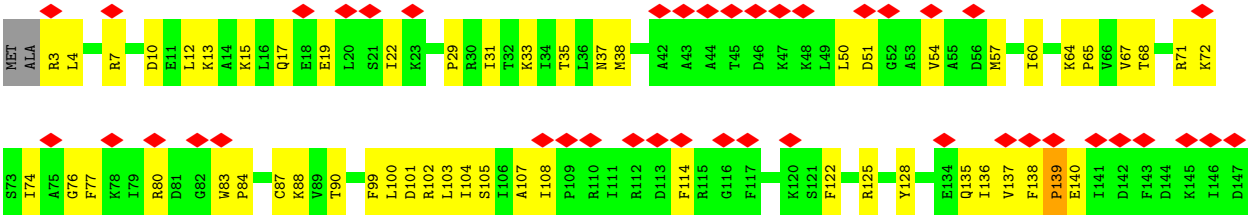


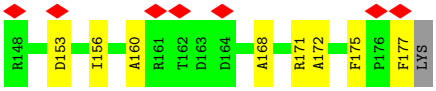
• Molecule 9: 50S ribosomal protein L4



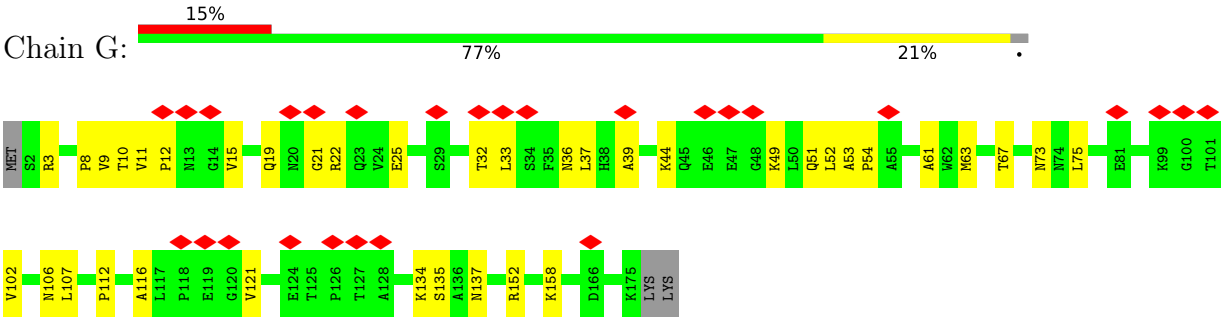


• Molecule 10: 50S ribosomal protein L5

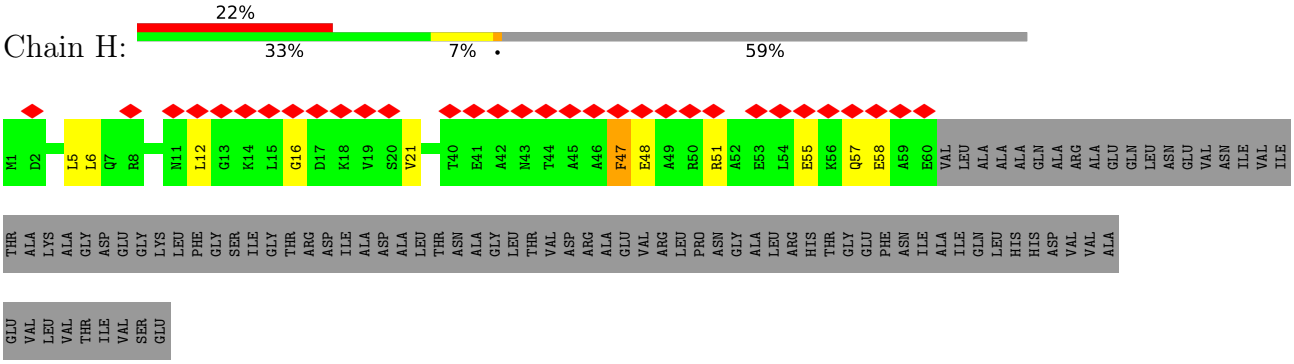




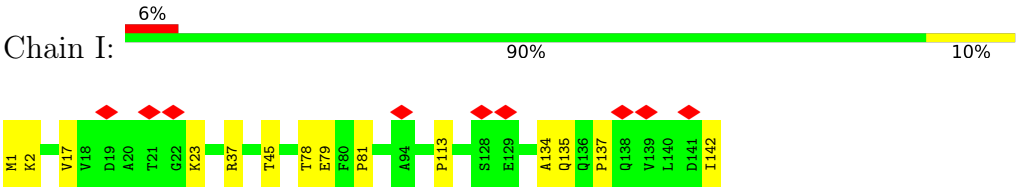
• Molecule 11: 50S ribosomal protein L6



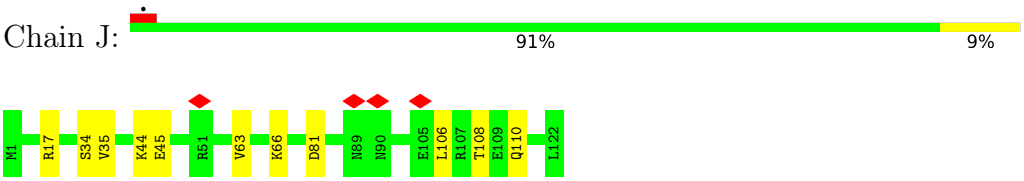
• Molecule 12: 50S ribosomal protein L9



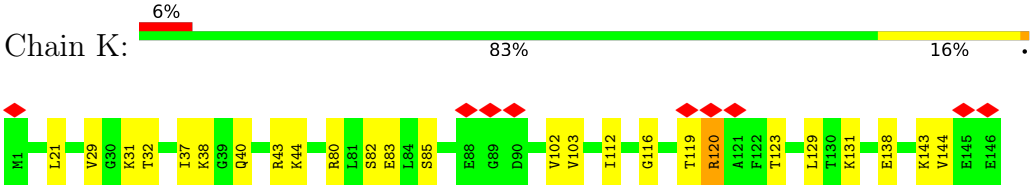
• Molecule 13: 50S ribosomal protein L13



• Molecule 14: 50S ribosomal protein L14

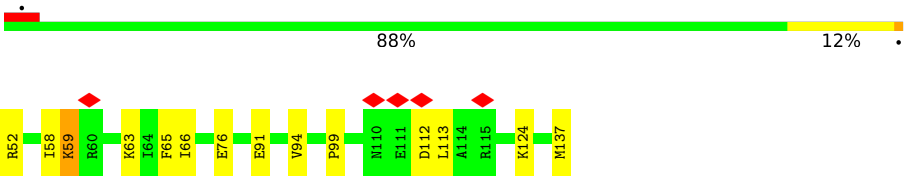


• Molecule 15: 50S ribosomal protein L15



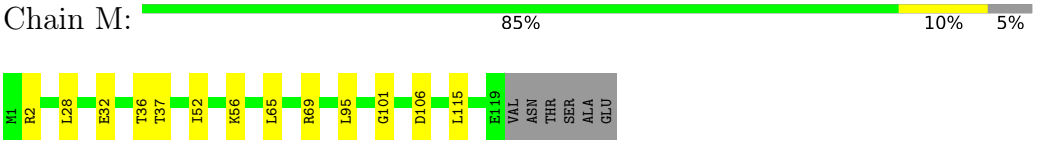
• Molecule 16: 50S ribosomal protein L16

Chain L:



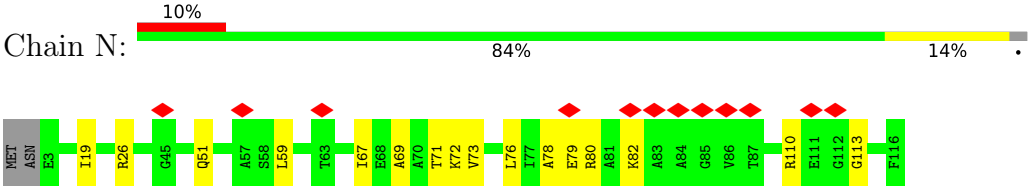
• Molecule 17: 50S ribosomal protein L17

Chain M:



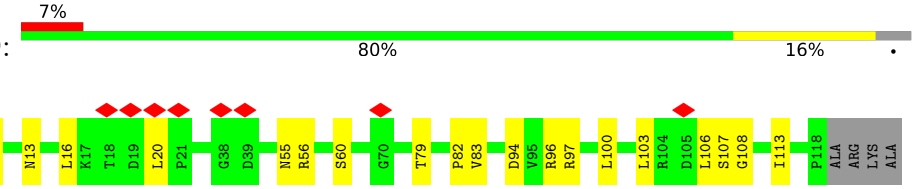
• Molecule 18: 50S ribosomal protein L18

Chain N:



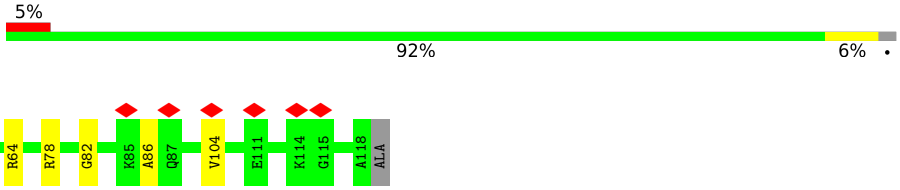
• Molecule 19: 50S ribosomal protein L19

Chain O:



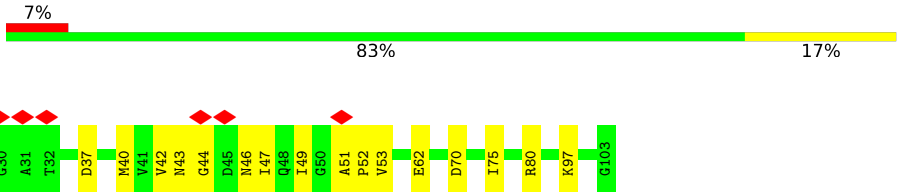
• Molecule 20: 50S ribosomal protein L20

Chain P:



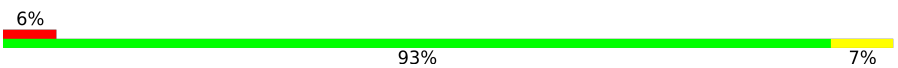
• Molecule 21: 50S ribosomal protein L21

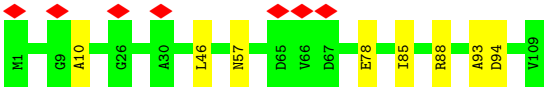
Chain Q:



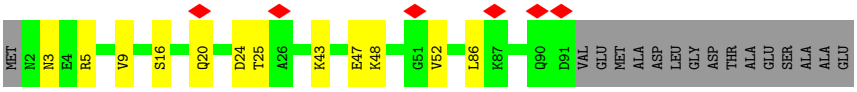
• Molecule 22: 50S ribosomal protein L22

Chain R:

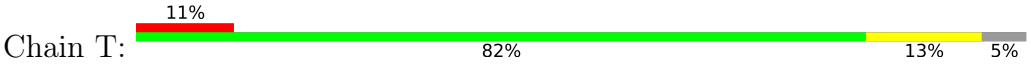


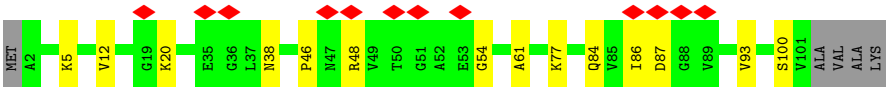


• Molecule 23: 50S ribosomal protein L23

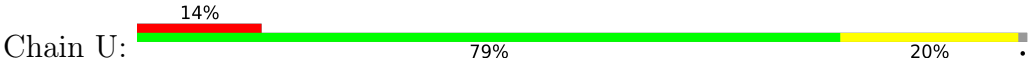


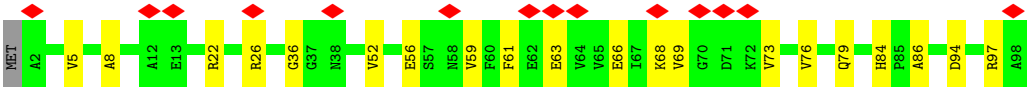
• Molecule 24: 50S ribosomal protein L24



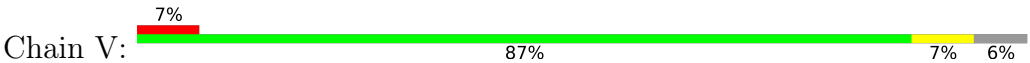


• Molecule 25: 50S ribosomal protein L25

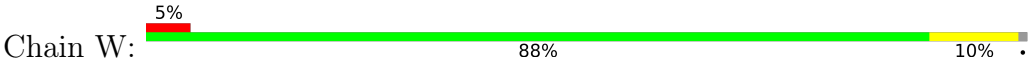


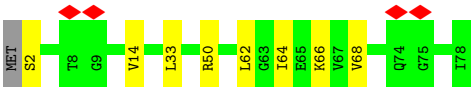


• Molecule 26: 50S ribosomal protein L27

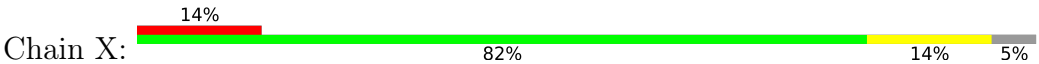


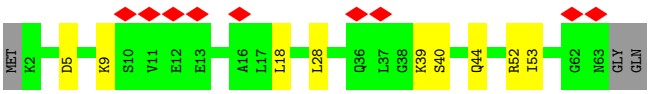
• Molecule 27: 50S ribosomal protein L28





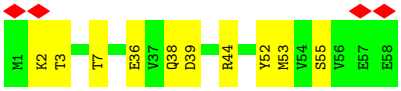
• Molecule 28: 50S ribosomal protein L29





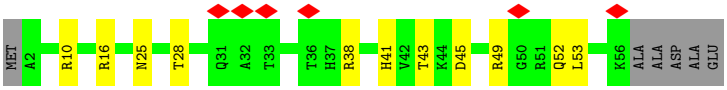
• Molecule 29: 50S ribosomal protein L30

Chain Y:



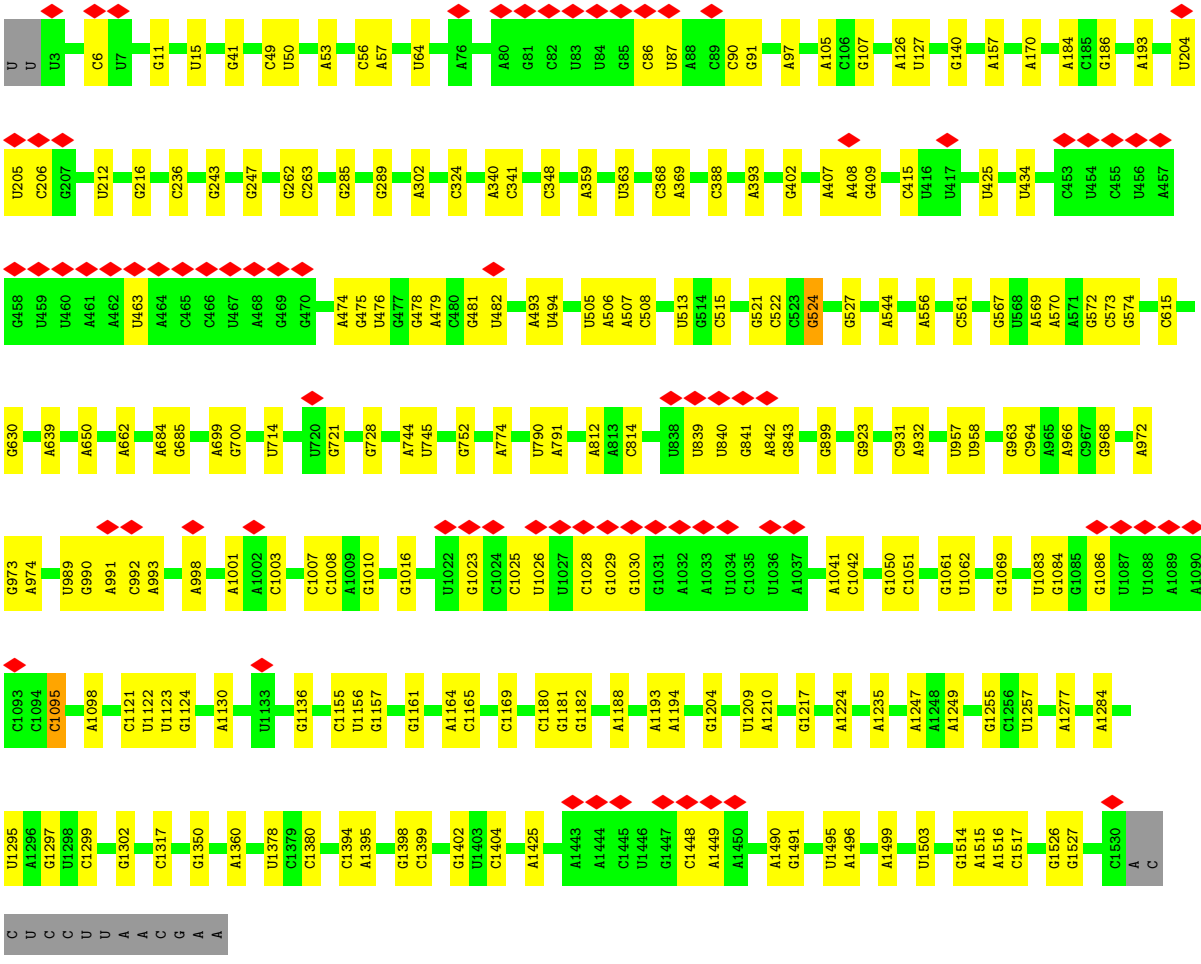
• Molecule 30: 50S ribosomal protein L32

Chain Z:



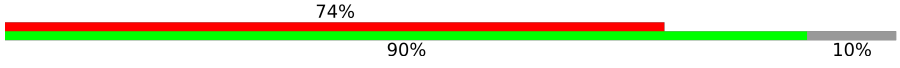
• Molecule 31: 16s Ribosomal RNA

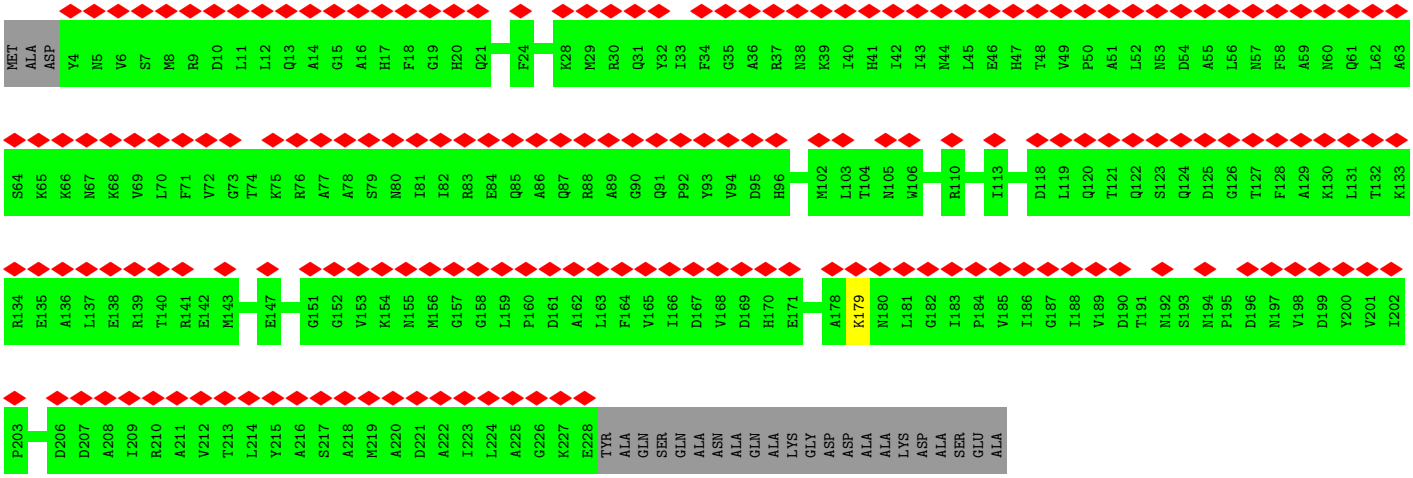
Chain sN1:



• Molecule 32: 30S ribosomal protein S2

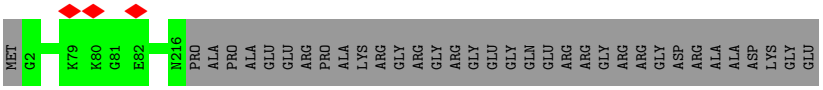
Chain b:





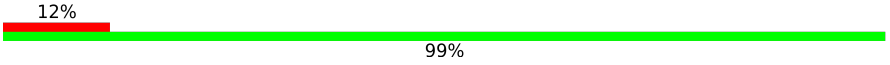
• Molecule 33: 30S ribosomal protein S3

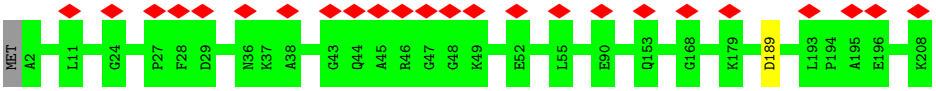
Chain c:



• Molecule 34: 30S ribosomal protein S4

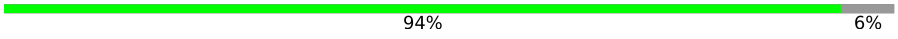
Chain d:

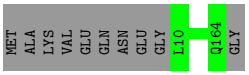




• Molecule 35: 30S ribosomal protein S5

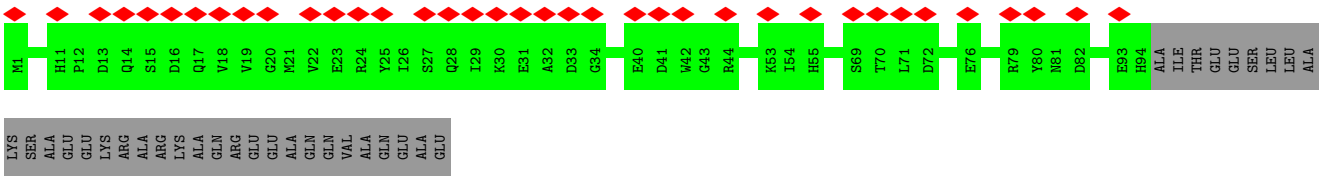
Chain e:





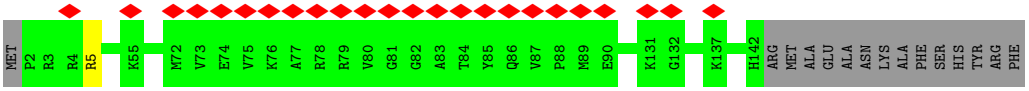
• Molecule 36: 30S ribosomal protein S6

Chain f:



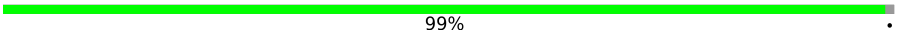
• Molecule 37: 30S ribosomal protein S7

Chain g:



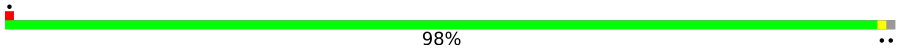
• Molecule 38: 30S ribosomal protein S8

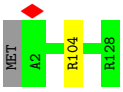
Chain h:



• Molecule 39: 30S ribosomal protein S9

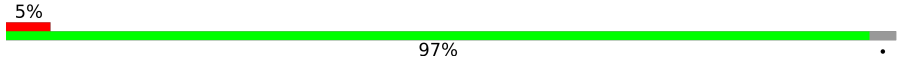
Chain i:

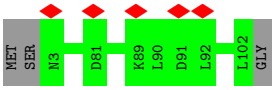




• Molecule 40: 30S ribosomal protein S10

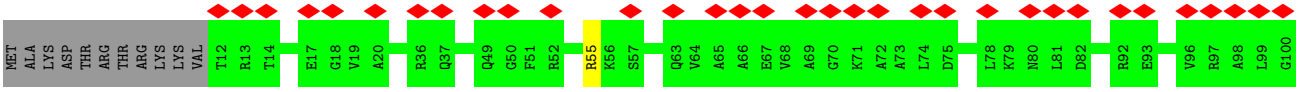
Chain j:

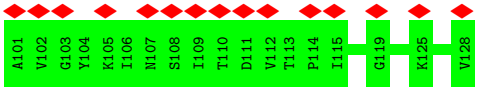




• Molecule 41: 30S ribosomal protein S11

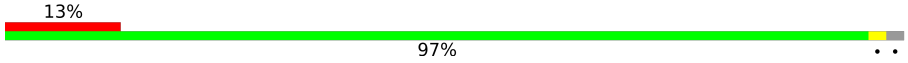
Chain k:

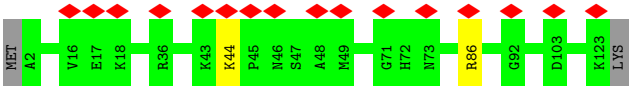




• Molecule 42: 30S ribosomal protein S12

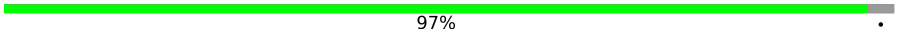
Chain l:

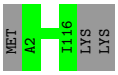




• Molecule 43: 30S ribosomal protein S13

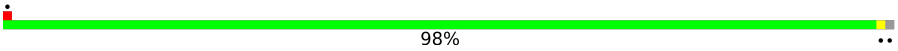
Chain m:

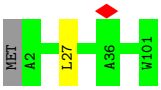




• Molecule 44: 30S ribosomal protein S14

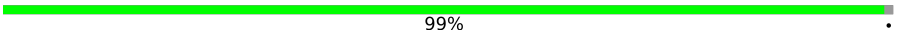
Chain n:





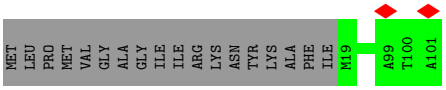
• Molecule 45: 30S ribosomal protein S15

Chain o:



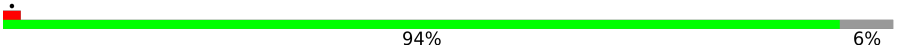
• Molecule 46: 30S ribosomal protein S16

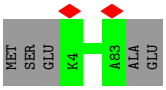
Chain p:



• Molecule 47: 30S ribosomal protein S17

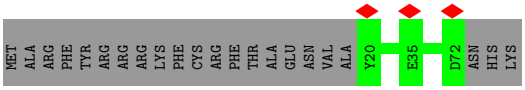
Chain q:





• Molecule 48: 30S ribosomal protein S18

Chain r:

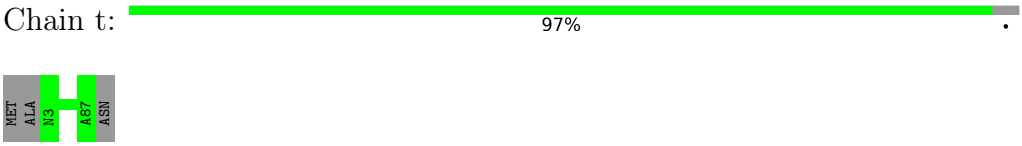


• Molecule 49: 30S ribosomal protein S19

Chain s:

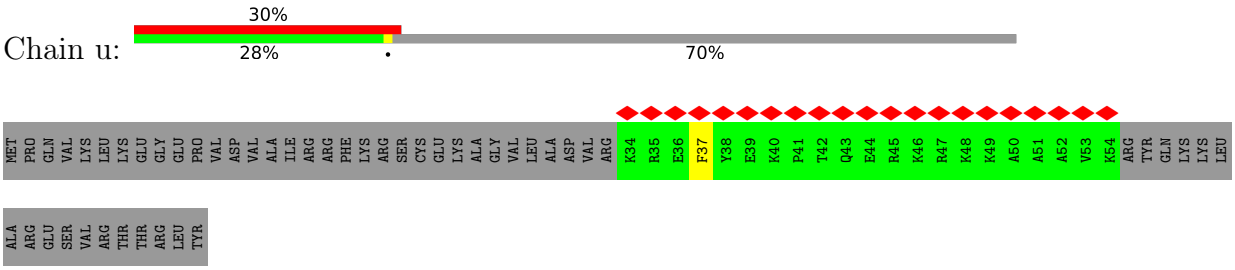
• Molecule 50: 30S ribosomal protein S20

Chain t:



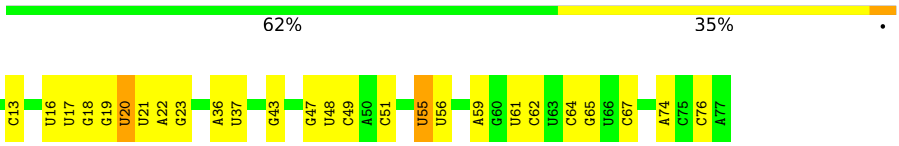
• Molecule 51: 30S ribosomal protein S21

Chain u:



• Molecule 52: tRNA-met

Chain v:



• Molecule 53: mRNA

Chain w:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90845	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	7.935	Depositor
Minimum map value	-2.795	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.45	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 7MG, PSU, OMG, ZN, OMU, UR3, MG, 2MG, 2MA, 4SU, 5MC, MA6, 6MZ, 5MU, 3TD, NA, H2U

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	0.24	0/434	0.40	0/573
2	1	0.23	0/367	0.39	0/481
3	2	0.24	0/515	0.55	1/678 (0.1%)
4	3	0.23	0/296	0.48	0/389
5	AN1	0.22	0/69101	0.77	19/107780 (0.0%)
6	B	0.19	0/2739	0.77	0/4266
7	C	0.24	0/2136	0.43	0/2869
8	D	0.24	0/1590	0.45	0/2142
9	E	0.24	0/1440	0.40	0/1944
10	F	0.26	0/1401	0.49	0/1877
11	G	0.25	0/1337	0.43	0/1807
12	H	0.25	0/461	0.51	0/616
13	I	0.25	0/1151	0.41	0/1551
14	J	0.24	0/956	0.44	0/1286
15	K	0.25	0/1097	0.44	0/1461
16	L	0.24	0/1104	0.44	0/1475
17	M	0.24	0/956	0.41	0/1282
18	N	0.24	0/865	0.46	0/1156
19	O	0.24	0/931	0.43	0/1249
20	P	0.25	0/947	0.34	0/1262
21	Q	0.23	0/818	0.45	0/1094
22	R	0.24	0/831	0.40	0/1113
23	S	0.25	0/708	0.41	0/947
24	T	0.24	0/753	0.48	0/1010
25	U	0.24	0/770	0.41	0/1036
26	V	0.25	0/606	0.44	0/810
27	W	0.22	0/642	0.41	0/856
28	X	0.24	0/499	0.39	0/662
29	Y	0.23	0/468	0.41	0/624
30	Z	0.22	0/462	0.41	0/615
31	sN1	0.19	0/36476	0.75	5/56895 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.26	0/1799	0.49	0/2429
33	c	0.23	0/1714	0.42	0/2304
34	d	0.24	0/1653	0.41	0/2213
35	e	0.24	0/1141	0.43	0/1537
36	f	0.24	0/808	0.47	0/1089
37	g	0.23	0/1127	0.40	0/1511
38	h	0.24	0/993	0.41	0/1331
39	i	0.24	0/1006	0.41	0/1346
40	j	0.23	0/811	0.42	0/1096
41	k	0.24	0/878	0.43	0/1189
42	l	0.23	0/958	0.46	0/1284
43	m	0.23	0/913	0.41	0/1226
44	n	0.24	0/803	0.38	0/1071
45	o	0.23	0/715	0.35	0/958
46	p	0.24	0/660	0.41	0/886
47	q	0.22	0/637	0.43	0/858
48	r	0.24	0/445	0.39	0/601
49	s	0.23	0/664	0.40	0/897
50	t	0.24	0/664	0.34	0/885
51	u	0.30	0/184	0.51	0/240
52	v	0.18	0/1739	0.76	0/2709
53	w	0.23	0/72	0.94	0/110
All	All	0.22	0/153241	0.69	25/229576 (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
51	u	0	1
All	All	0	3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AN1	1308	U	C2-N1-C1'	7.42	126.61	117.70
31	sN1	415	C	N3-C2-O2	-7.38	116.73	121.90
31	sN1	1095	C	N1-C2-O2	7.08	123.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2	32	LEU	CA-CB-CG	6.96	131.31	115.30
31	sN1	1095	C	N3-C2-O2	-6.58	117.29	121.90
5	AN1	788	U	C2-N1-C1'	6.53	125.53	117.70
5	AN1	1308	U	N1-C2-O2	6.43	127.30	122.80
5	AN1	2170	C	N1-C2-O2	6.37	122.72	118.90
5	AN1	2116	G	N1-C6-O6	-6.17	116.20	119.90
5	AN1	1603	C	N3-C2-O2	-6.01	117.69	121.90
5	AN1	1308	U	N3-C2-O2	-5.87	118.09	122.20
5	AN1	2473	U	C2-N1-C1'	5.86	124.73	117.70
5	AN1	788	U	N1-C2-O2	5.64	126.75	122.80
5	AN1	715	C	N1-C2-O2	5.56	122.23	118.90
5	AN1	2170	C	N3-C2-O2	-5.55	118.02	121.90
5	AN1	912	C	C2-N1-C1'	5.53	124.89	118.80
5	AN1	715	C	C2-N1-C1'	5.47	124.82	118.80
5	AN1	1889	C	N3-C2-O2	-5.46	118.08	121.90
5	AN1	1603	C	N1-C2-O2	5.45	122.17	118.90
5	AN1	979	C	C2-N1-C1'	5.33	124.66	118.80
31	sN1	1122	U	C2-N1-C1'	5.30	124.07	117.70
5	AN1	368	C	OP2-P-O3'	5.23	116.70	105.20
31	sN1	1155	C	C2-N1-C1'	5.16	124.48	118.80
5	AN1	2803	U	C2-N1-C1'	5.03	123.73	117.70
5	AN1	788	U	N3-C2-O2	-5.02	118.68	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	HIS	Peptide
12	H	47	PHE	Peptide
51	u	37	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	3	0
2	1	363	0	401	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	509	0	566	9	0
4	3	295	0	327	5	0
5	AN1	62023	0	31193	492	0
6	B	2450	0	1241	34	0
7	C	2096	0	2157	32	0
8	D	1572	0	1610	22	0
9	E	1419	0	1464	17	0
10	F	1381	0	1433	53	0
11	G	1318	0	1373	26	0
12	H	458	0	480	9	0
13	I	1125	0	1148	12	0
14	J	946	0	1007	6	0
15	K	1089	0	1159	15	0
16	L	1087	0	1162	10	0
17	M	942	0	987	8	0
18	N	857	0	899	12	0
19	O	919	0	973	14	0
20	P	934	0	997	6	0
21	Q	807	0	842	13	0
22	R	826	0	894	6	0
23	S	702	0	756	6	0
24	T	749	0	797	8	0
25	U	760	0	783	13	0
26	V	598	0	600	3	0
27	W	632	0	667	5	0
28	X	498	0	537	5	0
29	Y	463	0	488	7	0
30	Z	456	0	448	10	0
31	sN1	32782	0	16506	0	0
32	b	1769	0	1787	0	0
33	c	1690	0	1774	0	0
34	d	1631	0	1691	0	0
35	e	1129	0	1174	0	0
36	f	793	0	788	0	0
37	g	1111	0	1163	0	0
38	h	985	0	1047	0	0
39	i	995	0	1053	0	0
40	j	801	0	832	0	0
41	k	862	0	877	0	0
42	l	945	0	996	0	0
43	m	903	0	962	0	0
44	n	792	0	833	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	o	705	0	712	0	0
46	p	649	0	660	0	0
47	q	630	0	678	0	0
48	r	438	0	456	0	0
49	s	646	0	663	0	0
50	t	658	0	710	0	0
51	u	182	0	198	0	0
52	v	1636	0	832	0	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	AN1	49	0	0	0	0
55	sN1	44	0	0	0	0
56	AN1	1	0	0	0	0
57	AN1	319	0	0	1	0
57	B	4	0	0	0	0
57	C	5	0	0	0	0
57	D	3	0	0	0	0
57	E	3	0	0	0	0
57	K	3	0	0	0	0
57	O	1	0	0	0	0
57	P	3	0	0	0	0
57	Q	1	0	0	0	0
57	U	1	0	0	0	0
57	i	5	0	0	0	0
57	j	2	0	0	0	0
57	m	1	0	0	0	0
57	o	1	0	0	0	0
57	p	1	0	0	0	0
57	q	2	0	0	0	0
57	sN1	163	0	0	0	0
57	t	2	0	0	0	0
All	All	142113	0	94276	786	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 (786) 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	1.45	1.15
5:AN1:1463:A:N7	5:AN1:1544:G:O6	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:70:G:H21	6:B:101:A:H62	1.00	0.93
6:B:70:G:N2	6:B:101:A:H62	1.70	0.89
6:B:2:C:O2	6:B:113:G:N2	2.06	0.89
6:B:70:G:H21	6:B:101:A:N6	1.76	0.84
3:2:30:HIS:O	3:2:32:LEU:N	2.12	0.82
5:AN1:1462:G:O6	5:AN1:1543:A:H2	1.61	0.82
5:AN1:1846:G:N2	5:AN1:1888:C:O2	2.14	0.79
5:AN1:1523:A:N6	5:AN1:1541:G:C2	2.50	0.79
15:K:85:SER:OG	15:K:120:ARG:NH1	2.15	0.79
6:B:18:G:N1	6:B:61:C:N3	2.31	0.79
5:AN1:2311:C:HO2'	5:AN1:2312:G:H8	1.30	0.79
5:AN1:1523:A:N6	5:AN1:1541:G:N2	2.30	0.78
5:AN1:2112:G:O6	5:AN1:2166:A:N6	2.16	0.78
5:AN1:843:G:O2'	5:AN1:845:A:N7	2.18	0.77
5:AN1:873:G:N1	5:AN1:900:C:N3	2.29	0.77
5:AN1:873:G:N2	5:AN1:900:C:O2	2.16	0.77
5:AN1:1595:A:H5"	5:AN1:1596:A:H5'	1.65	0.76
5:AN1:1462:G:O6	5:AN1:1543:A:C2	2.39	0.76
5:AN1:1523:A:C6	5:AN1:1541:G:N2	2.54	0.75
5:AN1:52:G:H5"	5:AN1:53:G:H5'	1.70	0.74
6:B:18:G:N2	6:B:61:C:O2	2.16	0.73
5:AN1:879:G:O6	5:AN1:893:U:O2	2.08	0.72
5:AN1:1036:A:H61	5:AN1:1113:G:H1	1.37	0.71
5:AN1:34:G:N2	5:AN1:511:G:O2'	2.23	0.71
5:AN1:2804:A:O2'	5:AN1:2886:G:O6	2.09	0.71
8:D:6:VAL:H	8:D:33:ASN:HD21	1.39	0.71
3:2:24:LYS:NZ	3:2:46:CYS:SG	2.64	0.71
18:N:73:VAL:HA	18:N:76:LEU:HD23	1.72	0.71
11:G:11:VAL:HG13	11:G:15:VAL:HB	1.73	0.71
6:B:2:C:N3	6:B:113:G:N1	2.36	0.70
19:O:20:LEU:HD13	19:O:79:THR:HG22	1.73	0.70
5:AN1:875:U:O2	5:AN1:898:A:N7	2.25	0.69
5:AN1:1528:G:O2'	5:AN1:1536:A:N1	2.24	0.69
7:C:75:PRO:HB2	7:C:115:LYS:HD2	1.74	0.69
5:AN1:829:G:O2'	15:K:40:GLN:NE2	2.25	0.69
5:AN1:711:G:H8	5:AN1:716:A:H62	1.39	0.69
5:AN1:1463:A:C5	5:AN1:1544:G:O6	2.46	0.69
5:AN1:1533:U:N3	5:AN1:1534:G:N3	2.41	0.69
5:AN1:2372:A:N3	18:N:110:ARG:NH1	2.40	0.69
7:C:118:SER:OG	7:C:189:ARG:NH2	2.25	0.69
10:F:99:PHE:HD1	10:F:102:ARG:HH11	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2104:U:O2	5:AN1:2177:G:N2	2.27	0.68
5:AN1:2647:C:O2	5:AN1:2665:G:N2	2.19	0.68
5:AN1:2096:G:H1	5:AN1:2185:U:H3	0.78	0.68
5:AN1:293:U:H3	5:AN1:351:G:H1	1.41	0.68
9:E:20:ARG:NH1	9:E:106:CYS:SG	2.67	0.68
20:P:104:VAL:HG12	21:Q:47:ILE:HD11	1.76	0.68
5:AN1:322:G:N7	9:E:131:LYS:NZ	2.42	0.67
5:AN1:2159:U:OP1	5:AN1:2161:C:N4	2.27	0.67
5:AN1:342:A:O2'	9:E:161:ARG:NH1	2.27	0.67
5:AN1:1862:A:H61	5:AN1:1871:G:H2'	1.59	0.66
2:1:24:THR:HG23	2:1:27:GLY:H	1.61	0.66
5:AN1:364:A:OP2	5:AN1:424:G:O2'	2.13	0.66
10:F:57:MET:HA	10:F:60:ILE:HG12	1.76	0.66
5:AN1:1749:G:N2	5:AN1:1752:G:OP2	2.28	0.65
7:C:230:HIS:HD2	7:C:232:HIS:H	1.43	0.65
25:U:59:VAL:HG12	25:U:63:GLU:HG2	1.78	0.65
5:AN1:2879:A:OP2	30:Z:49:ARG:NH1	2.30	0.65
5:AN1:195:G:H5'	27:W:14:VAL:HG21	1.77	0.65
5:AN1:1041:A:O2'	5:AN1:1108:A:N6	2.30	0.65
7:C:6:CYS:SG	7:C:13:ARG:NH2	2.69	0.65
5:AN1:2130:A:H62	5:AN1:2153:G:H4'	1.62	0.65
5:AN1:2787:A:HO2'	5:AN1:2788:G:H8	1.41	0.65
5:AN1:2111:G:H4'	5:AN1:2113:A:H62	1.62	0.64
9:E:86:ALA:O	9:E:87:ARG:NH1	2.31	0.64
5:AN1:1816:U:O4	7:C:198:GLN:NE2	2.30	0.64
5:AN1:879:G:H2'	5:AN1:880:G:H8	1.62	0.64
5:AN1:1045:A:H61	11:G:3:ARG:HH12	1.43	0.64
7:C:38:LYS:NZ	7:C:39:ARG:O	2.31	0.64
5:AN1:1647:G:O2'	17:M:106:ASP:OD2	2.15	0.64
5:AN1:1413:G:N2	5:AN1:1577:A:OP2	2.29	0.64
5:AN1:474:C:O2	5:AN1:478:A:N6	2.31	0.63
5:AN1:1522:C:N4	5:AN1:1541:G:H22	1.97	0.63
9:E:97:ARG:HD3	9:E:101:ARG:HH21	1.62	0.63
5:AN1:198:A:H3'	5:AN1:199:G:H21	1.64	0.63
5:AN1:846:U:H2'	5:AN1:847:A:H8	1.63	0.63
14:J:66:LYS:HE2	14:J:81:ASP:HA	1.79	0.63
5:AN1:1311:A:H2'	5:AN1:1312:G:H8	1.64	0.63
5:AN1:1463:A:N7	5:AN1:1544:G:C6	2.67	0.62
8:D:20:GLY:HA2	19:O:82:PRO:HD2	1.82	0.62
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.80	0.62
18:N:59:LEU:HD21	18:N:72:LYS:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:40:C:OP1	10:F:64:LYS:NZ	2.33	0.62
5:AN1:70:A:H61	5:AN1:98:A:H61	1.47	0.62
5:AN1:410:G:OP2	5:AN1:2402:U:O2'	2.18	0.62
5:AN1:1865:G:O2'	5:AN1:1868:A:N6	2.34	0.61
5:AN1:527:A:H5'	13:I:113:PRO:HG3	1.82	0.61
11:G:33:LEU:HB2	11:G:75:LEU:HD11	1.81	0.61
3:2:30:HIS:O	3:2:32:LEU:HD22	2.00	0.61
11:G:21:GLY:O	11:G:22:ARG:NH2	2.33	0.61
4:3:18:ARG:HE	4:3:21:GLY:HA2	1.66	0.61
5:AN1:673:A:OP1	9:E:57:LYS:NZ	2.34	0.60
24:T:84:GLN:HE22	24:T:86:ILE:HD11	1.65	0.60
6:B:108:C:H2'	6:B:109:G:H8	1.66	0.60
5:AN1:280:A:H2	5:AN1:364:A:H62	1.47	0.60
10:F:103:LEU:O	10:F:107:ALA:HB2	2.01	0.60
15:K:80:ARG:HB2	15:K:83:GLU:HG3	1.83	0.60
5:AN1:93:G:HO2'	5:AN1:111:U:HO2'	1.47	0.60
5:AN1:1775:U:OP2	5:AN1:1780:A:N6	2.29	0.60
5:AN1:168:A:H3'	5:AN1:169:U:H5"	1.83	0.60
5:AN1:1462:G:H1	5:AN1:1520:A:H61	0.69	0.60
5:AN1:2109:U:O4	5:AN1:2163:U:O2'	2.20	0.60
5:AN1:879:G:N2	5:AN1:893:U:O2'	2.31	0.59
10:F:83:TRP:CE3	10:F:84:PRO:HD2	2.38	0.59
10:F:136:ILE:HG13	10:F:138:PHE:HD1	1.67	0.59
29:Y:39:ASP:OD1	29:Y:44:ARG:NH1	2.33	0.59
5:AN1:167:A:N3	5:AN1:2204:C:O2'	2.35	0.59
5:AN1:1870:C:H3'	5:AN1:1871:G:H4'	1.84	0.59
5:AN1:2123:G:N2	5:AN1:2158:G:O6	2.36	0.59
30:Z:43:THR:HG22	30:Z:45:ASP:H	1.66	0.59
6:B:18:G:O6	6:B:61:C:N4	2.35	0.59
7:C:137:ILE:HD12	7:C:166:GLY:HA2	1.85	0.59
5:AN1:1053:G:H21	5:AN1:1101:C:H41	1.51	0.59
5:AN1:2591:G:N2	5:AN1:2594:A:OP2	2.32	0.59
6:B:12:U:OP2	6:B:68:C:O2'	2.21	0.58
11:G:9:VAL:HG21	11:G:73:ASN:HA	1.84	0.58
26:V:11:LYS:O	26:V:14:ARG:NH1	2.33	0.58
5:AN1:2096:G:O6	5:AN1:2185:U:O4	2.21	0.58
5:AN1:2077:C:H2'	5:AN1:2078:A:H8	1.69	0.58
5:AN1:862:G:H2'	5:AN1:863:C:C6	2.39	0.58
5:AN1:579:C:H2'	5:AN1:580:A:C8	2.39	0.58
5:AN1:2151:U:OP2	5:AN1:2153:G:N2	2.36	0.58
5:AN1:2324:A:H2'	5:AN1:2325:A:C8	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2861:U:OP2	5:AN1:2862:G:O2'	2.21	0.58
3:2:31:ILE:O	3:2:33:THR:N	2.36	0.58
5:AN1:877:G:H2'	5:AN1:878:G:C8	2.38	0.58
12:H:47:PHE:O	12:H:51:ARG:HB3	2.03	0.58
18:N:73:VAL:HA	18:N:76:LEU:CD2	2.34	0.58
5:AN1:1535:U:H2'	5:AN1:1536:A:H8	1.69	0.57
5:AN1:2225:U:H2'	5:AN1:2226:G:H8	1.68	0.57
7:C:115:LYS:O	7:C:125:ARG:NH2	2.36	0.57
16:L:43:THR:HG22	16:L:94:VAL:HG12	1.86	0.57
24:T:86:ILE:HG22	24:T:87:ASP:H	1.68	0.57
5:AN1:2570:G:H1'	8:D:151:GLN:HG3	1.86	0.57
5:AN1:2309:C:O4'	10:F:37:ASN:ND2	2.37	0.57
5:AN1:2647:C:N3	5:AN1:2665:G:N1	2.34	0.57
5:AN1:1306:G:OP2	5:AN1:1306:G:N2	2.34	0.57
5:AN1:878:G:H2'	5:AN1:879:G:H8	1.70	0.57
10:F:83:TRP:HE3	10:F:84:PRO:HD2	1.69	0.57
25:U:68:LYS:HG3	25:U:73:VAL:HG12	1.87	0.57
5:AN1:1111:C:H2'	5:AN1:1112:G:C8	2.39	0.57
5:AN1:579:C:H2'	5:AN1:580:A:H8	1.70	0.57
5:AN1:2242:G:H2'	5:AN1:2243:A:H8	1.70	0.56
5:AN1:1361:A:OP1	27:W:2:SER:OG	2.21	0.56
5:AN1:1111:C:H2'	5:AN1:1112:G:H8	1.70	0.56
21:Q:70:ASP:OD2	21:Q:70:ASP:N	2.38	0.56
5:AN1:1535:U:H2'	5:AN1:1536:A:C8	2.41	0.56
5:AN1:148:A:N6	5:AN1:1593:G:O2'	2.24	0.56
5:AN1:2310:A:H4'	10:F:33:LYS:NZ	2.21	0.56
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.87	0.56
25:U:84:HIS:HD2	25:U:86:ALA:H	1.53	0.56
5:AN1:877:G:H2'	5:AN1:878:G:H8	1.71	0.56
5:AN1:1430:G:H2'	5:AN1:1431:G:C8	2.41	0.56
5:AN1:84:U:OP1	28:X:52:ARG:NH2	2.38	0.56
5:AN1:1052:G:H1'	5:AN1:1082:A:H2	1.71	0.56
6:B:64:A:N6	6:B:105:C:H2'	2.21	0.56
16:L:20:LEU:HD23	16:L:99:PRO:HG2	1.87	0.56
5:AN1:520:U:H2'	5:AN1:521:G:H8	1.71	0.56
5:AN1:719:A:H2'	5:AN1:720:A:C8	2.41	0.56
15:K:119:THR:HG22	15:K:120:ARG:HH21	1.69	0.56
5:AN1:2468:G:N2	5:AN1:2469:U:O2'	2.39	0.56
12:H:51:ARG:NH1	12:H:55:GLU:HB3	2.21	0.55
5:AN1:2287:U:H2'	5:AN1:2288:G:C8	2.41	0.55
5:AN1:2310:A:H4'	10:F:33:LYS:HZ1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:28:LEU:HD21	17:M:95:LEU:HD21	1.88	0.55
10:F:33:LYS:HD3	10:F:35:THR:HG23	1.88	0.55
5:AN1:552:U:H2'	5:AN1:553:G:O4'	2.06	0.55
5:AN1:570:A:OP2	21:Q:80:ARG:NH2	2.35	0.55
5:AN1:587:U:H2'	5:AN1:588:A:C8	2.41	0.55
5:AN1:887:C:H3'	5:AN1:888:C:H5"	1.89	0.55
5:AN1:2123:G:H2'	5:AN1:2124:G:C8	2.41	0.55
7:C:183:LYS:HG3	7:C:268:ILE:HD11	1.89	0.55
18:N:51:GLN:O	18:N:80:ARG:NH2	2.36	0.55
5:AN1:1042:U:H4'	5:AN1:1044:G:H1'	1.88	0.55
5:AN1:12:A:H2'	5:AN1:13:A:C8	2.42	0.55
5:AN1:1587:U:H2'	5:AN1:1588:A:H8	1.71	0.55
10:F:138:PHE:HB2	10:F:139:PRO:HD2	1.89	0.55
26:V:66:VAL:HG22	26:V:83:GLU:HB2	1.88	0.55
5:AN1:2743:G:H21	5:AN1:2753:A:H62	1.54	0.54
7:C:140:THR:OG1	7:C:161:SER:OG	2.25	0.54
5:AN1:86:C:H2'	5:AN1:87:G:H8	1.72	0.54
5:AN1:1004:C:OP1	13:I:37:ARG:NH1	2.39	0.54
5:AN1:1750:C:H5	19:O:97:ARG:HH11	1.55	0.54
5:AN1:2130:A:OP2	5:AN1:2152:G:N1	2.41	0.54
25:U:76:VAL:HG12	25:U:97:ARG:HA	1.88	0.54
5:AN1:2212:G:H2'	5:AN1:2213:G:H8	1.71	0.54
10:F:80:ARG:HB2	10:F:83:TRP:HD1	1.72	0.54
15:K:102:VAL:HG23	15:K:103:VAL:HG23	1.88	0.54
28:X:5:ASP:O	28:X:9:LYS:NZ	2.26	0.54
5:AN1:587:U:H2'	5:AN1:588:A:H8	1.73	0.54
5:AN1:876:A:H62	5:AN1:897:A:H2	1.55	0.54
5:AN1:1311:A:H2'	5:AN1:1312:G:C8	2.42	0.54
5:AN1:2311:C:O2'	5:AN1:2312:G:H8	1.91	0.54
5:AN1:2587:C:H2'	5:AN1:2588:G:H8	1.72	0.54
14:J:108:THR:HG22	14:J:110:GLN:H	1.71	0.54
5:AN1:303:C:H5"	5:AN1:336:U:H2'	1.90	0.54
5:AN1:2242:G:H2'	5:AN1:2243:A:C8	2.43	0.54
9:E:170:ASP:OD1	9:E:171:ALA:N	2.40	0.54
5:AN1:184:G:H3'	5:AN1:185:G:H8	1.71	0.54
5:AN1:1310:C:O2'	5:AN1:1387:A:N3	2.38	0.54
5:AN1:2021:C:OP1	8:D:157:ARG:NH2	2.41	0.54
10:F:51:ASP:HA	10:F:54:VAL:HG22	1.89	0.54
5:AN1:353:C:H2'	5:AN1:354:A:H8	1.73	0.54
5:AN1:873:G:O6	5:AN1:900:C:N4	2.31	0.53
18:N:19:ILE:HG21	18:N:26:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:327:G:H2'	5:AN1:328:G:H8	1.73	0.53
5:AN1:1717:G:N2	5:AN1:1734:G:O2'	2.41	0.53
8:D:127:ARG:HG3	8:D:168:LEU:HD13	1.89	0.53
5:AN1:372:U:H2'	5:AN1:373:A:H8	1.74	0.53
5:AN1:1068:G:N3	5:AN1:1086:A:O2'	2.39	0.53
8:D:180:ILE:HD13	8:D:192:VAL:HG22	1.89	0.53
10:F:15:LYS:O	10:F:19:GLU:HB2	2.08	0.53
5:AN1:1567:A:OP1	7:C:61:HIS:NE2	2.34	0.53
5:AN1:1844:A:H5"	5:AN1:1845:G:OP1	2.09	0.53
5:AN1:2107:U:O2	5:AN1:2111:G:N2	2.41	0.53
5:AN1:1679:G:N2	5:AN1:1759:G:OP2	2.33	0.53
11:G:44:LYS:NZ	11:G:53:ALA:O	2.42	0.53
5:AN1:1483:U:O2	5:AN1:1496:G:N2	2.40	0.53
5:AN1:2111:G:O2'	5:AN1:2113:A:N7	2.37	0.53
3:2:6:THR:HG22	3:2:62:PRO:HD2	1.90	0.52
5:AN1:1932:A:H2	5:AN1:1939:U:H3	1.57	0.52
5:AN1:31:G:N2	22:R:78:GLU:OE2	2.36	0.52
5:AN1:1199:A:H4'	5:AN1:1200:A:H5'	1.91	0.52
5:AN1:1472:A:N6	5:AN1:1510:G:O2'	2.43	0.52
5:AN1:1919:U:H2'	5:AN1:1920:C:C6	2.44	0.52
11:G:107:LEU:HB3	11:G:152:ARG:HD3	1.92	0.52
15:K:82:SER:HB3	15:K:116:GLY:HA3	1.92	0.52
7:C:133:ARG:HB3	7:C:186:VAL:HG22	1.92	0.52
7:C:137:ILE:HD11	7:C:167:ARG:HG2	1.91	0.52
10:F:108:ILE:HA	10:F:114:PHE:HZ	1.74	0.52
10:F:138:PHE:O	10:F:140:GLU:N	2.42	0.52
5:AN1:2301:U:C5	10:F:153:ASP:HB2	2.45	0.52
5:AN1:2830:G:H2'	5:AN1:2875:A:H61	1.75	0.52
30:Z:25:ASN:OD1	30:Z:38:ARG:NH2	2.41	0.52
5:AN1:1108:A:H8	5:AN1:1109:G:H4'	1.74	0.52
6:B:27:A:H2'	6:B:28:C:C6	2.45	0.52
10:F:10:ASP:HA	10:F:13:LYS:HG2	1.92	0.52
10:F:54:VAL:HG12	10:F:87:CYS:SG	2.50	0.52
5:AN1:719:A:H2'	5:AN1:720:A:H8	1.72	0.52
5:AN1:1310:C:H2'	5:AN1:1311:A:H8	1.74	0.52
5:AN1:1430:G:H2'	5:AN1:1431:G:H8	1.75	0.52
29:Y:3:THR:OG1	29:Y:36:GLU:OE2	2.26	0.52
23:S:43:LYS:O	23:S:47:GLU:HG2	2.09	0.51
5:AN1:1522:C:H41	5:AN1:1541:G:H22	1.59	0.51
4:3:10:ILE:HD13	4:3:33:HIS:HD2	1.75	0.51
5:AN1:878:G:H2'	5:AN1:879:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1424:G:H2'	5:AN1:1425:G:H8	1.76	0.51
5:AN1:2325:A:H2'	5:AN1:2326:G:C8	2.46	0.51
11:G:63:MET:O	11:G:67:THR:HG23	2.11	0.51
5:AN1:1589:C:H2'	5:AN1:1590:A:H8	1.75	0.51
5:AN1:2753:A:N1	11:G:67:THR:HG21	2.26	0.51
5:AN1:13:A:O2'	13:I:135:GLN:NE2	2.44	0.51
5:AN1:294:U:H3	5:AN1:350:G:H22	1.57	0.51
24:T:93:VAL:HG12	24:T:100:SER:HA	1.92	0.51
5:AN1:2315:U:H2'	5:AN1:2317:G:H1	1.76	0.51
10:F:50:LEU:HD21	10:F:84:PRO:HB2	1.91	0.51
24:T:38:ASN:HB3	24:T:61:ALA:HB3	1.91	0.51
4:3:11:CYS:SG	4:3:13:SER:OG	2.61	0.51
5:AN1:1487:G:H5"	5:AN1:1488:C:H5"	1.93	0.51
5:AN1:2096:G:N2	5:AN1:2185:U:O2	2.33	0.51
10:F:74:ILE:HG22	10:F:76:GLY:H	1.75	0.51
19:O:4:LYS:O	19:O:9:GLN:NE2	2.43	0.51
5:AN1:327:G:H2'	5:AN1:328:G:C8	2.46	0.50
5:AN1:1095:A:H2'	5:AN1:1096:G:H8	1.75	0.50
7:C:78:VAL:O	7:C:113:GLY:N	2.44	0.50
5:AN1:413:C:H2'	5:AN1:414:A:C8	2.47	0.50
5:AN1:1025:A:H2'	5:AN1:1026:A:C8	2.46	0.50
5:AN1:2049:G:H5'	8:D:152:ASN:O	2.12	0.50
6:B:28:C:H2'	6:B:29:C:O4'	2.11	0.50
5:AN1:1767:C:H2'	5:AN1:1768:A:H8	1.76	0.50
5:AN1:2116:G:H5"	5:AN1:2164:G:H22	1.75	0.50
5:AN1:2323:A:H2'	5:AN1:2324:A:C8	2.46	0.50
5:AN1:270:U:O2'	5:AN1:428:A:N3	2.37	0.50
5:AN1:2239:U:H2'	5:AN1:2240:U:C6	2.46	0.50
5:AN1:12:A:H2'	5:AN1:13:A:H8	1.77	0.50
11:G:102:VAL:HG12	11:G:116:ALA:HA	1.93	0.50
5:AN1:70:A:H61	5:AN1:98:A:N6	2.09	0.50
5:AN1:596:U:H2'	5:AN1:597:A:C8	2.46	0.50
5:AN1:1846:G:N1	5:AN1:1888:C:N3	2.44	0.50
21:Q:43:ASN:HB2	21:Q:46:ASN:HB3	1.94	0.50
5:AN1:909:A:H8	5:AN1:2273:G:H21	1.57	0.50
5:AN1:1911:3TD:N1	5:AN1:1938:C:O2	2.42	0.50
7:C:159:GLY:H	7:C:195:VAL:HB	1.76	0.50
29:Y:3:THR:HG22	29:Y:38:GLN:HA	1.94	0.50
5:AN1:1276:G:H2'	5:AN1:1277:U:C6	2.47	0.50
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.94	0.50
5:AN1:881:G:H2'	5:AN1:882:U:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1356:G:H2'	5:AN1:1357:C:C6	2.47	0.50
5:AN1:2654:C:H5"	11:G:158:LYS:HE3	1.94	0.50
5:AN1:2853:G:N1	5:AN1:2856:A:OP2	2.36	0.50
6:B:100:U:O2'	25:U:79:GLN:NE2	2.45	0.50
8:D:62:THR:O	8:D:66:LYS:HG2	2.12	0.50
11:G:25:GLU:OE2	11:G:32:THR:OG1	2.18	0.50
18:N:69:ALA:O	18:N:73:VAL:HG23	2.12	0.50
5:AN1:2070:U:H2'	5:AN1:2071:U:C6	2.47	0.49
5:AN1:2622:C:H2'	5:AN1:2623:G:C8	2.46	0.49
24:T:46:PRO:HB3	24:T:54:GLY:H	1.76	0.49
5:AN1:308:U:H2'	5:AN1:309:G:O4'	2.13	0.49
5:AN1:1583:C:H3'	5:AN1:1584:A:H8	1.78	0.49
5:AN1:2115:A:HO2'	5:AN1:2166:A:HO2'	1.61	0.49
5:AN1:2577:G:N2	5:AN1:2577:G:OP2	2.43	0.49
23:S:24:ASP:OD2	23:S:25:THR:HG23	2.11	0.49
25:U:94:ASP:OD1	25:U:94:ASP:N	2.44	0.49
5:AN1:663:U:H2'	5:AN1:664:A:H8	1.76	0.49
5:AN1:2119:G:H1'	5:AN1:2172:A:C2	2.48	0.49
5:AN1:2594:A:H5"	7:C:234:GLY:HA3	1.93	0.49
10:F:67:VAL:HG12	10:F:84:PRO:HB3	1.95	0.49
10:F:138:PHE:CZ	10:F:140:GLU:HB2	2.48	0.49
22:R:88:ARG:NH1	22:R:94:ASP:OD2	2.41	0.49
5:AN1:753:C:H2'	5:AN1:754:A:H8	1.78	0.49
5:AN1:2067:A:H2'	5:AN1:2068:C:C6	2.47	0.49
5:AN1:2479:C:N3	16:L:124:LYS:NZ	2.53	0.49
5:AN1:1543:A:O2'	5:AN1:1544:G:H5"	2.13	0.49
10:F:3:ARG:CZ	10:F:105:SER:HB3	2.43	0.49
30:Z:52:GLN:NE2	30:Z:53:LEU:O	2.45	0.49
2:1:12:ARG:HH11	2:1:44:VAL:HG21	1.78	0.49
5:AN1:1886:A:H3'	5:AN1:1887:G:H8	1.78	0.49
10:F:64:LYS:HG3	10:F:65:PRO:HD2	1.95	0.49
9:E:97:ARG:HG2	9:E:101:ARG:HE	1.77	0.49
2:1:29:GLN:NE2	5:AN1:217:C:OP1	2.46	0.49
5:AN1:184:G:H3'	5:AN1:185:G:C8	2.48	0.49
10:F:10:ASP:OD2	10:F:13:LYS:NZ	2.45	0.49
10:F:80:ARG:HB2	10:F:83:TRP:CD1	2.47	0.49
20:P:82:GLY:O	20:P:86:ALA:N	2.46	0.49
5:AN1:499:G:N1	5:AN1:502:A:OP2	2.37	0.49
5:AN1:518:C:H2'	5:AN1:519:A:H8	1.77	0.49
5:AN1:520:U:H2'	5:AN1:521:G:C8	2.48	0.49
5:AN1:1462:G:N1	5:AN1:1520:A:N6	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1798:A:H2'	5:AN1:1799:A:C8	2.48	0.49
5:AN1:1908:A:H2	5:AN1:1913:PSU:HN3	1.61	0.49
5:AN1:1478:G:H2'	5:AN1:1479:U:C6	2.48	0.49
5:AN1:2171:C:H2'	5:AN1:2172:A:N7	2.28	0.49
5:AN1:2852:A:H2'	5:AN1:2853:G:O4'	2.12	0.49
13:I:23:LYS:HD3	13:I:142:ILE:HD13	1.94	0.49
5:AN1:2306:A:H2'	5:AN1:2307:A:H5"	1.94	0.48
7:C:230:HIS:CD2	7:C:232:HIS:H	2.27	0.48
12:H:5:LEU:HB2	12:H:16:GLY:HA2	1.94	0.48
5:AN1:701:U:H2'	5:AN1:702:G:O4'	2.13	0.48
5:AN1:844:A:H61	5:AN1:929:C:H1'	1.77	0.48
6:B:101:A:H5'	25:U:79:GLN:HE22	1.78	0.48
10:F:3:ARG:NH1	10:F:101:ASP:O	2.46	0.48
5:AN1:2125:C:H2'	5:AN1:2155:G:H1	1.78	0.48
19:O:56:ARG:O	19:O:60:SER:OG	2.30	0.48
5:AN1:634:G:H5"	15:K:131:LYS:HE2	1.96	0.48
5:AN1:1591:C:H2'	5:AN1:1592:A:C8	2.48	0.48
5:AN1:1767:C:H2'	5:AN1:1768:A:C8	2.48	0.48
5:AN1:2119:G:N2	5:AN1:2120:G:O6	2.46	0.48
10:F:68:THR:OG1	10:F:88:LYS:HG2	2.13	0.48
5:AN1:1591:C:H2'	5:AN1:1592:A:H8	1.79	0.48
10:F:80:ARG:HD3	10:F:83:TRP:HE1	1.78	0.48
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.94	0.48
5:AN1:1356:G:H2'	5:AN1:1357:C:H6	1.78	0.48
5:AN1:2843:U:H2'	5:AN1:2844:G:O4'	2.13	0.48
5:AN1:1373:A:O2'	5:AN1:1375:G:OP2	2.32	0.48
7:C:135:MET:O	7:C:167:ARG:NH1	2.29	0.48
11:G:121:VAL:HG22	11:G:135:SER:HB2	1.95	0.48
17:M:2:ARG:HD2	17:M:2:ARG:O	2.13	0.48
5:AN1:1261:G:OP2	30:Z:16:ARG:NH1	2.47	0.48
5:AN1:176:U:H2'	5:AN1:177:G:H8	1.78	0.48
5:AN1:2082:U:H2'	5:AN1:2083:G:C8	2.49	0.48
12:H:51:ARG:HH12	12:H:55:GLU:HB3	1.78	0.48
5:AN1:462:G:N2	5:AN1:465:A:OP2	2.29	0.47
5:AN1:606:A:H2'	5:AN1:607:A:C8	2.49	0.47
21:Q:42:VAL:HG12	21:Q:44:GLY:H	1.79	0.47
5:AN1:103:U:H2'	5:AN1:104:C:O4'	2.15	0.47
5:AN1:718:U:O2'	5:AN1:719:A:H8	1.97	0.47
5:AN1:2622:C:H2'	5:AN1:2623:G:H8	1.79	0.47
5:AN1:2637:A:H5"	13:I:78:THR:HG21	1.96	0.47
19:O:94:ASP:OD2	19:O:94:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:28:LYS:HD3	3:2:32:LEU:HD11	1.95	0.47
5:AN1:578:U:H2'	5:AN1:579:C:C6	2.49	0.47
5:AN1:2060:C:H2'	5:AN1:2061:C:C6	2.50	0.47
5:AN1:2229:U:H2'	5:AN1:2230:G:C8	2.50	0.47
7:C:167:ARG:HA	7:C:172:ALA:HA	1.97	0.47
5:AN1:86:C:H2'	5:AN1:87:G:C8	2.49	0.47
5:AN1:158:U:H2'	5:AN1:159:G:H8	1.78	0.47
5:AN1:970:A:H5'	5:AN1:1183:U:H1'	1.96	0.47
5:AN1:1348:A:H2'	5:AN1:1349:A:C8	2.50	0.47
5:AN1:2119:G:H1	5:AN1:2169:A:N6	2.12	0.47
5:AN1:413:C:H2'	5:AN1:414:A:H8	1.78	0.47
5:AN1:1193:U:H2'	5:AN1:1194:U:C6	2.49	0.47
15:K:37:ILE:HG22	15:K:38:LYS:H	1.80	0.47
2:1:1:MET:N	5:AN1:1617:G:H21	2.13	0.47
5:AN1:31:G:O2'	22:R:78:GLU:O	2.31	0.47
5:AN1:34:G:H22	5:AN1:511:G:C2'	2.27	0.47
5:AN1:665:U:H2'	5:AN1:666:A:O4'	2.14	0.47
5:AN1:955:U:O2'	6:B:86:U:O4	2.29	0.47
5:AN1:2645:C:H2'	5:AN1:2646:U:H6	1.79	0.47
6:B:29:C:H2'	6:B:30:U:C5	2.50	0.47
7:C:53:HIS:HA	7:C:217:ARG:HB2	1.95	0.47
7:C:120:ASN:HD22	7:C:131:PRO:HG2	1.80	0.47
10:F:29:PRO:HB3	10:F:160:ALA:HB2	1.95	0.47
14:J:34:SER:OG	14:J:35:VAL:N	2.48	0.47
15:K:123:THR:HG22	15:K:143:LYS:HB2	1.97	0.47
5:AN1:678:A:H2'	5:AN1:679:G:C8	2.50	0.47
5:AN1:846:U:H2'	5:AN1:847:A:C8	2.48	0.47
5:AN1:879:G:C6	5:AN1:893:U:O2	2.68	0.47
5:AN1:2563:G:H2'	5:AN1:2564:A:C8	2.49	0.47
6:B:26:C:H2'	6:B:27:A:C8	2.49	0.47
9:E:20:ARG:HE	9:E:105:GLN:HG3	1.79	0.47
10:F:71:ARG:HG3	10:F:72:LYS:HG2	1.95	0.47
5:AN1:537:A:N6	5:AN1:553:G:O2'	2.44	0.47
5:AN1:1437:U:H2'	5:AN1:1438:C:C6	2.49	0.47
5:AN1:2172:A:H2'	5:AN1:2173:C:C6	2.50	0.47
9:E:82:LYS:HE2	9:E:82:LYS:HB3	1.78	0.47
5:AN1:498:U:H2'	5:AN1:499:G:O4'	2.15	0.47
5:AN1:1348:A:H2'	5:AN1:1349:A:H8	1.80	0.47
10:F:4:LEU:HB2	10:F:101:ASP:HB3	1.97	0.47
26:V:37:ILE:HG22	26:V:38:VAL:HG23	1.97	0.47
5:AN1:1538:A:O2'	5:AN1:1539:G:OP1	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2066:A:H2'	5:AN1:2067:A:C8	2.51	0.46
6:B:108:C:O2'	6:B:109:G:OP1	2.26	0.46
8:D:30:VAL:O	8:D:188:SER:OG	2.28	0.46
10:F:80:ARG:HD3	10:F:83:TRP:NE1	2.29	0.46
16:L:63:LYS:HD3	16:L:65:PHE:CZ	2.50	0.46
1:0:2:ARG:NE	5:AN1:2281:C:OP2	2.40	0.46
5:AN1:2312:G:H2'	5:AN1:2313:C:C6	2.50	0.46
6:B:68:C:H2'	6:B:69:U:H6	1.80	0.46
7:C:76:ALA:O	7:C:115:LYS:HD3	2.15	0.46
10:F:31:ILE:HD12	10:F:156:ILE:HB	1.98	0.46
10:F:37:ASN:OD1	10:F:38:MET:N	2.48	0.46
10:F:100:LEU:O	10:F:104:ILE:HG12	2.15	0.46
5:AN1:2295:G:H2'	5:AN1:2296:C:C6	2.51	0.46
10:F:108:ILE:HA	10:F:114:PHE:CZ	2.50	0.46
5:AN1:762:A:H5'	7:C:209:GLY:HA2	1.97	0.46
5:AN1:2187:A:O2'	5:AN1:2188:G:H8	1.99	0.46
5:AN1:2533:U:H2'	5:AN1:2534:C:H6	1.80	0.46
8:D:119:LYS:O	8:D:122:GLN:NE2	2.44	0.46
11:G:33:LEU:HD21	11:G:137:ASN:HB2	1.97	0.46
5:AN1:753:C:H2'	5:AN1:754:A:C8	2.50	0.46
5:AN1:1413:G:O2'	5:AN1:1577:A:N6	2.49	0.46
5:AN1:1413:G:H22	5:AN1:1576:U:H3'	1.80	0.46
13:I:17:VAL:HG23	13:I:137:PRO:HB2	1.98	0.46
5:AN1:720:A:H2'	5:AN1:721:C:C6	2.50	0.46
5:AN1:727:G:OP1	7:C:13:ARG:HG2	2.15	0.46
5:AN1:1411:G:H2'	5:AN1:1412:C:C6	2.50	0.46
5:AN1:1911:3TD:OP1	5:AN1:1911:3TD:O3'	2.34	0.46
5:AN1:2736:A:H2'	5:AN1:2737:A:C8	2.50	0.46
11:G:22:ARG:HH11	11:G:39:ALA:HA	1.80	0.46
16:L:76:GLU:HB3	16:L:91:GLU:HG3	1.98	0.46
5:AN1:2066:A:H2'	5:AN1:2067:A:H8	1.81	0.46
7:C:107:PRO:HD2	7:C:110:LEU:HD22	1.97	0.46
5:AN1:961:C:O2'	5:AN1:2269:A:N3	2.38	0.46
5:AN1:1226:U:H2'	5:AN1:1227:G:H8	1.81	0.46
5:AN1:1589:C:H2'	5:AN1:1590:A:C8	2.51	0.46
5:AN1:1844:A:H4'	5:AN1:1845:G:H8	1.81	0.46
5:AN1:1961:C:H5"	5:AN1:1962:A:H2'	1.98	0.46
5:AN1:2021:C:H2'	5:AN1:2022:U:C6	2.50	0.46
5:AN1:2212:G:H2'	5:AN1:2213:G:C8	2.50	0.46
23:S:52:VAL:HG21	23:S:86:LEU:HD23	1.97	0.46
5:AN1:272:A:N1	5:AN1:426:U:O2'	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:673:A:H4'	9:E:61:GLN:HE21	1.80	0.46
5:AN1:849:C:H2'	5:AN1:850:A:H8	1.80	0.46
5:AN1:1412:C:H3'	5:AN1:1413:G:H8	1.80	0.46
9:E:52:SER:O	9:E:73:ARG:NE	2.39	0.46
10:F:168:ALA:HA	10:F:171:ARG:HE	1.81	0.46
5:AN1:2543:A:H2'	5:AN1:2544:U:C6	2.50	0.45
5:AN1:2769:U:OP1	8:D:172:ARG:NH1	2.42	0.45
5:AN1:580:A:H2'	5:AN1:581:G:C8	2.51	0.45
5:AN1:831:A:H2'	5:AN1:832:G:C8	2.52	0.45
5:AN1:1052:G:H1'	5:AN1:1082:A:C2	2.51	0.45
5:AN1:1296:A:H2	5:AN1:1624:A:H2	1.65	0.45
5:AN1:596:U:H2'	5:AN1:597:A:H8	1.81	0.45
5:AN1:844:A:N6	5:AN1:929:C:O2'	2.49	0.45
5:AN1:997:A:H2'	5:AN1:998:A:C8	2.50	0.45
5:AN1:1680:G:H2'	5:AN1:1681:U:C6	2.52	0.45
5:AN1:1087:A:H2'	5:AN1:1088:G:C8	2.51	0.45
5:AN1:2104:U:H3	5:AN1:2177:G:H1	1.64	0.45
5:AN1:2568:A:H2'	8:D:152:ASN:HD21	1.81	0.45
5:AN1:2683:U:H2'	5:AN1:2684:G:O4'	2.17	0.45
5:AN1:2787:A:O2'	5:AN1:2788:G:H8	1.97	0.45
5:AN1:2815:C:H2'	5:AN1:2817:A:N7	2.32	0.45
11:G:36:ASN:OD1	11:G:37:LEU:N	2.48	0.45
18:N:76:LEU:O	18:N:79:GLU:HG3	2.16	0.45
5:AN1:358:A:HO2'	5:AN1:359:U:H6	1.64	0.45
5:AN1:494:G:N7	57:AN1:3126:HOH:O	2.36	0.45
5:AN1:805:U:OP2	15:K:43:ARG:NH2	2.50	0.45
5:AN1:2657:G:OP2	5:AN1:2657:G:H8	2.00	0.45
5:AN1:2694:U:H2'	5:AN1:2695:G:C8	2.51	0.45
5:AN1:1792:U:H2'	5:AN1:1793:C:C6	2.51	0.45
7:C:17:GLU:OE1	7:C:204:SER:HB3	2.16	0.45
7:C:107:PRO:HG2	7:C:110:LEU:HD13	1.98	0.45
16:L:58:ILE:O	16:L:59:LYS:HG3	2.16	0.45
24:T:86:ILE:HG22	24:T:87:ASP:N	2.31	0.45
29:Y:2:LYS:HG3	29:Y:3:THR:N	2.32	0.45
5:AN1:2633:U:H2'	5:AN1:2634:G:O4'	2.17	0.45
5:AN1:2639:G:H2'	5:AN1:2640:A:H8	1.81	0.45
6:B:61:C:H2'	6:B:62:U:C6	2.51	0.45
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.98	0.45
25:U:52:VAL:O	25:U:56:GLU:HG3	2.17	0.45
5:AN1:2324:A:H2'	5:AN1:2325:A:H8	1.80	0.45
8:D:159:PHE:HB3	13:I:81:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:137:MET:HB3	25:U:61:PHE:CE1	2.52	0.45
5:AN1:636:G:H2'	5:AN1:637:U:C6	2.52	0.45
5:AN1:2674:A:H2'	5:AN1:2675:A:C8	2.52	0.45
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.99	0.45
29:Y:7:THR:O	29:Y:55:SER:N	2.45	0.45
5:AN1:293:U:O4	5:AN1:351:G:O6	2.35	0.44
5:AN1:1310:C:H2'	5:AN1:1311:A:C8	2.52	0.44
5:AN1:1500:A:O2'	5:AN1:1502:U:O4'	2.27	0.44
5:AN1:2645:C:H2'	5:AN1:2646:U:C6	2.53	0.44
5:AN1:2744:A:H1'	11:G:67:THR:HG22	1.98	0.44
6:B:54:G:H4'	6:B:55:A:H8	1.81	0.44
11:G:8:PRO:HB2	11:G:49:LYS:HG2	1.98	0.44
14:J:44:LYS:HD3	14:J:44:LYS:HA	1.80	0.44
5:AN1:292:U:H2'	5:AN1:293:U:C6	2.52	0.44
5:AN1:1475:C:H2'	5:AN1:1476:A:C8	2.53	0.44
5:AN1:2727:G:H2'	5:AN1:2728:G:C8	2.52	0.44
5:AN1:2734:A:N1	5:AN1:2762:G:O6	2.50	0.44
6:B:54:G:H4'	6:B:55:A:C8	2.53	0.44
5:AN1:631:A:O2'	5:AN1:2400:U:OP1	2.29	0.44
5:AN1:1103:A:N6	5:AN1:1104:G:O6	2.50	0.44
5:AN1:2225:U:H2'	5:AN1:2226:G:C8	2.51	0.44
6:B:16:A:H1'	6:B:65:G:N2	2.32	0.44
6:B:108:C:HO2'	6:B:109:G:P	2.41	0.44
8:D:184:ASP:HB3	8:D:189:VAL:HG22	1.99	0.44
12:H:5:LEU:HD11	12:H:12:LEU:HD22	2.00	0.44
15:K:31:LYS:HE3	15:K:32:THR:HG23	1.99	0.44
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.99	0.44
5:AN1:8:A:H61	5:AN1:2898:U:H3	1.64	0.44
5:AN1:2149:A:H2'	5:AN1:2150:G:C8	2.52	0.44
5:AN1:2169:A:H2'	5:AN1:2170:C:C6	2.53	0.44
5:AN1:2373:A:H2'	5:AN1:2374:A:C8	2.52	0.44
5:AN1:2533:U:H2'	5:AN1:2534:C:C6	2.53	0.44
5:AN1:2639:G:H2'	5:AN1:2640:A:C8	2.53	0.44
6:B:64:A:H61	6:B:105:C:H2'	1.82	0.44
19:O:107:SER:OG	19:O:108:GLY:N	2.51	0.44
25:U:22:ARG:O	25:U:26:ARG:HD3	2.16	0.44
5:AN1:889:G:O2'	5:AN1:890:A:N7	2.50	0.44
5:AN1:1078:U:H2'	5:AN1:1079:U:C5	2.52	0.44
5:AN1:1381:A:H2'	5:AN1:1382:U:C6	2.52	0.44
5:AN1:2098:C:H2'	5:AN1:2099:C:O4'	2.16	0.44
21:Q:40:MET:HE3	21:Q:49:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:5:LYS:HE2	24:T:5:LYS:HB3	1.88	0.44
5:AN1:2287:U:H2'	5:AN1:2288:G:H8	1.81	0.44
7:C:232:HIS:CE1	7:C:244:PRO:HA	2.52	0.44
10:F:137:VAL:HG12	10:F:137:VAL:O	2.18	0.44
30:Z:38:ARG:HB3	30:Z:41:HIS:HB2	2.00	0.44
5:AN1:782:G:H5'	5:AN1:783:G:OP1	2.18	0.44
5:AN1:875:U:H2'	5:AN1:876:A:H8	1.81	0.44
5:AN1:1794:U:OP2	7:C:273:VAL:HG21	2.18	0.44
5:AN1:2127:U:OP1	5:AN1:2130:A:H5'	2.18	0.44
2:1:7:PRO:HB2	5:AN1:1304:G:H4'	1.99	0.44
5:AN1:1176:U:H2'	5:AN1:1177:A:C8	2.53	0.44
5:AN1:1569:A:H2'	5:AN1:1570:A:C8	2.52	0.44
5:AN1:1717:G:H21	5:AN1:1735:A:H62	1.65	0.44
5:AN1:2510:U:H2'	5:AN1:2511:C:C6	2.53	0.44
5:AN1:2795:A:H2'	5:AN1:2797:G:OP2	2.18	0.44
5:AN1:2880:U:H2'	5:AN1:2881:U:C6	2.52	0.44
5:AN1:278:U:H3	5:AN1:366:G:H22	1.65	0.44
8:D:109:ILE:HG22	8:D:209:THR:HG21	2.00	0.44
5:AN1:184:G:OP2	5:AN1:184:G:N2	2.26	0.43
5:AN1:2775:U:H5"	5:AN1:2776:A:H2'	2.00	0.43
8:D:20:GLY:HA3	19:O:83:VAL:HG13	1.98	0.43
1:0:22:ASN:HB3	1:0:25:THR:HB	2.01	0.43
5:AN1:593:C:H2'	5:AN1:594:A:H8	1.84	0.43
5:AN1:844:A:H1'	5:AN1:846:U:C4	2.53	0.43
5:AN1:1854:A:C2	5:AN1:1881:A:H1'	2.53	0.43
6:B:26:C:H2'	6:B:27:A:H8	1.83	0.43
6:B:111:C:H2'	6:B:112:A:H8	1.83	0.43
5:AN1:1909:A:O2'	5:AN1:1959:U:O4	2.25	0.43
5:AN1:1928:A:H2'	5:AN1:1929:G:O4'	2.18	0.43
5:AN1:2048:A:O3'	8:D:152:ASN:HA	2.18	0.43
5:AN1:2262:A:H4'	5:AN1:2263:A:N3	2.33	0.43
5:AN1:2553:G:H2'	5:AN1:2554:C:C6	2.54	0.43
8:D:54:GLY:HA3	8:D:78:ARG:HG2	1.99	0.43
28:X:40:SER:O	28:X:44:GLN:NE2	2.51	0.43
5:AN1:493:G:H21	22:R:57:ASN:HD21	1.66	0.43
5:AN1:630:A:H2'	5:AN1:631:A:C8	2.53	0.43
5:AN1:956:A:H2'	5:AN1:957:A:C8	2.53	0.43
5:AN1:2881:U:C4	30:Z:28:THR:HG21	2.53	0.43
18:N:67:ILE:O	18:N:71:THR:HG23	2.19	0.43
5:AN1:569:U:H3'	21:Q:80:ARG:NH2	2.34	0.43
5:AN1:627:A:N3	5:AN1:637:U:O2'	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:59:LEU:HD11	18:N:72:LYS:HD2	2.00	0.43
5:AN1:85:C:C2	5:AN1:86:C:C5	3.07	0.43
14:J:63:VAL:HG12	14:J:106:LEU:HD11	2.01	0.43
5:AN1:113:C:H2'	5:AN1:114:G:C8	2.54	0.43
5:AN1:880:G:C6	5:AN1:893:U:H1'	2.54	0.43
5:AN1:1436:A:H2'	5:AN1:1437:U:C6	2.54	0.43
5:AN1:1464:A:H2'	5:AN1:1465:A:C8	2.53	0.43
5:AN1:2232:U:H2'	5:AN1:2233:G:O4'	2.19	0.43
5:AN1:637:U:H2'	5:AN1:638:C:H6	1.84	0.43
5:AN1:1719:U:O4	5:AN1:1734:G:N2	2.52	0.43
5:AN1:2142:U:H4'	5:AN1:2143:A:C5	2.54	0.43
5:AN1:2229:U:H2'	5:AN1:2230:G:H8	1.84	0.43
7:C:125:ARG:HG2	7:C:126:PRO:HD2	2.00	0.43
5:AN1:849:C:H2'	5:AN1:850:A:C8	2.54	0.43
5:AN1:1230:G:O2'	5:AN1:1231:G:O4'	2.28	0.43
5:AN1:1427:G:H2'	5:AN1:1428:A:C8	2.54	0.43
5:AN1:1743:A:H2'	5:AN1:1744:C:C6	2.54	0.43
5:AN1:2115:A:N3	5:AN1:2166:A:H1'	2.34	0.43
16:L:112:ASP:OD1	16:L:113:LEU:N	2.52	0.43
3:2:50:HIS:HD2	3:2:52:SER:H	1.66	0.42
5:AN1:575:G:H2'	5:AN1:576:G:C8	2.54	0.42
5:AN1:580:A:H2'	5:AN1:581:G:H8	1.83	0.42
6:B:101:A:H2'	6:B:102:A:O4'	2.19	0.42
7:C:205:LEU:HB3	7:C:210:ALA:HB3	2.01	0.42
1:0:13:THR:HB	1:0:38:LYS:HD3	2.01	0.42
5:AN1:68:A:H2'	5:AN1:69:U:N3	2.33	0.42
5:AN1:667:G:H2'	5:AN1:667:G:N3	2.34	0.42
5:AN1:1108:A:H2'	5:AN1:1109:G:H4'	2.00	0.42
5:AN1:1389:U:H2'	5:AN1:1390:A:O4'	2.19	0.42
11:G:51:GLN:HE21	11:G:52:LEU:H	1.68	0.42
5:AN1:239:G:H8	5:AN1:239:G:OP2	2.02	0.42
5:AN1:342:A:HO2'	9:E:161:ARG:NH1	2.16	0.42
5:AN1:1792:U:H2'	5:AN1:1793:C:H6	1.84	0.42
5:AN1:2158:G:H2'	5:AN1:2159:U:O4'	2.19	0.42
5:AN1:2456:U:C2	5:AN1:2457:A:C8	3.07	0.42
19:O:103:LEU:HD11	19:O:113:ILE:HD11	2.00	0.42
23:S:5:ARG:O	23:S:9:VAL:HG13	2.19	0.42
5:AN1:609:C:H2'	5:AN1:610:G:O4'	2.20	0.42
10:F:175:PHE:HB3	10:F:177:PHE:HD1	1.84	0.42
23:S:3:ASN:HD21	23:S:48:LYS:HE2	1.84	0.42
5:AN1:898:A:H3'	5:AN1:899:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:976:A:H2'	5:AN1:979:C:N4	2.34	0.42
5:AN1:2115:A:O2'	5:AN1:2166:A:O2'	2.32	0.42
5:AN1:2169:A:H2'	5:AN1:2170:C:C5	2.54	0.42
5:AN1:2479:C:H1'	16:L:52:ARG:HH12	1.84	0.42
6:B:22:G:O2'	6:B:25:C:N4	2.50	0.42
9:E:116:ARG:NH2	9:E:182:PHE:O	2.52	0.42
11:G:106:ASN:ND2	11:G:112:PRO:HB3	2.35	0.42
5:AN1:437:G:H2'	5:AN1:438:A:C8	2.55	0.42
5:AN1:591:U:H2'	5:AN1:592:U:C6	2.54	0.42
5:AN1:990:G:OP2	20:P:51:ARG:NH1	2.52	0.42
5:AN1:1749:G:H5"	19:O:96:ARG:HD3	2.02	0.42
8:D:13:THR:OG1	8:D:14:ARG:N	2.50	0.42
8:D:31:ASP:OD1	8:D:31:ASP:N	2.49	0.42
10:F:168:ALA:O	10:F:171:ARG:HG2	2.19	0.42
11:G:19:GLN:HG3	11:G:21:GLY:H	1.85	0.42
15:K:21:LEU:HA	15:K:29:VAL:HG11	2.01	0.42
17:M:101:GLY:H	30:Z:41:HIS:HD2	1.66	0.42
5:AN1:592:U:H2'	5:AN1:593:C:C6	2.54	0.42
5:AN1:1025:A:H2'	5:AN1:1026:A:H8	1.85	0.42
5:AN1:1083:A:H1'	5:AN1:1100:A:H61	1.84	0.42
5:AN1:1506:U:H2'	5:AN1:1507:G:C8	2.55	0.42
28:X:28:LEU:HD22	28:X:39:LYS:HG2	2.02	0.42
5:AN1:1588:A:H2'	5:AN1:1589:C:H6	1.84	0.42
5:AN1:1862:A:H2	5:AN1:1872:A:C8	2.37	0.42
5:AN1:1879:U:H2'	5:AN1:1880:G:O4'	2.19	0.42
5:AN1:2573:A:H2'	5:AN1:2610:A:N6	2.35	0.42
12:H:57:GLN:NE2	12:H:58:GLU:HG3	2.35	0.42
17:M:65:LEU:O	17:M:69:ARG:HG3	2.20	0.42
19:O:13:ASN:HA	19:O:16:LEU:HG	2.02	0.42
5:AN1:944:A:H2'	5:AN1:945:C:C6	2.55	0.42
5:AN1:1412:C:H3'	5:AN1:1413:G:C8	2.55	0.42
5:AN1:1549:U:H2'	5:AN1:1550:G:O4'	2.19	0.42
5:AN1:1826:U:H2'	5:AN1:1827:G:H8	1.85	0.42
5:AN1:2127:U:O5'	5:AN1:2129:G:H4'	2.19	0.42
5:AN1:2182:U:H2'	5:AN1:2183:G:H8	1.85	0.42
13:I:45:THR:HG22	20:P:64:ARG:HH21	1.84	0.42
3:2:30:HIS:C	3:2:32:LEU:H	2.10	0.41
4:3:13:SER:OG	4:3:27:CYS:SG	2.78	0.41
5:AN1:1470:G:H5"	5:AN1:1510:G:O6	2.20	0.41
5:AN1:2379:G:O2'	5:AN1:2380:U:OP1	2.34	0.41
8:D:160:LYS:HE3	13:I:79:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:97:ARG:HB2	19:O:100:LEU:HD12	2.02	0.41
5:AN1:71:G:H2'	5:AN1:72:C:C6	2.56	0.41
5:AN1:86:C:C2	5:AN1:87:G:C8	3.08	0.41
5:AN1:1412:C:H2'	5:AN1:1413:G:O4'	2.20	0.41
10:F:12:LEU:HD22	10:F:172:ALA:HB1	2.02	0.41
10:F:99:PHE:CZ	10:F:103:LEU:HD11	2.55	0.41
18:N:78:ALA:O	18:N:82:LYS:HG2	2.20	0.41
25:U:36:GLY:HA3	25:U:97:ARG:HB2	2.02	0.41
5:AN1:2110:A:H3'	5:AN1:2111:G:H8	1.85	0.41
11:G:22:ARG:NH1	11:G:39:ALA:HA	2.36	0.41
15:K:31:LYS:HE2	15:K:31:LYS:HB3	1.84	0.41
20:P:78:ARG:HD3	20:P:78:ARG:HA	1.76	0.41
23:S:16:SER:O	23:S:20:GLN:HG2	2.20	0.41
5:AN1:323:U:O3'	9:E:161:ARG:NH1	2.45	0.41
5:AN1:1230:G:H2'	5:AN1:1231:G:C4	2.55	0.41
5:AN1:1259:G:OP1	30:Z:16:ARG:NH2	2.47	0.41
5:AN1:1860:U:H2'	5:AN1:1861:U:C6	2.56	0.41
6:B:108:C:H2'	6:B:109:G:C8	2.52	0.41
9:E:128:PRO:HB3	9:E:155:ASN:HA	2.03	0.41
17:M:36:THR:OG1	17:M:37:THR:N	2.53	0.41
5:AN1:727:G:O2'	5:AN1:761:G:H4'	2.20	0.41
5:AN1:1424:G:H2'	5:AN1:1425:G:C8	2.56	0.41
5:AN1:1842:G:H2'	5:AN1:1843:A:C8	2.55	0.41
5:AN1:2123:G:H2'	5:AN1:2124:G:H8	1.84	0.41
5:AN1:2130:A:H1'	5:AN1:2155:G:H1'	2.02	0.41
11:G:10:THR:HB	11:G:49:LYS:HD2	2.02	0.41
5:AN1:1164:G:H2'	5:AN1:1165:U:C6	2.56	0.41
5:AN1:1365:C:H2'	5:AN1:1366:G:O4'	2.21	0.41
5:AN1:1437:U:H2'	5:AN1:1438:C:H6	1.85	0.41
5:AN1:2111:G:OP1	5:AN1:2162:U:O2'	2.33	0.41
5:AN1:2127:U:H5'	5:AN1:2128:U:H5"	2.03	0.41
5:AN1:2308:U:H2'	10:F:37:ASN:HD21	1.85	0.41
6:B:111:C:H2'	6:B:112:A:C8	2.56	0.41
10:F:7:ARG:HA	10:F:7:ARG:HD2	1.91	0.41
27:W:33:LEU:HD22	27:W:50:ARG:HG2	2.03	0.41
5:AN1:355:C:O2'	5:AN1:356:A:H2'	2.20	0.41
5:AN1:412:C:H2'	5:AN1:413:C:H6	1.86	0.41
5:AN1:847:A:H2'	5:AN1:848:C:C6	2.56	0.41
5:AN1:1078:U:H2'	5:AN1:1079:U:H5	1.86	0.41
5:AN1:1277:U:H2'	5:AN1:1278:G:O4'	2.21	0.41
5:AN1:1355:G:N7	5:AN1:1356:G:C8	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2894:U:O2'	13:I:134:ALA:O	2.37	0.41
12:H:6:LEU:HD22	12:H:51:ARG:NH2	2.35	0.41
12:H:12:LEU:HD11	12:H:21:VAL:HG11	2.03	0.41
17:M:32:GLU:HG2	17:M:115:LEU:HD12	2.02	0.41
21:Q:62:GLU:HG2	21:Q:97:LYS:HB3	2.02	0.41
22:R:85:ILE:HD11	22:R:93:ALA:HB1	2.02	0.41
27:W:64:ILE:O	27:W:68:VAL:HG23	2.20	0.41
5:AN1:1490:A:H2'	5:AN1:1491:A:H8	1.85	0.41
5:AN1:1528:G:N2	5:AN1:1535:U:O4	2.53	0.41
5:AN1:1623:C:H2'	5:AN1:1624:A:O4'	2.21	0.41
10:F:17:GLN:HA	10:F:22:ILE:HD12	2.02	0.41
18:N:82:LYS:NZ	18:N:113:GLY:O	2.39	0.41
4:3:10:ILE:HD13	4:3:33:HIS:CD2	2.54	0.41
5:AN1:720:A:H2'	5:AN1:721:C:H6	1.86	0.41
5:AN1:825:U:O2'	5:AN1:2064:U:N3	2.53	0.41
5:AN1:854:G:H2'	5:AN1:855:G:C8	2.56	0.41
5:AN1:992:C:N4	13:I:1:MET:HA	2.36	0.41
5:AN1:1523:A:N1	5:AN1:1524:A:N6	2.69	0.41
5:AN1:2070:U:H2'	5:AN1:2071:U:H6	1.85	0.41
5:AN1:2120:G:H1	5:AN1:2171:C:H1'	1.86	0.41
5:AN1:2360:C:H2'	5:AN1:2361:G:O4'	2.21	0.41
5:AN1:2381:C:H2'	5:AN1:2382:U:C6	2.56	0.41
5:AN1:2587:C:H2'	5:AN1:2588:G:C8	2.53	0.41
5:AN1:2784:C:H2'	5:AN1:2785:C:C6	2.55	0.41
5:AN1:2841:U:H5"	19:O:55:ASN:O	2.21	0.41
12:H:5:LEU:HD21	12:H:12:LEU:HD22	2.03	0.41
17:M:52:ILE:O	17:M:56:LYS:HG3	2.21	0.41
21:Q:53:VAL:HG23	21:Q:53:VAL:O	4.88	0.41
25:U:8:ALA:HB3	25:U:69:VAL:HG22	2.02	0.41
29:Y:52:TYR:CE2	29:Y:53:MET:HG3	2.56	0.41
5:AN1:11:C:H2'	5:AN1:12:A:C8	2.56	0.41
5:AN1:199:G:O2'	5:AN1:675:A:N1	2.54	0.41
5:AN1:1081:A:O3'	5:AN1:1102:U:O2'	2.32	0.41
5:AN1:1410:U:O2	5:AN1:1585:G:O6	2.38	0.41
5:AN1:2306:A:H2	10:F:77:PHE:HE1	1.69	0.41
15:K:138:GLU:OE2	15:K:144:VAL:HG23	2.21	0.41
27:W:62:LEU:HD12	27:W:66:LYS:HD3	2.03	0.41
5:AN1:67:G:C2	5:AN1:68:A:N6	2.89	0.40
5:AN1:113:C:H2'	5:AN1:114:G:H8	1.85	0.40
5:AN1:1065:G:N2	5:AN1:1092:A:O2'	2.54	0.40
5:AN1:1441:C:H2'	5:AN1:1442:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1921:C:H2'	5:AN1:1922:U:C6	2.56	0.40
5:AN1:2119:G:H1	5:AN1:2169:A:H62	1.68	0.40
5:AN1:2845:G:H1'	5:AN1:2862:G:H21	1.86	0.40
11:G:12:PRO:HG2	11:G:15:VAL:HG21	2.03	0.40
24:T:12:VAL:HG22	24:T:20:LYS:O	2.21	0.40
3:2:31:ILE:H	3:2:31:ILE:HG13	1.42	0.40
5:AN1:157:U:H2'	5:AN1:158:U:C6	2.56	0.40
5:AN1:158:U:H2'	5:AN1:159:G:C8	2.55	0.40
5:AN1:418:U:H2'	5:AN1:419:C:C6	2.56	0.40
5:AN1:456:A:H61	5:AN1:469:A:H3'	1.85	0.40
5:AN1:981:A:H2'	5:AN1:981:A:N3	2.37	0.40
5:AN1:1029:A:H2'	5:AN1:1030:U:C6	2.56	0.40
5:AN1:1566:G:H4'	7:C:59:LYS:HB3	2.02	0.40
5:AN1:1568:A:H2'	5:AN1:1569:A:C8	2.57	0.40
5:AN1:2805:A:H2'	5:AN1:2806:A:C8	2.56	0.40
5:AN1:2894:U:H2'	5:AN1:2895:G:C8	2.57	0.40
19:O:103:LEU:HA	19:O:106:LEU:HD12	2.02	0.40
5:AN1:1569:A:H2'	5:AN1:1570:A:H8	1.86	0.40
5:AN1:1586:U:H2'	5:AN1:1587:U:C6	2.56	0.40
5:AN1:1862:A:H2	5:AN1:1872:A:H8	1.68	0.40
5:AN1:2010:A:H2'	5:AN1:2011:A:C8	2.57	0.40
10:F:35:THR:HG22	10:F:90:THR:HA	2.03	0.40
14:J:17:ARG:HB2	14:J:45:GLU:HG3	2.04	0.40
5:AN1:67:G:N1	5:AN1:81:A:C6	2.90	0.40
5:AN1:177:G:H2'	5:AN1:178:U:H6	1.85	0.40
5:AN1:516:C:OP2	30:Z:10:ARG:NH2	2.54	0.40
5:AN1:1166:A:H2'	5:AN1:1167:U:O4'	2.21	0.40
5:AN1:1681:U:H2'	5:AN1:1682:A:C8	2.57	0.40
5:AN1:2306:A:H2	10:F:77:PHE:CE1	2.39	0.40
5:AN1:2837:U:H2'	5:AN1:2838:G:C8	2.56	0.40
5:AN1:2837:U:H2'	5:AN1:2838:G:H8	1.86	0.40
10:F:135:GLN:HB3	10:F:140:GLU:OE1	2.22	0.40
21:Q:37:ASP:OD1	21:Q:37:ASP:N	2.50	0.40
25:U:5:VAL:HG12	25:U:66:GLU:HB3	2.02	0.40
5:AN1:291:G:O2'	5:AN1:292:U:H5"	2.22	0.40
5:AN1:324:A:OP2	9:E:162:ASN:HB2	2.21	0.40
5:AN1:553:G:HO2'	5:AN1:554:A:H8	1.63	0.40
5:AN1:916:A:N3	6:B:78:U:O2'	2.53	0.40
5:AN1:1713:U:H2'	5:AN1:1714:G:C8	2.56	0.40
5:AN1:2149:A:H2'	5:AN1:2150:G:H8	1.86	0.40
5:AN1:2572:G:H5'	5:AN1:2574:G:N7	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:184:ASP:OD1	8:D:187:ARG:NH1	2.53	0.40
10:F:122:PHE:CE2	10:F:128:TYR:HB2	2.57	0.40
11:G:53:ALA:HA	11:G:54:PRO:HD3	1.90	0.40
13:I:2:LYS:NZ	21:Q:13:ARG:H	2.19	0.40
29:Y:44:ARG:HA	29:Y:44:ARG:HD2	1.84	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%)	48 (98%)	1 (2%)	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%)	4	12
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%)	204 (98%)	5 (2%)	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%)	25	54
11	G	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
12	H	58/148 (39%)	56 (97%)	1 (2%)	1 (2%)	9	27
13	I	140/142 (99%)	138 (99%)	2 (1%)	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%)	133 (98%)	2 (2%)	0	100	100
17	M	117/125 (94%)	117 (100%)	0	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	O	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	94 (93%)	7 (7%)	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%)	94 (96%)	4 (4%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	78/85 (92%)	78 (100%)	0	0	100	100
27	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
28	X	60/65 (92%)	60 (100%)	0	0	100	100
29	Y	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	Z	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	207 (93%)	16 (7%)	0	100	100
33	c	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
34	d	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	92/127 (72%)	89 (97%)	3 (3%)	0	100	100
37	g	139/156 (89%)	138 (99%)	1 (1%)	0	100	100
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%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
42	l	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
43	m	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	p	81/101 (80%)	80 (99%)	1 (1%)	0	100	100
47	q	78/85 (92%)	78 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	u	19/71 (27%)	16 (84%)	3 (16%)	0	100 100
All	All	5361/5872 (91%)	5209 (97%)	148 (3%)	4 (0%)	54 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	PRO
12	H	48	GLU

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%)	46 (98%)	1 (2%)	53 82
2	1	36/36 (100%)	36 (100%)	0	100 100
3	2	52/53 (98%)	52 (100%)	0	100 100
4	3	33/33 (100%)	33 (100%)	0	100 100
7	C	216/220 (98%)	215 (100%)	1 (0%)	88 96
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%)	144 (99%)	1 (1%)	84 95
11	G	139/142 (98%)	138 (99%)	1 (1%)	84 95
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%)	106 (98%)	2 (2%)	57 84
16	L	113/113 (100%)	112 (99%)	1 (1%)	78 93
17	M	96/101 (95%)	96 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	80 (98%)	2 (2%)	49	80
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%)	88	96
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	169 (99%)	1 (1%)	86	95
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%)	115 (99%)	1 (1%)	78	93
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	98 (99%)	1 (1%)	76	92
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	87 (99%)	1 (1%)	73	91
42	l	104/106 (98%)	102 (98%)	2 (2%)	57	84
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	80 (99%)	1 (1%)	71	91
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	4419 (100%)	17 (0%)	91 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	LYS
7	C	272	ARG
10	F	125	ARG
11	G	134	LYS
15	K	44	LYS
15	K	120	ARG
16	L	59	LYS
24	T	48	ARG
24	T	77	LYS
32	b	179	LYS
34	d	189	ASP
37	g	5	ARG
39	i	104	ARG
41	k	55	ARG
42	l	44	LYS
42	l	86	ARG
44	n	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	22	ASN
3	2	50	HIS
7	C	48	HIS
7	C	58	HIS
7	C	60	GLN
7	C	90	HIS
7	C	117	GLN
7	C	120	ASN
7	C	230	HIS
7	C	250	GLN
8	D	33	ASN
8	D	50	GLN

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Mol	Chain	Res	Type
8	D	108	GLN
8	D	137	HIS
8	D	153	GLN
9	E	96	ASN
9	E	114	GLN
9	E	165	HIS
10	F	127	ASN
11	G	51	GLN
11	G	106	ASN
13	I	40	HIS
13	I	135	GLN
15	K	40	GLN
15	K	56	GLN
15	K	125	GLN
19	O	13	ASN
19	O	78	GLN
20	P	11	HIS
21	Q	87	GLN
22	R	57	ASN
22	R	60	HIS
24	T	38	ASN
25	U	16	GLN
25	U	79	GLN
25	U	84	HIS
26	V	29	GLN
27	W	6	GLN
29	Y	48	ASN
30	Z	41	HIS
32	b	17	HIS
32	b	80	ASN
32	b	105	ASN
32	b	122	GLN
33	c	6	HIS
33	c	19	ASN
33	c	176	HIS
34	d	42	HIS
34	d	102	ASN
34	d	138	GLN
34	d	154	GLN
35	e	121	ASN
36	f	11	HIS
36	f	17	GLN

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Mol	Chain	Res	Type
36	f	35	GLN
36	f	94	HIS
37	g	32	GLN
38	h	53	GLN
38	h	86	GLN
39	i	73	GLN
39	i	79	HIS
40	j	35	GLN
40	j	56	HIS
41	k	27	ASN
41	k	28	ASN
41	k	80	ASN
43	m	105	ASN
45	o	20	ASN
45	o	37	ASN
45	o	40	GLN
45	o	42	HIS
46	p	44	ASN
47	q	32	HIS
49	s	52	HIS
50	t	13	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	sN1	1524/1544 (98%)	204 (13%)	0
5	AN1	2888/2918 (98%)	494 (17%)	10 (0%)
52	v	76/77 (98%)	27 (35%)	0
53	w	2/3 (66%)	1 (50%)	0
6	B	114/115 (99%)	21 (18%)	1 (0%)
All	All	4604/4657 (98%)	747 (16%)	11 (0%)

All (747) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	21	A
5	AN1	22	G
5	AN1	34	G
5	AN1	41	U
5	AN1	50	G
5	AN1	53	G

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Mol	Chain	Res	Type
5	AN1	58	G
5	AN1	59	A
5	AN1	67	G
5	AN1	68	A
5	AN1	69	U
5	AN1	71	G
5	AN1	74	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	104	C
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
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	272	A
5	AN1	273	G
5	AN1	274	C
5	AN1	279	U
5	AN1	280	A

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Mol	Chain	Res	Type
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	416	C
5	AN1	423	G
5	AN1	434	C
5	AN1	455	C
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	541	C
5	AN1	543	U
5	AN1	544	U
5	AN1	545	C
5	AN1	547	U
5	AN1	554	A

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Mol	Chain	Res	Type
5	AN1	561	A
5	AN1	564	U
5	AN1	571	U
5	AN1	573	A
5	AN1	595	G
5	AN1	601	A
5	AN1	612	A
5	AN1	625	A
5	AN1	633	C
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	654	G
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	693	G
5	AN1	711	G
5	AN1	713	A
5	AN1	714	A
5	AN1	719	A
5	AN1	724	G
5	AN1	727	G
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

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Mol	Chain	Res	Type
5	AN1	825	U
5	AN1	828	G
5	AN1	843	G
5	AN1	855	G
5	AN1	857	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	904	U
5	AN1	908	A
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
5	AN1	1009	U
5	AN1	1010	C
5	AN1	1023	G
5	AN1	1028	G
5	AN1	1031	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	1043	A
5	AN1	1044	G
5	AN1	1054	A
5	AN1	1057	U
5	AN1	1058	U

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Mol	Chain	Res	Type
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	1129	U
5	AN1	1130	A
5	AN1	1131	A
5	AN1	1132	C
5	AN1	1140	A
5	AN1	1149	G
5	AN1	1167	U
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	1242	A
5	AN1	1245	G
5	AN1	1248	A
5	AN1	1251	G
5	AN1	1267	A
5	AN1	1296	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

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Mol	Chain	Res	Type
5	AN1	1374	U
5	AN1	1378	A
5	AN1	1390	A
5	AN1	1393	C
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	1433	U
5	AN1	1435	A
5	AN1	1447	G
5	AN1	1448	U
5	AN1	1449	U
5	AN1	1453	U
5	AN1	1455	U
5	AN1	1456	C
5	AN1	1470	G
5	AN1	1473	G
5	AN1	1477	U
5	AN1	1485	A
5	AN1	1501	C
5	AN1	1502	U
5	AN1	1504	U
5	AN1	1505	A
5	AN1	1509	U
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	1543	A
5	AN1	1544	G
5	AN1	1545	U
5	AN1	1564	A

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Mol	Chain	Res	Type
5	AN1	1567	A
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	1673	C
5	AN1	1691	U
5	AN1	1710	U
5	AN1	1712	U
5	AN1	1713	U
5	AN1	1714	G
5	AN1	1717	G
5	AN1	1718	A
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
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	1831	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

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Mol	Chain	Res	Type
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	1915	A
5	AN1	1916	C
5	AN1	1917	G
5	AN1	1918	G
5	AN1	1925	G
5	AN1	1926	G
5	AN1	1932	A
5	AN1	1933	A
5	AN1	1934	A
5	AN1	1936	U
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	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

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Mol	Chain	Res	Type
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
5	AN1	2127	U
5	AN1	2128	U
5	AN1	2129	G
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	2155	G
5	AN1	2157	C
5	AN1	2158	G
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

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Mol	Chain	Res	Type
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	2222	C
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	2284	A
5	AN1	2301	U
5	AN1	2304	G
5	AN1	2305	A
5	AN1	2308	U
5	AN1	2312	G
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	2418	C
5	AN1	2425	G
5	AN1	2426	A
5	AN1	2430	A
5	AN1	2431	A
5	AN1	2437	U
5	AN1	2443	G
5	AN1	2444	A
5	AN1	2455	A

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Mol	Chain	Res	Type
5	AN1	2468	G
5	AN1	2469	U
5	AN1	2470	U
5	AN1	2473	U
5	AN1	2474	A
5	AN1	2487	U
5	AN1	2494	C
5	AN1	2498	G
5	AN1	2500	PSU
5	AN1	2501	G
5	AN1	2503	C
5	AN1	2514	A
5	AN1	2516	C
5	AN1	2530	A
5	AN1	2543	A
5	AN1	2548	OMU
5	AN1	2550	U
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	2749	A
5	AN1	2753	A
5	AN1	2754	A

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Mol	Chain	Res	Type
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	2797	G
5	AN1	2800	C
5	AN1	2804	A
5	AN1	2816	G
5	AN1	2817	A
5	AN1	2829	U
5	AN1	2831	A
5	AN1	2845	G
5	AN1	2851	U
5	AN1	2853	G
5	AN1	2857	U
5	AN1	2863	A
5	AN1	2868	G
5	AN1	2875	A
5	AN1	2880	U
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	15	C
6	B	16	A
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

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Mol	Chain	Res	Type
6	B	87	A
6	B	105	C
6	B	106	A
6	B	108	C
6	B	109	G
31	sN1	6	C
31	sN1	11	G
31	sN1	15	U
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	86	C
31	sN1	87	U
31	sN1	90	C
31	sN1	91	G
31	sN1	97	A
31	sN1	105	A
31	sN1	107	G
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	243	G
31	sN1	247	G
31	sN1	262	G
31	sN1	263	C
31	sN1	285	G
31	sN1	289	G

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Mol	Chain	Res	Type
31	sN1	302	A
31	sN1	324	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	369	A
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	434	U
31	sN1	463	U
31	sN1	474	A
31	sN1	475	G
31	sN1	476	U
31	sN1	478	G
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

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Mol	Chain	Res	Type
31	sN1	572	G
31	sN1	573	C
31	sN1	574	G
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	699	A
31	sN1	700	G
31	sN1	714	U
31	sN1	721	G
31	sN1	728	G
31	sN1	744	A
31	sN1	745	U
31	sN1	752	G
31	sN1	774	A
31	sN1	790	U
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

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Mol	Chain	Res	Type
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
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	1121	C
31	sN1	1123	U
31	sN1	1124	G
31	sN1	1130	A
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

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Mol	Chain	Res	Type
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	1249	A
31	sN1	1255	G
31	sN1	1257	U
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
31	sN1	1350	G
31	sN1	1360	A
31	sN1	1378	U
31	sN1	1380	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	1448	C
31	sN1	1449	A
31	sN1	1490	A
31	sN1	1491	G
31	sN1	1496	A
31	sN1	1499	A
31	sN1	1503	U
31	sN1	1514	G
31	sN1	1517	C
31	sN1	1526	G
31	sN1	1527	G
52	v	4	U

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Mol	Chain	Res	Type
52	v	9	A
52	v	13	C
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	21	U
52	v	22	A
52	v	23	G
52	v	36	A
52	v	37	U
52	v	43	G
52	v	47	G
52	v	48	U
52	v	49	C
52	v	51	C
52	v	55	5MU
52	v	59	A
52	v	61	U
52	v	62	C
52	v	64	C
52	v	65	G
52	v	67	C
52	v	74	A
52	v	76	C
53	w	2	U

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)

28 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	PSU	AN1	2601	5	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
31	MA6	sN1	1516	31	19,26,27	1.02	2 (10%)	18,38,41	3.82	2 (11%)
52	4SU	v	8	52	18,21,22	4.31	8 (44%)	26,30,33	2.21	5 (19%)
5	PSU	AN1	2453	5	18,21,22	1.07	1 (5%)	22,30,33	1.80	6 (27%)
5	OMU	AN1	2548	5	19,22,23	3.05	8 (42%)	26,31,34	1.70	4 (15%)
5	6MZ	AN1	2026	5	18,25,26	1.87	3 (16%)	16,36,39	3.71	3 (18%)
31	PSU	sN1	513	31	18,21,22	1.14	1 (5%)	22,30,33	1.54	4 (18%)
5	PSU	AN1	2500	5	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
5	3TD	AN1	1911	5	18,22,23	4.21	7 (38%)	22,32,35	1.74	3 (13%)
31	4OC	sN1	1399	31	20,23,24	3.20	8 (40%)	26,32,35	0.93	1 (3%)
5	2MG	AN1	2441	5	18,26,27	2.50	7 (38%)	16,38,41	1.35	3 (18%)
5	PSU	AN1	1913	5	18,21,22	1.09	1 (5%)	22,30,33	1.67	5 (22%)
5	5MU	AN1	1935	5	19,22,23	4.93	7 (36%)	28,32,35	3.62	9 (32%)
5	OMG	AN1	2247	5	18,26,27	2.52	8 (44%)	19,38,41	1.50	4 (21%)
31	7MG	sN1	524	31	22,26,27	3.90	10 (45%)	29,39,42	2.04	9 (31%)
31	UR3	sN1	1495	31	19,22,23	2.91	6 (31%)	26,32,35	1.29	1 (3%)
5	PSU	AN1	2576	5	18,21,22	1.06	1 (5%)	22,30,33	1.80	6 (27%)
31	MA6	sN1	1515	31	19,26,27	1.03	2 (10%)	18,38,41	3.61	2 (11%)
52	PSU	v	56	52	18,21,22	1.07	1 (5%)	22,30,33	1.60	5 (22%)
5	PSU	AN1	1907	5	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
5	PSU	AN1	952	5	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
52	H2U	v	20	52	18,21,22	3.09	4 (22%)	21,30,33	1.91	5 (23%)
5	2MA	AN1	2499	55,5	17,25,26	2.54	5 (29%)	17,37,40	1.37	2 (11%)
52	5MU	v	55	52	19,22,23	4.99	7 (36%)	28,32,35	3.68	9 (32%)
31	2MG	sN1	1204	31	18,26,27	2.52	7 (38%)	16,38,41	1.38	3 (18%)
5	7MG	AN1	2065	5	22,26,27	3.81	10 (45%)	29,39,42	2.02	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	5MC	sN1	964	31	18,22,23	3.61	7 (38%)	26,32,35	1.00	2 (7%)
31	2MG	sN1	963	31	18,26,27	2.52	7 (38%)	16,38,41	1.40	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	AN1	2601	5	-	0/7/25/26	0/2/2/2
31	MA6	sN1	1516	31	-	3/7/29/30	0/3/3/3
52	4SU	v	8	52	-	4/7/25/26	0/2/2/2
5	PSU	AN1	2453	5	-	0/7/25/26	0/2/2/2
5	OMU	AN1	2548	5	-	2/9/27/28	0/2/2/2
5	6MZ	AN1	2026	5	-	2/5/27/28	0/3/3/3
31	PSU	sN1	513	31	-	0/7/25/26	0/2/2/2
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2
5	3TD	AN1	1911	5	-	5/7/25/26	0/2/2/2
31	4OC	sN1	1399	31	-	2/9/29/30	0/2/2/2
5	2MG	AN1	2441	5	-	1/5/27/28	0/3/3/3
5	PSU	AN1	1913	5	-	4/7/25/26	0/2/2/2
5	5MU	AN1	1935	5	-	0/7/25/26	0/2/2/2
5	OMG	AN1	2247	5	-	0/5/27/28	0/3/3/3
31	7MG	sN1	524	31	-	3/7/37/38	0/3/3/3
31	UR3	sN1	1495	31	-	0/7/25/26	0/2/2/2
5	PSU	AN1	2576	5	-	0/7/25/26	0/2/2/2
31	MA6	sN1	1515	31	-	3/7/29/30	0/3/3/3
52	PSU	v	56	52	-	0/7/25/26	0/2/2/2
5	PSU	AN1	1907	5	-	1/7/25/26	0/2/2/2
5	PSU	AN1	952	5	-	0/7/25/26	0/2/2/2
52	H2U	v	20	52	-	3/7/38/39	0/2/2/2
5	2MA	AN1	2499	55,5	-	2/3/25/26	0/3/3/3
52	5MU	v	55	52	-	6/7/25/26	0/2/2/2
31	2MG	sN1	1204	31	-	0/5/27/28	0/3/3/3
5	7MG	AN1	2065	5	-	3/7/37/38	0/3/3/3
31	5MC	sN1	964	31	-	0/7/25/26	0/2/2/2
31	2MG	sN1	963	31	-	0/5/27/28	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	1911	3TD	C6-C5	12.14	1.49	1.35
52	v	55	5MU	C2-N1	11.44	1.56	1.38
5	AN1	1935	5MU	C2-N1	11.34	1.56	1.38
52	v	55	5MU	C6-N1	11.11	1.57	1.38
5	AN1	1935	5MU	C6-N1	10.89	1.56	1.38
52	v	55	5MU	C4-C5	10.04	1.61	1.44
5	AN1	1935	5MU	C4-C5	9.96	1.61	1.44
31	sN1	524	7MG	C8-N9	9.92	1.51	1.46
52	v	8	4SU	C2-N1	9.81	1.54	1.38
52	v	20	H2U	C2-N1	9.72	1.49	1.35
5	AN1	2065	7MG	C8-N9	9.63	1.51	1.46
5	AN1	1911	3TD	C2-N1	9.54	1.49	1.37
31	sN1	964	5MC	C6-C5	9.21	1.49	1.34
52	v	8	4SU	C4-N3	8.17	1.46	1.37
31	sN1	524	7MG	C5-N7	7.86	1.44	1.35
5	AN1	2065	7MG	C5-N7	7.73	1.44	1.35
52	v	55	5MU	C4-N3	-7.37	1.25	1.38
5	AN1	2499	2MA	C2-N3	7.36	1.46	1.31
5	AN1	1935	5MU	C4-N3	-7.34	1.25	1.38
5	AN1	2548	OMU	C2-N1	7.13	1.49	1.38
31	sN1	1495	UR3	C2-N1	7.01	1.48	1.38
52	v	8	4SU	C2-N3	6.94	1.50	1.38
31	sN1	1399	4OC	C4-N3	6.92	1.44	1.32
31	sN1	1495	UR3	C6-C5	6.84	1.51	1.35
52	v	8	4SU	C5-C4	6.75	1.51	1.42
5	AN1	2548	OMU	C2-N3	6.72	1.49	1.38
5	AN1	1935	5MU	C6-C5	6.71	1.45	1.34
52	v	55	5MU	C6-C5	6.66	1.45	1.34
31	sN1	964	5MC	C4-N3	6.60	1.45	1.34
5	AN1	2026	6MZ	C6-N6	6.59	1.45	1.35
52	v	8	4SU	C6-C5	6.58	1.50	1.35
52	v	20	H2U	C2-N3	6.35	1.49	1.38
31	sN1	1399	4OC	C6-C5	6.31	1.49	1.35
31	sN1	1399	4OC	C2-N3	6.26	1.49	1.36
31	sN1	964	5MC	C2-N3	6.10	1.48	1.36
5	AN1	1911	3TD	C6-N1	6.00	1.46	1.36
31	sN1	524	7MG	C2-N3	5.99	1.47	1.33
5	AN1	2065	7MG	C2-N3	5.86	1.47	1.33
31	sN1	1495	UR3	C2-N3	5.85	1.50	1.39
5	AN1	2548	OMU	C6-C5	5.73	1.48	1.35
31	sN1	524	7MG	C4-N9	5.71	1.44	1.37
31	sN1	524	7MG	C4-N3	5.63	1.47	1.34
5	AN1	2065	7MG	C4-N3	5.54	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2247	OMG	C2-N3	5.52	1.46	1.33
31	sN1	1204	2MG	C2-N2	5.50	1.45	1.33
31	sN1	963	2MG	C2-N2	5.49	1.45	1.33
5	AN1	2065	7MG	C4-N9	5.45	1.44	1.37
5	AN1	2441	2MG	C2-N2	5.44	1.45	1.33
5	AN1	2499	2MA	C4-N3	5.25	1.50	1.37
31	sN1	1204	2MG	C4-N3	5.05	1.49	1.37
31	sN1	963	2MG	C4-N3	5.02	1.49	1.37
31	sN1	1399	4OC	C4-N4	4.96	1.46	1.35
5	AN1	2441	2MG	C4-N3	4.94	1.49	1.37
31	sN1	524	7MG	C2-N2	4.93	1.45	1.34
52	v	20	H2U	C4-N3	4.92	1.46	1.37
5	AN1	1911	3TD	C2-N3	4.90	1.49	1.38
5	AN1	2247	OMG	C4-N3	4.85	1.49	1.37
31	sN1	1204	2MG	C2-N1	4.85	1.44	1.36
31	sN1	963	2MG	C2-N1	4.84	1.44	1.36
5	AN1	2065	7MG	C2-N2	4.84	1.45	1.34
5	AN1	2441	2MG	C2-N1	4.75	1.44	1.36
31	sN1	964	5MC	C6-N1	4.63	1.45	1.38
31	sN1	964	5MC	C4-N4	4.38	1.45	1.34
31	sN1	1399	4OC	C2-N1	4.36	1.49	1.40
52	v	8	4SU	C4-S4	-4.35	1.60	1.68
31	sN1	964	5MC	C2-N1	4.30	1.49	1.40
5	AN1	2548	OMU	C4-N3	4.20	1.46	1.38
5	AN1	2247	OMG	C2-N2	4.05	1.43	1.34
31	sN1	1399	4OC	C5-C4	3.91	1.49	1.40
5	AN1	2247	OMG	C6-N1	3.85	1.43	1.37
31	sN1	524	7MG	C2-N1	3.84	1.47	1.37
5	AN1	2065	7MG	C2-N1	3.78	1.47	1.37
31	sN1	513	PSU	C6-C5	3.75	1.39	1.35
31	sN1	963	2MG	C6-N1	3.72	1.43	1.37
5	AN1	1913	PSU	C6-C5	3.65	1.39	1.35
52	v	56	PSU	C6-C5	3.62	1.39	1.35
31	sN1	1204	2MG	C6-N1	3.59	1.43	1.37
5	AN1	2441	2MG	C6-N1	3.58	1.43	1.37
31	sN1	524	7MG	C5-C6	3.56	1.52	1.43
5	AN1	1907	PSU	C6-C5	3.55	1.39	1.35
5	AN1	2500	PSU	C6-C5	3.53	1.39	1.35
5	AN1	2065	7MG	C5-C6	3.45	1.52	1.43
31	sN1	1495	UR3	C6-N1	3.40	1.46	1.38
5	AN1	952	PSU	C6-C5	3.39	1.39	1.35
5	AN1	2453	PSU	C6-C5	3.37	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2576	PSU	C6-C5	3.37	1.39	1.35
31	sN1	1399	4OC	C6-N1	3.36	1.46	1.38
5	AN1	2601	PSU	C6-C5	3.36	1.39	1.35
31	sN1	524	7MG	C6-N1	3.27	1.44	1.38
5	AN1	2065	7MG	C6-N1	3.25	1.44	1.38
52	v	55	5MU	O4-C4	-3.15	1.17	1.23
5	AN1	2441	2MG	C5-C6	3.13	1.53	1.47
31	sN1	1204	2MG	C5-C6	3.13	1.53	1.47
31	sN1	963	2MG	C5-C6	3.12	1.53	1.47
5	AN1	2247	OMG	C5-C6	2.97	1.53	1.47
5	AN1	2499	2MA	C6-N1	2.93	1.44	1.38
5	AN1	2548	OMU	C6-N1	2.92	1.45	1.38
5	AN1	2548	OMU	O4-C4	-2.92	1.18	1.24
52	v	8	4SU	C6-N1	2.87	1.44	1.38
5	AN1	1935	5MU	O4-C4	-2.87	1.18	1.23
31	sN1	964	5MC	O2-C2	-2.74	1.18	1.23
5	AN1	1911	3TD	C4-N3	2.73	1.46	1.40
5	AN1	2499	2MA	C5-C4	-2.66	1.36	1.43
31	sN1	1515	MA6	C2-N3	2.65	1.36	1.32
5	AN1	2026	6MZ	C5-C4	-2.65	1.33	1.40
5	AN1	2065	7MG	O6-C6	-2.59	1.18	1.23
31	sN1	1399	4OC	O2-C2	-2.58	1.18	1.23
31	sN1	1516	MA6	C5-C4	-2.58	1.34	1.40
52	v	8	4SU	O2-C2	-2.58	1.18	1.23
5	AN1	2499	2MA	C2-N1	2.57	1.44	1.36
31	sN1	1516	MA6	C2-N3	2.57	1.36	1.32
31	sN1	1515	MA6	C5-C4	-2.55	1.34	1.40
31	sN1	524	7MG	O6-C6	-2.55	1.18	1.23
5	AN1	2441	2MG	C5-C4	-2.55	1.36	1.43
5	AN1	2247	OMG	C5-C4	-2.55	1.36	1.43
31	sN1	963	2MG	C5-C4	-2.51	1.36	1.43
5	AN1	2247	OMG	O6-C6	-2.50	1.18	1.23
5	AN1	2247	OMG	C2-N1	2.49	1.43	1.37
31	sN1	1204	2MG	C5-C4	-2.47	1.36	1.43
5	AN1	1935	5MU	O2-C2	-2.46	1.18	1.23
52	v	20	H2U	O2-C2	-2.44	1.18	1.23
5	AN1	2548	OMU	C5-C4	2.42	1.49	1.43
52	v	55	5MU	O2-C2	-2.36	1.18	1.23
5	AN1	2548	OMU	O2-C2	-2.35	1.18	1.23
5	AN1	1911	3TD	O2-C2	-2.32	1.18	1.23
31	sN1	1495	UR3	C4-N3	2.32	1.46	1.40
31	sN1	1495	UR3	C5-C4	2.30	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2026	6MZ	C2-N3	2.26	1.35	1.32
5	AN1	2441	2MG	O6-C6	-2.20	1.18	1.23
31	sN1	963	2MG	O6-C6	-2.18	1.18	1.23
31	sN1	1204	2MG	O6-C6	-2.13	1.19	1.23
5	AN1	1911	3TD	O4-C4	-2.02	1.18	1.23

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	sN1	1516	MA6	N1-C6-N6	-14.99	101.28	117.06
31	sN1	1515	MA6	N1-C6-N6	-14.13	102.19	117.06
5	AN1	2026	6MZ	C1'-N9-C4	-13.18	103.48	126.64
52	v	55	5MU	C5-C4-N3	12.50	125.98	115.31
5	AN1	1935	5MU	C5-C4-N3	12.14	125.67	115.31
5	AN1	1935	5MU	C5-C6-N1	-10.20	112.84	123.34
52	v	55	5MU	C5-C6-N1	-9.94	113.11	123.34
52	v	8	4SU	C4-N3-C2	-7.60	119.96	127.34
52	v	20	H2U	C4-N3-C2	-6.64	120.28	125.79
31	sN1	1516	MA6	N3-C2-N1	-5.60	119.92	128.68
31	sN1	1515	MA6	N3-C2-N1	-5.45	120.16	128.68
5	AN1	2026	6MZ	N3-C2-N1	-5.28	120.42	128.68
5	AN1	2548	OMU	C4-N3-C2	-5.21	119.70	126.58
5	AN1	1911	3TD	N1-C2-N3	5.13	120.18	116.14
31	sN1	524	7MG	C5-C6-N1	5.06	119.91	110.99
52	v	8	4SU	C5-C4-N3	4.99	119.32	114.69
5	AN1	2065	7MG	C5-C6-N1	4.99	119.78	110.99
52	v	55	5MU	C4-N3-C2	-4.98	120.90	127.35
52	v	55	5MU	O4-C4-C5	-4.93	119.19	124.90
5	AN1	1935	5MU	C4-N3-C2	-4.91	121.00	127.35
5	AN1	1935	5MU	O4-C4-C5	-4.87	119.26	124.90
31	sN1	1495	UR3	C4-N3-C2	-4.79	120.06	124.56
5	AN1	2453	PSU	C4-N3-C2	-4.64	119.65	126.34
5	AN1	2500	PSU	C4-N3-C2	-4.60	119.71	126.34
5	AN1	2601	PSU	C4-N3-C2	-4.60	119.71	126.34
5	AN1	952	PSU	C4-N3-C2	-4.58	119.75	126.34
5	AN1	2453	PSU	N1-C2-N3	4.57	120.31	115.13
5	AN1	2576	PSU	C4-N3-C2	-4.57	119.76	126.34
52	v	55	5MU	N3-C2-N1	4.56	120.94	114.89
5	AN1	2576	PSU	N1-C2-N3	4.55	120.29	115.13
5	AN1	1907	PSU	C4-N3-C2	-4.54	119.80	126.34
5	AN1	952	PSU	N1-C2-N3	4.53	120.26	115.13
31	sN1	524	7MG	C2-N3-C4	4.47	120.27	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AN1	2500	PSU	N1-C2-N3	4.47	120.19	115.13
5	AN1	1935	5MU	N3-C2-N1	4.47	120.82	114.89
5	AN1	1907	PSU	N1-C2-N3	4.44	120.16	115.13
5	AN1	2601	PSU	N1-C2-N3	4.43	120.15	115.13
5	AN1	2065	7MG	C2-N3-C4	4.41	120.15	112.30
5	AN1	1911	3TD	C4-N3-C2	-4.33	119.91	124.61
5	AN1	1913	PSU	C4-N3-C2	-4.31	120.13	126.34
5	AN1	1913	PSU	N1-C2-N3	4.25	119.94	115.13
31	sN1	524	7MG	C5-C4-N3	-4.13	120.26	128.13
52	v	56	PSU	N1-C2-N3	4.10	119.77	115.13
52	v	56	PSU	C4-N3-C2	-4.07	120.48	126.34
52	v	8	4SU	N3-C2-N1	4.02	120.22	114.89
5	AN1	2065	7MG	C5-C4-N3	-4.02	120.47	128.13
31	sN1	513	PSU	C4-N3-C2	-3.92	120.69	126.34
31	sN1	513	PSU	N1-C2-N3	3.82	119.46	115.13
5	AN1	2548	OMU	N3-C2-N1	3.82	119.95	114.89
52	v	55	5MU	C5M-C5-C6	-3.75	117.84	122.85
52	v	55	5MU	C5M-C5-C4	3.73	122.87	118.77
5	AN1	1935	5MU	C5M-C5-C6	-3.71	117.89	122.85
5	AN1	2499	2MA	C5-C6-N1	3.52	120.10	114.02
31	sN1	963	2MG	C5-C6-N1	3.50	120.13	113.95
31	sN1	1204	2MG	C5-C6-N1	3.48	120.11	113.95
5	AN1	2247	OMG	C5-C6-N1	3.47	120.09	113.95
5	AN1	2441	2MG	C5-C6-N1	3.43	120.01	113.95
5	AN1	1935	5MU	C5M-C5-C4	3.39	122.50	118.77
5	AN1	2548	OMU	C5-C4-N3	3.35	119.86	114.84
31	sN1	964	5MC	C5-C6-N1	-3.26	119.99	123.34
5	AN1	2065	7MG	C4-C5-N7	3.19	109.96	105.53
31	sN1	524	7MG	C4-C5-N7	3.18	109.94	105.53
5	AN1	2026	6MZ	C2-N1-C6	3.12	119.27	116.59
5	AN1	2247	OMG	C2-N1-C6	-3.10	119.38	125.10
5	AN1	2499	2MA	C8-N7-C5	3.07	108.84	102.99
52	v	20	H2U	N3-C2-N1	3.06	119.89	116.65
31	sN1	524	7MG	C5-C4-N9	3.04	110.30	106.35
5	AN1	2065	7MG	C5-C4-N9	2.99	110.23	106.35
52	v	8	4SU	C5-C4-S4	-2.98	120.63	124.47
5	AN1	2548	OMU	O4-C4-C5	-2.83	120.18	125.16
31	sN1	524	7MG	C2-N1-C6	-2.81	119.98	125.10
31	sN1	524	7MG	O6-C6-C5	-2.78	120.71	127.54
5	AN1	2065	7MG	O6-C6-C5	-2.77	120.73	127.54
52	v	55	5MU	O4-C4-N3	-2.76	114.83	120.12
5	AN1	2065	7MG	C2-N1-C6	-2.74	120.09	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AN1	2247	OMG	C8-N7-C5	2.74	108.21	102.99
52	v	20	H2U	C5-C4-N3	2.70	119.69	116.65
52	v	20	H2U	C5-C6-N1	2.67	120.40	111.61
31	sN1	524	7MG	N9-C4-N3	2.66	129.44	125.47
31	sN1	1204	2MG	C8-N7-C5	2.65	108.05	102.99
5	AN1	1907	PSU	O2-C2-N1	-2.64	119.88	122.79
5	AN1	1935	5MU	O4-C4-N3	-2.63	115.07	120.12
5	AN1	2576	PSU	O2-C2-N1	-2.61	119.91	122.79
5	AN1	2500	PSU	O2-C2-N1	-2.61	119.92	122.79
5	AN1	952	PSU	O2-C2-N1	-2.58	119.94	122.79
31	sN1	963	2MG	C8-N7-C5	2.58	107.91	102.99
5	AN1	2441	2MG	C8-N7-C5	2.57	107.89	102.99
5	AN1	2065	7MG	N9-C4-N3	2.56	129.29	125.47
5	AN1	1913	PSU	O2-C2-N1	-2.48	120.06	122.79
5	AN1	2601	PSU	O2-C2-N1	-2.46	120.08	122.79
5	AN1	2453	PSU	O2-C2-N1	-2.46	120.08	122.79
52	v	55	5MU	O2-C2-N1	-2.41	119.59	122.79
31	sN1	1399	4OC	C6-C5-C4	2.37	119.86	116.96
5	AN1	1911	3TD	C6-C5-C4	2.36	119.85	118.22
5	AN1	1935	5MU	O2-C2-N1	-2.34	119.68	122.79
31	sN1	963	2MG	O6-C6-C5	-2.31	119.86	124.37
31	sN1	524	7MG	N9-C8-N7	2.31	106.68	103.38
52	v	8	4SU	C1'-N1-C2	2.31	121.75	117.57
31	sN1	1204	2MG	O6-C6-C5	-2.26	119.95	124.37
5	AN1	1913	PSU	C6-N1-C2	-2.26	120.37	122.68
5	AN1	2065	7MG	N9-C8-N7	2.26	106.60	103.38
5	AN1	2247	OMG	O6-C6-C5	-2.25	119.97	124.37
52	v	56	PSU	O2-C2-N1	-2.25	120.31	122.79
5	AN1	2576	PSU	C6-N1-C2	-2.24	120.39	122.68
5	AN1	2441	2MG	O6-C6-C5	-2.23	120.02	124.37
52	v	56	PSU	C6-N1-C2	-2.21	120.43	122.68
5	AN1	952	PSU	C6-N1-C2	-2.19	120.45	122.68
5	AN1	2453	PSU	C6-N1-C2	-2.17	120.47	122.68
5	AN1	1907	PSU	C6-N1-C2	-2.16	120.47	122.68
31	sN1	513	PSU	O4'-C1'-C2'	2.12	108.14	105.14
5	AN1	2500	PSU	C6-N1-C2	-2.09	120.55	122.68
5	AN1	2601	PSU	C6-N1-C2	-2.07	120.56	122.68
5	AN1	2453	PSU	O4'-C1'-C2'	2.04	108.02	105.14
5	AN1	2453	PSU	C6-C5-C4	2.03	119.62	118.20
52	v	20	H2U	O2-C2-N1	-2.03	120.56	123.11
31	sN1	964	5MC	CM5-C5-C6	-2.03	120.14	122.85
5	AN1	2576	PSU	O4'-C1'-C2'	2.02	108.00	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	sN1	513	PSU	C6-N1-C2	-2.02	120.61	122.68
52	v	56	PSU	O4'-C1'-C2'	2.01	107.98	105.14
5	AN1	2576	PSU	C6-C5-C4	2.01	119.60	118.20
5	AN1	1913	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	sN1	1515	MA6	C5-C6-N6-C9
31	sN1	1516	MA6	C5-C6-N6-C10
31	sN1	1516	MA6	N1-C6-N6-C10
5	AN1	1911	3TD	O4'-C4'-C5'-O5'
5	AN1	1913	PSU	O4'-C1'-C5-C4
5	AN1	1913	PSU	O4'-C1'-C5-C6
5	AN1	2499	2MA	O4'-C4'-C5'-O5'
5	AN1	2548	OMU	C3'-C4'-C5'-O5'
5	AN1	2548	OMU	O4'-C4'-C5'-O5'
52	v	8	4SU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C1'-N1-C6
31	sN1	524	7MG	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	C3'-C4'-C5'-O5'
5	AN1	2026	6MZ	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	C3'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
5	AN1	2065	7MG	O4'-C4'-C5'-O5'
5	AN1	2499	2MA	C3'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
31	sN1	1515	MA6	N1-C6-N6-C9
52	v	55	5MU	C2'-C1'-N1-C6
52	v	20	H2U	C3'-C4'-C5'-O5'
31	sN1	524	7MG	O4'-C4'-C5'-O5'
31	sN1	1399	4OC	O4'-C4'-C5'-O5'
5	AN1	2065	7MG	C3'-C4'-C5'-O5'
31	sN1	1515	MA6	C5-C6-N6-C10
52	v	8	4SU	O4'-C4'-C5'-O5'
5	AN1	1907	PSU	C4'-C5'-O5'-P
52	v	8	4SU	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C1'-N1-C6
52	v	55	5MU	C2'-C1'-N1-C2
31	sN1	524	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
31	sN1	1516	MA6	C5-C6-N6-C9
5	AN1	1913	PSU	O4'-C4'-C5'-O5'
52	v	55	5MU	O4'-C1'-N1-C2
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	1911	3TD	O4'-C1'-C5-C6
52	v	20	H2U	C2'-C1'-N1-C2
5	AN1	2065	7MG	C4'-C5'-O5'-P
5	AN1	1913	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AN1	1911	3TD	2	0
5	AN1	1913	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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.

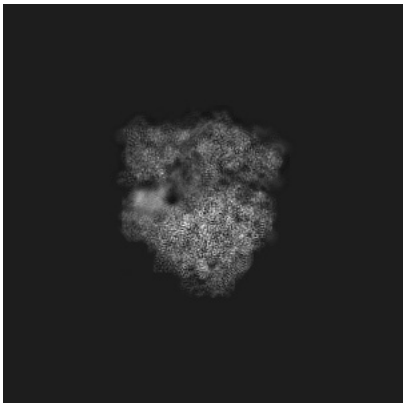
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21031. These allow visual inspection of the internal detail of the map and identification of artifacts.

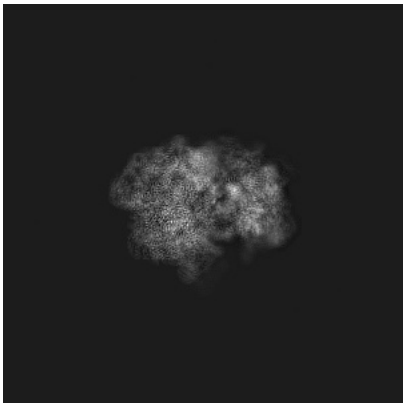
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

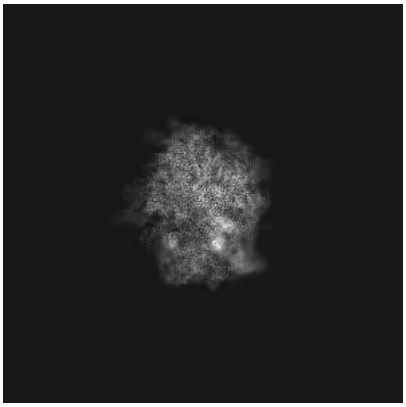
6.1.1 Primary map



X



Y



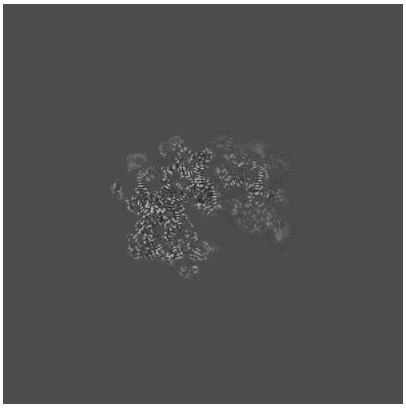
Z

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

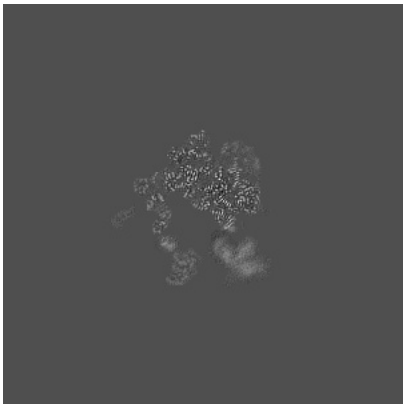
6.2 Central slices

6.2.1 Primary map

X Index: 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: 256

Y Index: 270

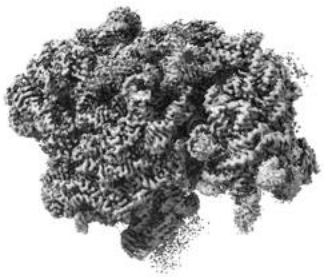
Z Index: 219

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

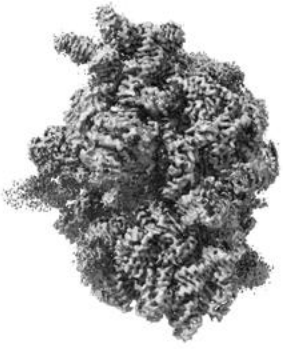
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

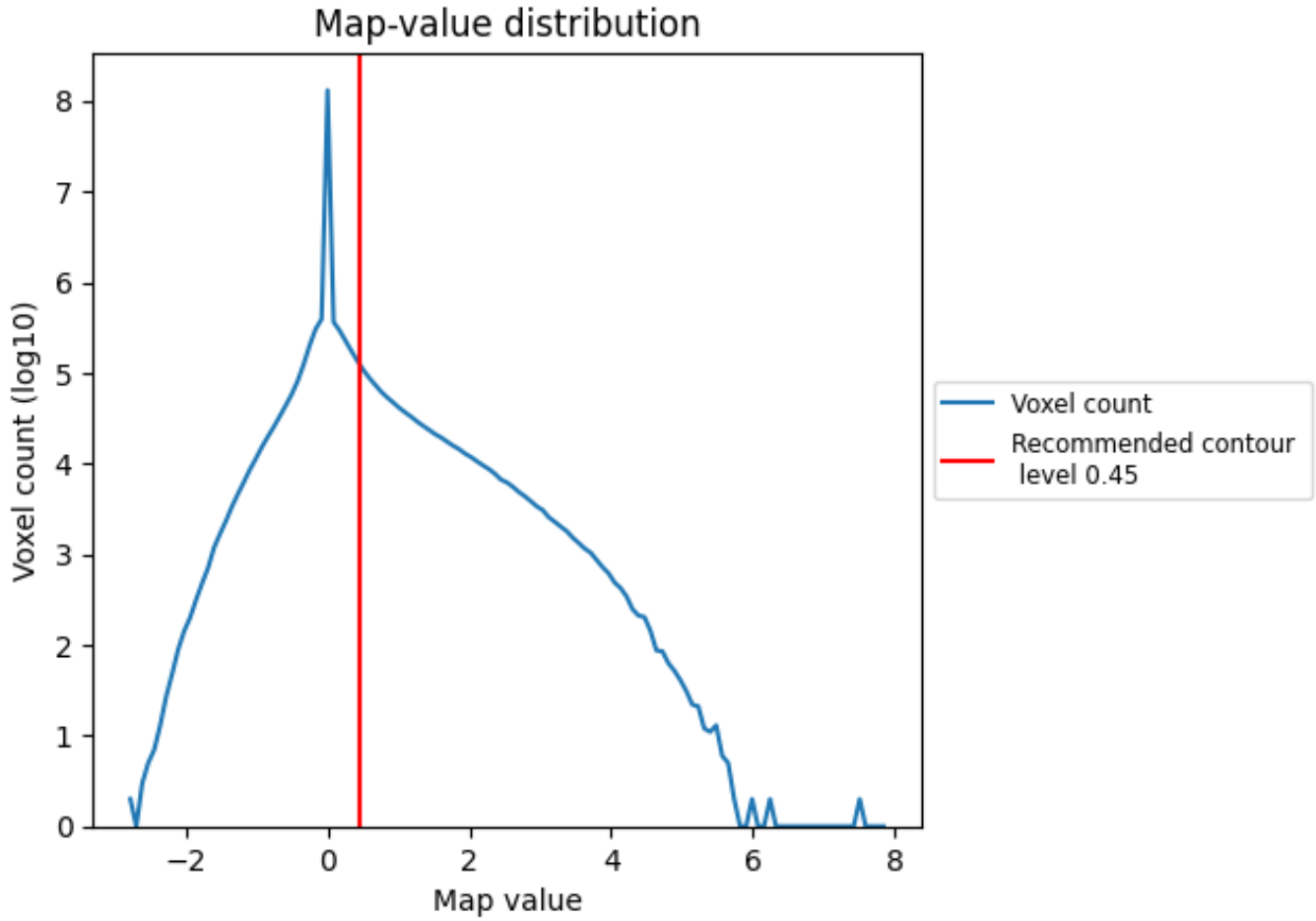
6.5 Mask visualisation (i)

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

7 Map analysis

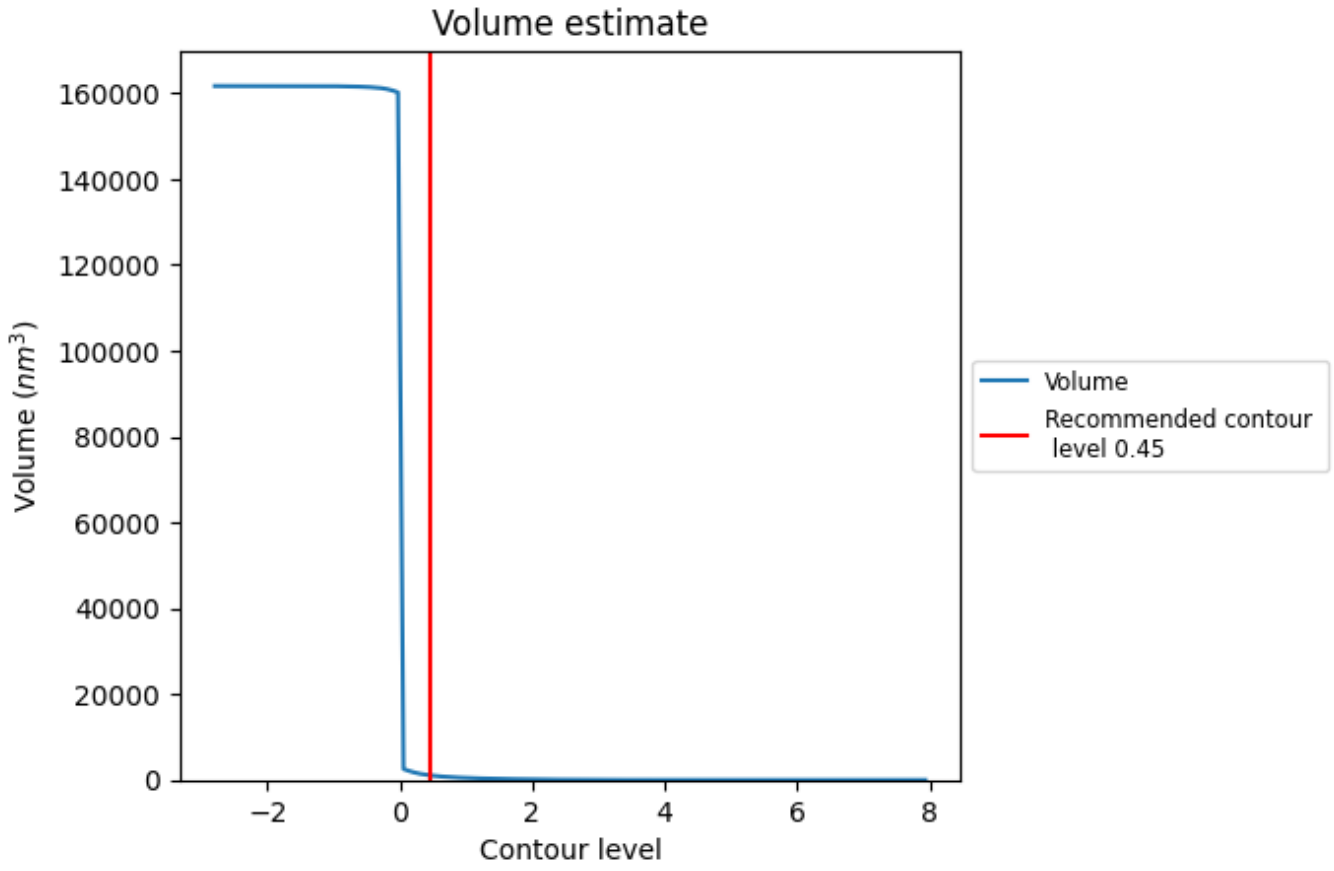
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

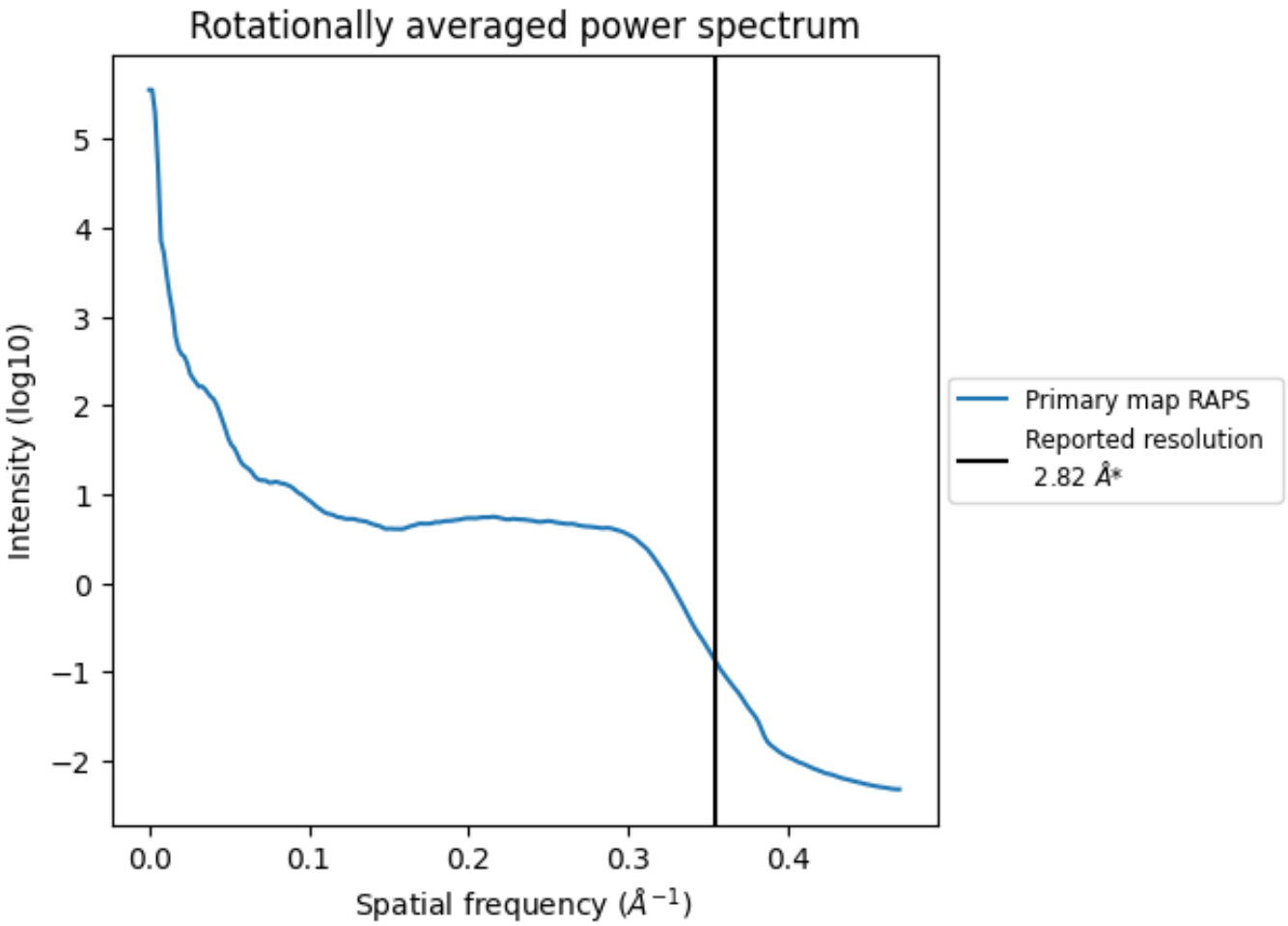
7.2 Volume estimate



The volume at the recommended contour level is 1088 nm^3; this corresponds to an approximate mass of 983 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 0.355 Å^{-1}

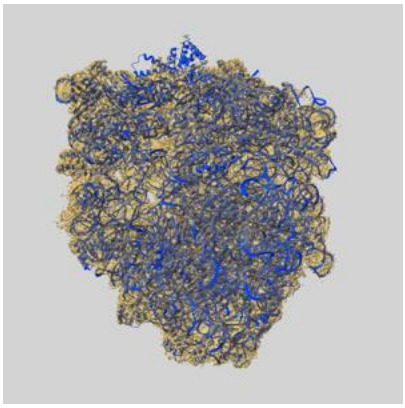
8 Fourier-Shell correlation (i)

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

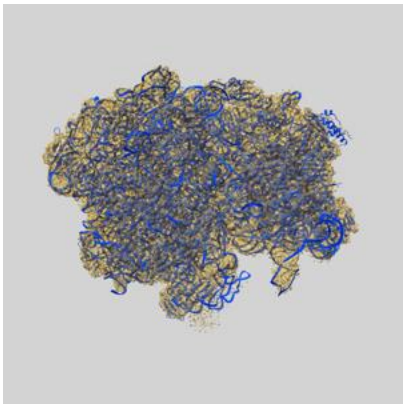
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21031 and PDB model 6V3A. Per-residue inclusion information can be found in section 3 on page 14.

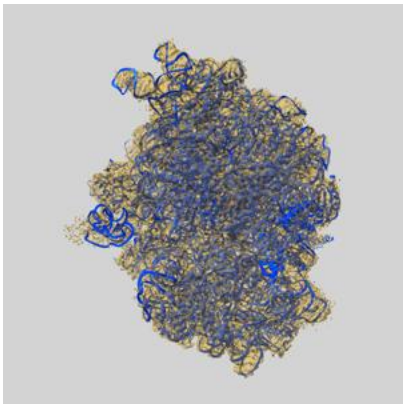
9.1 Map-model overlay



X



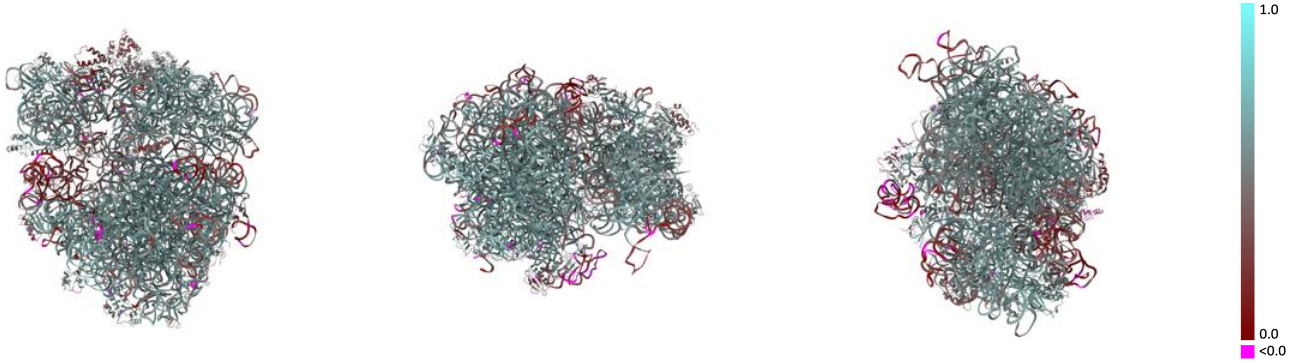
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

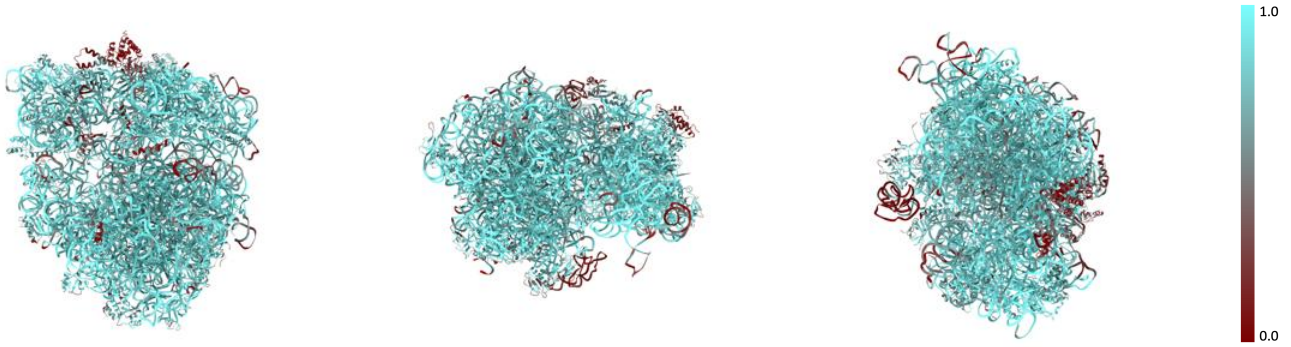
9.2 Q-score mapped to coordinate model



X Y Z

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

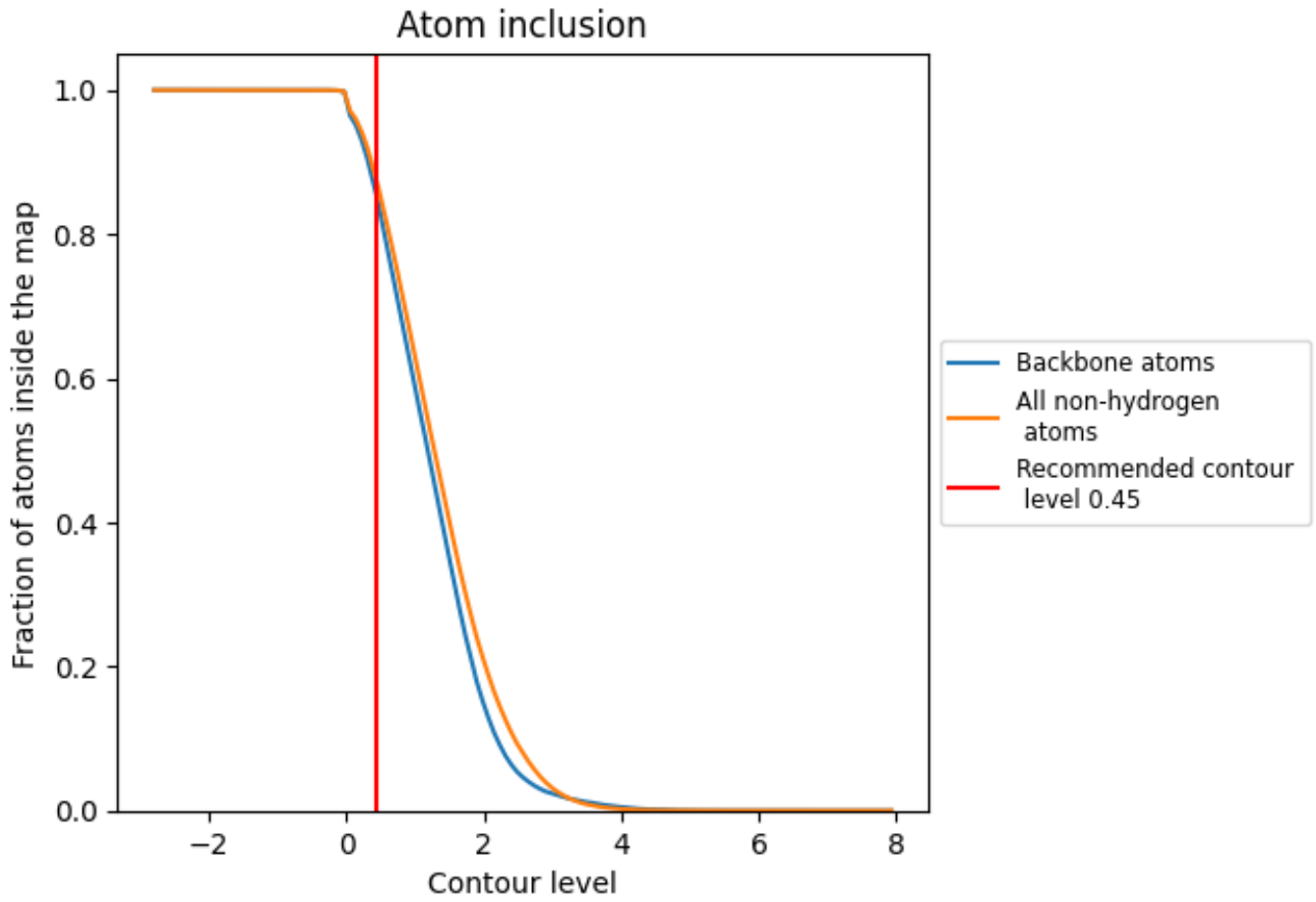
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

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

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8717	0.5310
0	0.8201	0.5320
1	0.9592	0.6400
2	0.9549	0.6160
3	0.8846	0.5580
AN1	0.9083	0.5450
B	0.9053	0.4910
C	0.8993	0.5900
D	0.8726	0.5680
E	0.8692	0.5660
F	0.5717	0.3150
G	0.6857	0.4060
H	0.3764	0.2810
I	0.8653	0.5610
J	0.8999	0.5900
K	0.8797	0.5680
L	0.8897	0.5740
M	0.9692	0.6260
N	0.8359	0.5020
O	0.8432	0.5540
P	0.9226	0.5990
Q	0.8782	0.5650
R	0.8492	0.5590
S	0.8565	0.5430
T	0.7835	0.4870
U	0.7900	0.5080
V	0.8818	0.5960
W	0.8858	0.5860
X	0.7377	0.4540
Y	0.8256	0.5280
Z	0.8322	0.5490
b	0.2028	0.3490
c	0.8659	0.5540
d	0.6946	0.4610
e	0.8840	0.5550

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Chain	Atom inclusion	Q-score
f	0.4876	0.3840
g	0.6410	0.4680
h	0.9141	0.5900
i	0.9185	0.5950
j	0.8241	0.5440
k	0.5054	0.3910
l	0.6915	0.5210
m	0.8884	0.5580
n	0.8954	0.5770
o	0.8799	0.5490
p	0.9250	0.5870
q	0.8555	0.5650
r	0.7052	0.4950
s	0.9444	0.5980
sN1	0.9039	0.5300
t	0.8995	0.5640
u	0.0914	0.2790
v	0.9444	0.3080
w	0.9538	0.2530