Full wwPDB EM Validation Report (i)

Feb 13, 2024 – 06:17 PM EST

PDB ID	:	3J6B
EMDB ID	:	EMD-2566
Title	:	Structure of the yeast mitochondrial large ribosomal subunit
Authors	:	Amunts, A.; Brown, A.; Bai, X.C.; Llacer, J.L.; Hussain, T.; Emsley, P.; Long, F.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-01-22
Resolution	:	3.20 Å(reported)

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

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

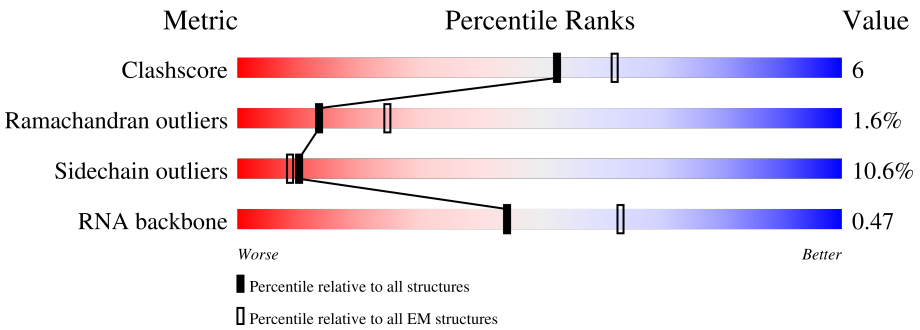
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	3296	48% 26% 8% 18%
2	B	393	55% 18% • 25%
3	C	269	74% 16% • 7%
4	D	286	62% 18% • 16%
5	E	292	78% 15% • 6%
6	F	214	66% 17% • 14%
7	G	139	35% 5% 60%

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Mol	Chain	Length	Quality of chain
8	H	163	74% 14% 9%
9	I	138	80% 10% 9%
10	J	322	57% 9% 32%
11	K	232	66% 15% 16%
12	L	238	81% 13%
13	M	169	73% 13% 11%
14	N	161	65% 9% 27%
15	O	309	57% 14% 28%
16	P	263	60% 17% 21%
17	Q	297	79% 13% 6%
18	R	371	68% 16% 14%
19	S	258	46% 10% 43%
20	T	319	53% 11% 34%
21	U	86	84% 12% 5%
22	V	177	34% 64%
23	W	183	48% 12% 39%
24	X	70	79% 11% 9%
25	Y	105	35% 6% 57%
26	Z	115	45% 7% 46%
27	0	93	38% 59%
28	1	367	74% 15% 10%
29	2	147	61% 14% 23%
30	3	146	75% 11% 14%
31	4	140	77% 18%
32	5	390	69% 13% 16%

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Mol	Chain	Length	Quality of chain
33	6	281	62% 11% 26%
34	7	146	53% 19% 27%
35	8	264	58% 10% 31%
36	9	253	62% 13% 23%
37	a	195	77% 12% 10%
38	b	157	84% 14%
39	c	131	84% 6% 10%
40	d	226	78% 12% 10%
41	e	20	70% 65% 35%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	ZN	0	100	-	-	X	-

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 195137 atoms, of which 83818 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 21S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2713	86569	25948	28898	10265	18752	2706	0	0

- Molecule 2 is a protein called 54S ribosomal protein RML2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	295	4603	1405	2343	459	387	9	0	0

- Molecule 3 is a protein called 54S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	249	3906	1217	1976	360	343	10	0	0

- Molecule 4 is a protein called 54S ribosomal protein YmL6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	239	3780	1187	1914	337	339	3	0	0

- Molecule 5 is a protein called 54S ribosomal protein L7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	274	4294	1363	2169	387	369	6	0	0

- Molecule 6 is a protein called 54S ribosomal protein L6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	185	2747	870	1392	236	246	3	0	0

- Molecule 7 is a protein called 54S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	55	929	293	471	86	78	1	0	0

- Molecule 8 is a protein called 54S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	148	2394	742	1218	225	205	4	0	0

- Molecule 9 is a protein called 54S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	125	1952	583	1015	175	168	11	0	0

- Molecule 10 is a protein called 54S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	220	3555	1109	1828	325	290	3	0	0

- Molecule 11 is a protein called 54S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	195	3208	1001	1635	297	270	5	0	0

- Molecule 12 is a protein called 54S ribosomal protein L8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	229	3698	1139	1883	333	335	8	0	0

- Molecule 13 is a protein called 54S ribosomal protein IMG1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	151	2492	766	1286	220	217	3	0	0

- Molecule 14 is a protein called 54S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	N	118	1958	598	1010	177	171	2	0	0

- Molecule 15 is a protein called 54S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	223	3684	1147	1895	328	309	5	0	0

- Molecule 16 is a protein called 54S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	P	207	3450	1101	1728	310	305	6	0	0

- Molecule 17 is a protein called 54S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	279	4287	1368	2161	375	375	8	0	0

- Molecule 18 is a protein called 54S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	R	318	4981	1571	2500	452	454	4	0	0

- Molecule 19 is a protein called 54S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	S	146	2440	763	1249	220	207	1	0	0

- Molecule 20 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	T	209	3264	1044	1618	307	292	3	0	0

- Molecule 21 is a protein called 54S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
21	U	82	1341	410	702	116	113	0	0

- Molecule 22 is a protein called 54S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	V	64	1083	332	555	105	90	1	0	0

- Molecule 23 is a protein called 54S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	W	112	1922	587	985	181	163	6	0	0

- Molecule 24 is a protein called 54S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
24	X	64	1077	330	565	96	86	0	0

- Molecule 25 is a protein called 54S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
25	Y	45	788	239	412	80	57	0	0

- Molecule 26 is a protein called mitochondrial ribosomal protein YNL122C.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Z	62	1054	322	546	111	74	1	0	0

- Molecule 27 is a protein called 54S ribosomal protein RTC6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	0	38	673	205	349	66	50	3	0	0

- Molecule 28 is a protein called 54S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	1	332	5397	1744	2690	467	490	6	0	0

- Molecule 29 is a protein called 54S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	2	113	1858	583	939	169	162	5	0	0

- Molecule 30 is a protein called 54S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	3	126	2025	643	1030	181	168	3	0	0

- Molecule 31 is a protein called 54S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	4	138	2263	700	1146	219	193	5	0	0

- Molecule 32 is a protein called 54S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	5	326	5026	1596	2541	425	453	11	0	0

- Molecule 33 is a protein called 54S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	6	209	3187	1046	1595	273	271	2	0	0

- Molecule 34 is a protein called 54S ribosomal protein IMG2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	7	106	1755	550	901	150	152	2	0	0

- Molecule 35 is a protein called 54S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	8	182	2829	898	1416	241	271	3	0	0

- Molecule 36 is a protein called 54S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	9	195	2865	919	1437	250	254	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	169	GLY	ASP	conflict	UNP P36523

- Molecule 37 is a protein called 54S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	a	176	2882	898	1455	264	259	6	0	0

- Molecule 38 is a protein called 54S ribosomal protein L25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	b	155	2671	850	1372	225	221	3	0	0

- Molecule 39 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	c	118	2066	643	1066	190	163	4	0	0

- Molecule 40 is a protein called Mitochondrial homologous recombination protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	d	204	3423	1099	1706	313	299	6	0	0

- Molecule 41 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
41	e	20	648	191	221	81	136	19	0	0

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
42	A	109	109	109	0
			Total	Mg	
42	N	1	1	1	0

- Molecule 43 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
43	B	1	1	1	0

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

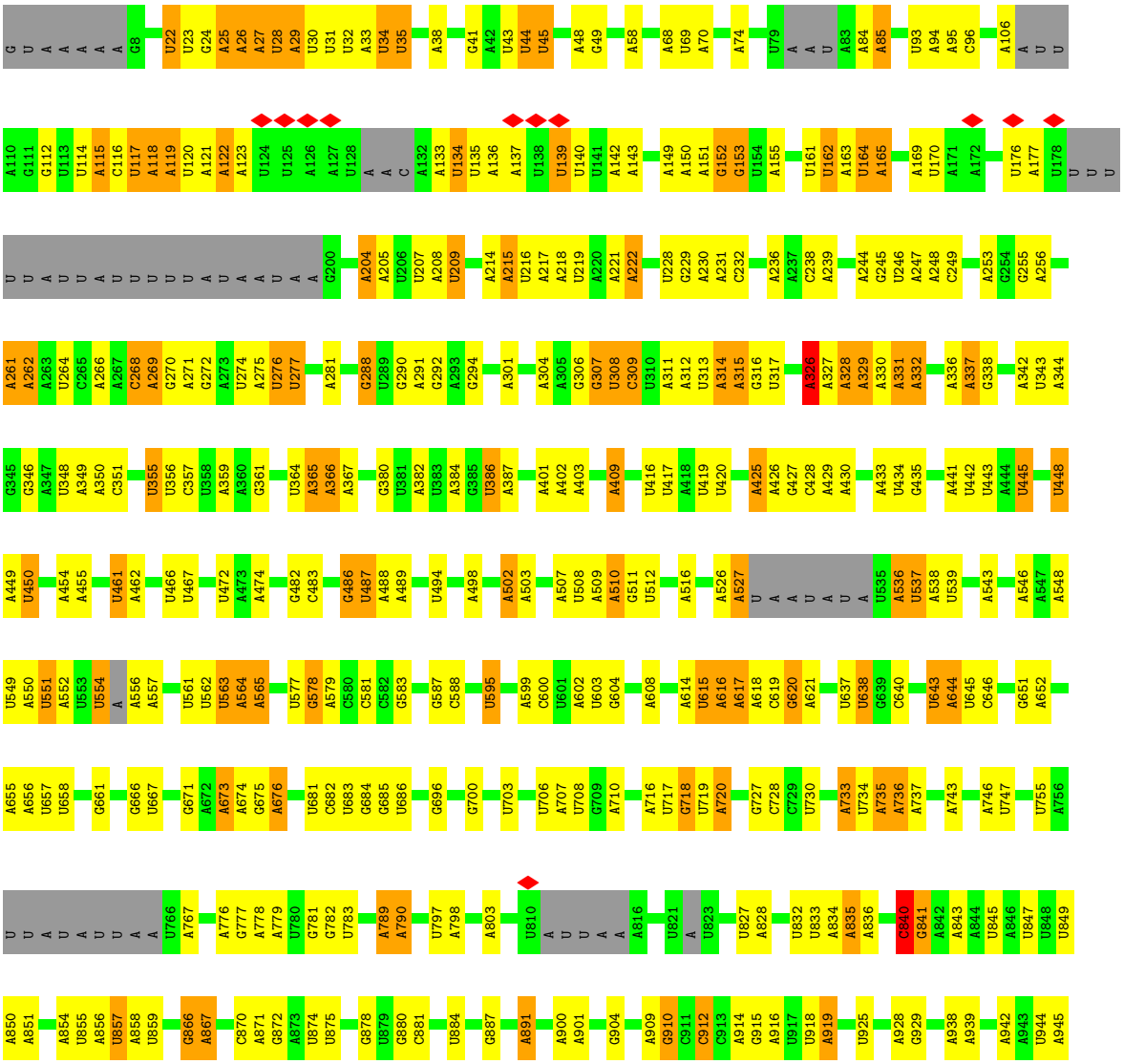
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
44	W	1	1	1	0
			Total	Zn	
44	0	1	1	1	0

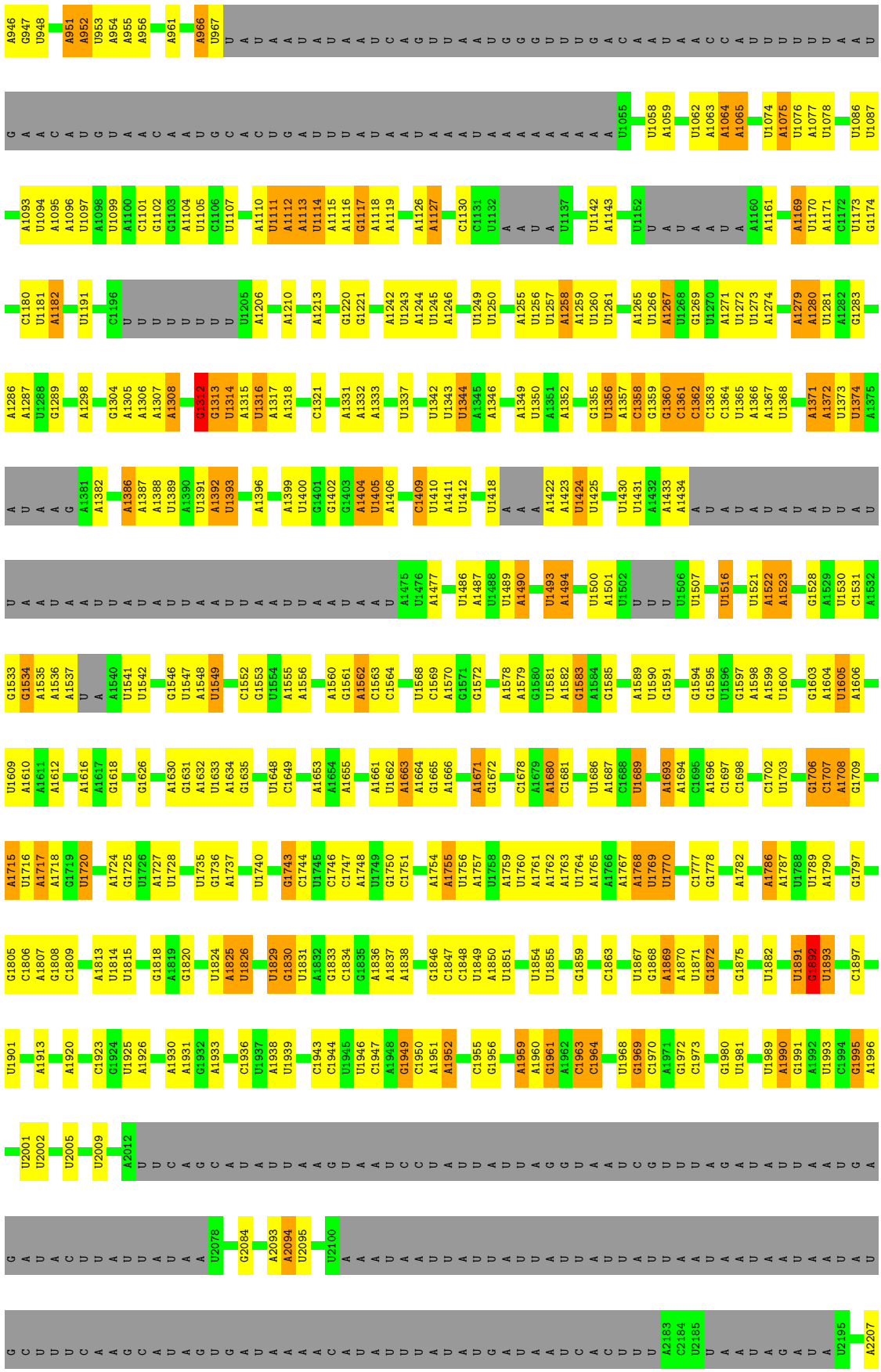
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 21S ribosomal RNA

Chain A: 48% 26% 8% 18%

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U1055 U1058 A1059 U1062 A1063 A1064 A1065 U1074 A1075 U1076 A1077 U1078 U1086 U1087
A1093 U1094 A1095 A1096 U1097 A1098 U1099 A1100 C1101 G1102 G1103 A1104 U1105 C1106 U1107 A1110 U1111 A1112 A1113 U1114 A1115 A1116 G1117 A1118 A1119 A1126 A1127 C1130 C1131 U1132 A A U A A1137 U1142 A1143 U1152 U A U A A1160 A1161 A1169 U1170 A1171 C1172 U1173 G1174
C1180 U1181 A1182 U1191 C1196 U U U U U U U U1205 A1206 A1210 A1213 G1220 G1221 A1242 U1243 A1244 U1245 A1246 U1249 U1250 A1255 U1256 U1257 A1258 A1259 U1260 U1261 A1265 U1266 A1267 U1268 G1269 U1270 A1271 U1272 U1273 A1274 A1279 A1280 U1281 A1282 G1283
A1286 A1287 U1288 G1289 A1298 G1304 A1305 A1306 A1307 A1308 G1312 G1313 U1314 A1315 U1316 A1317 A1318 C1321 A1331 A1332 A1333 U1337 U1342 U1343 U1344 A1345 A1346 A1349 U1350 A1351 A1352 G1355 U1356 A1357 C1358 G1359 G1360 C1361 C1362 C1363 C1364 U1365 A1366 A1367 U1368 A1371 A1372 U1373 U1374 A1375
A U A A G A1381 A1382 A1386 A1387 A1388 U1389 A1390 U1391 A1392 U1393 A1396 A1399 U1400 G1401 G1402 G1403 A1404 U1405 A1406 C1409 U1410 A1411 U1412 U1418 A A A A1422 A1423 U1424 U1425 U1430 U1431 A1432 A1433 A1434 A U A U A U A U A
U A A U A A U U A U U A A U U U A A U A A U A U A A U A1475 U1476 A1477 U1486 A1487 U1488 U1489 A1490 U1493 A1494 U1500 A1501 U1502 U U U U1506 U1507 U1516 U1521 A1522 A1523 G1528 A1529 U1530 C1531 A1532
G1533 G1534 A1535 A1536 A1537 U A A1540 U1541 U1542 G1546 U1547 A1548 U1549 C1552 G1553 U1554 A1555 A1556 A1560 G1561 A1562 C1563 C1564 U1568 C1569 A1570 G1571 G1572 A1578 A1579 G1580 U1581 A1582 G1583 A1584 G1585 A1589 U1590 G1591 G1594 G1595 U1596 G1597 A1598 A1599 U1600 G1603 A1604 U1605 A1606
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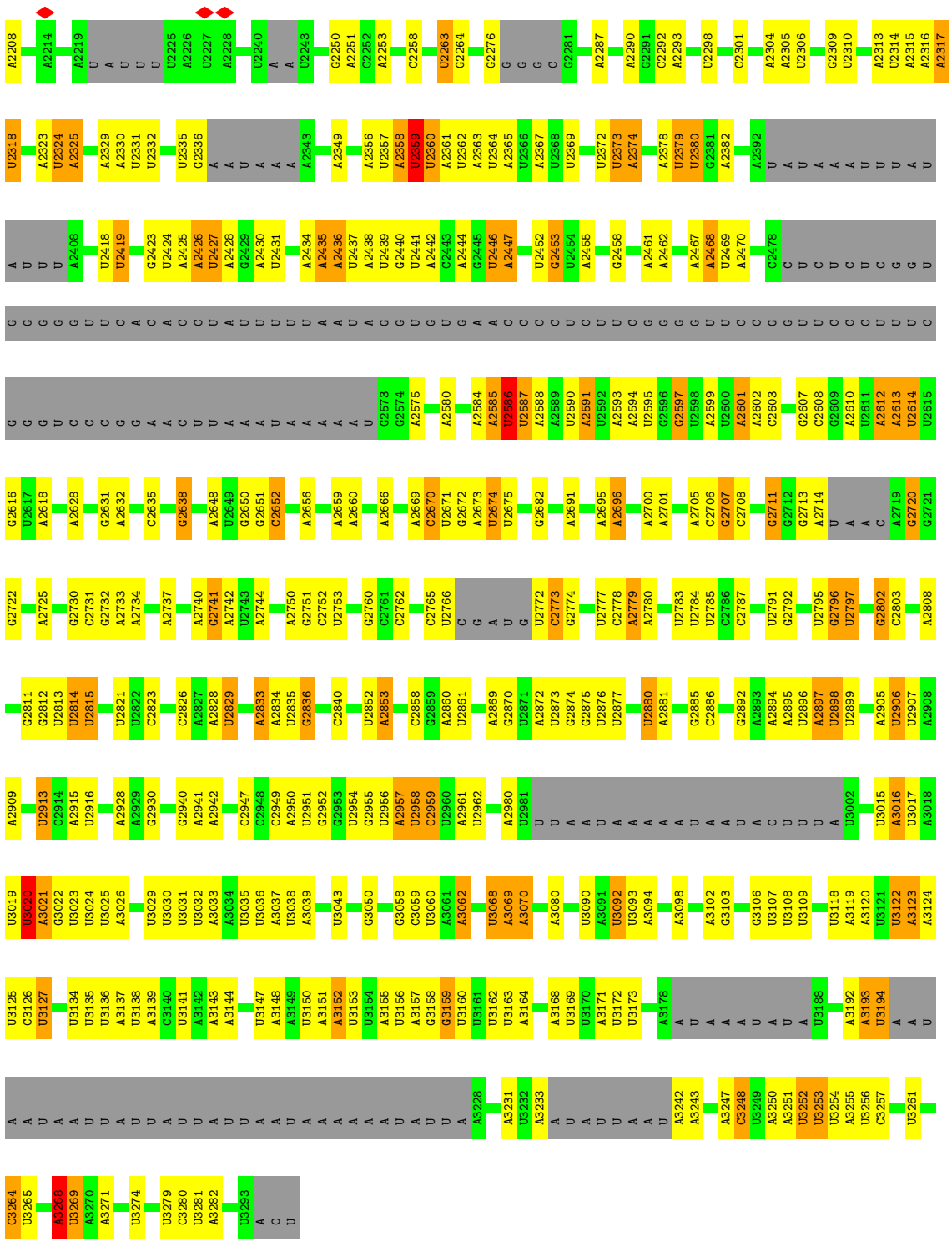
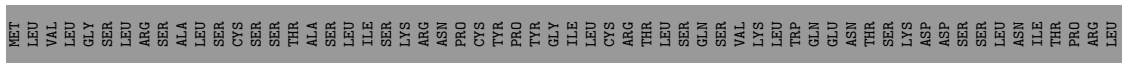
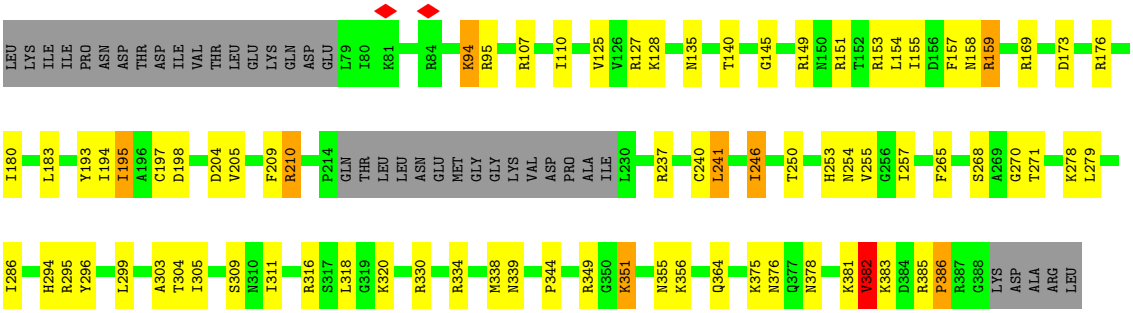
G1805 C1806 A1807 G1808 C1809 A1813 U1814 U1815 G1818 A1819 G1820 U1824 A1825 U1826 U1829 G1830 U1831 A1832 G1833 C1834 G1835 A1836 A1837 A1838 G1846 C1847 C1848 U1849 A1850 U1851 U1854 U1855 G1859 C1863 U1867 G1868 A1869 A1870 U1871 G1872 G1875 U1882 U1891 G1892 U1893 C1897
U1901 A1913 A1920 C1923 G1924 U1925 A1926 A1930 A1931 G1932 A1933 C1936 U1937 A1938 U1939 C1943 C1944 U1945 U1946 C1947 A1948 G1949 C1950 A1951 A1952 C1955 G1956 A1959 A1960 G1961 A1962 C1963 C1964 U1968 G1969 C1970 A1971 G1972 C1973 G1980 U1981 U1989 A1990 G1991 A1992 U1993 C1994 G1995 A1996
U2001 U2002 U2005 U2009 A2012 U U U C A G C A U A U U A A U U A U U A A U A A U U C C U A U U A U U A U U A U U A A A U C A U U A A U U A A A U U A A U U A A U U C A U U A A U U A A A U U A A A U U G A
G A U A C U U A U U A A A G U A A A U U A A U U A C A U U A A U U A A A U U A A A U U C A A U U A A A U U A A A U U A A A U U G A A U U A A A U U A A A U U A



• Molecule 2: 54S ribosomal protein RML2, mitochondrial

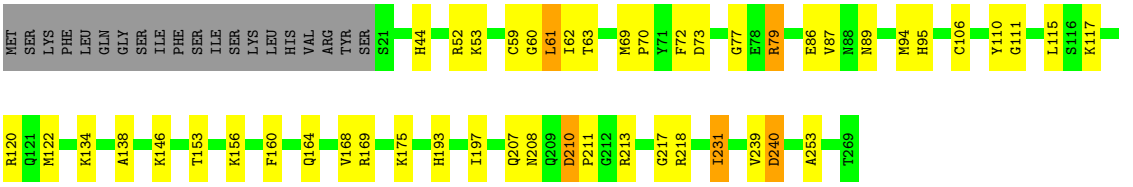
Chain B: 55% 18% • 25%





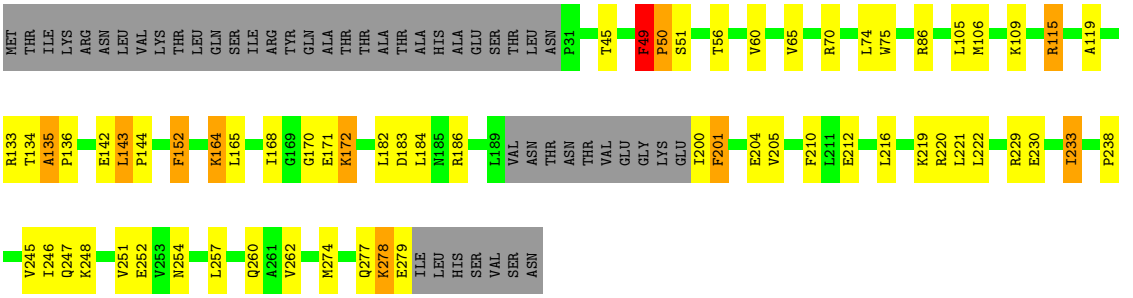
- Molecule 3: 54S ribosomal protein L9, mitochondrial

Chain C:



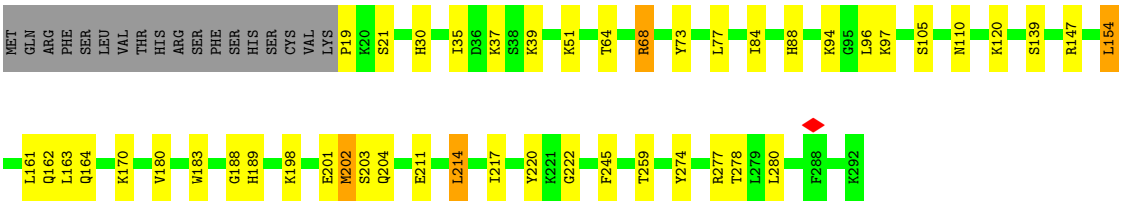
- Molecule 4: 54S ribosomal protein YmL6, mitochondrial

Chain D:



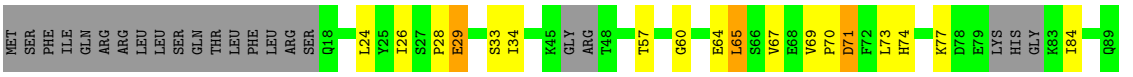
- Molecule 5: 54S ribosomal protein L7, mitochondrial

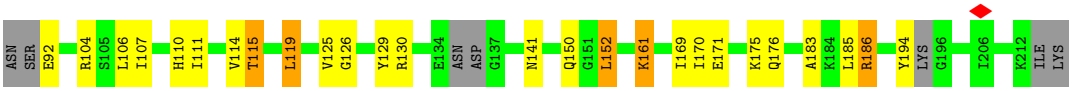
Chain E:



- Molecule 6: 54S ribosomal protein L6, mitochondrial

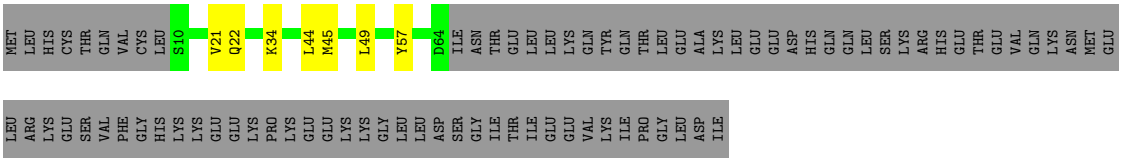
Chain F:





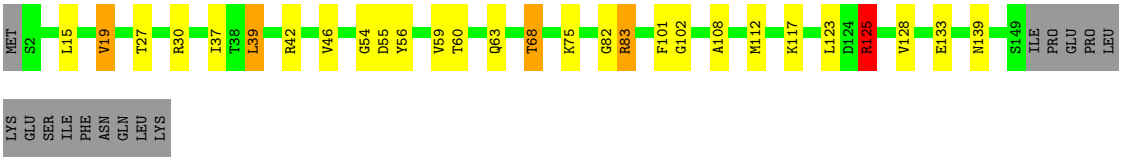
- Molecule 7: 54S ribosomal protein L50, mitochondrial

Chain G:



- Molecule 8: 54S ribosomal protein L23, mitochondrial

Chain H:

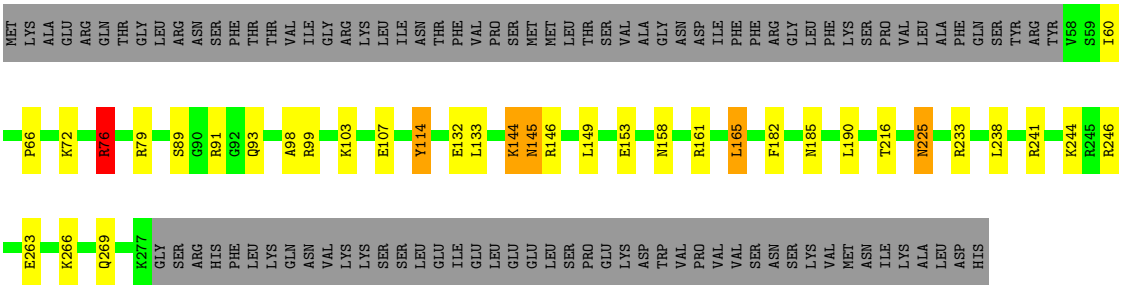


- Molecule 9: 54S ribosomal protein L38, mitochondrial

Chain I:

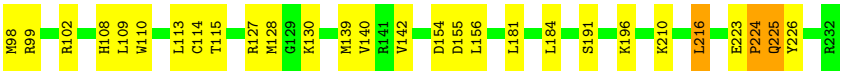
- Molecule 10: 54S ribosomal protein L10, mitochondrial

Chain J:



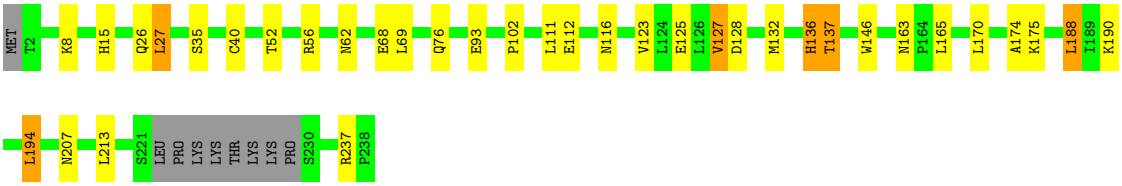
- Molecule 11: 54S ribosomal protein L16, mitochondrial

Chain K:



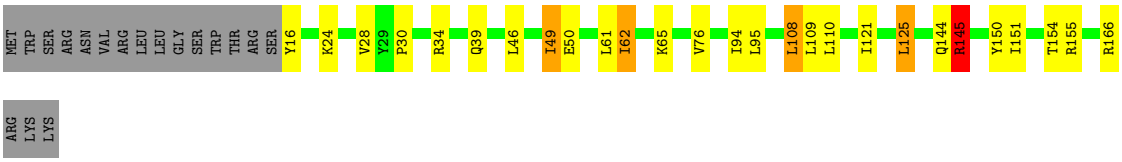
• Molecule 12: 54S ribosomal protein L8, mitochondrial

Chain L:



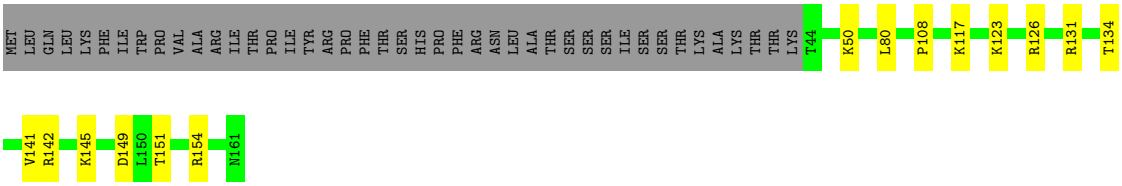
• Molecule 13: 54S ribosomal protein IMG1, mitochondrial

Chain M:



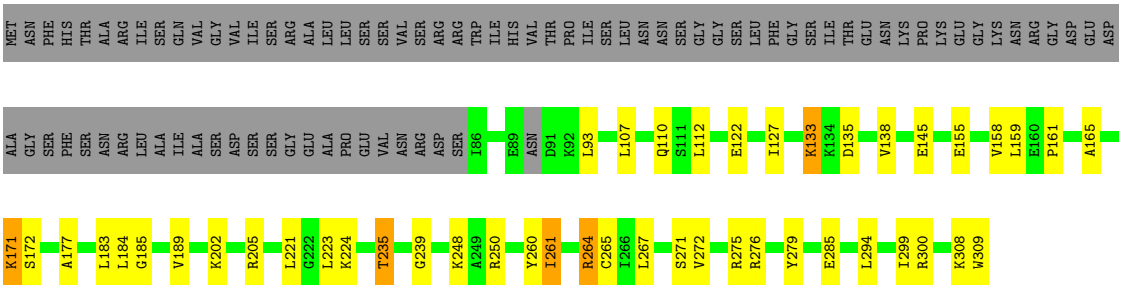
• Molecule 14: 54S ribosomal protein L49, mitochondrial

Chain N:



• Molecule 15: 54S ribosomal protein L22, mitochondrial

Chain O:



• Molecule 16: 54S ribosomal protein L41, mitochondrial

Chain P:

MET PRO ARG LEU THR VAL GLY THR LYS ASN MET LEU TYR PRO LEU GLN LYS THR LEU ALA VAL GLY SER CYS LYS PRO GLU GLN VAL PRO ILE ARG SER LEU ALA SER VAL VAL GLU SER SER SER LYS ILE LEU ASP LYS SER GLY SER ASP ARG GLU VAL D55 E60 W65

E71 Q72 N82 K83 K88 I92 L93 H100 Y103 K106 F107 F113 D117 L118 R119 D120 Y121 I125 L128 T134 T135 Q136 L137 L138 K141 M145 N146 L147 Q148 R151 I157 K158 K159 M160 T161 M164 P167 D177 F181 W182 D183

S184 T185 T186 P187 M190 E196 R197 I227 P228 R229 K232 R233 E234 I235 L255 N256 R257 D261 LEU HIS

- Molecule 17: 54S ribosomal protein L40, mitochondrial

Chain Q: 79% 13% • 6%

MET S2 Y5 S9 R14 L27 P28 T38 F55 K56 SER GLU K59 P65 R68 M72 S76 K77 G78 N79 I80 I83 F86 D87 K88 L95 D96 P100 T101 K102 T103 V104 P105 V124 L127 L131 R132 L133 V134 A135 ASP ILE ASP

ASP GLU LYS THR PRO GLY LYS THR ARG T148 V149 A163 ASP Y165 P170 V174 LYS GLY Q177 W184 P185 K186 N195 L196 R204 E205 Q206 D211 S212 V213 I218 R235 P252 L253 T254 R257 E271 V272 P273 R296 E297

- Molecule 18: 54S ribosomal protein L2, mitochondrial

Chain R: 68% 16% • 14%

MET TRP ASN PRO ILE LEU LEU ASP THR SER SER PHE SER PHE GLN LYS HIS VAL SER GLY VAL PHE LEU GLN VAL ARG ASN ALA THR LYS ARG ALA ALA GLY S35 R36 T37 S38 M39 K40 R45 R46 G54 T59 G60 E61 E75 N76 V77 I85 R104 L111 R112

R113 K116 L117 P118 S119 R128 F129 G130 E133 L134 T135 N136 K137 R138 E143 K155 P156 L159 K160 E163 K168 R169 L172 K175 L176 D182 E183 L184 D187 ILE LYS D190 I191 E192 L193 S196 Y197 L198 I199 R202 A203 S204 L205 I211 E212

D213 A214 R215 F216 K239 L254 N261 N262 K263 L264 E265 L266 L286 L304 F305 K306 L314 R322 K323 Y324 P330 GLU THR ASP SER THR VAL GLU THR LYS SER GLY LYS LYS SER ILE V346 K354 ASN LYS V357 R362 F367 L371

- Molecule 19: 54S ribosomal protein L24, mitochondrial

Chain S: 46% 10% • 43%

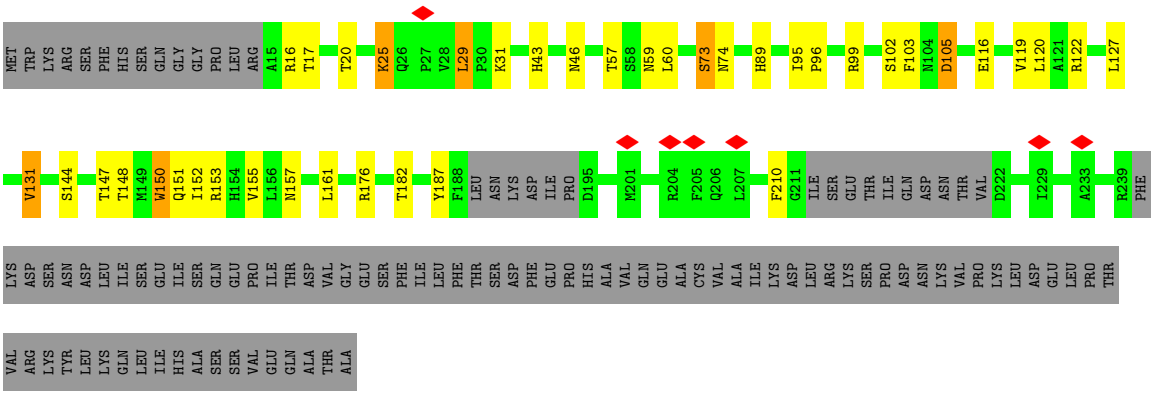
MET GLN LYS ILE PHE ARG PRO PHE GLN LEU THR ARG GLY PHE THR SER SER VAL LYS ASN PHE R22 Q23 W24 R25 I32 Q39 VAL GLY ASP ALA K44 E51 R52 Y58 I65 F66 L73 V79 T92 W96 V101 K102 K103 G104 L105 L110 S115

M118 V122 T125 I132 T137 K138 R155 V158 L159 K171 ASP ALA PRO ILE ILE GLU MET ALA GLY GLY LYS LYS ALA LYS ILE TYR TYR ASP GLU ILE VAL ASN GLY SER PRO ARG LYS ILE SER VAL GLY ARG ARG ARG LEU MET SER PHE LEU TYR PRO LEU

GLU LYS LEU GLU TYR ARG SER VAL GLY LYS ASP LEU ASN TYR LYS LYS PHE VAL GLU LEU PHE ALA ASP VAL PRO VAL LYS ASP ILE LEU ALA ARG LEU GLU ASP HIS LYS PHE ASP LEU SER THR ILE THR VAL

- Molecule 20: 54S ribosomal protein L4, mitochondrial

Chain T: 53% 11% • 34%

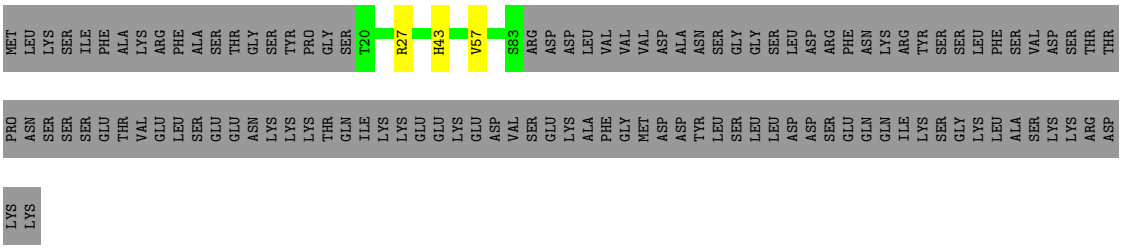


- Molecule 21: 54S ribosomal protein L33, mitochondrial

Chain U:

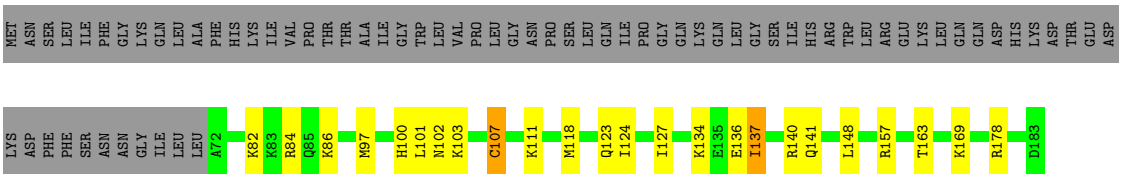
- Molecule 22: 54S ribosomal protein L36, mitochondrial

Chain V:



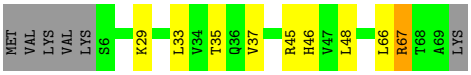
- Molecule 23: 54S ribosomal protein L32, mitochondrial

Chain W:



- Molecule 24: 54S ribosomal protein L39, mitochondrial

Chain X:



- Molecule 25: 54S ribosomal protein L34, mitochondrial

Chain Y: 35% 6% • 57%

MET PRO LEU PHE ALA ARG LEU CYS GLN PRO GLN SER ARG ARG MET PHE SER SER ILE SER SER PHE SER ALA LEU SER VAL LEU ARG PRO GLN THR GLY MET LEU LEU ASN SER SER PRO LEU LYS THR PRO SER PHE THR PRO LEU GLY PHE GLY LEU ILE GLY GLN ARG ARG TRP LYS

S61 L71 K72 R73 K74 R75 L80 R95 R100 L103 S104 H105

- Molecule 26: mitochondrial ribosomal protein YNL122C

Chain Z: 45% 7% • 46%

MET LYS ILE SER LEU HIS ASN LYS ARG GLN ARG GLY ASP GLN ASN GLN ASN MET SER VAL PHE ASN VAL LEU LYS PRO LEU LEU LYS GLY SER ASN SER PHE LYS VAL LYS LEU ASN GLY PHE LEU PHE ASN ASN VAL SER THR ILE THR ILE ARG THR L54 H58 K59 G60 R64

W65 R74 K92 T95 A100 L111 L112 H115

- Molecule 27: 54S ribosomal protein RTC6, mitochondrial

Chain 0: 38% • 59%

MET PHE LEU GLN THR LEU ARG LEU THR MET PRO ARG MET PHE LEU HIS MET LYS PRO SER PRO ILE THR ILE THR ARG ALA CYS THR VAL PRO SER LEU LEU SER VAL ALA ALA PRO GLN PRO ALA LEU VAL VAL ALA ALA ASN ARG PRO LEU VAL PHE ASN ARG GLY F56 R59 C66

G93

- Molecule 28: 54S ribosomal protein L35, mitochondrial

Chain 1: 74% 15% • 10%

MET LEU ARG ARG SER ILE HIS THR THR LYS ILE LEU GLN LYS PRO ASN ALA THR SER H20 Q45 LYS LYS ALA SER LEU ASP PRO P53 S54 I55 R58 I62 I70 I73 R84 E90 LEU ALA ASN LYS THR LYS N97 P98 D102 I110 P113 Q120

F121 N122 N123 K124 L125 V128 I131 V138 Y139 R140 H141 L142 G143 K144 L154 L155 M156 I165 P166 T171 L172 V173 P174 R175 A176 E177 I211 Q212 E213 Y214 E215 L216 V229 N230 P231 D232 V233 D239 K242 T243 Y247 G248 L249 D262 P263 R264 V291

I299 GLU ASP LYS Q303 L308 E314 F320 D321 I322 R323 Q324 K327 I334 G335 A336 H337 D344 A345 K346 R360 V361 R366 R367

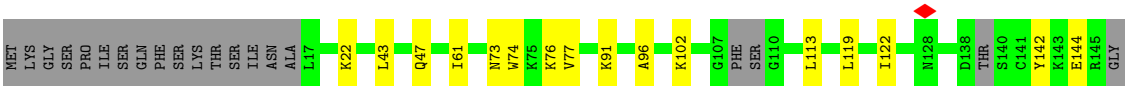
- Molecule 29: 54S ribosomal protein L28, mitochondrial

Chain 2: 61% 14% • 23%

MET LEU ALA GLN THR PHE LYS LYS PRO HIS ARG ALA VAL LEU GLU GLN VAL SER GLY THR THR VAL PHE ILE ARG ASN LYS ARG THR LYS SER LYS SER S34 R41 V42 V43 T44 Q45 V48 L58 L59 K60 D65 L66 I67 K68 T71 Q80 M102 R111

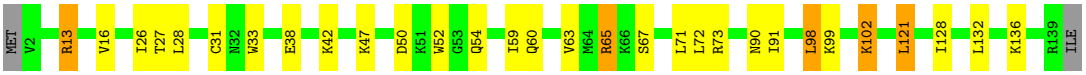
- Molecule 30: 54S ribosomal protein L27, mitochondrial

Chain 3:



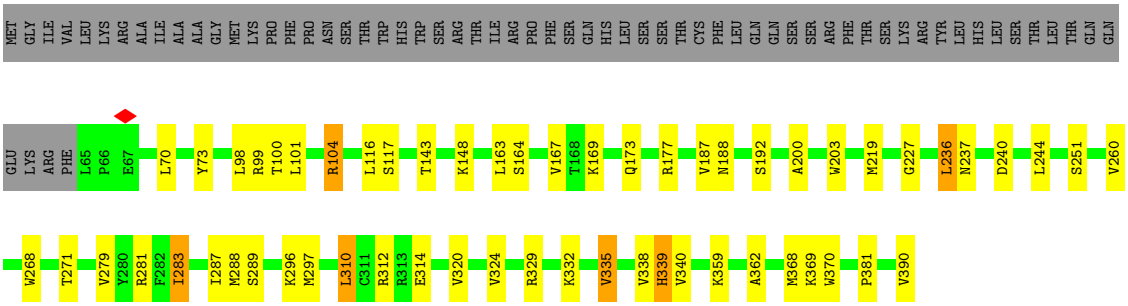
- Molecule 31: 54S ribosomal protein L51, mitochondrial

Chain 4:



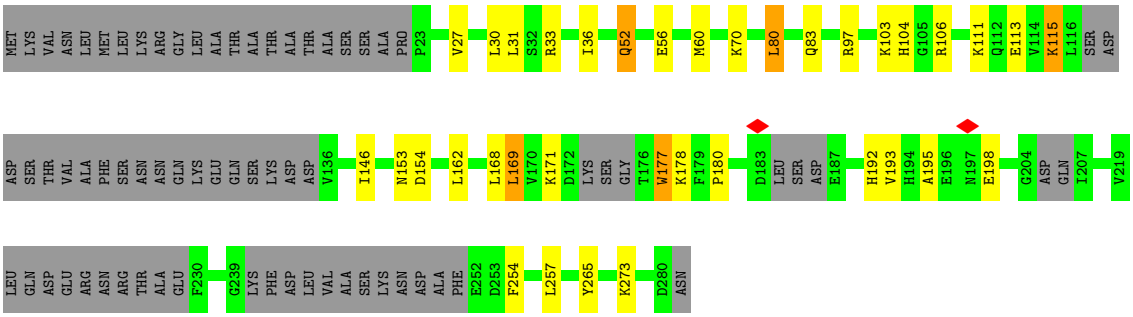
- Molecule 32: 54S ribosomal protein L3, mitochondrial

Chain 5:



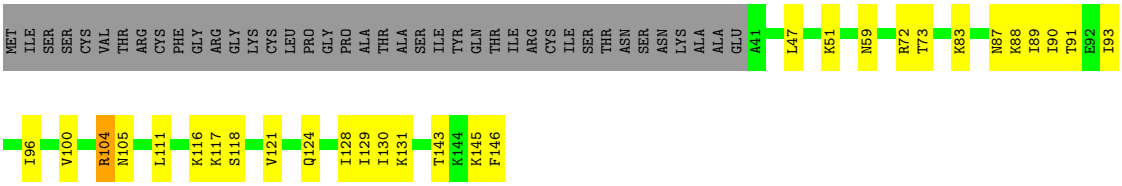
- Molecule 33: 54S ribosomal protein L17, mitochondrial

Chain 6:



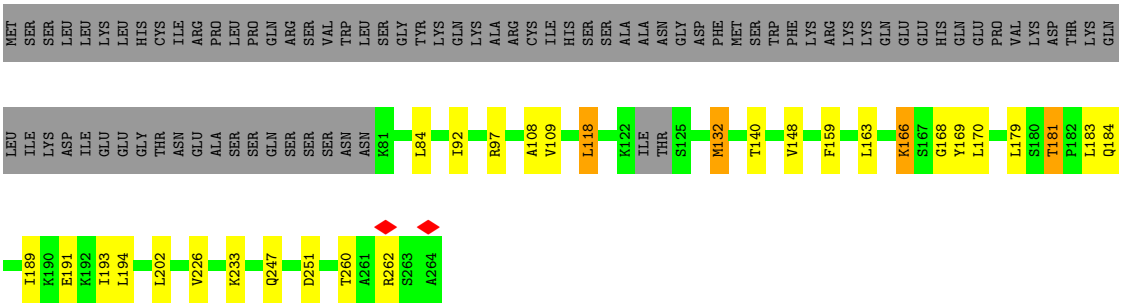
- Molecule 34: 54S ribosomal protein IMG2, mitochondrial

Chain 7:



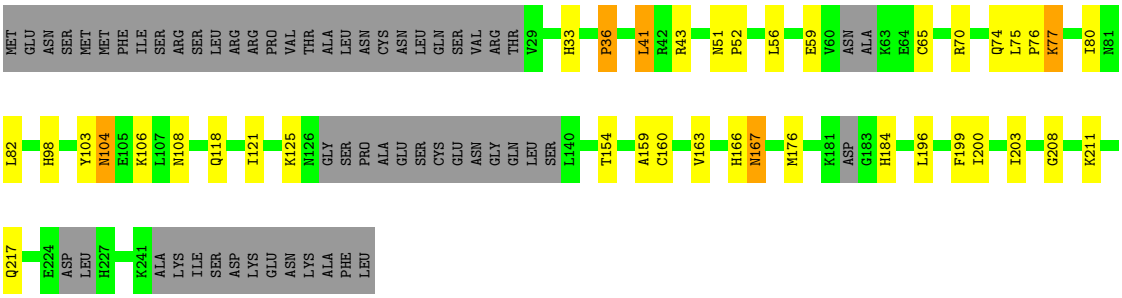
• Molecule 35: 54S ribosomal protein L13, mitochondrial

Chain 8:



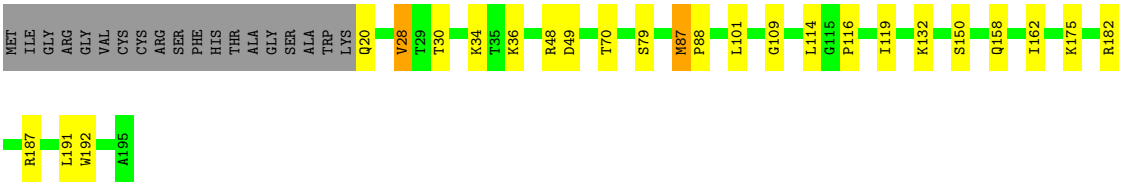
• Molecule 36: 54S ribosomal protein L15, mitochondrial

Chain 9:



• Molecule 37: 54S ribosomal protein L20, mitochondrial

Chain a:

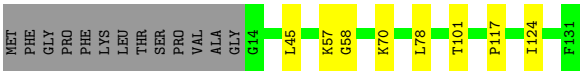


• Molecule 38: 54S ribosomal protein L25, mitochondrial

Chain b:

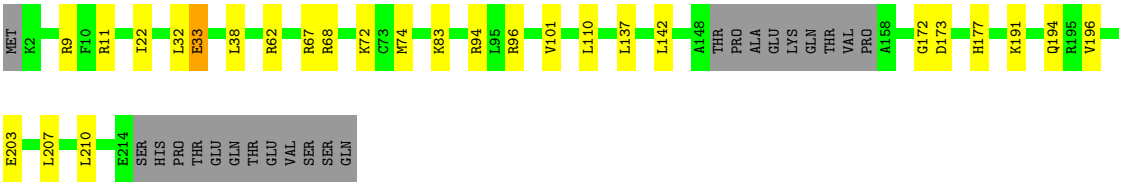
• Molecule 39: 54S ribosomal protein L31, mitochondrial

Chain c:



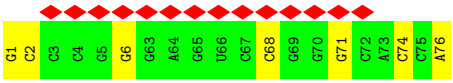
• Molecule 40: Mitochondrial homologous recombination protein 1

Chain d:



• Molecule 41: E-site tRNA

Chain e:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.687	Depositor
Minimum map value	-0.940	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.0681	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.24	0/64599	0.70	13/100487 (0.0%)
2	B	0.32	0/2305	0.66	0/3102
3	C	0.32	0/1973	0.59	0/2654
4	D	0.33	0/1904	0.65	0/2579
5	E	0.31	0/2181	0.54	0/2955
6	F	0.31	0/1376	0.58	0/1869
7	G	0.32	0/468	0.57	0/628
8	H	0.36	0/1200	0.63	1/1610 (0.1%)
9	I	0.30	0/943	0.58	0/1260
10	J	0.33	0/1764	0.66	2/2360 (0.1%)
11	K	0.33	0/1606	0.65	0/2148
12	L	0.35	0/1843	0.64	0/2486
13	M	0.30	0/1224	0.64	0/1651
14	N	0.30	0/961	0.61	0/1295
15	O	0.35	0/1821	0.68	0/2444
16	P	0.34	0/1766	0.63	0/2381
17	Q	0.31	0/2174	0.57	0/2946
18	R	0.36	0/2522	0.68	0/3392
19	S	0.34	0/1216	0.58	0/1626
20	T	0.36	0/1689	0.69	0/2297
21	U	0.38	0/648	0.67	0/870
22	V	0.28	0/539	0.54	0/726
23	W	0.33	0/955	0.65	0/1273
24	X	0.33	0/520	0.62	0/696
25	Y	0.44	0/383	0.69	0/504
26	Z	0.38	0/522	0.71	0/695
27	0	0.32	0/329	0.56	0/432
28	1	0.32	0/2777	0.61	0/3772
29	2	0.37	0/938	0.70	0/1264
30	3	0.31	0/1018	0.57	0/1368
31	4	0.33	0/1138	0.65	0/1526
32	5	0.34	0/2538	0.66	1/3451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.30	0/1631	0.54	0/2214
34	7	0.31	0/869	0.57	0/1166
35	8	0.35	0/1438	0.61	0/1945
36	9	0.34	0/1453	0.61	0/1969
37	a	0.33	0/1458	0.63	0/1961
38	b	0.34	0/1333	0.63	0/1783
39	c	0.35	0/1024	0.63	0/1367
40	d	0.34	0/1762	0.65	0/2381
41	e	0.21	0/476	0.73	2/739 (0.3%)
All	All	0.29	0/119284	0.67	19/174272 (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
1	A	1	0
3	C	0	1
4	D	0	1
10	J	0	1
20	T	0	1
37	a	0	1
All	All	1	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2897	A	C2'-C3'-O3'	7.88	126.83	109.50
1	A	1892	G	C2'-C3'-O3'	7.84	126.75	109.50
1	A	733	A	C2'-C3'-O3'	7.69	126.42	109.50
10	J	76	ARG	NE-CZ-NH1	7.44	124.02	120.30
8	H	125	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	2906	U	C2'-C3'-O3'	6.62	124.30	113.70
1	A	1312	G	C2'-C3'-O3'	6.52	124.13	113.70
1	A	3268	A	C2'-C3'-O3'	6.46	124.03	113.70
41	e	1	G	C5'-C4'-O4'	6.41	116.79	109.10
1	A	840	C	C2'-C3'-O3'	6.08	123.43	113.70
1	A	3020	U	C2'-C3'-O3'	6.04	123.37	113.70
1	A	1409	C	C2'-C3'-O3'	5.97	123.26	113.70
1	A	44	U	C2'-C3'-O3'	5.96	123.24	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	326	A	C2'-C3'-O3'	5.85	123.05	113.70
41	e	1	G	C5'-C4'-C3'	5.78	125.25	116.00
32	5	236	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	2359	U	C2'-C3'-O3'	5.06	121.79	113.70
10	J	76	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	2586	U	C2'-C3'-O3'	5.04	121.77	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1665	G	C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	210	ASP	Peptide
4	D	49	PHE	Peptide
10	J	93	GLN	Peptide
20	T	43	HIS	Peptide
37	a	87	MET	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	A	57671	28898	28934	625	0
2	B	2260	2343	2303	47	0
3	C	1930	1976	1964	21	0
4	D	1866	1914	1898	30	0
5	E	2125	2169	2125	23	0
6	F	1355	1392	1338	22	0
7	G	458	471	467	2	0
8	H	1176	1218	1210	19	0
9	I	937	1015	1013	10	0
10	J	1727	1828	1812	12	0
11	K	1573	1635	1629	9	0
12	L	1815	1883	1873	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1206	1286	1283	13	0
14	N	948	1010	1006	2	0
15	O	1789	1895	1877	21	0
16	P	1722	1728	1718	22	0
17	Q	2126	2161	2092	19	0
18	R	2481	2500	2413	25	0
19	S	1191	1249	1234	16	0
20	T	1646	1618	1557	22	0
21	U	639	702	699	11	0
22	V	528	555	553	3	0
23	W	937	985	974	9	0
24	X	512	565	563	3	0
25	Y	376	412	410	4	0
26	Z	508	546	539	6	0
27	0	324	349	345	4	0
28	1	2707	2690	2661	24	0
29	2	919	939	923	14	0
30	3	995	1030	1012	10	0
31	4	1117	1146	1142	18	0
32	5	2485	2541	2488	26	0
33	6	1592	1595	1511	13	0
34	7	854	901	897	10	0
35	8	1413	1416	1381	14	0
36	9	1428	1437	1368	19	0
37	a	1427	1455	1449	0	0
38	b	1299	1372	1367	0	0
39	c	1000	1066	1062	0	0
40	d	1717	1706	1691	0	0
41	e	427	221	222	0	0
42	A	109	0	0	0	0
42	N	1	0	0	0	0
43	B	1	0	0	0	0
44	0	1	0	0	2	0
44	W	1	0	0	0	0
All	All	111319	83818	83003	1022	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 (1022) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:U:O4	1:A:2895:A:N1	1.58	1.36
1:A:114:U:O4	1:A:118:A:N1	1.68	1.25
1:A:1913:A:N1	1:A:2880:U:O4	1.73	1.21
1:A:122:A:N6	1:A:139:U:N3	1.91	1.19
1:A:274:U:O4	1:A:367:A:N1	1.78	1.15
1:A:1344:U:O4	1:A:1555:A:N1	1.85	1.09
1:A:1344:U:C4	1:A:1555:A:N1	2.23	1.06
1:A:45:U:H3	1:A:2895:A:H61	1.04	1.00
1:A:123:A:C2	1:A:139:U:O2	2.20	0.94
1:A:1689:U:H3	1:A:2853:A:H61	1.15	0.94
1:A:230:A:H8	1:A:588:C:HO2'	1.08	0.93
27:0:66:CYS:SG	44:0:100:ZN:ZN	1.57	0.92
1:A:1913:A:N6	1:A:2880:U:H3	1.68	0.91
1:A:1361:C:O2'	1:A:1362:C:H6	1.53	0.91
1:A:2941:A:H2'	1:A:2942:A:C8	2.06	0.91
1:A:45:U:H3	1:A:2895:A:N6	1.67	0.90
1:A:944:U:HO2'	1:A:946:A:H2	1.20	0.89
1:A:274:U:H3	1:A:367:A:N6	1.70	0.88
1:A:315:A:H4'	1:A:315:A:OP1	1.72	0.88
1:A:1360:G:C6	1:A:1361:C:N3	2.43	0.87
1:A:1689:U:H3	1:A:2853:A:N6	1.73	0.86
1:A:2949:C:O2	3:C:79:ARG:NH2	2.08	0.86
26:Z:60:GLY:O	26:Z:64:ARG:HD2	1.75	0.86
1:A:152:G:O2'	1:A:153:G:O5'	1.94	0.85
1:A:1583:G:C2'	1:A:1585:G:H22	1.89	0.85
1:A:1361:C:O2'	1:A:1362:C:O5'	1.95	0.85
1:A:3160:U:H5"	12:L:52:THR:HG21	1.58	0.84
6:F:24:LEU:HD13	6:F:107:ILE:HD11	1.57	0.84
1:A:3242:A:H2'	1:A:3243:A:C8	2.14	0.82
1:A:1360:G:C5	1:A:1361:C:N3	2.48	0.82
32:5:104:ARG:NH1	32:5:203:TRP:O	2.13	0.82
1:A:274:U:H3	1:A:367:A:H61	1.24	0.81
1:A:2359:U:O3'	18:R:169:ARG:NH2	2.13	0.81
1:A:268:C:N4	1:A:2674:U:O2	2.13	0.81
1:A:122:A:N6	1:A:139:U:C2	2.48	0.81
1:A:3156:U:H2'	1:A:3157:A:C8	2.17	0.80
1:A:2792:G:HO2'	27:0:56:PHE:N	1.79	0.80
1:A:3162:U:H2'	1:A:3163:U:C6	2.15	0.80
1:A:114:U:C4	1:A:118:A:N1	2.50	0.80
1:A:45:U:O4	1:A:2895:A:C2	2.34	0.80
1:A:164:U:O2	16:P:82:ASN:HA	1.81	0.80
1:A:1913:A:N6	1:A:2880:U:N3	2.26	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2612:A:C8	1:A:2648:A:H2'	2.18	0.78
1:A:164:U:O2'	1:A:165:A:OP1	2.00	0.78
13:M:144:GLN:O	13:M:145:ARG:HB2	1.83	0.78
27:0:66:CYS:HG	44:0:100:ZN:ZN	0.95	0.78
1:A:238:C:H5	1:A:288:G:H1	1.32	0.78
1:A:1681:C:O2	1:A:1681:C:O5'	2.02	0.77
1:A:307:G:O2'	1:A:308:U:O5'	2.03	0.76
1:A:122:A:N6	1:A:139:U:H3	1.80	0.76
1:A:45:U:C4	1:A:2895:A:N1	2.53	0.76
1:A:1360:G:C2	1:A:1361:C:O2	2.39	0.76
33:6:36:ILE:HD11	33:6:162:LEU:HD22	1.68	0.75
1:A:849:U:H2'	1:A:850:A:C8	2.21	0.75
1:A:1583:G:H2'	1:A:1585:G:H22	1.54	0.73
1:A:3271:A:HO2'	13:M:16:TYR:N	1.86	0.73
1:A:307:G:HO2'	1:A:308:U:P	2.12	0.73
1:A:1913:A:N1	1:A:2880:U:C4	2.57	0.72
1:A:1313:G:H5'	1:A:1314:U:H2'	1.70	0.71
1:A:727:G:C6	1:A:728:C:N3	2.58	0.71
1:A:3159:G:N2	1:A:3248:C:C2	2.58	0.71
2:B:155:ILE:HD11	2:B:157:PHE:CZ	2.26	0.71
1:A:1344:U:C4	1:A:1555:A:C2	2.78	0.71
15:O:294:LEU:HD21	32:5:335:VAL:HG12	1.73	0.70
1:A:2373:U:O2'	1:A:2374:A:OP2	2.09	0.70
1:A:2597:G:N2	1:A:2652:C:C2	2.59	0.70
1:A:3159:G:N2	12:L:102:PRO:O	2.24	0.70
1:A:2957:A:H1'	1:A:2958:U:H5"	1.74	0.70
1:A:3025:U:H2'	1:A:3026:A:C8	2.26	0.70
1:A:563:U:O2'	1:A:564:A:OP1	2.08	0.70
1:A:1583:G:H2'	1:A:1585:G:N2	2.06	0.70
1:A:1075:A:C6	1:A:1076:U:H1'	2.27	0.69
1:A:2913:U:O4	1:A:2941:A:N1	2.26	0.69
6:F:119:LEU:HD11	6:F:169:ILE:HD11	1.73	0.69
1:A:114:U:N3	1:A:118:A:N6	2.39	0.69
31:4:60:GLN:HB3	32:5:100:THR:HG21	1.74	0.68
1:A:1312:G:H2'	1:A:1313:G:H5"	1.74	0.68
1:A:2913:U:H3	1:A:2941:A:H2	1.42	0.68
1:A:616:A:O2'	1:A:617:A:OP1	2.09	0.68
1:A:841:G:OP1	5:E:110:ASN:HB2	1.94	0.68
1:A:2670:C:N3	1:A:2682:G:C2	2.62	0.67
1:A:2613:A:O2'	1:A:2614:U:OP1	2.12	0.67
13:M:61:LEU:O	13:M:62:ILE:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361:C:O2'	1:A:1362:C:C5'	2.42	0.67
9:I:2:ILE:HD11	9:I:94:THR:HG21	1.76	0.67
1:A:268:C:O2'	1:A:269:A:OP2	2.12	0.67
1:A:1361:C:O2'	1:A:1362:C:C6	2.33	0.67
1:A:2814:U:H5'	1:A:2833:A:C2	2.30	0.66
16:P:181:PHE:HB3	20:T:127:LEU:HD11	1.78	0.66
1:A:115:A:OP2	17:Q:9:SER:OG	2.14	0.66
1:A:1180:C:OP1	21:U:72:ARG:NH1	2.29	0.66
1:A:3247:A:C2	1:A:3250:A:N6	2.63	0.66
1:A:1892:G:O2'	1:A:1893:U:OP2	2.10	0.66
3:C:59:CYS:SG	3:C:60:GLY:N	2.68	0.66
1:A:486:G:H22	10:J:91:ARG:NE	1.94	0.66
1:A:2913:U:C5	1:A:3068:U:H2'	2.30	0.66
17:Q:27:LEU:N	17:Q:28:PRO:HD2	2.10	0.66
1:A:1913:A:C2	1:A:2880:U:O4	2.49	0.66
1:A:3160:U:C5'	12:L:52:THR:HG21	2.26	0.66
1:A:743:A:O2'	21:U:42:ALA:O	2.15	0.65
1:A:1424:U:H2'	1:A:1425:U:O4'	1.96	0.65
1:A:1312:G:O2'	1:A:1313:G:OP1	2.13	0.65
1:A:1343:U:H1'	1:A:1344:U:C5	2.32	0.65
4:D:133:ARG:O	4:D:134:THR:HG22	1.97	0.65
9:I:79:ARG:O	9:I:80:ASN:CB	2.45	0.65
20:T:151:GLN:O	20:T:155:VAL:HG13	1.97	0.65
1:A:1392:A:O2'	1:A:1393:U:O5'	2.13	0.64
1:A:275:A:C2	1:A:367:A:C2	2.86	0.64
1:A:2094:A:N6	1:A:2250:G:O2'	2.30	0.64
1:A:1064:A:O2'	1:A:1065:A:OP2	2.12	0.64
17:Q:83:ILE:HG22	17:Q:95:LEU:HD22	1.79	0.64
30:3:61:ILE:HG23	30:3:77:VAL:HG22	1.78	0.64
1:A:1696:A:OP2	2:B:334:ARG:NH1	2.31	0.64
33:6:171:LYS:HA	33:6:177:TRP:HB2	1.79	0.64
1:A:114:U:O4	1:A:118:A:C2	2.50	0.64
1:A:2612:A:N3	1:A:2612:A:H5"	2.13	0.64
1:A:3247:A:H2	1:A:3250:A:H61	1.46	0.64
12:L:190:LYS:O	12:L:194:LEU:HD22	1.98	0.64
1:A:608:A:C2	1:A:1585:G:H8	2.15	0.63
1:A:608:A:C2	1:A:1585:G:C8	2.87	0.63
1:A:3159:G:C2	1:A:3248:C:N3	2.66	0.63
18:R:198:LEU:HD21	18:R:254:LEU:HD22	1.79	0.63
1:A:1344:U:O4	1:A:1555:A:C6	2.52	0.63
5:E:84:ILE:HD11	29:2:123:LYS:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:39:LEU:O	8:H:54:GLY:HA3	1.98	0.63
16:P:255:LEU:HD21	32:5:73:TYR:CE2	2.33	0.62
1:A:3242:A:H2'	1:A:3243:A:H8	1.60	0.62
14:N:80:LEU:HD12	14:N:151:THR:HG21	1.79	0.62
1:A:1761:A:H2'	1:A:1762:A:C8	2.35	0.62
1:A:2331:U:O2	1:A:2367:A:H1'	1.99	0.62
11:K:63:SER:O	11:K:64:ILE:HG22	1.98	0.62
34:7:96:ILE:HG21	34:7:100:VAL:HG12	1.82	0.62
1:A:1343:U:C1'	1:A:1344:U:C5	2.83	0.62
31:4:13:ARG:NH1	32:5:289:SER:O	2.33	0.61
36:9:76:PRO:O	36:9:77:LYS:CB	2.48	0.61
1:A:2913:U:H5	1:A:3068:U:H2'	1.64	0.61
3:C:213:ARG:NH2	8:H:82:GLY:O	2.33	0.61
10:J:76:ARG:HG3	10:J:76:ARG:HH11	1.64	0.61
1:A:2446:U:O2'	1:A:2447:A:O5'	2.17	0.61
1:A:238:C:O2	1:A:238:C:O5'	2.18	0.61
16:P:227:ILE:HD13	16:P:232:LYS:HD3	1.82	0.61
1:A:314:A:N6	1:A:361:G:C8	2.69	0.61
28:1:243:THR:OG1	28:1:320:PHE:O	2.18	0.61
1:A:2670:C:C2	1:A:2682:G:N2	2.68	0.61
1:A:2958:U:H3'	1:A:2958:U:O2	2.00	0.61
1:A:271:A:H2'	1:A:272:G:O4'	2.01	0.61
6:F:69:VAL:HG11	6:F:73:LEU:HD23	1.83	0.61
15:O:177:ALA:HB3	15:O:235:THR:HG21	1.83	0.60
5:E:217:ILE:HG23	5:E:220:TYR:HB2	1.81	0.60
12:L:111:LEU:HD21	12:L:123:VAL:HG23	1.83	0.60
12:L:111:LEU:HD22	23:W:118:MET:HE1	1.81	0.60
18:R:176:LEU:HD13	18:R:198:LEU:HB3	1.82	0.60
1:A:1696:A:H2'	1:A:1697:C:O4'	2.01	0.60
1:A:2913:U:N3	1:A:2941:A:C2	2.66	0.60
1:A:1361:C:O2	1:A:1361:C:O4'	2.19	0.60
18:R:77:VAL:HG13	18:R:85:ILE:HG23	1.84	0.60
1:A:486:G:H22	10:J:91:ARG:HE	1.48	0.60
1:A:274:U:C4	1:A:367:A:N1	2.66	0.60
31:4:99:LYS:O	31:4:102:LYS:HG3	2.02	0.59
1:A:1107:U:H2'	8:H:68:THR:HG21	1.84	0.59
1:A:34:U:HO2'	1:A:35:U:P	2.25	0.59
1:A:34:U:O2'	1:A:35:U:P	2.60	0.59
1:A:671:G:H2'	1:A:673:A:N7	2.18	0.59
2:B:241:LEU:HD11	2:B:305:ILE:HD11	1.85	0.59
2:B:254:ASN:O	2:B:303:ALA:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:G:C2	1:A:357:C:O2	2.55	0.59
1:A:2670:C:C2	1:A:2682:G:C2	2.91	0.59
24:X:35:THR:HB	24:X:48:LEU:HD11	1.85	0.59
1:A:1944:C:C2	1:A:2892:G:N2	2.71	0.59
1:A:461:U:H6	1:A:461:U:H5'	1.68	0.59
18:R:54:GLY:O	18:R:113:ARG:NH2	2.35	0.59
1:A:1358:C:H2'	1:A:1358:C:O2	2.03	0.59
1:A:2585:A:H4'	1:A:2586:U:OP1	2.03	0.59
1:A:1361:C:HO2'	1:A:1362:C:H6	0.72	0.58
1:A:1583:G:N3	1:A:1585:G:N2	2.51	0.58
2:B:278:LYS:HG2	2:B:299:LEU:HD11	1.85	0.58
16:P:227:ILE:HD12	16:P:227:ILE:O	2.03	0.58
1:A:1313:G:N2	1:A:1321:C:C2	2.71	0.58
1:A:122:A:N6	1:A:140:U:C4	2.72	0.58
1:A:543:A:N1	1:A:550:A:N1	2.51	0.58
1:A:850:A:H2'	1:A:851:A:C8	2.39	0.58
1:A:1564:C:C2	1:A:1572:G:C2	2.92	0.58
1:A:615:U:C2'	1:A:616:A:OP1	2.51	0.58
1:A:331:A:O2'	1:A:332:A:P	2.62	0.58
1:A:2597:G:C2	1:A:2652:C:C2	2.92	0.58
1:A:1549:U:OP1	16:P:119:ARG:NH2	2.36	0.58
36:9:51:ASN:HB2	36:9:52:PRO:HD2	1.86	0.58
36:9:103:TYR:O	36:9:104:ASN:CB	2.51	0.58
1:A:1173:U:H2'	1:A:1174:G:O4'	2.04	0.57
1:A:966:A:C2	1:A:1059:A:C2	2.92	0.57
1:A:2835:U:H2'	1:A:2836:G:O4'	2.05	0.57
1:A:2593:A:H2'	1:A:2594:A:C8	2.39	0.57
7:G:21:VAL:HG12	7:G:57:TYR:HA	1.86	0.57
9:I:24:VAL:HG22	9:I:34:ALA:HB2	1.85	0.57
6:F:28:PRO:O	6:F:29:GLU:CB	2.51	0.57
1:A:122:A:C6	1:A:139:U:N3	2.62	0.57
1:A:1944:C:C2	1:A:2892:G:C2	2.92	0.57
11:K:85:ILE:HD12	11:K:142:VAL:HG21	1.87	0.57
20:T:95:ILE:N	20:T:96:PRO:CD	2.68	0.57
1:A:23:U:H2'	1:A:24:G:C8	2.40	0.57
12:L:170:LEU:HD13	12:L:213:LEU:HD11	1.85	0.57
1:A:3107:U:OP1	3:C:52:ARG:NH1	2.37	0.57
1:A:2590:U:H3'	1:A:2591:A:H5'	1.86	0.57
1:A:1755:A:H2'	1:A:1756:U:C6	2.40	0.56
4:D:135:ALA:CB	4:D:136:PRO:CD	2.83	0.56
1:A:1360:G:N2	1:A:1552:C:C2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:U:O4	1:A:1075:A:N6	2.38	0.56
1:A:1344:U:H2'	1:A:1562:A:C2	2.40	0.56
1:A:2612:A:H2	1:A:2638:G:H1	1.52	0.56
1:A:3031:U:C4	1:A:3032:U:C4	2.92	0.56
1:A:3035:U:O2	1:A:3035:U:O4'	2.23	0.56
8:H:102:GLY:HA2	8:H:128:VAL:HG11	1.87	0.56
21:U:26:LEU:HD21	21:U:47:LEU:HD23	1.87	0.56
23:W:123:GLN:O	23:W:127:ILE:HG23	2.05	0.56
1:A:847:U:O2	1:A:847:U:O4'	2.23	0.56
1:A:2733:A:N6	1:A:2734:A:C6	2.73	0.56
16:P:184:SER:HA	20:T:131:VAL:HG23	1.86	0.56
31:4:27:THR:HB	31:4:73:ARG:HG3	1.87	0.56
15:O:133:LYS:HE3	15:O:279:TYR:CZ	2.40	0.56
1:A:1343:U:C2	1:A:1344:U:O4	2.59	0.56
1:A:1725:G:OP1	2:B:176:ARG:NH2	2.39	0.56
1:A:34:U:O2'	1:A:35:U:O5'	2.23	0.56
1:A:2335:U:O4'	1:A:2335:U:O2	2.23	0.56
6:F:152:LEU:HD21	6:F:185:LEU:HD23	1.88	0.56
1:A:1261:U:H5'	31:4:71:LEU:HD21	1.87	0.56
1:A:1362:C:H2'	1:A:1363:C:H6	1.70	0.56
1:A:1952:A:H4'	3:C:207:GLN:O	2.06	0.56
1:A:2958:U:O2'	1:A:2959:C:O4'	2.20	0.56
1:A:1344:U:C5	1:A:1555:A:C2	2.93	0.56
32:5:283:ILE:O	32:5:287:ILE:N	2.38	0.56
1:A:878:G:H22	1:A:891:A:H2	1.53	0.55
1:A:1360:G:C2	1:A:1552:C:C2	2.94	0.55
1:A:2711:G:OP1	4:D:115:ARG:NH2	2.38	0.55
8:H:108:ALA:O	8:H:112:MET:HG2	2.06	0.55
31:4:16:VAL:HG23	32:5:289:SER:HB2	1.88	0.55
1:A:23:U:HO2'	36:9:98:HIS:HD1	1.40	0.55
4:D:233:ILE:HG22	4:D:245:VAL:HG11	1.89	0.55
35:8:132:MET:SD	35:8:166:LYS:HB3	2.47	0.55
1:A:2597:G:C2	1:A:2652:C:N3	2.75	0.55
4:D:70:ARG:NH1	34:7:124:GLN:O	2.40	0.55
1:A:238:C:O2	1:A:238:C:O4'	2.24	0.55
1:A:386:U:O2	1:A:386:U:O4'	2.25	0.55
1:A:1833:G:C6	1:A:1834:C:C4	2.94	0.55
1:A:2360:U:P	18:R:169:ARG:HH22	2.30	0.55
1:A:2958:U:H2'	1:A:2959:C:C6	2.42	0.55
4:D:205:VAL:HG11	35:8:108:ALA:HB1	1.87	0.55
19:S:132:ILE:HD12	19:S:132:ILE:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:U:O4	25:Y:73:ARG:HB2	2.05	0.54
20:T:144:SER:O	20:T:147:THR:OG1	2.22	0.54
1:A:1698:C:O3'	2:B:318:LEU:O	2.26	0.54
1:A:1743:G:N2	1:A:1744:C:C2	2.75	0.54
1:A:602:A:O2'	1:A:1366:A:N3	2.37	0.54
1:A:2426:A:O2'	1:A:2427:U:O5'	2.20	0.54
1:A:3279:U:H2'	1:A:3280:C:C6	2.43	0.54
17:Q:218:ILE:HG22	20:T:103:PHE:CD1	2.43	0.54
1:A:509:A:H2'	1:A:510:A:O4'	2.07	0.54
31:4:28:LEU:HD13	31:4:72:LEU:CD2	2.38	0.54
1:A:2707:G:N1	1:A:2708:C:C4	2.76	0.54
12:L:146:TRP:CZ3	23:W:127:ILE:HD11	2.43	0.54
3:C:62:ILE:HD11	3:C:138:ALA:HB3	1.90	0.54
1:A:1358:C:H5	1:A:1553:G:H1	1.56	0.54
8:H:37:ILE:HG23	8:H:42:ARG:HB2	1.90	0.54
1:A:857:U:O2	1:A:857:U:O4'	2.22	0.54
18:R:204:SER:CB	18:R:214:ALA:HB1	2.38	0.54
5:E:214:LEU:O	5:E:217:ILE:HG22	2.08	0.54
1:A:1313:G:C2	1:A:1321:C:C2	2.95	0.53
1:A:1561:G:H3'	1:A:1561:G:N3	2.22	0.53
6:F:125:VAL:HG12	6:F:125:VAL:O	2.09	0.53
1:A:1405:U:O4'	1:A:1405:U:O2	2.26	0.53
1:A:2720:G:C6	1:A:2765:C:N3	2.77	0.53
1:A:3160:U:H5"	12:L:52:THR:CG2	2.33	0.53
1:A:176:U:H2'	1:A:177:A:C8	2.44	0.53
1:A:2707:G:N2	1:A:2708:C:C2	2.77	0.53
6:F:65:LEU:N	6:F:65:LEU:HD22	2.24	0.53
1:A:3156:U:H2'	1:A:3157:A:H8	1.70	0.53
32:5:163:LEU:HD12	32:5:283:ILE:HD11	1.90	0.53
1:A:536:A:H4'	1:A:537:U:OP1	2.07	0.53
8:H:27:THR:HG22	8:H:30:ARG:HD2	1.90	0.53
20:T:102:SER:N	20:T:105:ASP:OD2	2.42	0.53
1:A:331:A:O2'	1:A:332:A:OP2	2.25	0.53
1:A:554:U:H2'	1:A:556:A:C8	2.44	0.53
1:A:870:C:O2	1:A:870:C:O4'	2.22	0.53
1:A:2952:G:H1'	1:A:3062:A:C2	2.44	0.53
3:C:61:LEU:HD21	3:C:160:PHE:CE2	2.44	0.53
1:A:1750:G:C6	1:A:1751:C:C4	2.97	0.53
5:E:161:LEU:HD22	29:2:45:GLN:HB3	1.91	0.53
16:P:92:ILE:HG23	20:T:122:ARG:HA	1.91	0.53
1:A:595:U:H2'	1:A:595:U:O2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2287:A:OP1	18:R:45:ARG:NH2	2.41	0.53
1:A:2382:A:H4'	33:6:80:LEU:HD11	1.91	0.53
19:S:138:LYS:O	19:S:155:ARG:NH2	2.42	0.53
34:7:83:LYS:HB2	34:7:88:LYS:HG2	1.91	0.53
1:A:28:U:O2'	1:A:29:A:OP1	2.26	0.52
1:A:1373:U:O2	1:A:1373:U:O4'	2.25	0.52
1:A:1720:U:HO2'	2:B:135:ASN:H	1.57	0.52
1:A:2913:U:OP2	1:A:3069:A:OP1	2.27	0.52
15:O:172:SER:O	15:O:261:ILE:HG23	2.08	0.52
28:1:233:VAL:HG22	28:1:242:LYS:O	2.09	0.52
29:2:140:LEU:O	29:2:141:TRP:CB	2.56	0.52
32:5:324:VAL:HG21	32:5:339:HIS:ND1	2.24	0.52
16:P:186:THR:HG22	16:P:187:PRO:HD3	1.91	0.52
1:A:33:A:N6	1:A:34:U:C4	2.77	0.52
1:A:915:G:C5	21:U:13:ILE:HD12	2.44	0.52
1:A:1493:U:H2'	1:A:1494:A:C8	2.45	0.52
1:A:3247:A:H2	1:A:3250:A:N6	2.06	0.52
1:A:3264:C:O2'	32:5:332:LYS:O	2.26	0.52
3:C:240:ASP:OD1	3:C:240:ASP:N	2.43	0.52
5:E:202:MET:HG3	5:E:203:SER:N	2.24	0.52
18:R:204:SER:HB3	18:R:214:ALA:HB1	1.91	0.52
1:A:1486:U:H2'	1:A:1487:A:C8	2.45	0.52
17:Q:213:VAL:HG22	30:3:122:ILE:HD13	1.91	0.52
20:T:57:THR:HG21	23:W:148:LEU:HD12	1.92	0.52
20:T:96:PRO:O	20:T:99:ARG:HB2	2.09	0.52
1:A:247:A:H2'	1:A:248:A:O4'	2.09	0.52
1:A:2913:U:N3	1:A:2941:A:H2	2.06	0.52
25:Y:71:LEU:HD11	25:Y:75:ARG:NH2	2.24	0.52
1:A:581:C:C2	1:A:700:G:C2	2.97	0.52
1:A:1392:A:HO2'	1:A:1393:U:C5'	2.22	0.52
32:5:188:ASN:O	32:5:192:SER:N	2.43	0.52
1:A:3162:U:N3	1:A:3163:U:C4	2.78	0.52
1:A:27:A:HO2'	1:A:28:U:P	2.32	0.52
10:J:76:ARG:HH11	10:J:76:ARG:CG	2.23	0.52
1:A:511:G:H2'	1:A:512:U:C6	2.46	0.51
1:A:1681:C:O2	1:A:1681:C:O4'	2.26	0.51
1:A:2601:A:O2'	1:A:2602:A:C8	2.63	0.51
1:A:2720:G:C2	1:A:2765:C:O2	2.63	0.51
1:A:2741:G:N2	1:A:2796:G:H1	2.06	0.51
6:F:126:GLY:HA3	6:F:129:TYR:CD2	2.45	0.51
20:T:144:SER:O	20:T:148:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:A:C4	1:A:307:G:N7	2.79	0.51
1:A:2427:U:H3'	1:A:2427:U:O2	2.10	0.51
6:F:183:ALA:O	6:F:186:ARG:HG3	2.10	0.51
14:N:134:THR:HB	14:N:141:VAL:HG22	1.92	0.51
1:A:527:A:H62	1:A:539:U:H5'	1.74	0.51
1:A:2258:C:OP1	19:S:96:TRP:CZ3	2.64	0.51
1:A:2364:U:H2'	1:A:2365:A:H8	1.75	0.51
16:P:92:ILE:O	16:P:107:PHE:HA	2.11	0.51
29:2:117:ASN:O	29:2:118:ALA:C	2.48	0.51
1:A:441:A:N1	1:A:448:U:H5	2.09	0.51
15:O:155:GLU:O	15:O:158:VAL:HG12	2.10	0.51
20:T:89:HIS:O	30:3:96:ALA:HB2	2.11	0.51
1:A:23:U:O2'	36:9:98:HIS:ND1	2.33	0.51
1:A:3068:U:H4'	1:A:3069:A:OP2	2.10	0.51
1:A:904:G:C2	1:A:912:C:C2	2.98	0.51
1:A:2435:A:H3'	1:A:2436:A:H5"	1.91	0.51
1:A:1355:G:O2'	1:A:1356:U:P	2.69	0.51
1:A:1960:A:C2	1:A:1961:G:C8	2.99	0.51
1:A:2594:A:H2'	1:A:2595:U:C6	2.46	0.51
13:M:108:LEU:HG	13:M:125:LEU:HD23	1.93	0.51
32:5:169:LYS:O	32:5:173:GLN:HG2	2.11	0.51
36:9:82:LEU:HD11	36:9:203:ILE:HG22	1.92	0.51
1:A:834:A:HO2'	1:A:835:A:H8	1.58	0.51
17:Q:83:ILE:HG22	17:Q:95:LEU:CD2	2.41	0.51
23:W:124:ILE:O	23:W:127:ILE:HG12	2.10	0.51
1:A:122:A:N6	1:A:139:U:C4	2.56	0.51
1:A:1582:A:H2'	1:A:1583:G:O4'	2.11	0.51
4:D:70:ARG:HG2	4:D:70:ARG:HH11	1.76	0.51
11:K:69:LEU:HD23	11:K:69:LEU:H	1.76	0.51
19:S:105:LEU:HB3	19:S:132:ILE:HD11	1.93	0.51
1:A:164:U:HO2'	1:A:165:A:P	2.30	0.51
1:A:1830:G:O2'	1:A:1868:G:N1	2.44	0.51
1:A:3233:A:O5'	1:A:3233:A:H8	1.94	0.51
1:A:117:U:O4'	1:A:117:U:O2	2.30	0.50
9:I:79:ARG:O	9:I:80:ASN:HB3	2.10	0.50
28:1:120:GLN:HB3	28:1:121:PHE:CD1	2.47	0.50
1:A:1392:A:O2'	1:A:1393:U:P	2.69	0.50
11:K:223:GLU:HG2	11:K:224:PRO:HD2	1.93	0.50
15:O:127:ILE:HD12	15:O:138:VAL:HG23	1.93	0.50
16:P:138:LEU:HD11	16:P:159:LYS:HD2	1.92	0.50
1:A:1386:A:O2'	19:S:65:ILE:O	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2612:A:OP1	24:X:46:HIS:NE2	2.42	0.50
4:D:143:LEU:HD23	4:D:144:PRO:HD2	1.93	0.50
4:D:246:ILE:HG21	4:D:251:VAL:HA	1.93	0.50
1:A:1806:C:H2'	1:A:1830:G:C8	2.46	0.50
2:B:209:PHE:HB2	2:B:241:LEU:HB3	1.94	0.50
23:W:118:MET:HA	23:W:118:MET:HE2	1.94	0.50
1:A:1535:A:H2'	1:A:1536:A:C8	2.47	0.50
1:A:419:U:H2'	1:A:420:U:O4'	2.12	0.50
1:A:2317:A:O2'	1:A:2318:U:P	2.69	0.50
1:A:2898:U:H2'	1:A:2899:U:C6	2.45	0.50
1:A:488:A:H2'	1:A:489:A:C8	2.47	0.50
1:A:1993:U:H1'	19:S:101:VAL:HG11	1.93	0.50
1:A:2258:C:OP1	19:S:96:TRP:HZ3	1.95	0.50
18:R:286:LEU:HD12	18:R:324:TYR:CG	2.46	0.50
1:A:3069:A:O2'	1:A:3070:A:OP2	2.21	0.50
1:A:3192:A:H2'	1:A:3193:A:O4'	2.11	0.50
2:B:286:ILE:HD11	2:B:296:TYR:CE1	2.46	0.50
33:6:171:LYS:HA	33:6:177:TRP:CB	2.41	0.50
1:A:502:A:C8	1:A:563:U:C5	3.00	0.50
1:A:1972:G:C6	1:A:1973:C:C4	3.00	0.50
1:A:275:A:N6	1:A:276:U:O4	2.45	0.49
1:A:346:G:C6	1:A:357:C:N3	2.80	0.49
1:A:645:U:H2'	1:A:646:C:C6	2.47	0.49
1:A:2958:U:O2	1:A:2958:U:C3'	2.60	0.49
1:A:3069:A:C8	1:A:3108:U:H1'	2.46	0.49
8:H:139:ASN:HB3	32:5:329:ARG:O	2.12	0.49
1:A:3159:G:C2	1:A:3248:C:C2	3.00	0.49
4:D:200:ILE:O	4:D:201:PHE:CB	2.59	0.49
1:A:238:C:O2	1:A:238:C:C5'	2.60	0.49
1:A:365:A:N3	1:A:365:A:H2'	2.28	0.49
1:A:1318:A:N7	12:L:116:ASN:ND2	2.59	0.49
33:6:27:VAL:HG11	33:6:195:ALA:HB2	1.94	0.49
36:9:118:GLN:O	36:9:121:ILE:HG22	2.13	0.49
1:A:2648:A:O3'	5:E:19:PRO:N	2.45	0.49
1:A:2706:C:OP2	2:B:349:ARG:NH2	2.42	0.49
15:O:271:SER:O	15:O:275:ARG:HD3	2.13	0.49
1:A:3164:A:N1	1:A:3233:A:C2	2.81	0.49
29:2:41:ARG:O	29:2:44:THR:OG1	2.27	0.49
32:5:167:VAL:HG13	32:5:288:MET:HE1	1.94	0.49
1:A:366:A:C6	1:A:367:A:N6	2.81	0.49
1:A:789:A:N7	1:A:840:C:C4	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2607:G:C6	1:A:2608:C:C4	3.00	0.49
1:A:2814:U:C2	1:A:2815:U:C5	3.01	0.49
13:M:61:LEU:O	13:M:62:ILE:CB	2.60	0.49
20:T:116:GLU:O	20:T:119:VAL:HG22	2.13	0.49
20:T:147:THR:HA	20:T:150:TRP:CD1	2.48	0.49
1:A:207:U:C2	1:A:208:A:C8	3.01	0.49
1:A:538:A:N1	1:A:556:A:C2	2.81	0.49
35:8:189:ILE:HG22	35:8:194:LEU:HD23	1.95	0.49
1:A:304:A:H1'	1:A:365:A:H2	1.78	0.49
1:A:543:A:C2	1:A:550:A:N1	2.81	0.49
15:O:294:LEU:HD21	32:5:335:VAL:CG1	2.42	0.49
26:Z:65:TRP:CZ3	26:Z:100:ALA:HB2	2.48	0.49
1:A:133:A:C6	1:A:134:U:C2	3.00	0.49
1:A:1846:G:C6	1:A:1847:C:C4	3.00	0.49
11:K:225:GLN:HG2	11:K:226:TYR:N	2.28	0.49
15:O:112:LEU:HD21	16:P:227:ILE:HG21	1.95	0.49
15:O:171:LYS:HD2	15:O:260:TYR:CZ	2.48	0.49
34:7:104:ARG:HG3	34:7:105:ASN:N	2.26	0.49
1:A:1743:G:N1	1:A:1744:C:C4	2.81	0.48
16:P:186:THR:N	16:P:187:PRO:CD	2.76	0.48
33:6:192:HIS:CE1	33:6:193:VAL:HG23	2.48	0.48
1:A:735:A:H4'	1:A:736:A:OP1	2.11	0.48
1:A:119:A:H2'	1:A:119:A:N3	2.28	0.48
1:A:2468:A:OP1	5:E:97:LYS:NZ	2.46	0.48
6:F:77:LYS:HA	6:F:84:ILE:HG22	1.95	0.48
18:R:155:LYS:N	18:R:156:PRO:CD	2.76	0.48
34:7:93:ILE:HD12	34:7:128:ILE:HD11	1.95	0.48
36:9:200:ILE:O	36:9:203:ILE:HG12	2.13	0.48
1:A:708:U:O2'	1:A:730:U:H5"	2.14	0.48
1:A:2590:U:H3'	1:A:2591:A:C5'	2.43	0.48
1:A:3158:G:H2'	1:A:3159:G:O4'	2.13	0.48
23:W:137:ILE:O	23:W:137:ILE:HG23	2.13	0.48
35:8:118:LEU:HB3	35:8:168:GLY:HA2	1.95	0.48
1:A:1360:G:H2'	1:A:1361:C:H5'	1.95	0.48
1:A:1382:A:C6	1:A:1392:A:N6	2.81	0.48
1:A:1901:U:OP1	12:L:8:LYS:NZ	2.46	0.48
1:A:3163:U:C2	1:A:3164:A:C8	3.02	0.48
10:J:114:TYR:O	26:Z:64:ARG:HD3	2.13	0.48
29:2:44:THR:O	29:2:48:VAL:HG23	2.13	0.48
30:3:74:TRP:C	30:3:76:LYS:H	2.16	0.48
31:4:121:LEU:N	31:4:121:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:U:O2'	1:A:365:A:C8	2.66	0.48
1:A:409:A:N3	1:A:409:A:H2'	2.29	0.48
1:A:2802:G:C6	1:A:2803:C:C4	3.02	0.48
8:H:19:VAL:HG13	8:H:59:VAL:HG22	1.94	0.48
1:A:448:U:O4'	1:A:448:U:O2	2.28	0.48
1:A:3122:U:O2'	1:A:3123:A:OP2	2.29	0.48
4:D:50:PRO:CD	4:D:183:ASP:HB2	2.43	0.48
5:E:154:LEU:HG	29:2:42:VAL:HG11	1.95	0.48
5:E:274:TYR:HA	5:E:277:ARG:HG2	1.95	0.48
18:R:205:LEU:HD21	18:R:211:ILE:HG22	1.95	0.48
28:1:174:PRO:O	28:1:334:ILE:O	2.31	0.48
1:A:25:A:O2'	1:A:26:A:P	2.71	0.48
1:A:27:A:O2'	1:A:28:U:P	2.72	0.48
1:A:364:U:O2'	1:A:365:A:H8	1.97	0.48
1:A:945:A:N1	1:A:1107:U:O2'	2.32	0.48
2:B:180:ILE:HD12	2:B:193:TYR:CD1	2.49	0.48
1:A:615:U:O2'	1:A:616:A:OP1	2.29	0.48
1:A:1969:G:C6	1:A:1970:C:C4	3.02	0.48
6:F:24:LEU:CD1	6:F:107:ILE:HD11	2.37	0.48
36:9:103:TYR:O	36:9:104:ASN:HB2	2.13	0.48
1:A:119:A:N3	1:A:119:A:C2'	2.76	0.48
1:A:1981:U:O4	1:A:2263:U:C4	2.67	0.48
1:A:2601:A:HO2'	1:A:2602:A:H8	1.60	0.48
1:A:651:G:H2'	1:A:652:A:O4'	2.14	0.47
1:A:880:G:OP2	11:K:55:ARG:NH1	2.44	0.47
1:A:1555:A:H2'	1:A:1556:A:O4'	2.13	0.47
1:A:2452:U:H2'	1:A:2453:G:O4'	2.14	0.47
1:A:2707:G:C2	1:A:2708:C:C6	3.02	0.47
8:H:56:TYR:CD2	8:H:125:ARG:HG3	2.49	0.47
16:P:103:TYR:CE1	16:P:167:PRO:HB3	2.49	0.47
18:R:77:VAL:CG1	18:R:85:ILE:HG23	2.44	0.47
32:5:98:LEU:HG	32:5:227:GLY:HA2	1.96	0.47
32:5:340:VAL:HG23	32:5:362:ALA:HB1	1.95	0.47
1:A:169:A:H2'	1:A:170:U:O4'	2.14	0.47
1:A:275:A:C6	1:A:276:U:O4	2.67	0.47
1:A:1541:U:H2'	1:A:1542:U:C6	2.49	0.47
1:A:2947:C:H5'	3:C:253:ALA:HA	1.96	0.47
3:C:63:THR:HG22	3:C:87:VAL:HG22	1.96	0.47
4:D:135:ALA:HB1	4:D:136:PRO:HD3	1.95	0.47
5:E:245:PHE:CD1	5:E:245:PHE:N	2.82	0.47
21:U:11:SER:OG	21:U:13:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:166:HIS:O	36:9:167:ASN:CB	2.62	0.47
1:A:274:U:O4	1:A:367:A:C2	2.62	0.47
1:A:880:G:C6	1:A:881:C:C4	3.02	0.47
1:A:1142:U:H2'	1:A:1143:A:O4'	2.15	0.47
1:A:1756:U:C2	1:A:1757:A:C8	3.02	0.47
2:B:173:ASP:OD2	2:B:176:ARG:NH1	2.44	0.47
15:O:299:ILE:HD11	31:4:128:ILE:HG23	1.97	0.47
36:9:118:GLN:HA	36:9:121:ILE:HG22	1.95	0.47
36:9:199:PHE:O	36:9:203:ILE:HG23	2.13	0.47
1:A:275:A:N1	1:A:367:A:C2	2.81	0.47
1:A:954:A:O2'	1:A:955:A:OP2	2.27	0.47
1:A:3137:A:H1'	1:A:3143:A:C2	2.50	0.47
1:A:3261:U:O2	1:A:3261:U:O4'	2.31	0.47
17:Q:195:ASN:O	30:3:91:LYS:HG2	2.14	0.47
28:1:176:ALA:HB3	28:1:334:ILE:HD12	1.95	0.47
1:A:231:A:H2'	1:A:232:C:C6	2.50	0.47
1:A:718:G:H2'	1:A:1968:U:C2	2.48	0.47
1:A:2885:G:C6	1:A:2886:C:C4	3.02	0.47
2:B:268:SER:O	2:B:271:THR:HG22	2.13	0.47
1:A:832:U:H4'	11:K:70:GLN:HG3	1.97	0.47
1:A:1630:A:O2'	1:A:1891:U:H4'	2.14	0.47
6:F:60:GLY:HA3	6:F:114:VAL:HB	1.97	0.47
15:O:183:LEU:HD11	23:W:97:MET:HG3	1.97	0.47
19:S:66:PHE:CE1	19:S:79:VAL:HG23	2.50	0.47
1:A:643:U:H4'	1:A:644:A:O5'	2.13	0.47
1:A:1258:A:H2'	1:A:1259:A:O4'	2.15	0.47
1:A:2785:U:C5	1:A:2808:A:C6	3.02	0.47
1:A:2951:U:O2'	9:I:80:ASN:HA	2.15	0.47
2:B:385:ARG:HG3	2:B:386:PRO:HD2	1.96	0.47
6:F:24:LEU:HB2	6:F:84:ILE:HG13	1.95	0.47
8:H:46:VAL:HG13	15:O:299:ILE:HG23	1.96	0.47
8:H:125:ARG:CG	8:H:125:ARG:HH11	2.28	0.47
1:A:1116:A:N6	1:A:1117:G:C6	2.82	0.47
1:A:1535:A:OP1	2:B:151:ARG:NH2	2.47	0.47
1:A:2741:G:N2	1:A:2796:G:N1	2.62	0.47
18:R:117:LEU:O	18:R:119:SER:N	2.47	0.47
1:A:328:A:H2'	1:A:329:A:H5'	1.96	0.47
1:A:716:A:H2'	1:A:717:U:O4'	2.14	0.47
1:A:1938:A:H2'	1:A:1939:U:O4'	2.15	0.47
1:A:2954:U:H2'	1:A:2955:G:O4'	2.15	0.47
1:A:3109:U:OP1	3:C:169:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3122:U:O2'	1:A:3123:A:P	2.73	0.47
1:A:221:A:H2'	1:A:222:A:C8	2.50	0.47
1:A:789:A:H2'	1:A:790:A:C8	2.50	0.47
18:R:196:SER:HA	18:R:199:ILE:HG12	1.96	0.47
1:A:1805:G:C6	1:A:1806:C:C4	3.03	0.46
1:A:1995:G:H2'	1:A:1996:A:O4'	2.14	0.46
1:A:3254:U:OP1	23:W:102:ASN:HB2	2.15	0.46
5:E:161:LEU:HD22	29:2:45:GLN:CB	2.45	0.46
1:A:2207:A:C5	1:A:2208:A:N7	2.83	0.46
1:A:2446:U:H4'	1:A:2447:A:OP1	2.15	0.46
2:B:183:LEU:HG	2:B:194:ILE:HG12	1.97	0.46
19:S:132:ILE:N	19:S:132:ILE:CD1	2.78	0.46
1:A:1392:A:HO2'	1:A:1393:U:P	2.39	0.46
1:A:1493:U:O2'	1:A:1494:A:OP1	2.32	0.46
1:A:1833:G:C5	1:A:1834:C:C5	3.04	0.46
1:A:2597:G:N1	1:A:2652:C:C4	2.84	0.46
1:A:2732:G:OP1	27:0:59:ARG:HB2	2.16	0.46
1:A:3029:U:C4	1:A:3030:U:C4	3.03	0.46
18:R:216:PHE:CZ	28:1:264:ARG:HD2	2.51	0.46
28:1:171:THR:HG22	28:1:172:LEU:N	2.30	0.46
33:6:30:LEU:HD12	33:6:30:LEU:O	2.14	0.46
1:A:28:U:O2'	1:A:29:A:P	2.73	0.46
1:A:308:U:C2'	1:A:309:C:O5'	2.63	0.46
1:A:1245:U:O4	1:A:1267:A:N1	2.49	0.46
1:A:1706:G:O2'	2:B:295:ARG:NH1	2.48	0.46
1:A:1808:G:C6	1:A:1809:C:C4	3.04	0.46
1:A:2317:A:C2	1:A:2318:U:C2	3.04	0.46
35:8:169:TYR:CD2	35:8:193:ILE:HG21	2.50	0.46
1:A:836:A:N3	1:A:2290:A:O2'	2.40	0.46
1:A:914:A:C5	21:U:13:ILE:HD13	2.50	0.46
1:A:1765:A:C6	1:A:1786:A:C2	3.03	0.46
1:A:3120:A:N1	1:A:3261:U:C4	2.84	0.46
16:P:146:ASN:O	16:P:147:LEU:CB	2.63	0.46
1:A:840:C:O2	1:A:840:C:H3'	2.16	0.46
3:C:69:MET:HB2	3:C:70:PRO:CD	2.45	0.46
3:C:115:LEU:HD11	13:M:28:VAL:HG21	1.97	0.46
4:D:230:GLU:O	4:D:233:ILE:HG13	2.15	0.46
1:A:1261:U:C5'	31:4:71:LEU:HD21	2.46	0.46
1:A:1312:G:C2'	1:A:1313:G:H5"	2.45	0.46
1:A:1362:C:H2'	1:A:1363:C:C6	2.51	0.46
1:A:1364:C:C2	1:A:1402:G:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3268:A:H2'	1:A:3269:U:H6	1.81	0.46
1:A:123:A:C2	1:A:139:U:C2	3.02	0.46
1:A:2874:G:H2'	1:A:2875:G:O4'	2.16	0.46
12:L:127:VAL:HG12	12:L:128:ASP:N	2.31	0.46
18:R:128:ARG:O	28:1:239:ASP:O	2.33	0.46
20:T:147:THR:O	20:T:151:GLN:HG2	2.16	0.46
1:A:328:A:C2'	1:A:329:A:H5'	2.45	0.46
1:A:673:A:C2	2:B:338:MET:HG2	2.51	0.46
1:A:1759:A:H2'	1:A:1760:U:O4'	2.16	0.46
2:B:294:HIS:O	2:B:382:VAL:HG23	2.16	0.46
6:F:161:LYS:HG2	6:F:169:ILE:CG2	2.46	0.46
1:A:549:U:O2	1:A:2635:C:O2'	2.16	0.46
1:A:581:C:C2	1:A:700:G:N2	2.83	0.46
1:A:1274:A:C8	31:4:33:TRP:CH2	3.04	0.46
1:A:2730:G:C6	1:A:2731:C:C4	3.03	0.46
22:V:57:VAL:HB	29:2:133:THR:HG22	1.98	0.46
32:5:200:ALA:HB2	32:5:260:VAL:HG23	1.97	0.46
34:7:118:SER:HB2	34:7:131:LYS:HB2	1.97	0.46
1:A:1220:G:H2'	1:A:1221:G:O4'	2.16	0.45
1:A:2796:G:H2'	1:A:2797:U:OP1	2.15	0.45
1:A:2898:U:H2'	1:A:2899:U:H6	1.79	0.45
1:A:3143:A:H2'	1:A:3144:A:O4'	2.16	0.45
5:E:73:TYR:HA	5:E:77:LEU:HB2	1.97	0.45
13:M:95:LEU:HD12	13:M:109:LEU:HD13	1.97	0.45
18:R:129:PHE:HB3	28:1:239:ASP:O	2.16	0.45
1:A:346:G:N1	1:A:357:C:C2	2.85	0.45
1:A:416:U:H2'	1:A:417:U:C6	2.52	0.45
1:A:910:G:N3	1:A:910:G:H2'	2.32	0.45
1:A:1356:U:OP2	1:A:1358:C:O2	2.33	0.45
1:A:1360:G:N3	1:A:1361:C:O2	2.48	0.45
1:A:1392:A:N3	1:A:1392:A:H2'	2.31	0.45
1:A:1702:C:H2'	1:A:1703:U:O4'	2.15	0.45
1:A:1925:U:H2'	1:A:1926:A:C8	2.51	0.45
1:A:2607:G:C2	1:A:2608:C:C2	3.04	0.45
13:M:76:VAL:HG21	13:M:94:ILE:HD11	1.97	0.45
15:O:155:GLU:HG2	16:P:235:ILE:HD11	1.98	0.45
16:P:121:TYR:O	16:P:125:ILE:HG12	2.16	0.45
1:A:114:U:H3	1:A:118:A:N6	2.13	0.45
1:A:275:A:C2	1:A:367:A:N3	2.84	0.45
1:A:291:A:P	26:Z:58:HIS:HE2	2.39	0.45
1:A:1116:A:H2'	1:A:1117:G:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:U:H2'	1:A:1246:A:C8	2.52	0.45
1:A:2373:U:O2'	1:A:2374:A:P	2.73	0.45
1:A:2631:G:H2'	1:A:2632:A:O4'	2.16	0.45
1:A:3160:U:OP1	12:L:52:THR:HG21	2.15	0.45
6:F:26:ILE:HD11	6:F:84:ILE:HG12	1.98	0.45
19:S:137:THR:OG1	19:S:159:LEU:HD11	2.16	0.45
36:9:159:ALA:HB1	36:9:196:LEU:HD23	1.97	0.45
1:A:1111:U:H3'	1:A:1112:A:H5"	1.98	0.45
1:A:2777:U:H2'	1:A:2778:C:O4'	2.16	0.45
1:A:3281:U:C2	1:A:3282:A:C8	3.04	0.45
2:B:240:CYS:CB	2:B:304:THR:HG22	2.46	0.45
36:9:36:PRO:O	36:9:43:ARG:NH2	2.49	0.45
1:A:2324:U:H4'	1:A:2325:A:OP1	2.17	0.45
1:A:1391:U:H2'	1:A:1392:A:H5'	1.98	0.45
1:A:1825:A:H3'	1:A:1826:U:H5"	1.99	0.45
1:A:2913:U:C4	1:A:2941:A:N1	2.85	0.45
1:A:779:A:N1	1:A:847:U:H5	2.13	0.45
1:A:1678:C:O2'	1:A:1693:A:H1'	2.16	0.45
1:A:2586:U:H1'	1:A:2587:U:C6	2.52	0.45
1:A:2730:G:C2	1:A:2731:C:C2	3.05	0.45
2:B:270:GLY:HA2	2:B:311:ILE:HG22	1.98	0.45
1:A:261:A:C8	1:A:307:G:O6	2.70	0.45
1:A:536:A:C2	1:A:557:A:C2	3.05	0.45
1:A:1364:C:O2'	1:A:1536:A:N3	2.42	0.45
1:A:1371:A:H3'	1:A:1372:A:C5'	2.47	0.45
1:A:3138:U:H2'	1:A:3139:A:H5"	1.98	0.45
19:S:32:ILE:HD12	19:S:32:ILE:N	2.32	0.45
34:7:91:THR:OG1	34:7:130:ILE:HB	2.17	0.45
35:8:181:THR:HG23	35:8:184:GLN:HB2	1.99	0.45
1:A:58:A:OP1	15:O:264:ARG:NH2	2.49	0.45
1:A:482:G:C6	1:A:483:C:C4	3.05	0.45
1:A:603:U:OP2	2:B:149:ARG:NH1	2.50	0.45
1:A:685:G:H2'	1:A:686:U:O4'	2.17	0.45
12:L:132:MET:HB3	12:L:188:LEU:HD13	1.99	0.45
16:P:186:THR:CG2	16:P:187:PRO:HD3	2.47	0.45
19:S:104:GLY:HA2	19:S:115:SER:HA	1.99	0.45
20:T:152:ILE:O	20:T:155:VAL:HG22	2.17	0.45
26:Z:92:LYS:HA	26:Z:92:LYS:HE2	1.99	0.45
1:A:355:U:H2'	1:A:356:U:O4'	2.17	0.45
1:A:2811:G:H2'	1:A:2812:G:O4'	2.17	0.45
1:A:3279:U:H2'	1:A:3280:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:G:C2	1:A:1751:C:C2	3.05	0.44
1:A:2872:A:C6	1:A:2873:U:O4	2.70	0.44
1:A:2915:A:H2'	1:A:2916:U:C6	2.52	0.44
2:B:194:ILE:HG22	2:B:195:ILE:N	2.32	0.44
18:R:38:SER:O	18:R:39:MET:CB	2.65	0.44
1:A:551:U:H2'	1:A:552:A:H8	1.81	0.44
1:A:840:C:H2'	1:A:841:G:H5"	1.99	0.44
1:A:2860:A:C6	1:A:2861:U:C4	3.05	0.44
2:B:240:CYS:HA	2:B:304:THR:HA	1.99	0.44
5:E:68:ARG:NH2	22:V:57:VAL:HG21	2.32	0.44
28:1:229:VAL:HG21	28:1:322:ILE:HD12	2.00	0.44
1:A:307:G:O2'	1:A:308:U:C5'	2.65	0.44
1:A:2951:U:O2	9:I:80:ASN:OD1	2.36	0.44
4:D:60:VAL:HG21	4:D:65:VAL:HG21	1.99	0.44
32:5:268:TRP:HA	32:5:279:VAL:CG2	2.47	0.44
34:7:90:ILE:HD13	34:7:129:ILE:HG23	1.99	0.44
1:A:918:U:H2'	1:A:919:A:O4'	2.18	0.44
1:A:1743:G:C6	1:A:1744:C:C4	3.05	0.44
1:A:2584:A:C2	1:A:2585:A:H1'	2.52	0.44
22:V:43:HIS:HA	33:6:60:MET:SD	2.58	0.44
1:A:1430:U:H2'	1:A:1431:U:O4'	2.18	0.44
2:B:125:VAL:HG23	2:B:154:LEU:HD11	1.99	0.44
2:B:158:ASN:O	2:B:210:ARG:NH1	2.50	0.44
5:E:30:HIS:HB2	28:1:165:ILE:HD12	2.00	0.44
8:H:125:ARG:HH11	8:H:125:ARG:HG2	1.82	0.44
19:S:110:LEU:HD23	19:S:158:VAL:HG22	1.99	0.44
21:U:13:ILE:O	21:U:13:ILE:HG23	2.17	0.44
31:4:63:VAL:HB	35:8:226:VAL:HG22	1.99	0.44
1:A:276:U:H1'	1:A:277:U:OP1	2.17	0.44
1:A:461:U:C6	1:A:461:U:C5'	3.01	0.44
1:A:727:G:C5	1:A:728:C:C4	3.06	0.44
1:A:3268:A:H2'	1:A:3269:U:C6	2.53	0.44
20:T:73:SER:OG	20:T:74:ASN:N	2.50	0.44
1:A:640:C:O2	1:A:1570:A:H2'	2.17	0.44
1:A:2601:A:O2'	1:A:2602:A:H8	1.99	0.44
1:A:2696:A:N3	1:A:2696:A:H2'	2.33	0.44
6:F:67:VAL:HG22	6:F:110:HIS:CE1	2.52	0.44
28:1:121:PHE:CE1	29:2:67:ILE:HD11	2.53	0.44
1:A:583:G:O2'	4:D:115:ARG:HD2	2.18	0.44
1:A:1848:C:C2	1:A:1859:G:C2	3.06	0.44
8:H:139:ASN:CB	32:5:329:ARG:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:27:LEU:N	17:Q:28:PRO:CD	2.77	0.44
33:6:168:LEU:HD23	33:6:169:LEU:N	2.33	0.44
1:A:74:A:O2'	4:D:238:PRO:O	2.36	0.44
1:A:208:A:H2'	1:A:209:U:C6	2.53	0.44
1:A:315:A:O2'	1:A:317:U:C1'	2.65	0.44
1:A:1833:G:C2	1:A:1834:C:C2	3.06	0.44
1:A:2373:U:HO2'	1:A:2374:A:P	2.37	0.44
1:A:2787:C:C2	1:A:2812:G:N2	2.86	0.44
1:A:2905:A:O2'	3:C:44:HIS:O	2.35	0.44
2:B:253:HIS:O	2:B:255:VAL:HG23	2.18	0.44
1:A:136:A:H2'	1:A:137:A:C8	2.53	0.43
1:A:673:A:N3	2:B:338:MET:HG2	2.33	0.43
1:A:1366:A:O4'	1:A:1534:G:N2	2.51	0.43
1:A:2814:U:C5'	1:A:2833:A:C2	3.00	0.43
16:P:157:ILE:HD12	17:Q:5:TYR:HB3	1.99	0.43
32:5:324:VAL:HG21	32:5:339:HIS:CG	2.53	0.43
1:A:466:U:H2'	1:A:467:U:O4'	2.18	0.43
1:A:1210:A:O2'	31:4:90:ASN:ND2	2.51	0.43
1:A:1754:A:N1	1:A:1755:A:C6	2.86	0.43
1:A:2336:G:C4	28:1:62:ILE:HD13	2.53	0.43
1:A:2364:U:H2'	1:A:2365:A:C8	2.52	0.43
1:A:2584:A:H3'	1:A:2585:A:H5"	1.99	0.43
1:A:3193:A:H2'	1:A:3194:U:H4'	2.00	0.43
4:D:164:LYS:HG2	4:D:260:GLN:O	2.18	0.43
10:J:91:ARG:HD3	10:J:98:ALA:HA	1.99	0.43
1:A:443:U:H4'	1:A:445:U:OP1	2.19	0.43
1:A:1279:A:H2'	1:A:1280:A:O4'	2.18	0.43
1:A:1631:G:N2	1:A:1671:A:O2'	2.51	0.43
1:A:1846:G:C2	1:A:1847:C:C2	3.07	0.43
6:F:26:ILE:HD11	6:F:84:ILE:HG23	1.99	0.43
28:1:113:PRO:HG3	29:2:71:THR:HG21	1.99	0.43
1:A:827:U:C2	1:A:828:A:C8	3.06	0.43
1:A:915:G:OP2	21:U:11:SER:OG	2.31	0.43
1:A:1693:A:N6	1:A:2873:U:O4'	2.50	0.43
1:A:1717:A:H2'	1:A:1718:A:C8	2.52	0.43
1:A:1763:A:H2'	1:A:1990:A:H1'	2.00	0.43
1:A:2722:G:C2	1:A:2762:C:C2	3.05	0.43
7:G:44:LEU:CD2	7:G:49:LEU:HD13	2.48	0.43
34:7:89:ILE:O	34:7:131:LYS:O	2.36	0.43
1:A:95:A:H2'	1:A:96:C:C6	2.54	0.43
1:A:866:G:H5'	1:A:867:A:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:A:N3	1:A:1113:A:O5'	2.52	0.43
1:A:1698:C:H5	1:A:1736:G:H21	1.65	0.43
1:A:1769:U:C2'	1:A:1770:U:OP1	2.66	0.43
2:B:344:PRO:HB3	2:B:356:LYS:HD3	2.01	0.43
4:D:165:LEU:HD12	4:D:262:VAL:HG23	2.00	0.43
10:J:146:ARG:CZ	34:7:73:THR:HG23	2.48	0.43
35:8:247:GLN:O	35:8:251:ASP:HB2	2.18	0.43
1:A:1786:A:H2'	1:A:1787:A:C8	2.53	0.43
1:A:1949:G:C6	1:A:1950:C:C4	3.07	0.43
1:A:3231:A:OP1	12:L:56:ARG:NH2	2.52	0.43
4:D:152:PHE:HZ	4:D:251:VAL:HG13	1.84	0.43
25:Y:95:ARG:CZ	25:Y:100:ARG:HD3	2.48	0.43
35:8:166:LYS:N	35:8:166:LYS:HD2	2.33	0.43
36:9:80:ILE:HG22	36:9:82:LEU:CD1	2.49	0.43
1:A:2607:G:H2'	1:A:2608:C:O4'	2.19	0.43
5:E:64:THR:HA	33:6:52:GLN:HB3	2.00	0.43
6:F:111:ILE:O	6:F:115:THR:HG22	2.19	0.43
12:L:237:ARG:NH1	13:M:30:PRO:O	2.52	0.43
1:A:577:U:C4	1:A:579:A:C8	3.06	0.43
1:A:676:A:H4'	1:A:1686:U:H4'	2.00	0.43
1:A:1750:G:H2'	1:A:1751:C:O4'	2.19	0.43
1:A:3058:G:C6	1:A:3059:C:C4	3.06	0.43
1:A:3118:U:C4	1:A:3119:A:N7	2.87	0.43
1:A:3159:G:N1	1:A:3248:C:C4	2.87	0.43
4:D:229:ARG:O	4:D:233:ILE:HG23	2.18	0.43
28:1:247:TYR:CZ	28:1:249:LEU:HD21	2.53	0.43
1:A:1104:A:O2'	8:H:108:ALA:O	2.37	0.43
1:A:1113:A:O2'	1:A:1114:U:OP1	2.29	0.43
1:A:2292:C:H1'	1:A:2298:U:O4	2.19	0.43
1:A:2440:G:H2'	1:A:2441:U:O4'	2.19	0.43
1:A:3058:G:H2'	1:A:3059:C:O4'	2.18	0.43
2:B:94:LYS:HB2	2:B:110:ILE:HD11	2.00	0.43
3:C:73:ASP:O	3:C:77:GLY:N	2.52	0.43
17:Q:80:ILE:HD11	35:8:84:LEU:CD1	2.49	0.43
28:1:128:VAL:HG23	28:1:131:ILE:HB	2.00	0.43
32:5:268:TRP:HA	32:5:279:VAL:HG21	2.01	0.43
1:A:486:G:H4'	1:A:487:U:O5'	2.18	0.43
1:A:1374:U:C6	1:A:1374:U:OP1	2.72	0.43
1:A:1848:C:C2	1:A:1859:G:N2	2.87	0.43
2:B:246:ILE:HG22	2:B:250:THR:HG21	2.01	0.43
1:A:536:A:C2	1:A:557:A:H2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:U:H2'	1:A:658:U:O4'	2.19	0.42
1:A:2586:U:H4'	1:A:2587:U:OP1	2.19	0.42
1:A:2651:G:H5'	5:E:19:PRO:CG	2.49	0.42
5:E:245:PHE:N	5:E:245:PHE:HD1	2.15	0.42
1:A:142:A:H2'	1:A:143:A:O4'	2.18	0.42
1:A:294:G:H4'	1:A:328:A:C5	2.54	0.42
1:A:1490:A:C2	1:A:1523:A:H2	2.37	0.42
1:A:1743:G:C2	1:A:1744:C:C2	3.08	0.42
12:L:35:SER:HG	12:L:40:CYS:HG	1.64	0.42
18:R:143:GLU:HB3	28:1:361:VAL:HG11	2.01	0.42
1:A:121:A:H3'	1:A:122:A:H5"	2.02	0.42
1:A:1314:U:O2	1:A:1316:U:H2'	2.18	0.42
1:A:1516:U:C2	1:A:3022:G:N2	2.87	0.42
1:A:2674:U:H2'	1:A:2675:U:C6	2.53	0.42
2:B:257:ILE:CD1	2:B:265:PHE:CE2	3.03	0.42
15:O:107:LEU:HD21	15:O:161:PRO:HB3	2.01	0.42
15:O:165:ALA:HB3	15:O:265:CYS:SG	2.60	0.42
21:U:11:SER:CB	21:U:13:ILE:HG22	2.49	0.42
28:1:211:ILE:N	28:1:211:ILE:HD12	2.34	0.42
1:A:720:A:N3	1:A:720:A:H2'	2.34	0.42
1:A:951:A:O2'	1:A:952:A:O5'	2.32	0.42
1:A:1680:A:H2'	1:A:1681:C:O4'	2.19	0.42
1:A:2858:C:OP1	2:B:351:LYS:HD3	2.19	0.42
1:A:3147:U:OP2	3:C:117:LYS:HE3	2.18	0.42
2:B:197:CYS:SG	2:B:198:ASP:N	2.92	0.42
4:D:50:PRO:HG2	4:D:183:ASP:CB	2.50	0.42
9:I:11:ILE:HD11	9:I:74:VAL:HG21	2.01	0.42
17:Q:65:PRO:HA	17:Q:83:ILE:HG13	2.00	0.42
1:A:268:C:OP1	10:J:216:THR:HG21	2.19	0.42
1:A:1589:A:C5	1:A:1590:U:C5	3.07	0.42
1:A:1605:U:O4	12:L:8:LYS:HB3	2.19	0.42
1:A:1869:A:O2'	1:A:1872:G:N3	2.45	0.42
1:A:1946:U:H2'	1:A:1947:C:C6	2.54	0.42
2:B:294:HIS:HB2	2:B:383:LYS:HB2	2.02	0.42
21:U:4:TYR:O	21:U:36:TYR:HA	2.19	0.42
1:A:230:A:O4'	1:A:230:A:N3	2.51	0.42
1:A:231:A:H2'	1:A:232:C:H6	1.83	0.42
1:A:904:G:N2	1:A:912:C:C2	2.88	0.42
1:A:1706:G:O2'	1:A:1707:C:OP2	2.29	0.42
1:A:1826:U:H4'	1:A:1826:U:OP1	2.20	0.42
1:A:2418:U:H2'	1:A:2419:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2751:G:C6	1:A:2752:C:C4	3.08	0.42
2:B:145:GLY:HA3	2:B:330:ARG:HG3	2.02	0.42
3:C:168:VAL:HB	3:C:231:ILE:HG23	2.01	0.42
6:F:161:LYS:HG2	6:F:169:ILE:HG23	2.01	0.42
13:M:46:LEU:O	13:M:49:ILE:HG13	2.19	0.42
19:S:105:LEU:HD12	19:S:118:MET:CE	2.50	0.42
1:A:587:G:C6	1:A:588:C:C4	3.07	0.42
1:A:720:A:N3	1:A:720:A:C2'	2.82	0.42
1:A:1581:U:H2'	1:A:1582:A:H5'	2.01	0.42
1:A:2669:A:H4'	1:A:2670:C:H5"	2.01	0.42
1:A:204:A:C2	1:A:205:A:C8	3.08	0.42
1:A:261:A:H4'	1:A:262:A:O5'	2.19	0.42
1:A:274:U:N3	1:A:367:A:N6	2.43	0.42
1:A:1181:U:C4	1:A:1182:A:N7	2.88	0.42
1:A:2707:G:C6	1:A:2708:C:C4	3.07	0.42
1:A:3019:U:O4	1:A:3033:A:C2	2.72	0.42
1:A:3127:U:OP1	3:C:120:ARG:HB2	2.20	0.42
2:B:125:VAL:CG2	2:B:154:LEU:HD11	2.50	0.42
4:D:74:LEU:HG	4:D:257:LEU:HD11	2.00	0.42
6:F:26:ILE:HD11	6:F:84:ILE:CG2	2.50	0.42
9:I:24:VAL:HG11	9:I:27:LYS:HD2	2.01	0.42
17:Q:149:VAL:HG13	35:8:92:ILE:HD12	2.01	0.42
1:A:315:A:H2'	1:A:317:U:C6	2.55	0.42
1:A:536:A:H2	1:A:557:A:C2	2.37	0.42
1:A:551:U:H2'	1:A:552:A:C8	2.55	0.42
1:A:1127:A:OP2	1:A:1169:A:O3'	2.37	0.42
1:A:1391:U:C2'	1:A:1392:A:H5'	2.50	0.42
1:A:2434:A:N3	5:E:188:GLY:HA2	2.35	0.42
1:A:3015:U:C4	1:A:3016:A:N6	2.88	0.42
1:A:3163:U:C4	1:A:3164:A:N7	2.87	0.42
4:D:75:TRP:CZ3	10:J:66:PRO:HB3	2.55	0.42
5:E:220:TYR:CZ	5:E:222:GLY:HA2	2.54	0.42
29:2:126:PRO:O	29:2:127:MET:CB	2.67	0.42
1:A:1360:G:H2'	1:A:1361:C:C5'	2.49	0.42
1:A:2359:U:C2'	1:A:2360:U:O5'	2.68	0.42
1:A:2802:G:C2	1:A:2803:C:C2	3.08	0.42
1:A:3162:U:C2	1:A:3243:A:N1	2.88	0.42
3:C:217:GLY:HA3	8:H:83:ARG:NH1	2.35	0.42
11:K:115:THR:HA	11:K:140:VAL:HB	2.01	0.42
12:L:27:LEU:HD21	12:L:125:GLU:HA	2.01	0.42
18:R:128:ARG:O	18:R:130:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:321:ASP:HB2	28:1:324:GLN:HB3	2.01	0.42
29:2:140:LEU:O	29:2:141:TRP:HB2	2.19	0.42
31:4:52:TRP:HH2	31:4:99:LYS:HA	1.85	0.42
33:6:83:GLN:OE1	33:6:115:LYS:N	2.48	0.42
1:A:578:G:N2	1:A:579:A:C2	2.88	0.41
1:A:1697:C:H2'	1:A:1698:C:C6	2.55	0.41
1:A:1769:U:H3'	1:A:1770:U:H5"	2.01	0.41
4:D:49:PHE:HB2	4:D:168:ILE:HG12	2.01	0.41
6:F:119:LEU:HA	6:F:170:ILE:O	2.20	0.41
10:J:144:LYS:O	10:J:145:ASN:HB2	2.19	0.41
11:K:216:LEU:HD22	11:K:216:LEU:HA	1.93	0.41
15:O:189:VAL:HG11	15:O:267:LEU:HD13	2.01	0.41
20:T:95:ILE:HB	20:T:96:PRO:HD3	2.02	0.41
28:1:334:ILE:HG13	28:1:335:GLY:N	2.35	0.41
31:4:31:CYS:SG	31:4:67:SER:HA	2.60	0.41
1:A:22:U:C4	1:A:23:U:C5	3.08	0.41
1:A:84:A:H2'	1:A:85:A:C8	2.55	0.41
1:A:162:U:C2	30:3:76:LYS:HE2	2.56	0.41
1:A:308:U:H2'	1:A:309:C:O5'	2.20	0.41
1:A:1530:U:H3	1:A:1533:G:H1	1.68	0.41
1:A:1594:G:H2'	1:A:1595:G:O4'	2.20	0.41
1:A:1663:A:H3'	13:M:150:TYR:CD1	2.55	0.41
2:B:198:ASP:HA	2:B:309:SER:HA	2.01	0.41
1:A:350:A:H2'	1:A:351:C:C6	2.55	0.41
1:A:434:U:O3'	15:O:300:ARG:HB2	2.20	0.41
1:A:620:G:C5	2:B:320:LYS:HB2	2.56	0.41
1:A:1521:U:H2'	1:A:1522:A:C8	2.56	0.41
1:A:2787:C:C2	1:A:2812:G:C2	3.07	0.41
30:3:119:LEU:HA	30:3:122:ILE:HD12	2.02	0.41
36:9:118:GLN:O	36:9:121:ILE:CG2	2.69	0.41
1:A:119:A:N6	20:T:153:ARG:HH11	2.19	0.41
1:A:1344:U:C5	1:A:1555:A:H2	2.36	0.41
1:A:1564:C:C2	1:A:1572:G:N2	2.88	0.41
1:A:1735:U:OP2	2:B:334:ARG:NE	2.51	0.41
2:B:257:ILE:HD11	2:B:265:PHE:CZ	2.54	0.41
10:J:225:ASN:CG	10:J:225:ASN:O	2.58	0.41
21:U:26:LEU:HD21	21:U:47:LEU:CD2	2.51	0.41
1:A:1112:A:O4'	1:A:1112:A:OP1	2.38	0.41
1:A:1846:G:C6	1:A:1847:C:N3	2.88	0.41
1:A:2828:A:H2'	1:A:2829:U:O4'	2.20	0.41
16:P:100:HIS:CE1	16:P:106:LYS:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:148:GLN:OE1	16:P:148:GLN:N	2.54	0.41
17:Q:76:SER:O	17:Q:79:ASN:HB2	2.20	0.41
17:Q:131:LEU:O	17:Q:131:LEU:HD12	2.20	0.41
18:R:261:ASN:HD21	18:R:265:GLU:HB2	1.85	0.41
19:S:122:VAL:O	19:S:125:THR:OG1	2.28	0.41
1:A:874:U:H2'	1:A:875:U:C6	2.55	0.41
1:A:955:A:H2'	1:A:956:A:C8	2.55	0.41
1:A:1249:U:H2'	1:A:1250:U:C6	2.56	0.41
1:A:1493:U:O2'	1:A:1494:A:P	2.78	0.41
1:A:1768:A:H2'	1:A:1769:U:C6	2.55	0.41
1:A:1808:G:C2	1:A:1809:C:C2	3.09	0.41
1:A:3152:A:H4'	1:A:3152:A:OP1	2.20	0.41
12:L:174:ALA:O	12:L:175:LYS:C	2.59	0.41
17:Q:213:VAL:CG2	30:3:122:ILE:HD13	2.51	0.41
17:Q:252:PRO:HG2	19:S:159:LEU:HB3	2.03	0.41
20:T:127:LEU:O	20:T:131:VAL:HG13	2.19	0.41
1:A:425:A:H5"	8:H:117:LYS:HG3	2.02	0.41
1:A:1265:A:H2'	1:A:1266:U:C6	2.56	0.41
2:B:278:LYS:C	2:B:279:LEU:HD12	2.40	0.41
4:D:212:GLU:OE1	35:8:109:VAL:HG13	2.21	0.41
5:E:217:ILE:HG23	5:E:220:TYR:CB	2.46	0.41
8:H:63:GLN:HA	8:H:101:PHE:CD1	2.55	0.41
12:L:136:HIS:O	12:L:137:THR:CB	2.69	0.41
25:Y:103:LEU:O	25:Y:104:SER:CB	2.68	0.41
35:8:140:THR:HG21	35:8:159:PHE:HA	2.02	0.41
1:A:228:U:H2'	1:A:229:G:O4'	2.21	0.41
1:A:2001:U:H2'	1:A:2002:U:O4'	2.21	0.41
1:A:2358:A:C6	1:A:2359:U:C4	3.09	0.41
4:D:171:GLU:O	4:D:172:LYS:CB	2.69	0.41
6:F:24:LEU:HD11	6:F:104:ARG:HG2	2.02	0.41
30:3:74:TRP:C	30:3:76:LYS:N	2.74	0.41
1:A:26:A:C6	36:9:41:LEU:HD12	2.55	0.41
1:A:402:A:H2'	1:A:403:A:O4'	2.20	0.41
1:A:449:A:H2'	1:A:450:U:C6	2.56	0.41
1:A:564:A:O2'	1:A:565:A:C8	2.69	0.41
1:A:1433:A:H2'	1:A:1434:A:C8	2.56	0.41
1:A:1609:U:H2'	1:A:1610:A:C8	2.56	0.41
1:A:1959:A:N6	1:A:1960:A:C2	2.89	0.41
1:A:1963:C:H2'	1:A:1964:C:O4'	2.20	0.41
1:A:2441:U:H2'	1:A:2442:A:C8	2.55	0.41
1:A:2772:U:O2'	1:A:2773:C:OP2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ILE:HD11	2:B:157:PHE:CE1	2.55	0.41
2:B:378:ASN:O	2:B:381:LYS:HB2	2.21	0.41
3:C:110:TYR:CD1	3:C:110:TYR:C	2.94	0.41
4:D:45:THR:O	4:D:45:THR:HG23	2.21	0.41
4:D:105:LEU:HD11	4:D:119:ALA:HB2	2.02	0.41
15:O:107:LEU:HD13	15:O:221:LEU:HD13	2.03	0.41
18:R:160:LYS:O	18:R:163:GLU:HG3	2.21	0.41
24:X:66:LEU:O	24:X:67:ARG:C	2.58	0.41
29:2:68:LYS:O	29:2:71:THR:OG1	2.29	0.41
1:A:214:A:H2'	1:A:215:A:C4'	2.51	0.41
1:A:602:A:H1'	1:A:1367:A:H1'	2.03	0.41
1:A:2628:A:OP1	26:Z:74:ARG:NH1	2.54	0.41
1:A:3090:U:H2'	1:A:3092:U:OP1	2.21	0.41
17:Q:104:VAL:HG13	17:Q:105:PRO:HD2	2.02	0.41
17:Q:170:PRO:O	17:Q:184:TRP:NE1	2.52	0.41
31:4:28:LEU:HD13	31:4:72:LEU:HD21	2.02	0.41
32:5:70:LEU:O	32:5:70:LEU:HD23	2.21	0.41
1:A:274:U:O2	1:A:274:U:C2'	2.68	0.40
1:A:337:A:N6	1:A:338:G:C2	2.89	0.40
1:A:1808:G:N2	1:A:1809:C:C2	2.89	0.40
1:A:1849:U:H2'	1:A:1850:A:O4'	2.20	0.40
1:A:2779:A:H2'	1:A:2780:A:C8	2.56	0.40
1:A:2796:G:O2'	1:A:2797:U:P	2.80	0.40
1:A:3020:U:C2'	1:A:3021:A:O5'	2.69	0.40
5:E:180:VAL:O	5:E:183:TRP:O	2.39	0.40
8:H:15:LEU:O	8:H:55:ASP:HB3	2.22	0.40
13:M:151:ILE:O	13:M:154:THR:HG22	2.20	0.40
17:Q:100:PRO:HB2	17:Q:124:VAL:HG23	2.01	0.40
28:1:140:ARG:HG3	28:1:214:TYR:HD1	1.86	0.40
36:9:80:ILE:HG22	36:9:82:LEU:HD12	2.02	0.40
1:A:164:U:H3	16:P:82:ASN:C	2.25	0.40
1:A:248:A:H2'	1:A:249:C:C6	2.56	0.40
1:A:638:U:O2'	15:O:248:LYS:HE3	2.21	0.40
1:A:1361:C:H2'	1:A:1362:C:C5	2.56	0.40
1:A:1404:A:C2'	1:A:1405:U:OP1	2.69	0.40
1:A:1609:U:H2'	1:A:1610:A:H8	1.86	0.40
1:A:1707:C:H4'	1:A:1708:A:H3'	2.04	0.40
1:A:1833:G:C4	1:A:1834:C:C6	3.09	0.40
1:A:1972:G:C2	1:A:1973:C:C2	3.09	0.40
1:A:2941:A:H2'	1:A:2942:A:H8	1.75	0.40
4:D:152:PHE:CZ	4:D:251:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:257:LEU:HD22	10:J:60:ILE:CG2	2.51	0.40
28:1:174:PRO:O	28:1:176:ALA:N	2.54	0.40
30:3:102:LYS:O	30:3:142:TYR:HB2	2.21	0.40
32:5:163:LEU:CD1	32:5:283:ILE:HD11	2.51	0.40
1:A:326:A:H3'	1:A:326:A:N3	2.37	0.40
1:A:859:U:O2	1:A:859:U:O4'	2.37	0.40
1:A:1747:C:C4	1:A:1748:A:N7	2.90	0.40
1:A:1829:U:O2	1:A:1829:U:O4'	2.36	0.40
1:A:2379:U:O2'	1:A:2380:U:O5'	2.33	0.40
1:A:3233:A:O5'	1:A:3233:A:C8	2.73	0.40
1:A:3252:U:O2'	1:A:3253:U:OP2	2.24	0.40
3:C:72:PHE:CE1	3:C:79:ARG:HG3	2.56	0.40
18:R:135:THR:O	18:R:136:ASN:C	2.58	0.40
32:5:338:VAL:HG21	32:5:359:LYS:HA	2.03	0.40
1:A:142:A:O3'	20:T:157:ASN:ND2	2.54	0.40
1:A:1361:C:C2'	1:A:1362:C:C6	3.04	0.40
1:A:1388:A:N6	1:A:1715:A:C2	2.89	0.40
1:A:3058:G:C2	1:A:3059:C:C2	3.09	0.40
5:E:30:HIS:CD2	28:1:166:PRO:HB3	2.56	0.40
9:I:138:ILE:HG22	13:M:121:ILE:HD11	2.02	0.40
20:T:95:ILE:HG23	20:T:155:VAL:HG12	2.03	0.40
31:4:26:ILE:HD13	31:4:98:LEU:CD2	2.51	0.40
33:6:27:VAL:CG1	33:6:195:ALA:HB2	2.51	0.40
1:A:599:A:H2'	1:A:600:C:O4'	2.21	0.40
1:A:1308:A:OP2	1:A:1597:G:O2'	2.34	0.40
1:A:2952:G:H4'	9:I:79:ARG:HG3	2.04	0.40
1:A:2961:A:H2'	1:A:2962:U:O4'	2.21	0.40
1:A:3069:A:H4'	1:A:3070:A:O5'	2.22	0.40
2:B:159:ARG:NE	2:B:194:ILE:HD12	2.37	0.40
2:B:381:LYS:O	2:B:382:VAL:C	2.60	0.40
18:R:262:ASN:ND2	18:R:314:LEU:HA	2.37	0.40
28:1:291:VAL:CG1	28:1:337:HIS:HB3	2.52	0.40
31:4:65:ARG:HD2	31:4:65:ARG:C	2.42	0.40
32:5:310:LEU:HD11	32:5:370:TRP:CG	2.56	0.40
33:6:257:LEU:HD21	33:6:265:TYR:CD2	2.57	0.40
35:8:189:ILE:HG22	35:8:194:LEU:CD2	2.50	0.40
36:9:70:ARG:HG2	36:9:75:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	291/393 (74%)	272 (94%)	16 (6%)	3 (1%)	15	54
3	C	247/269 (92%)	226 (92%)	15 (6%)	6 (2%)	6	34
4	D	235/286 (82%)	211 (90%)	15 (6%)	9 (4%)	3	22
5	E	272/292 (93%)	246 (90%)	22 (8%)	4 (2%)	10	44
6	F	173/214 (81%)	163 (94%)	7 (4%)	3 (2%)	9	42
7	G	53/139 (38%)	50 (94%)	3 (6%)	0	100	100
8	H	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
9	I	121/138 (88%)	110 (91%)	10 (8%)	1 (1%)	19	58
10	J	218/322 (68%)	202 (93%)	14 (6%)	2 (1%)	17	56
11	K	193/232 (83%)	182 (94%)	7 (4%)	4 (2%)	7	37
12	L	225/238 (94%)	208 (92%)	14 (6%)	3 (1%)	12	47
13	M	149/169 (88%)	138 (93%)	9 (6%)	2 (1%)	12	47
14	N	116/161 (72%)	109 (94%)	6 (5%)	1 (1%)	17	56
15	O	219/309 (71%)	199 (91%)	18 (8%)	2 (1%)	17	56
16	P	205/263 (78%)	189 (92%)	14 (7%)	2 (1%)	15	54
17	Q	269/297 (91%)	243 (90%)	22 (8%)	4 (2%)	10	44
18	R	310/371 (84%)	288 (93%)	17 (6%)	5 (2%)	9	43
19	S	142/258 (55%)	136 (96%)	6 (4%)	0	100	100
20	T	203/319 (64%)	184 (91%)	13 (6%)	6 (3%)	4	28
21	U	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
22	V	62/177 (35%)	57 (92%)	5 (8%)	0	100	100
23	W	110/183 (60%)	100 (91%)	6 (6%)	4 (4%)	3	23
24	X	62/70 (89%)	55 (89%)	6 (10%)	1 (2%)	9	43
25	Y	43/105 (41%)	41 (95%)	1 (2%)	1 (2%)	6	34
26	Z	60/115 (52%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	36/93 (39%)	34 (94%)	2 (6%)	0	100	100
28	1	324/367 (88%)	293 (90%)	26 (8%)	5 (2%)	10	44
29	2	111/147 (76%)	103 (93%)	5 (4%)	3 (3%)	5	30
30	3	120/146 (82%)	103 (86%)	16 (13%)	1 (1%)	19	58
31	4	136/140 (97%)	128 (94%)	8 (6%)	0	100	100
32	5	324/390 (83%)	299 (92%)	23 (7%)	2 (1%)	25	64
33	6	195/281 (69%)	179 (92%)	12 (6%)	4 (2%)	7	37
34	7	104/146 (71%)	99 (95%)	5 (5%)	0	100	100
35	8	178/264 (67%)	168 (94%)	10 (6%)	0	100	100
36	9	185/253 (73%)	163 (88%)	14 (8%)	8 (4%)	2	20
37	a	174/195 (89%)	161 (92%)	7 (4%)	6 (3%)	3	24
38	b	153/157 (98%)	139 (91%)	12 (8%)	2 (1%)	12	47
39	c	116/131 (88%)	108 (93%)	5 (4%)	3 (3%)	5	31
40	d	200/226 (88%)	179 (90%)	16 (8%)	5 (2%)	5	32
All	All	6560/8505 (77%)	6037 (92%)	421 (6%)	102 (2%)	13	43

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	382	VAL
3	C	211	PRO
4	D	49	PHE
4	D	50	PRO
4	D	135	ALA
4	D	248	LYS
6	F	70	PRO
6	F	71	ASP
10	J	165	LEU
11	K	154	ASP
13	M	62	ILE
13	M	145	ARG
14	N	108	PRO
20	T	31	LYS
23	W	100	HIS
28	1	55	ILE
29	2	141	TRP
36	9	77	LYS

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Mol	Chain	Res	Type
38	b	83	GLU
38	b	151	ASN
3	C	193	HIS
3	C	208	ASN
4	D	172	LYS
4	D	278	LYS
6	F	29	GLU
10	J	145	ASN
11	K	59	ARG
12	L	127	VAL
12	L	137	THR
15	O	185	GLY
15	O	239	GLY
16	P	177	ASP
17	Q	96	ASP
18	R	129	PHE
18	R	262	ASN
20	T	20	THR
20	T	29	LEU
20	T	46	ASN
24	X	67	ARG
28	1	110	ILE
28	1	125	LEU
28	1	175	ARG
29	2	127	MET
36	9	33	HIS
36	9	104	ASN
36	9	167	ASN
37	a	79	SER
40	d	67	ARG
40	d	172	GLY
40	d	196	VAL
4	D	201	PHE
5	E	37	LYS
9	I	80	ASN
12	L	136	HIS
16	P	147	LEU
18	R	184	LEU
18	R	306	LYS
20	T	73	SER
25	Y	104	SER
29	2	118	ALA

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Mol	Chain	Res	Type
32	5	219	MET
33	6	153	ASN
33	6	180	PRO
36	9	59	GLU
37	a	88	PRO
37	a	109	GLY
2	B	355	ASN
4	D	51	SER
5	E	21	SER
5	E	88	HIS
11	K	64	ILE
17	Q	211	ASP
17	Q	235	ARG
23	W	136	GLU
39	c	124	ILE
40	d	33	GLU
40	d	68	ARG
4	D	170	GLY
17	Q	273	PRO
18	R	39	MET
20	T	25	LYS
23	W	107	CYS
23	W	137	ILE
30	3	144	GLU
36	9	36	PRO
36	9	74	GLN
39	c	117	PRO
2	B	386	PRO
3	C	197	ILE
3	C	210	ASP
5	E	35	ILE
32	5	381	PRO
33	6	154	ASP
37	a	116	PRO
28	1	98	PRO
3	C	111	GLY
11	K	224	PRO
33	6	146	ILE
37	a	28	VAL
37	a	87	MET
36	9	208	GLY
39	c	58	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	233/337 (69%)	210 (90%)	23 (10%)	8	30
3	C	209/229 (91%)	190 (91%)	19 (9%)	9	34
4	D	200/248 (81%)	173 (86%)	27 (14%)	4	18
5	E	225/260 (86%)	201 (89%)	24 (11%)	6	27
6	F	141/190 (74%)	120 (85%)	21 (15%)	3	14
7	G	50/129 (39%)	47 (94%)	3 (6%)	19	54
8	H	126/141 (89%)	117 (93%)	9 (7%)	14	47
9	I	106/117 (91%)	101 (95%)	5 (5%)	26	62
10	J	175/274 (64%)	147 (84%)	28 (16%)	2	11
11	K	167/200 (84%)	138 (83%)	29 (17%)	2	10
12	L	202/212 (95%)	188 (93%)	14 (7%)	15	49
13	M	136/153 (89%)	124 (91%)	12 (9%)	10	36
14	N	107/147 (73%)	98 (92%)	9 (8%)	11	39
15	O	191/270 (71%)	169 (88%)	22 (12%)	5	24
16	P	183/236 (78%)	155 (85%)	28 (15%)	2	13
17	Q	219/268 (82%)	198 (90%)	21 (10%)	8	32
18	R	250/337 (74%)	218 (87%)	32 (13%)	4	20
19	S	126/231 (54%)	116 (92%)	10 (8%)	12	43
20	T	171/298 (57%)	156 (91%)	15 (9%)	10	36
21	U	73/77 (95%)	71 (97%)	2 (3%)	44	75
22	V	59/161 (37%)	58 (98%)	1 (2%)	60	83
23	W	104/167 (62%)	90 (86%)	14 (14%)	4	18
24	X	56/62 (90%)	52 (93%)	4 (7%)	14	47
25	Y	39/93 (42%)	37 (95%)	2 (5%)	24	60
26	Z	50/100 (50%)	45 (90%)	5 (10%)	7	30
27	0	36/84 (43%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	1	299/341 (88%)	269 (90%)	30 (10%)	7	30
29	2	99/137 (72%)	90 (91%)	9 (9%)	9	34
30	3	102/126 (81%)	97 (95%)	5 (5%)	25	61
31	4	121/123 (98%)	107 (88%)	14 (12%)	5	24
32	5	263/345 (76%)	234 (89%)	29 (11%)	6	26
33	6	153/252 (61%)	134 (88%)	19 (12%)	4	21
34	7	94/128 (73%)	81 (86%)	13 (14%)	3	16
35	8	149/240 (62%)	134 (90%)	15 (10%)	7	29
36	9	140/221 (63%)	127 (91%)	13 (9%)	9	33
37	a	156/171 (91%)	136 (87%)	20 (13%)	4	20
38	b	144/146 (99%)	122 (85%)	22 (15%)	2	13
39	c	110/120 (92%)	105 (96%)	5 (4%)	27	63
40	d	185/210 (88%)	162 (88%)	23 (12%)	4	21
All	All	5649/7581 (74%)	5053 (89%)	596 (11%)	10	27

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	LYS
2	B	95	ARG
2	B	107	ARG
2	B	127	ARG
2	B	128	LYS
2	B	140	THR
2	B	153	ARG
2	B	159	ARG
2	B	169	ARG
2	B	195	ILE
2	B	204	ASP
2	B	205	VAL
2	B	210	ARG
2	B	237	ARG
2	B	241	LEU
2	B	246	ILE
2	B	316	ARG
2	B	339	ASN
2	B	351	LYS

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Mol	Chain	Res	Type
2	B	364	GLN
2	B	375	LYS
2	B	376	ASN
2	B	382	VAL
3	C	53	LYS
3	C	61	LEU
3	C	79	ARG
3	C	86	GLU
3	C	89	ASN
3	C	94	MET
3	C	95	HIS
3	C	106	CYS
3	C	122	MET
3	C	134	LYS
3	C	146	LYS
3	C	153	THR
3	C	156	LYS
3	C	164	GLN
3	C	175	LYS
3	C	218	ARG
3	C	231	ILE
3	C	239	VAL
3	C	240	ASP
4	D	56	THR
4	D	86	ARG
4	D	106	MET
4	D	109	LYS
4	D	115	ARG
4	D	142	GLU
4	D	143	LEU
4	D	152	PHE
4	D	164	LYS
4	D	182	LEU
4	D	184	LEU
4	D	186	ARG
4	D	204	GLU
4	D	210	PHE
4	D	216	LEU
4	D	219	LYS
4	D	220	ARG
4	D	221	LEU
4	D	222	LEU

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Mol	Chain	Res	Type
4	D	233	ILE
4	D	247	GLN
4	D	252	GLU
4	D	254	ASN
4	D	274	MET
4	D	277	GLN
4	D	278	LYS
4	D	279	GLU
5	E	39	LYS
5	E	51	LYS
5	E	68	ARG
5	E	94	LYS
5	E	96	LEU
5	E	105	SER
5	E	120	LYS
5	E	139	SER
5	E	147	ARG
5	E	154	LEU
5	E	162	GLN
5	E	163	LEU
5	E	164	GLN
5	E	170	LYS
5	E	189	HIS
5	E	198	LYS
5	E	201	GLU
5	E	202	MET
5	E	204	GLN
5	E	211	GLU
5	E	214	LEU
5	E	259	THR
5	E	278	THR
5	E	280	LEU
6	F	33	SER
6	F	34	ILE
6	F	57	THR
6	F	64	GLU
6	F	65	LEU
6	F	71	ASP
6	F	74	HIS
6	F	92	GLU
6	F	106	LEU
6	F	115	THR

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Mol	Chain	Res	Type
6	F	119	LEU
6	F	130	ARG
6	F	141	ASN
6	F	150	GLN
6	F	152	LEU
6	F	161	LYS
6	F	171	GLU
6	F	175	LYS
6	F	176	GLN
6	F	186	ARG
6	F	194	TYR
7	G	22	GLN
7	G	34	LYS
7	G	45	MET
8	H	19	VAL
8	H	39	LEU
8	H	60	THR
8	H	68	THR
8	H	75	LYS
8	H	83	ARG
8	H	123	LEU
8	H	125	ARG
8	H	133	GLU
9	I	4	LEU
9	I	17	GLN
9	I	48	LYS
9	I	115	ASP
9	I	129	LYS
10	J	72	LYS
10	J	76	ARG
10	J	79	ARG
10	J	89	SER
10	J	99	ARG
10	J	103	LYS
10	J	107	GLU
10	J	114	TYR
10	J	132	GLU
10	J	133	LEU
10	J	144	LYS
10	J	149	LEU
10	J	153	GLU
10	J	158	ASN

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Mol	Chain	Res	Type
10	J	161	ARG
10	J	165	LEU
10	J	182	PHE
10	J	185	ASN
10	J	190	LEU
10	J	225	ASN
10	J	233	ARG
10	J	238	LEU
10	J	241	ARG
10	J	244	LYS
10	J	246	ARG
10	J	263	GLU
10	J	266	LYS
10	J	269	GLN
11	K	39	HIS
11	K	44	ARG
11	K	59	ARG
11	K	69	LEU
11	K	71	PHE
11	K	76	LEU
11	K	86	SER
11	K	90	LEU
11	K	98	MET
11	K	99	ARG
11	K	102	ARG
11	K	108	HIS
11	K	109	LEU
11	K	110	TRP
11	K	113	LEU
11	K	114	CYS
11	K	127	ARG
11	K	128	MET
11	K	130	LYS
11	K	139	MET
11	K	155	ASP
11	K	156	LEU
11	K	181	LEU
11	K	184	LEU
11	K	191	SER
11	K	196	LYS
11	K	210	LYS
11	K	216	LEU

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Mol	Chain	Res	Type
11	K	225	GLN
12	L	15	HIS
12	L	26	GLN
12	L	27	LEU
12	L	62	ASN
12	L	68	GLU
12	L	69	LEU
12	L	76	GLN
12	L	93	GLU
12	L	112	GLU
12	L	163	ASN
12	L	165	LEU
12	L	188	LEU
12	L	194	LEU
12	L	207	ASN
13	M	24	LYS
13	M	34	ARG
13	M	39	GLN
13	M	49	ILE
13	M	50	GLU
13	M	65	LYS
13	M	108	LEU
13	M	110	LEU
13	M	125	LEU
13	M	145	ARG
13	M	155	ARG
13	M	166	ARG
14	N	50	LYS
14	N	117	LYS
14	N	123	LYS
14	N	126	ARG
14	N	131	ARG
14	N	142	ARG
14	N	145	LYS
14	N	149	ASP
14	N	154	ARG
15	O	93	LEU
15	O	110	GLN
15	O	122	GLU
15	O	133	LYS
15	O	135	ASP
15	O	145	GLU

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Mol	Chain	Res	Type
15	O	159	LEU
15	O	171	LYS
15	O	184	LEU
15	O	202	LYS
15	O	205	ARG
15	O	223	LEU
15	O	224	LYS
15	O	235	THR
15	O	250	ARG
15	O	261	ILE
15	O	264	ARG
15	O	272	VAL
15	O	276	ARG
15	O	285	GLU
15	O	308	LYS
15	O	309	TRP
16	P	60	GLU
16	P	65	TRP
16	P	71	GLU
16	P	72	GLN
16	P	83	LYS
16	P	88	LYS
16	P	93	LEU
16	P	106	LYS
16	P	113	PHE
16	P	117	ASP
16	P	119	ARG
16	P	128	LEU
16	P	134	THR
16	P	136	GLN
16	P	137	LEU
16	P	141	LYS
16	P	145	MET
16	P	151	ARG
16	P	157	ILE
16	P	161	THR
16	P	164	MET
16	P	182	TRP
16	P	190	MET
16	P	196	GLU
16	P	197	ARG
16	P	229	ARG

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Mol	Chain	Res	Type
16	P	233	ARG
16	P	257	ARG
17	Q	14	ARG
17	Q	38	THR
17	Q	55	PHE
17	Q	65	PRO
17	Q	68	ARG
17	Q	72	MET
17	Q	77	LYS
17	Q	79	ASN
17	Q	86	PHE
17	Q	88	LYS
17	Q	102	LYS
17	Q	124	VAL
17	Q	127	LEU
17	Q	133	LEU
17	Q	186	LYS
17	Q	196	LEU
17	Q	204	ARG
17	Q	206	GLN
17	Q	213	VAL
17	Q	254	THR
17	Q	257	ARG
18	R	40	LYS
18	R	46	ARG
18	R	59	THR
18	R	61	GLU
18	R	75	GLU
18	R	104	ARG
18	R	111	LEU
18	R	116	LYS
18	R	133	GLU
18	R	137	LYS
18	R	138	ARG
18	R	159	LEU
18	R	163	GLU
18	R	168	LYS
18	R	172	LEU
18	R	175	LYS
18	R	182	ASP
18	R	191	ILE
18	R	193	LEU

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Mol	Chain	Res	Type
18	R	198	LEU
18	R	202	ARG
18	R	205	LEU
18	R	213	ASP
18	R	239	LYS
18	R	263	LYS
18	R	266	LEU
18	R	304	LEU
18	R	305	PHE
18	R	314	LEU
18	R	322	ARG
18	R	362	ARG
18	R	367	PHE
19	S	23	GLN
19	S	25	ARG
19	S	51	GLU
19	S	52	ARG
19	S	58	TYR
19	S	65	ILE
19	S	73	LEU
19	S	92	THR
19	S	102	LYS
19	S	118	MET
20	T	16	ARG
20	T	17	THR
20	T	25	LYS
20	T	29	LEU
20	T	59	ASN
20	T	60	LEU
20	T	105	ASP
20	T	120	LEU
20	T	131	VAL
20	T	150	TRP
20	T	161	LEU
20	T	176	ARG
20	T	182	THR
20	T	187	TYR
20	T	210	PHE
21	U	8	LEU
21	U	43	ILE
22	V	27	ARG
23	W	82	LYS

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Mol	Chain	Res	Type
23	W	84	ARG
23	W	86	LYS
23	W	101	LEU
23	W	103	LYS
23	W	107	CYS
23	W	111	LYS
23	W	134	LYS
23	W	140	ARG
23	W	141	GLN
23	W	157	ARG
23	W	163	THR
23	W	169	LYS
23	W	178	ARG
24	X	29	LYS
24	X	33	LEU
24	X	37	VAL
24	X	45	ARG
25	Y	73	ARG
25	Y	80	LEU
26	Z	64	ARG
26	Z	74	ARG
26	Z	95	THR
26	Z	111	LEU
26	Z	112	LEU
28	1	58	ARG
28	1	70	ILE
28	1	73	ILE
28	1	84	ARG
28	1	102	ASP
28	1	120	GLN
28	1	123	ASN
28	1	128	VAL
28	1	138	VAL
28	1	142	LEU
28	1	144	LYS
28	1	154	LEU
28	1	156	MET
28	1	165	ILE
28	1	175	ARG
28	1	177	GLU
28	1	212	GLN
28	1	216	LEU

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Mol	Chain	Res	Type
28	1	230	ASN
28	1	232	ASP
28	1	239	ASP
28	1	262	ASP
28	1	264	ARG
28	1	308	LEU
28	1	314	GLU
28	1	327	LYS
28	1	344	ASP
28	1	346	LYS
28	1	360	ARG
28	1	366	ARG
29	2	58	LEU
29	2	59	LEU
29	2	60	LYS
29	2	65	ASP
29	2	80	GLN
29	2	102	MET
29	2	111	ARG
29	2	121	LYS
29	2	133	THR
30	3	22	LYS
30	3	43	LEU
30	3	47	GLN
30	3	73	ASN
30	3	113	LEU
31	4	13	ARG
31	4	38	GLU
31	4	42	LYS
31	4	47	LYS
31	4	50	ASP
31	4	54	GLN
31	4	59	ILE
31	4	65	ARG
31	4	91	ILE
31	4	98	LEU
31	4	102	LYS
31	4	121	LEU
31	4	132	LEU
31	4	136	LYS
32	5	99	ARG
32	5	101	LEU

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Mol	Chain	Res	Type
32	5	104	ARG
32	5	116	LEU
32	5	117	SER
32	5	143	THR
32	5	148	LYS
32	5	164	SER
32	5	177	ARG
32	5	187	VAL
32	5	236	LEU
32	5	237	ASN
32	5	240	ASP
32	5	244	LEU
32	5	251	SER
32	5	271	THR
32	5	281	ARG
32	5	283	ILE
32	5	296	LYS
32	5	297	MET
32	5	310	LEU
32	5	312	ARG
32	5	314	GLU
32	5	320	VAL
32	5	335	VAL
32	5	339	HIS
32	5	368	MET
32	5	369	LYS
32	5	390	VAL
33	6	31	LEU
33	6	33	ARG
33	6	52	GLN
33	6	56	GLU
33	6	70	LYS
33	6	80	LEU
33	6	97	ARG
33	6	103	LYS
33	6	104	HIS
33	6	106	ARG
33	6	111	LYS
33	6	113	GLU
33	6	115	LYS
33	6	169	LEU
33	6	177	TRP

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Mol	Chain	Res	Type
33	6	178	LYS
33	6	198	GLU
33	6	254	PHE
33	6	273	LYS
34	7	47	LEU
34	7	51	LYS
34	7	59	ASN
34	7	72	ARG
34	7	87	ASN
34	7	104	ARG
34	7	111	LEU
34	7	116	LYS
34	7	117	LYS
34	7	121	VAL
34	7	143	THR
34	7	145	LYS
34	7	146	PHE
35	8	97	ARG
35	8	118	LEU
35	8	132	MET
35	8	148	VAL
35	8	163	LEU
35	8	166	LYS
35	8	170	LEU
35	8	179	LEU
35	8	181	THR
35	8	183	LEU
35	8	191	GLU
35	8	202	LEU
35	8	233	LYS
35	8	260	THR
35	8	262	ARG
36	9	41	LEU
36	9	56	LEU
36	9	65	CYS
36	9	106	LYS
36	9	108	ASN
36	9	125	LYS
36	9	154	THR
36	9	160	CYS
36	9	163	VAL
36	9	176	MET

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Mol	Chain	Res	Type
36	9	184	HIS
36	9	211	LYS
36	9	217	GLN
37	a	20	GLN
37	a	28	VAL
37	a	30	THR
37	a	34	LYS
37	a	36	LYS
37	a	48	ARG
37	a	49	ASP
37	a	70	THR
37	a	101	LEU
37	a	114	LEU
37	a	119	ILE
37	a	132	LYS
37	a	150	SER
37	a	158	GLN
37	a	162	ILE
37	a	175	LYS
37	a	182	ARG
37	a	187	ARG
37	a	191	LEU
37	a	192	TRP
38	b	5	GLN
38	b	14	LEU
38	b	19	GLN
38	b	32	THR
38	b	35	LYS
38	b	52	ARG
38	b	57	LYS
38	b	63	MET
38	b	65	ASP
38	b	71	LEU
38	b	83	GLU
38	b	105	LEU
38	b	107	LYS
38	b	117	GLU
38	b	119	LEU
38	b	123	GLU
38	b	129	VAL
38	b	130	ASP
38	b	132	LEU

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Mol	Chain	Res	Type
38	b	136	LYS
38	b	137	LYS
38	b	146	GLU
39	c	45	LEU
39	c	57	LYS
39	c	70	LYS
39	c	78	LEU
39	c	101	THR
40	d	9	ARG
40	d	11	ARG
40	d	22	ILE
40	d	32	LEU
40	d	33	GLU
40	d	38	LEU
40	d	62	ARG
40	d	72	LYS
40	d	74	MET
40	d	83	LYS
40	d	94	ARG
40	d	96	ARG
40	d	101	VAL
40	d	110	LEU
40	d	137	LEU
40	d	142	LEU
40	d	173	ASP
40	d	177	HIS
40	d	191	LYS
40	d	194	GLN
40	d	203	GLU
40	d	207	LEU
40	d	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	378	ASN
3	C	207	GLN
16	P	256	ASN
19	S	84	ASN
22	V	81	ASN
35	8	235	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2682/3296 (81%)	692 (25%)	132 (4%)
41	e	18/20 (90%)	6 (33%)	0
All	All	2700/3316 (81%)	698 (25%)	132 (4%)

All (698) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	29	A
1	A	30	U
1	A	31	U
1	A	32	U
1	A	35	U
1	A	38	A
1	A	41	G
1	A	43	U
1	A	45	U
1	A	48	A
1	A	49	G
1	A	68	A
1	A	69	U
1	A	70	A
1	A	85	A
1	A	93	U
1	A	94	A
1	A	106	A
1	A	112	G
1	A	115	A
1	A	116	C
1	A	117	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	A
1	A	134	U
1	A	135	U
1	A	139	U
1	A	149	A

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Mol	Chain	Res	Type
1	A	150	A
1	A	151	A
1	A	152	G
1	A	153	G
1	A	155	A
1	A	161	U
1	A	162	U
1	A	163	A
1	A	164	U
1	A	165	A
1	A	204	A
1	A	209	U
1	A	215	A
1	A	216	U
1	A	217	A
1	A	218	A
1	A	219	U
1	A	222	A
1	A	236	A
1	A	239	A
1	A	244	A
1	A	245	G
1	A	246	U
1	A	253	A
1	A	255	G
1	A	256	A
1	A	261	A
1	A	262	A
1	A	264	U
1	A	266	A
1	A	269	A
1	A	270	G
1	A	276	U
1	A	277	U
1	A	281	A
1	A	288	G
1	A	290	G
1	A	292	G
1	A	301	A
1	A	307	G
1	A	308	U
1	A	309	C

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Mol	Chain	Res	Type
1	A	311	A
1	A	312	A
1	A	313	U
1	A	314	A
1	A	315	A
1	A	316	G
1	A	327	A
1	A	328	A
1	A	329	A
1	A	330	A
1	A	331	A
1	A	332	A
1	A	336	A
1	A	337	A
1	A	342	A
1	A	343	U
1	A	344	A
1	A	348	U
1	A	349	A
1	A	355	U
1	A	359	A
1	A	365	A
1	A	366	A
1	A	380	G
1	A	382	A
1	A	384	A
1	A	386	U
1	A	387	A
1	A	401	A
1	A	425	A
1	A	427	G
1	A	428	C
1	A	429	A
1	A	430	A
1	A	433	A
1	A	435	G
1	A	442	U
1	A	445	U
1	A	448	U
1	A	450	U
1	A	455	A
1	A	461	U

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Mol	Chain	Res	Type
1	A	462	A
1	A	472	U
1	A	474	A
1	A	486	G
1	A	487	U
1	A	494	U
1	A	498	A
1	A	502	A
1	A	503	A
1	A	507	A
1	A	508	U
1	A	510	A
1	A	516	A
1	A	526	A
1	A	527	A
1	A	536	A
1	A	537	U
1	A	546	A
1	A	548	A
1	A	551	U
1	A	554	U
1	A	561	U
1	A	562	U
1	A	563	U
1	A	564	A
1	A	565	A
1	A	578	G
1	A	595	U
1	A	604	G
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	618	A
1	A	619	C
1	A	620	G
1	A	621	A
1	A	637	U
1	A	638	U
1	A	644	A
1	A	655	A
1	A	656	A

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Mol	Chain	Res	Type
1	A	661	G
1	A	666	G
1	A	667	U
1	A	673	A
1	A	674	A
1	A	675	G
1	A	676	A
1	A	681	U
1	A	682	C
1	A	683	U
1	A	684	G
1	A	696	G
1	A	703	U
1	A	706	U
1	A	707	A
1	A	710	A
1	A	718	G
1	A	719	U
1	A	720	A
1	A	733	A
1	A	734	U
1	A	736	A
1	A	737	A
1	A	747	U
1	A	755	U
1	A	767	A
1	A	776	A
1	A	777	G
1	A	778	A
1	A	782	G
1	A	783	U
1	A	789	A
1	A	790	A
1	A	797	U
1	A	798	A
1	A	803	A
1	A	833	U
1	A	835	A
1	A	840	C
1	A	841	G
1	A	843	A
1	A	845	U

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Mol	Chain	Res	Type
1	A	854	A
1	A	855	U
1	A	856	A
1	A	857	U
1	A	858	A
1	A	866	G
1	A	867	A
1	A	871	A
1	A	872	G
1	A	884	U
1	A	887	G
1	A	891	A
1	A	900	A
1	A	901	A
1	A	909	A
1	A	910	G
1	A	912	C
1	A	916	A
1	A	919	A
1	A	925	U
1	A	928	A
1	A	929	G
1	A	938	A
1	A	939	A
1	A	942	A
1	A	947	G
1	A	948	U
1	A	951	A
1	A	952	A
1	A	953	U
1	A	961	A
1	A	966	A
1	A	967	U
1	A	1058	U
1	A	1063	A
1	A	1065	A
1	A	1075	A
1	A	1077	A
1	A	1078	U
1	A	1086	U
1	A	1087	U
1	A	1094	U

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Mol	Chain	Res	Type
1	A	1095	A
1	A	1096	A
1	A	1097	U
1	A	1099	U
1	A	1101	C
1	A	1102	G
1	A	1105	U
1	A	1110	A
1	A	1111	U
1	A	1112	A
1	A	1113	A
1	A	1114	U
1	A	1115	A
1	A	1117	G
1	A	1118	A
1	A	1119	A
1	A	1126	A
1	A	1127	A
1	A	1130	C
1	A	1161	A
1	A	1169	A
1	A	1170	U
1	A	1171	A
1	A	1182	A
1	A	1191	U
1	A	1206	A
1	A	1213	A
1	A	1242	A
1	A	1243	U
1	A	1244	A
1	A	1255	A
1	A	1256	U
1	A	1257	U
1	A	1258	A
1	A	1260	U
1	A	1267	A
1	A	1269	G
1	A	1271	A
1	A	1272	U
1	A	1273	U
1	A	1279	A
1	A	1280	A

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Mol	Chain	Res	Type
1	A	1281	U
1	A	1283	G
1	A	1286	A
1	A	1287	A
1	A	1289	G
1	A	1298	A
1	A	1304	G
1	A	1305	A
1	A	1306	A
1	A	1307	A
1	A	1308	A
1	A	1313	G
1	A	1314	U
1	A	1315	A
1	A	1316	U
1	A	1317	A
1	A	1331	A
1	A	1332	A
1	A	1333	A
1	A	1337	U
1	A	1342	U
1	A	1344	U
1	A	1346	A
1	A	1349	A
1	A	1350	U
1	A	1352	A
1	A	1356	U
1	A	1357	A
1	A	1358	C
1	A	1359	G
1	A	1360	G
1	A	1361	C
1	A	1362	C
1	A	1365	U
1	A	1368	U
1	A	1371	A
1	A	1372	A
1	A	1374	U
1	A	1386	A
1	A	1387	A
1	A	1389	U
1	A	1392	A

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Mol	Chain	Res	Type
1	A	1393	U
1	A	1396	A
1	A	1399	A
1	A	1400	U
1	A	1404	A
1	A	1405	U
1	A	1406	A
1	A	1409	C
1	A	1410	U
1	A	1411	A
1	A	1412	U
1	A	1418	U
1	A	1423	A
1	A	1424	U
1	A	1477	A
1	A	1490	A
1	A	1493	U
1	A	1494	A
1	A	1500	U
1	A	1501	A
1	A	1507	U
1	A	1516	U
1	A	1523	A
1	A	1528	G
1	A	1531	C
1	A	1534	G
1	A	1537	A
1	A	1546	G
1	A	1548	A
1	A	1549	U
1	A	1560	A
1	A	1562	A
1	A	1563	C
1	A	1568	U
1	A	1569	C
1	A	1578	A
1	A	1579	A
1	A	1583	G
1	A	1598	A
1	A	1599	A
1	A	1600	U
1	A	1603	G

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Mol	Chain	Res	Type
1	A	1604	A
1	A	1605	U
1	A	1606	A
1	A	1612	A
1	A	1616	A
1	A	1618	G
1	A	1626	G
1	A	1632	A
1	A	1633	U
1	A	1634	A
1	A	1635	G
1	A	1648	U
1	A	1649	C
1	A	1653	A
1	A	1655	A
1	A	1661	A
1	A	1662	U
1	A	1663	A
1	A	1664	A
1	A	1665	G
1	A	1666	A
1	A	1671	A
1	A	1672	G
1	A	1680	A
1	A	1687	A
1	A	1689	U
1	A	1693	A
1	A	1694	A
1	A	1706	G
1	A	1707	C
1	A	1708	A
1	A	1709	G
1	A	1715	A
1	A	1716	U
1	A	1717	A
1	A	1720	U
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1737	A
1	A	1740	U
1	A	1743	G

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Mol	Chain	Res	Type
1	A	1746	C
1	A	1755	A
1	A	1764	U
1	A	1767	A
1	A	1768	A
1	A	1769	U
1	A	1770	U
1	A	1777	C
1	A	1778	G
1	A	1782	A
1	A	1786	A
1	A	1789	U
1	A	1790	A
1	A	1797	G
1	A	1807	A
1	A	1813	A
1	A	1814	U
1	A	1815	U
1	A	1818	G
1	A	1820	G
1	A	1824	U
1	A	1825	A
1	A	1826	U
1	A	1829	U
1	A	1830	G
1	A	1831	U
1	A	1836	A
1	A	1837	A
1	A	1838	A
1	A	1851	U
1	A	1855	U
1	A	1863	C
1	A	1867	U
1	A	1869	A
1	A	1870	A
1	A	1871	U
1	A	1872	G
1	A	1875	G
1	A	1882	U
1	A	1891	U
1	A	1892	G
1	A	1893	U

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Mol	Chain	Res	Type
1	A	1897	C
1	A	1920	A
1	A	1923	C
1	A	1930	A
1	A	1931	A
1	A	1933	A
1	A	1936	C
1	A	1943	C
1	A	1949	G
1	A	1951	A
1	A	1952	A
1	A	1955	C
1	A	1956	G
1	A	1959	A
1	A	1961	G
1	A	1963	C
1	A	1964	C
1	A	1969	G
1	A	1980	G
1	A	1989	U
1	A	1990	A
1	A	1991	G
1	A	1995	G
1	A	2005	U
1	A	2009	U
1	A	2084	G
1	A	2093	A
1	A	2094	A
1	A	2095	U
1	A	2251	A
1	A	2253	A
1	A	2263	U
1	A	2264	G
1	A	2276	G
1	A	2293	A
1	A	2301	C
1	A	2305	A
1	A	2306	U
1	A	2309	G
1	A	2310	U
1	A	2313	A
1	A	2315	A

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Mol	Chain	Res	Type
1	A	2316	A
1	A	2317	A
1	A	2318	U
1	A	2323	A
1	A	2324	U
1	A	2325	A
1	A	2330	A
1	A	2332	U
1	A	2349	A
1	A	2356	A
1	A	2358	A
1	A	2360	U
1	A	2361	A
1	A	2362	U
1	A	2363	A
1	A	2369	U
1	A	2372	U
1	A	2373	U
1	A	2374	A
1	A	2379	U
1	A	2380	U
1	A	2419	U
1	A	2423	G
1	A	2424	U
1	A	2425	A
1	A	2427	U
1	A	2428	A
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2436	A
1	A	2438	A
1	A	2439	U
1	A	2444	A
1	A	2447	A
1	A	2453	G
1	A	2455	A
1	A	2458	G
1	A	2461	A
1	A	2462	A
1	A	2467	A
1	A	2468	A

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Mol	Chain	Res	Type
1	A	2469	U
1	A	2470	A
1	A	2575	A
1	A	2580	A
1	A	2585	A
1	A	2586	U
1	A	2587	U
1	A	2588	A
1	A	2591	A
1	A	2597	G
1	A	2599	A
1	A	2601	A
1	A	2603	C
1	A	2610	A
1	A	2612	A
1	A	2613	A
1	A	2614	U
1	A	2616	G
1	A	2618	A
1	A	2638	G
1	A	2650	G
1	A	2652	C
1	A	2656	A
1	A	2659	A
1	A	2660	A
1	A	2666	A
1	A	2670	C
1	A	2671	U
1	A	2672	G
1	A	2673	A
1	A	2674	U
1	A	2691	A
1	A	2695	A
1	A	2696	A
1	A	2700	A
1	A	2701	A
1	A	2705	A
1	A	2707	G
1	A	2711	G
1	A	2713	G
1	A	2714	A
1	A	2720	G

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Mol	Chain	Res	Type
1	A	2725	A
1	A	2737	A
1	A	2740	A
1	A	2741	G
1	A	2742	A
1	A	2744	A
1	A	2750	A
1	A	2753	U
1	A	2760	G
1	A	2766	U
1	A	2773	C
1	A	2774	G
1	A	2779	A
1	A	2784	U
1	A	2791	U
1	A	2795	U
1	A	2796	G
1	A	2797	U
1	A	2802	G
1	A	2813	U
1	A	2814	U
1	A	2815	U
1	A	2821	U
1	A	2823	C
1	A	2826	C
1	A	2829	U
1	A	2833	A
1	A	2834	A
1	A	2836	G
1	A	2840	C
1	A	2852	U
1	A	2853	A
1	A	2869	A
1	A	2870	G
1	A	2876	U
1	A	2877	U
1	A	2880	U
1	A	2881	A
1	A	2894	A
1	A	2896	U
1	A	2897	A
1	A	2898	U

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Mol	Chain	Res	Type
1	A	2907	U
1	A	2909	A
1	A	2913	U
1	A	2928	A
1	A	2930	G
1	A	2940	G
1	A	2950	A
1	A	2956	U
1	A	2957	A
1	A	2958	U
1	A	2959	C
1	A	2980	A
1	A	3016	A
1	A	3017	U
1	A	3021	A
1	A	3023	U
1	A	3024	U
1	A	3037	A
1	A	3038	U
1	A	3039	A
1	A	3043	U
1	A	3050	G
1	A	3060	U
1	A	3062	A
1	A	3069	A
1	A	3070	A
1	A	3080	A
1	A	3092	U
1	A	3093	U
1	A	3094	A
1	A	3098	A
1	A	3102	A
1	A	3103	G
1	A	3106	G
1	A	3122	U
1	A	3123	A
1	A	3124	A
1	A	3125	U
1	A	3126	C
1	A	3127	U
1	A	3134	U
1	A	3135	U

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Mol	Chain	Res	Type
1	A	3136	U
1	A	3141	U
1	A	3148	A
1	A	3150	U
1	A	3151	A
1	A	3152	A
1	A	3153	U
1	A	3155	A
1	A	3159	G
1	A	3168	A
1	A	3169	U
1	A	3171	A
1	A	3172	U
1	A	3173	U
1	A	3193	A
1	A	3194	U
1	A	3248	C
1	A	3251	A
1	A	3252	U
1	A	3253	U
1	A	3255	A
1	A	3256	U
1	A	3257	C
1	A	3264	C
1	A	3265	U
1	A	3268	A
1	A	3269	U
1	A	3274	U
41	e	2	C
41	e	6	G
41	e	68	C
41	e	71	G
41	e	74	C
41	e	76	A

All (132) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	25	A
1	A	27	A
1	A	34	U
1	A	44	U

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Mol	Chain	Res	Type
1	A	93	U
1	A	134	U
1	A	162	U
1	A	164	U
1	A	216	U
1	A	217	A
1	A	236	A
1	A	239	A
1	A	261	A
1	A	268	C
1	A	276	U
1	A	306	G
1	A	313	U
1	A	326	A
1	A	329	A
1	A	365	A
1	A	409	A
1	A	426	A
1	A	429	A
1	A	454	A
1	A	461	U
1	A	486	G
1	A	507	A
1	A	526	A
1	A	536	A
1	A	561	U
1	A	563	U
1	A	564	A
1	A	578	G
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	637	U
1	A	643	U
1	A	655	A
1	A	666	G
1	A	675	G
1	A	682	C
1	A	696	G
1	A	733	A
1	A	735	A

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Mol	Chain	Res	Type
1	A	746	A
1	A	781	G
1	A	840	C
1	A	856	A
1	A	909	A
1	A	951	A
1	A	1062	U
1	A	1064	A
1	A	1093	A
1	A	1113	A
1	A	1126	A
1	A	1272	U
1	A	1306	A
1	A	1312	G
1	A	1313	G
1	A	1316	U
1	A	1331	A
1	A	1349	A
1	A	1409	C
1	A	1410	U
1	A	1422	A
1	A	1489	U
1	A	1493	U
1	A	1522	A
1	A	1547	U
1	A	1560	A
1	A	1591	G
1	A	1662	U
1	A	1663	A
1	A	1664	A
1	A	1665	G
1	A	1693	A
1	A	1706	G
1	A	1707	C
1	A	1708	A
1	A	1727	A
1	A	1818	G
1	A	1829	U
1	A	1830	G
1	A	1854	U
1	A	1892	G
1	A	1990	A

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Mol	Chain	Res	Type
1	A	2301	C
1	A	2304	A
1	A	2309	G
1	A	2314	U
1	A	2316	A
1	A	2324	U
1	A	2329	A
1	A	2357	U
1	A	2359	U
1	A	2372	U
1	A	2373	U
1	A	2378	A
1	A	2426	A
1	A	2427	U
1	A	2437	U
1	A	2446	U
1	A	2467	A
1	A	2585	A
1	A	2587	U
1	A	2591	A
1	A	2612	A
1	A	2613	A
1	A	2713	G
1	A	2783	U
1	A	2796	G
1	A	2880	U
1	A	2897	A
1	A	2906	U
1	A	2956	U
1	A	3020	U
1	A	3023	U
1	A	3036	U
1	A	3068	U
1	A	3069	A
1	A	3122	U
1	A	3124	A
1	A	3125	U
1	A	3126	C
1	A	3135	U
1	A	3150	U
1	A	3171	A
1	A	3193	A

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Mol	Chain	Res	Type
1	A	3252	U
1	A	3268	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 113 ligands modelled in this entry, 113 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
41	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2226:A	O3'	2227:U	P	17.43
1	A	2197:A	O3'	2198:U	P	17.36
1	e	6:G	O3'	63:G	P	15.82
1	A	2344:A	O3'	2345:A	P	15.67
1	A	1374:U	O3'	1375:A	P	11.56
1	A	558:A	O3'	559:U	P	8.70

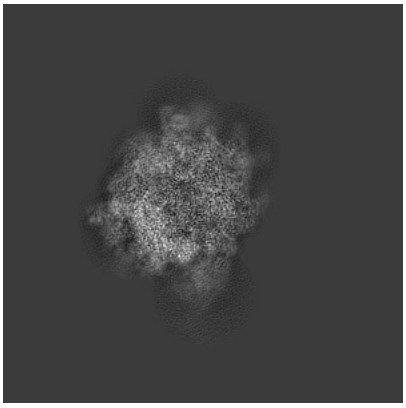
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2566. These allow visual inspection of the internal detail of the map and identification of artifacts.

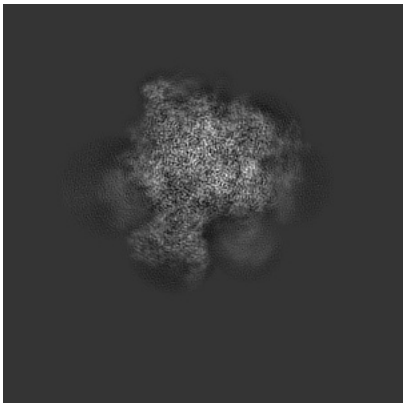
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

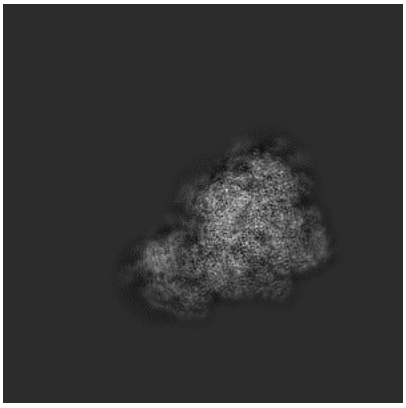
6.1.1 Primary map



X



Y

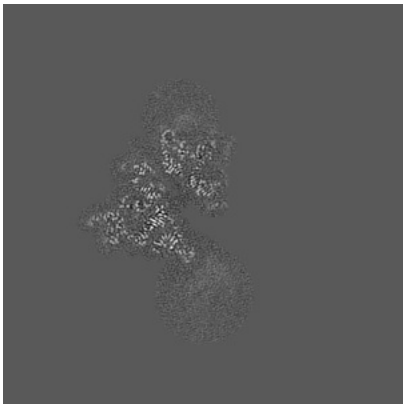


Z

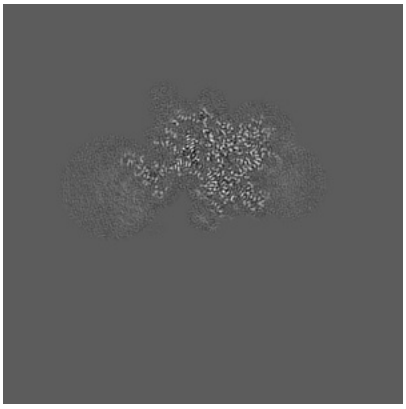
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

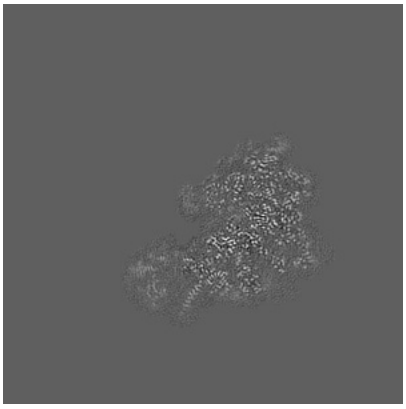
6.2.1 Primary map



X Index: 180



Y Index: 180

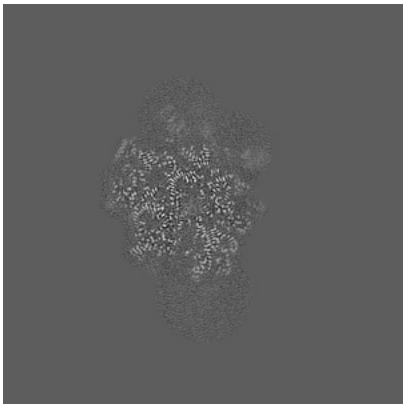


Z Index: 180

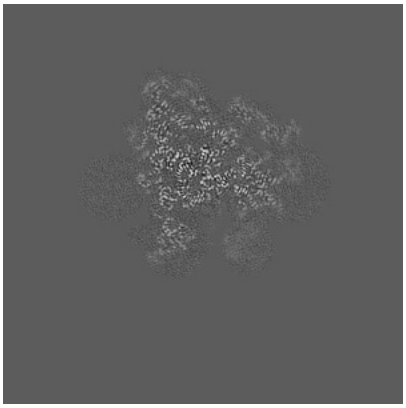
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

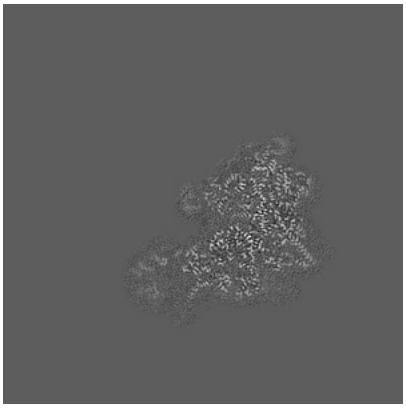
6.3.1 Primary map



X Index: 212



Y Index: 145

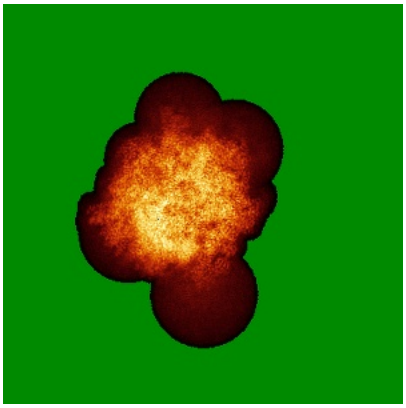


Z Index: 182

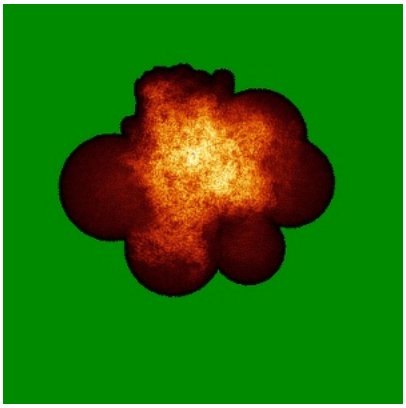
The images above show the largest variance slices of the map in three orthogonal directions.

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

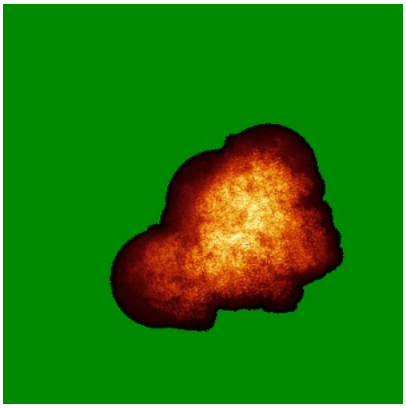
6.4.1 Primary map



X



Y

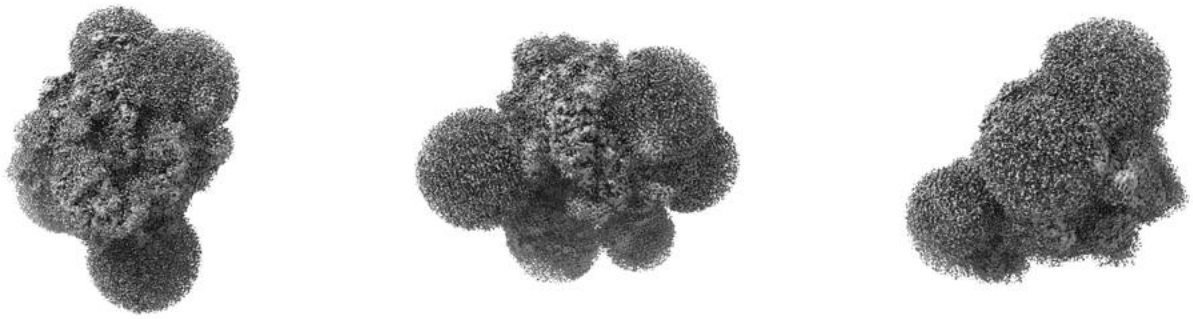


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0681. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

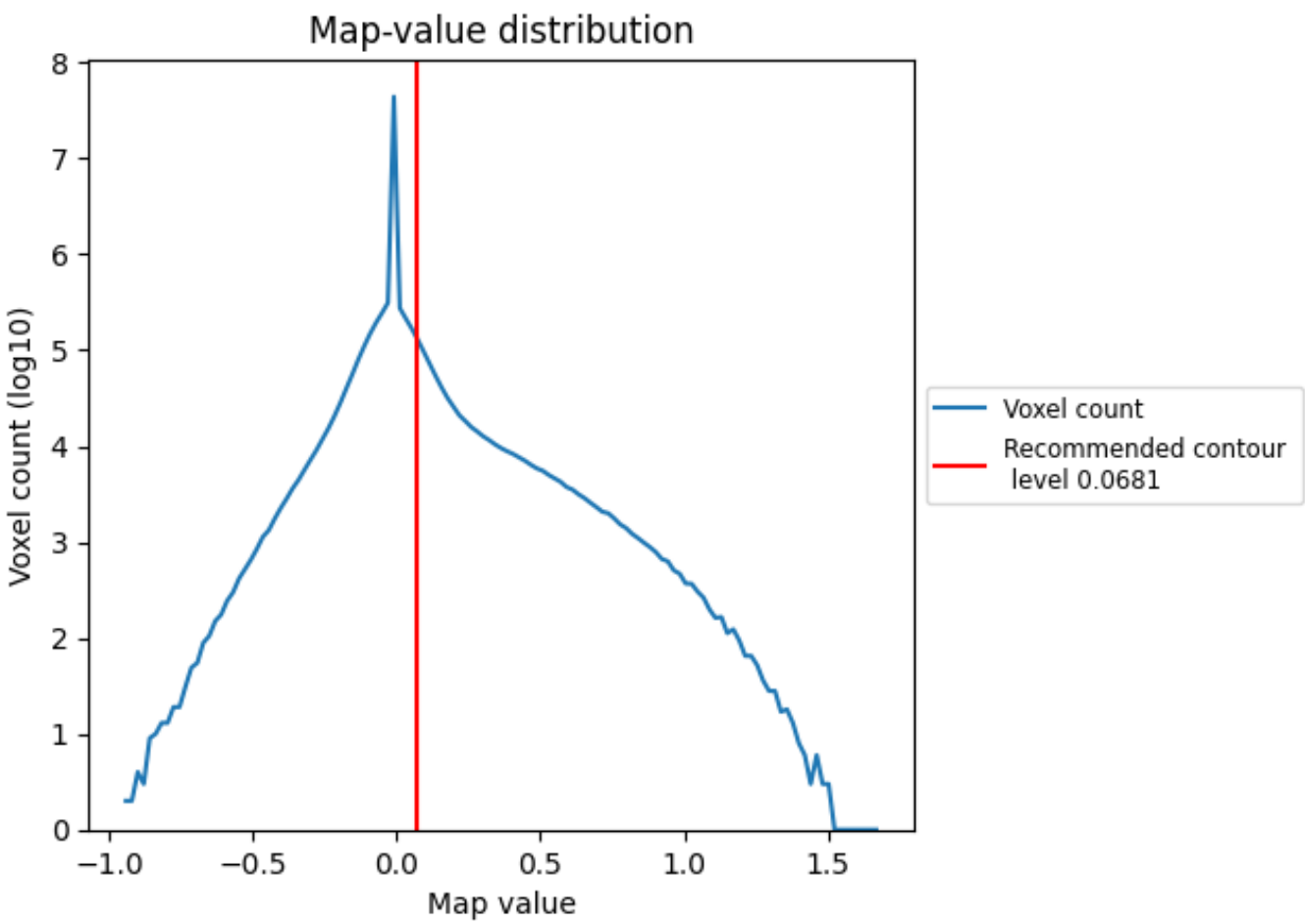
6.6 Mask visualisation (i)

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

7 Map analysis (i)

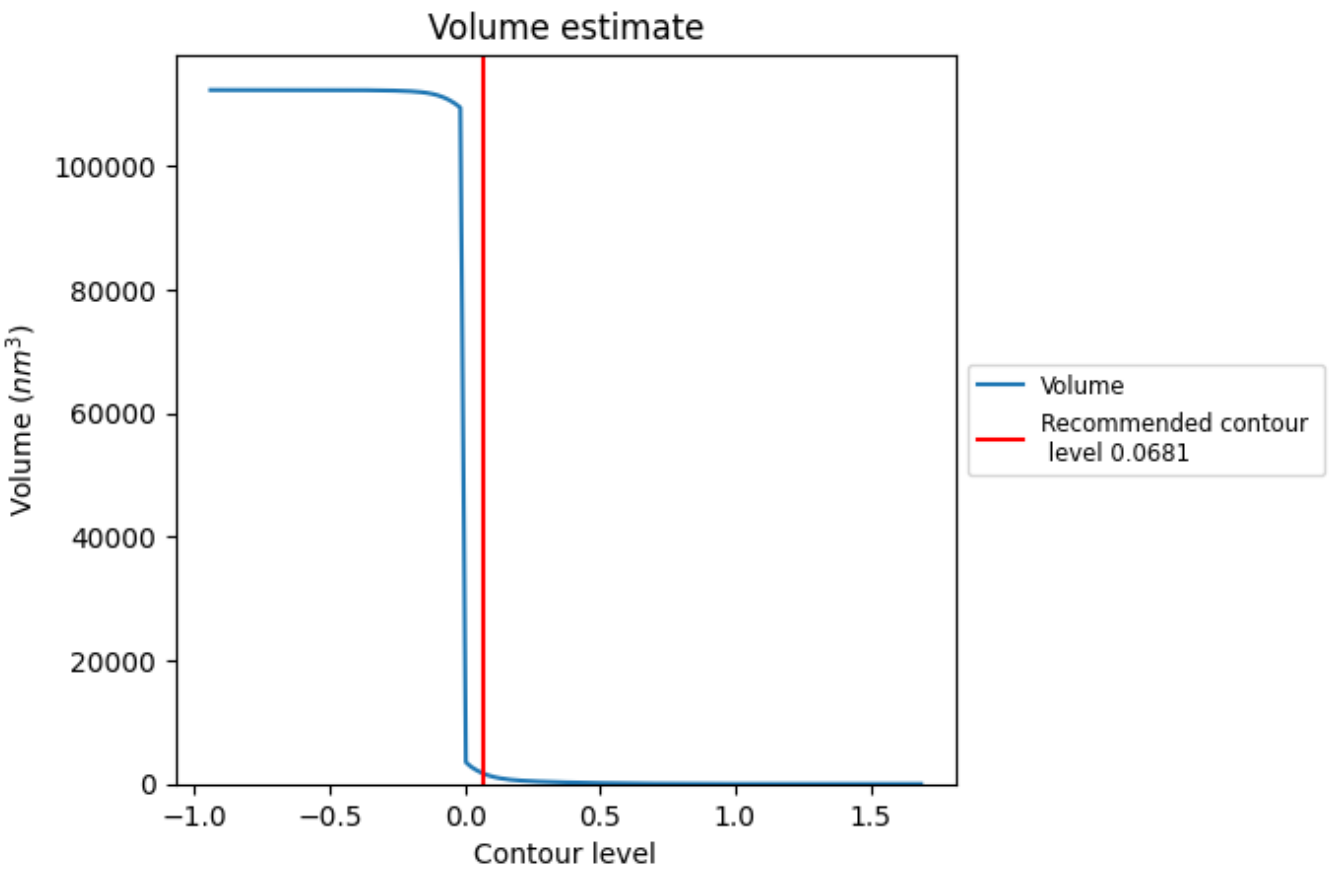
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

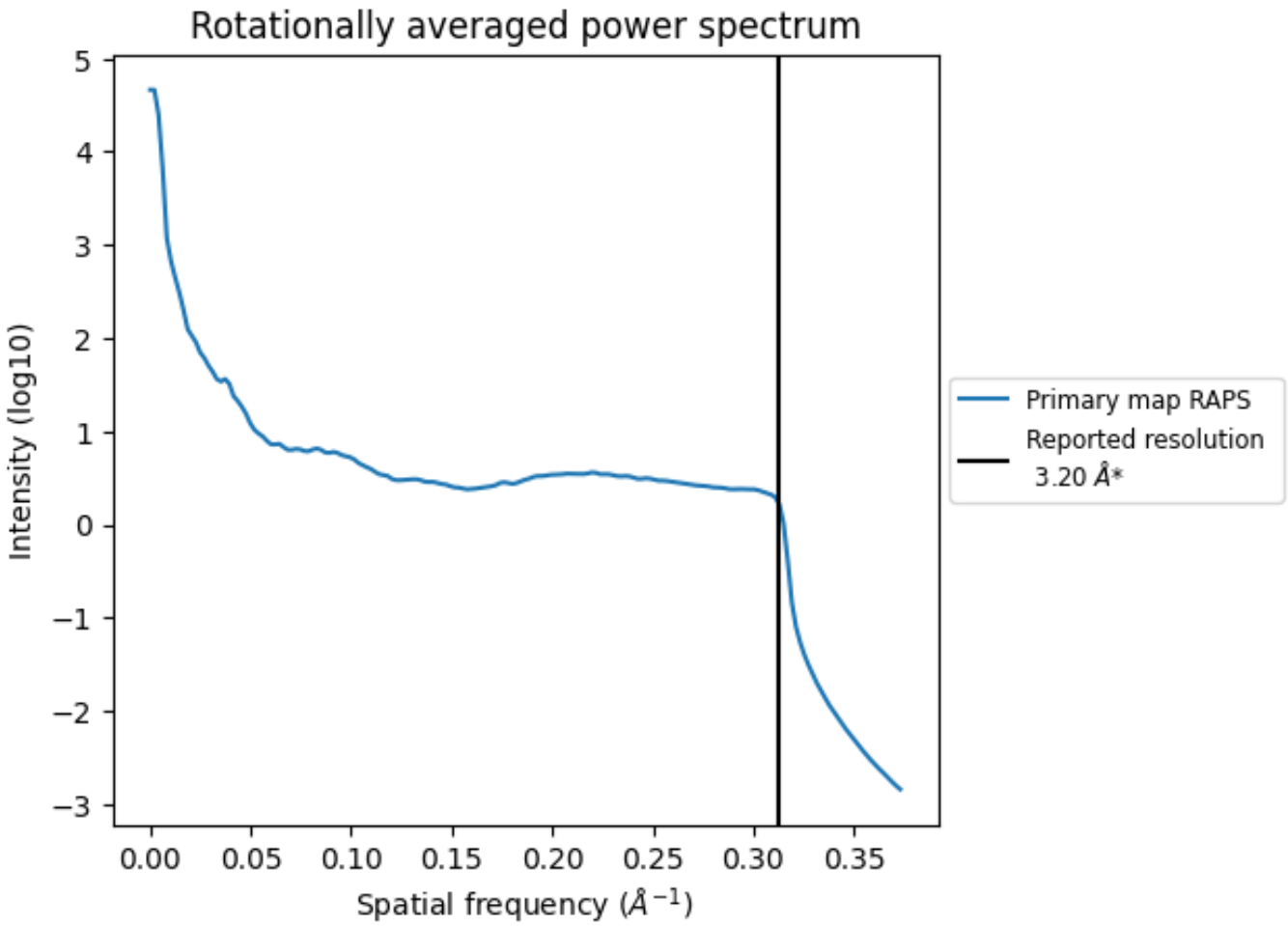
7.2 Volume estimate (i)



The volume at the recommended contour level is 1704 nm^3; this corresponds to an approximate mass of 1539 kDa.

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

7.3 Rotationally averaged power spectrum (i)

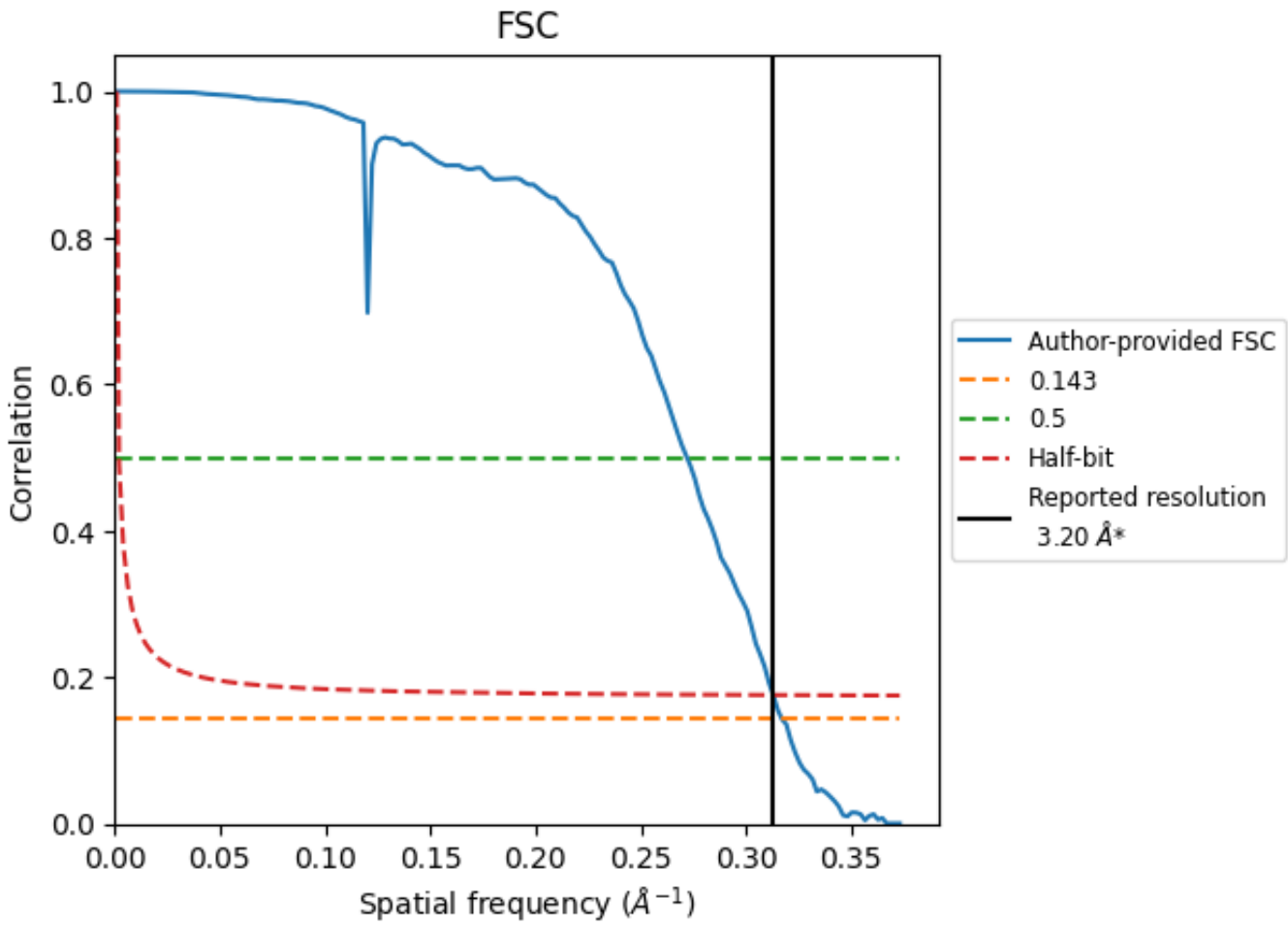


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

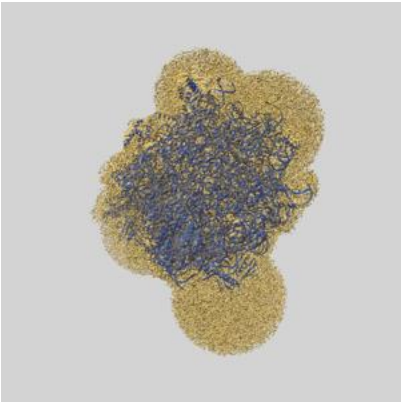
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.68	3.19
Unmasked-calculated*	-	-	-

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

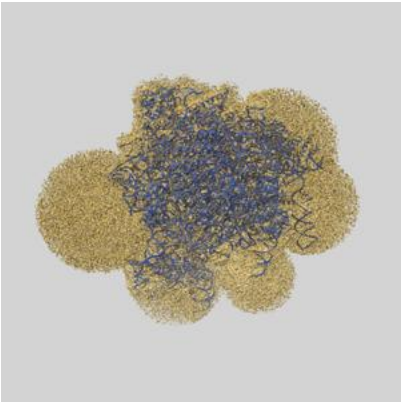
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2566 and PDB model 3J6B. Per-residue inclusion information can be found in section 3 on page 12.

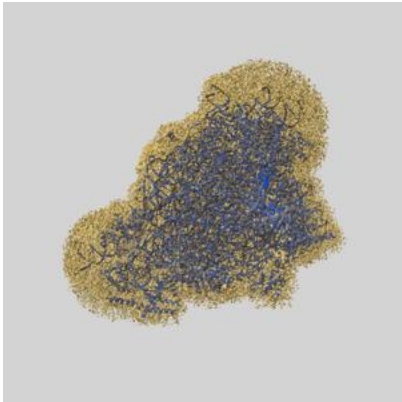
9.1 Map-model overlay (i)



X



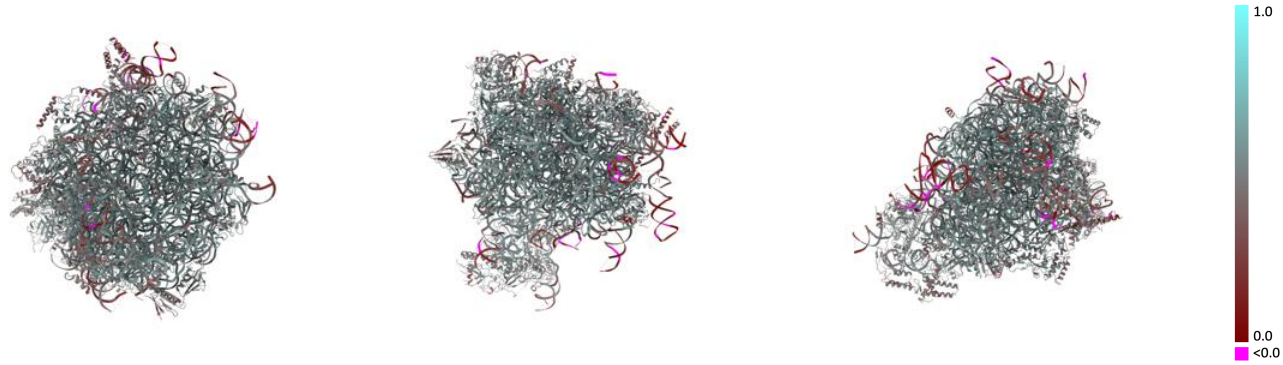
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0681 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

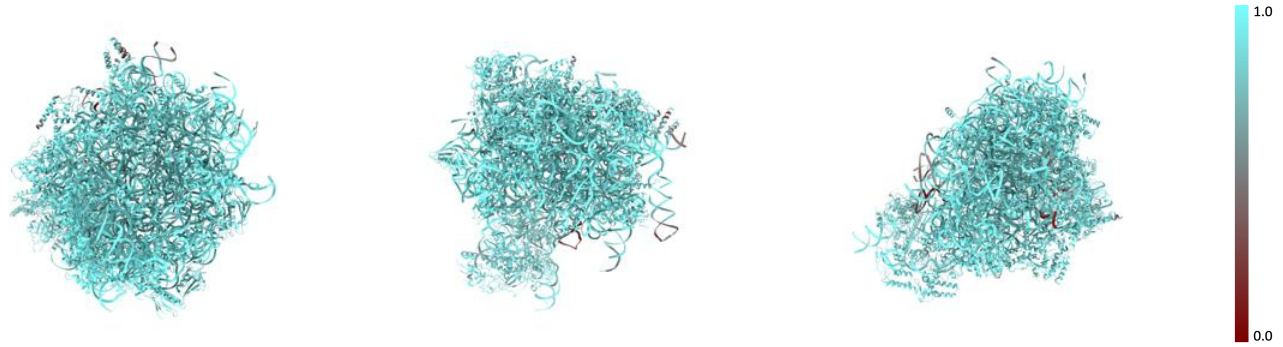
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

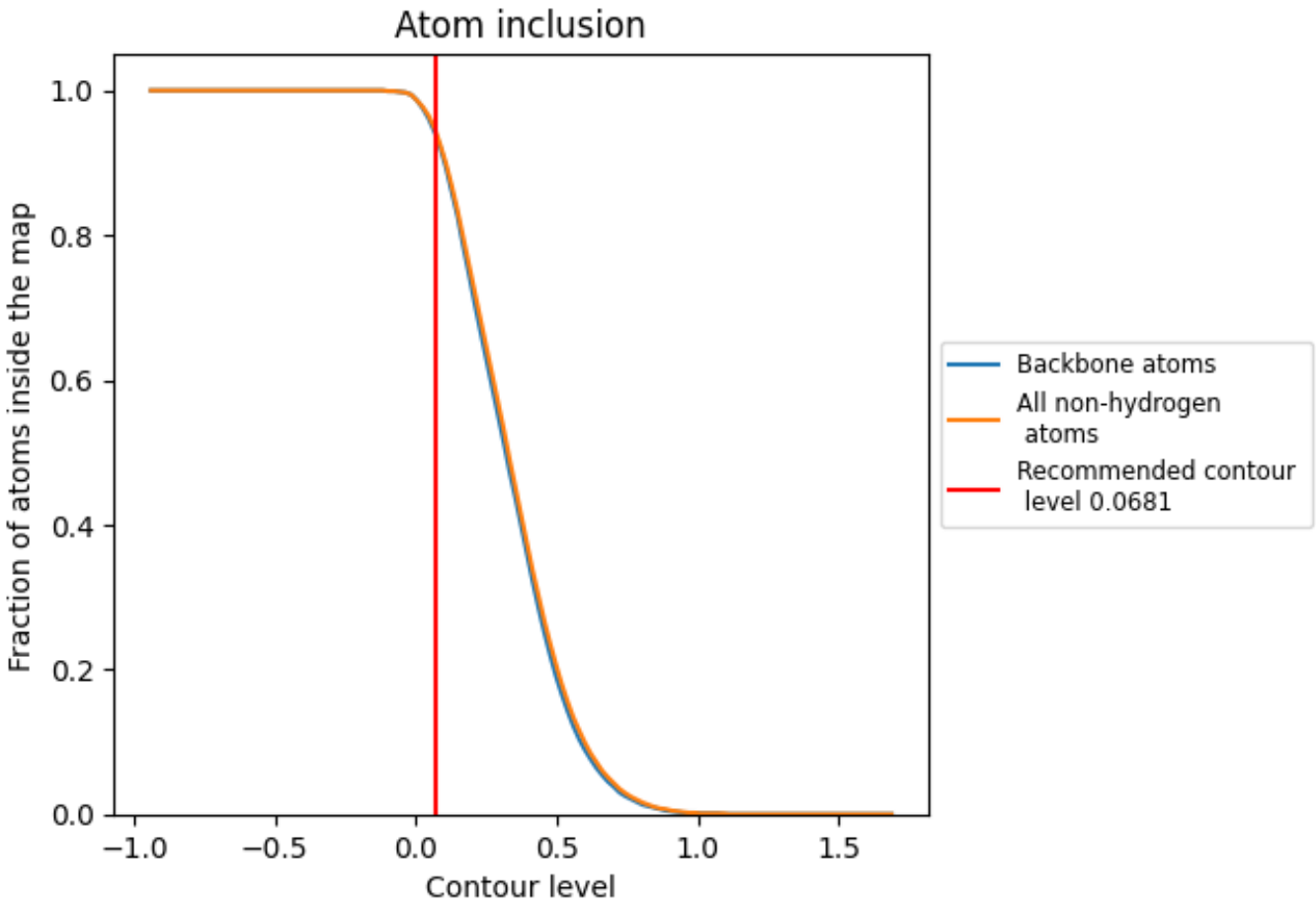
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0681).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0681) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.5070
0	0.9550	0.5600
1	0.9440	0.5060
2	0.9420	0.4870
3	0.9400	0.5180
4	0.9500	0.5420
5	0.9400	0.5190
6	0.9260	0.4600
7	0.9420	0.5170
8	0.8880	0.4180
9	0.9420	0.4650
A	0.9600	0.5070
B	0.9490	0.5350
C	0.9580	0.5580
D	0.9310	0.5210
E	0.9350	0.5150
F	0.9140	0.4500
G	0.9580	0.5080
H	0.9470	0.5580
I	0.9150	0.5150
J	0.9570	0.5360
K	0.9390	0.5240
L	0.9380	0.5230
M	0.9380	0.5120
N	0.9520	0.5500
O	0.9350	0.5230
P	0.9280	0.5110
Q	0.8950	0.4610
R	0.9300	0.4700
S	0.9430	0.5270
T	0.8780	0.4520
U	0.9490	0.5350
V	0.9330	0.5010
W	0.9440	0.5330
X	0.9260	0.5300

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Chain	Atom inclusion	Q-score
Y	0.9190	0.5590
Z	0.9610	0.5640
a	0.9390	0.5060
b	0.9180	0.4930
c	0.9370	0.5390
d	0.9390	0.5240
e	0.2880	0.1130