Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 06:44 pm GMT

PDB ID	:	6QDW
EMDB ID	:	EMD-4531
Title	:	Cryo-EM structure of the 50S ribosomal subunit at 2.83 Angstroms with modeled GBC SecM peptide
Authors	:	Schulte, L.; Reitz, J.; Hodirnau, V.V.; Kudlinzki, D.; Mao, J.; Glaubitz, C.; Frangakis, A.; Schwalbe, H.
Deposited on	:	2019-01-03
Resolution	:	2.83 Å(reported)
Based on initial model	:	3JBU

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

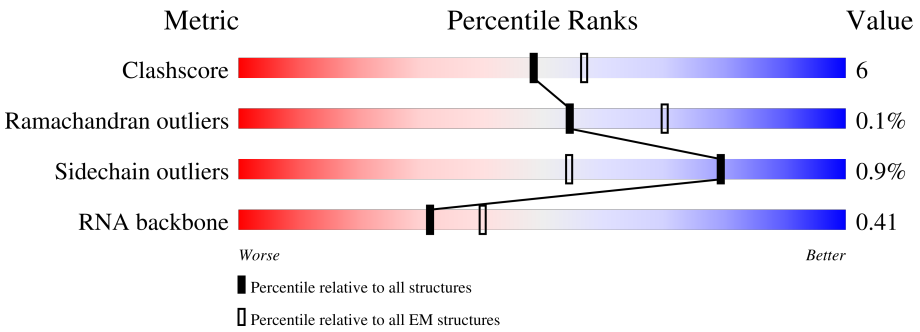
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.83 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	78	92% 6% •
2	1	63	81% 16% •
3	2	59	90% 7% •
4	3	57	84% 12% •
5	4	55	73% 16% • 9%
6	6	46	93% 7%
7	7	65	91% 5% • •

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Mol	Chain	Length	Quality of chain
8	8	38	95% 5%
9	a	120	64% 31%
10	b	2906	67% 29%
11	c	273	99%
12	d	209	99%
13	e	201	99%
14	f	179	96%
15	g	177	99%
16	h	149	26% 74%
17	j	142	100%
18	k	123	98%
19	l	144	99%
20	m	136	99%
21	n	127	94% 6%
22	o	117	99%
23	p	115	98%
24	q	118	99%
25	r	103	96%
26	s	110	98%
27	t	100	92% 7%
28	u	104	98%
29	v	75	48% 44% 8%
30	w	94	99%
31	y	85	86% 13%
32	z	61	36% 7% 57%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	77	625	388	129	106	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	61	495	305	97	92	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	57	439	276	86	75	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	55	434	263	92	78	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	4	50	409	263	75	71	0	0

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	46	377	228	90	57	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	64	504	323	105	74	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	38	302	185	65	48	4	0	0

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	a	118	2528	1126	464	821	117	0	0

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	b	2888	62008	27660	11413	20047	2888	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	271	2082	1288	423	364	7	0	0

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	209	1565	979	288	294	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	f	177	1410	899	249	256	6	0	0

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	g	176	1323	832	243	246	2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	h	39	287	184	51	51	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	j	142	1129	714	212	199	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	k	122	938	587	180	165	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	l	143	1042	648	206	186	2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	m	136	1074	686	205	177	6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	o	116	892	552	178	162	0	0

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	p	113	908	570	177	160	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	r	99	791	500	149	140	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	s	109	845	526	162	154	3	0	0

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	t	93	738	466	139	131	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	u	102	779	492	146	141	0	0

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	v	75	1583	707	270	531	75	0	0

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	w	94	753	479	137	134	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	y	74	559	348	112	98	1	0	0

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	z	26	412	266	74	70	2	26	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-32	MET	-	initiating methionine	UNP P02526
z	-31	GLY	-	expression tag	UNP P02526
z	-30	HIS	-	expression tag	UNP P02526
z	-29	HIS	-	expression tag	UNP P02526
z	-28	HIS	-	expression tag	UNP P02526
z	-27	HIS	-	expression tag	UNP P02526
z	-26	HIS	-	expression tag	UNP P02526
z	-25	HIS	-	expression tag	UNP P02526
z	-24	HIS	-	expression tag	UNP P02526
z	-23	HIS	-	expression tag	UNP P02526
z	-22	HIS	-	expression tag	UNP P02526
z	-21	HIS	-	expression tag	UNP P02526

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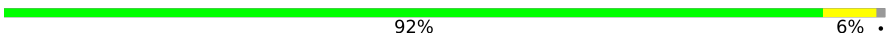
Chain	Residue	Modelled	Actual	Comment	Reference
z	13	PHE	ASN	conflict	UNP P02526
z	15	THR	ILE	conflict	UNP P02526
z	16	PRO	ARG	conflict	UNP P02526
z	18	TRP	-	expression tag	UNP P02526
z	19	ILE	-	expression tag	UNP P02526
z	20	SER	-	expression tag	UNP P02526
z	21	GLN	-	expression tag	UNP P02526
z	22	ALA	-	expression tag	UNP P02526
z	23	GLN	-	expression tag	UNP P02526
z	24	GLY	-	expression tag	UNP P02526
z	25	ILE	-	expression tag	UNP P02526
z	26	ARG	-	expression tag	UNP P02526
z	27	ALA	-	expression tag	UNP P02526
z	28	GLY	-	expression tag	UNP P02526

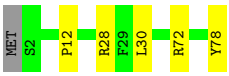
3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L28

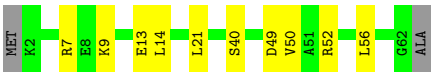
Chain 0:





- Molecule 2: 50S ribosomal protein L29

Chain 1:

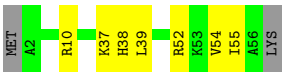


- Molecule 3: 50S ribosomal protein L30

Chain 2:

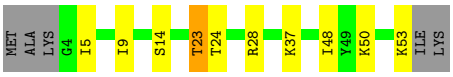
- Molecule 4: 50S ribosomal protein L32

Chain 3:



- Molecule 5: 50S ribosomal protein L33

Chain 4:



- Molecule 6: 50S ribosomal protein L34

Chain 6: 93% 7%

M1 K2 R3 K25 K46

- Molecule 7: 50S ribosomal protein L35

Chain 7: 91% 5%

MET P2 R30 H31 I32 S51 K52 A65

- Molecule 8: 50S ribosomal protein L36

Chain 8: 95% 5%

M1 R4 G38

- Molecule 9: 5S rRNA

Chain a: 64% 31%

U G2 C3 C4 U5 G6 G7 C8 G9 G13 U14 A15 G16 C17 G24 U25 C26 A29 C30 C31 U32 C35 A39 C42 C43 G44 A52 A53 G56 A66 G67 U77 U87 C88 U89 C90 C91 C92 C93 C97 G98 A99 U103 A109 G112

C113 C114 G117 C118 A119 U

- Molecule 10: 23S rRNA

Chain b: 67% 29%

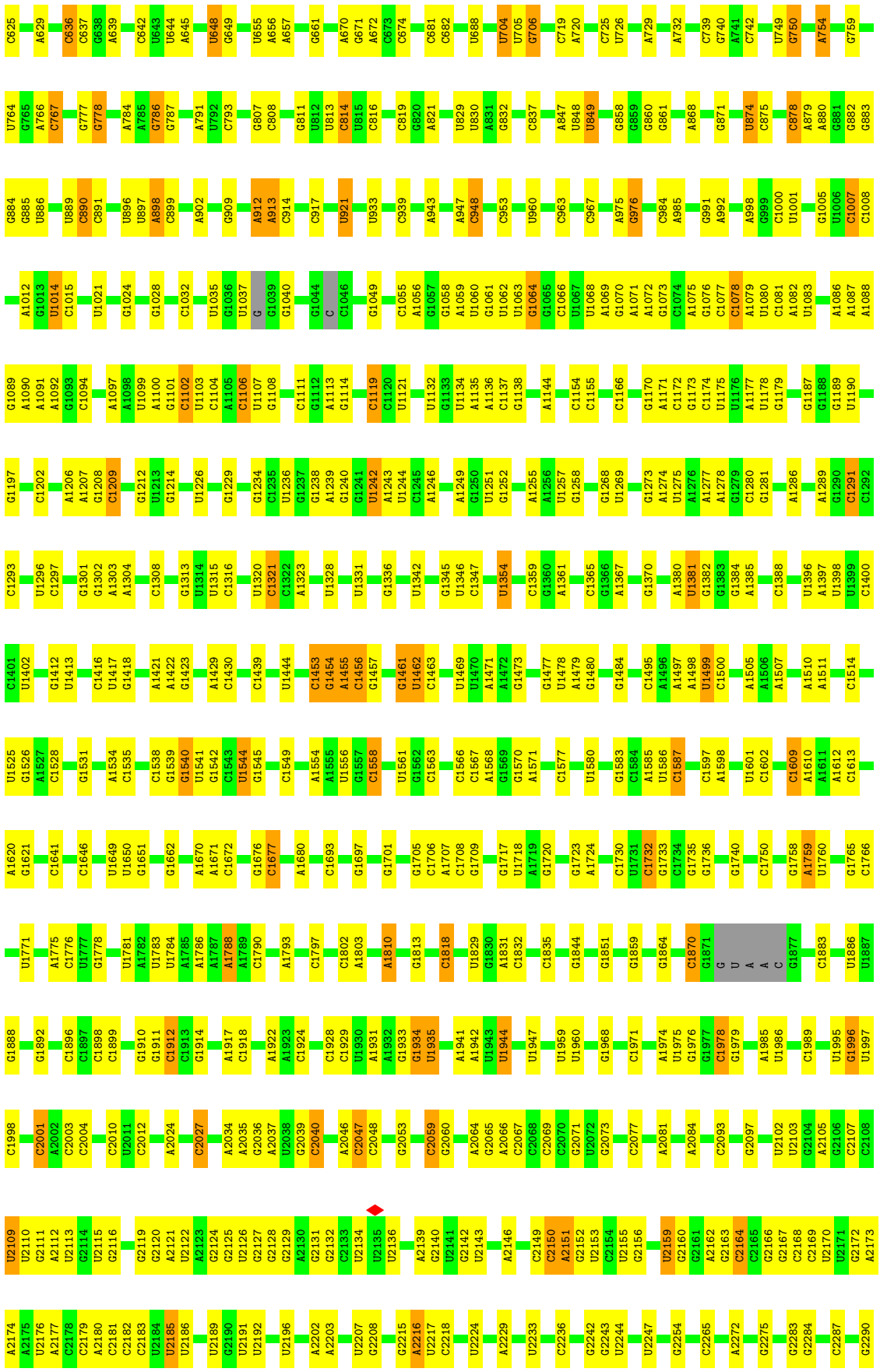
G1 U4 G9 A10 C11 U12 G15 C22 G27 A28 U34 G35 G46 C47 G51 C61 U62 A63 C66 C69 G70 A71 A74 G75 A84 A91 U92 G93 U99 U100 A101 U102 A103 U114 A118 A119 U120 G121 G122 A125 G136

U137 A142 C143 A144 G159 A160 C163 C164 A165 U166 U174 G175 A176 G177 A196 A197 C198 A199 U200 C201 U202 G205 C209 A213 G214 G215 A216 A221 A222 A223 U224 C225 C228 C229 G230 A233 C239 G245 G248 G252 C253 G254 A255 C264

A265 G266 C267 C268 G271 U276 G277 A278 A279 U280 C281 A294 G298 A299 A300 G301 C302 G317 C318 A322 C323 G329 A330 C331 A332 C341 A342 C343 A344 A345 A346 A347 A352 C353 A354 U355 U358 G359 U360 G361 A362 G363 C366 G367 A371 G372 U373

C378 G386 U387 U390 A391 U395 G396 U405 G406 C413 C417 C418 A439 G442 G446 U451 A457 G458 U459 U464 G467 A471 A472 G473 G474 G481 C484 C485 C486 C487 C490 G491 A501 A502 A503 A504 A505 G506 A507 A508 C509 C510

C527 A528 A529 G530 C531 A532 A538 C542 A543 G A G C A A U C U G553 U554 A558 C559 C562 A565 U570 U575 A576 A577 U578 G579 C583 C586 U590 C597 A604 A605 G606 G607 U608 C612 A615 A616 U617 G624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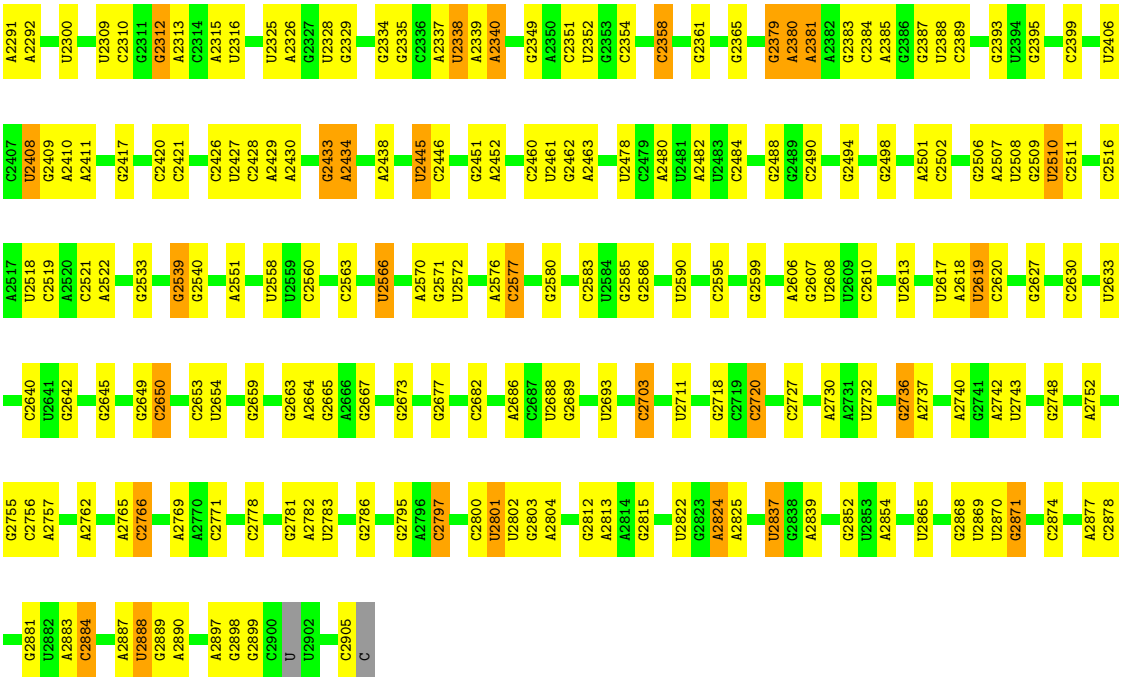
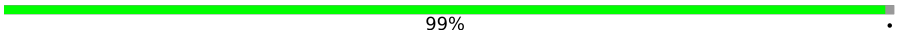
U764 G765 A766 C767 G777 G778 A784 A785 G786 G787 A791 U792 C793 G807 C808 G811 U812 U813 C814 U815 C816 C819 G820 A821 U829 U830 A831 G832 C837 A847 U848 U849 G858 G859 G860 G861 A868 G871 U874 C875 C878 A879 A880 G881 G882 G883
G884 G885 U886 U889 C890 C891 U896 U897 A898 C899 A902 G909 A912 A913 C914 C917 U921 U933 C939 A943 A947 C948 C953 U960 C963 C967 A975 G976 C984 A985 G991 A992 A998 G999 C1000 U1001 G1005 U1006 C1007 C1008
A1012 G1013 U1014 C1015 U1021 G1024 G1028 C1032 U1035 G1036 U1037 G 1039 G1040 G1044 C C1046 G1049 C1055 A1056 G1057 G1058 A1059 U1060 G1061 U1062 U1063 G1064 G1065 C1066 U1067 U1068 A1069 G1070 A1071 A1072 G1073 C1074 A1075 G1076 C1077 C1078 A1079 U1080 C1081 A1082 U1083 A1086 A1087 A1088
G1089 A1090 A1091 A1092 G1093 C1094 A1097 A1098 U1099 A1100 G1101 C1102 U1103 C1104 A1105 C1106 U1107 G1108 C1111 G1112 A1113 G1114 C1119 C1120 U1121 U1132 G1133 U1134 A1135 A1136 C1137 G1138 A1144 C1154 C1155 C1166 G1170 A1171 C1172 G1173 C1174 U1175 U1176 A1177 U1178 G1179 G1187 G1188 G1189 U1190
G1197 C1202 A1206 A1207 G1208 C1209 G1212 U1213 G1214 U1226 G1229 G1234 C1235 U1236 G1237 G1238 A1239 G1240 G1241 U1242 A1243 U1244 C1245 A1246 A1249 G1250 U1251 G1252 A1255 A1256 U1257 G1258 G1268 U1269 G1273 A1274 U1275 A1276 A1277 A1278 G1279 C1280 G1281 A1286 A1289 G1290 C1291 C1292
C1293 U1296 C1297 G1301 G1302 A1303 A1304 C1308 G1313 U1314 U1315 C1316 U1320 C1321 C1322 A1323 U1328 U1331 G1336 U1342 G1345 U1346 C1347 U1354 C1359 G1360 A1361 C1365 G1366 A1367 G1370 A1380 U1381 G1382 G1383 G1384 A1385 C1388 U1396 A1397 U1398 U1399 C1400
C1401 U1402 G1412 U1413 C1416 U1417 G1418 A1421 A1422 G1423 A1429 C1430 C1439 U1444 C1453 G1454 A1455 C1456 G1457 G1461 U1462 C1463 U1469 U1470 A1471 A1472 G1473 G1477 U1478 A1479 G1480 G1484 C1495 A1496 A1497 A1498 U1499 C1500 A1505 A1506 A1507 A1510 A1511 C1514
U1525 G1526 A1527 C1528 G1531 A1534 C1535 C1538 G1539 G1540 U1541 G1542 C1543 U1544 G1545 C1549 A1554 A1555 U1556 G1557 C1558 U1561 G1562 C1563 C1566 C1567 A1568 G1569 G1570 A1571 C1577 U1580 G1583 C1584 A1585 U1586 C1587 C1597 A1598 U1601 C1602 C1609 A1610 A1611 A1612 C1613
A1620 G1621 C1641 C1646 U1649 U1650 G1651 G1662 A1670 A1671 C1672 G1676 C1677 A1680 C1693 G1697 G1701 G1705 C1706 A1707 C1708 G1709 G1717 U1718 A1719 G1720 G1723 A1724 C1730 U1731 C1732 G1733 C1734 G1735 G1736 G1740 C1750 G1758 A1759 U1760 G1765 C1766
U1771 A1775 C1776 U1777 G1778 U1781 A1782 U1783 U1784 A1785 A1786 A1787 A1788 A1789 C1790 A1793 C1797 C1802 A1803 A1810 G1813 C1818 U1829 G1830 A1831 C1832 C1835 G1844 G1851 G1859 G1864 C1870 G1871 G U A A C G1877 C1883 U1886 U1887
G1888 G1892 C1896 C1897 C1898 C1899 G1910 G1911 C1912 C1913 G1914 A1917 C1918 A1922 A1923 C1924 C1928 C1929 U1930 A1931 A1932 G1933 G1934 U1935 A1941 A1942 U1943 U1944 U1947 U1959 U1960 G1968 C1971 A1974 U1975 G1976 G1977 C1978 G1979 A1985 U1986 C1989 U1995 G1996 U1997
C1998 C2001 A2002 C2003 C2004 C2010 U2011 C2012 A2024 C2027 A2034 A2035 G2036 A2037 U2038 G2039 C2040 A2046 C2047 C2048 G2053 C2059 G2060 A2064 G2065 A2066 C2067 C2068 C2069 C2070 G2071 U2072 G2073 C2077 A2081 A2084 C2093 G2097 U2102 U2103 G2104 A2105 G2106 C2107 C2108
U2109 U2110 G2111 A2112 U2113 G2114 U2115 G2116 G2119 G2120 A2121 U2122 A2123 G2124 G2125 U2126 G2127 G2128 G2129 A2130 G2131 G2132 C2133 U2134 U2135 U2136 A2139 G2140 U2141 G2142 U2143 A2146 C2149 C2150 A2151 G2152 U2153 C2154 U2155 G2156 U2159 G2160 G2161 A2162 G2163 C2164 C2165 G2166 G2167 C2168 C2169 U2170 U2171 G2172 A2173
A2174 A2175 U2176 A2177 C2178 C2179 A2180 C2181 C2182 C2183 U2184 U2185 U2186 U2189 G2190 U2191 U2192 U2196 A2202 A2203 U2207 G2208 G2215 A2216 U2217 C2218 U2224 A2229 U2233 C2236 G2242 G2243 U2244 U2247 G2254 C2265 A2272 G2275 G2283 G2284 C2287 G2290



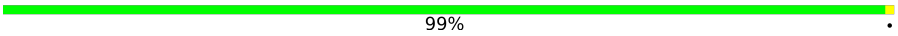
- Molecule 11: 50S ribosomal protein L2

Chain c:



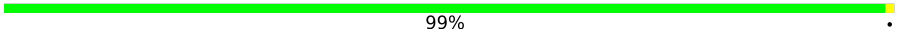
- Molecule 12: 50S ribosomal protein L3

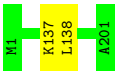
Chain d:



- Molecule 13: 50S ribosomal protein L4

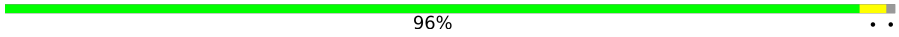
Chain e:

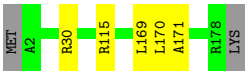




- Molecule 14: 50S ribosomal protein L5

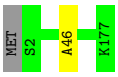
Chain f:





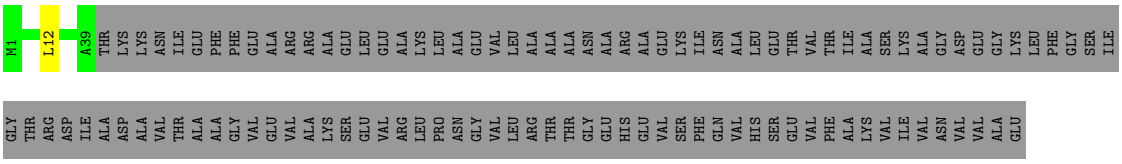
- Molecule 15: 50S ribosomal protein L6

Chain g: 99%



• Molecule 16: 50S ribosomal protein L9

Chain h: 26% 74%



• Molecule 17: 50S ribosomal protein L13

Chain j: 100%

There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L14

Chain k: 98%

• Molecule 19: 50S ribosomal protein L15

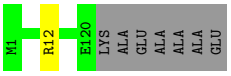
Chain l: 99%

• Molecule 20: 50S ribosomal protein L16

Chain m: 99%

• Molecule 21: 50S ribosomal protein L17

Chain n: 94% 6%



• Molecule 22: 50S ribosomal protein L18

Chain o: 99%

• Molecule 23: 50S ribosomal protein L19

Chain p: 98%

• Molecule 24: 50S ribosomal protein L20

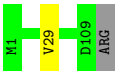
Chain q: 99%

• Molecule 25: 50S ribosomal protein L21

Chain r: 96%

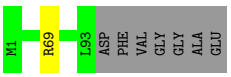
• Molecule 26: 50S ribosomal protein L22

Chain s: 98%



• Molecule 27: 50S ribosomal protein L23

Chain t: 92% 7%

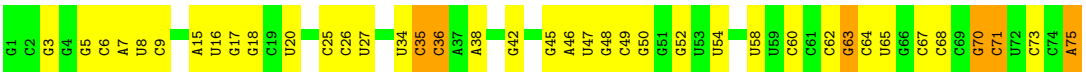


• Molecule 28: 50S ribosomal protein L24

Chain u: 98%

• Molecule 29: glycine-tRNA glyT

Chain v: 48% 44% 8%



- Molecule 30: 50S ribosomal protein L25

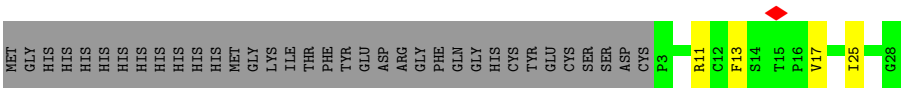
Chain w: 99%

- Molecule 31: 50S ribosomal protein L27

Chain y: 86% 13%

- Molecule 32: Gamma-crystallin B

Chain z: 36% 7% 57%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	0	0.57	0/635	0.58	0/848
2	1	0.45	0/496	0.55	0/660
3	2	0.53	0/443	0.62	0/593
4	3	0.69	0/440	0.62	0/588
5	4	0.47	0/416	0.62	0/554
6	6	0.69	0/380	0.56	0/498
7	7	0.61	0/513	0.57	0/676
8	8	0.67	0/303	0.68	0/397
9	a	1.00	0/2824	1.14	17/4402 (0.4%)
10	b	1.42	1/69444 (0.0%)	1.22	534/108322 (0.5%)
11	c	0.66	0/2121	0.64	0/2852
12	d	0.65	0/1586	0.62	0/2134
13	e	0.60	0/1571	0.65	0/2113
14	f	0.40	0/1434	0.63	0/1926
15	g	0.43	0/1343	0.62	0/1816
16	h	0.44	0/290	0.74	0/392
17	j	0.63	0/1152	0.58	0/1551
18	k	0.62	0/947	0.64	0/1268
19	l	0.61	0/1051	0.65	0/1400
20	m	0.63	0/1093	0.58	0/1460
21	n	0.63	0/973	0.65	0/1301
22	o	0.44	0/902	0.62	0/1209
23	p	0.58	0/920	0.57	0/1231
24	q	0.76	0/960	0.63	0/1278
25	r	0.64	0/803	0.61	0/1070
26	s	0.60	0/852	0.58	0/1142
27	t	0.54	0/744	0.60	0/994
28	u	0.50	0/787	0.65	0/1051
29	v	0.64	0/1764	1.29	17/2744 (0.6%)
30	w	0.51	0/766	0.60	0/1025
31	y	0.63	0/566	0.61	0/750
32	z	0.42	0/426	0.72	0/578
All	All	1.24	1/98945 (0.0%)	1.11	568/148823 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	1	G	OP3-P	-10.17	1.49	1.61

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2027	C	N1-C2-O2	10.25	125.05	118.90
10	b	819	C	C6-N1-C2	-10.20	116.22	120.30
10	b	2888	U	N3-C2-O2	-10.20	115.06	122.20
10	b	1315	U	N1-C2-O2	10.01	129.81	122.80
10	b	2462	G	O4'-C1'-N9	9.90	116.12	108.20
10	b	878	C	N1-C2-O2	9.71	124.73	118.90
10	b	2462	G	N7-C8-N9	9.71	117.95	113.10
10	b	849	U	N3-C2-O2	-9.66	115.44	122.20
10	b	976	G	N7-C8-N9	9.64	117.92	113.10
10	b	1315	U	C2-N1-C1'	9.62	129.24	117.70
10	b	1315	U	N3-C2-O2	-9.56	115.51	122.20
10	b	265	A	O4'-C1'-N9	9.37	115.70	108.20
10	b	2059	C	C6-N1-C2	-9.35	116.56	120.30
10	b	2577	C	N1-C2-O2	9.24	124.44	118.90
10	b	2462	G	C8-N9-C4	-9.23	102.71	106.40
10	b	2577	C	C2-N1-C1'	9.09	128.80	118.80
10	b	2650	C	C6-N1-C2	-8.96	116.71	120.30
10	b	960	U	N1-C2-O2	8.89	129.02	122.80
10	b	2164	C	C5-C6-N1	8.84	125.42	121.00
10	b	1781	U	C5-C6-N1	-8.81	118.30	122.70
29	v	36	C	N1-C2-O2	8.76	124.15	118.90
10	b	1818	C	N1-C2-O2	8.66	124.10	118.90
10	b	2358	C	N1-C2-O2	8.63	124.08	118.90
10	b	849	U	N1-C2-O2	8.57	128.80	122.80
10	b	2164	C	C6-N1-C2	-8.49	116.91	120.30
10	b	2462	G	C5-N7-C8	-8.47	100.06	104.30
10	b	1776	C	C6-N1-C2	-8.41	116.93	120.30
10	b	1514	C	N1-C2-O2	8.34	123.91	118.90
10	b	878	C	C2-N1-C1'	8.31	127.95	118.80
10	b	976	G	C5-N7-C8	-8.31	100.14	104.30
10	b	2159	U	N1-C2-O2	8.29	128.60	122.80
29	v	73	C	N1-C2-O2	8.23	123.84	118.90
10	b	976	G	C8-N9-C4	-8.14	103.14	106.40
10	b	2069	C	C6-N1-C2	-8.11	117.06	120.30
29	v	58	U	N1-C2-O2	8.09	128.46	122.80
10	b	2650	C	C5-C6-N1	8.02	125.01	121.00
10	b	1641	C	N1-C2-O2	8.01	123.70	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	960	U	N3-C2-O2	-7.94	116.64	122.20
10	b	830	U	C2-N1-C1'	7.91	127.19	117.70
10	b	830	U	N3-C2-O2	-7.90	116.67	122.20
10	b	2510	U	N3-C2-O2	-7.89	116.68	122.20
10	b	2358	C	N3-C2-O2	-7.78	116.46	121.90
10	b	1947	U	N3-C2-O2	-7.76	116.77	122.20
10	b	830	U	N1-C2-O2	7.74	128.22	122.80
10	b	2290	G	C4-C5-N7	7.60	113.84	110.80
10	b	201	C	C6-N1-C2	-7.59	117.26	120.30
10	b	2837	U	N1-C2-O2	7.59	128.11	122.80
10	b	2159	U	N3-C2-O2	-7.59	116.89	122.20
10	b	1456	C	N1-C2-O2	7.58	123.45	118.90
10	b	1587	C	N1-C2-O2	7.57	123.44	118.90
10	b	1960	U	N3-C2-O2	-7.54	116.92	122.20
10	b	2837	U	N3-C2-O2	-7.54	116.92	122.20
10	b	2027	C	N3-C2-O2	-7.54	116.62	121.90
10	b	2446	C	C6-N1-C2	-7.53	117.29	120.30
10	b	2379	G	C4-N9-C1'	7.52	136.27	126.50
10	b	2510	U	N1-C2-O2	7.49	128.04	122.80
10	b	1456	C	O4'-C1'-N1	7.48	114.19	108.20
10	b	2254	G	N3-C4-C5	7.47	132.34	128.60
10	b	750	G	O4'-C1'-N9	7.46	114.17	108.20
10	b	976	G	C4-C5-N7	7.46	113.78	110.80
10	b	1456	C	N3-C2-O2	-7.46	116.68	121.90
10	b	390	U	N3-C2-O2	-7.42	117.00	122.20
10	b	2577	C	N3-C2-O2	-7.41	116.71	121.90
10	b	874	U	C5-C6-N1	7.40	126.40	122.70
10	b	912	A	O4'-C1'-N9	7.37	114.10	108.20
10	b	984	C	N3-C2-O2	-7.33	116.77	121.90
10	b	2379	G	N3-C4-C5	-7.33	124.94	128.60
10	b	1008	C	C6-N1-C2	-7.32	117.37	120.30
29	v	36	C	N3-C2-O2	-7.31	116.78	121.90
10	b	1316	C	C6-N1-C2	-7.31	117.38	120.30
10	b	1641	C	N3-C2-O2	-7.31	116.78	121.90
29	v	35	C	N3-C2-O2	-7.31	116.78	121.90
10	b	2837	U	C2-N1-C1'	7.27	126.42	117.70
10	b	2608	U	N3-C2-O2	-7.26	117.11	122.20
10	b	2338	U	C2-N1-C1'	7.26	126.41	117.70
10	b	2254	G	C2-N3-C4	-7.21	108.30	111.90
10	b	47	C	C6-N1-C2	-7.20	117.42	120.30
10	b	625	C	C6-N1-C2	-7.19	117.42	120.30
10	b	1316	C	C5-C6-N1	7.19	124.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1209	C	N1-C2-O2	7.19	123.21	118.90
10	b	346	A	N7-C8-N9	7.19	117.39	113.80
10	b	1106	C	C6-N1-C2	-7.18	117.43	120.30
10	b	268	C	N1-C2-O2	7.13	123.18	118.90
10	b	264	C	N1-C2-O2	7.12	123.17	118.90
10	b	2379	G	N3-C4-N9	7.11	130.27	126.00
29	v	35	C	N1-C2-O2	7.11	123.16	118.90
10	b	1646	C	N1-C2-O2	7.10	123.16	118.90
10	b	481	G	O4'-C1'-N9	7.09	113.88	108.20
10	b	1291	C	N1-C2-O2	7.09	123.16	118.90
10	b	917	C	N1-C2-O2	7.08	123.15	118.90
10	b	1119	C	C6-N1-C2	-7.07	117.47	120.30
10	b	2608	U	N1-C2-O2	7.06	127.74	122.80
10	b	890	C	C6-N1-C2	-7.05	117.48	120.30
9	a	97	C	N3-C2-O2	-7.05	116.97	121.90
10	b	2888	U	N1-C2-O2	7.04	127.72	122.80
10	b	343	C	N1-C2-O2	7.02	123.11	118.90
10	b	1094	C	C5-C6-N1	7.00	124.50	121.00
10	b	1892	G	O4'-C1'-N9	6.97	113.78	108.20
10	b	2871	G	C4-C5-N7	6.97	113.59	110.80
10	b	1461	G	N3-C4-C5	6.96	132.08	128.60
10	b	2040	C	N1-C2-O2	6.95	123.07	118.90
10	b	1202	C	C6-N1-C2	-6.94	117.52	120.30
10	b	878	C	N3-C2-O2	-6.94	117.05	121.90
10	b	1730	C	C5-C6-N1	6.93	124.47	121.00
10	b	1269	U	N3-C2-O2	-6.92	117.36	122.20
10	b	99	U	C2-N1-C1'	6.90	125.98	117.70
10	b	2059	C	C5-C6-N1	6.90	124.45	121.00
10	b	2563	C	N1-C2-O2	6.87	123.03	118.90
10	b	102	U	N1-C2-O2	6.87	127.61	122.80
10	b	1514	C	N3-C2-O2	-6.87	117.09	121.90
10	b	1007	C	N1-C2-O2	6.84	123.00	118.90
29	v	58	U	C2-N1-C1'	6.83	125.90	117.70
10	b	373	U	N3-C2-O2	-6.81	117.43	122.20
10	b	268	C	N3-C2-O2	-6.81	117.13	121.90
10	b	1646	C	N3-C2-O2	-6.78	117.15	121.90
10	b	2583	C	C6-N1-C2	-6.77	117.59	120.30
10	b	417	C	O4'-C1'-N1	6.75	113.60	108.20
10	b	239	C	N1-C2-O2	6.73	122.94	118.90
29	v	58	U	N3-C2-O2	-6.72	117.49	122.20
10	b	559	C	C6-N1-C2	-6.72	117.61	120.30
10	b	2610	C	C6-N1-C2	-6.71	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1315	U	C6-N1-C1'	-6.70	111.83	121.20
10	b	2340	A	C5-N7-C8	-6.67	100.56	103.90
10	b	2871	G	C4-N9-C1'	6.66	135.16	126.50
10	b	1321	C	C6-N1-C2	-6.65	117.64	120.30
10	b	253	C	N1-C2-O2	6.63	122.88	118.90
10	b	767	C	N1-C2-O2	6.61	122.87	118.90
10	b	2640	C	N1-C2-O2	6.61	122.87	118.90
10	b	1316	C	N1-C2-O2	6.61	122.86	118.90
10	b	976	G	C4-N9-C1'	6.59	135.07	126.50
29	v	73	C	C2-N1-C1'	6.59	126.05	118.80
10	b	209	C	C6-N1-C2	-6.58	117.67	120.30
29	v	73	C	N3-C2-O2	-6.56	117.31	121.90
10	b	2325	U	C2-N1-C1'	6.56	125.57	117.70
10	b	2290	G	C5-N7-C8	-6.56	101.02	104.30
10	b	2727	C	C6-N1-C2	-6.55	117.68	120.30
10	b	637	C	C6-N1-C2	-6.55	117.68	120.30
10	b	1316	C	C2-N1-C1'	6.55	126.00	118.80
10	b	2254	G	C4-C5-N7	6.54	113.42	110.80
10	b	562	C	C6-N1-C2	-6.53	117.69	120.30
10	b	1732	C	N1-C2-O2	6.53	122.81	118.90
10	b	264	C	N3-C2-O2	-6.52	117.34	121.90
10	b	2703	C	C6-N1-C2	-6.52	117.69	120.30
10	b	2510	U	C2-N1-C1'	6.51	125.51	117.70
10	b	625	C	C5-C6-N1	6.49	124.25	121.00
10	b	1384	G	O4'-C1'-N9	6.46	113.37	108.20
10	b	1301	G	C2'-C3'-O3'	6.46	124.03	113.70
10	b	2069	C	C5-C6-N1	6.46	124.23	121.00
10	b	2408	U	N1-C2-O2	6.45	127.31	122.80
10	b	1014	U	N3-C4-O4	-6.44	114.89	119.40
10	b	1934	G	P-O3'-C3'	6.44	127.42	119.70
10	b	2610	C	C5-C6-N1	6.43	124.22	121.00
10	b	1456	C	C2-N1-C1'	6.43	125.87	118.80
10	b	2577	C	C6-N1-C1'	-6.42	113.09	120.80
10	b	559	C	C5-C6-N1	6.42	124.21	121.00
10	b	2254	G	C5-N7-C8	-6.41	101.09	104.30
10	b	22	C	C6-N1-C2	-6.39	117.74	120.30
9	a	97	C	C6-N1-C2	-6.39	117.74	120.30
10	b	2507	A	C2-N3-C4	6.39	113.79	110.60
10	b	2743	U	N1-C2-O2	6.38	127.27	122.80
10	b	586	C	C6-N1-C2	-6.37	117.75	120.30
10	b	1106	C	N1-C2-O2	6.37	122.72	118.90
10	b	891	C	N1-C2-O2	6.36	122.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1577	C	N1-C2-O2	6.36	122.72	118.90
10	b	604	A	N7-C8-N9	6.36	116.98	113.80
10	b	2871	G	C6-C5-N7	-6.35	126.59	130.40
10	b	346	A	C8-N9-C4	-6.34	103.26	105.80
10	b	341	C	C6-N1-C2	-6.32	117.77	120.30
10	b	69	C	N1-C2-O2	6.32	122.69	118.90
10	b	706	G	O4'-C1'-N9	6.32	113.25	108.20
10	b	2040	C	N3-C2-O2	-6.32	117.48	121.90
10	b	2801	U	C5-C6-N1	6.31	125.86	122.70
10	b	767	C	N3-C2-O2	-6.31	117.48	121.90
10	b	1365	C	C6-N1-C2	-6.31	117.78	120.30
10	b	1001	U	N3-C2-O2	-6.30	117.79	122.20
10	b	102	U	N3-C2-O2	-6.30	117.79	122.20
10	b	343	C	N3-C2-O2	-6.30	117.49	121.90
10	b	2182	C	C2-N1-C1'	6.30	125.73	118.80
9	a	103	U	N3-C2-O2	-6.29	117.79	122.20
10	b	323	C	C2-N1-C1'	6.29	125.72	118.80
10	b	830	U	C6-N1-C1'	-6.29	112.40	121.20
10	b	198	C	C5-C6-N1	6.28	124.14	121.00
10	b	1935	U	N1-C2-O2	6.27	127.19	122.80
9	a	89	U	C5-C6-N1	6.27	125.83	122.70
10	b	1978	C	N1-C2-O2	6.27	122.66	118.90
10	b	2159	U	C2-N1-C1'	6.25	125.21	117.70
10	b	849	U	C2-N1-C1'	6.25	125.20	117.70
10	b	2379	G	C2-N3-C4	6.25	115.02	111.90
10	b	1609	C	C2-N1-C1'	6.24	125.66	118.80
10	b	1453	C	C2-N1-C1'	6.23	125.65	118.80
10	b	1829	U	N1-C2-O2	6.23	127.16	122.80
10	b	2150	C	C6-N1-C2	-6.22	117.81	120.30
10	b	343	C	C6-N1-C2	-6.22	117.81	120.30
10	b	2047	C	C5-C6-N1	6.22	124.11	121.00
10	b	2358	C	C6-N1-C2	-6.22	117.81	120.30
10	b	2340	A	N7-C8-N9	6.21	116.91	113.80
10	b	2736	G	O4'-C1'-N9	6.21	113.17	108.20
10	b	341	C	C5-C6-N1	6.20	124.10	121.00
10	b	1321	C	N1-C2-O2	6.20	122.62	118.90
10	b	1776	C	C5-C6-N1	6.20	124.10	121.00
10	b	847	A	C8-N9-C4	-6.20	103.32	105.80
10	b	2379	G	C8-N9-C1'	-6.20	118.94	127.00
10	b	1818	C	N3-C2-O2	-6.20	117.56	121.90
10	b	921	U	N1-C2-O2	6.19	127.14	122.80
10	b	2874	C	C6-N1-C2	-6.19	117.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2824	A	OP1-P-O3'	6.19	118.82	105.20
10	b	878	C	C6-N1-C1'	-6.19	113.37	120.80
10	b	2888	U	C2-N1-C1'	6.17	125.11	117.70
10	b	99	U	N3-C2-O2	-6.14	117.90	122.20
9	a	14	U	N3-C2-O2	-6.13	117.91	122.20
10	b	1347	C	C6-N1-C2	-6.11	117.86	120.30
10	b	1094	C	C6-N1-C2	-6.11	117.86	120.30
10	b	390	U	P-O3'-C3'	6.08	127.00	119.70
10	b	542	C	N1-C2-O2	6.08	122.55	118.90
10	b	1321	C	C2-N1-C1'	6.08	125.49	118.80
10	b	976	G	C6-C5-N7	-6.07	126.76	130.40
10	b	1797	C	C6-N1-C2	-6.06	117.88	120.30
10	b	2736	G	C4-C5-N7	6.06	113.22	110.80
10	b	1462	U	N3-C2-O2	-6.06	117.96	122.20
10	b	2640	C	C2-N1-C1'	6.05	125.46	118.80
10	b	2519	C	C6-N1-C2	-6.04	117.88	120.30
29	v	36	C	C2-N1-C1'	6.03	125.44	118.80
10	b	739	C	C6-N1-C2	-6.03	117.89	120.30
10	b	2381	A	O5'-P-OP2	-6.03	100.28	105.70
10	b	159	G	P-O3'-C3'	6.02	126.92	119.70
10	b	742	C	N1-C2-O2	6.02	122.51	118.90
10	b	2577	C	C5-C6-N1	6.00	124.00	121.00
10	b	1365	C	C5-C6-N1	6.00	124.00	121.00
10	b	1701	G	C4-C5-N7	6.00	113.20	110.80
10	b	510	C	N1-C2-O2	6.00	122.50	118.90
10	b	1732	C	C2-N1-C1'	5.98	125.38	118.80
10	b	2048	C	C6-N1-C2	-5.98	117.91	120.30
10	b	1730	C	C6-N1-C2	-5.98	117.91	120.30
9	a	17	C	N1-C2-O2	5.98	122.49	118.90
10	b	984	C	C2-N1-C1'	5.97	125.37	118.80
10	b	1453	C	C4-C5-C6	5.97	120.39	117.40
10	b	2151	A	C2-N3-C4	5.95	113.58	110.60
10	b	1832	C	C6-N1-C2	-5.95	117.92	120.30
10	b	174	U	N3-C2-O2	-5.95	118.04	122.20
10	b	2630	C	C6-N1-C2	-5.94	117.92	120.30
10	b	1870	C	N1-C2-O2	5.94	122.46	118.90
10	b	1960	U	N1-C2-O2	5.93	126.95	122.80
10	b	1898	C	N1-C2-O2	5.93	122.46	118.90
10	b	1296	U	N3-C2-O2	-5.92	118.06	122.20
10	b	1400	C	N1-C2-O2	5.91	122.44	118.90
10	b	917	C	C2-N1-C1'	5.90	125.29	118.80
10	b	705	U	P-O3'-C3'	5.90	126.78	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	66	A	P-O3'-C3'	5.90	126.78	119.70
10	b	1007	C	C6-N1-C2	-5.90	117.94	120.30
10	b	490	C	N1-C2-O2	5.89	122.44	118.90
10	b	1001	U	N1-C2-O2	5.89	126.93	122.80
10	b	948	C	C6-N1-C2	-5.89	117.94	120.30
10	b	917	C	N3-C2-O2	-5.88	117.78	121.90
10	b	1646	C	C6-N1-C2	-5.88	117.95	120.30
10	b	890	C	C5-C6-N1	5.87	123.94	121.00
10	b	2766	C	C6-N1-C2	-5.87	117.95	120.30
10	b	1106	C	C5-C6-N1	5.87	123.94	121.00
10	b	681	C	N1-C2-O2	5.86	122.42	118.90
10	b	681	C	N3-C2-O2	-5.86	117.80	121.90
10	b	1781	U	C4-C5-C6	5.85	123.21	119.70
10	b	1892	G	N7-C8-N9	5.85	116.03	113.10
10	b	2743	U	N3-C2-O2	-5.85	118.10	122.20
9	a	97	C	N1-C2-O2	5.85	122.41	118.90
10	b	1706	C	P-O3'-C3'	5.84	126.71	119.70
10	b	604	A	C5-N7-C8	-5.84	100.98	103.90
10	b	816	C	N1-C2-O2	5.84	122.40	118.90
10	b	2502	C	N1-C2-O2	5.84	122.40	118.90
10	b	967	C	N1-C2-O2	5.83	122.40	118.90
10	b	1912	C	N1-C2-O2	5.83	122.40	118.90
10	b	554	U	N3-C2-O2	-5.83	118.12	122.20
10	b	228	C	P-O3'-C3'	5.83	126.69	119.70
10	b	1384	G	C4-C5-N7	5.83	113.13	110.80
10	b	346	A	C5-N7-C8	-5.81	100.99	103.90
10	b	1008	C	C5-C6-N1	5.81	123.91	121.00
10	b	2408	U	N3-C2-O2	-5.81	118.13	122.20
10	b	2010	C	N3-C2-O2	-5.80	117.84	121.90
10	b	1321	C	N3-C2-O2	-5.80	117.84	121.90
10	b	268	C	C6-N1-C2	-5.79	117.98	120.30
10	b	2516	C	C6-N1-C2	-5.79	117.98	120.30
10	b	1236	U	N1-C2-O2	5.79	126.86	122.80
10	b	1155	C	C6-N1-C2	-5.79	117.98	120.30
10	b	1829	U	N3-C2-O2	-5.78	118.15	122.20
29	v	71	C	N1-C2-O2	5.78	122.37	118.90
10	b	542	C	N3-C2-O2	-5.77	117.86	121.90
10	b	1677	C	N3-C2-O2	-5.77	117.86	121.90
10	b	1014	U	C5-C4-O4	5.76	129.36	125.90
10	b	2004	C	N1-C2-O2	5.76	122.36	118.90
10	b	2736	G	C5-N7-C8	-5.76	101.42	104.30
10	b	960	U	C5-C6-N1	5.75	125.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	837	C	N1-C2-O2	5.75	122.35	118.90
10	b	1236	U	N3-C2-O2	-5.75	118.17	122.20
10	b	1453	C	N3-C2-O2	-5.75	117.88	121.90
10	b	2720	C	N1-C2-O2	5.75	122.35	118.90
10	b	2871	G	N7-C8-N9	5.74	115.97	113.10
10	b	1007	C	N3-C2-O2	-5.74	117.88	121.90
10	b	913	A	N7-C8-N9	5.73	116.67	113.80
10	b	967	C	N3-C2-O2	-5.73	117.89	121.90
10	b	1154	C	C6-N1-C2	-5.73	118.01	120.30
10	b	1883	C	C6-N1-C2	-5.73	118.01	120.30
10	b	413	C	C6-N1-C2	-5.72	118.01	120.30
10	b	1269	U	N1-C2-O2	5.72	126.81	122.80
10	b	209	C	C5-C6-N1	5.72	123.86	121.00
10	b	1646	C	C2-N1-C1'	5.71	125.08	118.80
10	b	786	G	C5-N7-C8	-5.71	101.45	104.30
10	b	1788	A	O4'-C1'-N9	5.71	112.77	108.20
29	v	75	A	OP1-P-OP2	-5.71	111.04	119.60
10	b	917	C	C6-N1-C2	-5.70	118.02	120.30
10	b	2566	U	N3-C2-O2	-5.70	118.21	122.20
9	a	103	U	N1-C2-O2	5.70	126.79	122.80
10	b	1996	G	O4'-C1'-N9	-5.70	103.64	108.20
10	b	2507	A	N1-C2-N3	-5.70	126.45	129.30
9	a	77	U	N3-C2-O2	-5.69	118.22	122.20
10	b	2001	C	N1-C2-O2	5.69	122.31	118.90
29	v	63	G	C4-N9-C1'	5.69	133.89	126.50
10	b	2110	U	P-O3'-C3'	5.68	126.52	119.70
10	b	1461	G	C6-N1-C2	5.68	128.51	125.10
10	b	786	G	C4-C5-N7	5.68	113.07	110.80
10	b	2328	U	OP2-P-O3'	5.67	117.68	105.20
10	b	373	U	O5'-P-OP2	-5.67	100.60	105.70
10	b	69	C	N3-C2-O2	-5.67	117.93	121.90
10	b	1454	G	C4-C5-N7	5.67	113.07	110.80
10	b	1236	U	C2-N1-C1'	5.66	124.49	117.70
10	b	2460	C	N3-C2-O2	-5.66	117.94	121.90
10	b	2619	U	C5-C6-N1	5.66	125.53	122.70
10	b	2563	C	N3-C2-O2	-5.65	117.94	121.90
10	b	99	U	N1-C2-O2	5.65	126.76	122.80
10	b	1892	G	C4-N9-C1'	5.65	133.85	126.50
10	b	2801	U	C2-N1-C1'	5.65	124.48	117.70
10	b	1354	U	N3-C2-O2	-5.65	118.25	122.20
10	b	921	U	N3-C2-O2	-5.63	118.26	122.20
10	b	1978	C	N3-C2-O2	-5.63	117.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2340	A	C4-C5-N7	5.62	113.51	110.70
10	b	2046	A	N1-C6-N6	5.62	121.97	118.60
10	b	953	C	N1-C2-O2	5.62	122.27	118.90
10	b	1119	C	N1-C2-O2	5.62	122.27	118.90
10	b	1514	C	C2-N1-C1'	5.62	124.98	118.80
10	b	413	C	C5-C6-N1	5.61	123.81	121.00
10	b	542	C	C6-N1-C2	-5.60	118.06	120.30
10	b	2338	U	N1-C2-O2	5.59	126.71	122.80
29	v	73	C	C6-N1-C2	-5.59	118.06	120.30
10	b	1587	C	N3-C2-O2	-5.59	117.99	121.90
10	b	1759	A	O4'-C1'-N9	5.58	112.67	108.20
10	b	510	C	N3-C2-O2	-5.58	118.00	121.90
10	b	164	C	N1-C2-O2	5.57	122.24	118.90
10	b	2778	C	C6-N1-C2	-5.57	118.07	120.30
10	b	205	G	O4'-C1'-N9	5.57	112.65	108.20
10	b	984	C	C6-N1-C2	-5.54	118.08	120.30
10	b	2577	C	C6-N1-C2	-5.54	118.08	120.30
10	b	847	A	N7-C8-N9	5.54	116.57	113.80
10	b	1461	G	N3-C4-N9	-5.54	122.68	126.00
10	b	166	U	C5-C6-N1	5.53	125.47	122.70
10	b	1577	C	N3-C2-O2	-5.53	118.03	121.90
10	b	2460	C	N1-C2-O2	5.53	122.22	118.90
10	b	2771	C	N1-C2-O2	5.53	122.22	118.90
10	b	114	U	C2-N1-C1'	5.52	124.33	117.70
10	b	1384	G	C5-N7-C8	-5.52	101.54	104.30
10	b	1587	C	C5-C6-N1	5.52	123.76	121.00
10	b	2109	U	N1-C2-O2	5.52	126.66	122.80
10	b	674	C	C6-N1-C2	-5.51	118.09	120.30
10	b	2420	C	C5-C6-N1	5.51	123.76	121.00
10	b	1293	C	C6-N1-C2	-5.51	118.10	120.30
10	b	1064	G	N3-C4-N9	5.50	129.30	126.00
10	b	1345	G	C4-N9-C1'	5.50	133.65	126.50
10	b	1209	C	N3-C2-O2	-5.50	118.05	121.90
10	b	636	C	C6-N1-C2	-5.50	118.10	120.30
10	b	2642	G	O4'-C1'-N9	5.50	112.60	108.20
10	b	198	C	C6-N1-C2	-5.49	118.10	120.30
10	b	1381	U	N1-C2-O2	5.49	126.64	122.80
10	b	2445	U	N1-C2-O2	5.49	126.64	122.80
10	b	1499	U	N3-C2-O2	-5.48	118.36	122.20
10	b	1102	C	C5-C6-N1	5.47	123.74	121.00
10	b	2884	C	N1-C2-O2	5.47	122.18	118.90
10	b	1455	A	N7-C8-N9	5.47	116.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2185	U	P-O3'-C3'	5.47	126.27	119.70
10	b	682	C	C6-N1-C2	-5.47	118.11	120.30
10	b	253	C	N3-C2-O2	-5.46	118.08	121.90
10	b	1944	U	N3-C2-O2	-5.46	118.38	122.20
10	b	1320	U	C5-C6-N1	5.45	125.42	122.70
29	v	63	G	C8-N9-C1'	-5.45	119.92	127.00
10	b	1771	U	N1-C2-O2	5.45	126.61	122.80
10	b	819	C	C5-C6-N1	5.44	123.72	121.00
10	b	486	C	N1-C2-O2	5.43	122.16	118.90
10	b	612	C	C5-C6-N1	5.43	123.72	121.00
10	b	1701	G	C5-N7-C8	-5.43	101.58	104.30
10	b	1308	C	N1-C2-O2	5.43	122.16	118.90
10	b	1832	C	C5-C6-N1	5.43	123.71	121.00
10	b	1935	U	N3-C2-O2	-5.42	118.41	122.20
10	b	2047	C	C6-N1-C2	-5.42	118.13	120.30
10	b	1587	C	C2-N1-C1'	5.41	124.76	118.80
10	b	2868	G	P-O3'-C3'	5.41	126.19	119.70
10	b	1781	U	C2-N3-C4	-5.41	123.75	127.00
10	b	2338	U	C6-N1-C1'	-5.41	113.62	121.20
10	b	1354	U	N1-C2-O2	5.41	126.59	122.80
10	b	1672	C	N1-C2-O2	5.41	122.14	118.90
10	b	66	C	N1-C2-O2	5.41	122.14	118.90
10	b	847	A	C5-N7-C8	-5.41	101.20	103.90
10	b	1771	U	N3-C2-O2	-5.40	118.42	122.20
10	b	2012	C	C6-N1-C2	-5.40	118.14	120.30
10	b	2399	C	C6-N1-C2	-5.40	118.14	120.30
10	b	2871	G	C8-N9-C1'	-5.40	119.98	127.00
10	b	953	C	N3-C2-O2	-5.39	118.13	121.90
10	b	1000	C	C6-N1-C2	-5.39	118.14	120.30
10	b	2290	G	C6-C5-N7	-5.39	127.17	130.40
10	b	268	C	C2-N1-C1'	5.38	124.71	118.80
10	b	1989	C	N1-C2-O2	5.38	122.13	118.90
10	b	1308	C	N3-C2-O2	-5.38	118.14	121.90
10	b	1912	C	N3-C2-O2	-5.38	118.14	121.90
10	b	1381	U	N3-C2-O2	-5.37	118.44	122.20
10	b	1528	C	C6-N1-C2	-5.37	118.15	120.30
10	b	484	C	C5-C6-N1	5.37	123.68	121.00
10	b	2871	G	C5-N7-C8	-5.37	101.62	104.30
10	b	1007	C	C5-C6-N1	5.36	123.68	121.00
10	b	1566	C	C5-C6-N1	5.36	123.68	121.00
10	b	2328	U	P-O3'-C3'	5.36	126.14	119.70
10	b	814	C	C5-C6-N1	5.36	123.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1064	G	C4-N9-C1'	5.36	133.46	126.50
10	b	2216	A	N7-C8-N9	5.36	116.48	113.80
10	b	2511	C	N1-C2-O2	5.35	122.11	118.90
10	b	2462	G	C4-N9-C1'	5.35	133.46	126.50
10	b	114	U	C5-C6-N1	5.35	125.37	122.70
10	b	1602	C	C6-N1-C2	-5.35	118.16	120.30
10	b	2003	C	C5-C6-N1	5.35	123.67	121.00
10	b	1320	U	N1-C2-O2	5.34	126.54	122.80
10	b	2312	G	C8-N9-C4	-5.33	104.27	106.40
10	b	1609	C	N1-C2-O2	5.33	122.10	118.90
10	b	2077	C	C6-N1-C2	-5.33	118.17	120.30
10	b	2539	G	P-O3'-C3'	5.32	126.09	119.70
10	b	1202	C	C5-C6-N1	5.32	123.66	121.00
10	b	2107	C	C6-N1-C2	-5.32	118.17	120.30
10	b	2358	C	C2-N1-C1'	5.32	124.65	118.80
9	a	117	G	N3-C4-N9	-5.31	122.81	126.00
10	b	27	G	P-O3'-C3'	5.31	126.07	119.70
10	b	1998	C	N1-C2-O2	5.31	122.08	118.90
10	b	2446	C	C5-C6-N1	5.31	123.65	121.00
10	b	2338	U	N3-C2-O2	-5.31	118.49	122.20
10	b	1928	C	C6-N1-C2	-5.30	118.18	120.30
10	b	360	U	N1-C2-O2	5.30	126.51	122.80
9	a	89	U	C6-N1-C2	-5.30	117.82	121.00
10	b	213	A	C8-N9-C4	5.29	107.91	105.80
10	b	2462	G	C4-C5-N7	5.28	112.91	110.80
10	b	510	C	C6-N1-C2	-5.28	118.19	120.30
10	b	1892	G	C6-C5-N7	-5.27	127.24	130.40
10	b	373	U	N1-C2-O2	5.26	126.49	122.80
10	b	2047	C	N1-C2-O2	5.26	122.06	118.90
10	b	590	U	C2-N1-C1'	5.26	124.01	117.70
10	b	2236	C	C6-N1-C2	-5.26	118.20	120.30
10	b	2736	G	C5-C6-N1	5.26	114.13	111.50
10	b	2649	G	N3-C4-C5	5.25	131.22	128.60
10	b	704	U	N1-C2-O2	5.24	126.47	122.80
10	b	1166	C	C6-N1-C2	-5.24	118.20	120.30
10	b	778	G	C6-C5-N7	-5.24	127.26	130.40
10	b	276	U	C5-C6-N1	5.23	125.32	122.70
10	b	2682	C	N1-C2-O2	5.23	122.04	118.90
10	b	1291	C	N3-C2-O2	-5.23	118.24	121.90
10	b	2433	G	OP2-P-O3'	5.23	116.71	105.20
29	v	70	G	C4-N9-C1'	5.23	133.30	126.50
10	b	2244	U	N1-C2-O2	5.23	126.46	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	648	U	C6-N1-C2	-5.23	117.86	121.00
10	b	1119	C	N3-C2-O2	-5.23	118.24	121.90
10	b	174	U	N1-C2-O2	5.22	126.46	122.80
9	a	3	C	C5-C4-N4	-5.22	116.55	120.20
10	b	1892	G	C8-N9-C4	-5.22	104.31	106.40
10	b	2408	U	C2-N1-C1'	5.22	123.96	117.70
10	b	2265	C	N1-C2-O2	5.22	122.03	118.90
10	b	2595	C	C6-N1-C2	-5.22	118.21	120.30
10	b	1597	C	P-O3'-C3'	5.22	125.96	119.70
10	b	1892	G	C5-N7-C8	-5.21	101.69	104.30
10	b	1396	U	C5-C6-N1	5.21	125.31	122.70
10	b	2109	U	N3-C2-O2	-5.21	118.55	122.20
10	b	1119	C	C5-C6-N1	5.21	123.60	121.00
10	b	1308	C	C6-N1-C2	-5.21	118.22	120.30
10	b	1898	C	N3-C2-O2	-5.21	118.25	121.90
10	b	590	U	C5-C6-N1	5.21	125.30	122.70
10	b	967	C	C6-N1-C2	-5.21	118.22	120.30
10	b	1810	A	C5-C6-N6	-5.21	119.54	123.70
10	b	1032	C	C6-N1-C2	-5.20	118.22	120.30
10	b	1453	C	C6-N1-C1'	-5.20	114.56	120.80
10	b	1672	C	N3-C2-O2	-5.20	118.26	121.90
10	b	2797	C	N1-C2-O2	5.19	122.02	118.90
10	b	1297	C	N3-C2-O2	-5.19	118.27	121.90
10	b	1345	G	C8-N9-C1'	-5.19	120.25	127.00
10	b	102	U	C5-C6-N1	5.19	125.30	122.70
10	b	2619	U	C2-N1-C1'	5.19	123.93	117.70
10	b	202	U	N3-C2-O2	-5.19	118.57	122.20
10	b	562	C	C5-C6-N1	5.19	123.59	121.00
10	b	2620	C	C6-N1-C2	-5.19	118.22	120.30
10	b	1540	G	P-O3'-C3'	5.19	125.92	119.70
10	b	2224	U	N3-C2-O2	-5.19	118.57	122.20
10	b	750	G	N1-C6-O6	-5.18	116.79	119.90
10	b	786	G	N7-C8-N9	5.18	115.69	113.10
10	b	1297	C	N1-C2-O2	5.18	122.01	118.90
10	b	1929	C	C6-N1-C2	-5.18	118.23	120.30
10	b	1558	C	N3-C2-O2	-5.18	118.27	121.90
10	b	814	C	C6-N1-C2	-5.18	118.23	120.30
10	b	1280	C	N1-C2-O2	5.17	122.00	118.90
9	a	15	A	O4'-C1'-N9	5.17	112.34	108.20
10	b	754	A	C5-N7-C8	-5.17	101.32	103.90
10	b	1416	C	C5-C6-N1	5.17	123.58	121.00
10	b	2580	G	C4-N9-C1'	5.16	133.21	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2727	C	C5-C6-N1	5.16	123.58	121.00
10	b	9	G	P-O3'-C3'	5.16	125.89	119.70
10	b	459	U	N3-C2-O2	-5.16	118.59	122.20
10	b	645	A	O4'-C1'-N9	5.16	112.33	108.20
10	b	898	A	C4-N9-C1'	5.15	135.58	126.30
9	a	32	U	N1-C2-O2	5.15	126.41	122.80
10	b	583	C	N3-C2-O2	-5.15	118.29	121.90
10	b	1078	C	C6-N1-C2	-5.15	118.24	120.30
10	b	2254	G	N3-C4-N9	-5.15	122.91	126.00
10	b	1671	A	C8-N9-C4	-5.15	103.74	105.80
10	b	1896	C	C5-C6-N1	5.14	123.57	121.00
10	b	2884	C	N3-C2-O2	-5.14	118.30	121.90
10	b	481	G	C4-N9-C1'	-5.14	119.82	126.50
10	b	1587	C	C6-N1-C2	-5.14	118.25	120.30
10	b	69	C	C6-N1-C2	-5.14	118.25	120.30
10	b	2888	U	C5-C4-O4	5.13	128.98	125.90
10	b	597	C	C6-N1-C2	-5.13	118.25	120.30
10	b	2093	C	N3-C2-O2	-5.13	118.31	121.90
10	b	1563	C	C5-C6-N1	5.13	123.56	121.00
10	b	239	C	N3-C2-O2	-5.12	118.32	121.90
10	b	1455	A	C5-N7-C8	-5.12	101.34	103.90
10	b	61	C	N1-C2-O2	5.11	121.97	118.90
10	b	939	C	C6-N1-C2	-5.11	118.26	120.30
10	b	2518	U	C6-N1-C2	-5.10	117.94	121.00
10	b	2801	U	N1-C2-O2	5.10	126.37	122.80
10	b	2878	C	N1-C2-O2	5.10	121.96	118.90
10	b	2428	C	N1-C2-O2	5.10	121.96	118.90
10	b	786	G	C8-N9-C4	-5.10	104.36	106.40
10	b	1672	C	C6-N1-C2	-5.09	118.26	120.30
10	b	2484	C	N3-C2-O2	-5.09	118.33	121.90
10	b	390	U	N1-C2-O2	5.09	126.36	122.80
10	b	2254	G	C6-N1-C2	5.09	128.16	125.10
10	b	391	A	N7-C8-N9	5.09	116.34	113.80
10	b	1106	C	N3-C2-O2	-5.09	118.34	121.90
10	b	1968	G	O4'-C1'-N9	-5.08	104.13	108.20
10	b	2421	C	C6-N1-C2	-5.08	118.27	120.30
10	b	2511	C	N3-C2-O2	-5.08	118.34	121.90
10	b	726	U	C2-N1-C1'	5.08	123.79	117.70
10	b	2518	U	C5-C6-N1	5.07	125.24	122.70
10	b	1718	U	N1-C2-O2	5.07	126.35	122.80
10	b	2610	C	N1-C2-O2	5.07	121.94	118.90
10	b	2182	C	N1-C2-O2	5.06	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1613	C	N1-C2-O2	5.06	121.94	118.90
10	b	1321	C	C5-C6-N1	5.06	123.53	121.00
10	b	2510	U	C6-N1-C2	-5.06	117.97	121.00
10	b	2736	G	N7-C8-N9	5.06	115.63	113.10
9	a	93	C	N1-C2-O2	5.05	121.93	118.90
10	b	1242	U	C2-N1-C1'	5.05	123.76	117.70
10	b	1439	C	N1-C2-O2	5.04	121.92	118.90
10	b	378	C	C6-N1-C2	-5.03	118.29	120.30
10	b	1693	C	C6-N1-C2	-5.03	118.29	120.30
10	b	2420	C	C6-N1-C2	-5.03	118.29	120.30
10	b	225	C	N1-C2-O2	5.02	121.91	118.90
10	b	1790	C	C6-N1-C2	-5.02	118.29	120.30
10	b	2380	A	C2-N3-C4	5.02	113.11	110.60
10	b	705	U	C2'-C3'-O3'	5.02	121.73	113.70
10	b	976	G	O4'-C1'-N9	5.02	112.21	108.20
10	b	2434	A	O4'-C1'-N9	5.01	112.21	108.20
10	b	1280	C	N3-C2-O2	-5.01	118.39	121.90
10	b	1359	C	N1-C2-O2	5.01	121.91	118.90
9	a	117	G	N3-C4-C5	5.01	131.10	128.60
10	b	323	C	C6-N1-C1'	-5.01	114.79	120.80
10	b	1912	C	C6-N1-C2	-5.01	118.30	120.30
10	b	2001	C	N3-C2-O2	-5.01	118.39	121.90
10	b	223	A	O4'-C1'-N9	5.01	112.21	108.20
10	b	2143	U	N1-C2-O2	5.01	126.30	122.80
10	b	1544	U	N1-C2-O2	5.00	126.30	122.80
10	b	2566	U	N1-C2-O2	5.00	126.30	122.80
10	b	604	A	C8-N9-C4	-5.00	103.80	105.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	2	0
2	1	495	0	526	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	439	0	482	2	0
4	3	434	0	445	4	0
5	4	409	0	440	5	0
6	6	377	0	418	3	0
7	7	504	0	572	5	0
8	8	302	0	341	1	0
9	a	2528	0	1283	0	0
10	b	62008	0	31189	0	0
11	c	2082	0	2154	0	0
12	d	1565	0	1616	0	0
13	e	1552	0	1619	0	0
14	f	1410	0	1444	0	0
15	g	1323	0	1371	0	0
16	h	287	0	307	0	0
17	j	1129	0	1162	0	0
18	k	938	0	1012	0	0
19	l	1042	0	1121	0	0
20	m	1074	0	1157	0	0
21	n	960	0	1000	0	0
22	o	892	0	923	0	0
23	p	908	0	956	0	0
24	q	947	0	1019	0	0
25	r	791	0	811	0	0
26	s	845	0	909	0	0
27	t	738	0	807	0	0
28	u	779	0	831	0	0
29	v	1583	0	807	0	0
30	w	753	0	780	0	0
31	y	559	0	575	0	0
32	z	412	0	398	0	0
All	All	90690	0	59127	28	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 (28) 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)
1:0:12:PRO:HB3	1:0:30:LEU:HD23	1.68	0.74
1:0:72:ARG:NH1	1:0:78:TYR:OH	2.33	0.59
2:1:7:ARG:HG3	2:1:56:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:6:LYS:NZ	3:2:37:GLU:OE1	2.37	0.58
3:2:12:SER:HB3	3:2:32:ILE:HD11	1.88	0.56
5:4:5:ILE:O	5:4:28:ARG:NH1	2.41	0.53
2:1:9:LYS:HE3	2:1:13:GLU:HG2	1.91	0.52
2:1:49:ASP:OD1	2:1:52:ARG:NH2	2.44	0.51
6:6:1:MET:SD	6:6:1:MET:N	2.74	0.50
2:1:21:LEU:HB3	2:1:50:VAL:HG12	1.94	0.50
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.92	0.50
5:4:37:LYS:HG2	5:4:48:ILE:HG13	1.93	0.50
5:4:14:SER:OG	5:4:50:LYS:NZ	2.45	0.49
2:1:14:LEU:HD11	2:1:56:LEU:HD23	1.95	0.48
4:3:52:ARG:HH11	4:3:54:VAL:HA	1.80	0.46
7:7:32:ILE:HG22	7:7:32:ILE:O	2.16	0.46
6:6:25:LYS:HB3	6:6:25:LYS:HE3	1.82	0.45
8:8:4:ARG:O	8:8:38:GLY:N	2.49	0.45
4:3:38:HIS:ND1	4:3:39:LEU:O	2.37	0.44
7:7:31:HIS:H	7:7:31:HIS:CD2	2.36	0.44
5:4:23:THR:OG1	5:4:24:THR:N	2.52	0.43
4:3:37:LYS:HB2	4:3:37:LYS:HE3	1.84	0.42
7:7:30:ARG:HD2	7:7:30:ARG:HA	1.75	0.41
7:7:51:SER:OG	7:7:52:LYS:N	2.54	0.41
5:4:9:ILE:HA	5:4:53:LYS:HB2	2.02	0.41
6:6:3:ARG:HA	6:6:3:ARG:HD3	1.85	0.41
7:7:31:HIS:H	7:7:31:HIS:HD2	1.69	0.40
2:1:40:SER:O	2:1:40:SER:OG	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	29	51
14	f	175/179 (98%)	154 (88%)	20 (11%)	1 (1%)	25	46
15	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	25	46
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	14	30
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	48/61 (79%)	38 (79%)	10 (21%)	0	100	100
All	All	3091/3328 (93%)	2867 (93%)	220 (7%)	4 (0%)	54	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	e	138	LEU
14	f	171	ALA
30	w	66	ASP
15	g	46	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	66 (98%)	1 (2%)	65	82
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	47 (100%)	0	100	100
4	3	46/48 (96%)	45 (98%)	1 (2%)	52	75
5	4	45/49 (92%)	44 (98%)	1 (2%)	52	75
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	49 (96%)	2 (4%)	32	58
8	8	34/34 (100%)	34 (100%)	0	100	100
11	c	216/218 (99%)	216 (100%)	0	100	100
12	d	164/164 (100%)	162 (99%)	2 (1%)	71	85
13	e	165/165 (100%)	164 (99%)	1 (1%)	86	93
14	f	148/150 (99%)	144 (97%)	4 (3%)	44	69
15	g	137/138 (99%)	137 (100%)	0	100	100
16	h	30/114 (26%)	29 (97%)	1 (3%)	38	63
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	102 (99%)	1 (1%)	76	88
19	l	102/103 (99%)	102 (100%)	0	100	100
20	m	109/109 (100%)	108 (99%)	1 (1%)	78	89
21	n	100/103 (97%)	99 (99%)	1 (1%)	76	88
22	o	86/87 (99%)	86 (100%)	0	100	100
23	p	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	82/84 (98%)	82 (100%)	0	100	100
26	s	92/93 (99%)	91 (99%)	1 (1%)	73	86
27	t	80/84 (95%)	79 (99%)	1 (1%)	69	84
28	u	83/85 (98%)	83 (100%)	0	100	100
30	w	78/78 (100%)	78 (100%)	0	100	100
31	y	55/63 (87%)	54 (98%)	1 (2%)	59	78
32	z	44/53 (83%)	36 (82%)	8 (18%)	1	2
All	All	2559/2694 (95%)	2532 (99%)	27 (1%)	79	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
4	3	10	ARG
5	4	23	THR
7	7	30	ARG
7	7	31	HIS
12	d	121	THR
12	d	184	ARG
13	e	137	LYS
14	f	30	ARG
14	f	115	ARG
14	f	169	LEU
14	f	170	LEU
16	h	12	LEU
18	k	49	ARG
20	m	75	GLU
21	n	12	ARG
26	s	29	VAL
27	t	69	ARG
31	y	51	VAL
32	z	11[A]	ARG
32	z	11[B]	ARG
32	z	13[A]	PHE
32	z	13[B]	PHE
32	z	17[A]	VAL
32	z	17[B]	VAL
32	z	25[A]	ILE

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Mol	Chain	Res	Type
32	z	25[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	6	GLN
1	0	16	ASN
1	0	17	ASN
2	1	36	GLN
4	3	6	ASN
11	c	142	HIS
11	c	260	ASN
12	d	32	ASN
12	d	150	GLN
14	f	5	HIS
14	f	27	GLN
14	f	127	ASN
14	f	135	GLN
15	g	20	ASN
15	g	73	ASN
16	h	28	ASN
18	k	90	ASN
19	l	99	ASN
19	l	104	GLN
24	q	52	GLN
24	q	81	ASN
26	s	15	GLN
26	s	40	ASN
28	u	66	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2880/2906 (99%)	764 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3070/3101 (99%)	834 (27%)	0

All (834) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G
9	a	24	G
9	a	25	U
9	a	26	C
9	a	29	A
9	a	30	C
9	a	35	C
9	a	39	A
9	a	42	C
9	a	43	C
9	a	44	G
9	a	52	A
9	a	53	A
9	a	56	G
9	a	66	A
9	a	67	G
9	a	87	U
9	a	88	C
9	a	89	U
9	a	90	C
9	a	91	C
9	a	93	C
9	a	99	A
9	a	109	A
9	a	112	G
9	a	113	C
9	a	114	C
9	a	117	G
9	a	118	C
10	b	4	U
10	b	10	A
10	b	12	U
10	b	15	G
10	b	28	A
10	b	34	U
10	b	35	G
10	b	46	G
10	b	51	G
10	b	62	U

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Mol	Chain	Res	Type
10	b	63	A
10	b	71	A
10	b	74	A
10	b	75	G
10	b	84	A
10	b	91	A
10	b	92	U
10	b	93	G
10	b	100	U
10	b	101	A
10	b	102	U
10	b	103	A
10	b	118	A
10	b	119	A
10	b	120	U
10	b	121	G
10	b	122	G
10	b	125	A
10	b	136	G
10	b	137	U
10	b	142	A
10	b	144	A
10	b	159	G
10	b	160	A
10	b	163	C
10	b	174	U
10	b	175	G
10	b	177	G
10	b	196	A
10	b	199	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A
10	b	223	A
10	b	224	U
10	b	229	C
10	b	230	G
10	b	233	A
10	b	245	G
10	b	248	G
10	b	252	G

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Mol	Chain	Res	Type
10	b	255	A
10	b	264	C
10	b	265	A
10	b	266	G
10	b	271	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	294	A
10	b	298	G
10	b	300	A
10	b	302	C
10	b	317	G
10	b	318	C
10	b	322	A
10	b	329	G
10	b	330	A
10	b	331	C
10	b	332	A
10	b	343	C
10	b	345	A
10	b	346	A
10	b	347	A
10	b	352	A
10	b	353	C
10	b	355	U
10	b	358	U
10	b	359	G
10	b	362	A
10	b	363	G
10	b	366	C
10	b	367	G
10	b	371	A
10	b	372	G
10	b	373	U
10	b	386	G
10	b	387	U
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G

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Mol	Chain	Res	Type
10	b	405	U
10	b	406	G
10	b	417	C
10	b	418	C
10	b	439	A
10	b	442	G
10	b	446	G
10	b	451	U
10	b	457	A
10	b	464	U
10	b	467	G
10	b	471	A
10	b	472	A
10	b	474	G
10	b	481	G
10	b	487	C
10	b	491	G
10	b	501	A
10	b	503	A
10	b	505	A
10	b	507	A
10	b	508	A
10	b	509	C
10	b	510	C
10	b	527	C
10	b	529	A
10	b	531	C
10	b	532	A
10	b	538	A
10	b	558	A
10	b	559	C
10	b	565	A
10	b	570	U
10	b	575	U
10	b	577	A
10	b	579	G
10	b	590	U
10	b	604	A
10	b	605	A
10	b	606	G
10	b	608	U
10	b	615	A

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Mol	Chain	Res	Type
10	b	616	A
10	b	617	U
10	b	624	G
10	b	629	A
10	b	636	C
10	b	639	A
10	b	642	C
10	b	644	U
10	b	648	U
10	b	649	G
10	b	655	U
10	b	656	A
10	b	657	A
10	b	661	G
10	b	670	A
10	b	671	G
10	b	672	A
10	b	688	U
10	b	704	U
10	b	706	G
10	b	719	C
10	b	720	A
10	b	725	C
10	b	729	A
10	b	732	A
10	b	740	G
10	b	749	U
10	b	750	G
10	b	754	A
10	b	759	G
10	b	764	U
10	b	766	A
10	b	767	C
10	b	777	G
10	b	778	G
10	b	784	A
10	b	786	G
10	b	787	G
10	b	791	A
10	b	793	C
10	b	807	G
10	b	808	C

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Mol	Chain	Res	Type
10	b	811	G
10	b	813	U
10	b	814	C
10	b	821	A
10	b	829	U
10	b	832	G
10	b	848	U
10	b	849	U
10	b	858	G
10	b	860	G
10	b	861	G
10	b	868	A
10	b	871	G
10	b	874	U
10	b	875	C
10	b	878	C
10	b	879	A
10	b	880	A
10	b	882	G
10	b	883	G
10	b	884	G
10	b	885	G
10	b	886	U
10	b	889	U
10	b	890	C
10	b	896	U
10	b	897	U
10	b	898	A
10	b	899	C
10	b	902	A
10	b	909	G
10	b	912	A
10	b	913	A
10	b	914	C
10	b	921	U
10	b	933	U
10	b	943	A
10	b	947	A
10	b	948	C
10	b	963	C
10	b	975	A
10	b	976	G

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Mol	Chain	Res	Type
10	b	985	A
10	b	991	G
10	b	992	A
10	b	998	A
10	b	1005	G
10	b	1007	C
10	b	1012	A
10	b	1014	U
10	b	1015	C
10	b	1021	U
10	b	1024	G
10	b	1028	G
10	b	1035	U
10	b	1037	U
10	b	1040	G
10	b	1049	G
10	b	1055	C
10	b	1056	A
10	b	1058	G
10	b	1059	A
10	b	1060	U
10	b	1061	G
10	b	1062	U
10	b	1063	U
10	b	1064	G
10	b	1066	C
10	b	1068	U
10	b	1069	A
10	b	1070	G
10	b	1071	A
10	b	1072	A
10	b	1073	G
10	b	1075	A
10	b	1076	G
10	b	1077	C
10	b	1078	C
10	b	1079	A
10	b	1080	U
10	b	1081	C
10	b	1082	A
10	b	1083	U
10	b	1086	A

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Mol	Chain	Res	Type
10	b	1087	A
10	b	1088	A
10	b	1089	G
10	b	1090	A
10	b	1091	A
10	b	1092	A
10	b	1097	A
10	b	1099	U
10	b	1100	A
10	b	1101	G
10	b	1102	C
10	b	1103	U
10	b	1104	C
10	b	1106	C
10	b	1107	U
10	b	1108	G
10	b	1111	C
10	b	1113	A
10	b	1114	G
10	b	1119	C
10	b	1121	U
10	b	1132	U
10	b	1134	U
10	b	1135	A
10	b	1136	A
10	b	1137	C
10	b	1138	G
10	b	1144	A
10	b	1170	G
10	b	1171	A
10	b	1172	C
10	b	1173	G
10	b	1174	C
10	b	1175	U
10	b	1177	A
10	b	1178	U
10	b	1179	G
10	b	1187	G
10	b	1189	G
10	b	1190	U
10	b	1197	G
10	b	1206	A

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Mol	Chain	Res	Type
10	b	1207	A
10	b	1208	G
10	b	1209	C
10	b	1212	G
10	b	1214	G
10	b	1226	U
10	b	1229	G
10	b	1234	G
10	b	1238	G
10	b	1239	A
10	b	1240	G
10	b	1242	U
10	b	1243	A
10	b	1244	U
10	b	1246	A
10	b	1249	A
10	b	1251	U
10	b	1252	G
10	b	1255	A
10	b	1257	U
10	b	1258	G
10	b	1268	G
10	b	1273	G
10	b	1274	A
10	b	1275	U
10	b	1277	A
10	b	1278	A
10	b	1281	G
10	b	1286	A
10	b	1289	A
10	b	1291	C
10	b	1302	G
10	b	1303	A
10	b	1304	A
10	b	1313	G
10	b	1321	C
10	b	1323	A
10	b	1328	U
10	b	1331	U
10	b	1336	G
10	b	1342	U
10	b	1346	U

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Mol	Chain	Res	Type
10	b	1354	U
10	b	1361	A
10	b	1367	A
10	b	1370	G
10	b	1380	A
10	b	1381	U
10	b	1382	G
10	b	1385	A
10	b	1388	C
10	b	1397	A
10	b	1398	U
10	b	1402	U
10	b	1412	G
10	b	1413	U
10	b	1417	U
10	b	1418	G
10	b	1421	A
10	b	1422	A
10	b	1423	G
10	b	1429	A
10	b	1430	C
10	b	1444	U
10	b	1453	C
10	b	1454	G
10	b	1455	A
10	b	1456	C
10	b	1457	G
10	b	1461	G
10	b	1462	U
10	b	1463	C
10	b	1469	U
10	b	1471	A
10	b	1473	G
10	b	1477	G
10	b	1478	U
10	b	1479	A
10	b	1480	G
10	b	1484	G
10	b	1495	C
10	b	1497	A
10	b	1498	A
10	b	1499	U

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Mol	Chain	Res	Type
10	b	1500	C
10	b	1505	A
10	b	1507	A
10	b	1510	A
10	b	1511	A
10	b	1525	U
10	b	1526	G
10	b	1531	G
10	b	1534	A
10	b	1535	C
10	b	1538	C
10	b	1539	G
10	b	1540	G
10	b	1541	U
10	b	1542	G
10	b	1544	U
10	b	1545	G
10	b	1549	C
10	b	1554	A
10	b	1556	U
10	b	1558	C
10	b	1561	U
10	b	1567	C
10	b	1568	A
10	b	1570	G
10	b	1571	A
10	b	1580	U
10	b	1583	G
10	b	1585	A
10	b	1586	U
10	b	1587	C
10	b	1598	A
10	b	1601	U
10	b	1609	C
10	b	1610	A
10	b	1612	A
10	b	1620	A
10	b	1621	G
10	b	1649	U
10	b	1650	U
10	b	1651	G
10	b	1662	G

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Mol	Chain	Res	Type
10	b	1670	A
10	b	1676	G
10	b	1677	C
10	b	1680	A
10	b	1697	G
10	b	1705	G
10	b	1707	A
10	b	1708	C
10	b	1709	G
10	b	1717	G
10	b	1720	G
10	b	1723	G
10	b	1724	A
10	b	1732	C
10	b	1733	G
10	b	1735	G
10	b	1736	G
10	b	1740	G
10	b	1750	C
10	b	1758	G
10	b	1759	A
10	b	1760	U
10	b	1765	G
10	b	1766	C
10	b	1775	A
10	b	1778	G
10	b	1783	U
10	b	1784	U
10	b	1786	A
10	b	1788	A
10	b	1793	A
10	b	1802	C
10	b	1803	A
10	b	1810	A
10	b	1813	G
10	b	1818	C
10	b	1831	A
10	b	1835	C
10	b	1844	G
10	b	1851	G
10	b	1859	G
10	b	1864	G

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Mol	Chain	Res	Type
10	b	1870	C
10	b	1886	U
10	b	1888	G
10	b	1899	C
10	b	1910	G
10	b	1911	G
10	b	1912	C
10	b	1914	G
10	b	1917	A
10	b	1918	C
10	b	1922	A
10	b	1924	C
10	b	1931	A
10	b	1933	G
10	b	1934	G
10	b	1935	U
10	b	1941	A
10	b	1942	A
10	b	1944	U
10	b	1959	U
10	b	1971	C
10	b	1974	A
10	b	1975	U
10	b	1976	G
10	b	1978	C
10	b	1979	G
10	b	1985	A
10	b	1986	U
10	b	1995	U
10	b	1996	G
10	b	1997	U
10	b	2001	C
10	b	2024	A
10	b	2027	C
10	b	2034	A
10	b	2035	A
10	b	2036	G
10	b	2037	A
10	b	2039	G
10	b	2040	C
10	b	2047	C
10	b	2053	G

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Mol	Chain	Res	Type
10	b	2059	C
10	b	2060	G
10	b	2064	A
10	b	2065	G
10	b	2066	A
10	b	2067	C
10	b	2071	G
10	b	2073	G
10	b	2081	A
10	b	2084	A
10	b	2097	G
10	b	2102	U
10	b	2103	U
10	b	2105	A
10	b	2109	U
10	b	2111	G
10	b	2112	A
10	b	2113	U
10	b	2115	U
10	b	2116	G
10	b	2119	G
10	b	2120	G
10	b	2121	A
10	b	2122	U
10	b	2124	G
10	b	2125	G
10	b	2126	U
10	b	2127	G
10	b	2128	G
10	b	2129	G
10	b	2131	G
10	b	2132	G
10	b	2134	U
10	b	2136	U
10	b	2139	A
10	b	2140	G
10	b	2142	G
10	b	2146	A
10	b	2149	C
10	b	2150	C
10	b	2151	A
10	b	2152	G

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Mol	Chain	Res	Type
10	b	2153	U
10	b	2155	U
10	b	2156	G
10	b	2159	U
10	b	2160	G
10	b	2162	A
10	b	2163	G
10	b	2164	C
10	b	2166	G
10	b	2167	G
10	b	2168	C
10	b	2169	C
10	b	2170	U
10	b	2172	G
10	b	2173	A
10	b	2174	A
10	b	2176	U
10	b	2177	A
10	b	2179	C
10	b	2180	A
10	b	2181	C
10	b	2183	C
10	b	2185	U
10	b	2186	U
10	b	2189	U
10	b	2191	U
10	b	2192	U
10	b	2196	U
10	b	2202	A
10	b	2203	A
10	b	2207	U
10	b	2208	G
10	b	2215	G
10	b	2216	A
10	b	2217	U
10	b	2218	C
10	b	2229	A
10	b	2233	U
10	b	2242	G
10	b	2243	G
10	b	2247	U
10	b	2272	A

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Mol	Chain	Res	Type
10	b	2275	G
10	b	2283	G
10	b	2284	G
10	b	2287	C
10	b	2291	A
10	b	2292	A
10	b	2300	U
10	b	2309	U
10	b	2310	C
10	b	2312	G
10	b	2313	A
10	b	2315	A
10	b	2316	U
10	b	2326	A
10	b	2329	G
10	b	2334	G
10	b	2335	G
10	b	2337	A
10	b	2338	U
10	b	2339	A
10	b	2340	A
10	b	2349	G
10	b	2351	C
10	b	2352	U
10	b	2354	C
10	b	2358	C
10	b	2361	G
10	b	2365	G
10	b	2379	G
10	b	2380	A
10	b	2381	A
10	b	2383	G
10	b	2384	C
10	b	2385	A
10	b	2387	G
10	b	2388	U
10	b	2389	C
10	b	2393	G
10	b	2395	G
10	b	2406	U
10	b	2408	U
10	b	2409	G

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Mol	Chain	Res	Type
10	b	2410	A
10	b	2411	A
10	b	2417	G
10	b	2426	C
10	b	2427	U
10	b	2429	A
10	b	2430	A
10	b	2433	G
10	b	2434	A
10	b	2438	A
10	b	2445	U
10	b	2451	G
10	b	2452	A
10	b	2461	U
10	b	2463	A
10	b	2478	U
10	b	2480	A
10	b	2482	A
10	b	2488	G
10	b	2490	C
10	b	2494	G
10	b	2498	G
10	b	2501	A
10	b	2506	G
10	b	2508	U
10	b	2509	G
10	b	2510	U
10	b	2521	C
10	b	2522	A
10	b	2533	G
10	b	2539	G
10	b	2540	G
10	b	2551	A
10	b	2558	U
10	b	2560	C
10	b	2566	U
10	b	2570	A
10	b	2571	G
10	b	2572	U
10	b	2576	A
10	b	2577	C
10	b	2585	G

Continued on next page...

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Mol	Chain	Res	Type
10	b	2586	G
10	b	2590	U
10	b	2599	G
10	b	2606	A
10	b	2607	G
10	b	2613	U
10	b	2617	U
10	b	2618	A
10	b	2619	U
10	b	2627	G
10	b	2633	U
10	b	2645	G
10	b	2650	C
10	b	2653	C
10	b	2654	U
10	b	2659	G
10	b	2663	G
10	b	2664	A
10	b	2665	G
10	b	2667	G
10	b	2673	G
10	b	2677	G
10	b	2686	A
10	b	2688	U
10	b	2689	G
10	b	2693	U
10	b	2703	C
10	b	2711	U
10	b	2718	G
10	b	2720	C
10	b	2730	A
10	b	2732	U
10	b	2736	G
10	b	2737	A
10	b	2740	A
10	b	2742	A
10	b	2748	G
10	b	2752	A
10	b	2755	G
10	b	2756	C
10	b	2757	A
10	b	2762	A

Continued on next page...

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Mol	Chain	Res	Type
10	b	2765	A
10	b	2766	C
10	b	2769	A
10	b	2781	G
10	b	2782	A
10	b	2783	U
10	b	2786	G
10	b	2795	G
10	b	2797	C
10	b	2800	C
10	b	2801	U
10	b	2802	U
10	b	2803	G
10	b	2804	A
10	b	2812	G
10	b	2813	A
10	b	2815	G
10	b	2822	U
10	b	2824	A
10	b	2825	A
10	b	2837	U
10	b	2839	A
10	b	2852	G
10	b	2854	A
10	b	2865	U
10	b	2869	U
10	b	2870	U
10	b	2871	G
10	b	2877	A
10	b	2881	G
10	b	2883	A
10	b	2884	C
10	b	2887	A
10	b	2888	U
10	b	2889	G
10	b	2890	A
10	b	2897	A
10	b	2898	G
10	b	2899	G
10	b	2905	C
29	v	3	G
29	v	5	G

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Mol	Chain	Res	Type
29	v	6	C
29	v	7	A
29	v	8	U
29	v	9	C
29	v	15	A
29	v	16	U
29	v	17	G
29	v	18	G
29	v	20	U
29	v	25	C
29	v	26	C
29	v	27	U
29	v	34	U
29	v	35	C
29	v	36	C
29	v	38	A
29	v	42	G
29	v	45	G
29	v	46	A
29	v	47	U
29	v	48	G
29	v	49	C
29	v	50	G
29	v	52	G
29	v	54	U
29	v	60	C
29	v	62	C
29	v	63	G
29	v	64	C
29	v	65	U
29	v	67	C
29	v	68	C
29	v	70	G
29	v	71	C
29	v	75	A

There are no RNA pucker outliers to report.

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)

There are no ligands in this entry.

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
10	b	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	511:U	O3'	512:G	P	2.42
1	b	512:G	O3'	513:A	P	2.26

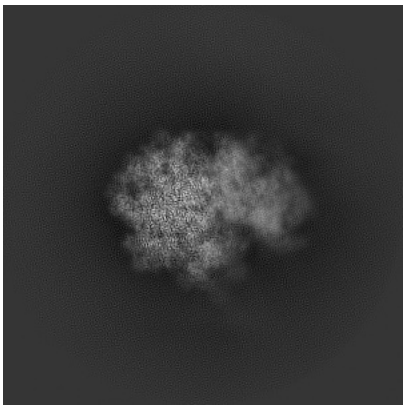
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4531. These allow visual inspection of the internal detail of the map and identification of artifacts.

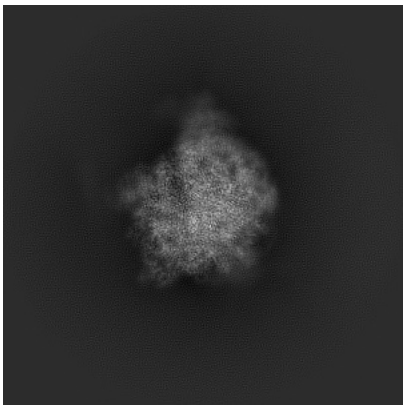
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

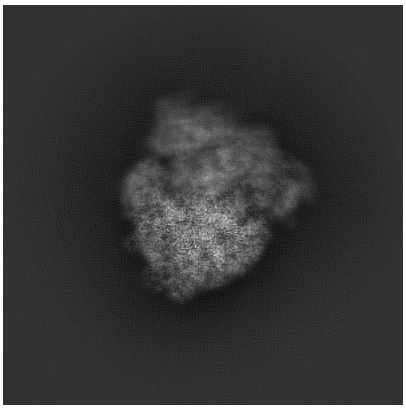
6.1.1 Primary map



X

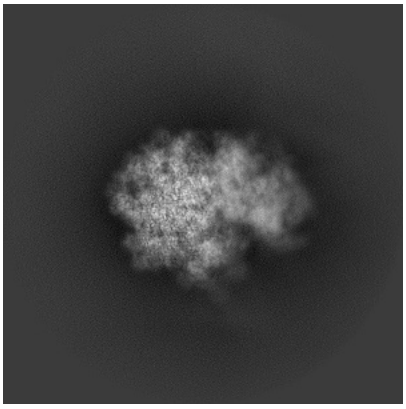


Y

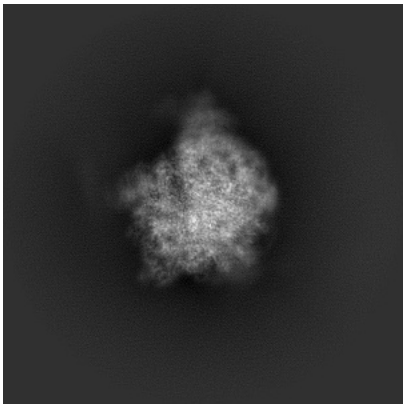


Z

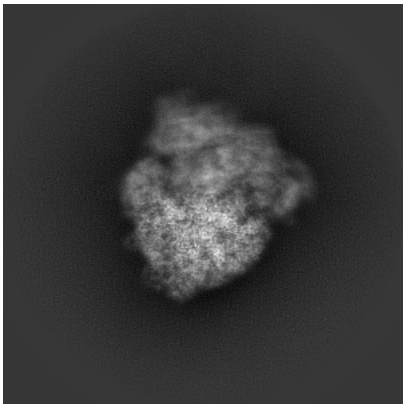
6.1.2 Raw map



X



Y

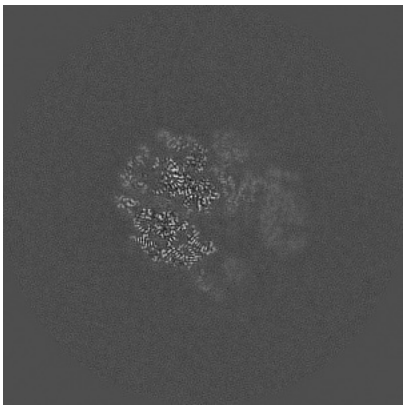


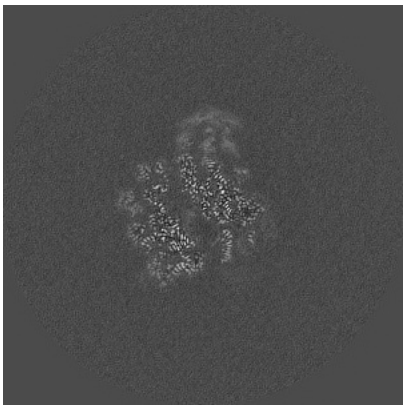
Z

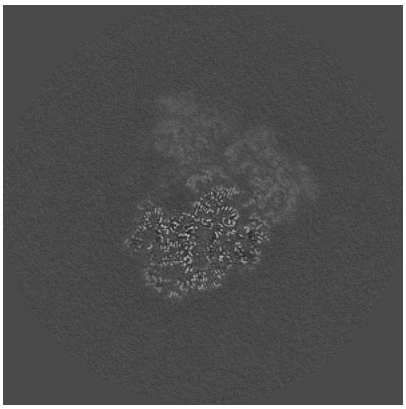
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

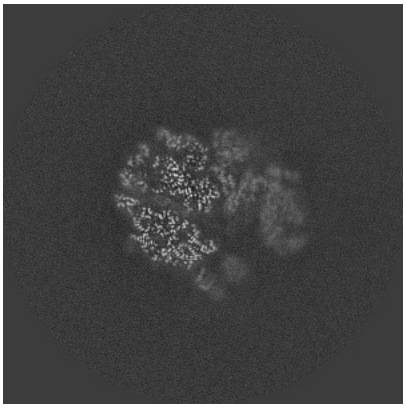
6.2.1 Primary map

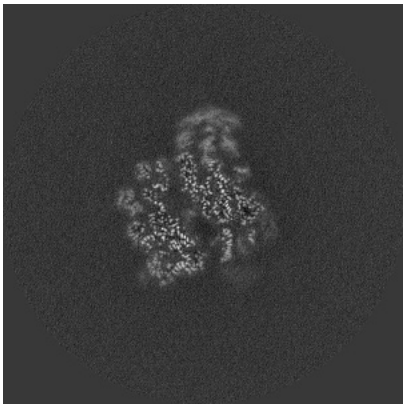

X Index: 240

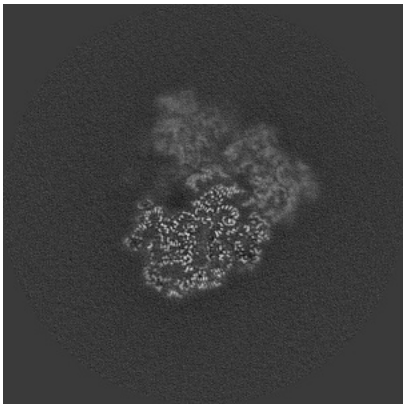

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

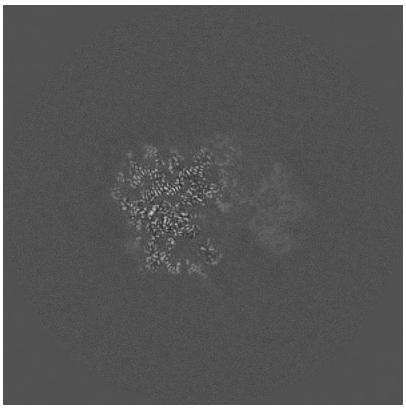

Y Index: 240

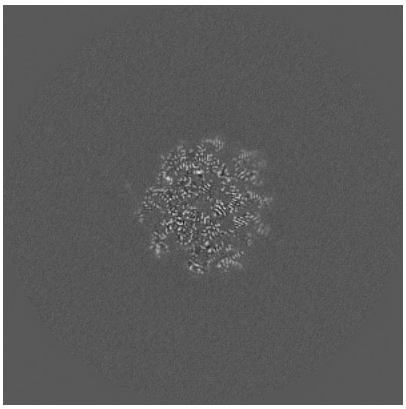

Z Index: 240

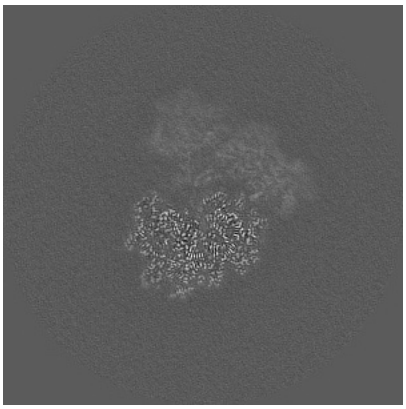
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

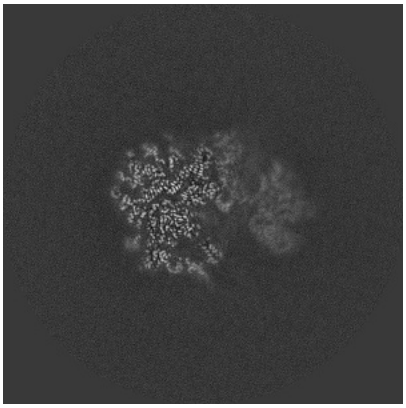
6.3.1 Primary map

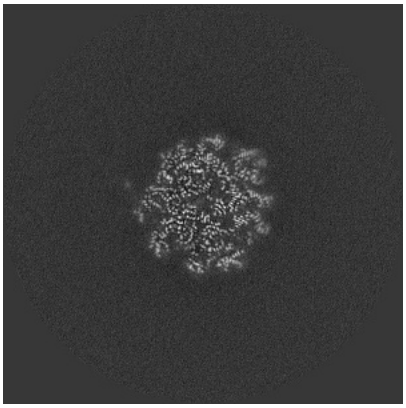

X Index: 229

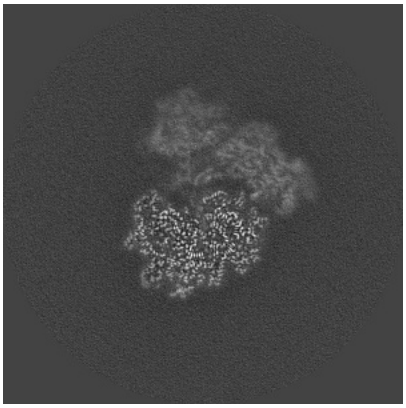

Y Index: 207


Z Index: 231

6.3.2 Raw map


X Index: 230

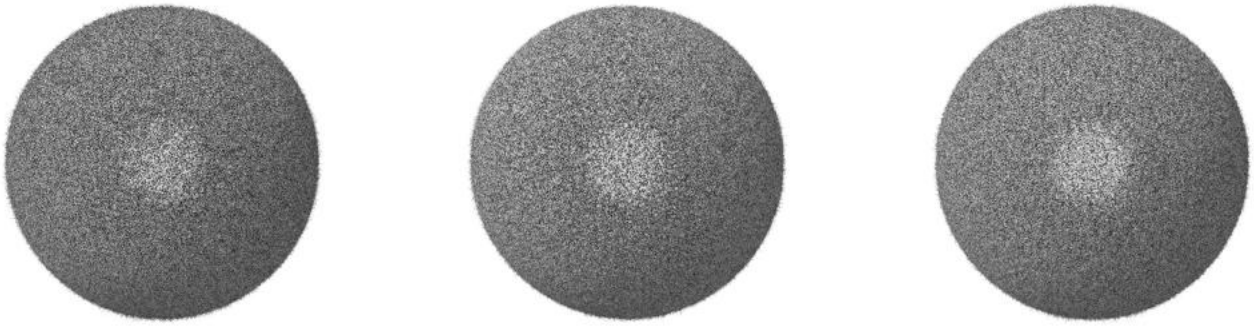

Y Index: 207


Z Index: 231

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

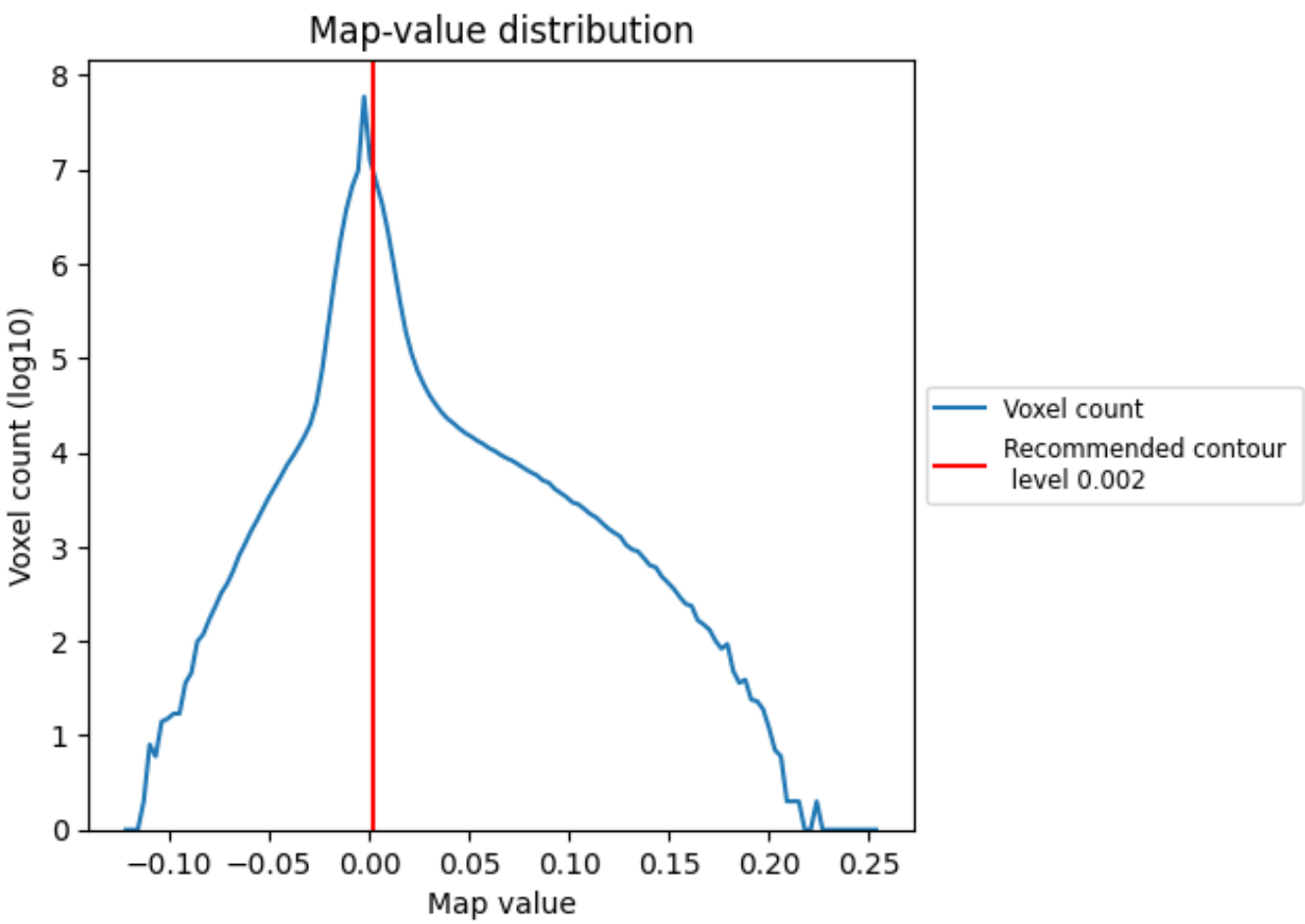
6.5 Mask visualisation (i)

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

7 Map analysis (i)

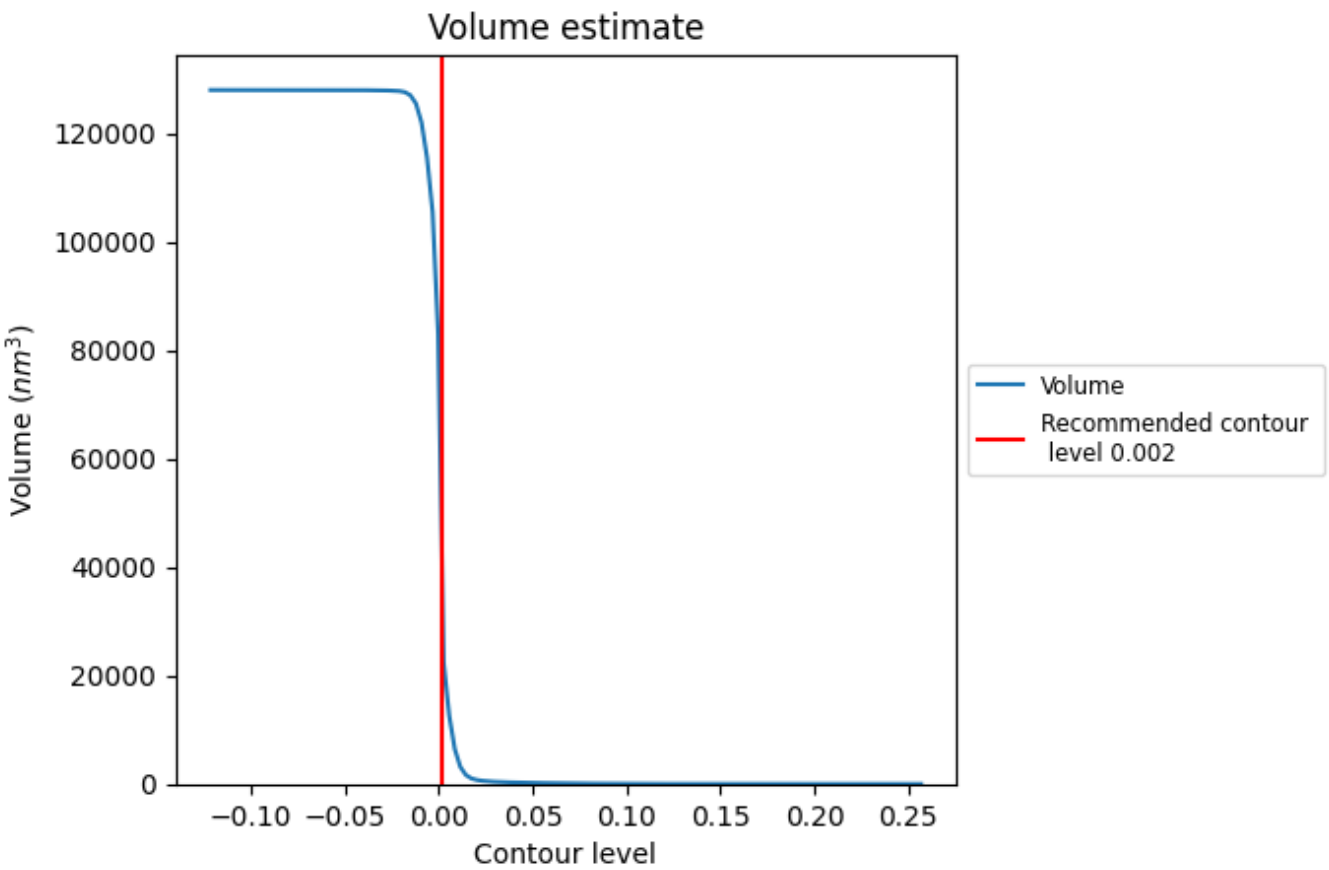
This section contains the results of statistical analysis of the map.

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.

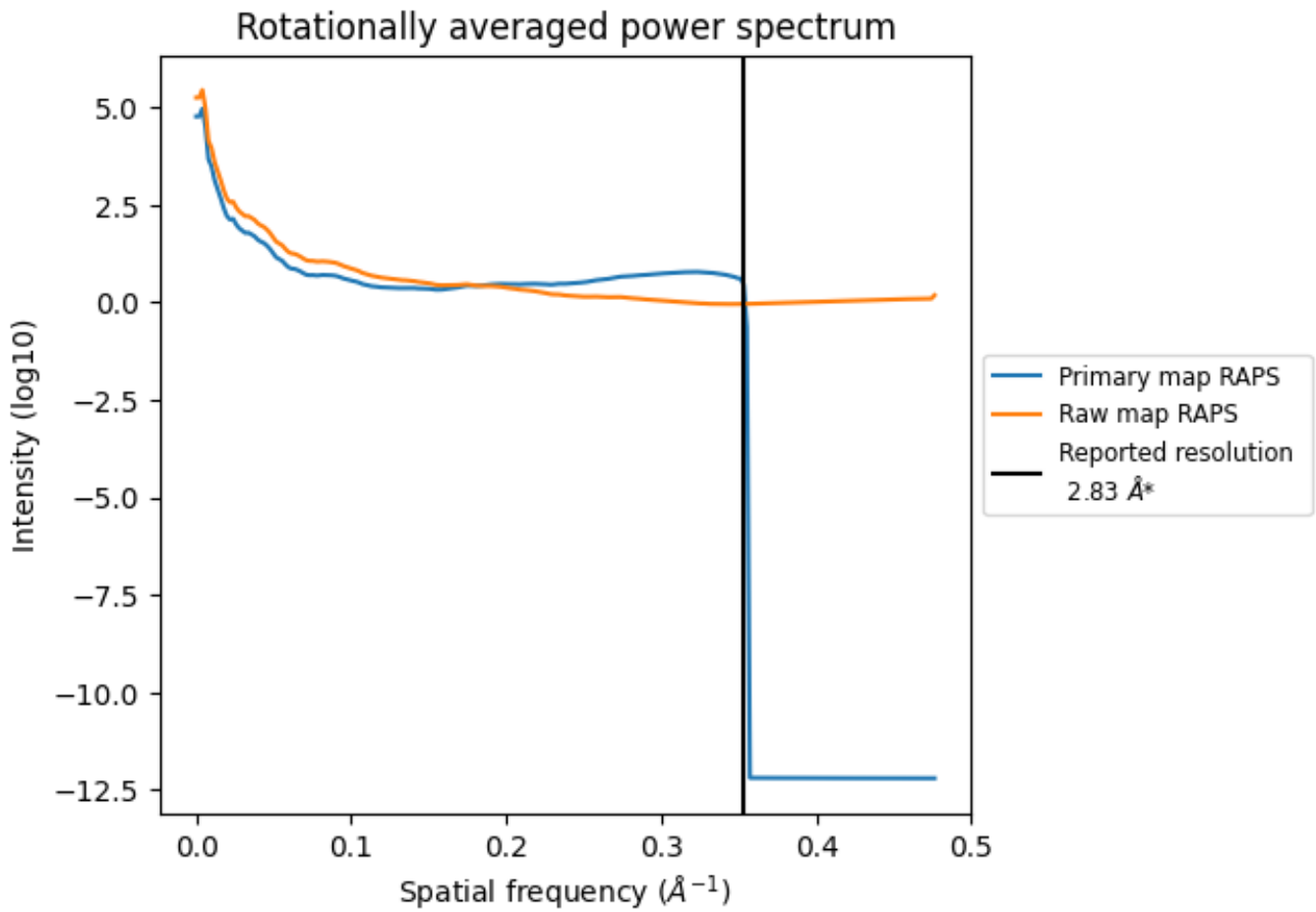
7.2 Volume estimate (i)



The volume at the recommended contour level is 35519 nm^3; this corresponds to an approximate mass of 32085 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)

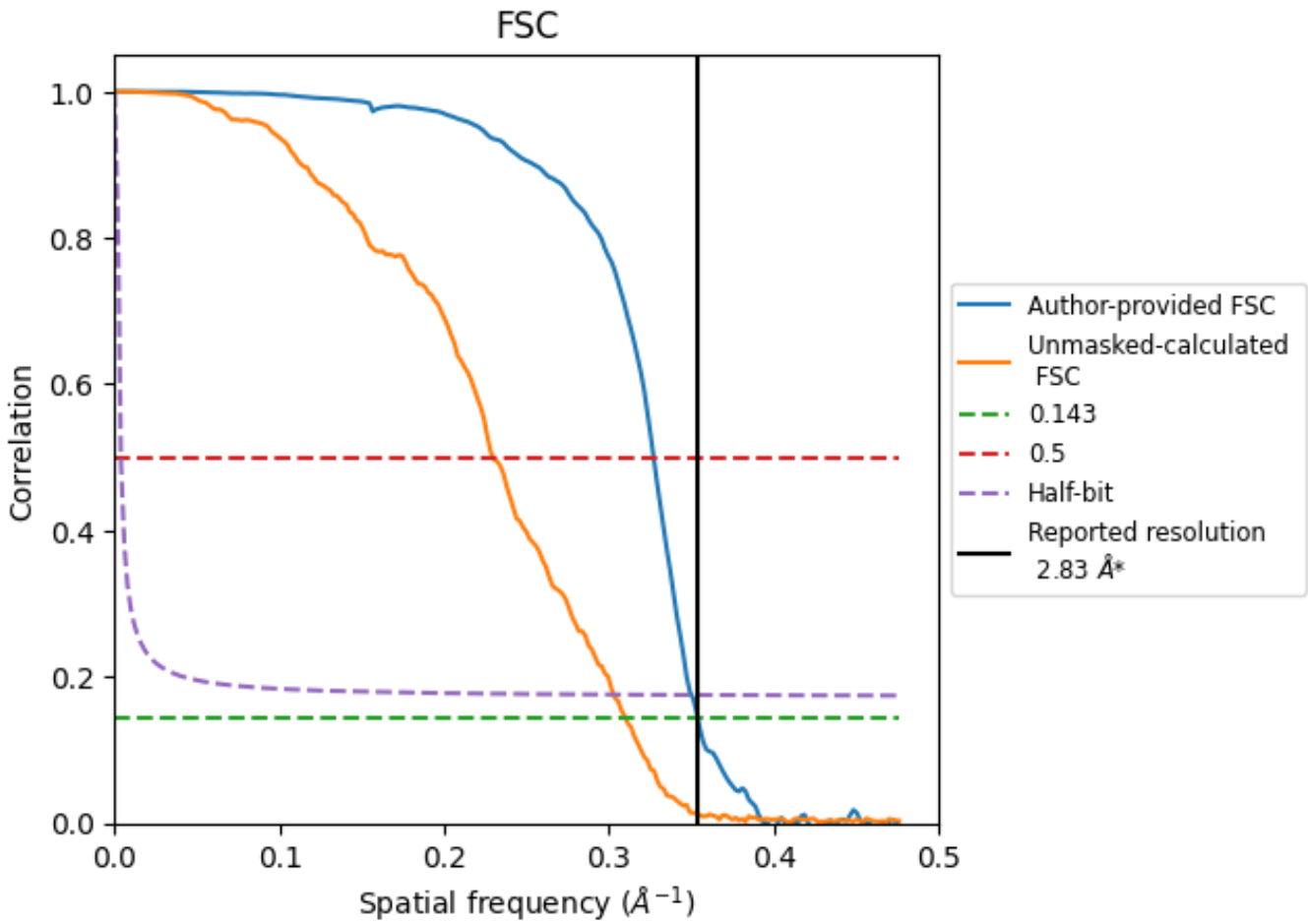


*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

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 0.353 Å^{-1}

8.2 Resolution estimates (i)

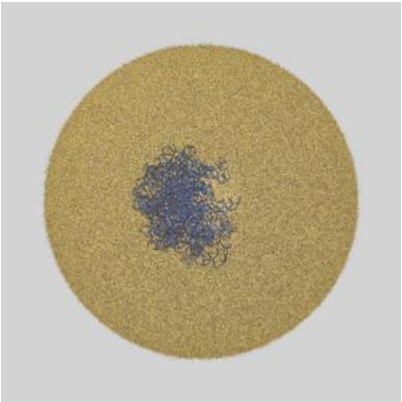
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.06	2.86
Unmasked-calculated*	3.22	4.36	3.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.83 by more than 10 %

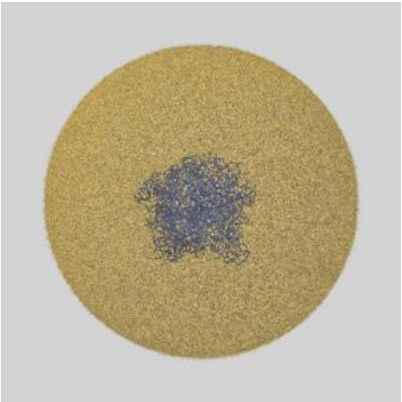
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4531 and PDB model 6QDW. Per-residue inclusion information can be found in section 3 on page 10.

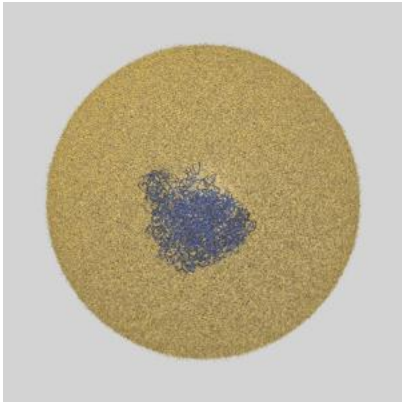
9.1 Map-model overlay (i)



X



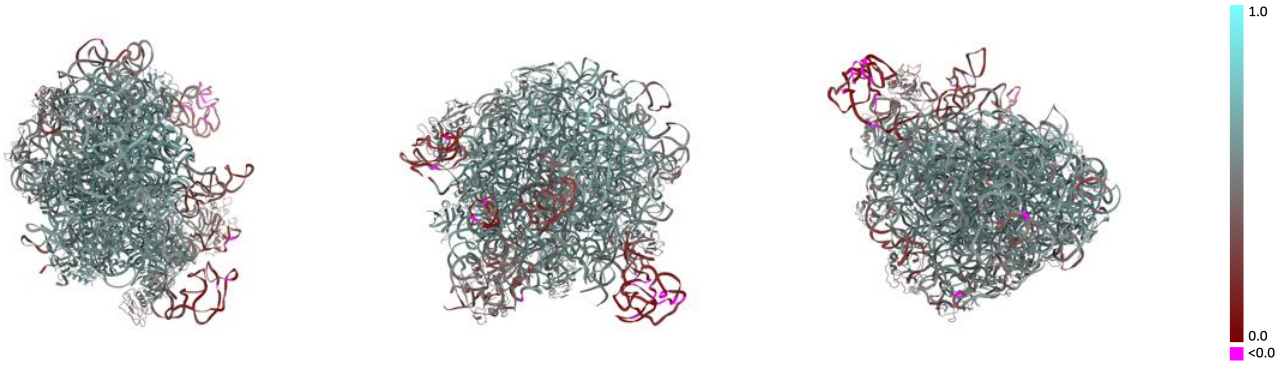
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002 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.

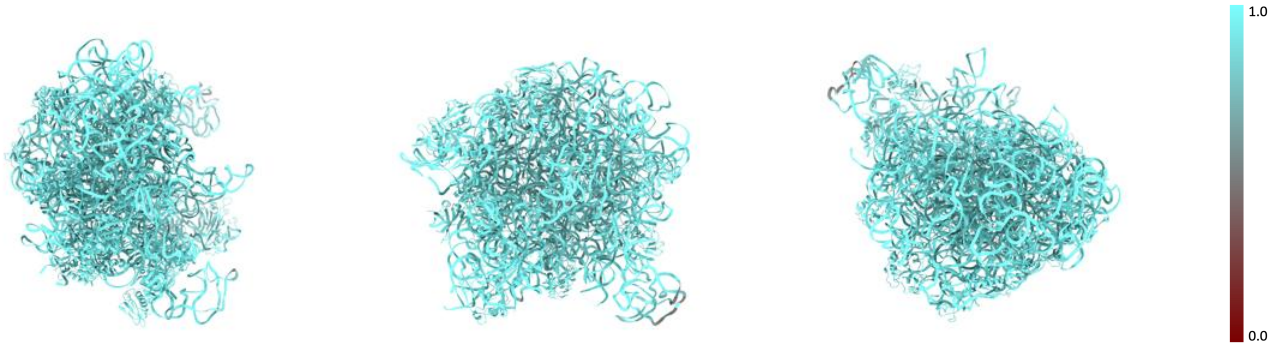
9.2 Q-score mapped to coordinate model (i)



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.

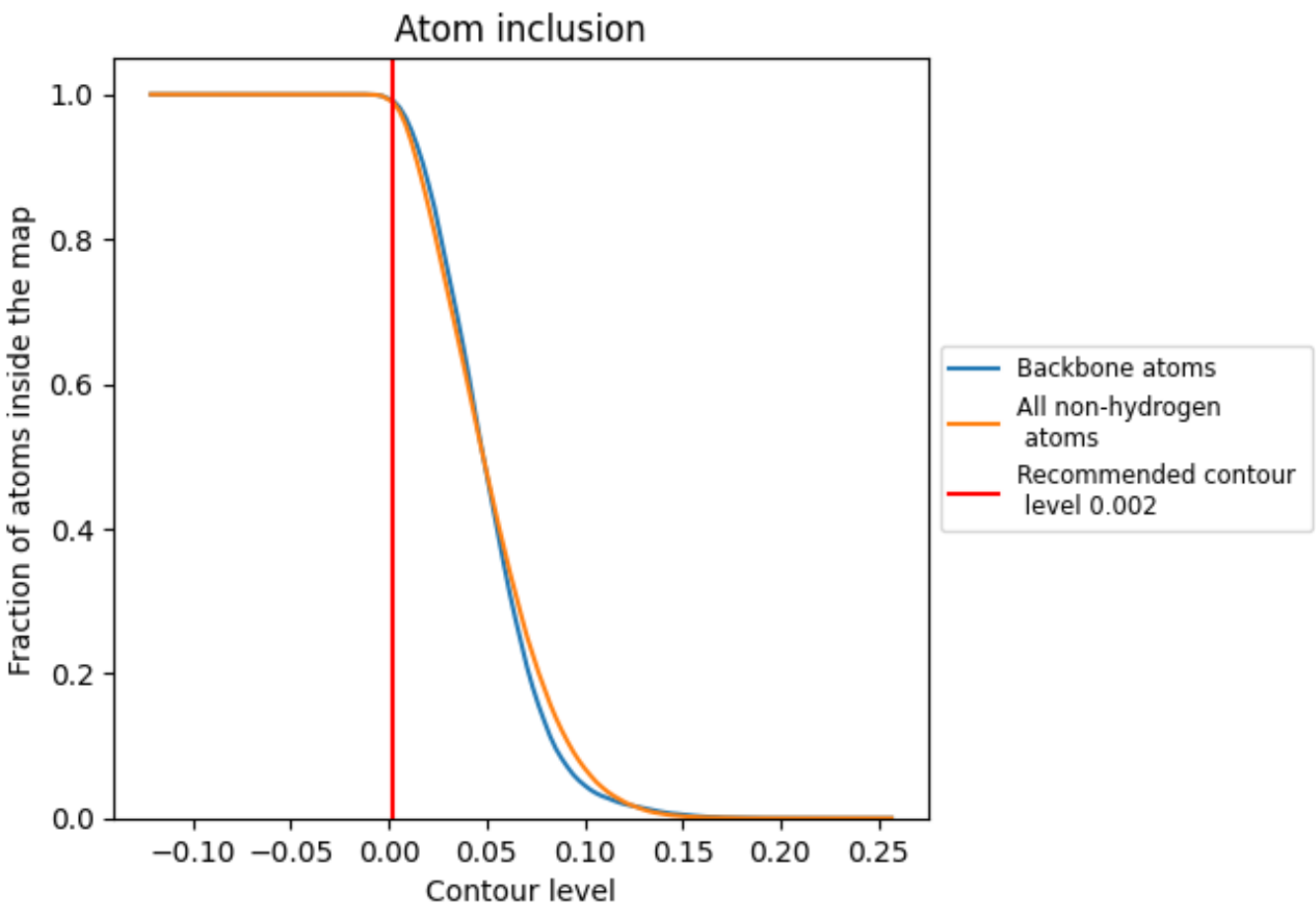
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.002).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9894	0.5410
0	0.9884	0.5580
1	0.9772	0.4710
2	0.9977	0.5990
3	0.9952	0.5550
4	0.9676	0.5120
6	0.9915	0.6080
7	0.9959	0.6150
8	1.0000	0.5820
a	0.9933	0.5000
b	0.9913	0.5510
c	0.9926	0.5910
d	0.9889	0.5650
e	0.9849	0.5240
f	0.9832	0.3410
g	0.9869	0.4600
h	0.9789	0.4550
j	0.9945	0.5910
k	0.9923	0.5730
l	0.9852	0.5590
m	0.9942	0.5920
n	0.9935	0.5660
o	0.9884	0.4670
p	0.9841	0.5340
q	0.9967	0.6130
r	0.9896	0.5800
s	0.9927	0.5770
t	0.9889	0.5100
u	0.9844	0.4570
v	0.9261	0.2810
w	0.9932	0.5560
y	0.9908	0.5980
z	0.8500	0.2500