Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:17 pm GMT

PDB ID	:	7AQD
EMDB ID	:	EMD-11864
Title	:	Structure of the bacterial RQC complex (Translocating State)
Authors	:	Filbeck, S.; Pfeffer, S.
Deposited on	:	2020-10-21
Resolution	:	3.10 Å(reported)
Based on initial models	:	5H3W, 3J9W, 5H3X

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

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

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

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

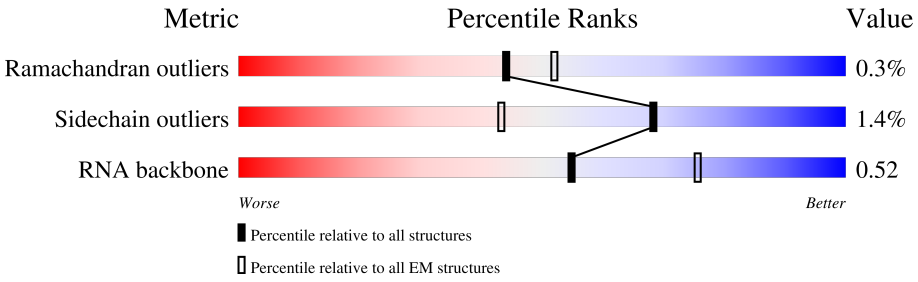
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 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)
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	R	570	29% 67% 5% 24%
2	A	2918	75% 23%
3	B	112	67% 31%
4	C	277	99%
5	D	209	99%
6	E	207	99%
7	F	179	9% 98%
8	G	179	97%

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Mol	Chain	Length	Quality of chain
9	I	141	63% 94% 6%
10	J	145	97%
11	K	122	100%
12	L	146	99%
13	M	144	94%
14	N	120	98%
15	O	120	100%
16	Q	119	97%
17	S	113	96%
18	T	76	34% 39% 22%
19	U	103	97%
20	V	94	87% 13%
21	W	7	100%
22	X	62	90% 6%
23	Z	59	98%
24	a	115	99%
25	b	59	92% 8%
26	c	49	98%
27	d	44	98%
28	e	66	97%
29	f	37	97%
30	g	102	99%
31	h	95	98%
32	i	66	97%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 94357 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 Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	433	3519	2239	612	658	10	0	0

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	2918	62663	27955	11572	20218	2918	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	112	2395	1068	435	780	112	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	275	2111	1312	416	377	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	207	1575	988	290	292	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	205	1561	980	289	290	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	178	Total	C	N	O	S	0	0
			1404	893	245	259	7		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	133	Total	C	N	O	S	0	0
			981	617	173	185	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1097	703	208	181	5		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total 953	C 583	N 186	O 180	S 4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total 912	C 564	N 176	O 171	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	117	Total 940	C 591	N 189	O 156	S 4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	109	Total 842	C 525	N 164	O 150	S 3	0	0

- Molecule 18 is a RNA chain called Ala-tRNA (A/P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	76	Total 1622	C 722	N 290	O 534	P 76	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	100	Total 754	C 473	N 141	O 137	S 3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	82	Total 630	C 390	N 123	O 117	0	0

- Molecule 21 is a protein called nascent polyalanine.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	114	Total	C	N	O	0	0
			936	595	184	157		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 26 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	36	Total	C	N	O	S	0	0
			288	181	59	44	4		

- Molecule 30 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	93	Total	C	N	O	S	0	0
			752	472	137	139	4		

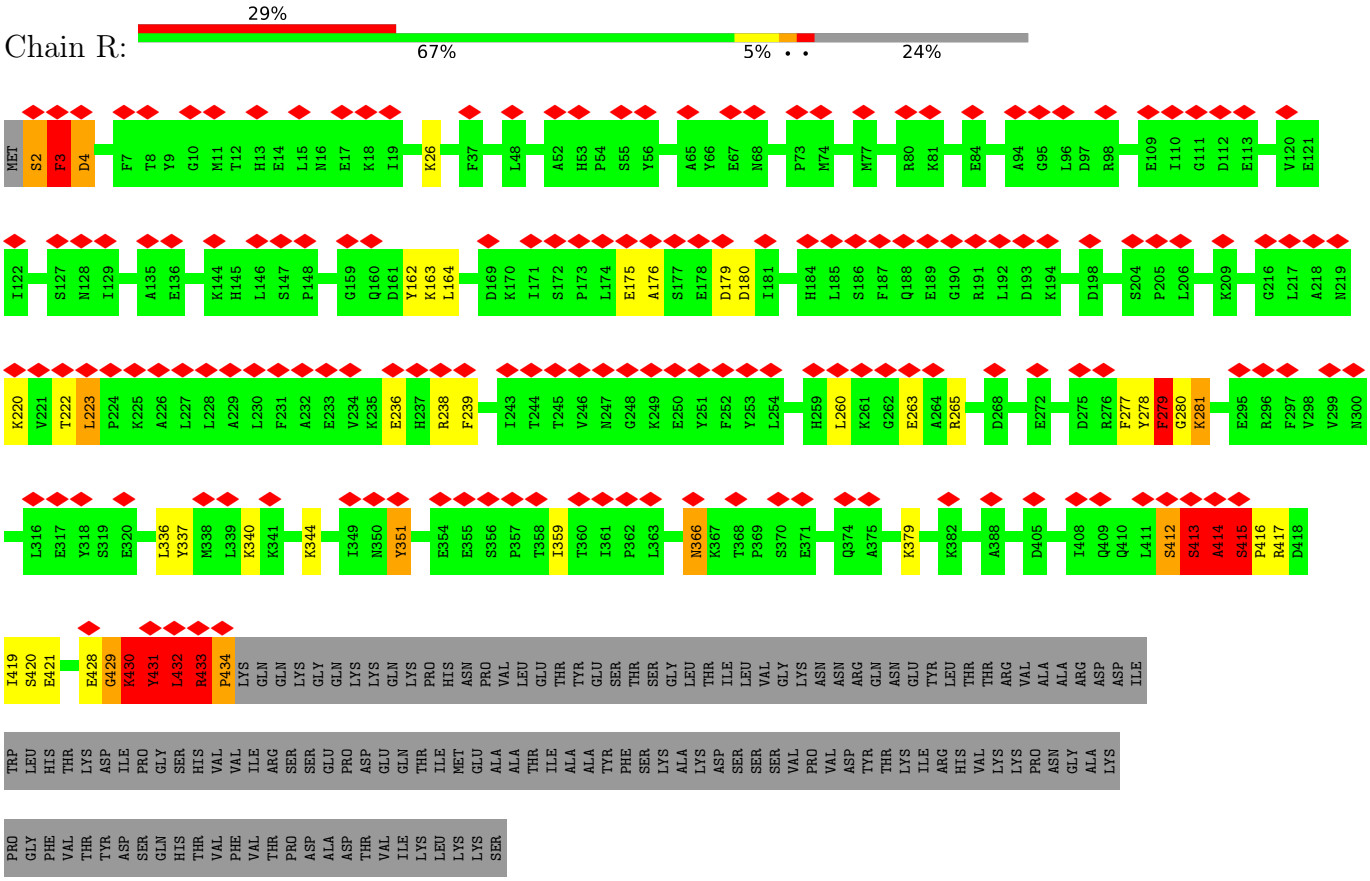
- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

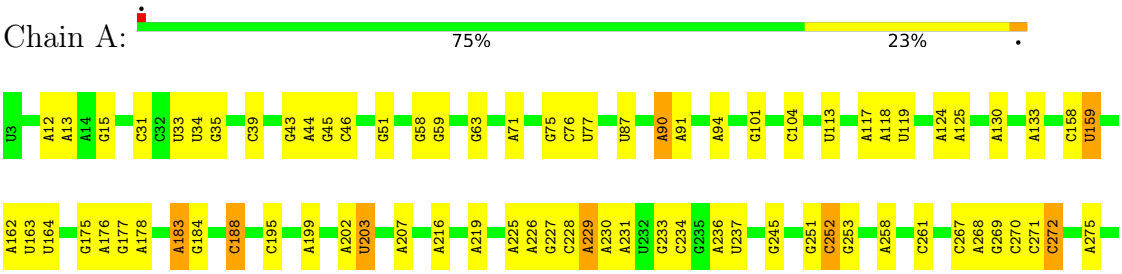
3 Residue-property plots (i)

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: Rqc2 homolog RqcH



• Molecule 2: 23S ribosomal RNA



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U386 C387 A390 A391 C392 U393 U394 U405 G406 G410 G411 A412 U413 C414 G417 A418 C422 C430 A431 C432 G433 U434 G435 A436 A437 A438 C442 G443 U444 A459 U474 U478 C482 C483 C484 U485 A490 A494 U498 C502 C503 A504 G514
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G680 A683 G684 U691 U700 G701 G713 U714 A715 G716 A717 C718 C719 U733 A762 A763 G773 C777 A781 A782 C785 A786 G792 U793 U794 G795 A796 A797 G822 G823 G824 A829 A830 U831 G832 A836 U837 C838 G839 G852 C853 U858 C859
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A987 G988 U989 C990 A991 G992 A999 A1005 A1006 G1007 A1019 A1020 A1025 A1026 A1027 C1028 A1029 G1030 C1031 A1034 C1037 A1055 U1058 A1059 G1068 U1069 A1072 U1079 U1091 A1092 G1093 A1094 C1095 G1102 A1103 U1104 G1105 U1106 U1107 G1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115
A1116 G1117 C1122 A1123 C1124 U1127 U1128 U1129 A1130 A1131 G1135 G1139 U1140 A1141 A1142 U1143 A1144 C1148 G1152 A1157 G1158 U1159 U1176 G1177 U1178 A1179 C1180 C1181 G1182 G1185 C1186 U1187 A1188 A1194 A1201 A1202 G1209 U1217 U1218 C1219 G1220 U1229 G1245 G1246 G1247
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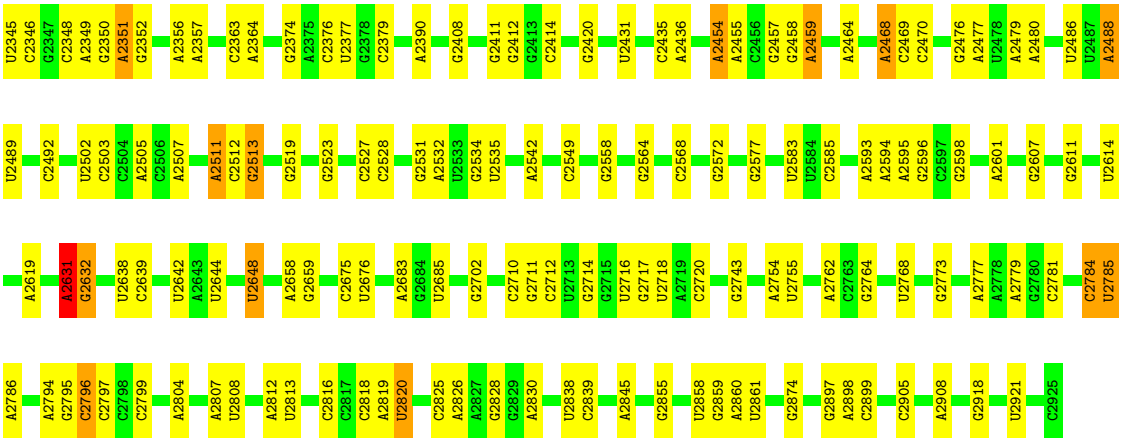
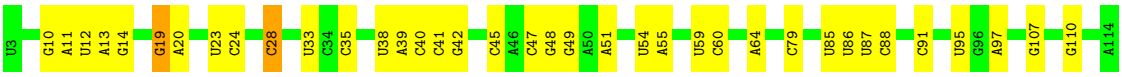
U1418 A1423 A1424 C1425 G1431 A1432 U1433 A1434 U1435 U1436 C1437 C1438 U1439 G1440 U1441 A1442 C1450 A1456 G1460 A1464 G1472 A1473 C1474 A1490 G1497 U1498 A1499 U1507 U1513 C1514 C1515 C1519 A1520 A1524 U1528 A1536 C1539 C1544 C1550 A1553 U1554
A1555 G1561 A1562 G1563 C1564 A1569 U1570 G1571 G1572 C1573 A1581 U1582 A1583 U1584 A1585 G1586 U1595 U1596 C1607 A1608 A1614 A1617 C1622 U1626 G1630 A1631 G1632 G1633 U1634 C1652 A1653 A1654 A1655 C1656 C1657 G1658 A1659 C1660 A1667 G1674 A1679 A1691 U1692 C1693
G1696 A1697 C1705 A1709 G1712 G1719 A1727 G1744 A1745 G1752 C1755 U1756 G1757 U1758 C1770 C1771 A1774 G1777 A1778 G1779 C1780 C1781 G1782 C1783 A1784 G1785 A1788 A1791 G1792 G1793 C1794 A1802 C1803 U1804 G1805 A1809 G1810 C1811 C1829 G1830 A1845 A1858
C1859 A1877 U1881 A1895 G1898 A1901 G1902 G1912 A1913 U1916 G1917 A1918 C1922 G1935 G1936 C1937 A1941 A1947 A1948 C1949 G1958 G1959 C1963 A1966 A1967 U1968 U1969 C1970 C1971 U1972 U1984 U1985 C1990 G1993 C1996 A1999 A2000 G2001 A2010 U2011
U2020 G2021 U2022 C2023 U2024 C2025 A2026 C2035 G2050 U2051 A2052 A2060 G2061 A2062 G2068 C2072 C2084 G2085 A2088 A2089 G2090 A2091 C2092 C2093 G2098 C2110 A2111 U2121 G2122 A2123 C2133 U2140 A2141 C2142 A2143 G2144 G2145 A2146 U2147 A2148 G2149 A2155 G2156 C2157 U2160 G2161
G2162 A2165 C2175 A2176 G2177 G2186 A2187 G2188 C2193 G2194 G2195 U2196 G2197 G2198 G2199 A2200 G2232 C2233 C2234 G2235 U2240 A2241 U2242 C2243 A2254 C2255 G2267 G2268 G2280 G2281 G2282 C2283 G2308 G2311 C2312 A2315 A2316 A2317 C2323 G2333 U2334 U2335 G2336 G2337 A2338

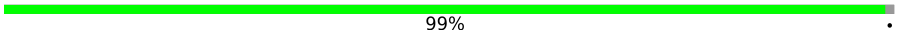


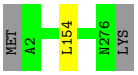
• Molecule 3: 5S ribosomal RNA

Chain B: 

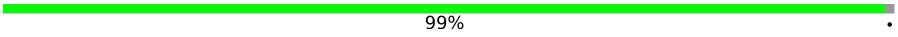


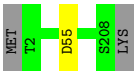
• Molecule 4: 50S ribosomal protein L2

Chain C: 

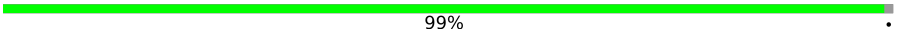


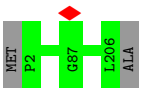
• Molecule 5: 50S ribosomal protein L3

Chain D: 

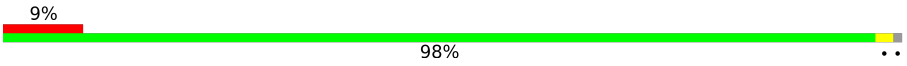


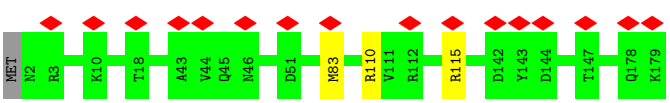
• Molecule 6: 50S ribosomal protein L4

Chain E: 



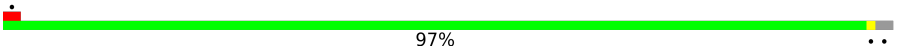
• Molecule 7: 50S ribosomal protein L5

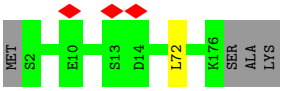
Chain F: 



• Molecule 8: 50S ribosomal protein L6

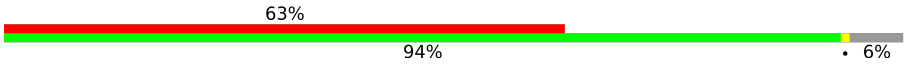
Chain G:

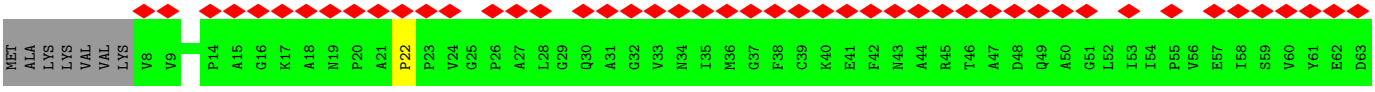


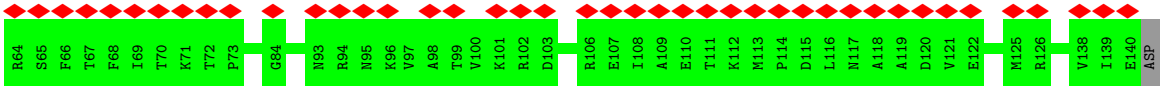


• Molecule 9: 50S ribosomal protein L11

Chain I:

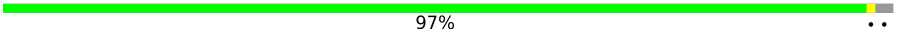


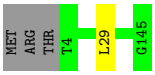




• Molecule 10: 50S ribosomal protein L13

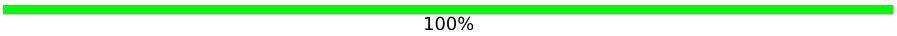
Chain J:





• Molecule 11: 50S ribosomal protein L14

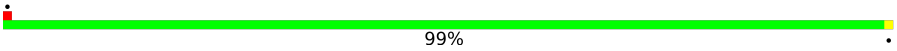
Chain K:

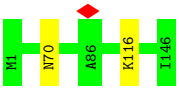


There are no outlier residues recorded for this chain.

• Molecule 12: 50S ribosomal protein L15

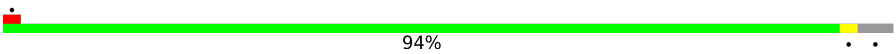
Chain L:

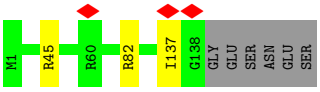




• Molecule 13: 50S ribosomal protein L16

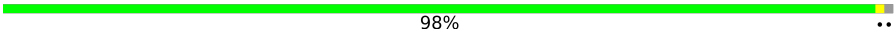
Chain M:

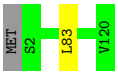




• Molecule 14: 50S ribosomal protein L17

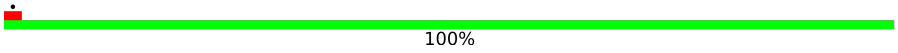
Chain N:

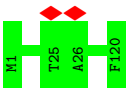




• Molecule 15: 50S ribosomal protein L18

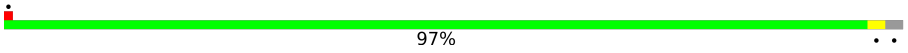
Chain O:

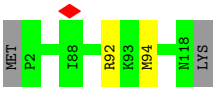




• Molecule 16: 50S ribosomal protein L20

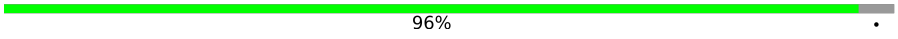
Chain Q:

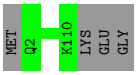




• Molecule 17: 50S ribosomal protein L22

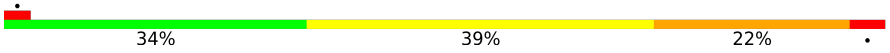
Chain S:

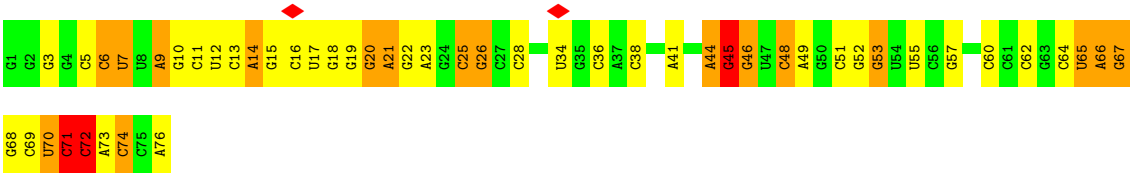




• Molecule 18: Ala-tRNA (A/P-site)

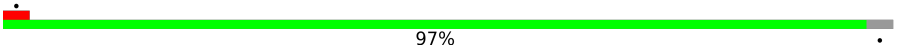
Chain T:

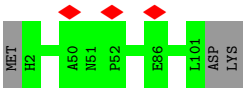




• Molecule 19: 50S ribosomal protein L24

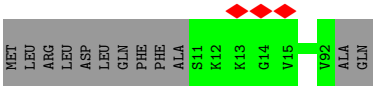
Chain U:





• Molecule 20: 50S ribosomal protein L27

Chain V:



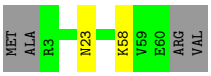
• Molecule 21: nascent polyalanine

Chain W: 

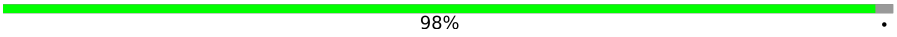
There are no outlier residues recorded for this chain.

• Molecule 22: 50S ribosomal protein L28

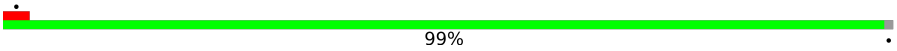
Chain X: 

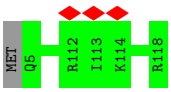


• Molecule 23: 50S ribosomal protein L30

Chain Z: 

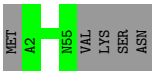
• Molecule 24: 50S ribosomal protein L19

Chain a: 

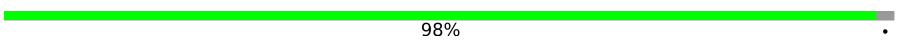


• Molecule 25: 50S ribosomal protein L32

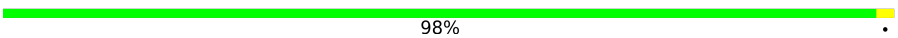
Chain b: 



• Molecule 26: 50S ribosomal protein L33 1

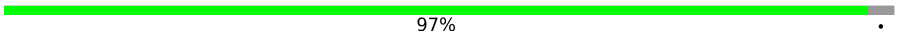
Chain c: 

• Molecule 27: 50S ribosomal protein L34

Chain d: 

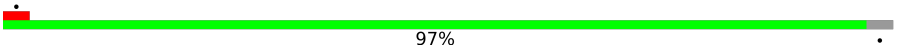
• Molecule 28: 50S ribosomal protein L35

Chain e:



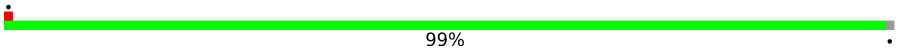
• Molecule 29: 50S ribosomal protein L36

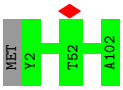
Chain f:



• Molecule 30: 50S ribosomal protein L21

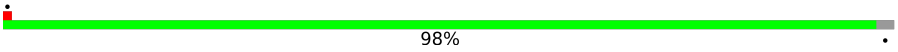
Chain g:

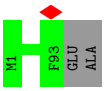




• Molecule 31: 50S ribosomal protein L23

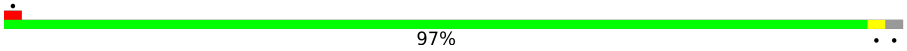
Chain h:

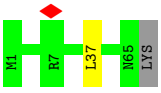




• Molecule 32: 50S ribosomal protein L29

Chain i:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24348	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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	R	0.84	18/3590 (0.5%)	3.03	68/4835 (1.4%)
2	A	0.34	1/70190 (0.0%)	1.05	279/109503 (0.3%)
3	B	0.32	0/2678	1.10	19/4174 (0.5%)
4	C	0.27	0/2148	0.54	0/2881
5	D	0.28	0/1597	0.55	1/2140 (0.0%)
6	E	0.28	0/1580	0.56	0/2132
7	F	0.30	0/1423	0.65	1/1910 (0.1%)
8	G	0.29	0/1360	0.56	1/1832 (0.1%)
9	I	0.29	0/995	0.59	0/1346
10	J	0.30	0/1146	0.60	1/1542 (0.1%)
11	K	0.28	0/927	0.58	0/1245
12	L	0.29	0/1093	0.52	0/1457
13	M	0.34	0/1120	0.63	3/1496 (0.2%)
14	N	0.26	0/960	0.51	1/1284 (0.1%)
15	O	0.27	0/921	0.58	0/1236
16	Q	0.28	0/952	0.54	1/1266 (0.1%)
17	S	0.27	0/851	0.57	0/1146
18	T	1.13	1/1811 (0.1%)	1.90	74/2822 (2.6%)
19	U	0.27	0/764	0.53	0/1022
20	V	0.32	0/638	0.59	0/847
21	W	0.31	0/34	0.86	0/46
22	X	0.28	0/448	0.68	1/596 (0.2%)
23	Z	0.28	0/457	0.54	0/613
24	a	0.25	0/949	0.51	0/1269
25	b	0.29	0/433	0.61	0/574
26	c	0.27	0/406	0.53	0/540
27	d	0.24	0/370	0.45	0/483
28	e	0.28	0/519	0.55	0/680
29	f	0.24	0/291	0.44	0/383
30	g	0.30	0/797	0.66	0/1070
31	h	0.26	0/759	0.49	0/1011
32	i	0.28	0/531	0.65	1/707 (0.1%)
All	All	0.38	20/102738 (0.0%)	1.11	451/154088 (0.3%)

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	R	0	15
2	A	0	7
4	C	0	1
9	I	0	1
18	T	0	14
All	All	0	38

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	430	LYS	CA-CB	14.59	1.86	1.53
1	R	429	GLY	C-N	13.71	1.65	1.34
1	R	3	PHE	CB-CG	11.71	1.71	1.51
1	R	3	PHE	CG-CD1	9.22	1.52	1.38
18	T	72	C	C4-N4	-8.93	1.25	1.33
1	R	431	TYR	CB-CG	-8.80	1.38	1.51
1	R	431	TYR	CE2-CZ	-8.72	1.27	1.38
1	R	431	TYR	C-O	-8.34	1.07	1.23
1	R	431	TYR	C-N	7.99	1.52	1.34
1	R	412	SER	C-N	7.59	1.51	1.34
1	R	434	PRO	CA-CB	7.15	1.67	1.53
1	R	431	TYR	CD1-CE1	6.96	1.49	1.39
1	R	415	SER	C-N	6.88	1.47	1.34
1	R	4	ASP	N-CA	6.86	1.60	1.46
1	R	433	ARG	C-N	-5.67	1.23	1.34
1	R	434	PRO	CA-C	5.50	1.63	1.52
1	R	434	PRO	N-CD	-5.48	1.40	1.47
2	A	2010	A	N9-C4	5.13	1.41	1.37
1	R	433	ARG	CA-CB	-5.03	1.42	1.53
1	R	431	TYR	CZ-OH	5.02	1.46	1.37

All (451) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	431	TYR	CD1-CG-CD2	-78.07	32.02	117.90
1	R	431	TYR	CG-CD2-CE2	-71.48	64.12	121.30
1	R	3	PHE	CD1-CE1-CZ	-71.22	34.63	120.10
1	R	431	TYR	CG-CD1-CE1	-71.09	64.43	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	3	PHE	CB-CG-CD1	58.90	162.03	120.80
1	R	3	PHE	CG-CD1-CE1	-57.69	57.34	120.80
1	R	3	PHE	CD1-CG-CD2	-40.51	65.63	118.30
1	R	430	LYS	N-CA-CB	-39.03	40.35	110.60
1	R	3	PHE	CZ-CE2-CD2	-37.46	75.15	120.10
1	R	3	PHE	CG-CD2-CE2	-34.79	82.53	120.80
1	R	3	PHE	CE1-CZ-CE2	-32.96	60.68	120.00
1	R	431	TYR	CB-CG-CD1	-29.58	103.25	121.00
1	R	431	TYR	CZ-CE2-CD2	-25.08	97.23	119.80
1	R	431	TYR	CE1-CZ-CE2	-23.90	81.56	119.80
1	R	429	GLY	C-N-CA	-20.51	70.44	121.70
1	R	431	TYR	CB-CG-CD2	18.53	132.12	121.00
1	R	431	TYR	N-CA-CB	-16.81	80.34	110.60
1	R	433	ARG	C-N-CD	-14.99	87.62	120.60
1	R	414	ALA	CB-CA-C	-14.89	87.77	110.10
1	R	2	SER	C-N-CA	-13.85	87.08	121.70
1	R	431	TYR	CE1-CZ-OH	11.89	152.20	120.10
1	R	433	ARG	CB-CG-CD	-11.24	82.38	111.60
2	A	2511	A	N1-C6-N6	-10.95	112.03	118.60
1	R	351	TYR	CG-CD1-CE1	-10.90	112.58	121.30
1	R	3	PHE	N-CA-CB	10.89	130.20	110.60
1	R	3	PHE	CB-CG-CD2	10.85	128.39	120.80
2	A	2479	A	N1-C6-N6	-10.38	112.37	118.60
18	T	76	A	N1-C6-N6	-10.18	112.49	118.60
18	T	21	A	N1-C6-N6	-10.17	112.50	118.60
2	A	2489	U	O4'-C1'-N1	10.11	116.28	108.20
1	R	415	SER	CB-CA-C	-9.98	91.13	110.10
1	R	351	TYR	CD1-CE1-CZ	9.84	128.65	119.80
18	T	14	A	N1-C6-N6	-9.81	112.71	118.60
1	R	3	PHE	CA-C-O	-9.79	99.54	120.10
2	A	2631	A	N1-C6-N6	-9.67	112.80	118.60
2	A	272	C	C2-N1-C1'	9.62	129.38	118.80
2	A	1281	C	N1-C2-O2	9.55	124.63	118.90
2	A	483	C	C2-N1-C1'	9.39	129.13	118.80
2	A	1352	U	C2-N1-C1'	9.36	128.94	117.70
2	A	914	C	N1-C2-O2	9.35	124.51	118.90
1	R	430	LYS	C-N-CA	9.35	145.06	121.70
2	A	2480	A	N1-C6-N6	-9.28	113.03	118.60
2	A	1657	C	C5-C6-N1	9.23	125.61	121.00
2	A	1281	C	N3-C2-O2	-9.20	115.46	121.90
1	R	3	PHE	CA-C-N	9.17	137.38	117.20
1	R	433	ARG	CB-CA-C	-9.13	92.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1352	U	N1-C2-O2	9.00	129.10	122.80
1	R	3	PHE	CB-CA-C	-8.98	92.44	110.40
1	R	413	SER	C-N-CA	8.93	144.03	121.70
2	A	1564	C	N1-C2-O2	8.87	124.22	118.90
2	A	1352	U	N3-C2-O2	-8.83	116.02	122.20
2	A	2488	A	P-O3'-C3'	8.83	130.29	119.70
2	A	2712	C	N1-C2-O2	8.77	124.16	118.90
2	A	2480	A	C5-C6-N1	8.66	122.03	117.70
2	A	1281	C	C2-N1-C1'	8.62	128.28	118.80
1	R	4	ASP	CB-CG-OD1	-8.61	110.56	118.30
18	T	66	A	N1-C6-N6	-8.56	113.46	118.60
1	R	279	PHE	CD1-CE1-CZ	8.55	130.36	120.10
2	A	1246	G	O4'-C1'-N9	8.44	114.95	108.20
1	R	279	PHE	CG-CD1-CE1	-8.29	111.69	120.80
1	R	430	LYS	CB-CG-CD	8.24	133.03	111.60
18	T	9	A	N1-C6-N6	-8.23	113.67	118.60
1	R	434	PRO	N-CA-CB	-8.19	93.48	103.30
18	T	23	A	C5-C6-N1	8.09	121.75	117.70
2	A	716	G	C4-N9-C1'	7.99	136.88	126.50
2	A	914	C	C2-N1-C1'	7.94	127.53	118.80
18	T	44	A	C5-C6-N1	7.88	121.64	117.70
1	R	430	LYS	CD-CE-NZ	-7.87	93.59	111.70
18	T	62	C	N3-C2-O2	-7.86	116.40	121.90
18	T	44	A	N1-C6-N6	-7.86	113.89	118.60
3	B	28	C	N1-C2-O2	7.84	123.60	118.90
2	A	1281	C	C6-N1-C2	-7.80	117.18	120.30
2	A	442	C	C2-N1-C1'	7.79	127.37	118.80
2	A	1622	C	C2-N1-C1'	7.78	127.36	118.80
2	A	2489	U	N3-C2-O2	-7.72	116.80	122.20
1	R	3	PHE	C-N-CA	7.71	140.97	121.70
1	R	4	ASP	O-C-N	-7.69	110.12	123.20
2	A	203	U	C2-N1-C1'	7.67	126.90	117.70
2	A	203	U	N1-C2-O2	7.64	128.15	122.80
2	A	2712	C	C2-N1-C1'	7.61	127.17	118.80
13	M	45	ARG	NE-CZ-NH1	7.58	124.09	120.30
18	T	66	A	C5-C6-N1	7.57	121.49	117.70
7	F	83	MET	CA-CB-CG	7.54	126.11	113.30
18	T	69	C	N3-C2-O2	-7.50	116.65	121.90
2	A	1564	C	N3-C2-O2	-7.49	116.66	121.90
2	A	914	C	N3-C2-O2	-7.46	116.68	121.90
1	R	433	ARG	CA-C-N	-7.44	96.28	117.10
2	A	2480	A	C4-C5-C6	-7.38	113.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	483	C	C6-N1-C2	-7.36	117.36	120.30
2	A	1345	U	O4'-C1'-N1	7.33	114.07	108.20
18	T	11	C	N3-C2-O2	-7.33	116.77	121.90
2	A	272	C	C6-N1-C2	-7.31	117.38	120.30
2	A	2376	C	O4'-C1'-N1	7.30	114.04	108.20
2	A	1515	C	C2-N1-C1'	7.29	126.82	118.80
18	T	22	G	O4'-C1'-N9	7.26	114.00	108.20
2	A	2631	A	C5-C6-N1	7.23	121.31	117.70
2	A	237	U	N1-C2-O2	7.15	127.81	122.80
1	R	4	ASP	CB-CG-OD2	7.14	124.73	118.30
2	A	2785	U	P-O3'-C3'	7.14	128.27	119.70
18	T	48	C	O4'-C1'-N1	7.14	113.91	108.20
2	A	203	U	N3-C2-O2	-7.13	117.20	122.20
18	T	9	A	C5-C6-N1	7.13	121.27	117.70
18	T	64	C	N3-C2-O2	-7.12	116.91	121.90
18	T	76	A	C5-C6-N1	7.12	121.26	117.70
2	A	1544	C	N1-C2-O2	7.12	123.17	118.90
2	A	1696	G	O4'-C1'-N9	7.09	113.87	108.20
2	A	1550	C	N1-C2-O2	7.08	123.15	118.90
2	A	1963	C	C2-N1-C1'	7.08	126.59	118.80
18	T	14	A	C5-C6-N1	7.07	121.24	117.70
2	A	2010	A	C2-N3-C4	7.07	114.14	110.60
2	A	234	C	C2-N1-C1'	7.03	126.53	118.80
18	T	14	A	C4-C5-C6	-7.00	113.50	117.00
18	T	6	C	N3-C2-O2	-7.00	117.00	121.90
2	A	1515	C	N1-C2-O2	6.99	123.09	118.90
2	A	716	G	N3-C4-N9	6.98	130.19	126.00
2	A	716	G	N3-C4-C5	-6.93	125.14	128.60
2	A	1564	C	C2-N1-C1'	6.92	126.41	118.80
1	R	434	PRO	CB-CG-CD	-6.92	79.53	106.50
2	A	2093	C	N3-C2-O2	-6.90	117.07	121.90
2	A	1245	G	P-O3'-C3'	6.88	127.96	119.70
2	A	377	G	P-O3'-C3'	6.88	127.95	119.70
2	A	2255	C	N1-C2-O2	6.85	123.01	118.90
18	T	69	C	O4'-C1'-N1	6.85	113.68	108.20
1	R	4	ASP	CA-C-N	6.82	129.84	116.20
1	R	278	TYR	CB-CG-CD1	-6.82	116.91	121.00
18	T	74	C	C2'-C3'-O3'	6.82	124.61	113.70
2	A	716	G	C8-N9-C1'	-6.80	118.15	127.00
2	A	1657	C	C6-N1-C2	-6.78	117.59	120.30
2	A	2712	C	N3-C2-O2	-6.77	117.16	121.90
18	T	70	U	O4'-C1'-N1	6.77	113.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1110	C	C2-N1-C1'	6.75	126.23	118.80
2	A	2459	A	C2-N3-C4	6.75	113.97	110.60
2	A	936	C	P-O3'-C3'	6.74	127.79	119.70
2	A	1028	C	N1-C2-O2	6.72	122.93	118.90
18	T	13	C	N3-C4-N4	-6.72	113.29	118.00
2	A	1351	U	P-O3'-C3'	6.71	127.75	119.70
18	T	66	A	C4-C5-C6	-6.68	113.66	117.00
2	A	2568	C	C2-N1-C1'	6.67	126.14	118.80
2	A	1229	U	N1-C2-O2	6.66	127.47	122.80
2	A	1803	C	C6-N1-C2	-6.66	117.64	120.30
18	T	71	C	N3-C2-O2	-6.66	117.24	121.90
2	A	683	A	P-O3'-C3'	6.65	127.68	119.70
2	A	1362	G	P-O3'-C3'	6.64	127.67	119.70
2	A	1652	C	P-O3'-C3'	6.63	127.66	119.70
2	A	1985	U	N1-C2-O2	6.63	127.44	122.80
2	A	237	U	N3-C2-O2	-6.62	117.56	122.20
2	A	483	C	C5-C6-N1	6.61	124.31	121.00
2	A	188	C	C5-C6-N1	6.61	124.30	121.00
18	T	25	C	N3-C2-O2	-6.61	117.28	121.90
18	T	11	C	N1-C2-O2	6.61	122.86	118.90
2	A	1803	C	N1-C2-O2	6.57	122.84	118.90
2	A	1110	C	N1-C2-O2	6.56	122.84	118.90
18	T	13	C	N3-C2-O2	-6.54	117.32	121.90
2	A	113	U	C2-N1-C1'	6.54	125.54	117.70
2	A	1353	C	C2-N1-C1'	6.53	125.98	118.80
2	A	484	C	C2-N1-C1'	6.53	125.98	118.80
2	A	2479	A	C4-C5-C6	-6.52	113.74	117.00
18	T	44	A	C5'-C4'-C3'	-6.52	105.57	116.00
18	T	76	A	C4-C5-C6	-6.50	113.75	117.00
2	A	914	C	C6-N1-C2	-6.50	117.70	120.30
2	A	1245	G	O4'-C1'-N9	6.49	113.39	108.20
1	R	433	ARG	N-CA-C	6.49	128.53	111.00
18	T	44	A	C5'-C4'-O4'	6.49	116.89	109.10
3	B	28	C	C2-N1-C1'	6.48	125.92	118.80
1	R	260	LEU	CA-CB-CG	6.46	130.17	115.30
2	A	1564	C	C6-N1-C2	-6.46	117.71	120.30
2	A	2503	C	C2-N1-C1'	6.46	125.91	118.80
2	A	1771	C	C2-N1-C1'	6.46	125.90	118.80
18	T	23	A	N1-C6-N6	-6.44	114.73	118.60
2	A	195	C	N1-C2-O2	6.44	122.76	118.90
1	R	277	PHE	CB-CG-CD1	-6.40	116.32	120.80
1	R	430	LYS	N-CA-C	-6.40	93.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	272	C	C6-N1-C1'	-6.39	113.14	120.80
2	A	272	C	N1-C2-O2	6.38	122.73	118.90
2	A	1970	C	N1-C2-O2	6.38	122.73	118.90
2	A	717	A	P-O3'-C3'	6.38	127.35	119.70
18	T	51	C	N3-C2-O2	-6.37	117.44	121.90
18	T	62	C	N1-C2-O2	6.37	122.72	118.90
14	N	83	LEU	CA-CB-CG	6.34	129.88	115.30
2	A	104	C	C2-N1-C1'	6.33	125.76	118.80
2	A	2511	A	C5-C6-N1	6.33	120.86	117.70
2	A	483	C	N1-C2-O2	6.30	122.68	118.90
3	B	28	C	N3-C2-O2	-6.29	117.50	121.90
18	T	21	A	C4-C5-C6	-6.28	113.86	117.00
2	A	1970	C	C2-N1-C1'	6.25	125.67	118.80
2	A	1985	U	N3-C2-O2	-6.24	117.83	122.20
3	B	79	C	N1-C2-O2	6.22	122.63	118.90
18	T	7	U	C3'-C2'-C1'	6.22	106.48	101.50
18	T	7	U	O4'-C1'-N1	6.22	113.17	108.20
2	A	2512	C	N3-C2-O2	-6.21	117.55	121.90
2	A	1572	G	O4'-C1'-N9	6.20	113.16	108.20
2	A	188	C	C6-N1-C2	-6.18	117.83	120.30
2	A	1922	C	N3-C2-O2	-6.18	117.58	121.90
2	A	1803	C	N3-C2-O2	-6.17	117.58	121.90
1	R	412	SER	C-N-CA	-6.17	106.29	121.70
2	A	1922	C	N1-C2-O2	6.16	122.60	118.90
2	A	1411	U	N3-C2-O2	-6.16	117.89	122.20
2	A	261	C	N1-C2-O2	6.16	122.59	118.90
13	M	82	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	A	2585	C	N1-C2-O2	6.14	122.58	118.90
2	A	1069	U	N1-C2-O2	6.14	127.10	122.80
3	B	35	C	N1-C2-O2	6.14	122.58	118.90
2	A	483	C	C6-N1-C1'	-6.13	113.44	120.80
2	A	2712	C	C6-N1-C2	-6.13	117.85	120.30
2	A	719	C	C2-N1-C1'	6.12	125.53	118.80
2	A	2468	A	P-O3'-C3'	6.11	127.04	119.70
2	A	2838	U	N3-C2-O2	-6.11	117.92	122.20
2	A	437	A	P-O3'-C3'	6.11	127.03	119.70
2	A	272	C	C5-C6-N1	6.06	124.03	121.00
18	T	51	C	O4'-C1'-N1	6.06	113.05	108.20
1	R	351	TYR	CB-CG-CD1	-6.06	117.36	121.00
2	A	2511	A	C4-C5-C6	-6.06	113.97	117.00
2	A	252	C	N1-C2-O2	6.05	122.53	118.90
2	A	981	C	C2-N1-C1'	6.05	125.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	49	A	N1-C6-N6	-6.04	114.98	118.60
2	A	2072	C	C2-N1-C1'	6.03	125.44	118.80
18	T	20	G	P-O3'-C3'	6.00	126.90	119.70
2	A	2631	A	O4'-C1'-N9	5.98	112.98	108.20
1	R	413	SER	CB-CA-C	-5.97	98.76	110.10
2	A	2648	U	N3-C2-O2	-5.96	118.03	122.20
2	A	588	C	C2-N1-C1'	5.95	125.34	118.80
2	A	90	A	P-O3'-C3'	5.95	126.84	119.70
2	A	1368	U	N3-C2-O2	-5.95	118.04	122.20
2	A	2839	C	N1-C2-O2	5.95	122.47	118.90
2	A	288	C	N3-C2-O2	-5.94	117.74	121.90
18	T	72	C	N3-C2-O2	-5.94	117.74	121.90
2	A	1028	C	C2-N1-C1'	5.92	125.31	118.80
2	A	1963	C	C6-N1-C2	-5.91	117.93	120.30
3	B	91	C	C2-N1-C1'	5.91	125.30	118.80
3	B	45	C	N1-C2-O2	5.91	122.44	118.90
1	R	278	TYR	CB-CG-CD2	5.90	124.54	121.00
2	A	183	A	OP1-P-O3'	5.89	118.15	105.20
18	T	22	G	N3-C2-N2	-5.88	115.78	119.90
2	A	1352	U	C6-N1-C1'	-5.87	112.98	121.20
2	A	1515	C	C6-N1-C2	-5.87	117.95	120.30
2	A	962	C	C2-N1-C1'	5.86	125.24	118.80
2	A	2796	C	P-O3'-C3'	5.85	126.72	119.70
2	A	1859	C	C5-C6-N1	5.84	123.92	121.00
2	A	77	U	C2-N1-C1'	5.84	124.71	117.70
2	A	979	U	N1-C2-O2	5.83	126.88	122.80
2	A	1859	C	C6-N1-C2	-5.83	117.97	120.30
2	A	2454	A	P-O3'-C3'	5.82	126.68	119.70
2	A	537	A	P-O3'-C3'	5.81	126.67	119.70
32	i	37	LEU	CA-CB-CG	5.81	128.66	115.30
2	A	945	C	N1-C2-O2	5.80	122.38	118.90
2	A	1794	C	C2-N1-C1'	5.80	125.18	118.80
2	A	1515	C	N3-C2-O2	-5.79	117.84	121.90
3	B	28	C	C6-N1-C2	-5.79	117.98	120.30
2	A	310	C	C2-N1-C1'	5.79	125.17	118.80
2	A	1544	C	N3-C2-O2	-5.79	117.85	121.90
2	A	1246	G	C4-N9-C1'	5.78	134.02	126.50
2	A	1755	C	P-O3'-C3'	5.78	126.63	119.70
3	B	24	C	N1-C2-O2	5.77	122.36	118.90
2	A	482	C	C2-N1-C1'	5.76	125.13	118.80
18	T	21	A	C5-C6-N1	5.75	120.58	117.70
1	R	2	SER	CB-CA-C	5.75	121.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	26	G	N1-C6-O6	-5.75	116.45	119.90
2	A	413	U	N3-C2-O2	-5.74	118.18	122.20
2	A	924	U	N1-C2-O2	5.74	126.82	122.80
18	T	65	U	N3-C2-O2	-5.73	118.19	122.20
2	A	2022	U	N3-C2-O2	-5.73	118.19	122.20
2	A	1069	U	C2-N1-C1'	5.70	124.54	117.70
2	A	1916	U	N1-C2-O2	5.70	126.79	122.80
18	T	44	A	C4-C5-C6	-5.69	114.15	117.00
2	A	1550	C	C2-N1-C1'	5.68	125.05	118.80
2	A	183	A	P-O3'-C3'	5.68	126.52	119.70
2	A	413	U	N1-C2-O2	5.68	126.78	122.80
2	A	549	A	P-O3'-C3'	5.67	126.51	119.70
3	B	19	G	C4-N9-C1'	5.67	133.87	126.50
2	A	104	C	N1-C2-O2	5.66	122.30	118.90
2	A	1437	C	C2-N1-C1'	5.66	125.02	118.80
18	T	71	C	N1-C2-O2	5.65	122.29	118.90
1	R	280	GLY	O-C-N	5.65	131.74	122.70
2	A	2568	C	C6-N1-C2	-5.64	118.05	120.30
2	A	77	U	N1-C2-O2	5.63	126.74	122.80
18	T	9	A	C4-C5-C6	-5.62	114.19	117.00
2	A	2503	C	N1-C2-O2	5.61	122.27	118.90
18	T	65	U	O4'-C1'-N1	5.61	112.69	108.20
2	A	892	U	C2-N1-C1'	5.61	124.43	117.70
1	R	4	ASP	CA-CB-CG	-5.60	101.07	113.40
2	A	899	C	N3-C2-O2	-5.60	117.98	121.90
2	A	2351	A	P-O3'-C3'	5.60	126.42	119.70
2	A	2712	C	C5-C6-N1	5.60	123.80	121.00
2	A	1229	U	N3-C2-O2	-5.60	118.28	122.20
2	A	2781	C	N1-C2-O2	5.59	122.25	118.90
16	Q	94	MET	CA-CB-CG	5.58	122.79	113.30
2	A	1069	U	N3-C2-O2	-5.58	118.30	122.20
2	A	288	C	N1-C2-O2	5.57	122.24	118.90
18	T	53	G	C4-N9-C1'	5.56	133.73	126.50
2	A	1031	C	C2-N1-C1'	5.56	124.91	118.80
2	A	2255	C	N3-C2-O2	-5.55	118.01	121.90
2	A	1368	U	C2-N1-C1'	5.55	124.36	117.70
2	A	1411	U	C2-N1-C1'	5.55	124.36	117.70
18	T	71	C	O4'-C1'-N1	5.55	112.64	108.20
18	T	49	A	C5-C6-N1	5.54	120.47	117.70
2	A	1438	C	P-O3'-C3'	5.54	126.35	119.70
2	A	442	C	C6-N1-C2	-5.54	118.09	120.30
18	T	28	C	C2-N1-C1'	5.53	124.88	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2685	U	N1-C2-O2	5.52	126.67	122.80
2	A	1691	A	C2-N3-C4	5.52	113.36	110.60
2	A	899	C	N1-C2-O2	5.51	122.21	118.90
2	A	2784	C	P-O3'-C3'	5.51	126.31	119.70
18	T	5	C	N3-C2-O2	-5.50	118.05	121.90
2	A	2838	U	N1-C2-O2	5.50	126.65	122.80
1	R	432	LEU	C-N-CA	5.50	135.44	121.70
2	A	252	C	C2-N1-C1'	5.49	124.84	118.80
2	A	309	U	C2-N1-C1'	5.48	124.28	117.70
1	R	414	ALA	N-CA-C	5.47	125.78	111.00
2	A	234	C	N1-C2-O2	5.47	122.18	118.90
2	A	2072	C	C6-N1-C2	-5.47	118.11	120.30
2	A	1859	C	C2-N1-C1'	5.46	124.80	118.80
2	A	2010	A	N3-C4-C5	-5.45	122.99	126.80
2	A	2816	C	C2-N1-C1'	5.44	124.79	118.80
2	A	1622	C	C6-N1-C2	-5.42	118.13	120.30
8	G	72	LEU	CA-CB-CG	5.42	127.75	115.30
2	A	1803	C	C2-N1-C1'	5.41	124.76	118.80
1	R	432	LEU	CB-CA-C	-5.41	99.92	110.20
2	A	1916	U	N3-C2-O2	-5.41	118.41	122.20
18	T	25	C	O4'-C1'-N1	5.41	112.53	108.20
2	A	2480	A	C6-C5-N7	5.40	136.08	132.30
18	T	6	C	N1-C2-O2	5.40	122.14	118.90
18	T	69	C	N1-C2-O2	5.39	122.13	118.90
2	A	662	U	P-O3'-C3'	5.38	126.16	119.70
2	A	195	C	C6-N1-C2	-5.37	118.15	120.30
3	B	35	C	N3-C2-O2	-5.37	118.14	121.90
2	A	2334	U	P-O3'-C3'	5.37	126.14	119.70
2	A	1622	C	N1-C2-O2	5.36	122.12	118.90
2	A	2283	C	O4'-C1'-N1	5.36	112.49	108.20
18	T	48	C	N3-C2-O2	-5.36	118.15	121.90
2	A	1963	C	N1-C2-O2	5.36	122.11	118.90
18	T	53	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	924	U	N3-C2-O2	-5.35	118.45	122.20
2	A	924	U	C2-N1-C1'	5.34	124.11	117.70
2	A	442	C	C6-N1-C1'	-5.34	114.39	120.80
18	T	62	C	N3-C4-N4	-5.34	114.27	118.00
2	A	2323	C	C2-N1-C1'	5.33	124.67	118.80
2	A	1622	C	C6-N1-C1'	-5.33	114.41	120.80
2	A	2489	U	C5'-C4'-C3'	-5.31	107.51	116.00
2	A	484	C	C6-N1-C2	-5.30	118.18	120.30
2	A	1916	U	C2-N1-C1'	5.30	124.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	77	U	N3-C2-O2	-5.30	118.49	122.20
18	T	60	C	C2-N1-C1'	5.29	124.62	118.80
2	A	252	C	C6-N1-C2	-5.29	118.18	120.30
2	A	2283	C	N3-C2-O2	-5.29	118.19	121.90
2	A	2839	C	N3-C2-O2	-5.29	118.20	121.90
2	A	229	A	P-O3'-C3'	5.29	126.04	119.70
2	A	1657	C	C2-N1-C1'	5.28	124.61	118.80
13	M	137	ILE	C-N-CA	5.28	133.38	122.30
1	R	412	SER	O-C-N	-5.27	114.27	122.70
3	B	19	G	OP1-P-O3'	5.26	116.78	105.20
2	A	1539	C	N1-C2-O2	5.26	122.06	118.90
2	A	2010	A	N3-C4-N9	5.25	131.60	127.40
2	A	1411	U	N1-C2-O2	5.25	126.47	122.80
2	A	413	U	C2-N1-C1'	5.25	123.99	117.70
18	T	70	U	C3'-C2'-C1'	5.24	105.69	101.50
2	A	228	C	C6-N1-C2	-5.23	118.21	120.30
2	A	1353	C	N1-C2-O2	5.23	122.04	118.90
2	A	2513	G	C5'-C4'-C3'	-5.23	107.63	116.00
2	A	837	U	P-O3'-C3'	5.23	125.97	119.70
2	A	1281	C	C6-N1-C1'	-5.23	114.53	120.80
1	R	4	ASP	CB-CA-C	5.22	120.85	110.40
2	A	310	C	N1-C2-O2	5.22	122.03	118.90
18	T	25	C	N1-C2-O2	5.22	122.03	118.90
2	A	2492	C	C2-N1-C1'	5.22	124.54	118.80
2	A	1352	U	C5-C6-N1	5.22	125.31	122.70
2	A	195	C	N3-C2-O2	-5.21	118.25	121.90
2	A	979	U	N3-C2-O2	-5.21	118.55	122.20
18	T	26	G	C5-C6-N1	5.21	114.11	111.50
2	A	936	C	OP1-P-O3'	5.21	116.66	105.20
2	A	2632	G	N1-C6-O6	-5.21	116.78	119.90
2	A	1544	C	C6-N1-C2	-5.20	118.22	120.30
2	A	228	C	C2-N1-C1'	5.19	124.51	118.80
2	A	2631	A	C4-C5-C6	-5.19	114.41	117.00
1	R	433	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	A	1544	C	C2-N1-C1'	5.19	124.50	118.80
2	A	2479	A	C5-C6-N1	5.18	120.29	117.70
2	A	1937	C	N1-C2-O2	5.17	122.00	118.90
18	T	15	G	N1-C6-O6	-5.17	116.80	119.90
2	A	1095	C	N1-C2-O2	5.16	122.00	118.90
2	A	1437	C	C6-N1-C2	-5.16	118.23	120.30
3	B	35	C	C6-N1-C2	-5.16	118.23	120.30
2	A	1229	U	C5-C6-N1	5.16	125.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2337	G	N3-C4-C5	-5.16	126.02	128.60
1	R	337	TYR	CD1-CE1-CZ	-5.15	115.16	119.80
2	A	1937	C	C2-N1-C1'	5.15	124.47	118.80
2	A	158	C	C2-N1-C1'	5.15	124.46	118.80
2	A	1028	C	N3-C2-O2	-5.14	118.30	121.90
18	T	72	C	C6-N1-C2	-5.14	118.24	120.30
2	A	831	U	N3-C2-O2	-5.14	118.60	122.20
2	A	1246	G	C8-N9-C1'	-5.14	120.32	127.00
2	A	1794	C	C6-N1-C2	-5.14	118.24	120.30
2	A	271	C	C2-N1-C1'	5.14	124.45	118.80
2	A	1550	C	N3-C2-O2	-5.14	118.30	121.90
1	R	279	PHE	CZ-CE2-CD2	-5.14	113.94	120.10
2	A	785	C	P-O3'-C3'	5.14	125.86	119.70
5	D	55	ASP	CB-CG-OD1	5.13	122.92	118.30
10	J	29	LEU	CA-CB-CG	5.13	127.11	115.30
3	B	79	C	N3-C2-O2	-5.13	118.31	121.90
2	A	159	U	N1-C2-O2	5.12	126.39	122.80
2	A	1691	A	C4-N9-C1'	5.12	135.52	126.30
2	A	1963	C	C5-C6-N1	5.12	123.56	121.00
2	A	2323	C	N1-C2-O2	5.12	121.97	118.90
2	A	2820	U	C2-N1-C1'	5.12	123.84	117.70
3	B	95	U	N1-C2-O2	5.12	126.38	122.80
1	R	431	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
18	T	70	U	N3-C2-O2	-5.11	118.62	122.20
2	A	309	U	N1-C2-O2	5.11	126.38	122.80
2	A	482	C	N1-C2-O2	5.10	121.96	118.90
2	A	1622	C	C5-C6-N1	5.10	123.55	121.00
2	A	2267	G	P-O3'-C3'	5.10	125.82	119.70
22	X	23	ASN	C-N-CA	5.08	134.41	121.70
2	A	2632	G	C5-C6-N1	5.08	114.04	111.50
2	A	914	C	C6-N1-C1'	-5.08	114.71	120.80
2	A	1368	U	N1-C2-O2	5.08	126.35	122.80
2	A	2511	A	C6-C5-N7	5.07	135.85	132.30
2	A	1362	G	OP1-P-O3'	5.07	116.35	105.20
2	A	2035	C	C2-N1-C1'	5.07	124.38	118.80
18	T	74	C	C4'-C3'-O3'	5.07	123.14	113.00
2	A	1333	C	C2-N1-C1'	5.07	124.37	118.80
2	A	2092	C	C2-N3-C4	-5.07	117.37	119.90
18	T	51	C	N1-C2-O2	5.07	121.94	118.90
2	A	203	U	C5-C6-N1	5.06	125.23	122.70
2	A	2480	A	O4'-C1'-N9	5.06	112.25	108.20
18	T	45	G	N3-C4-C5	-5.05	126.07	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1970	C	N3-C2-O2	-5.05	118.36	121.90
3	B	19	G	P-O3'-C3'	5.05	125.76	119.70
2	A	570	C	C2-N1-C1'	5.05	124.36	118.80
2	A	1148	C	N1-C2-O2	5.05	121.93	118.90
2	A	405	U	P-O3'-C3'	5.04	125.75	119.70
3	B	19	G	C8-N9-C1'	-5.04	120.45	127.00
2	A	442	C	N1-C2-O2	5.04	121.92	118.90
2	A	898	U	N3-C2-O2	-5.04	118.67	122.20
2	A	1770	C	C2-N1-C1'	5.03	124.34	118.80
2	A	261	C	N3-C2-O2	-5.03	118.38	121.90
18	T	72	C	C4'-C3'-C2'	-5.03	97.57	102.60
2	A	1948	A	P-O3'-C3'	5.03	125.73	119.70
2	A	159	U	N3-C2-O2	-5.02	118.68	122.20
1	R	434	PRO	CA-CB-CG	-5.02	94.46	104.00
2	A	1281	C	O4'-C1'-N1	5.02	112.22	108.20
3	B	95	U	C2-N1-C1'	5.02	123.72	117.70
3	B	19	G	N3-C4-N9	5.02	129.01	126.00
2	A	422	C	C2-N1-C1'	5.01	124.32	118.80
2	A	2092	C	O4'-C1'-N1	5.01	112.21	108.20
2	A	2110	C	C2-N1-C1'	5.01	124.31	118.80
18	T	12	U	N3-C2-O2	-5.01	118.69	122.20
2	A	383	U	N3-C2-O2	-5.01	118.69	122.20
2	A	2255	C	C6-N1-C2	-5.01	118.30	120.30
2	A	2093	C	C4'-C3'-C2'	-5.01	97.59	102.60
1	R	280	GLY	CA-C-N	-5.00	106.19	117.20
2	A	2585	C	N3-C2-O2	-5.00	118.40	121.90
18	T	64	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2280	G	Sidechain
2	A	2281	G	Sidechain
2	A	2282	G	Sidechain
2	A	2511	A	Sidechain
2	A	2513	G	Sidechain
2	A	2614	U	Sidechain
2	A	2631	A	Sidechain
4	C	154	LEU	Peptide
9	I	22	PRO	Peptide
1	R	2	SER	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	R	279	PHE	Peptide
1	R	281	LYS	Peptide
1	R	3	PHE	Sidechain
1	R	412	SER	Mainchain,Peptide
1	R	413	SER	Peptide
1	R	414	ALA	Peptide
1	R	415	SER	Peptide
1	R	430	LYS	Mainchain
1	R	431	TYR	Sidechain,Peptide
1	R	432	LEU	Peptide
1	R	433	ARG	Sidechain
18	T	10	G	Sidechain
18	T	14	A	Sidechain
18	T	21	A	Sidechain
18	T	25	C	Sidechain
18	T	26	G	Sidechain
18	T	3	G	Sidechain
18	T	45	G	Sidechain
18	T	46	G	Sidechain
18	T	52	G	Sidechain
18	T	6	C	Sidechain
18	T	67	G	Sidechain
18	T	68	G	Sidechain
18	T	71	C	Sidechain
18	T	72	C	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	R	431/570 (76%)	397 (92%)	22 (5%)	12 (3%)	5	25
4	C	273/277 (99%)	261 (96%)	12 (4%)	0	100	100
5	D	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
6	E	203/207 (98%)	189 (93%)	14 (7%)	0	100	100
7	F	176/179 (98%)	163 (93%)	13 (7%)	0	100	100
8	G	173/179 (97%)	166 (96%)	7 (4%)	0	100	100
9	I	131/141 (93%)	126 (96%)	5 (4%)	0	100	100
10	J	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
12	L	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
13	M	136/144 (94%)	133 (98%)	3 (2%)	0	100	100
14	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
15	O	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
16	Q	115/119 (97%)	110 (96%)	5 (4%)	0	100	100
17	S	107/113 (95%)	94 (88%)	13 (12%)	0	100	100
19	U	98/103 (95%)	87 (89%)	11 (11%)	0	100	100
20	V	80/94 (85%)	80 (100%)	0	0	100	100
21	W	5/7 (71%)	5 (100%)	0	0	100	100
22	X	56/62 (90%)	51 (91%)	5 (9%)	0	100	100
23	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
24	a	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
25	b	52/59 (88%)	48 (92%)	4 (8%)	0	100	100
26	c	46/49 (94%)	46 (100%)	0	0	100	100
27	d	42/44 (96%)	42 (100%)	0	0	100	100
28	e	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
29	f	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
30	g	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
31	h	91/95 (96%)	87 (96%)	4 (4%)	0	100	100
32	i	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
All	All	3485/3749 (93%)	3292 (94%)	181 (5%)	12 (0%)	44	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	414	ALA
1	R	431	TYR
1	R	432	LEU
1	R	433	ARG
1	R	223	LEU
1	R	413	SER
1	R	429	GLY
1	R	366	ASN
1	R	416	PRO
1	R	164	LEU
1	R	176	ALA
1	R	415	SER

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	R	383/505 (76%)	348 (91%)	35 (9%)	9 33
4	C	223/225 (99%)	223 (100%)	0	100 100
5	D	168/170 (99%)	168 (100%)	0	100 100
6	E	169/170 (99%)	169 (100%)	0	100 100
7	F	153/154 (99%)	151 (99%)	2 (1%)	69 87
8	G	148/151 (98%)	148 (100%)	0	100 100
9	I	103/110 (94%)	103 (100%)	0	100 100
10	J	120/123 (98%)	120 (100%)	0	100 100
11	K	101/101 (100%)	101 (100%)	0	100 100
12	L	110/110 (100%)	108 (98%)	2 (2%)	59 82
13	M	111/116 (96%)	111 (100%)	0	100 100
14	N	99/100 (99%)	99 (100%)	0	100 100
15	O	93/93 (100%)	93 (100%)	0	100 100
16	Q	96/98 (98%)	95 (99%)	1 (1%)	76 90
17	S	90/93 (97%)	90 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	U	84/87 (97%)	84 (100%)	0	100 100
20	V	64/74 (86%)	64 (100%)	0	100 100
22	X	47/50 (94%)	46 (98%)	1 (2%)	53 79
23	Z	52/53 (98%)	52 (100%)	0	100 100
24	a	99/100 (99%)	99 (100%)	0	100 100
25	b	48/53 (91%)	48 (100%)	0	100 100
26	c	46/47 (98%)	46 (100%)	0	100 100
27	d	39/39 (100%)	38 (97%)	1 (3%)	46 74
28	e	54/56 (96%)	54 (100%)	0	100 100
29	f	34/35 (97%)	34 (100%)	0	100 100
30	g	83/84 (99%)	83 (100%)	0	100 100
31	h	84/85 (99%)	84 (100%)	0	100 100
32	i	56/57 (98%)	56 (100%)	0	100 100
All	All	2957/3139 (94%)	2915 (99%)	42 (1%)	68 86

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	3	PHE
1	R	4	ASP
1	R	26	LYS
1	R	162	TYR
1	R	163	LYS
1	R	175	GLU
1	R	179	ASP
1	R	180	ASP
1	R	220	LYS
1	R	222	THR
1	R	223	LEU
1	R	236	GLU
1	R	238	ARG
1	R	239	PHE
1	R	263	GLU
1	R	265	ARG
1	R	279	PHE
1	R	281	LYS
1	R	336	LEU

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Mol	Chain	Res	Type
1	R	340	LYS
1	R	344	LYS
1	R	351	TYR
1	R	359	ILE
1	R	366	ASN
1	R	379	LYS
1	R	413	SER
1	R	417	ARG
1	R	419	ILE
1	R	420	SER
1	R	421	GLU
1	R	428	GLU
1	R	430	LYS
1	R	431	TYR
1	R	432	LEU
1	R	434	PRO
7	F	110	ARG
7	F	115	ARG
12	L	70	ASN
12	L	116	LYS
16	Q	92	ARG
22	X	58	LYS
27	d	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	335	ASN
1	R	366	ASN
1	R	372	ASN
1	R	381	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	T	75/76 (98%)	23 (30%)	6 (8%)
2	A	2916/2918 (99%)	643 (22%)	44 (1%)
3	B	111/112 (99%)	30 (27%)	2 (1%)
All	All	3102/3106 (99%)	696 (22%)	52 (1%)

All (696) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	13	A
2	A	15	G
2	A	31	C
2	A	33	U
2	A	34	U
2	A	35	G
2	A	39	C
2	A	44	A
2	A	45	G
2	A	46	C
2	A	51	G
2	A	59	G
2	A	63	G
2	A	71	A
2	A	75	G
2	A	76	C
2	A	87	U
2	A	91	A
2	A	94	A
2	A	101	G
2	A	117	A
2	A	118	A
2	A	119	U
2	A	124	A
2	A	125	A
2	A	130	A
2	A	133	A
2	A	159	U
2	A	162	A
2	A	163	U
2	A	164	U
2	A	176	A
2	A	177	G
2	A	178	A
2	A	183	A
2	A	184	G
2	A	188	C
2	A	199	A
2	A	202	A
2	A	203	U
2	A	207	A
2	A	216	A

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Mol	Chain	Res	Type
2	A	219	A
2	A	225	A
2	A	226	A
2	A	227	G
2	A	230	A
2	A	231	A
2	A	233	G
2	A	236	A
2	A	245	G
2	A	251	G
2	A	252	C
2	A	253	G
2	A	258	A
2	A	267	C
2	A	268	A
2	A	269	G
2	A	270	C
2	A	272	C
2	A	275	A
2	A	282	G
2	A	289	C
2	A	290	U
2	A	291	C
2	A	295	G
2	A	298	U
2	A	299	U
2	A	300	G
2	A	301	U
2	A	302	A
2	A	310	C
2	A	312	G
2	A	313	U
2	A	314	A
2	A	315	C
2	A	321	U
2	A	322	A
2	A	324	A
2	A	325	A
2	A	331	C
2	A	337	A
2	A	345	A
2	A	346	G

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Mol	Chain	Res	Type
2	A	348	U
2	A	352	G
2	A	354	A
2	A	355	A
2	A	360	C
2	A	367	G
2	A	373	A
2	A	374	A
2	A	376	A
2	A	378	C
2	A	382	G
2	A	386	U
2	A	387	C
2	A	390	A
2	A	392	C
2	A	393	U
2	A	394	U
2	A	405	U
2	A	406	G
2	A	410	G
2	A	411	G
2	A	414	C
2	A	417	G
2	A	418	A
2	A	430	C
2	A	432	C
2	A	433	G
2	A	434	U
2	A	435	G
2	A	438	A
2	A	443	G
2	A	444	U
2	A	459	A
2	A	474	U
2	A	478	U
2	A	482	C
2	A	483	C
2	A	484	C
2	A	485	U
2	A	490	A
2	A	494	A
2	A	498	U

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Mol	Chain	Res	Type
2	A	502	C
2	A	503	C
2	A	504	A
2	A	514	G
2	A	528	G
2	A	538	A
2	A	548	A
2	A	550	G
2	A	551	A
2	A	552	G
2	A	554	U
2	A	555	C
2	A	556	C
2	A	558	G
2	A	562	C
2	A	564	G
2	A	572	A
2	A	576	G
2	A	577	U
2	A	578	A
2	A	592	A
2	A	593	A
2	A	594	C
2	A	595	G
2	A	607	G
2	A	617	G
2	A	619	A
2	A	631	G
2	A	647	A
2	A	648	G
2	A	649	G
2	A	650	U
2	A	651	U
2	A	660	G
2	A	663	G
2	A	666	G
2	A	667	A
2	A	673	A
2	A	674	G
2	A	680	G
2	A	683	A
2	A	684	G

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Mol	Chain	Res	Type
2	A	691	U
2	A	700	U
2	A	701	G
2	A	713	G
2	A	715	A
2	A	717	A
2	A	718	C
2	A	719	C
2	A	733	U
2	A	773	G
2	A	777	C
2	A	781	A
2	A	782	A
2	A	786	A
2	A	792	G
2	A	794	U
2	A	795	G
2	A	797	A
2	A	822	G
2	A	823	G
2	A	824	G
2	A	829	A
2	A	831	U
2	A	832	G
2	A	836	A
2	A	837	U
2	A	838	C
2	A	839	G
2	A	852	G
2	A	853	C
2	A	858	U
2	A	859	C
2	A	866	A
2	A	874	U
2	A	875	U
2	A	877	G
2	A	892	U
2	A	893	A
2	A	895	G
2	A	913	A
2	A	914	C
2	A	924	U

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Mol	Chain	Res	Type
2	A	925	A
2	A	927	G
2	A	928	G
2	A	931	C
2	A	935	A
2	A	937	C
2	A	942	U
2	A	943	A
2	A	944	C
2	A	948	A
2	A	951	C
2	A	952	A
2	A	954	U
2	A	957	A
2	A	959	C
2	A	961	C
2	A	962	C
2	A	964	A
2	A	973	G
2	A	977	U
2	A	978	A
2	A	981	C
2	A	987	A
2	A	988	G
2	A	990	C
2	A	991	A
2	A	992	G
2	A	999	A
2	A	1005	A
2	A	1007	G
2	A	1019	A
2	A	1020	A
2	A	1025	A
2	A	1026	A
2	A	1027	A
2	A	1028	C
2	A	1029	A
2	A	1031	C
2	A	1034	A
2	A	1037	C
2	A	1055	A
2	A	1058	U

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Mol	Chain	Res	Type
2	A	1059	A
2	A	1068	G
2	A	1072	A
2	A	1079	U
2	A	1091	U
2	A	1092	A
2	A	1093	G
2	A	1102	G
2	A	1104	U
2	A	1105	G
2	A	1107	U
2	A	1108	G
2	A	1110	C
2	A	1111	U
2	A	1112	U
2	A	1113	A
2	A	1115	A
2	A	1116	A
2	A	1117	G
2	A	1123	A
2	A	1124	C
2	A	1127	U
2	A	1128	U
2	A	1129	U
2	A	1131	A
2	A	1135	G
2	A	1139	G
2	A	1140	U
2	A	1141	A
2	A	1142	A
2	A	1143	U
2	A	1144	A
2	A	1152	G
2	A	1157	A
2	A	1158	G
2	A	1159	U
2	A	1176	U
2	A	1178	U
2	A	1179	A
2	A	1181	C
2	A	1182	G
2	A	1185	G

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Mol	Chain	Res	Type
2	A	1187	U
2	A	1188	A
2	A	1194	A
2	A	1201	A
2	A	1202	A
2	A	1209	G
2	A	1217	U
2	A	1218	U
2	A	1219	C
2	A	1220	G
2	A	1246	G
2	A	1247	G
2	A	1251	U
2	A	1252	G
2	A	1260	A
2	A	1276	G
2	A	1278	G
2	A	1289	U
2	A	1293	A
2	A	1295	U
2	A	1296	G
2	A	1311	G
2	A	1312	A
2	A	1313	A
2	A	1314	A
2	A	1315	G
2	A	1327	U
2	A	1339	A
2	A	1340	A
2	A	1345	U
2	A	1346	A
2	A	1352	U
2	A	1363	G
2	A	1364	C
2	A	1376	G
2	A	1381	A
2	A	1382	G
2	A	1384	C
2	A	1388	A
2	A	1404	A
2	A	1417	A
2	A	1418	U

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Mol	Chain	Res	Type
2	A	1423	A
2	A	1424	A
2	A	1425	C
2	A	1431	G
2	A	1433	U
2	A	1435	U
2	A	1436	U
2	A	1439	U
2	A	1441	U
2	A	1442	A
2	A	1450	C
2	A	1456	A
2	A	1460	G
2	A	1464	A
2	A	1472	G
2	A	1473	A
2	A	1474	C
2	A	1490	A
2	A	1497	G
2	A	1498	U
2	A	1499	A
2	A	1507	U
2	A	1513	U
2	A	1519	C
2	A	1520	A
2	A	1524	A
2	A	1528	U
2	A	1536	A
2	A	1539	C
2	A	1553	A
2	A	1555	A
2	A	1561	G
2	A	1563	G
2	A	1564	C
2	A	1569	A
2	A	1571	G
2	A	1572	G
2	A	1573	C
2	A	1581	A
2	A	1582	U
2	A	1584	U
2	A	1586	G

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Mol	Chain	Res	Type
2	A	1596	U
2	A	1607	C
2	A	1608	A
2	A	1614	A
2	A	1617	A
2	A	1626	U
2	A	1631	A
2	A	1632	G
2	A	1634	U
2	A	1652	C
2	A	1653	A
2	A	1655	A
2	A	1657	C
2	A	1658	G
2	A	1660	C
2	A	1667	A
2	A	1674	G
2	A	1679	A
2	A	1691	A
2	A	1692	U
2	A	1693	C
2	A	1696	G
2	A	1697	A
2	A	1705	C
2	A	1709	A
2	A	1712	G
2	A	1719	G
2	A	1727	A
2	A	1744	G
2	A	1745	A
2	A	1752	G
2	A	1756	U
2	A	1757	G
2	A	1758	U
2	A	1770	C
2	A	1774	A
2	A	1777	G
2	A	1778	A
2	A	1779	G
2	A	1780	C
2	A	1781	C
2	A	1782	G

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Mol	Chain	Res	Type
2	A	1785	G
2	A	1788	A
2	A	1791	A
2	A	1792	G
2	A	1793	G
2	A	1802	A
2	A	1805	G
2	A	1809	A
2	A	1811	C
2	A	1829	C
2	A	1830	G
2	A	1845	A
2	A	1858	A
2	A	1877	A
2	A	1881	U
2	A	1895	A
2	A	1898	G
2	A	1901	A
2	A	1902	G
2	A	1912	G
2	A	1913	A
2	A	1918	A
2	A	1935	G
2	A	1941	A
2	A	1949	C
2	A	1958	G
2	A	1959	G
2	A	1966	A
2	A	1968	U
2	A	1972	U
2	A	1984	U
2	A	1990	C
2	A	1993	G
2	A	1996	C
2	A	1999	A
2	A	2000	A
2	A	2001	G
2	A	2011	U
2	A	2020	U
2	A	2021	G
2	A	2022	U
2	A	2024	U

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Mol	Chain	Res	Type
2	A	2026	A
2	A	2050	G
2	A	2052	A
2	A	2060	A
2	A	2061	G
2	A	2062	A
2	A	2068	G
2	A	2072	C
2	A	2084	C
2	A	2085	G
2	A	2088	A
2	A	2089	A
2	A	2090	G
2	A	2091	A
2	A	2098	G
2	A	2110	C
2	A	2111	A
2	A	2121	U
2	A	2123	A
2	A	2140	U
2	A	2142	C
2	A	2143	A
2	A	2145	G
2	A	2147	U
2	A	2149	G
2	A	2155	A
2	A	2156	G
2	A	2157	C
2	A	2161	G
2	A	2162	G
2	A	2165	A
2	A	2175	C
2	A	2176	A
2	A	2177	G
2	A	2187	A
2	A	2195	G
2	A	2197	G
2	A	2200	A
2	A	2232	G
2	A	2233	C
2	A	2235	G
2	A	2240	U

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Mol	Chain	Res	Type
2	A	2241	A
2	A	2243	C
2	A	2254	A
2	A	2255	C
2	A	2267	G
2	A	2268	G
2	A	2308	G
2	A	2311	G
2	A	2312	C
2	A	2315	A
2	A	2317	A
2	A	2333	G
2	A	2334	U
2	A	2335	U
2	A	2336	G
2	A	2337	G
2	A	2338	A
2	A	2345	U
2	A	2346	C
2	A	2348	C
2	A	2349	A
2	A	2350	G
2	A	2351	A
2	A	2352	G
2	A	2356	A
2	A	2357	A
2	A	2363	C
2	A	2364	A
2	A	2374	G
2	A	2377	U
2	A	2379	C
2	A	2390	A
2	A	2408	G
2	A	2411	G
2	A	2412	G
2	A	2414	C
2	A	2420	G
2	A	2431	U
2	A	2435	C
2	A	2436	A
2	A	2454	A
2	A	2455	A

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Mol	Chain	Res	Type
2	A	2457	G
2	A	2458	G
2	A	2459	A
2	A	2464	A
2	A	2468	A
2	A	2469	C
2	A	2470	C
2	A	2476	G
2	A	2477	A
2	A	2486	U
2	A	2488	A
2	A	2502	U
2	A	2505	A
2	A	2507	A
2	A	2519	G
2	A	2523	G
2	A	2527	C
2	A	2528	C
2	A	2531	G
2	A	2532	A
2	A	2534	G
2	A	2535	U
2	A	2542	A
2	A	2549	C
2	A	2558	G
2	A	2564	G
2	A	2572	G
2	A	2577	G
2	A	2583	U
2	A	2593	A
2	A	2594	A
2	A	2595	A
2	A	2596	G
2	A	2598	G
2	A	2601	A
2	A	2607	G
2	A	2611	G
2	A	2619	A
2	A	2631	A
2	A	2632	G
2	A	2638	U
2	A	2639	C

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Mol	Chain	Res	Type
2	A	2642	U
2	A	2644	U
2	A	2648	U
2	A	2658	A
2	A	2659	G
2	A	2675	C
2	A	2676	U
2	A	2683	A
2	A	2702	G
2	A	2710	C
2	A	2711	G
2	A	2714	G
2	A	2717	G
2	A	2718	U
2	A	2720	C
2	A	2743	G
2	A	2754	A
2	A	2755	U
2	A	2762	A
2	A	2764	G
2	A	2768	U
2	A	2773	G
2	A	2777	A
2	A	2779	A
2	A	2785	U
2	A	2786	A
2	A	2794	A
2	A	2795	G
2	A	2797	C
2	A	2799	C
2	A	2804	A
2	A	2807	A
2	A	2808	U
2	A	2813	U
2	A	2818	C
2	A	2819	A
2	A	2820	U
2	A	2825	C
2	A	2826	A
2	A	2828	G
2	A	2830	A
2	A	2845	A

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Mol	Chain	Res	Type
2	A	2855	G
2	A	2858	U
2	A	2859	G
2	A	2860	A
2	A	2861	U
2	A	2874	G
2	A	2897	G
2	A	2898	A
2	A	2899	C
2	A	2905	C
2	A	2908	A
2	A	2918	G
2	A	2921	U
3	B	10	G
3	B	11	A
3	B	12	U
3	B	13	A
3	B	14	G
3	B	19	G
3	B	20	A
3	B	23	U
3	B	28	C
3	B	33	U
3	B	38	U
3	B	39	A
3	B	40	C
3	B	41	C
3	B	42	G
3	B	48	G
3	B	49	G
3	B	51	A
3	B	54	U
3	B	55	A
3	B	59	U
3	B	60	C
3	B	64	A
3	B	85	U
3	B	86	U
3	B	87	U
3	B	88	C
3	B	97	A
3	B	107	G

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Mol	Chain	Res	Type
3	B	110	G
18	T	16	C
18	T	17	U
18	T	18	G
18	T	19	G
18	T	20	G
18	T	34	U
18	T	36	C
18	T	38	C
18	T	41	A
18	T	44	A
18	T	45	G
18	T	46	G
18	T	48	C
18	T	53	G
18	T	55	U
18	T	57	G
18	T	65	U
18	T	66	A
18	T	67	G
18	T	70	U
18	T	71	C
18	T	73	A
18	T	74	C

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	12	A
2	A	43	G
2	A	58	G
2	A	90	A
2	A	175	G
2	A	183	A
2	A	229	A
2	A	288	C
2	A	377	G
2	A	405	U
2	A	437	A
2	A	537	A
2	A	549	A
2	A	649	G

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Mol	Chain	Res	Type
2	A	662	U
2	A	683	A
2	A	717	A
2	A	785	C
2	A	837	U
2	A	936	C
2	A	1111	U
2	A	1245	G
2	A	1250	G
2	A	1351	U
2	A	1362	G
2	A	1438	C
2	A	1595	U
2	A	1630	G
2	A	1652	C
2	A	1755	C
2	A	1779	G
2	A	1784	A
2	A	1948	A
2	A	2267	G
2	A	2334	U
2	A	2351	A
2	A	2454	A
2	A	2468	A
2	A	2710	C
2	A	2716	U
2	A	2784	C
2	A	2785	U
2	A	2796	C
2	A	2812	A
3	B	47	C
3	B	59	U
18	T	7	U
18	T	9	A
18	T	65	U
18	T	70	U
18	T	72	C
18	T	74	C

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
2	A	1
1	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1941:A	O3'	1947:A	P	13.89
1	R	429:GLY	C	430:LYS	N	1.65

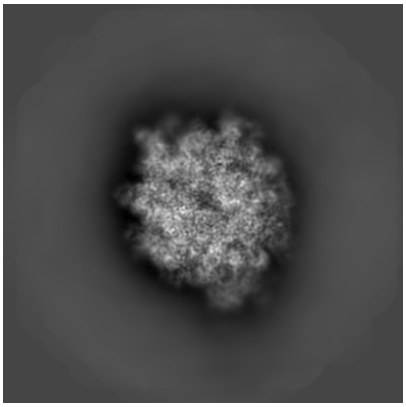
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11864. These allow visual inspection of the internal detail of the map and identification of artifacts.

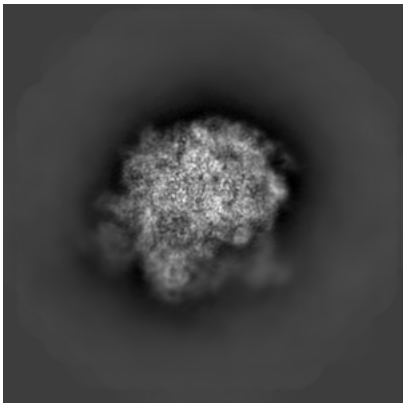
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

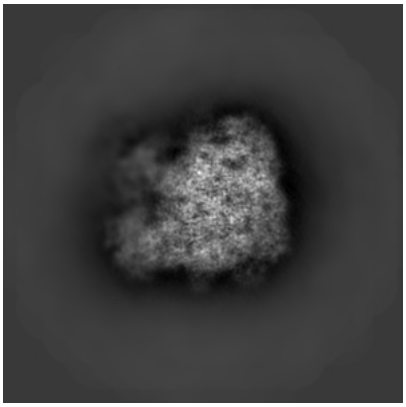
6.1.1 Primary map



X



Y

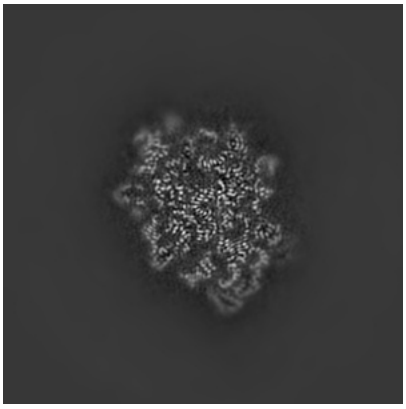


Z

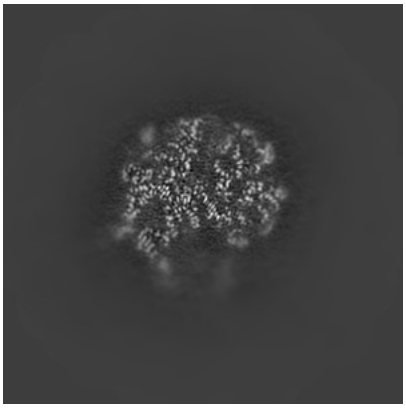
The images above show the map projected in three orthogonal directions.

6.2 Central slices

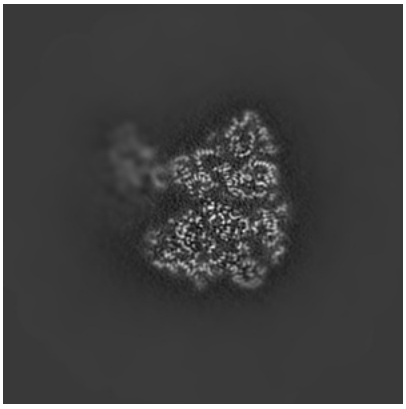
6.2.1 Primary map



X Index: 192



Y Index: 192

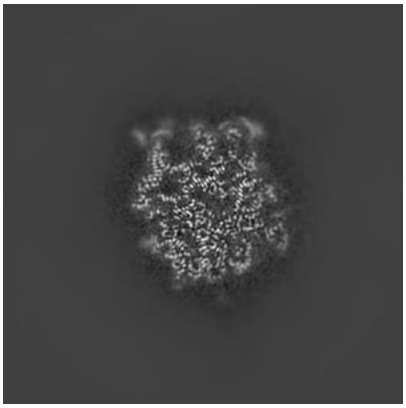


Z Index: 192

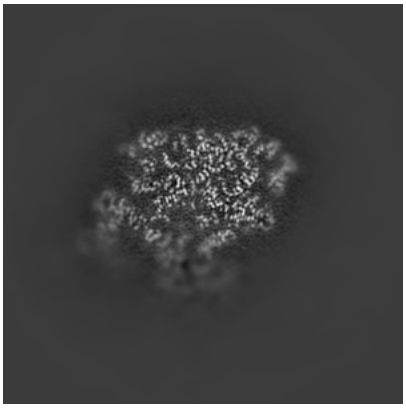
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

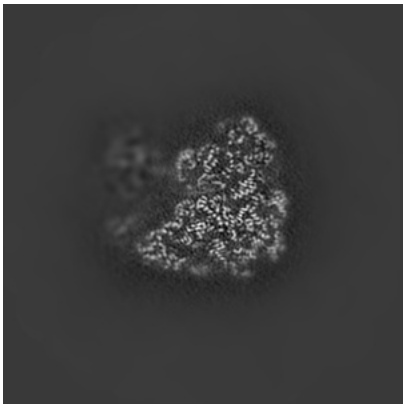
6.3.1 Primary map



X Index: 207



Y Index: 211

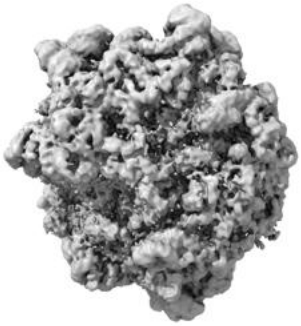


Z Index: 183

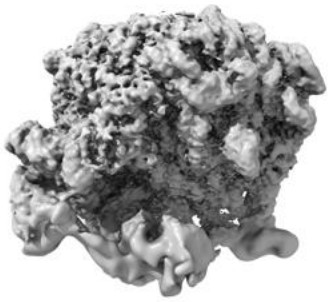
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

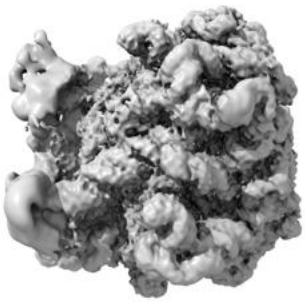
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

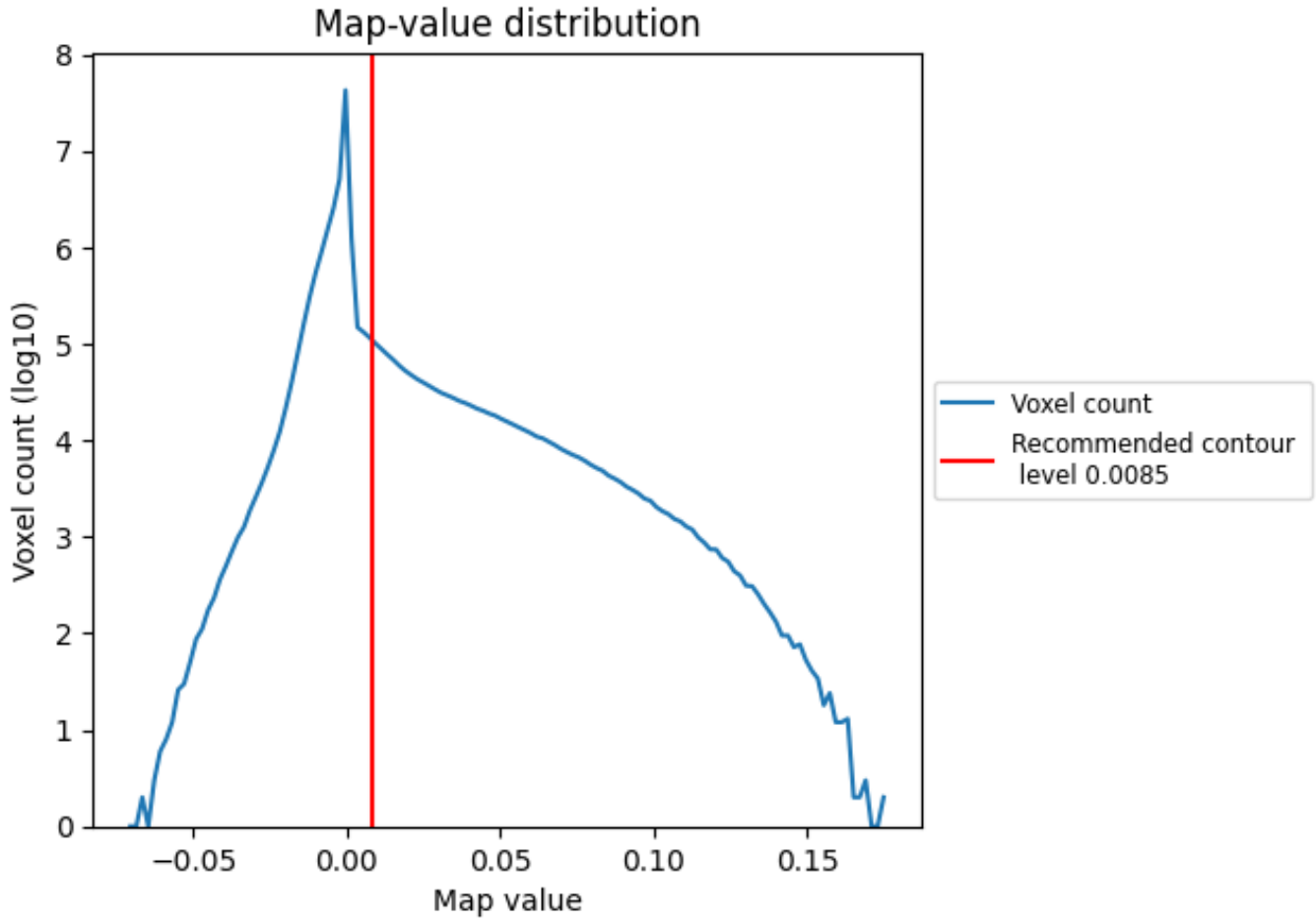
6.5 Mask visualisation (i)

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

7 Map analysis

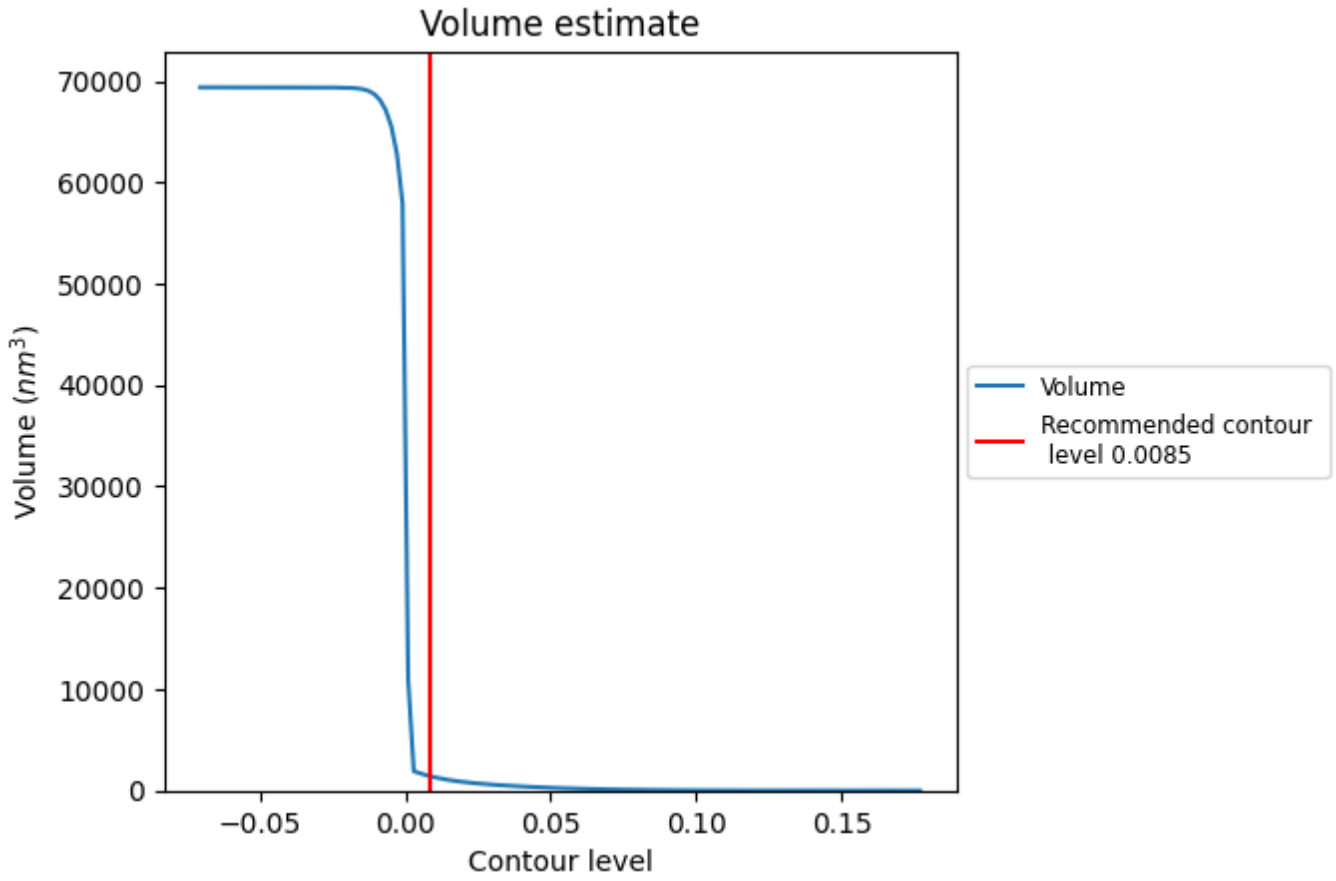
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

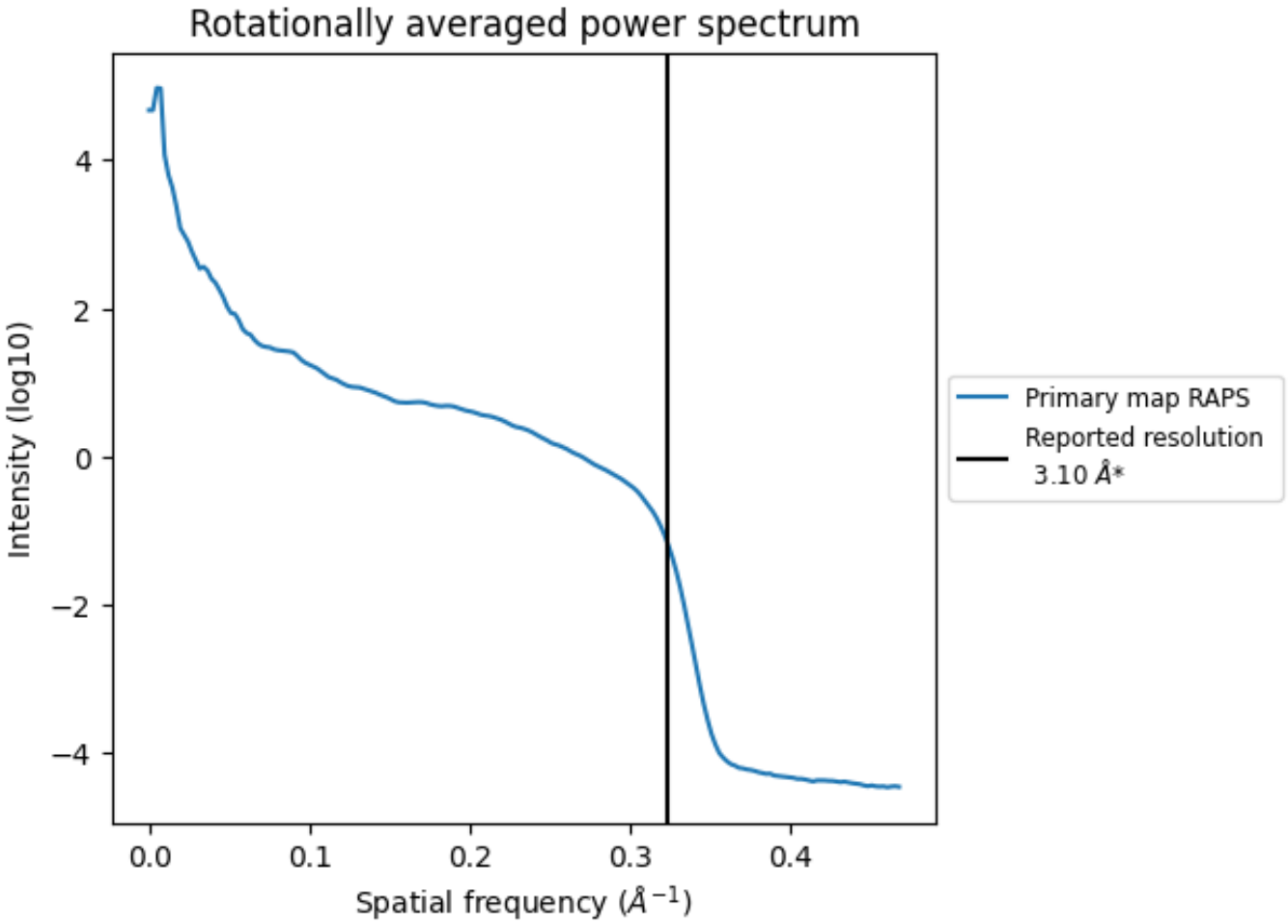
7.2 Volume estimate



The volume at the recommended contour level is 1417 nm^3; this corresponds to an approximate mass of 1280 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 0.323 Å^{-1}

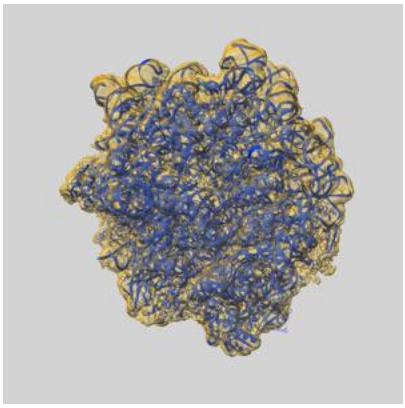
8 Fourier-Shell correlation

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

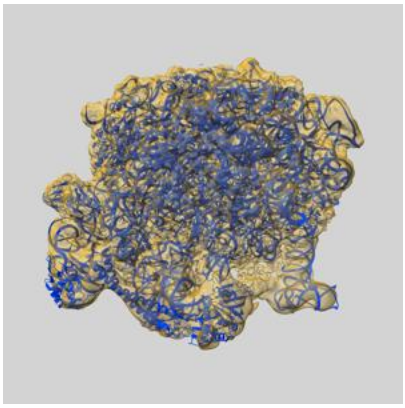
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11864 and PDB model 7AQD. Per-residue inclusion information can be found in section 3 on page 9.

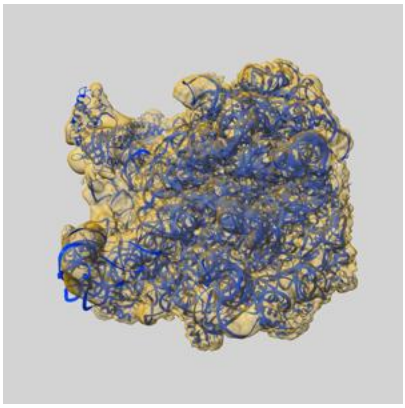
9.1 Map-model overlay



X



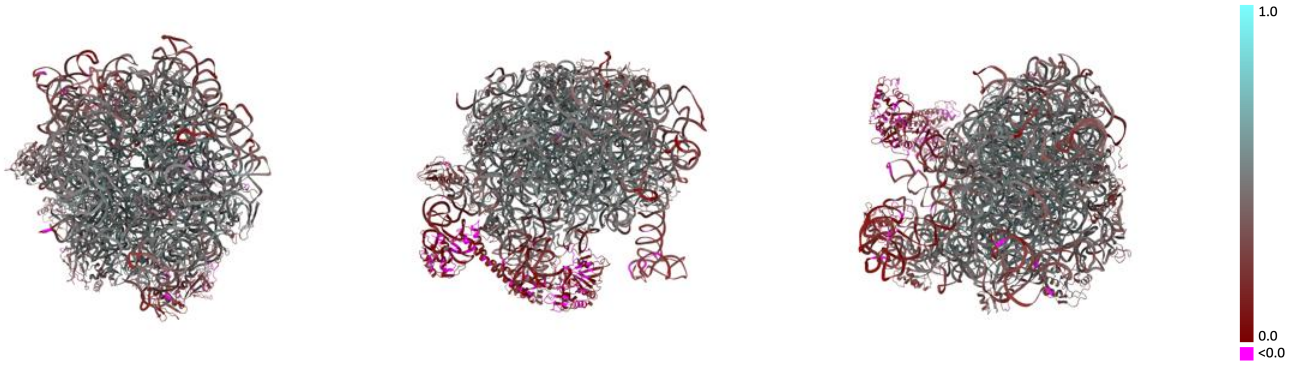
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085 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.

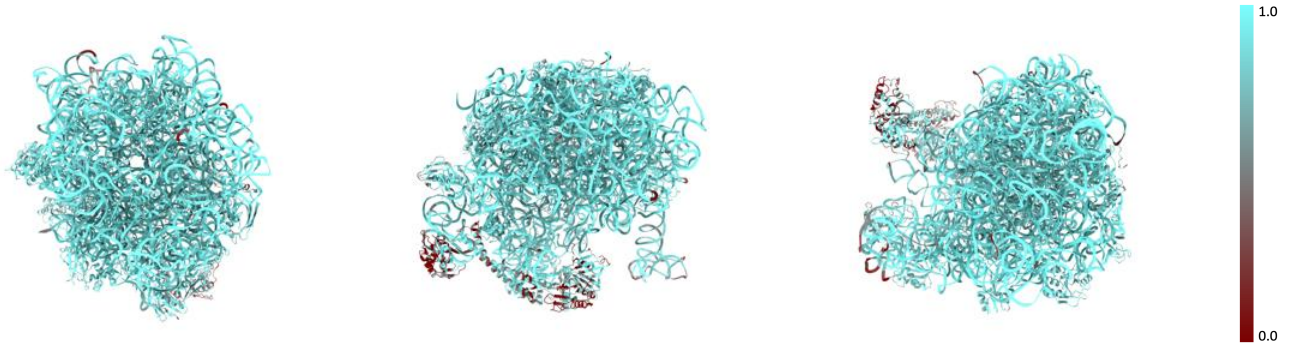
9.2 Q-score mapped to coordinate model (i)



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.

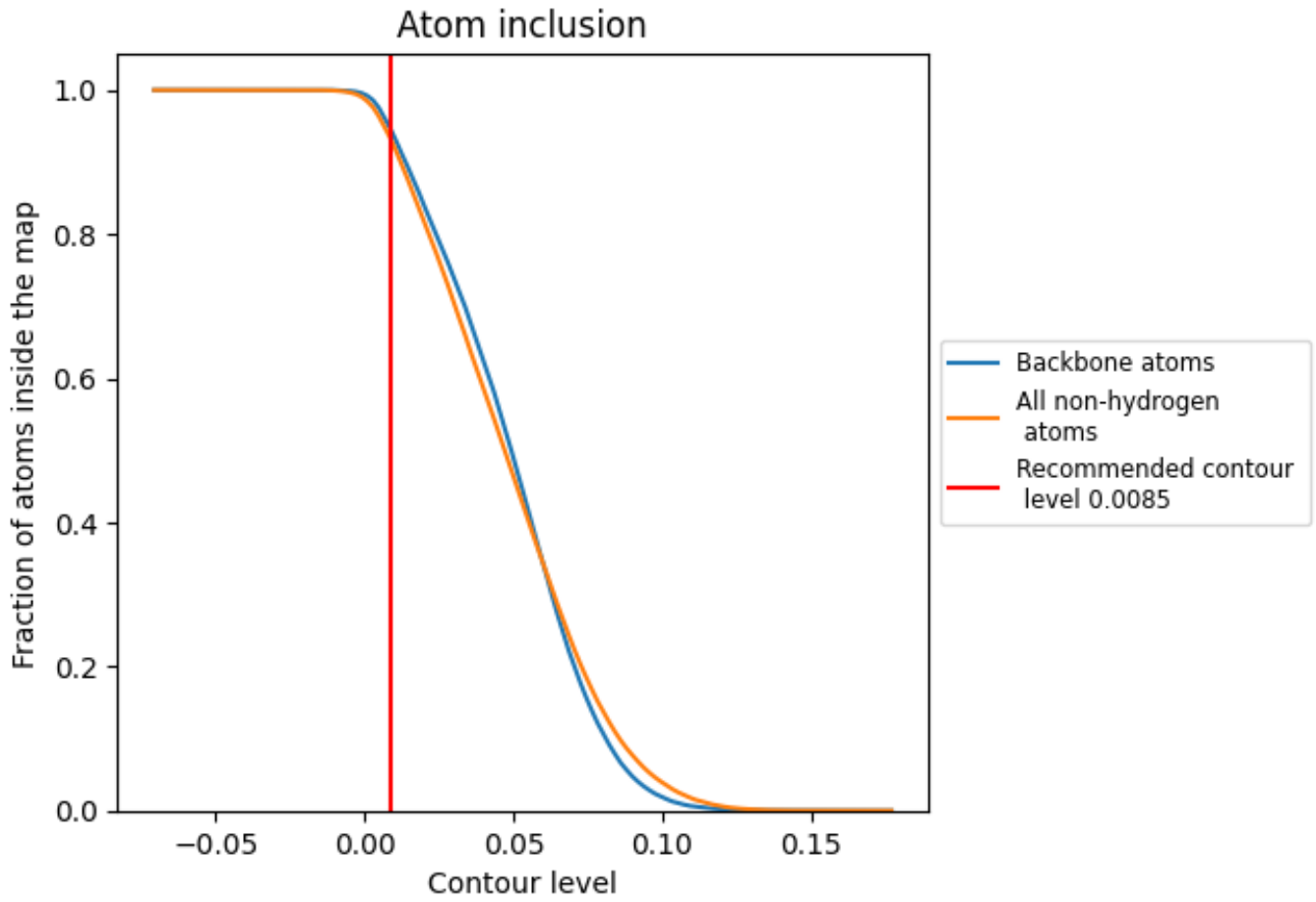
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0085).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9349	0.4100
A	0.9767	0.4440
B	0.9912	0.3430
C	0.9455	0.4690
D	0.9257	0.4670
E	0.9182	0.4290
F	0.7527	0.1490
G	0.8674	0.2700
I	0.2702	0.0450
J	0.9317	0.4600
K	0.9242	0.4510
L	0.9143	0.4340
M	0.9078	0.4340
N	0.9193	0.4590
O	0.8579	0.2800
Q	0.9329	0.4580
R	0.5426	0.0770
S	0.9426	0.4780
T	0.9007	0.1850
U	0.8956	0.3700
V	0.8867	0.4450
W	0.9429	0.3940
X	0.9190	0.4060
Z	0.9124	0.4400
a	0.8898	0.4200
b	0.9467	0.4660
c	0.9276	0.4190
d	0.9652	0.5350
e	0.9499	0.4980
f	0.9113	0.4320
g	0.8918	0.4090
h	0.8906	0.4040
i	0.8774	0.3100