Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:56 pm GMT

PDB ID	:	5O60
EMDB ID	:	EMD-3750
Title	:	Structure of the 50S large ribosomal subunit from Mycobacterium smegmatis
Authors	:	Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2017-06-02
Resolution	:	3.20 Å(reported)

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

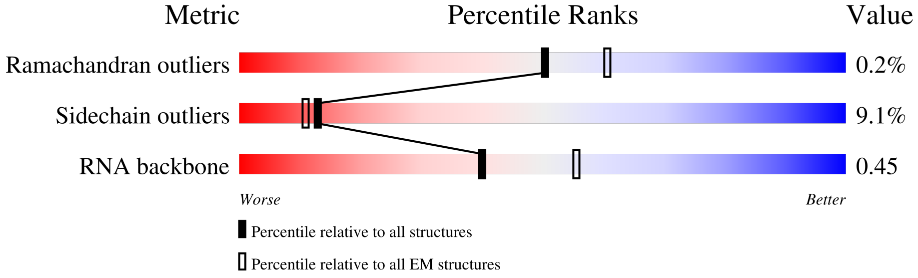
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

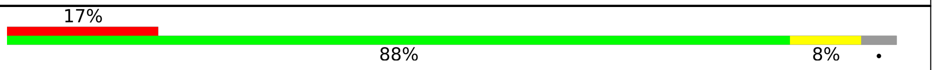
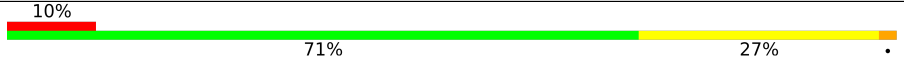
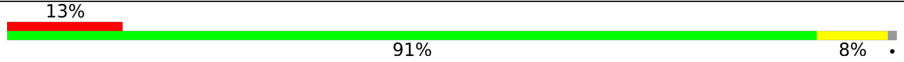
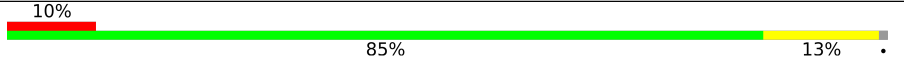
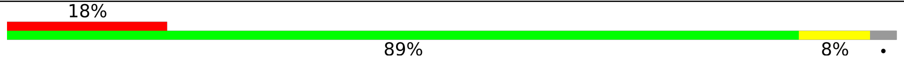
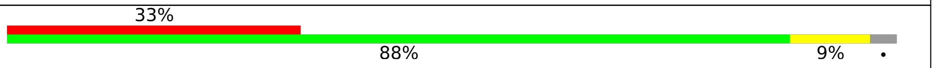
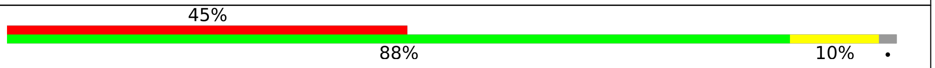
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	3	24	
2	A	3120	
3	B	118	
4	C	278	
5	D	217	
6	E	215	
7	F	187	
8	G	179	

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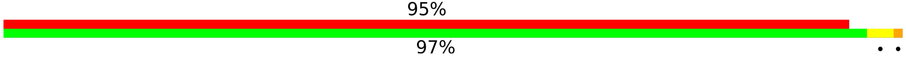
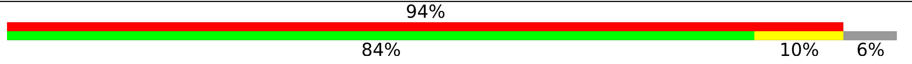
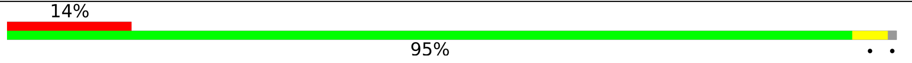
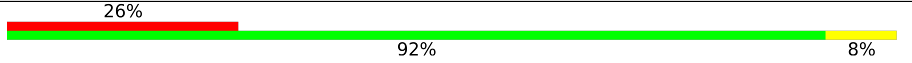
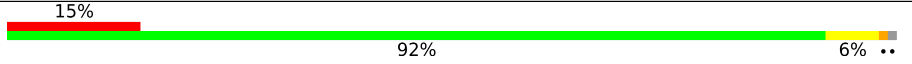
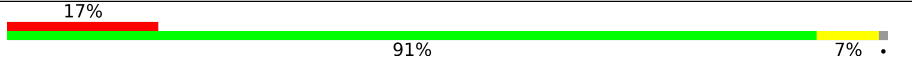
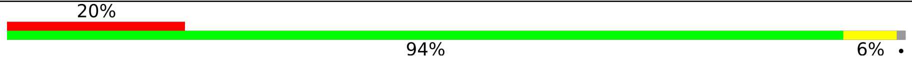
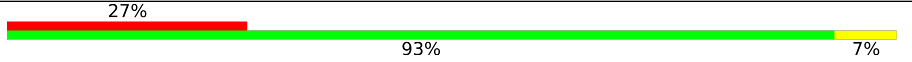
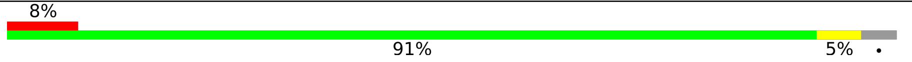
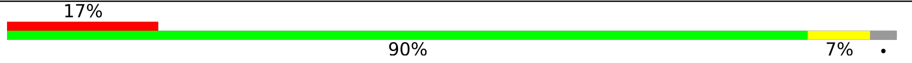
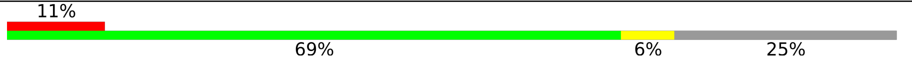
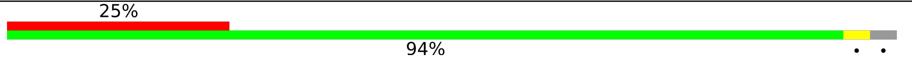
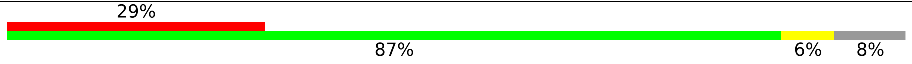
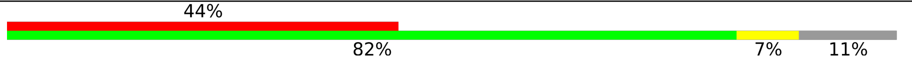
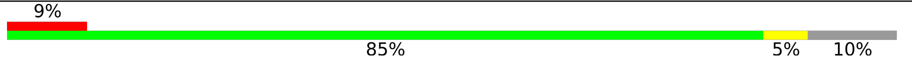
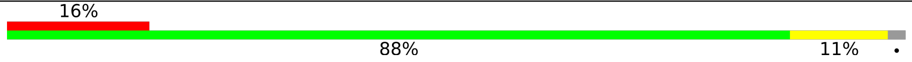
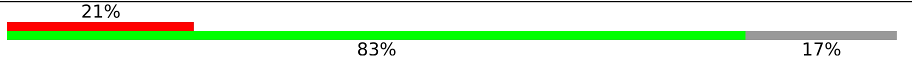
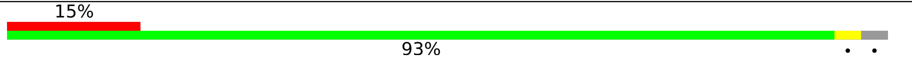
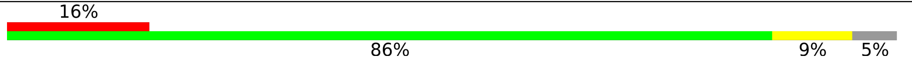
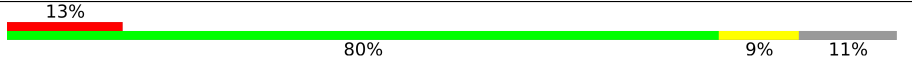
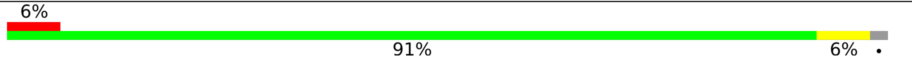
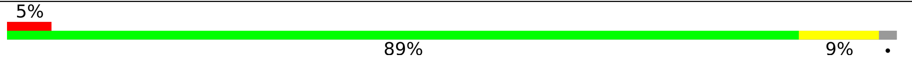
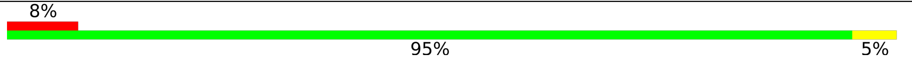
Mol	Chain	Length	Quality of chain
9	H	151	
10	I	175	
11	J	142	
12	K	147	
13	L	122	
14	M	147	
15	N	138	
16	O	199	
17	P	127	
18	Q	113	
19	R	129	
20	S	103	
21	T	153	
22	U	100	
23	V	105	
24	W	215	
25	X	88	
26	Y	64	
27	Z	77	
28	a	61	
29	b	57	
30	c	55	
31	d	47	
32	e	64	
33	f	37	

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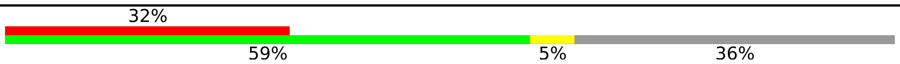
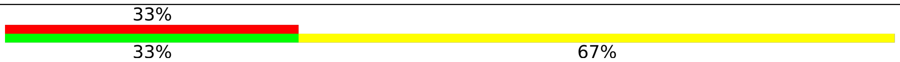
Mol	Chain	Length	Quality of chain
34	g	75	
35	2	3	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98153 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 bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	3	23	189	111	50	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	3119	66981	29854	12313	21695	3119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	118	2522	1126	468	810	118	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	2110	1298	438	370	4	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	214	1587	982	310	290	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	209	1569	969	295	303	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	126	Total	C	N	O	0	0
			956	586	199	171		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	124	Total	C	N	O	0	0
			988	613	203	172		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	T	114	873	543	171	159	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	U	97	756	479	138	139	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	97	732	456	137	137	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	W	192	1428	881	255	292	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	X	79	586	361	123	102	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	63	470	283	103	80	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	64	531	324	103	103	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 35 is a RNA chain called tRNA CCA-end acetylated (Phe).

Mol	Chain	Residues	Atoms	AltConf	Trace
35	2	3	Total C N O P 62 28 11 20 3	0	0

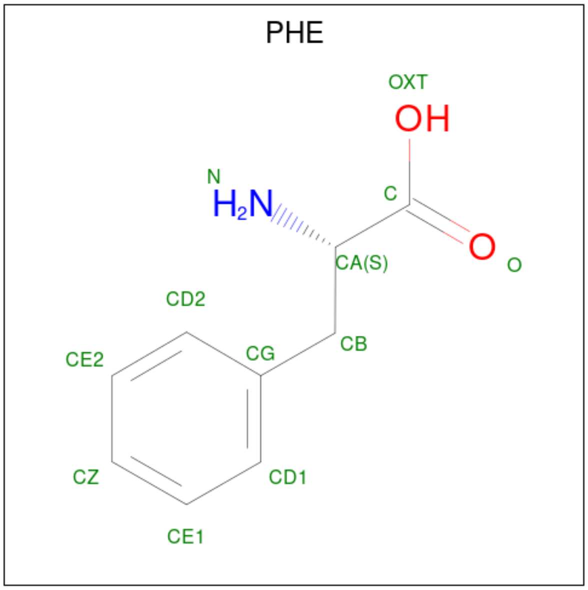
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	A	388	Total Mg 388 388	0
36	B	9	Total Mg 9 9	0
36	C	4	Total Mg 4 4	0
36	D	1	Total Mg 1 1	0
36	F	1	Total Mg 1 1	0
36	N	2	Total Mg 2 2	0
36	T	1	Total Mg 1 1	0
36	c	1	Total Mg 1 1	0
36	2	1	Total Mg 1 1	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
37	Y	1	Total Zn 1 1	0
37	c	1	Total Zn 1 1	0
37	f	1	Total Zn 1 1	0
37	g	1	Total Zn 1 1	0

- Molecule 38 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



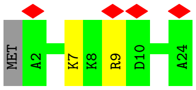
Mol	Chain	Residues	Atoms	AltConf
38	2	1	Total C N O 11 9 1 1	0

3 Residue-property plots ⓘ

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.

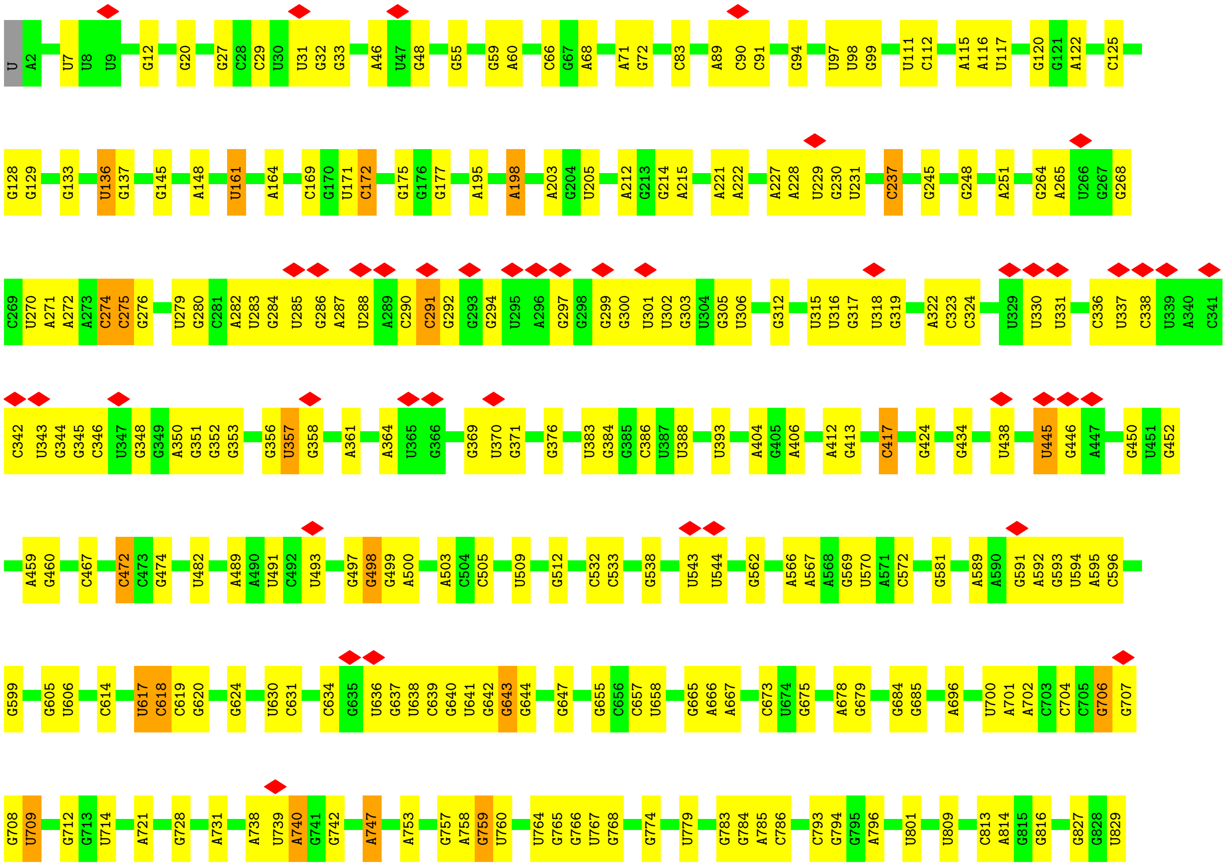
- Molecule 1: 50S ribosomal protein bL37

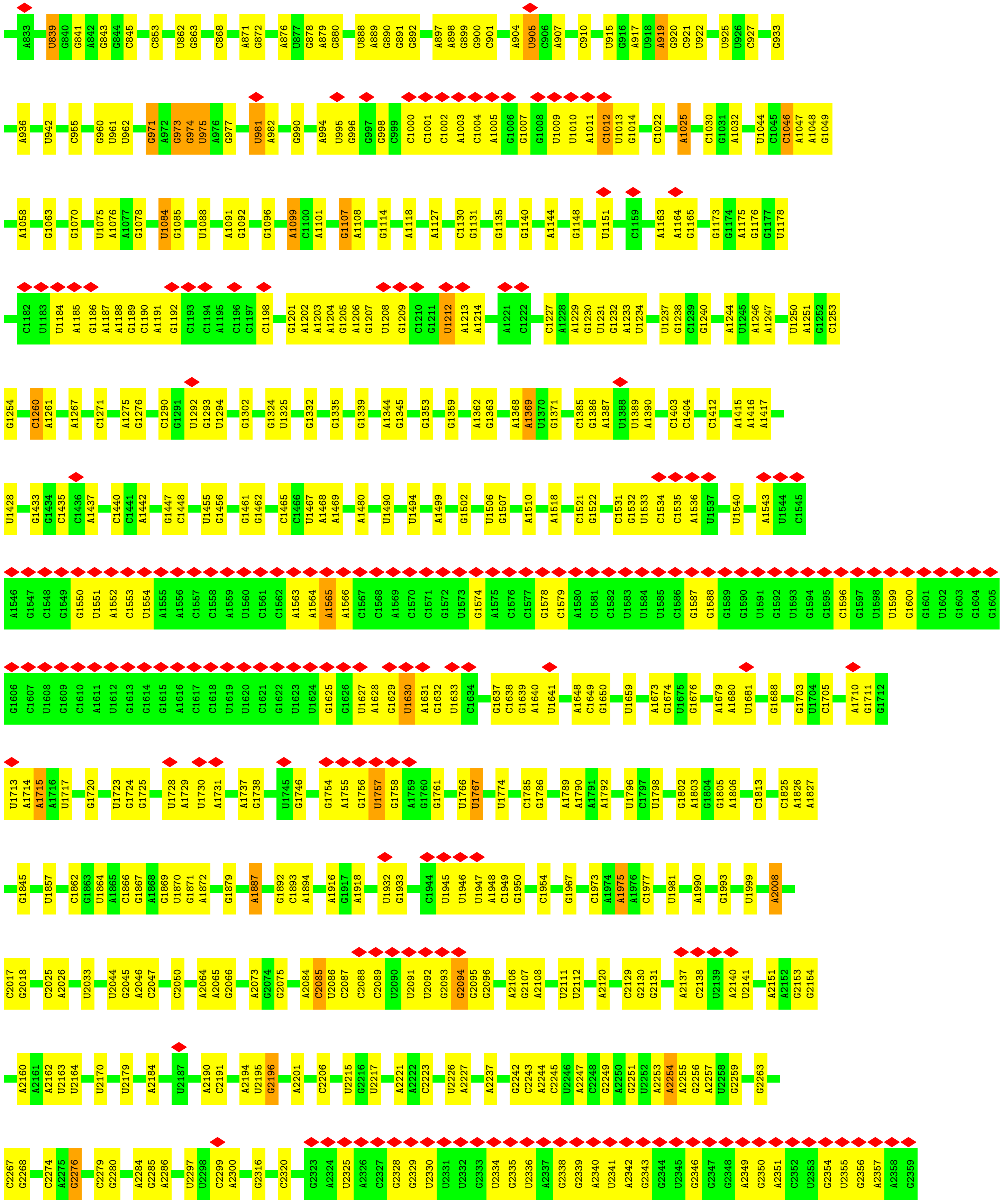
Chain 3:



- Molecule 2: 23S rRNA

Chain A:




A833 U839 G840 G841 A842 G843 G844 C845 C853 U862 G863 C868 A871 G872 A876 U877 G878 A879 G880 U888 A889 G890 G891 G892 A897 A898 G899 G900 C901 A904 U905 C906 A907 C910 U915 G916 A917 U918 A919 G920 C921 U922 U925 U926 C927 G933
A936 U942 C955 G960 U961 U962 G971 A972 G973 G974 U975 A976 G977 U981 A982 G990 A994 U995 G996 G997 G998 C999 C1000 C1001 C1002 A1003 C1004 A1005 G1006 G1007 G1008 U1009 U1010 A1011 C1012 U1013 G1014 C1022 A1025 C1030 G1031 A1032 U1044 C1045 C1046 A1047 A1048 G1049
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C1182 U1183 U1184 A1185 G1186 A1187 A1188 G1189 C1190 A1191 G1192 C1193 C1194 A1195 C1196 C1197 C1198 G1201 A1202 A1203 A1204 G1205 A1206 G1207 U1208 G1209 C1210 G1211 U1212 A1213 A1214 A1221 C1222 C1227 A1228 A1229 G1230 U1231 G1232 A1233 U1234 U1237 G1238 C1239 G1240 A1244 U1245 A1246 A1247 U1250 A1251 G1252 C1253
G1254 C1260 A1261 A1267 C1271 A1275 G1276 C1290 G1291 U1292 G1293 U1294 G1302 G1324 U1325 G1332 G1335 G1339 A1344 G1345 G1353 G1359 A1362 G1363 A1368 A1369 U1370 G1371 C1385 G1386 A1387 U1388 U1389 A1390 C1403 C1404 C1412 A1415 A1416 A1417
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A1546 G1547 C1548 G1549 G1550 U1551 A1552 C1553 U1554 A1555 A1556 C1557 G1558 A1559 U1560 C1561 C1562 A1563 A1564 A1565 A1566 C1567 C1568 A1569 C1570 G1571 G1572 U1573 G1574 A1575 C1576 C1577 G1578 C1579 A1580 C1581 C1582 U1583 U1584 U1585 C1586 G1587 G1588 G1589 G1590 U1591 G1592 U1593 G1594 G1595 C1596 G1597 U1598 U1599 G1600 G1601 U1602 G1603 G1604 G1605
G1606 C1607 U1608 G1609 C1610 A1611 U1612 G1613 G1614 G1615 A1616 C1617 C1618 U1619 U1620 C1621 G1622 U1623 U1624 G1625 G1626 U1627 A1628 G1629 U1630 A1631 G1632 U1633 C1634 G1637 C1638 G1639 A1640 U1641 A1648 C1649 G1650 U1659 A1673 G1674 U1675 G1676 A1679 A1680 U1681 G1688 G1703 U1704 C1705 A1710 G1711 G1712
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G1845 U1857 C1862 G1863 U1864 A1865 C1866 G1867 A1868 G1869 U1870 G1871 A1872 G1879 A1887 G1892 C1893 A1894 A1916 G1917 A1918 U1932 G1933 C1944 U1945 G1946 U1947 A1948 C1949 G1950 C1954 G1967 C1973 A1974 A1975 A1976 C1977 U1981 A1990 G1993 U1999 A2008
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A2160 A2161 A2162 U2163 U2164 U2170 U2179 A2184 U2187 A2190 C2191 A2194 U2195 G2196 A2201 C2206 U2215 G2216 U2217 A2221 A2222 C2223 U2226 A2227 A2237 G2242 C2243 A2244 C2245 U2246 A2247 G2248 G2249 A2250 G2251 U2252 A2253 A2254 A2255 G2256 A2257 U2258 G2259 G2263
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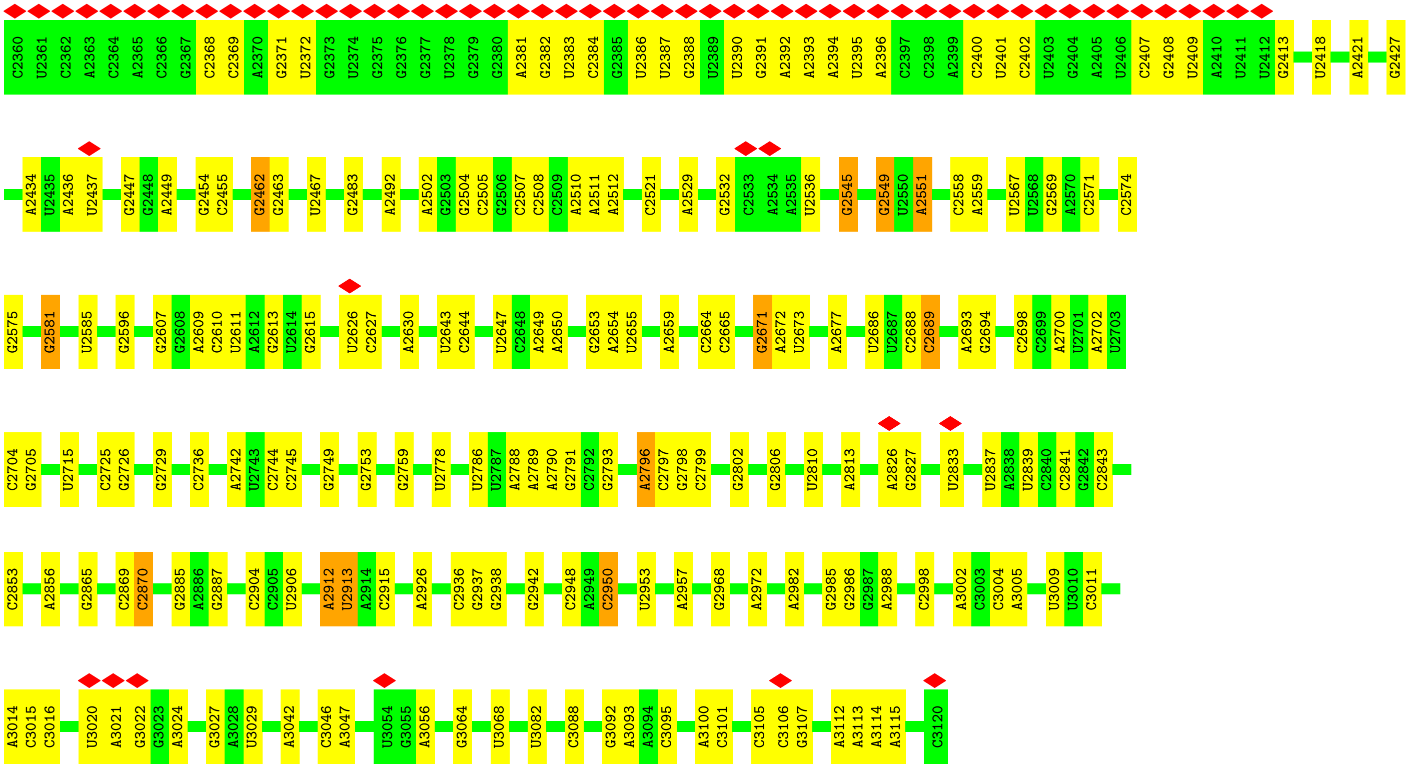
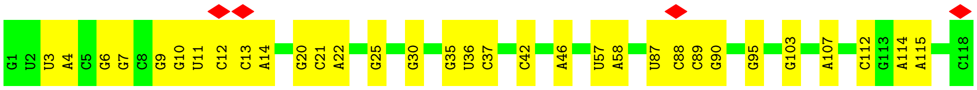


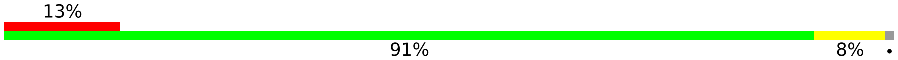
- Molecule 3: 5S rRNA

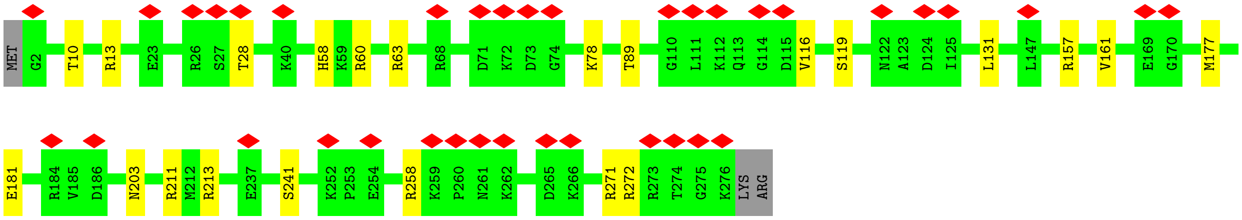
Chain B:



- Molecule 4: 50S ribosomal protein L2

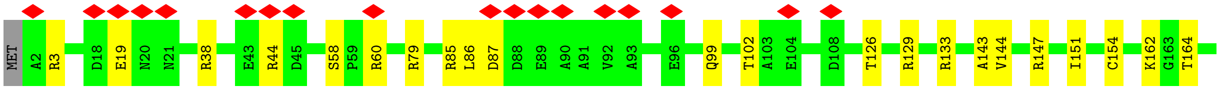
Chain C:

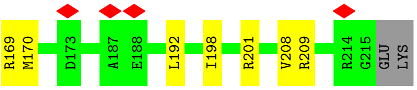




- Molecule 5: 50S ribosomal protein L3

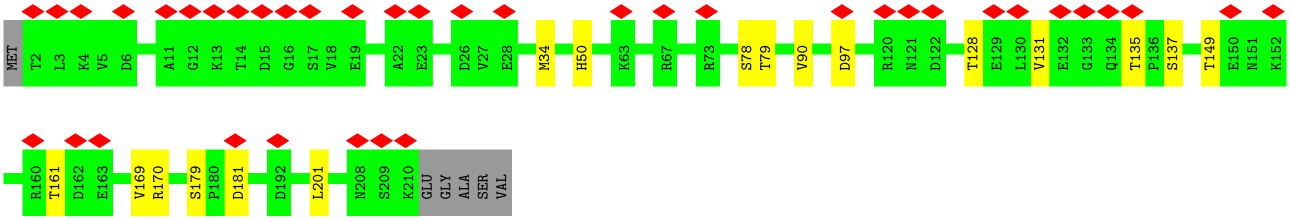
Chain D:





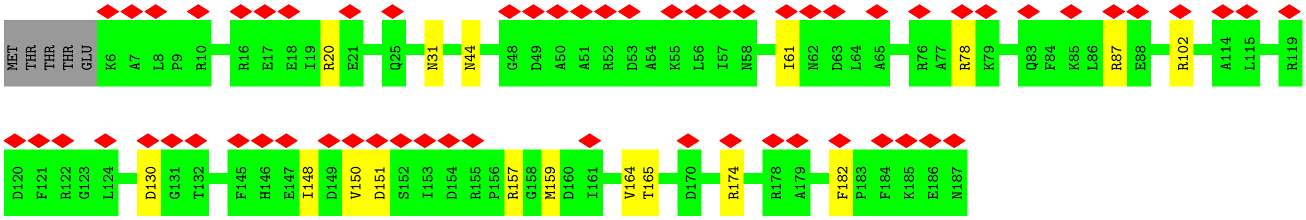
- Molecule 6: 50S ribosomal protein L4

Chain E:



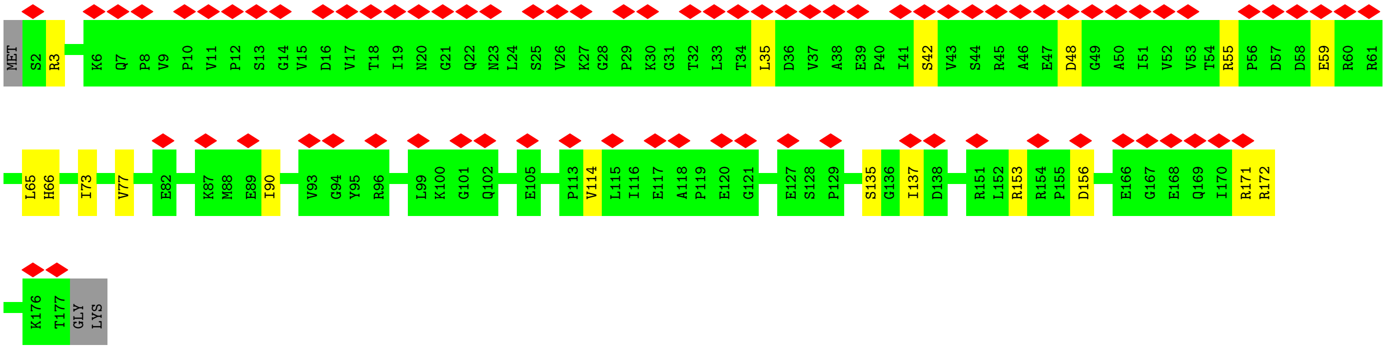
- Molecule 7: 50S ribosomal protein L5

Chain F:



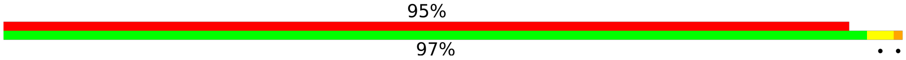
- Molecule 8: 50S ribosomal protein L6

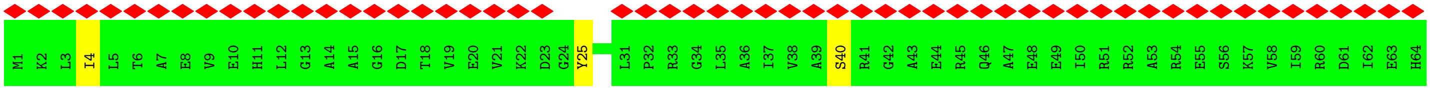
Chain G:

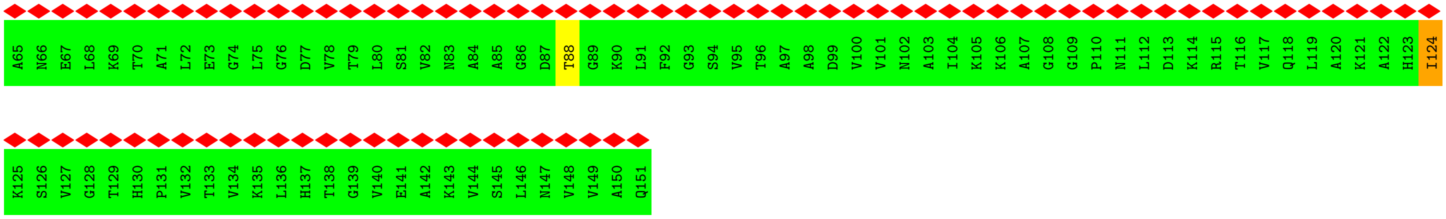


- Molecule 9: 50S ribosomal protein L9

Chain H:

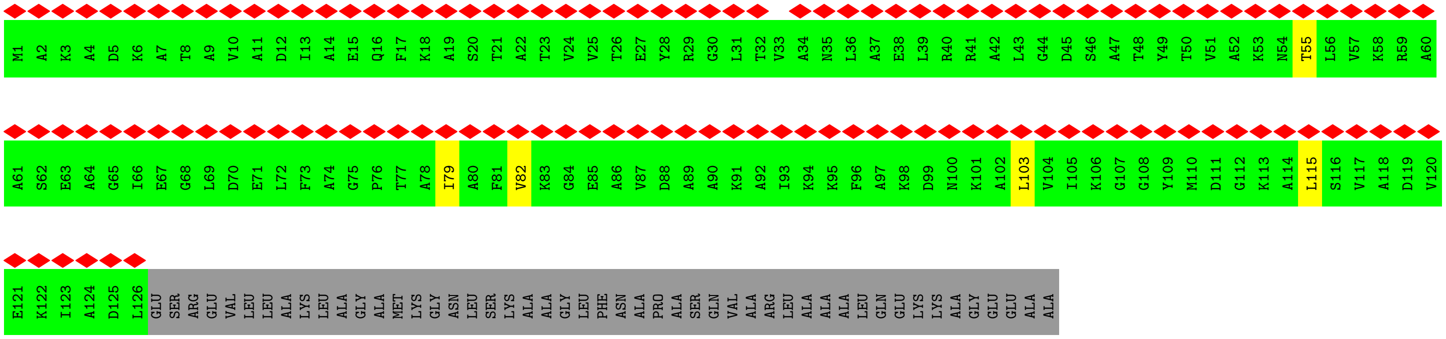






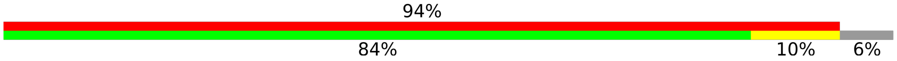
- Molecule 10: 50S ribosomal protein L10

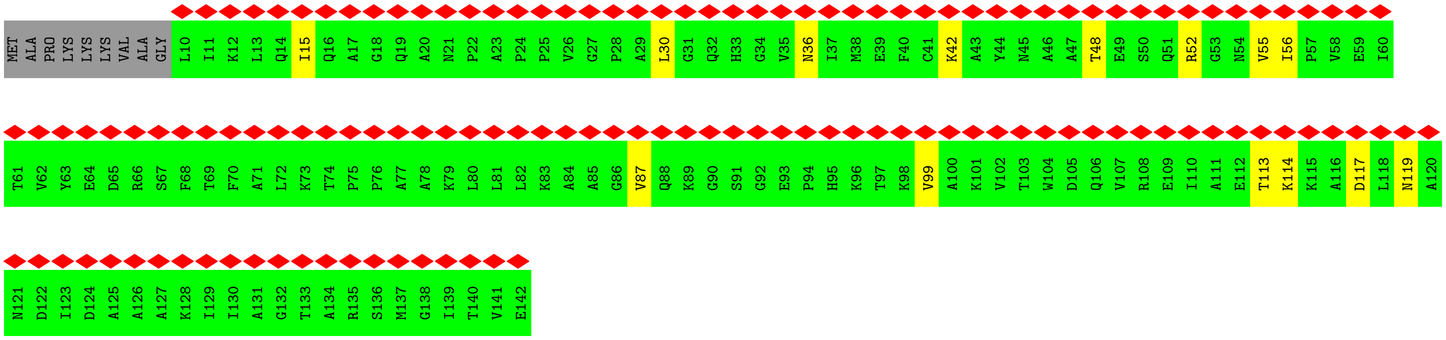
Chain I:



- Molecule 11: 50S ribosomal protein L11

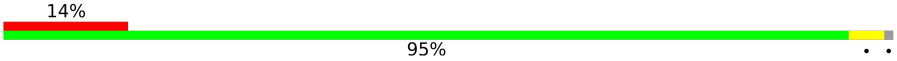
Chain J:

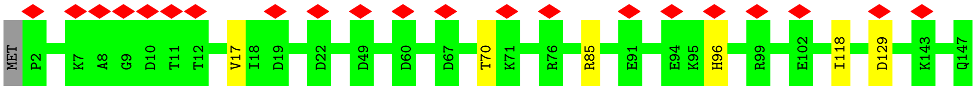




- Molecule 12: 50S ribosomal protein L13

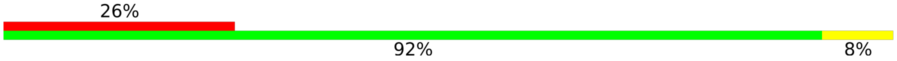
Chain K:

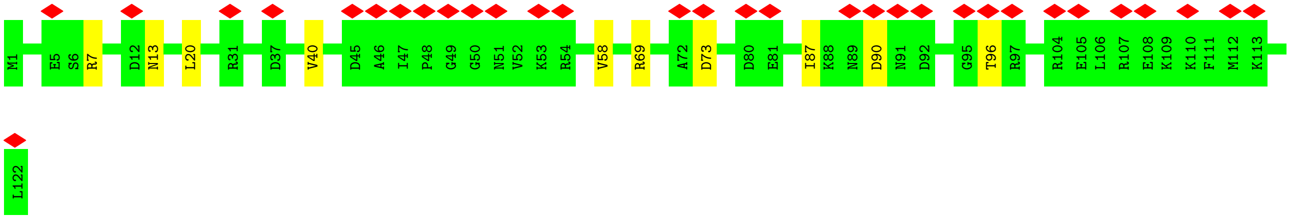




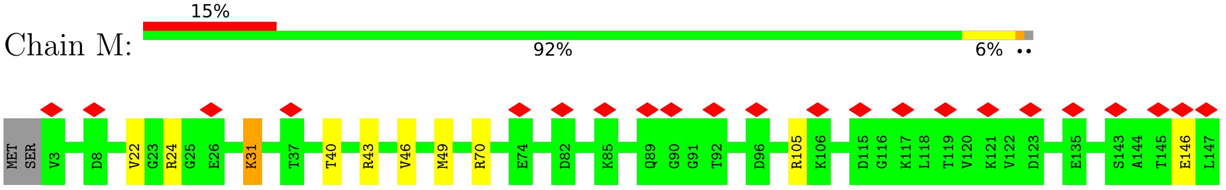
- Molecule 13: 50S ribosomal protein L14

Chain L:

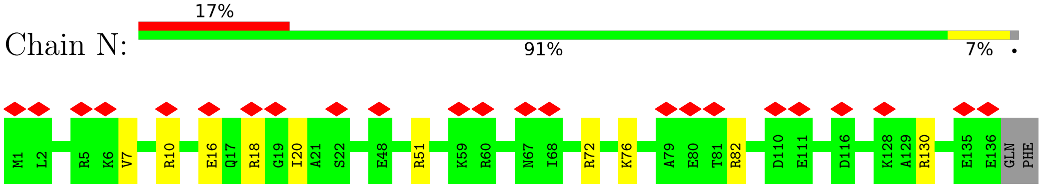




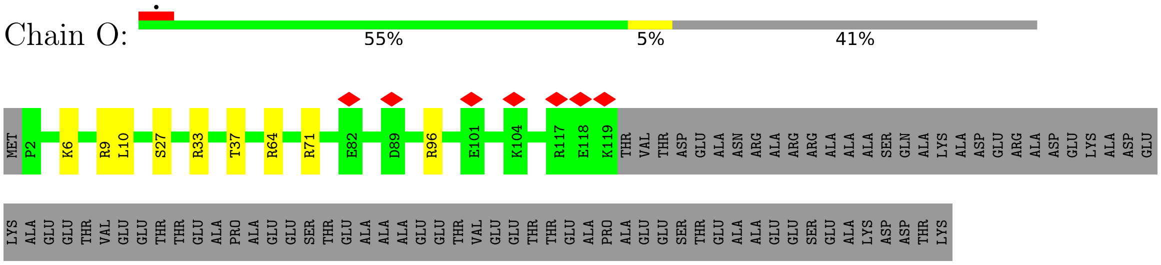
- Molecule 14: 50S ribosomal protein L15



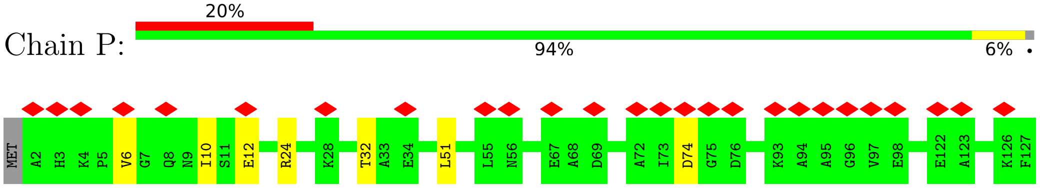
- Molecule 15: 50S ribosomal protein L16



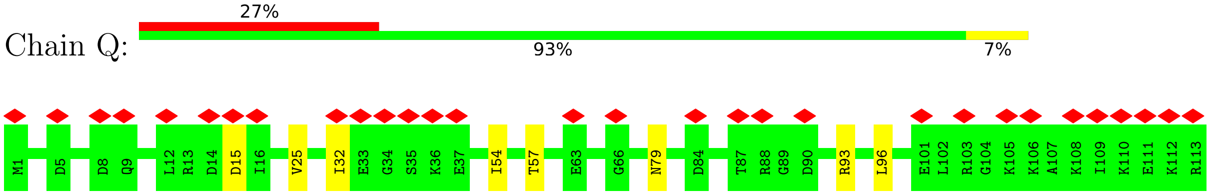
- Molecule 16: 50S ribosomal protein L17



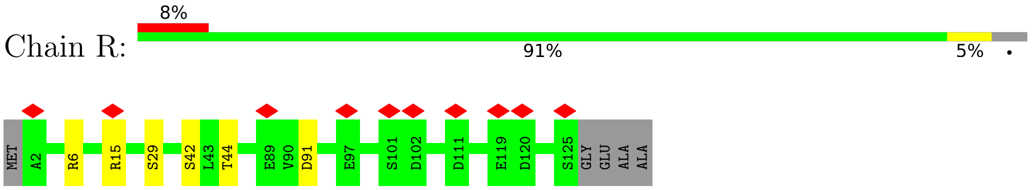
- Molecule 17: 50S ribosomal protein L18



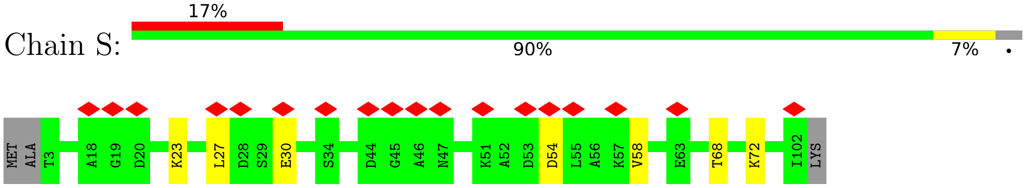
- Molecule 18: 50S ribosomal protein L19



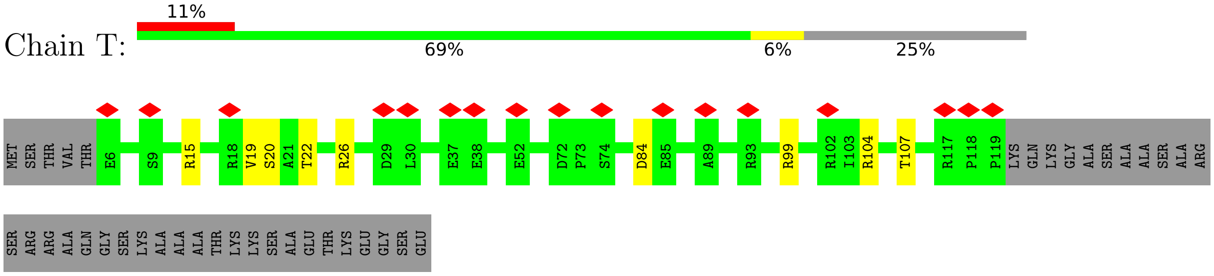
- Molecule 19: 50S ribosomal protein L20



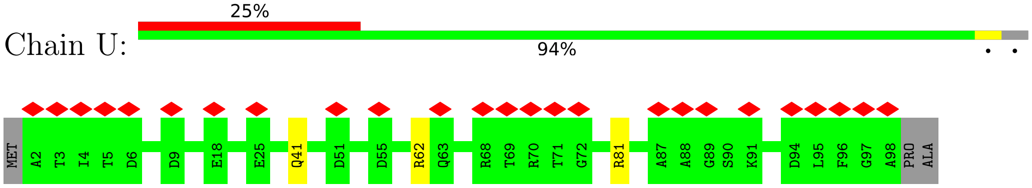
- Molecule 20: 50S ribosomal protein L21



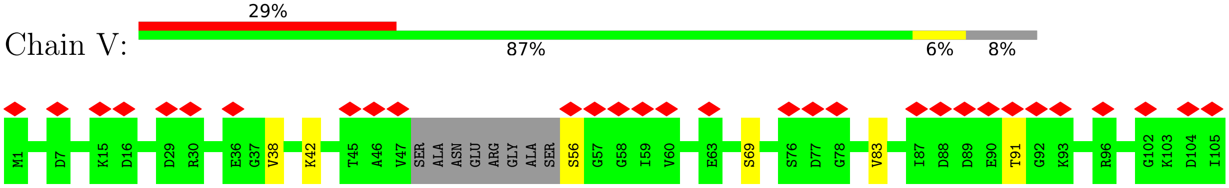
- Molecule 21: 50S ribosomal protein L22



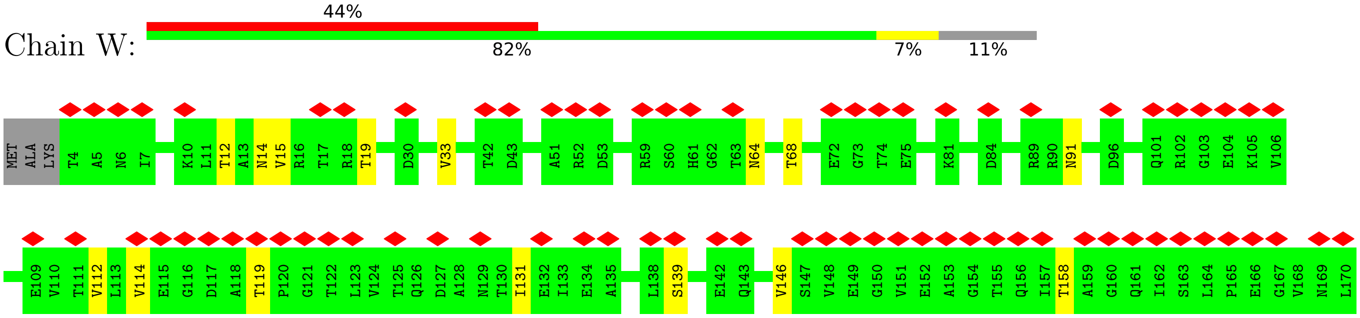
- Molecule 22: 50S ribosomal protein L23

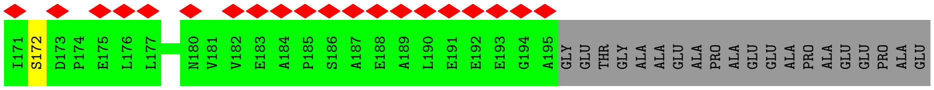


- Molecule 23: 50S ribosomal protein L24



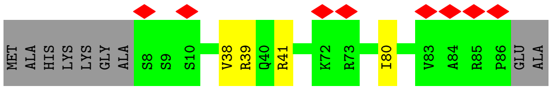
- Molecule 24: 50S ribosomal protein L25





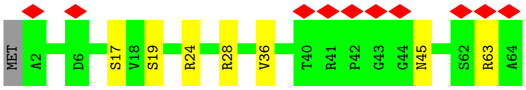
- Molecule 25: 50S ribosomal protein L27

Chain X:



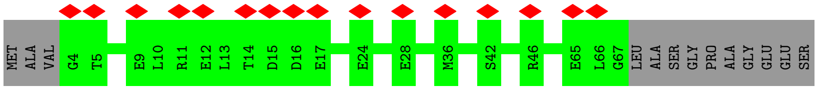
- Molecule 26: 50S ribosomal protein L28

Chain Y:



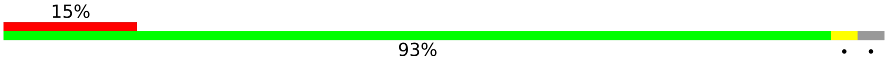
- Molecule 27: 50S ribosomal protein L29

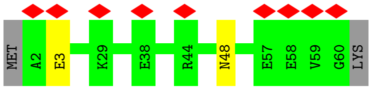
Chain Z:



- Molecule 28: 50S ribosomal protein L30

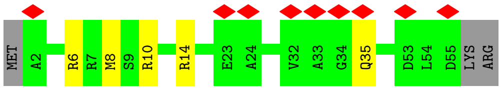
Chain a:





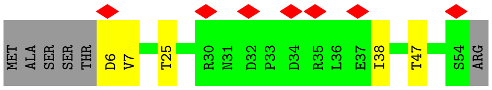
- Molecule 29: 50S ribosomal protein L32

Chain b:



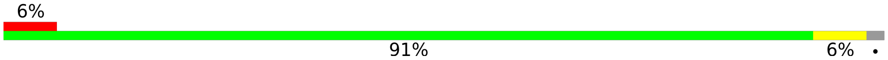
- Molecule 30: 50S ribosomal protein L33 1

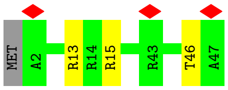
Chain c:



- Molecule 31: 50S ribosomal protein L34

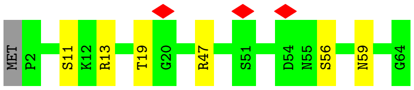
Chain d:





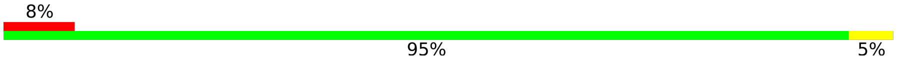
- Molecule 32: 50S ribosomal protein L35

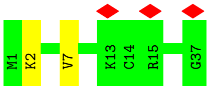
Chain e:



- Molecule 33: 50S ribosomal protein L36

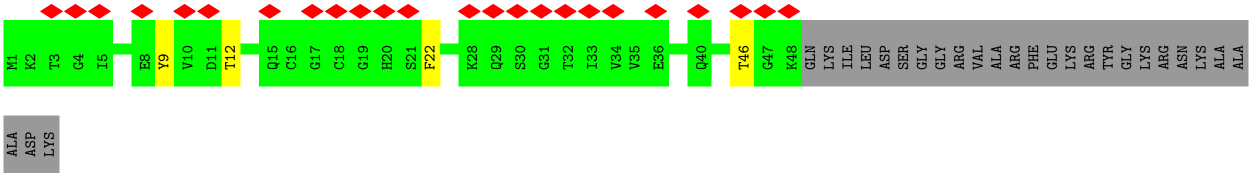
Chain f:





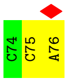
- Molecule 34: 50S ribosomal protein L31

Chain g:



- Molecule 35: tRNA CCA-end acetylated (Phe)

Chain 2:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.570	Depositor
Minimum map value	-0.255	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	3	0.56	0/191	0.60	0/247
2	A	0.83	29/75001 (0.0%)	1.19	238/117027 (0.2%)
3	B	0.53	0/2821	1.04	4/4396 (0.1%)
4	C	0.54	0/2153	0.67	0/2895
5	D	0.55	0/1609	0.71	0/2165
6	E	0.47	0/1592	0.61	0/2153
7	F	0.35	0/1467	0.53	0/1973
8	G	0.36	0/1369	0.52	0/1848
9	H	0.33	0/1027	0.52	0/1398
10	I	0.41	0/925	0.54	0/1246
11	J	0.42	0/1006	0.57	0/1364
12	K	0.50	0/1157	0.63	0/1567
13	L	0.52	0/946	0.66	0/1268
14	M	0.51	0/1091	0.71	0/1457
15	N	0.54	0/1118	0.64	0/1506
16	O	0.52	0/945	0.73	0/1267
17	P	0.37	0/966	0.55	0/1298
18	Q	0.50	0/921	0.65	0/1236
19	R	0.63	0/1000	0.67	0/1341
20	S	0.48	0/764	0.65	0/1030
21	T	0.57	0/887	0.69	0/1204
22	U	0.49	0/766	0.57	0/1030
23	V	0.55	1/738 (0.1%)	0.62	0/987
24	W	0.42	0/1443	0.61	0/1970
25	X	0.56	0/595	0.63	0/798
26	Y	0.64	0/478	0.75	1/641 (0.2%)
27	Z	0.44	0/534	0.57	0/713
28	a	0.53	0/477	0.64	0/640
29	b	0.51	0/427	0.67	0/572
30	c	0.45	0/413	0.57	0/553
31	d	0.54	0/380	0.70	0/500
32	e	0.51	0/507	0.69	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.58	0/303	0.66	0/401
34	g	0.36	0/372	0.50	0/503
35	2	0.65	0/68	1.16	0/103
All	All	0.75	30/106457 (0.0%)	1.08	243/159969 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	936	A	N9-C4	-8.24	1.32	1.37
2	A	889	A	N3-C4	-7.64	1.30	1.34
23	V	56	SER	CB-OG	7.10	1.51	1.42
2	A	889	A	N9-C4	-6.90	1.33	1.37
2	A	1630	U	C1'-N1	6.59	1.58	1.48
2	A	673	C	N1-C6	-5.98	1.33	1.37
2	A	2912	A	N9-C4	-5.91	1.34	1.37
2	A	786	C	N1-C6	-5.79	1.33	1.37
2	A	251	A	N9-C4	-5.66	1.34	1.37
2	A	2789	A	N9-C4	-5.65	1.34	1.37
2	A	1385	C	N1-C6	-5.57	1.33	1.37
2	A	1469	A	C5-C4	-5.57	1.34	1.38
2	A	1565	A	N9-C4	5.56	1.41	1.37
2	A	2045	G	N1-C2	-5.35	1.33	1.37
2	A	2249	G	C5-C4	-5.31	1.34	1.38
2	A	2551	A	N3-C4	-5.31	1.31	1.34
2	A	876	A	N9-C4	-5.31	1.34	1.37
2	A	1469	A	N9-C4	-5.31	1.34	1.37
2	A	2725	C	N1-C6	-5.27	1.33	1.37
2	A	2799	C	N1-C6	-5.27	1.33	1.37
2	A	1244	A	N3-C4	-5.25	1.31	1.34
2	A	901	C	N1-C6	-5.19	1.34	1.37
2	A	2904	C	N1-C6	-5.18	1.34	1.37
2	A	2736	C	N1-C6	-5.14	1.34	1.37
2	A	759	G	N9-C4	-5.13	1.33	1.38
2	A	814	A	N3-C4	-5.12	1.31	1.34
2	A	1025	A	C5-C4	-5.10	1.35	1.38
2	A	975	U	C4-C5	-5.07	1.39	1.43
2	A	1790	A	N3-C4	-5.04	1.31	1.34
2	A	1099	A	C5-C6	-5.03	1.36	1.41

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	975	U	C5-C4-O4	-10.81	119.42	125.90
2	A	981	U	C5-C6-N1	10.39	127.89	122.70
2	A	975	U	N3-C4-O4	8.32	125.22	119.40
2	A	2245	C	N1-C2-O2	8.12	123.77	118.90
2	A	1403	C	C4-C5-C6	8.06	121.43	117.40
2	A	1032	A	N1-C2-N3	7.95	133.27	129.30
2	A	981	U	C5-C4-O4	-7.78	121.23	125.90
2	A	759	G	N3-C4-C5	7.58	132.39	128.60
2	A	617	U	C2-N1-C1’	7.55	126.75	117.70
2	A	275	C	C5-C6-N1	7.37	124.68	121.00
2	A	981	U	C2-N1-C1’	7.12	126.24	117.70
2	A	2796	A	O5’-P-OP2	-7.03	99.38	105.70
2	A	1302	G	N1-C6-O6	7.00	124.10	119.90
2	A	919	A	C5-N7-C8	-7.00	100.40	103.90
2	A	2551	A	C8-N9-C4	-6.97	103.01	105.80
2	A	2950	C	C6-N1-C2	6.96	123.09	120.30
2	A	445	U	C2-N1-C1’	6.96	126.05	117.70
2	A	2551	A	N9-C4-C5	6.95	108.58	105.80
2	A	981	U	C6-N1-C2	-6.88	116.87	121.00
3	B	88	C	C2-N1-C1’	6.87	126.36	118.80
2	A	66	C	C6-N1-C2	-6.87	117.55	120.30
2	A	1302	G	C6-C5-N7	-6.87	126.28	130.40
2	A	599	G	O4’-C1’-N9	6.86	113.69	108.20
2	A	2025	C	N3-C2-O2	-6.82	117.13	121.90
2	A	1403	C	N3-C2-O2	-6.81	117.13	121.90
2	A	2912	A	C5-N7-C8	-6.78	100.51	103.90
2	A	2505	C	C6-N1-C2	6.72	122.99	120.30
2	A	975	U	C2-N1-C1’	6.61	125.63	117.70
2	A	868	C	C5-C6-N1	6.61	124.30	121.00
2	A	1766	U	N3-C4-C5	-6.61	110.64	114.60
2	A	2259	G	N3-C4-C5	-6.57	125.31	128.60
2	A	740	A	O4’-C1’-N9	6.57	113.46	108.20
2	A	759	G	P-O3’-C3’	6.57	127.58	119.70
2	A	786	C	C4-C5-C6	6.55	120.68	117.40
2	A	2581	G	N3-C4-C5	6.55	131.87	128.60
2	A	275	C	C6-N1-C2	-6.45	117.72	120.30
2	A	974	G	N7-C8-N9	-6.42	109.89	113.10
2	A	925	U	C5-C6-N1	-6.41	119.50	122.70
2	A	657	C	C5-C4-N4	-6.39	115.72	120.20
2	A	237	C	C5-C6-N1	6.39	124.20	121.00
2	A	868	C	C6-N1-C2	-6.38	117.75	120.30
2	A	905	U	C2-N1-C1’	6.37	125.34	117.70
2	A	888	U	C5-C6-N1	-6.34	119.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	169	C	C2-N1-C1'	6.30	125.72	118.80
2	A	618	C	C6-N1-C2	6.27	122.81	120.30
2	A	1650	G	N3-C4-C5	-6.27	125.47	128.60
2	A	2245	C	N3-C2-O2	-6.19	117.57	121.90
3	B	88	C	N1-C2-O2	6.15	122.59	118.90
2	A	2245	C	C2-N1-C1'	6.14	125.56	118.80
2	A	1766	U	C6-N1-C2	-6.08	117.35	121.00
2	A	973	G	N3-C4-C5	-6.07	125.57	128.60
2	A	1369	A	O5'-P-OP2	-6.06	100.24	105.70
2	A	1455	U	C5-C6-N1	-6.04	119.68	122.70
2	A	161	U	O4'-C1'-N1	6.03	113.02	108.20
2	A	2870	C	C6-N1-C2	-6.00	117.90	120.30
2	A	876	A	C5-N7-C8	-5.99	100.91	103.90
2	A	2223	C	C2-N3-C4	-5.97	116.91	119.90
2	A	2437	U	N1-C2-O2	5.94	126.96	122.80
2	A	809	U	C5-C6-N1	-5.93	119.74	122.70
2	A	786	C	N1-C2-N3	5.90	123.33	119.20
2	A	1758	G	C5-C6-O6	-5.90	125.06	128.60
2	A	538	G	C6-C5-N7	-5.89	126.87	130.40
2	A	962	U	C2-N1-C1'	5.87	124.75	117.70
2	A	2615	G	O4'-C1'-N9	5.87	112.90	108.20
2	A	974	G	C8-N9-C4	5.87	108.75	106.40
2	A	643	G	C4-N9-C1'	5.87	134.12	126.50
2	A	417	C	C6-N1-C2	-5.86	117.95	120.30
2	A	2505	C	C5-C6-N1	-5.86	118.07	121.00
2	A	1302	G	C5-C6-O6	-5.84	125.10	128.60
2	A	1032	A	C6-N1-C2	-5.83	115.10	118.60
2	A	1403	C	C5-C6-N1	-5.83	118.08	121.00
2	A	1894	A	C2-N3-C4	-5.83	107.69	110.60
2	A	2575	G	N3-C4-C5	-5.83	125.69	128.60
2	A	2689	C	N3-C2-O2	-5.81	117.83	121.90
2	A	467	C	C5-C6-N1	-5.81	118.10	121.00
2	A	971	G	N3-C4-C5	-5.81	125.70	128.60
2	A	974	G	OP2-P-O3'	5.81	117.98	105.20
2	A	1096	G	N9-C4-C5	-5.80	103.08	105.40
2	A	1455	U	C2-N1-C1'	-5.80	110.74	117.70
2	A	2455	C	C5-C6-N1	-5.79	118.10	121.00
2	A	981	U	N3-C4-O4	5.79	123.45	119.40
2	A	357	U	P-O3'-C3'	5.79	126.65	119.70
2	A	2008	A	N1-C2-N3	5.79	132.19	129.30
2	A	2843	C	N1-C2-O2	-5.79	115.43	118.90
2	A	1766	U	C6-N1-C1'	5.79	129.30	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1758	G	N1-C6-O6	5.76	123.36	119.90
2	A	853	C	C6-N1-C2	-5.75	118.00	120.30
2	A	2094	G	P-O3'-C3'	5.74	126.58	119.70
2	A	2521	C	C6-N1-C2	-5.74	118.00	120.30
2	A	2437	U	C2-N1-C1'	5.73	124.58	117.70
2	A	1107	G	C8-N9-C4	5.73	108.69	106.40
2	A	2551	A	N1-C6-N6	-5.72	115.17	118.60
2	A	1827	A	C8-N9-C4	5.72	108.09	105.80
2	A	1650	G	C4-N9-C1'	5.72	133.94	126.50
2	A	2841	C	N3-C4-C5	5.70	124.18	121.90
2	A	657	C	N3-C4-C5	5.70	124.18	121.90
2	A	3068	U	N1-C2-N3	5.70	118.32	114.90
2	A	915	U	C2-N1-C1'	-5.69	110.87	117.70
2	A	1766	U	C5-C4-O4	5.68	129.31	125.90
2	A	593	G	O4'-C1'-N9	5.68	112.74	108.20
2	A	1088	U	N1-C2-N3	5.67	118.30	114.90
2	A	2813	A	C8-N9-C4	5.65	108.06	105.80
2	A	3046	C	N3-C2-O2	-5.64	117.95	121.90
2	A	445	U	N1-C2-O2	5.63	126.74	122.80
2	A	1046	C	C6-N1-C2	-5.63	118.05	120.30
2	A	922	U	C2-N3-C4	-5.63	123.62	127.00
2	A	1212	U	C5-C6-N1	5.62	125.51	122.70
2	A	973	G	N3-C4-N9	5.61	129.37	126.00
3	B	95	G	N3-C4-C5	-5.61	125.80	128.60
2	A	161	U	C2-N1-C1'	5.60	124.42	117.70
2	A	2455	C	C4-C5-C6	5.59	120.20	117.40
2	A	759	G	N3-C4-N9	-5.59	122.65	126.00
2	A	498	G	C4-N9-C1'	5.58	133.76	126.50
2	A	3092	G	C8-N9-C4	5.58	108.63	106.40
2	A	706	G	C4-C5-N7	5.57	113.03	110.80
2	A	1048	A	C8-N9-C4	-5.56	103.57	105.80
2	A	1767	U	C5-C6-N1	5.56	125.48	122.70
2	A	1887	A	C6-N1-C2	-5.55	115.27	118.60
2	A	1012	C	C2-N1-C1'	5.54	124.89	118.80
2	A	624	G	N3-C4-N9	5.53	129.32	126.00
2	A	839	U	C2-N1-C1'	5.53	124.34	117.70
2	A	876	A	C4-C5-N7	5.53	113.47	110.70
2	A	112	C	C6-N1-C2	-5.53	118.09	120.30
2	A	2254	A	C8-N9-C4	5.52	108.01	105.80
2	A	2201	A	C8-N9-C4	5.52	108.01	105.80
2	A	1428	U	C2-N1-C1'	5.52	124.32	117.70
2	A	2297	U	C2-N3-C4	-5.52	123.69	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2988	A	N1-C6-N6	-5.52	115.29	118.60
2	A	1084	U	C5-C6-N1	5.51	125.46	122.70
2	A	1993	G	C4-N9-C1'	5.51	133.66	126.50
3	B	88	C	C6-N1-C1'	-5.51	114.19	120.80
2	A	2788	A	N1-C2-N3	5.50	132.05	129.30
2	A	1096	G	C8-N9-C4	5.50	108.60	106.40
2	A	2799	C	N1-C2-O2	-5.48	115.61	118.90
2	A	1260	C	C6-N1-C2	-5.47	118.11	120.30
2	A	2206	C	C4-C5-C6	5.47	120.14	117.40
2	A	3068	U	C5-C4-O4	5.47	129.18	125.90
2	A	714	U	N3-C2-O2	-5.47	118.37	122.20
2	A	291	C	C6-N1-C2	-5.46	118.11	120.30
2	A	974	G	C5-N7-C8	5.45	107.03	104.30
2	A	971	G	C4-N9-C1'	5.44	133.57	126.50
2	A	1302	G	C4-N9-C1'	5.43	133.55	126.50
2	A	2610	C	C6-N1-C2	-5.42	118.13	120.30
2	A	2664	C	N3-C4-C5	5.42	124.07	121.90
2	A	2913	U	C5-C6-N1	-5.42	119.99	122.70
2	A	2094	G	N7-C8-N9	5.41	115.81	113.10
2	A	274	C	C5-C6-N1	5.41	123.70	121.00
2	A	2950	C	C5-C6-N1	-5.41	118.30	121.00
2	A	1977	C	C6-N1-C2	-5.40	118.14	120.30
2	A	910	C	C6-N1-C2	-5.39	118.14	120.30
26	Y	63	ARG	NE-CZ-NH1	-5.38	117.61	120.30
2	A	2671	G	C8-N9-C4	5.37	108.55	106.40
2	A	1879	G	N9-C4-C5	5.37	107.55	105.40
2	A	1099	A	N1-C6-N6	5.36	121.82	118.60
2	A	2462	G	N1-C6-O6	-5.36	116.69	119.90
2	A	1030	C	N3-C2-O2	-5.35	118.16	121.90
2	A	1118	A	N9-C4-C5	5.35	107.94	105.80
2	A	1993	G	C8-N9-C1'	-5.34	120.06	127.00
2	A	2998	C	C6-N1-C2	-5.34	118.16	120.30
2	A	2237	A	C8-N9-C4	-5.34	103.67	105.80
2	A	796	A	N9-C4-C5	5.33	107.93	105.80
2	A	1442	A	N1-C6-N6	5.32	121.79	118.60
2	A	1676	G	N3-C4-N9	5.32	129.19	126.00
2	A	3092	G	N7-C8-N9	-5.32	110.44	113.10
2	A	1975	A	C5-N7-C8	-5.32	101.24	103.90
2	A	2611	U	C2-N1-C1'	-5.32	111.32	117.70
2	A	1271	C	C5-C6-N1	-5.31	118.34	121.00
2	A	706	G	C5-N7-C8	-5.31	101.64	104.30
2	A	617	U	N1-C2-O2	5.31	126.52	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	445	U	P-O3'-C3'	5.30	126.06	119.70
2	A	975	U	C6-N1-C2	-5.30	117.82	121.00
2	A	617	U	N3-C2-O2	-5.29	118.50	122.20
2	A	136	U	C5-C6-N1	5.27	125.33	122.70
2	A	709	U	C2-N1-C1'	5.26	124.02	117.70
2	A	955	C	N3-C4-C5	-5.26	119.80	121.90
2	A	747	A	O4'-C1'-N9	5.25	112.40	108.20
2	A	2259	G	C8-N9-C4	-5.25	104.30	106.40
2	A	2611	U	C5-C6-N1	-5.25	120.08	122.70
2	A	567	A	O4'-C1'-N9	5.24	112.39	108.20
2	A	2196	G	N3-C4-C5	-5.24	125.98	128.60
2	A	1118	A	C8-N9-C4	-5.22	103.71	105.80
2	A	2549	G	C8-N9-C4	-5.21	104.32	106.40
2	A	796	A	N1-C6-N6	-5.21	115.48	118.60
2	A	2268	G	C8-N9-C4	-5.21	104.32	106.40
2	A	2454	G	N3-C4-N9	5.20	129.12	126.00
2	A	2437	U	N3-C2-O2	-5.19	118.57	122.20
2	A	1468	A	C6-N1-C2	-5.18	115.49	118.60
2	A	1030	C	N1-C2-O2	5.18	122.01	118.90
2	A	2025	C	N1-C2-O2	5.18	122.00	118.90
2	A	445	U	N3-C2-O2	-5.17	118.58	122.20
2	A	919	A	C4-C5-N7	5.16	113.28	110.70
2	A	1012	C	N1-C2-O2	5.16	122.00	118.90
2	A	975	U	C5-C6-N1	5.16	125.28	122.70
2	A	2044	U	C6-N1-C2	-5.15	117.91	121.00
2	A	1758	G	C4-C5-N7	5.15	112.86	110.80
2	A	2869	C	C6-N1-C2	-5.15	118.24	120.30
2	A	198	A	N1-C6-N6	-5.14	115.52	118.60
2	A	2170	U	C5-C6-N1	5.14	125.27	122.70
2	A	1260	C	C2-N1-C1'	5.13	124.44	118.80
2	A	172	C	C2-N1-C1'	5.13	124.44	118.80
2	A	1715	A	C8-N9-C4	-5.12	103.75	105.80
2	A	1975	A	C4-C5-N7	5.12	113.26	110.70
2	A	111	U	C2-N1-C1'	5.12	123.84	117.70
2	A	1650	G	N3-C4-N9	5.12	129.07	126.00
2	A	2686	U	N1-C2-O2	5.11	126.38	122.80
2	A	169	C	C6-N1-C1'	-5.11	114.67	120.80
2	A	889	A	N1-C2-N3	5.11	131.86	129.30
2	A	2050	C	C5-C6-N1	-5.11	118.44	121.00
2	A	3046	C	C2-N1-C1'	5.10	124.41	118.80
2	A	1490	U	C5-C6-N1	-5.10	120.15	122.70
2	A	977	G	N1-C6-O6	-5.10	116.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2276	G	O5'-P-OP1	-5.10	101.11	105.70
2	A	933	G	C4-N9-C1'	5.09	133.12	126.50
2	A	1212	U	C6-N1-C2	-5.09	117.95	121.00
2	A	796	A	N1-C2-N3	5.09	131.84	129.30
2	A	2798	G	C8-N9-C4	-5.08	104.37	106.40
2	A	1276	G	C4-N9-C1'	5.08	133.11	126.50
2	A	2245	C	C6-N1-C1'	-5.07	114.72	120.80
2	A	532	C	N1-C2-O2	-5.05	115.87	118.90
2	A	2545	G	C4-N9-C1'	5.05	133.07	126.50
2	A	2253	A	C8-N9-C4	5.05	107.82	105.80
2	A	1099	A	C6-C5-N7	-5.05	128.76	132.30
2	A	2912	A	C4-C5-N7	5.05	113.23	110.70
2	A	2085	C	P-O3'-C3'	5.05	125.76	119.70
2	A	1757	U	C2-N1-C1'	5.05	123.76	117.70
2	A	2300	A	C6-N1-C2	-5.05	115.57	118.60
2	A	482	U	C5-C6-N1	-5.04	120.18	122.70
2	A	2237	A	N1-C6-N6	-5.04	115.58	118.60
2	A	472	C	N3-C2-O2	-5.04	118.38	121.90
2	A	2745	C	C5-C6-N1	-5.03	118.48	121.00
2	A	1879	G	N1-C2-N3	5.03	126.92	123.90
2	A	2942	G	N3-C4-C5	-5.03	126.08	128.60
2	A	2671	G	C6-N1-C2	-5.03	122.08	125.10
2	A	1412	C	C6-N1-C2	-5.02	118.29	120.30
2	A	1766	U	N1-C2-N3	5.02	117.91	114.90
2	A	27	G	N3-C4-N9	5.02	129.01	126.00
2	A	1918	A	N1-C6-N6	5.01	121.61	118.60
2	A	1302	G	C8-N9-C1'	-5.01	120.48	127.00
2	A	1535	C	C2-N1-C1'	5.01	124.31	118.80
2	A	1993	G	N3-C4-N9	5.01	129.01	126.00
2	A	2243	C	C6-N1-C2	5.01	122.30	120.30
2	A	1918	A	C5-C6-N6	-5.01	119.69	123.70
2	A	1887	A	C5-C6-N1	5.01	120.20	117.70

There are no chirality outliers.

There are no planarity outliers.

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	3	21/24 (88%)	21 (100%)	0	0	100	100
4	C	273/278 (98%)	259 (95%)	14 (5%)	0	100	100
5	D	212/217 (98%)	199 (94%)	12 (6%)	1 (0%)	29	67
6	E	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	29	67
7	F	180/187 (96%)	164 (91%)	15 (8%)	1 (1%)	25	64
8	G	174/179 (97%)	166 (95%)	7 (4%)	1 (1%)	25	64
9	H	149/151 (99%)	140 (94%)	8 (5%)	1 (1%)	22	61
10	I	124/175 (71%)	117 (94%)	7 (6%)	0	100	100
11	J	131/142 (92%)	124 (95%)	7 (5%)	0	100	100
12	K	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
13	L	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
14	M	143/147 (97%)	135 (94%)	7 (5%)	1 (1%)	22	61
15	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
16	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100
17	P	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
18	Q	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
19	R	122/129 (95%)	116 (95%)	6 (5%)	0	100	100
20	S	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
21	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
22	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
23	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
24	W	190/215 (88%)	186 (98%)	4 (2%)	0	100	100
25	X	77/88 (88%)	73 (95%)	4 (5%)	0	100	100
26	Y	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
27	Z	62/77 (80%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
29	b	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
30	c	47/55 (86%)	44 (94%)	2 (4%)	1 (2%)	7	37
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
32	e	61/64 (95%)	61 (100%)	0	0	100	100
33	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	g	46/75 (61%)	46 (100%)	0	0	100	100
All	All	3615/3991 (91%)	3457 (96%)	151 (4%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	c	7	VAL
5	D	143	ALA
14	M	31	LYS
8	G	66	HIS
6	E	90	VAL
9	H	124	ILE
7	F	61	ILE

5.3.2 Protein sidechains ⓘ

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	3	18/19 (95%)	16 (89%)	2 (11%)	6	25
4	C	215/218 (99%)	193 (90%)	22 (10%)	7	29
5	D	160/163 (98%)	132 (82%)	28 (18%)	2	9
6	E	169/173 (98%)	153 (90%)	16 (10%)	8	32
7	F	151/156 (97%)	135 (89%)	16 (11%)	6	27
8	G	148/150 (99%)	131 (88%)	17 (12%)	5	24
9	H	90/116 (78%)	85 (94%)	5 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	89/120 (74%)	84 (94%)	5 (6%)	21	57
11	J	102/108 (94%)	88 (86%)	14 (14%)	3	17
12	K	119/120 (99%)	113 (95%)	6 (5%)	24	60
13	L	100/100 (100%)	90 (90%)	10 (10%)	7	30
14	M	112/114 (98%)	102 (91%)	10 (9%)	9	35
15	N	114/116 (98%)	104 (91%)	10 (9%)	10	36
16	O	97/158 (61%)	88 (91%)	9 (9%)	9	33
17	P	93/94 (99%)	86 (92%)	7 (8%)	13	45
18	Q	100/100 (100%)	92 (92%)	8 (8%)	12	42
19	R	97/99 (98%)	91 (94%)	6 (6%)	18	53
20	S	81/83 (98%)	74 (91%)	7 (9%)	10	38
21	T	90/117 (77%)	81 (90%)	9 (10%)	7	30
22	U	83/85 (98%)	80 (96%)	3 (4%)	35	69
23	V	81/86 (94%)	76 (94%)	5 (6%)	18	53
24	W	155/168 (92%)	139 (90%)	16 (10%)	7	29
25	X	58/63 (92%)	54 (93%)	4 (7%)	15	49
26	Y	50/51 (98%)	44 (88%)	6 (12%)	5	22
27	Z	58/66 (88%)	58 (100%)	0	100	100
28	a	52/54 (96%)	50 (96%)	2 (4%)	33	67
29	b	43/46 (94%)	38 (88%)	5 (12%)	5	24
30	c	47/52 (90%)	43 (92%)	4 (8%)	10	38
31	d	35/36 (97%)	32 (91%)	3 (9%)	10	38
32	e	53/54 (98%)	47 (89%)	6 (11%)	6	25
33	f	35/35 (100%)	33 (94%)	2 (6%)	20	56
34	g	43/63 (68%)	39 (91%)	4 (9%)	9	33
All	All	2938/3183 (92%)	2671 (91%)	267 (9%)	13	34

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	7	LYS
1	3	9	ARG
4	C	10	THR

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Mol	Chain	Res	Type
4	C	13	ARG
4	C	28	THR
4	C	58	HIS
4	C	60	ARG
4	C	63	ARG
4	C	78	LYS
4	C	89	THR
4	C	116	VAL
4	C	119	SER
4	C	131	LEU
4	C	157	ARG
4	C	161	VAL
4	C	177	MET
4	C	181	GLU
4	C	203	ASN
4	C	211	ARG
4	C	213	ARG
4	C	241	SER
4	C	258	ARG
4	C	271	ARG
4	C	272	ARG
5	D	3	ARG
5	D	19	GLU
5	D	38	ARG
5	D	44	ARG
5	D	58	SER
5	D	60	ARG
5	D	79	ARG
5	D	85	ARG
5	D	86	LEU
5	D	87	ASP
5	D	99	GLN
5	D	102	THR
5	D	126	THR
5	D	129	ARG
5	D	133	ARG
5	D	144	VAL
5	D	147	ARG
5	D	151	ILE
5	D	154	CYS
5	D	162	LYS
5	D	164	THR

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Mol	Chain	Res	Type
5	D	169	ARG
5	D	170	MET
5	D	192	LEU
5	D	198	ILE
5	D	201	ARG
5	D	208	VAL
5	D	209	ARG
6	E	34	MET
6	E	50	HIS
6	E	78	SER
6	E	79	THR
6	E	97	ASP
6	E	128	THR
6	E	131	VAL
6	E	135	THR
6	E	137	SER
6	E	149	THR
6	E	161	THR
6	E	169	VAL
6	E	170	ARG
6	E	179	SER
6	E	181	ASP
6	E	201	LEU
7	F	20	ARG
7	F	31	ASN
7	F	44	ASN
7	F	78	ARG
7	F	87	ARG
7	F	102	ARG
7	F	130	ASP
7	F	148	ILE
7	F	150	VAL
7	F	151	ASP
7	F	157	ARG
7	F	159	MET
7	F	164	VAL
7	F	165	THR
7	F	174	ARG
7	F	182	PHE
8	G	3	ARG
8	G	35	LEU
8	G	42	SER

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Mol	Chain	Res	Type
8	G	48	ASP
8	G	55	ARG
8	G	59	GLU
8	G	65	LEU
8	G	73	ILE
8	G	77	VAL
8	G	90	ILE
8	G	114	VAL
8	G	135	SER
8	G	137	ILE
8	G	153	ARG
8	G	156	ASP
8	G	171	ARG
8	G	172	ARG
9	H	4	ILE
9	H	25	TYR
9	H	40	SER
9	H	88	THR
9	H	124	ILE
10	I	55	THR
10	I	79	ILE
10	I	82	VAL
10	I	103	LEU
10	I	115	LEU
11	J	15	ILE
11	J	30	LEU
11	J	36	ASN
11	J	42	LYS
11	J	48	THR
11	J	52	ARG
11	J	55	VAL
11	J	56	ILE
11	J	87	VAL
11	J	99	VAL
11	J	113	THR
11	J	114	LYS
11	J	117	ASP
11	J	119	ASN
12	K	17	VAL
12	K	70	THR
12	K	85	ARG
12	K	96	HIS

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Mol	Chain	Res	Type
12	K	118	ILE
12	K	129	ASP
13	L	7	ARG
13	L	13	ASN
13	L	20	LEU
13	L	40	VAL
13	L	58	VAL
13	L	69	ARG
13	L	73	ASP
13	L	87	ILE
13	L	90	ASP
13	L	96	THR
14	M	22	VAL
14	M	24	ARG
14	M	31	LYS
14	M	40	THR
14	M	43	ARG
14	M	46	VAL
14	M	49	MET
14	M	70	ARG
14	M	105	ARG
14	M	146	GLU
15	N	7	VAL
15	N	10	ARG
15	N	16	GLU
15	N	18	ARG
15	N	20	ILE
15	N	51	ARG
15	N	72	ARG
15	N	76	LYS
15	N	82	ARG
15	N	130	ARG
16	O	6	LYS
16	O	9	ARG
16	O	10	LEU
16	O	27	SER
16	O	33	ARG
16	O	37	THR
16	O	64	ARG
16	O	71	ARG
16	O	96	ARG
17	P	6	VAL

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Mol	Chain	Res	Type
17	P	10	ILE
17	P	12	GLU
17	P	24	ARG
17	P	32	THR
17	P	51	LEU
17	P	74	ASP
18	Q	15	ASP
18	Q	25	VAL
18	Q	32	ILE
18	Q	54	ILE
18	Q	57	THR
18	Q	79	ASN
18	Q	93	ARG
18	Q	96	LEU
19	R	6	ARG
19	R	15	ARG
19	R	29	SER
19	R	42	SER
19	R	44	THR
19	R	91	ASP
20	S	23	LYS
20	S	27	LEU
20	S	30	GLU
20	S	54	ASP
20	S	58	VAL
20	S	68	THR
20	S	72	LYS
21	T	15	ARG
21	T	19	VAL
21	T	20	SER
21	T	22	THR
21	T	26	ARG
21	T	84	ASP
21	T	99	ARG
21	T	104	ARG
21	T	107	THR
22	U	41	GLN
22	U	62	ARG
22	U	81	ARG
23	V	38	VAL
23	V	42	LYS
23	V	69	SER

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Mol	Chain	Res	Type
23	V	83	VAL
23	V	91	THR
24	W	12	THR
24	W	14	ASN
24	W	15	VAL
24	W	19	THR
24	W	33	VAL
24	W	64	ASN
24	W	68	THR
24	W	91	ASN
24	W	112	VAL
24	W	114	VAL
24	W	119	THR
24	W	131	ILE
24	W	139	SER
24	W	146	VAL
24	W	158	THR
24	W	172	SER
25	X	38	VAL
25	X	39	ARG
25	X	41	ARG
25	X	80	ILE
26	Y	17	SER
26	Y	19	SER
26	Y	24	ARG
26	Y	28	ARG
26	Y	36	VAL
26	Y	45	ASN
28	a	3	GLU
28	a	48	ASN
29	b	6	ARG
29	b	8	MET
29	b	10	ARG
29	b	14	ARG
29	b	35	GLN
30	c	6	ASP
30	c	25	THR
30	c	38	ILE
30	c	47	THR
31	d	13	ARG
31	d	15	ARG
31	d	46	THR

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Mol	Chain	Res	Type
32	e	11	SER
32	e	13	ARG
32	e	19	THR
32	e	47	ARG
32	e	56	SER
32	e	59	ASN
33	f	2	LYS
33	f	7	VAL
34	g	9	TYR
34	g	12	THR
34	g	22	PHE
34	g	46	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
1	3	18	HIS
4	C	38	HIS
4	C	76	ASN
4	C	129	ASN
4	C	205	ASN
5	D	34	ASN
5	D	51	GLN
5	D	99	GLN
5	D	179	ASN
6	E	125	HIS
6	E	171	ASN
6	E	202	ASN
7	F	62	ASN
7	F	146	HIS
8	G	66	HIS
8	G	86	GLN
9	H	11	HIS
9	H	147	ASN
11	J	33	HIS
12	K	77	HIS
12	K	103	ASN
12	K	132	HIS
13	L	3	GLN
13	L	13	ASN
14	M	58	HIS

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Mol	Chain	Res	Type
14	M	76	GLN
14	M	127	ASN
15	N	13	HIS
15	N	123	HIS
16	O	17	GLN
17	P	22	HIS
17	P	41	ASN
17	P	53	ASN
18	Q	28	HIS
18	Q	50	GLN
18	Q	79	ASN
19	R	11	GLN
19	R	41	HIS
19	R	94	ASN
19	R	122	ASN
20	S	76	HIS
20	S	85	HIS
21	T	67	ASN
22	U	41	GLN
22	U	58	ASN
22	U	61	ASN
23	V	31	ASN
23	V	67	HIS
23	V	101	ASN
24	W	46	HIS
24	W	61	HIS
24	W	76	GLN
24	W	94	HIS
25	X	29	GLN
25	X	44	HIS
26	Y	22	HIS
26	Y	45	ASN
29	b	36	GLN
30	c	22	ASN
30	c	48	HIS
31	d	36	ASN
32	e	25	GLN
32	e	31	HIS
32	e	63	ASN
33	f	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	784 (25%)	30 (0%)
3	B	117/118 (99%)	28 (23%)	2 (1%)
35	2	2/3 (66%)	2 (100%)	0
All	All	3237/3241 (99%)	814 (25%)	32 (0%)

All (814) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	33	G
2	A	46	A
2	A	48	G
2	A	55	G
2	A	59	G
2	A	60	A
2	A	68	A
2	A	71	A
2	A	72	G
2	A	83	C
2	A	89	A
2	A	90	C
2	A	91	C
2	A	94	G
2	A	98	U
2	A	99	G
2	A	115	A
2	A	116	A
2	A	117	U
2	A	120	G
2	A	122	A
2	A	125	C
2	A	128	G
2	A	129	G
2	A	133	G
2	A	136	U
2	A	137	G
2	A	145	G
2	A	148	A

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Mol	Chain	Res	Type
2	A	161	U
2	A	164	A
2	A	171	U
2	A	172	C
2	A	175	G
2	A	177	G
2	A	195	A
2	A	198	A
2	A	203	A
2	A	205	U
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	237	C
2	A	245	G
2	A	248	G
2	A	264	G
2	A	265	A
2	A	268	G
2	A	270	U
2	A	271	A
2	A	272	A
2	A	274	C
2	A	275	C
2	A	276	G
2	A	279	U
2	A	280	G
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C

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Mol	Chain	Res	Type
2	A	292	G
2	A	294	G
2	A	297	G
2	A	299	G
2	A	300	G
2	A	301	U
2	A	302	U
2	A	303	G
2	A	305	G
2	A	306	U
2	A	312	G
2	A	315	U
2	A	316	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	322	A
2	A	323	C
2	A	324	C
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	343	U
2	A	344	G
2	A	345	G
2	A	346	C
2	A	348	G
2	A	350	A
2	A	351	G
2	A	352	G
2	A	353	G
2	A	356	G
2	A	357	U
2	A	358	G
2	A	361	A
2	A	364	A
2	A	369	G
2	A	370	U
2	A	371	G

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Mol	Chain	Res	Type
2	A	376	G
2	A	383	U
2	A	384	G
2	A	386	C
2	A	388	U
2	A	393	U
2	A	404	A
2	A	406	A
2	A	412	A
2	A	413	G
2	A	417	C
2	A	424	G
2	A	434	G
2	A	438	U
2	A	445	U
2	A	446	G
2	A	450	G
2	A	452	G
2	A	459	A
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	491	U
2	A	493	U
2	A	497	G
2	A	498	G
2	A	499	G
2	A	500	A
2	A	503	A
2	A	505	C
2	A	509	U
2	A	512	G
2	A	533	C
2	A	543	U
2	A	544	U
2	A	562	G
2	A	566	A
2	A	569	G
2	A	570	U
2	A	572	C
2	A	581	G

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Mol	Chain	Res	Type
2	A	589	A
2	A	591	G
2	A	592	A
2	A	594	U
2	A	595	A
2	A	596	C
2	A	605	G
2	A	606	U
2	A	614	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	630	U
2	A	631	C
2	A	634	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	643	G
2	A	644	G
2	A	647	G
2	A	655	G
2	A	658	U
2	A	665	G
2	A	666	A
2	A	667	A
2	A	675	G
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	700	U
2	A	701	A
2	A	702	A
2	A	704	C
2	A	706	G

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Mol	Chain	Res	Type
2	A	707	G
2	A	708	G
2	A	709	U
2	A	712	G
2	A	721	A
2	A	728	G
2	A	731	A
2	A	738	A
2	A	739	U
2	A	740	A
2	A	742	G
2	A	747	A
2	A	753	A
2	A	757	G
2	A	758	A
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	767	U
2	A	768	G
2	A	774	G
2	A	779	U
2	A	783	G
2	A	784	G
2	A	785	A
2	A	793	C
2	A	794	G
2	A	801	U
2	A	813	C
2	A	816	G
2	A	827	G
2	A	829	U
2	A	839	U
2	A	841	G
2	A	843	G
2	A	845	C
2	A	862	U
2	A	863	G
2	A	871	A
2	A	872	G
2	A	878	G

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Mol	Chain	Res	Type
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	892	G
2	A	897	A
2	A	898	A
2	A	899	G
2	A	900	G
2	A	904	A
2	A	905	U
2	A	907	A
2	A	917	A
2	A	919	A
2	A	920	G
2	A	921	C
2	A	927	C
2	A	942	U
2	A	960	G
2	A	961	U
2	A	971	G
2	A	973	G
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A
2	A	990	G
2	A	994	A
2	A	995	U
2	A	996	G
2	A	998	G
2	A	1000	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1005	A
2	A	1007	G
2	A	1009	U
2	A	1011	A
2	A	1012	C
2	A	1013	U
2	A	1014	G

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Mol	Chain	Res	Type
2	A	1022	C
2	A	1025	A
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1058	A
2	A	1063	G
2	A	1070	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G
2	A	1091	A
2	A	1092	G
2	A	1099	A
2	A	1101	A
2	A	1107	G
2	A	1108	A
2	A	1114	G
2	A	1127	A
2	A	1130	C
2	A	1131	G
2	A	1135	G
2	A	1140	G
2	A	1144	A
2	A	1148	G
2	A	1151	U
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1175	A
2	A	1176	G
2	A	1178	U
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G

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Mol	Chain	Res	Type
2	A	1190	C
2	A	1191	A
2	A	1192	G
2	A	1198	C
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1204	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1227	C
2	A	1229	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1234	U
2	A	1237	U
2	A	1238	G
2	A	1240	G
2	A	1246	A
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1267	A
2	A	1275	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1294	U
2	A	1324	G
2	A	1325	U
2	A	1332	G

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Mol	Chain	Res	Type
2	A	1335	G
2	A	1339	G
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1359	G
2	A	1362	A
2	A	1363	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1390	A
2	A	1404	C
2	A	1415	A
2	A	1416	A
2	A	1417	A
2	A	1433	G
2	A	1435	C
2	A	1437	A
2	A	1440	C
2	A	1447	G
2	A	1448	C
2	A	1456	G
2	A	1461	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U
2	A	1499	A
2	A	1502	G
2	A	1506	U
2	A	1507	G
2	A	1510	A
2	A	1518	A
2	A	1521	C
2	A	1522	G
2	A	1531	C
2	A	1532	G

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Mol	Chain	Res	Type
2	A	1533	U
2	A	1534	C
2	A	1536	A
2	A	1540	U
2	A	1543	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1574	G
2	A	1578	G
2	A	1579	C
2	A	1587	G
2	A	1588	G
2	A	1596	C
2	A	1599	U
2	A	1600	G
2	A	1625	G
2	A	1627	U
2	A	1628	A
2	A	1629	G
2	A	1630	U
2	A	1631	A
2	A	1632	G
2	A	1633	U
2	A	1637	G
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1659	U
2	A	1673	A
2	A	1674	G
2	A	1679	A
2	A	1680	A

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Mol	Chain	Res	Type
2	A	1681	U
2	A	1688	G
2	A	1703	G
2	A	1705	C
2	A	1710	A
2	A	1711	G
2	A	1714	A
2	A	1715	A
2	A	1717	U
2	A	1720	G
2	A	1723	U
2	A	1724	G
2	A	1725	G
2	A	1728	U
2	A	1729	A
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1738	G
2	A	1746	G
2	A	1754	G
2	A	1755	A
2	A	1756	G
2	A	1757	U
2	A	1761	G
2	A	1767	U
2	A	1774	U
2	A	1785	C
2	A	1786	G
2	A	1789	A
2	A	1792	A
2	A	1796	U
2	A	1798	U
2	A	1802	G
2	A	1803	A
2	A	1805	G
2	A	1806	A
2	A	1813	C
2	A	1825	C
2	A	1826	A
2	A	1845	G
2	A	1857	U

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Mol	Chain	Res	Type
2	A	1862	C
2	A	1864	U
2	A	1866	C
2	A	1867	G
2	A	1869	G
2	A	1870	U
2	A	1871	G
2	A	1872	A
2	A	1887	A
2	A	1892	G
2	A	1893	C
2	A	1916	A
2	A	1932	U
2	A	1933	G
2	A	1945	U
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1949	C
2	A	1950	G
2	A	1954	C
2	A	1967	G
2	A	1973	C
2	A	1975	A
2	A	1981	U
2	A	1990	A
2	A	1999	U
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2047	C
2	A	2064	A
2	A	2065	A
2	A	2066	G
2	A	2073	A
2	A	2075	G
2	A	2084	A
2	A	2085	C
2	A	2086	U

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Mol	Chain	Res	Type
2	A	2087	C
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A
2	A	2107	G
2	A	2108	A
2	A	2111	U
2	A	2112	U
2	A	2120	A
2	A	2129	C
2	A	2130	G
2	A	2131	G
2	A	2137	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2151	A
2	A	2153	G
2	A	2154	G
2	A	2160	A
2	A	2162	A
2	A	2163	U
2	A	2164	U
2	A	2179	U
2	A	2184	A
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2226	U
2	A	2227	A
2	A	2242	G

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Mol	Chain	Res	Type
2	A	2244	A
2	A	2247	A
2	A	2251	G
2	A	2254	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2274	C
2	A	2276	G
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2299	C
2	A	2316	G
2	A	2320	C
2	A	2325	U
2	A	2328	G
2	A	2329	G
2	A	2330	U
2	A	2334	U
2	A	2335	G
2	A	2336	U
2	A	2338	G
2	A	2339	G
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2368	C
2	A	2369	C
2	A	2371	G

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Mol	Chain	Res	Type
2	A	2372	U
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2390	U
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2413	G
2	A	2418	U
2	A	2421	A
2	A	2427	G
2	A	2434	A
2	A	2436	A
2	A	2447	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2483	G
2	A	2492	A
2	A	2502	A
2	A	2504	G
2	A	2507	C
2	A	2508	C
2	A	2510	A
2	A	2511	A
2	A	2512	A
2	A	2529	A
2	A	2532	G

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Mol	Chain	Res	Type
2	A	2536	U
2	A	2545	G
2	A	2549	G
2	A	2551	A
2	A	2558	C
2	A	2559	A
2	A	2567	U
2	A	2569	G
2	A	2571	C
2	A	2574	C
2	A	2581	G
2	A	2585	U
2	A	2596	G
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2626	U
2	A	2627	C
2	A	2630	A
2	A	2643	U
2	A	2644	C
2	A	2647	U
2	A	2649	A
2	A	2650	A
2	A	2653	G
2	A	2654	A
2	A	2655	U
2	A	2659	A
2	A	2665	C
2	A	2671	G
2	A	2672	A
2	A	2673	U
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2702	A
2	A	2704	C
2	A	2705	G

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Mol	Chain	Res	Type
2	A	2715	U
2	A	2726	G
2	A	2729	G
2	A	2742	A
2	A	2744	C
2	A	2749	G
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2793	G
2	A	2796	A
2	A	2797	C
2	A	2802	G
2	A	2806	G
2	A	2810	U
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2839	U
2	A	2853	C
2	A	2856	A
2	A	2865	G
2	A	2870	C
2	A	2885	G
2	A	2887	G
2	A	2906	U
2	A	2912	A
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2937	G
2	A	2938	G
2	A	2948	C
2	A	2950	C
2	A	2953	U
2	A	2957	A
2	A	2968	G

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Mol	Chain	Res	Type
2	A	2972	A
2	A	2982	A
2	A	2985	G
2	A	2986	G
2	A	3002	A
2	A	3004	C
2	A	3005	A
2	A	3009	U
2	A	3011	C
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3020	U
2	A	3021	A
2	A	3022	G
2	A	3024	A
2	A	3027	G
2	A	3029	U
2	A	3042	A
2	A	3047	A
2	A	3056	A
2	A	3064	G
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3095	C
2	A	3100	A
2	A	3101	C
2	A	3105	C
2	A	3106	C
2	A	3107	G
2	A	3112	A
2	A	3113	A
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	6	G
3	B	7	G
3	B	9	G
3	B	11	U
3	B	12	C
3	B	13	C

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Mol	Chain	Res	Type
3	B	14	A
3	B	20	G
3	B	21	C
3	B	22	A
3	B	25	G
3	B	30	G
3	B	35	G
3	B	36	U
3	B	37	C
3	B	42	C
3	B	46	A
3	B	57	U
3	B	58	A
3	B	87	U
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	112	C
3	B	114	A
3	B	115	A
35	2	75	C
35	2	76	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	284	G
2	A	287	A
2	A	316	U
2	A	357	U
2	A	445	U
2	A	759	G
2	A	919	A
2	A	974	G
2	A	981	U
2	A	1004	C
2	A	1010	U
2	A	1046	C
2	A	1084	U

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Mol	Chain	Res	Type
2	A	1186	G
2	A	1231	U
2	A	1344	A
2	A	1368	A
2	A	1713	U
2	A	1730	U
2	A	1947	U
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2350	G
2	A	2381	A
2	A	2407	C
2	A	2626	U
2	A	3113	A
3	B	3	U
3	B	10	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 413 ligands modelled in this entry, 412 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	PHE	2	1002	35	10,11,12	0.66	0	10,13,15	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PHE	2	1002	35	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

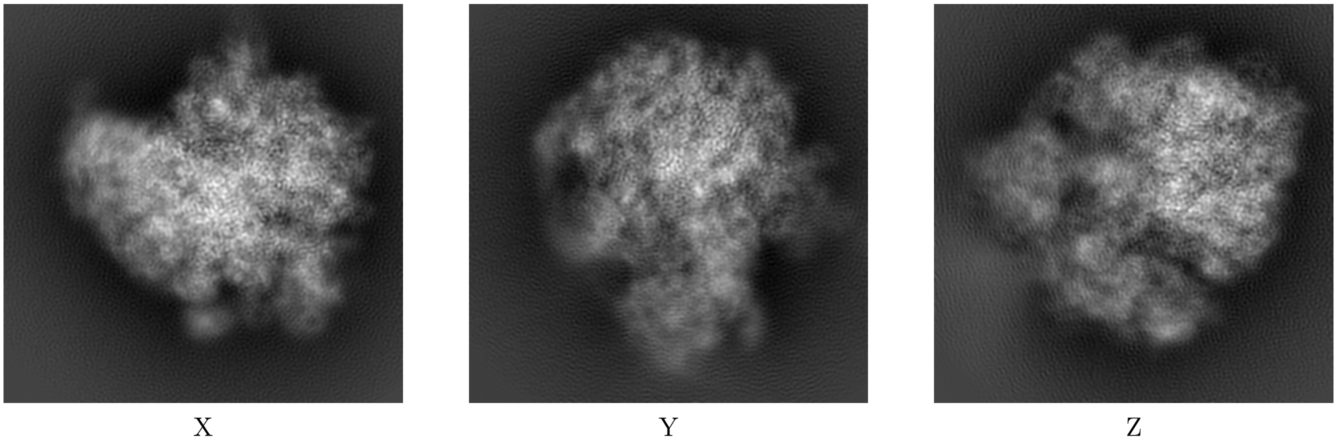
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3750. 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 ⓘ

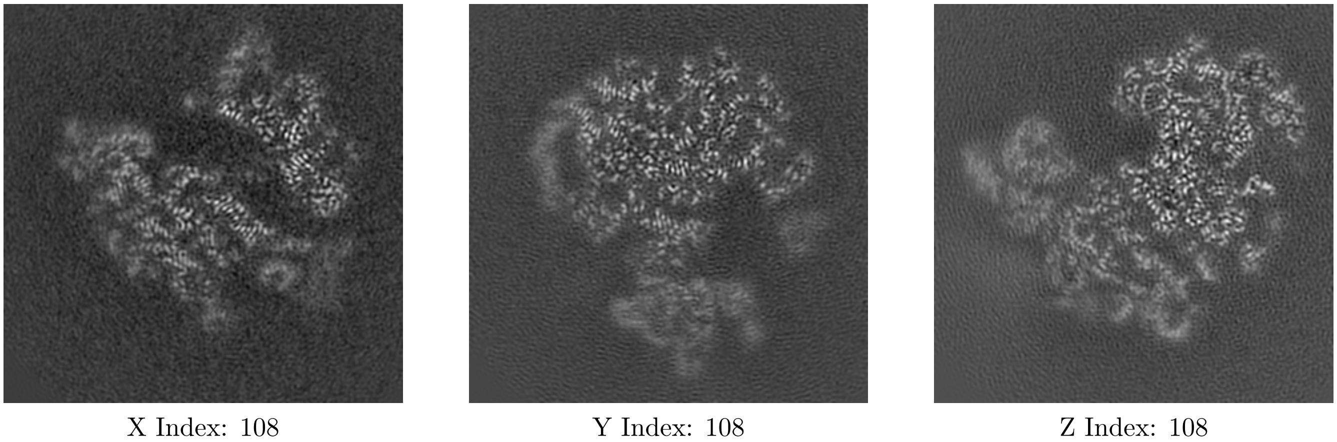
6.1.1 Primary map



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

6.2 Central slices ⓘ

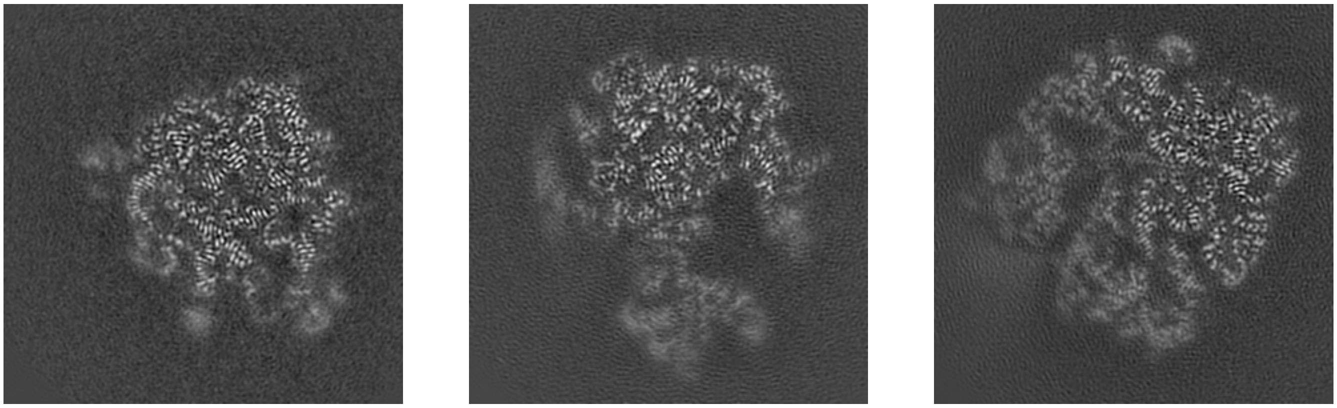
6.2.1 Primary map



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

6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 148 Y Index: 114 Z Index: 124

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

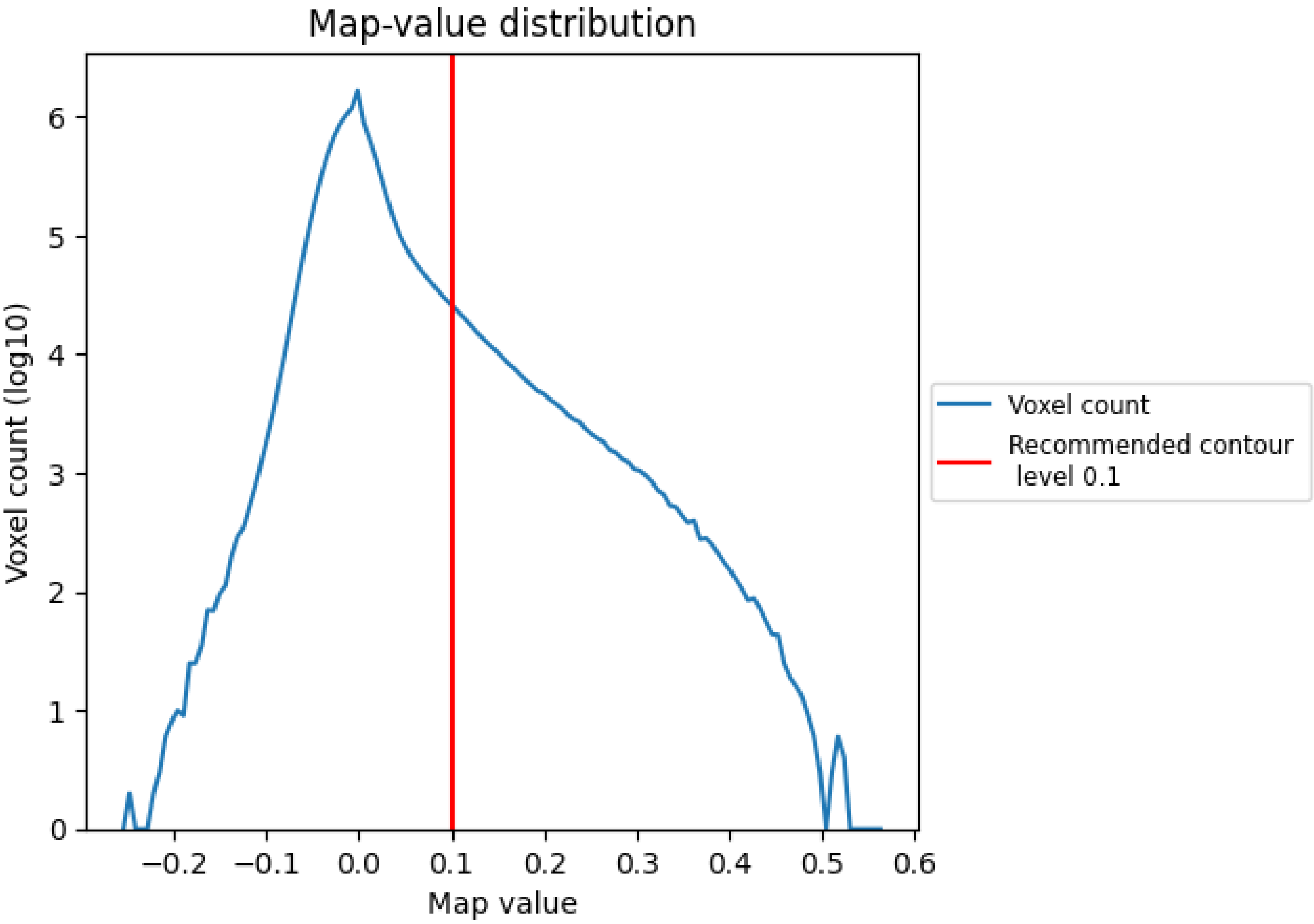
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

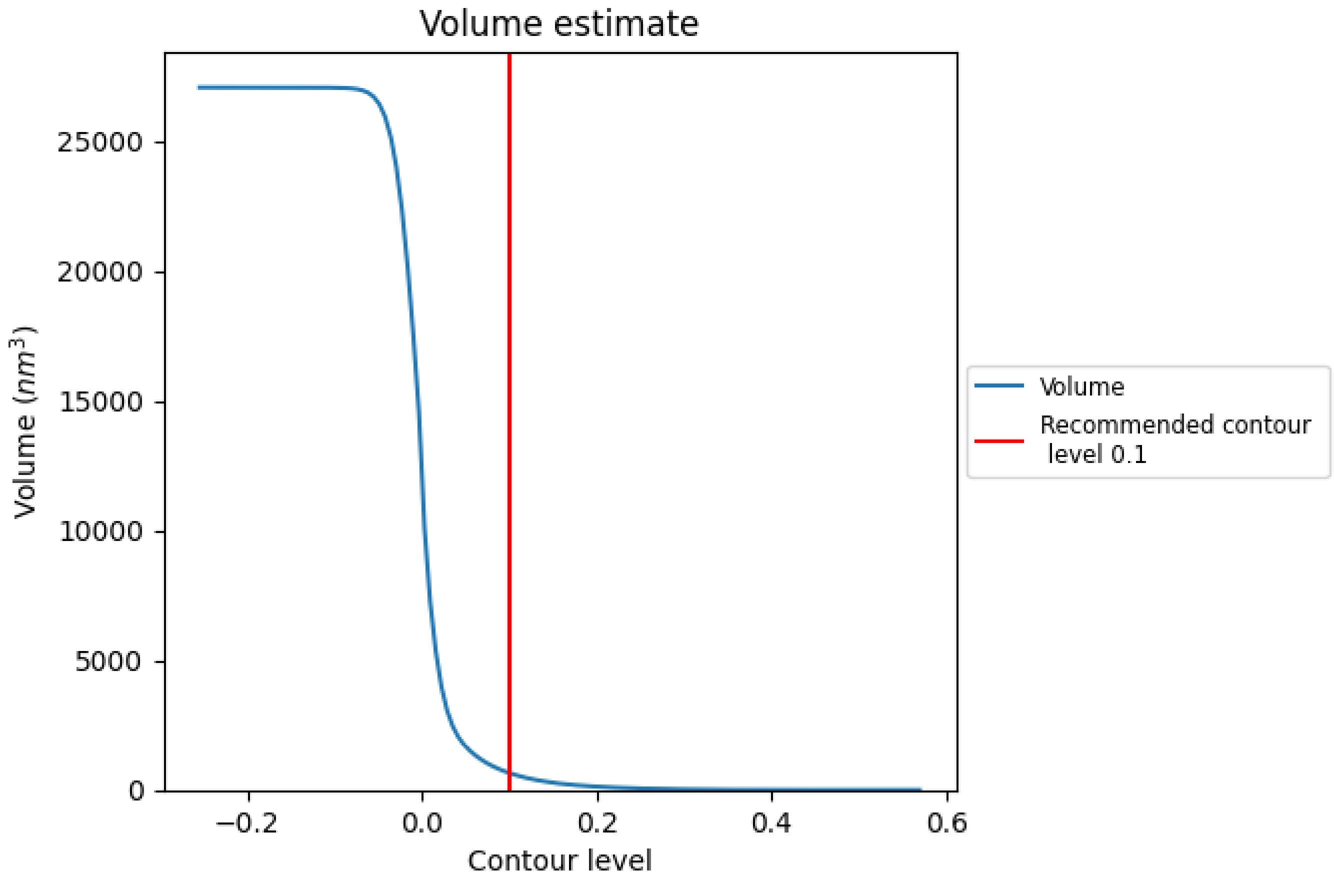
This section contains the results of statistical analysis of the map.

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.

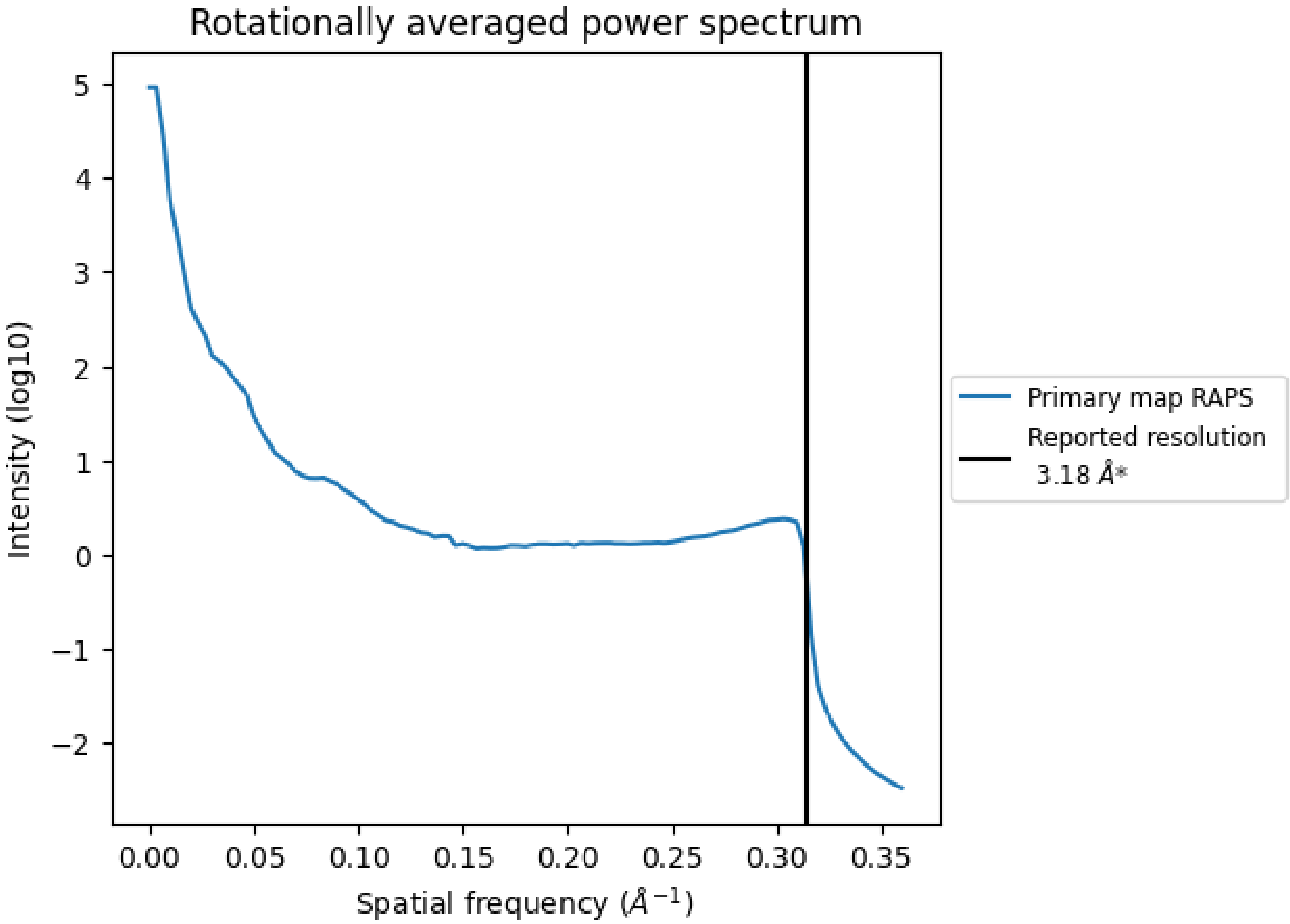
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 651 nm^3; this corresponds to an approximate mass of 588 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)

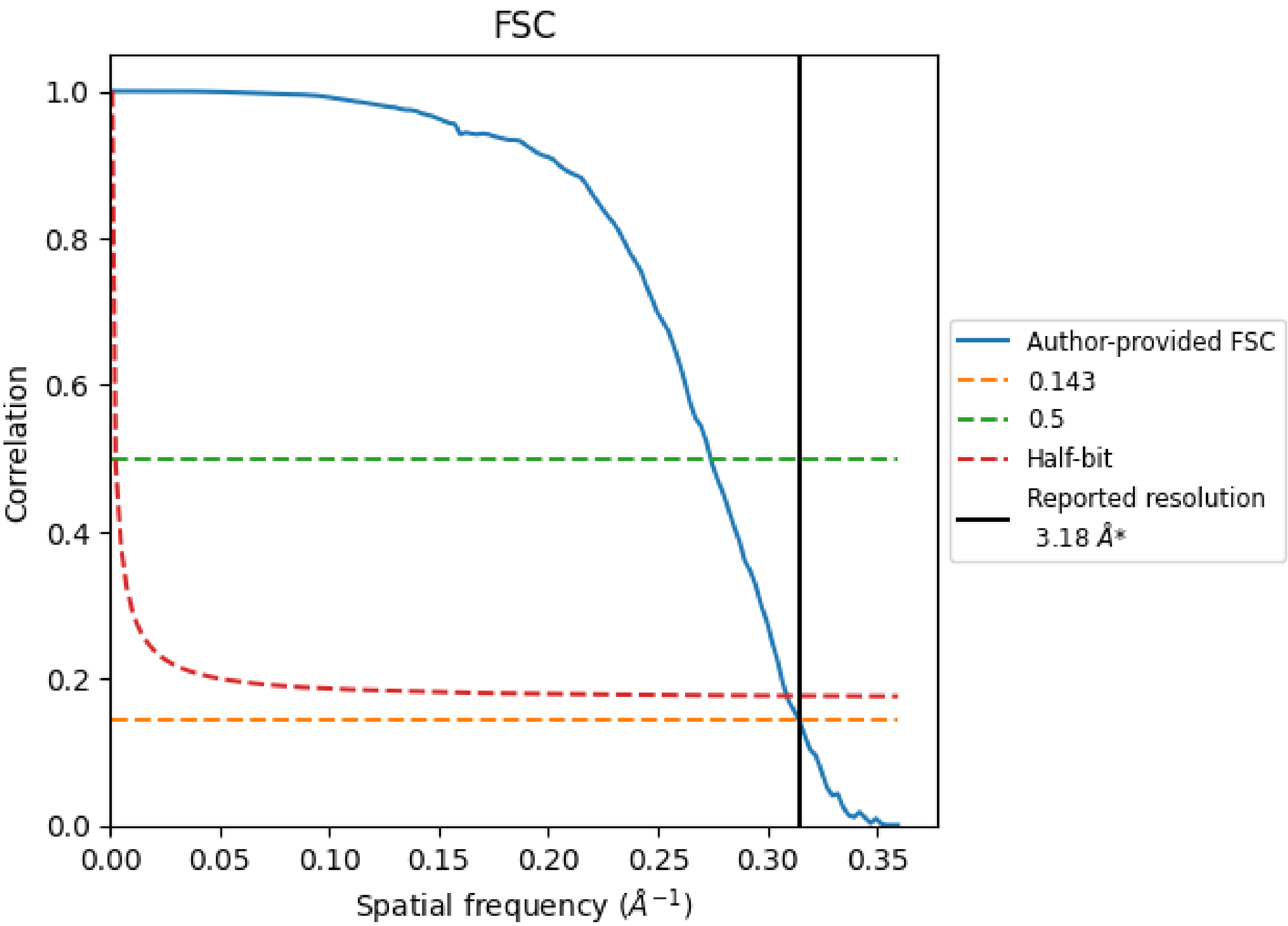


*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8.2 Resolution estimates ⓘ

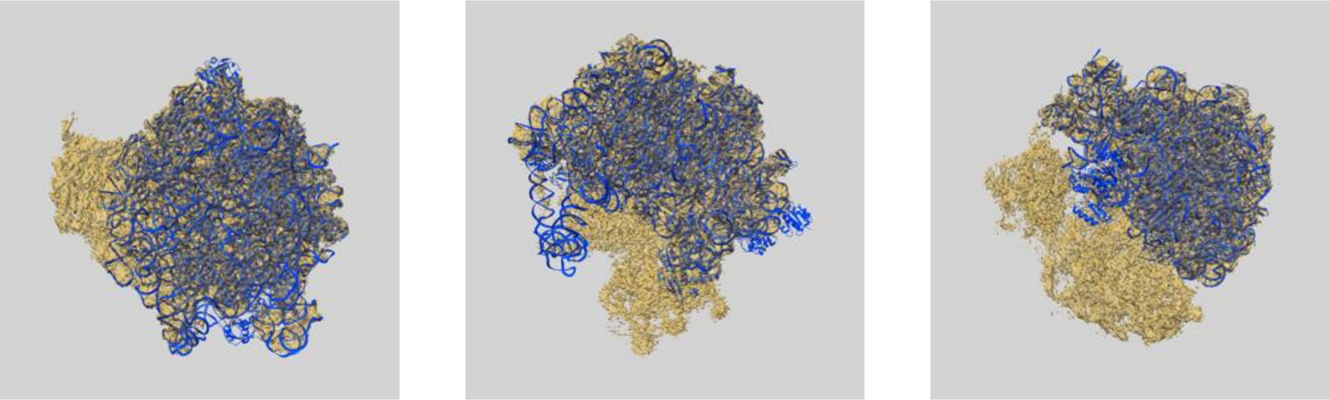
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.65	3.24
Unmasked-calculated*	-	-	-

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3750 and PDB model 5O60. Per-residue inclusion information can be found in section 3 on page 12.

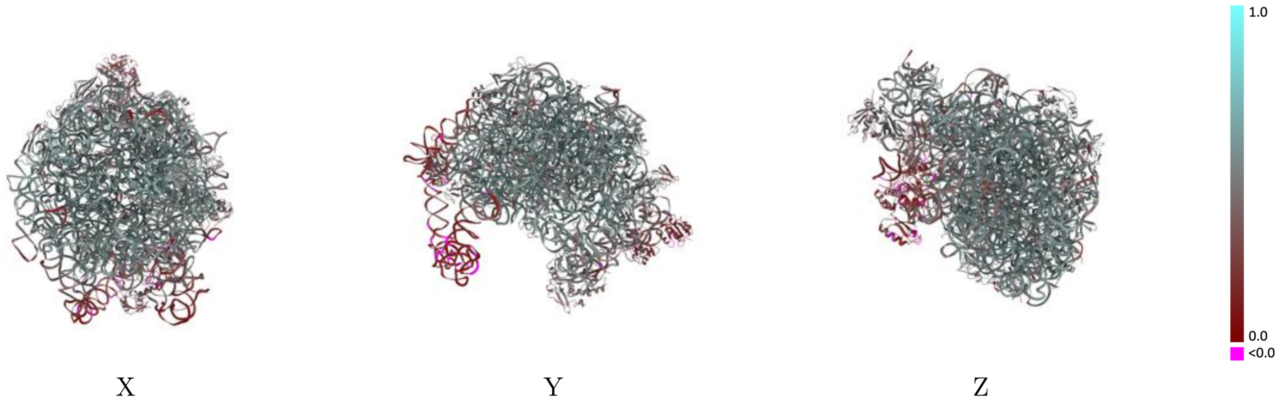
9.1 Map-model overlay



X Y Z

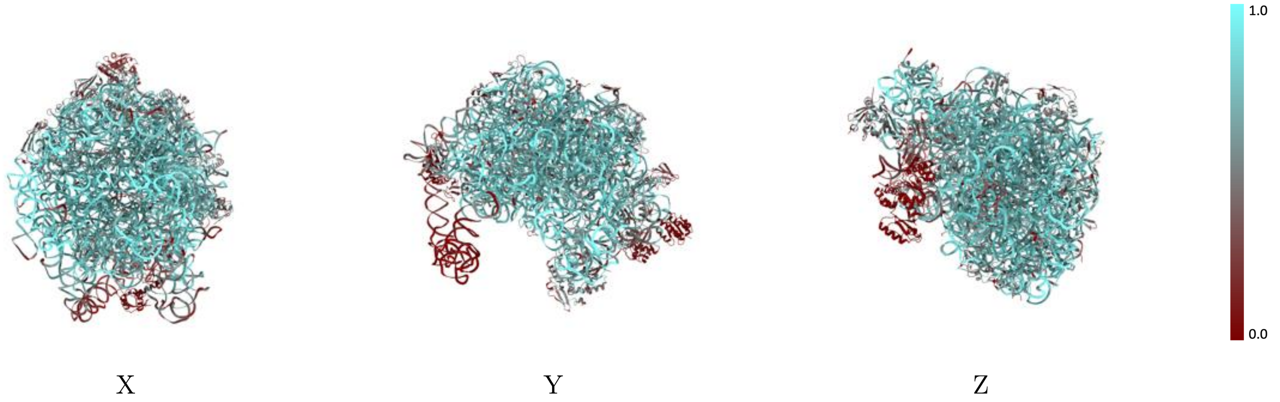
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



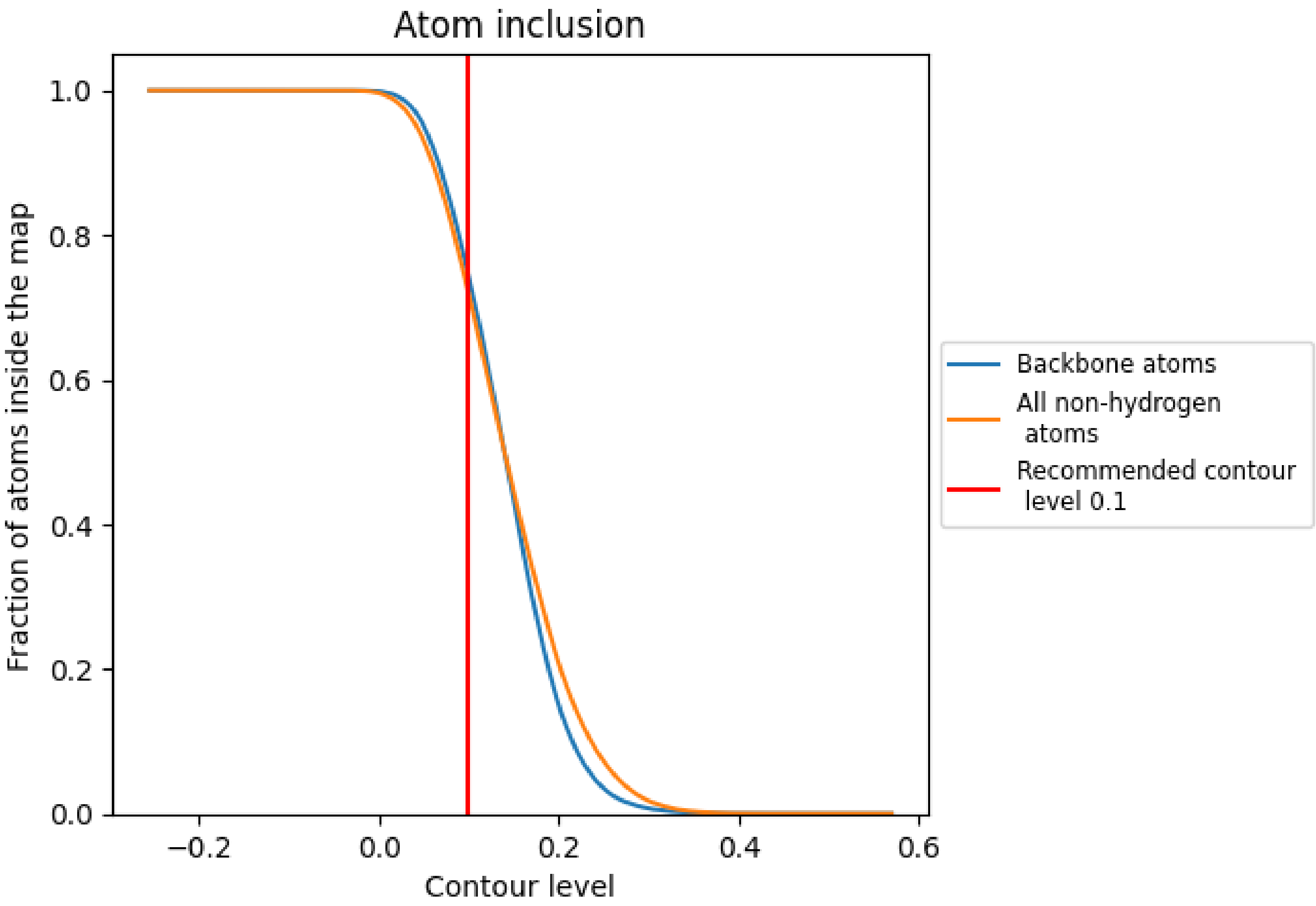
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 72% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7186	0.4870
2	0.3919	0.4480
3	0.6927	0.5360
A	0.7888	0.4960
B	0.8297	0.5010
C	0.6484	0.5250
D	0.6772	0.5280
E	0.6038	0.4950
F	0.4793	0.4130
G	0.4440	0.4210
H	0.1032	0.3400
I	0.0165	0.1790
J	0.0327	0.1890
K	0.6426	0.5110
L	0.5560	0.4970
M	0.6138	0.4920
N	0.6113	0.5130
O	0.7021	0.5290
P	0.6085	0.4780
Q	0.5625	0.4740
R	0.7061	0.5300
S	0.6040	0.5160
T	0.6275	0.5110
U	0.5459	0.4750
V	0.4847	0.4470
W	0.4051	0.4260
X	0.6961	0.5410
Y	0.6454	0.5160
Z	0.5784	0.4500
a	0.6601	0.5110
b	0.6144	0.5060
c	0.6364	0.4970
d	0.6934	0.5490
e	0.6750	0.5310
f	0.7049	0.5250
g	0.4321	0.4090