Full wwPDB EM Validation Report (i)

Mar 4, 2024 – 07:30 PM EST

PDB ID	:	6DZI
EMDB ID	:	EMD-8932
Title	:	Cryo-EM Structure of Mycobacterium smegmatis 70S C(minus) ribosome 70S-MPY complex
Authors	:	Sharma, M.R.; Li, Y.; Korripella, R.; Yang, Y.; Kaushal, P.S.; Lin, Q.; Wade, J.T.; Gray, A.G.; Derbyshire, K.M.; Agrawal, R.K.; Ojha, A.
Deposited on	:	2018-07-05
Resolution	:	3.46 Å(reported)

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

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

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

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

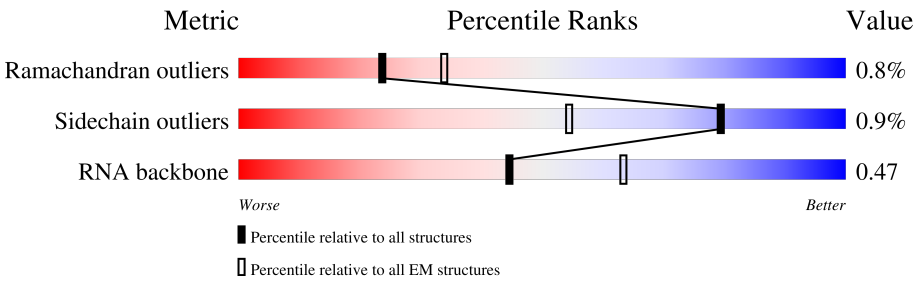
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.46 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	h	1511	72% 26% •
2	j	32	• 100%
3	k	208	• 99% •
4	l	200	• 100%
5	m	180	• 98% •
6	n	96	98% •
7	p	155	• 99% •
8	q	131	98% •

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Mol	Chain	Length	Quality of chain
9	4	126	97%
10	s	99	100%
11	t	115	99%
12	u	122	98%
13	v	116	100%
14	x	88	99%
15	z	113	100%
16	5	94	97%
17	6	82	5%, 100%
18	7	85	95%, 5%
19	8	228	34%, 83%, 13%
20	r	84	17%, 100%
21	Y	103	30%, 100%
22	9	100	100%
23	A	3119	69%, 29%
24	B	118	79%, 20%
25	C	275	98%
26	D	214	98%
27	E	209	99%
28	F	182	98%
29	G	176	99%
30	H	151	33%, 99%
31	I	126	17%, 99%
32	J	133	5%, 98%
33	K	146	100%

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Mol	Chain	Length	Quality of chain
34	L	122	100%
35	M	145	98%
36	N	136	99%
37	O	118	100%
38	P	126	98%
39	Q	113	96%
40	R	124	100%
41	S	100	99%
42	T	114	97%
43	U	97	100%
44	V	105	91% 8%
45	W	192	99%
46	X	79	97%
47	Z	64	98%
48	a	59	100%
49	b	54	94% 6%
50	c	53	19% 79% 19%
51	d	46	98%
52	e	63	100%
53	f	37	100%
54	g	82	82% 10% 9%
55	y	77	83% 14%
56	3	23	100%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 150868 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	h	1511	32439	14448	5930	10550	1511	0	0

- Molecule 2 is a protein called CONSERVED PROTEIN DOMAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	j	32	280	172	71	36	1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	k	208	1660	1036	322	298	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	l	200	1641	1028	316	295	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	m	180	1296	812	245	235	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	n	96	771	486	138	145	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	p	155	1232	768	241	221	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	q	131	1010	633	189	187	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	4	126	994	630	194	170	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	s	99	788	495	146	144	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	t	115	855	528	170	156	1	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	u	122	958	594	197	165	2	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	v	116	935	572	191	169	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	x	88	720	449	147	124	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	z	113	891	570	162	159	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	5	94	748	469	142	135	2	0	0

- Molecule 17 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	6	82	662	425	124	112	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	7	85	660	402	139	119	0	0

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	8	228	1793	1132	322	330	9	0	0

- Molecule 20 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	r	84	659	408	131	116	4	0	0

- Molecule 21 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Y	103	861	529	175	155	2	0	0

- Molecule 22 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	9	100	819	497	183	138	1	0	0

- Molecule 23 is a RNA chain called 23 S rRNA (3119-MER).

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

- Molecule 24 is a RNA chain called 5S RNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	B	118	2522	1126	468	810	118	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	C	275	2110	1298	438	370	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	D	214	1587	982	310	290	5	0	0

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	E	209	1569	969	295	303	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	H	151	1119	695	209	214	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L10.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

- Molecule 50 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	c	53	456	281	97	78	0	0

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	g	75	593	379	103	110	1	0	0

- Molecule 55 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	y	77	617	377	132	106	2	0	0

- Molecule 56 is a protein called Uncharacterized protein.

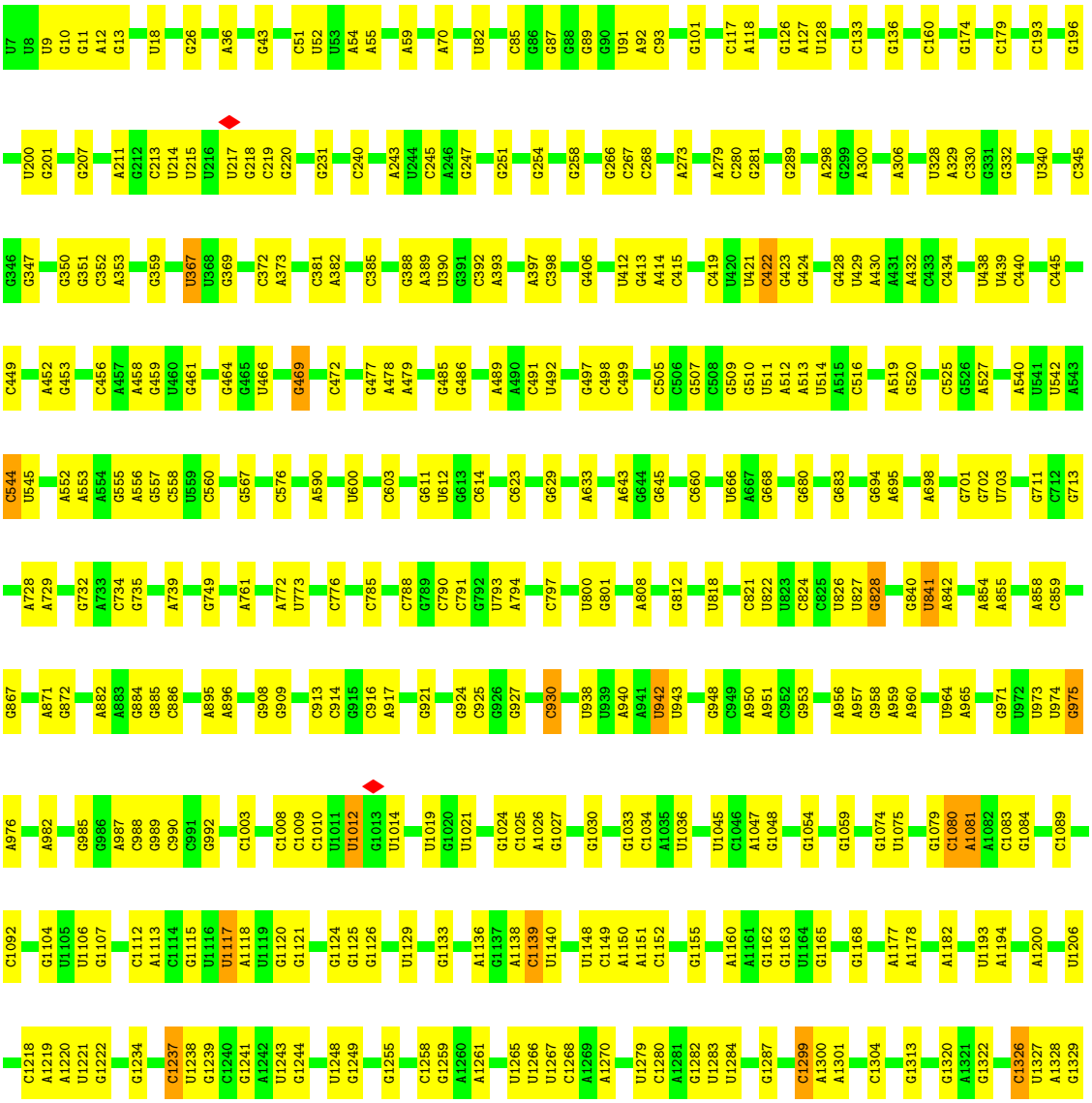
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
56	3	23	189	111	50	28	0	0

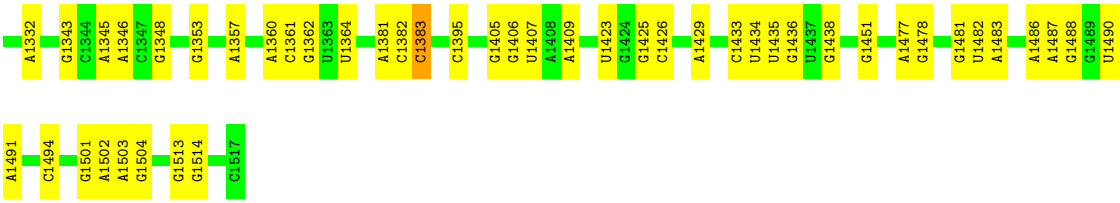
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

Chain h: 72% 26%



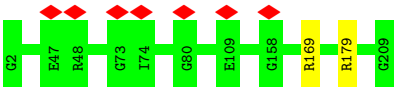


• Molecule 2: CONSERVED PROTEIN DOMAIN

Chain j: 100%

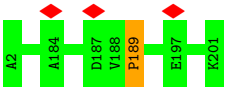
• Molecule 3: 30S ribosomal protein S3

Chain k: 99%



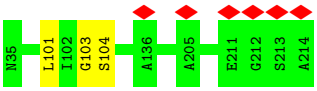
• Molecule 4: 30S ribosomal protein S4

Chain l: 100%



• Molecule 5: 30S ribosomal protein S5

Chain m: 98%

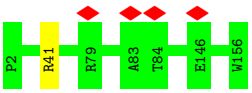


• Molecule 6: 30S ribosomal protein S6

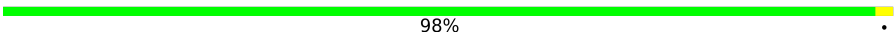
Chain n: 98%

• Molecule 7: 30S ribosomal protein S7

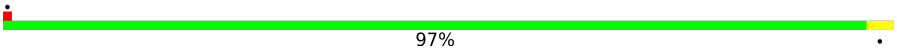
Chain p: 99%



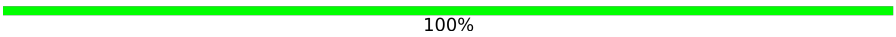
• Molecule 8: 30S ribosomal protein S8

Chain q: 

• Molecule 9: 30S ribosomal protein S9

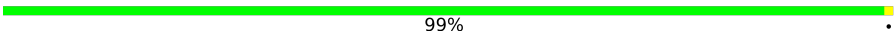
Chain 4: 

• Molecule 10: 30S ribosomal protein S10

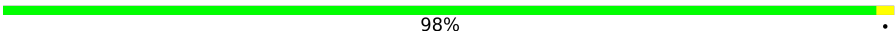
Chain s: 

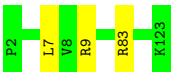
There are no outlier residues recorded for this chain.

• Molecule 11: 30S ribosomal protein S11

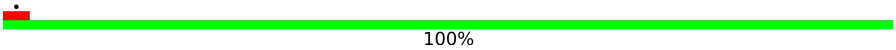
Chain t: 

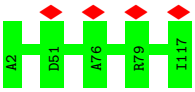
• Molecule 12: 30S ribosomal protein S12

Chain u: 

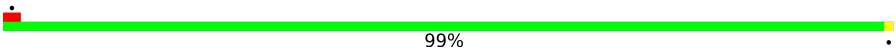


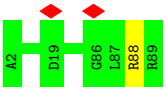
• Molecule 13: 30S ribosomal protein S13

Chain v: 



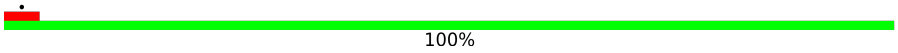
• Molecule 14: 30S ribosomal protein S15

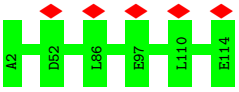
Chain x: 



• Molecule 15: 30S ribosomal protein S16

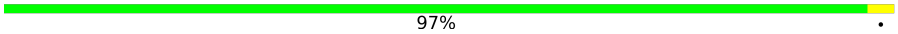
Chain z:

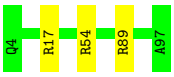




• Molecule 16: 30S ribosomal protein S17

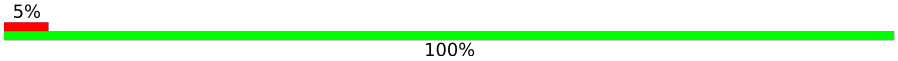
Chain 5:

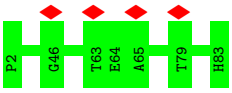




• Molecule 17: 30S ribosomal protein S19

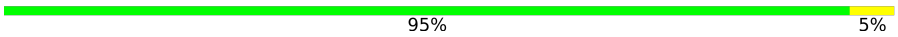
Chain 6:





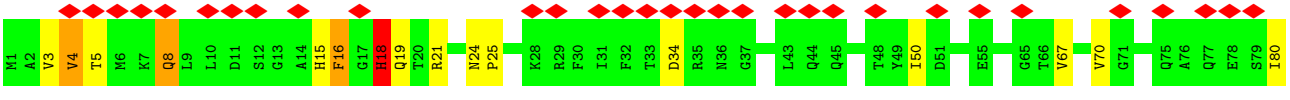
• Molecule 18: 30S ribosomal protein S20

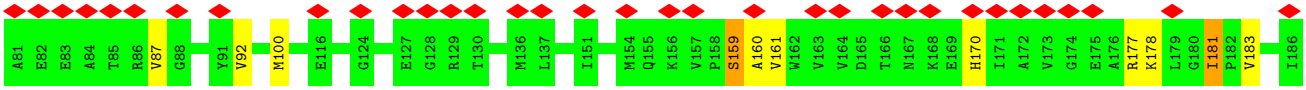
Chain 7:



• Molecule 19: 30S ribosomal protein S2

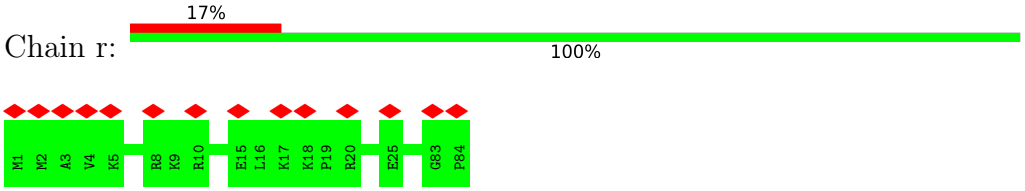
Chain 8:





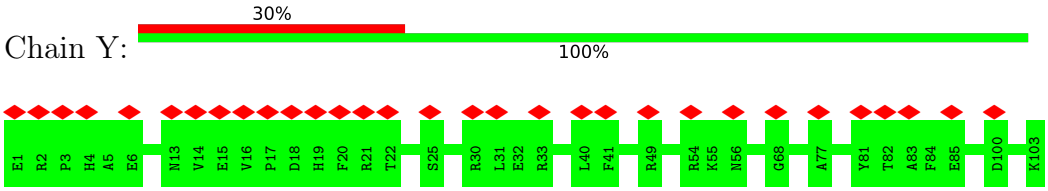
• Molecule 20: 30S ribosomal protein S18 1

Chain r:



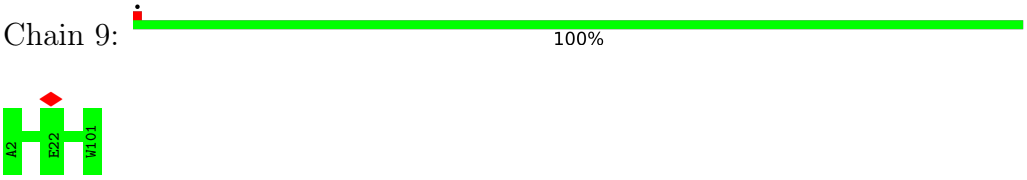
• Molecule 21: Ribosome hibernation promoting factor

Chain Y:



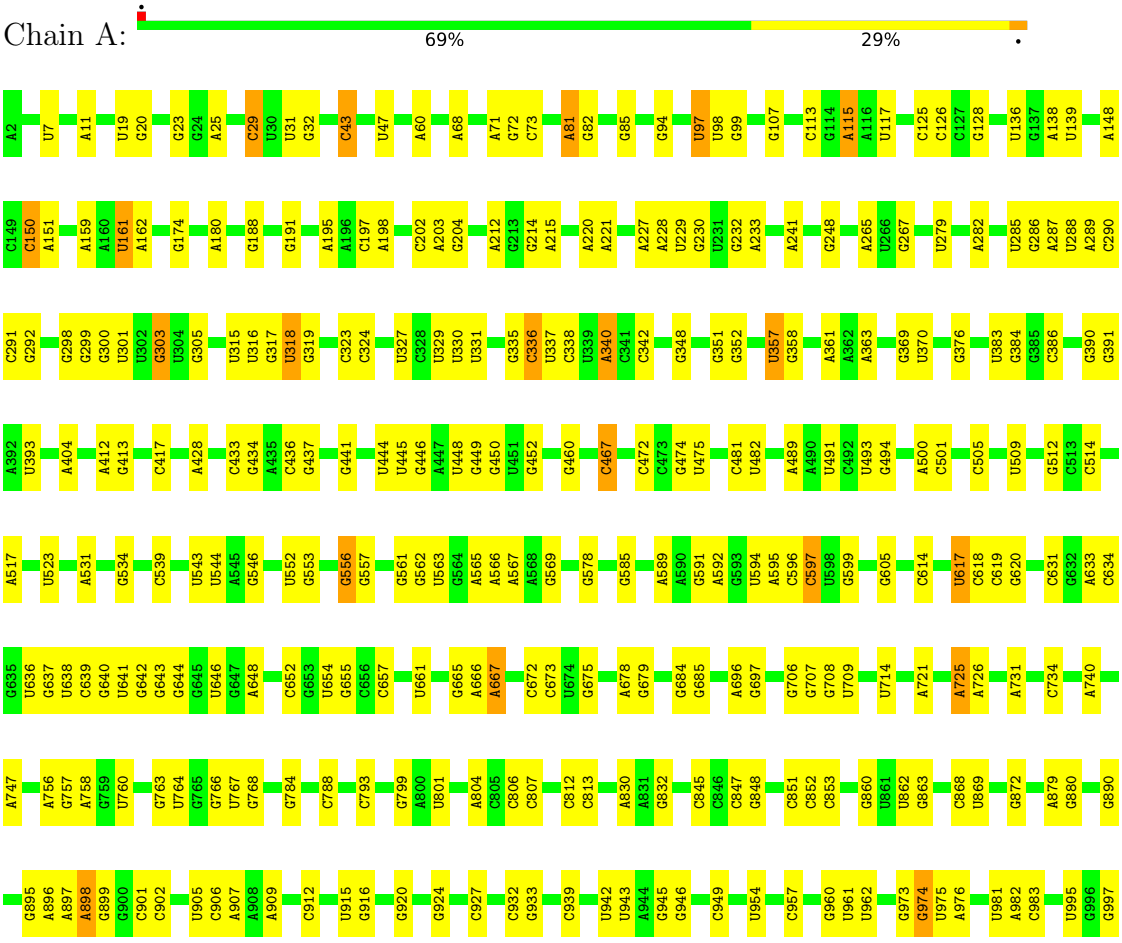
• Molecule 22: 30S ribosomal protein S14

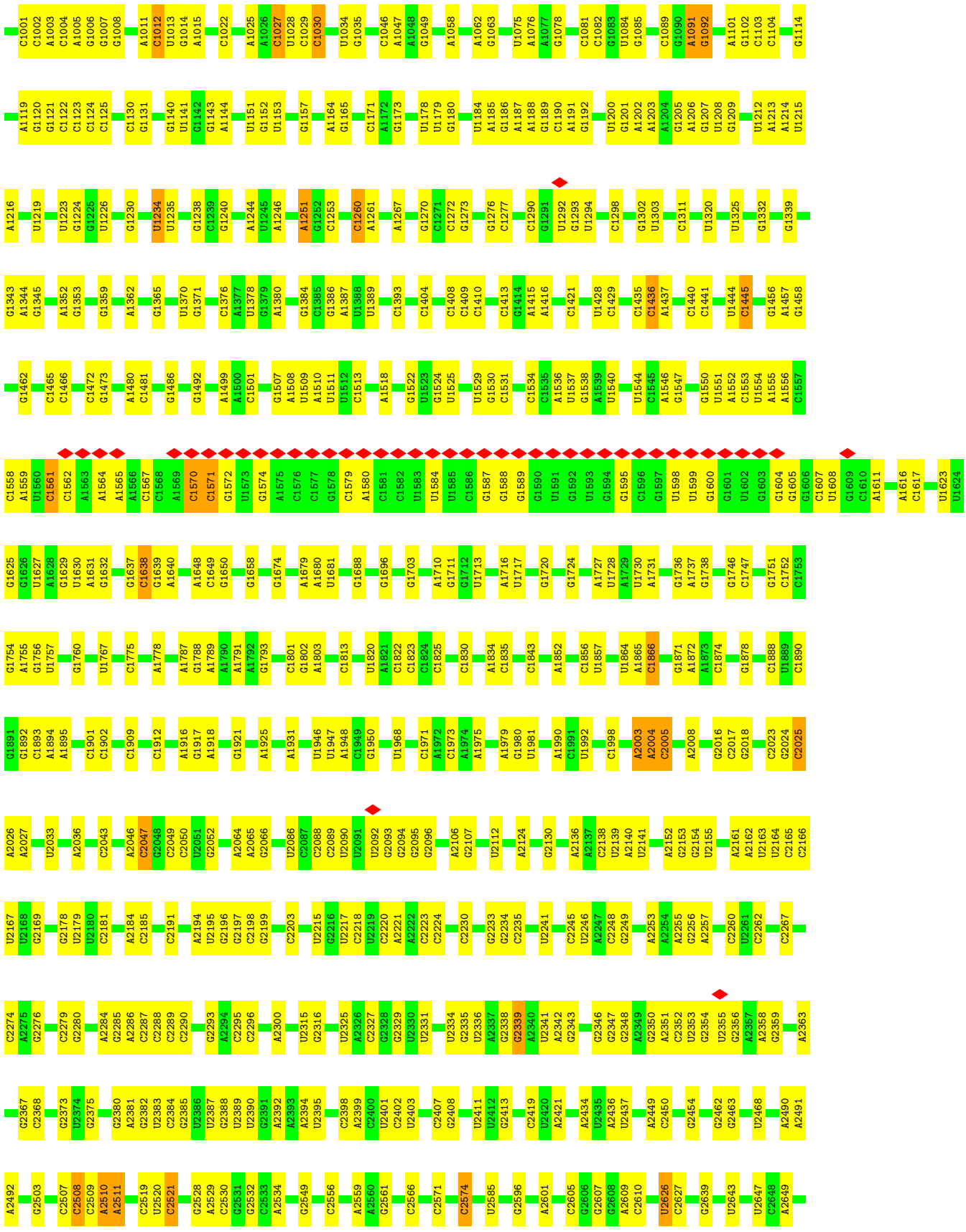
Chain 9:



• Molecule 23: 23 S rRNA (3119-MER)

Chain A:

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C1022
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U1034 G1035
C1046 A1047 A1048 G1049
A1058
A1062 G1063
U1075 A1076 A1077 G1078
C1081 C1082 G1083 U1084 G1085
C1089 G1090 A1091 G1092
A1101 G1102 C1103 C1104
G1114
A1119 G1120 G1121 C1122 C1123 C1124 C1125
C1130 G1131
G1140 U1141 G1142 G1143 A1144
U1151 G1152 U1153
G1157
A1164 G1165
C1171 A1172 G1173
U1178 U1179 G1180
U1184 A1185 G1186 A1187 A1188 G1189 C1190 A1191 G1192
U1200 G1201 A1202 A1203 A1204 G1205 A1206 G1207 U1208 G1209
U1212 A1213 A1214 U1215
A1216
U1219
U1223 G1224 G1225 U1226
G1230
U1234 U1235
G1238 C1239 G1240
A1244 U1245 A1246
A1251 G1252 C1253
C1260 A1261
A1267
G1270 C1271 C1272 G1273
G1276 C1277
C1290 G1291 U1292 G1293 U1294
C1298
G1302 U1303
C1311
U1320
U1325
G1332
G1339
G1343 A1344 G1345
A1352 G1353
G1359
A1362
G1365
U1370 G1371
C1376 A1377 U1378 G1379 A1380
G1384 C1385 G1386 A1387 U1388 U1389
C1393
C1404
C1408 C1409 C1410
C1413 C1414 A1415 A1416
C1421
U1428 C1429
C1435 C1436 A1437
C1440 C1441
U1444 C1445
G1456 A1457 G1458
G1462
C1465 C1466
C1472 G1473
A1480 C1481
G1486
G1492
A1499 A1500 C1501
G1507 A1508 A1509 A1510 U1511 U1512 C1513
A1518
G1522 U1523 G1524 U1525
U1529 G1530 C1531
C1534 C1535 A1536 U1537 G1538 A1539 U1540
U1544 C1545 A1546 G1547
G1550 U1551 A1552 C1553 U1554 A1555 A1556 C1557
C1558 A1559 U1560 C1561 C1562 A1563 A1564 A1565 A1566 C1567 C1568 A1569 C1570 C1571 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 A1616 C1617 U1623 U1624
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G1637 C1638 G1639 A1640
A1648 C1649 G1650
G1658
G1674
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G1688
G1696
G1703
A1710 G1711 G1712 U1713
A1716 U1717
G1720
G1724
A1727 U1728 A1729 U1730 A1731
G1736 A1737 G1738
G1746 C1747
G1751 C1752 C1753
G1754 A1755 G1756 U1757
G1760
U1767
C1775
A1778
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C1813
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C1830
A1834 C1835
C1843
A1852
C1856 U1857
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G1878
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C1909
C1912
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U1968
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A1990 C1991 U1992
C1998
A2003 A2004 C2005
A2008
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C2043
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U2112
A2124
G2130
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A2152 G2153 G2154 U2155
A2161 A2162 U2163 U2164 C2165 C2166
U2167 U2168 G2169
G2178 U2179 U2180 C2181
A2184 C2185
C2191
A2194 A2195 G2196 G2197 C2198 G2199
C2203
U2215 G2216 U2217 C2218 U2219 C2220 A2221 A2222 C2223 C2224
C2230
G2233 G2234 C2235
U2241
C2245 U2246 A2247 C2248 G2249
A2253 A2254 A2255 G2256 A2257
C2260 U2261 C2262
C2267
C2274 A2275 G2276
C2279 G2280
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U2325
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U2355 G2356 A2357 A2358 G2359
A2363
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C2407 G2408
U2411 U2412 G2413
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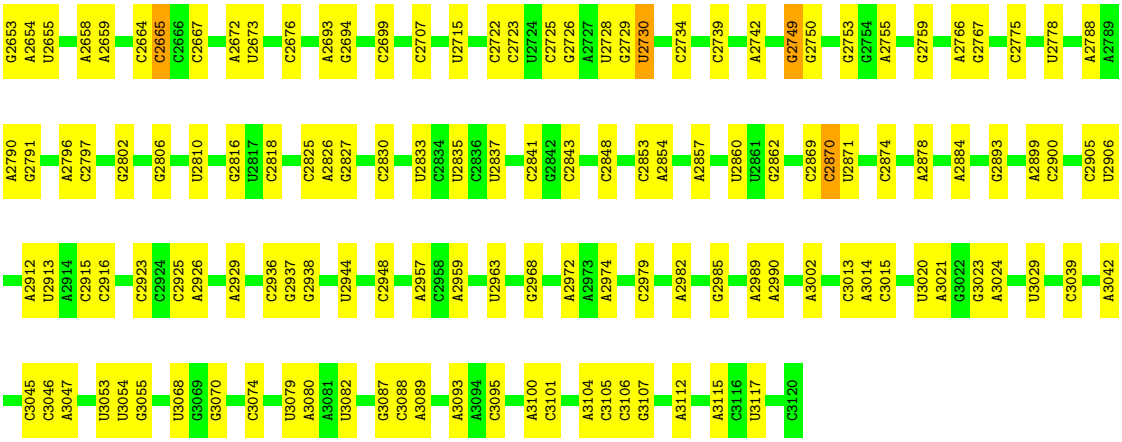
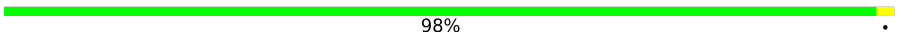


- Molecule 24: 5S RNA (118-MER)

Chain B:

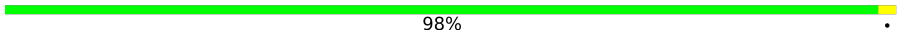
- Molecule 25: 50S ribosomal protein L2

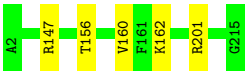
Chain C:



- Molecule 26: 50S ribosomal protein L3

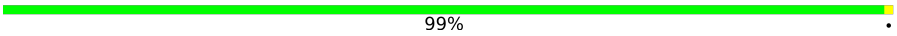
Chain D:





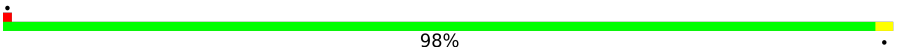
- Molecule 27: 50S ribosomal protein L4

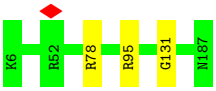
Chain E:



- Molecule 28: 50S ribosomal protein L5

Chain F:





- Molecule 29: 50S ribosomal protein L6

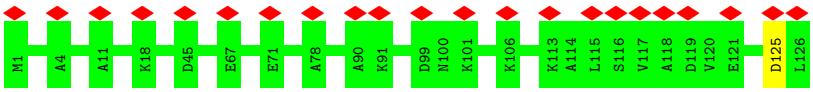
Chain G: 99%

• Molecule 30: 50S ribosomal protein L9

Chain H: 33% 99%

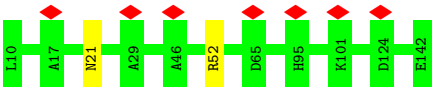
• Molecule 31: 50S ribosomal protein L10

Chain I: 17% 99%



• Molecule 32: 50S ribosomal protein L11

Chain J: 5% 98%



• Molecule 33: 50S ribosomal protein L13

Chain K: 100%

There are no outlier residues recorded for this chain.

• Molecule 34: 50S ribosomal protein L14

Chain L: 100%

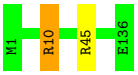
There are no outlier residues recorded for this chain.

• Molecule 35: 50S ribosomal protein L15

Chain M: 98%

• Molecule 36: 50S ribosomal protein L16

Chain N: 99%



• Molecule 37: 50S ribosomal protein L17

Chain O: 100%

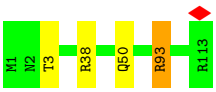
There are no outlier residues recorded for this chain.

• Molecule 38: 50S ribosomal protein L18

Chain P: 98%

• Molecule 39: 50S ribosomal protein L19

Chain Q: 96%



• Molecule 40: 50S ribosomal protein L20

Chain R: 100%

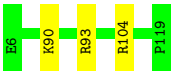
There are no outlier residues recorded for this chain.

• Molecule 41: 50S ribosomal protein L21

Chain S: 99%

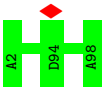
• Molecule 42: 50S ribosomal protein L22

Chain T: 97%

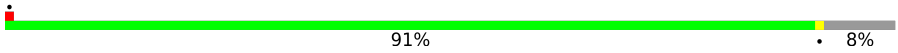


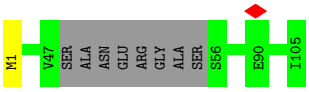
• Molecule 43: 50S ribosomal protein L23

Chain U: 100%

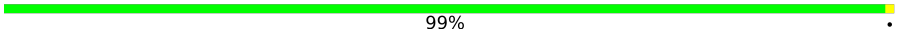


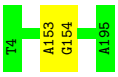
• Molecule 44: 50S ribosomal protein L24

Chain V: 

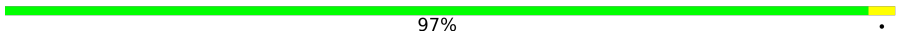


• Molecule 45: 50S ribosomal protein L25

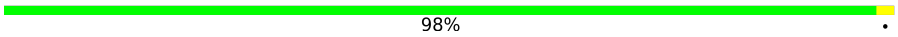
Chain W: 



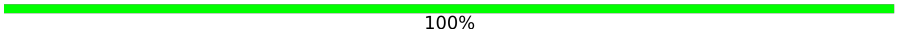
• Molecule 46: 50S ribosomal protein L27

Chain X: 

• Molecule 47: 50S ribosomal protein L29

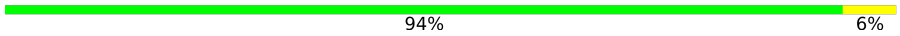
Chain Z: 

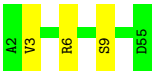
• Molecule 48: 50S ribosomal protein L30

Chain a: 

There are no outlier residues recorded for this chain.

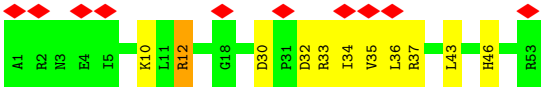
• Molecule 49: 50S ribosomal protein L32

Chain b: 

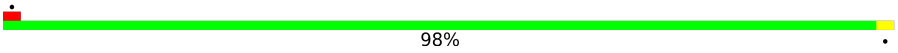


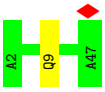
• Molecule 50: 50S ribosomal protein L33 2

Chain c:

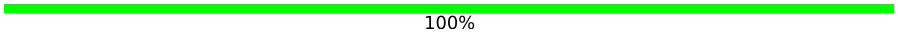


• Molecule 51: 50S ribosomal protein L34

Chain d: 

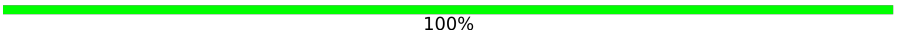


• Molecule 52: 50S ribosomal protein L35

Chain e: 

There are no outlier residues recorded for this chain.

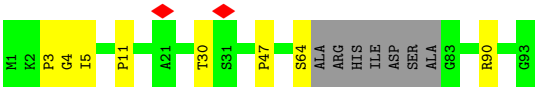
• Molecule 53: 50S ribosomal protein L36

Chain f: 

There are no outlier residues recorded for this chain.

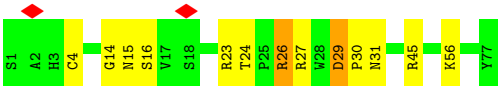
• Molecule 54: 50S ribosomal protein L31

Chain g:

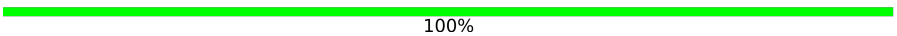


• Molecule 55: 50S ribosomal protein L28

Chain y:



• Molecule 56: Uncharacterized protein

Chain 3: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	66840	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 ($e^-/Å^2$)	67.10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.313	Depositor
Minimum map value	-0.175	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	485.78003, 485.78003, 485.78003	wwPDB
Map dimensions	454, 454, 454	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	h	0.75	0/36309	1.06	78/56657 (0.1%)
2	j	0.54	0/280	0.87	0/359
3	k	0.37	0/1684	0.62	0/2261
4	l	0.38	0/1672	0.65	0/2251
5	m	0.42	0/1312	0.63	0/1772
6	n	0.44	0/782	0.61	0/1059
7	p	0.35	0/1252	0.67	0/1690
8	q	0.44	0/1025	0.65	1/1385 (0.1%)
9	4	0.34	0/1012	0.66	0/1362
10	s	0.35	0/802	0.62	0/1086
11	t	0.42	0/873	0.65	0/1180
12	u	0.47	0/969	0.79	2/1294 (0.2%)
13	v	0.35	0/942	0.72	0/1260
14	x	0.47	0/729	0.73	0/977
15	z	0.41	0/908	0.65	0/1226
16	5	0.42	0/759	0.69	0/1016
17	6	0.37	0/680	0.62	0/915
18	7	0.44	0/663	0.65	0/882
19	8	0.46	0/1822	1.21	28/2457 (1.1%)
20	r	0.41	0/665	0.72	0/889
21	Y	0.36	0/875	0.67	0/1169
22	9	0.36	0/830	0.65	0/1106
23	A	1.26	88/75001 (0.1%)	1.23	313/117027 (0.3%)
24	B	0.99	0/2821	1.12	5/4396 (0.1%)
25	C	0.76	1/2153 (0.0%)	0.77	4/2895 (0.1%)
26	D	0.80	0/1609	0.79	1/2165 (0.0%)
27	E	0.66	0/1592	0.67	1/2153 (0.0%)
28	F	0.49	0/1467	0.67	0/1973
29	G	0.53	0/1369	0.70	1/1848 (0.1%)
30	H	0.42	0/1129	0.75	0/1524
31	I	0.34	0/925	0.58	0/1246
32	J	0.34	0/1006	0.62	0/1364
33	K	0.71	0/1157	0.65	0/1567
34	L	0.80	0/946	0.74	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	M	0.70	0/1091	0.76	1/1457 (0.1%)
36	N	0.70	0/1118	0.75	2/1506 (0.1%)
37	O	0.75	0/945	0.73	0/1267
38	P	0.60	0/966	0.74	1/1298 (0.1%)
39	Q	0.80	1/921 (0.1%)	0.73	1/1236 (0.1%)
40	R	0.86	0/1000	0.75	0/1341
41	S	0.69	0/764	0.63	0/1030
42	T	0.76	0/887	0.76	0/1204
43	U	0.68	0/766	0.64	0/1030
44	V	0.55	0/738	0.63	0/987
45	W	0.52	0/1443	0.64	0/1970
46	X	0.80	0/595	0.73	0/798
47	Z	0.60	0/534	0.74	1/713 (0.1%)
48	a	0.70	0/477	0.69	0/640
49	b	0.67	0/427	0.79	1/572 (0.2%)
50	c	0.50	0/463	0.88	1/621 (0.2%)
51	d	0.84	0/380	0.99	2/500 (0.4%)
52	e	0.69	0/507	0.75	0/672
53	f	0.85	0/303	0.71	0/401
54	g	0.42	0/613	0.76	2/835 (0.2%)
55	y	0.53	0/629	0.82	1/843 (0.1%)
56	3	0.72	0/191	0.79	0/247
All	All	0.98	90/163778 (0.1%)	1.07	447/244847 (0.2%)

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
4	l	0	1
19	8	0	10
26	D	0	1
32	J	0	1
45	W	0	1
All	All	0	14

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	50	GLN	CA-CB	-8.43	1.35	1.53
23	A	1081	C	N1-C6	-6.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2841	C	N1-C6	-6.26	1.33	1.37
23	A	901	C	N1-C6	-6.19	1.33	1.37
23	A	202	C	N1-C6	-6.10	1.33	1.37
23	A	2008	A	N9-C4	-6.04	1.34	1.37
23	A	1376	C	N1-C6	-6.04	1.33	1.37
23	A	1822	C	N1-C6	-6.03	1.33	1.37
23	A	1125	C	N1-C6	-5.97	1.33	1.37
23	A	2223	C	N1-C6	-5.96	1.33	1.37
23	A	2905	C	N1-C6	-5.88	1.33	1.37
23	A	902	C	N1-C6	-5.84	1.33	1.37
23	A	1888	C	C4-C5	-5.80	1.38	1.43
23	A	2915	C	C4-C5	-5.78	1.38	1.43
23	A	1027	C	N1-C6	-5.77	1.33	1.37
23	A	847	C	C4-C5	-5.76	1.38	1.43
23	A	678	A	N7-C5	-5.76	1.35	1.39
23	A	2005	C	C4-C5	-5.72	1.38	1.43
23	A	2667	C	N1-C6	-5.70	1.33	1.37
23	A	197	C	C4-C5	-5.69	1.38	1.43
23	A	2233	G	N9-C8	-5.68	1.33	1.37
23	A	2923	C	N1-C6	-5.68	1.33	1.37
23	A	2830	C	N1-C6	-5.68	1.33	1.37
23	A	799	G	N9-C4	-5.65	1.33	1.38
23	A	793	C	C4-C5	-5.65	1.38	1.43
23	A	2248	C	C4-C5	-5.64	1.38	1.43
23	A	2916	C	N1-C6	-5.62	1.33	1.37
23	A	813	C	N1-C6	-5.60	1.33	1.37
23	A	1413	C	C4-C5	-5.58	1.38	1.43
23	A	848	G	C6-N1	-5.56	1.35	1.39
23	A	2224	C	N1-C6	-5.54	1.33	1.37
23	A	906	C	C4-C5	-5.51	1.38	1.43
23	A	2766	A	C6-N6	-5.50	1.29	1.33
23	A	949	C	N1-C6	-5.47	1.33	1.37
23	A	1866	C	N1-C6	-5.46	1.33	1.37
23	A	678	A	N9-C8	-5.43	1.33	1.37
23	A	675	G	N9-C8	-5.41	1.34	1.37
23	A	1856	C	C4-C5	-5.40	1.38	1.43
23	A	2870	C	C4-C5	-5.40	1.38	1.43
23	A	725	A	N9-C4	-5.38	1.34	1.37
23	A	852	C	C4-C5	-5.38	1.38	1.43
23	A	1874	C	C4-C5	-5.38	1.38	1.43
23	A	2235	C	C4-C5	-5.37	1.38	1.43
23	A	2218	C	C4-C5	-5.30	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2274	C	C4-C5	-5.27	1.38	1.43
23	A	939	C	C4-C5	-5.26	1.38	1.43
23	A	2043	C	N1-C6	-5.23	1.34	1.37
23	A	2220	C	N1-C6	-5.22	1.34	1.37
23	A	1311	C	C4-C5	-5.22	1.38	1.43
23	A	847	C	N1-C6	-5.21	1.34	1.37
23	A	1441	C	C4-C5	-5.21	1.38	1.43
23	A	2049	C	N1-C6	-5.20	1.34	1.37
23	A	788	C	N1-C6	-5.20	1.34	1.37
23	A	1277	C	C4-C5	-5.20	1.38	1.43
23	A	2230	C	C4-C5	-5.18	1.38	1.43
23	A	879	A	C6-N6	-5.18	1.29	1.33
23	A	924	G	N9-C8	-5.18	1.34	1.37
23	A	1466	C	N1-C6	-5.18	1.34	1.37
23	A	2948	C	N1-C6	-5.17	1.34	1.37
25	C	34	VAL	C-N	-5.16	1.22	1.34
23	A	807	C	C4-C5	-5.16	1.38	1.43
23	A	2295	C	N1-C6	-5.16	1.34	1.37
23	A	2260	C	C4-C5	-5.15	1.38	1.43
23	A	2274	C	N3-C4	-5.14	1.30	1.33
23	A	2218	C	N1-C6	-5.14	1.34	1.37
23	A	2234	G	N9-C8	-5.13	1.34	1.37
23	A	678	A	C5-C6	-5.12	1.36	1.41
23	A	932	C	C4-C5	-5.11	1.38	1.43
23	A	939	C	N1-C6	-5.10	1.34	1.37
23	A	2739	C	N1-C6	-5.10	1.34	1.37
23	A	2915	C	N1-C6	-5.09	1.34	1.37
23	A	1445	C	N1-C6	-5.09	1.34	1.37
23	A	1124	C	N1-C6	-5.09	1.34	1.37
23	A	2289	C	C4-C5	-5.08	1.38	1.43
23	A	1272	C	N1-C6	-5.08	1.34	1.37
23	A	1413	C	N1-C6	-5.07	1.34	1.37
23	A	657	C	N1-C6	-5.07	1.34	1.37
23	A	1104	C	N1-C6	-5.07	1.34	1.37
23	A	672	C	C4-C5	-5.07	1.38	1.43
23	A	1124	C	C4-C5	-5.07	1.38	1.43
23	A	806	C	N1-C6	-5.06	1.34	1.37
23	A	2848	C	C4-C5	-5.05	1.39	1.43
23	A	2004	A	N7-C5	-5.04	1.36	1.39
23	A	2253	A	N9-C4	-5.03	1.34	1.37
23	A	1429	C	C4-C5	-5.02	1.39	1.43
23	A	2830	C	C4-C5	-5.02	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	807	C	N1-C6	-5.02	1.34	1.37
23	A	1856	C	N1-C6	-5.01	1.34	1.37
23	A	2004	A	C5-C6	-5.01	1.36	1.41
23	A	2816	G	N9-C8	-5.01	1.34	1.37

All (447) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	8	213	LEU	CA-CB-CG	14.81	149.37	115.30
1	h	1081	A	O4'-C1'-N9	11.00	117.00	108.20
23	A	2509	C	O4'-C1'-N1	10.71	116.77	108.20
23	A	1012	C	C2-N1-C1'	10.54	130.39	118.80
23	A	2245	C	C2-N1-C1'	10.28	130.10	118.80
19	8	213	LEU	CB-CG-CD2	9.79	127.64	111.00
23	A	1012	C	N1-C2-O2	9.62	124.67	118.90
23	A	2245	C	N1-C2-O2	9.13	124.38	118.90
19	8	187	LEU	C-N-CA	9.07	144.38	121.70
23	A	2025	C	C6-N1-C2	-9.04	116.68	120.30
23	A	2274	C	N1-C2-O2	8.99	124.30	118.90
23	A	2025	C	N3-C2-O2	-8.61	115.88	121.90
23	A	2025	C	N1-C2-O2	8.20	123.82	118.90
19	8	18	HIS	C-N-CA	7.96	141.60	121.70
23	A	2245	C	C6-N1-C1'	-7.88	111.34	120.80
23	A	1441	C	C5-C4-N4	-7.85	114.70	120.20
24	B	87	U	N3-C2-O2	-7.75	116.78	122.20
1	h	85	C	N1-C2-O2	7.72	123.53	118.90
23	A	2468	U	N3-C4-O4	7.66	124.76	119.40
23	A	197	C	C6-N1-C2	-7.65	117.24	120.30
23	A	2491	A	N1-C6-N6	-7.63	114.02	118.60
23	A	1012	C	N3-C2-O2	-7.61	116.57	121.90
23	A	848	G	N1-C2-N2	-7.58	109.38	116.20
23	A	2511	A	O4'-C1'-N9	7.57	114.25	108.20
23	A	1012	C	C6-N1-C1'	-7.53	111.77	120.80
23	A	1421	C	C5-C4-N4	-7.52	114.94	120.20
23	A	336	C	N3-C2-O2	-7.52	116.64	121.90
23	A	2521	C	C6-N1-C2	-7.47	117.31	120.30
23	A	2248	C	N1-C2-O2	7.43	123.36	118.90
1	h	841	U	C5'-C4'-O4'	7.41	117.99	109.10
23	A	1888	C	C5-C4-N4	-7.39	115.02	120.20
23	A	3045	C	C5-C4-N4	-7.38	115.03	120.20
23	A	1747	C	N3-C2-O2	-7.36	116.75	121.90
1	h	544	C	C6-N1-C2	-7.33	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	8	212	LEU	CA-CB-CG	7.32	132.13	115.30
23	A	962	U	C2-N1-C1'	7.31	126.47	117.70
1	h	85	C	C2-N1-C1'	7.30	126.83	118.80
23	A	2944	U	C5-C4-O4	-7.29	121.53	125.90
19	8	92	VAL	CG1-CB-CG2	7.25	122.51	110.90
23	A	1992	U	C5-C4-O4	-7.24	121.56	125.90
23	A	2245	C	N3-C2-O2	-7.23	116.84	121.90
23	A	597	C	C5-C4-N4	-7.21	115.15	120.20
23	A	2185	C	C5-C4-N4	-7.19	115.16	120.20
1	h	1139	C	C2-N1-C1'	7.19	126.71	118.80
23	A	318	U	C2-N1-C1'	7.18	126.31	117.70
23	A	1429	C	C6-N1-C2	-7.14	117.44	120.30
23	A	318	U	N1-C2-O2	7.14	127.80	122.80
1	h	415	C	N1-C2-O2	7.13	123.18	118.90
23	A	2730	U	C2-N1-C1'	7.09	126.21	117.70
23	A	932	C	C5-C4-N4	-7.08	115.24	120.20
23	A	2509	C	C6-N1-C2	-7.08	117.47	120.30
23	A	1277	C	C5-C4-N4	-7.06	115.26	120.20
23	A	726	A	C5-C6-N6	-7.05	118.06	123.70
23	A	652	C	C5-C4-N4	-7.03	115.28	120.20
19	8	183	VAL	CG1-CB-CG2	7.01	122.12	110.90
23	A	2944	U	N3-C4-O4	7.01	124.31	119.40
23	A	2900	C	N1-C2-O2	6.97	123.08	118.90
23	A	336	C	N1-C2-O2	6.94	123.06	118.90
1	h	560	C	C5-C4-N4	-6.94	115.34	120.20
19	8	178	LYS	C-N-CA	6.93	139.03	121.70
1	h	1326	C	N3-C2-O2	-6.88	117.09	121.90
19	8	3	VAL	CG1-CB-CG2	6.83	121.82	110.90
23	A	2766	A	C5-C6-N6	-6.82	118.24	123.70
1	h	415	C	N3-C2-O2	-6.82	117.13	121.90
1	h	1383	C	C2-N1-C1'	6.82	126.30	118.80
19	8	50	ILE	CG1-CB-CG2	6.82	126.39	111.40
23	A	879	A	C5-C6-N1	6.81	121.10	117.70
1	h	1299	C	C2-N1-C1'	6.80	126.28	118.80
1	h	1383	C	N1-C2-O2	6.77	122.96	118.90
23	A	673	C	N1-C2-O2	6.77	122.96	118.90
23	A	2519	C	C5-C4-N4	-6.77	115.46	120.20
23	A	1513	C	C5-C4-N4	-6.73	115.49	120.20
23	A	197	C	C5-C6-N1	6.71	124.36	121.00
23	A	318	U	N3-C2-O2	-6.69	117.52	122.20
23	A	557	G	C2-N3-C4	-6.69	108.56	111.90
1	h	1012	U	C2-N1-C1'	6.68	125.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	1299	C	N1-C2-O2	6.67	122.90	118.90
23	A	2905	C	C5-C4-N4	-6.65	115.54	120.20
23	A	2468	U	C5-C4-O4	-6.63	121.92	125.90
23	A	1843	C	C5-C4-N4	-6.60	115.58	120.20
19	8	195	VAL	CG1-CB-CG2	6.60	121.46	110.90
19	8	80	ILE	CG1-CB-CG2	6.58	125.88	111.40
19	8	181	ILE	CG1-CB-CG2	6.58	125.88	111.40
39	Q	93	ARG	C-N-CA	6.58	138.14	121.70
23	A	2825	C	C5-C4-N4	-6.57	115.60	120.20
23	A	1030	C	C5-C4-N4	-6.57	115.60	120.20
23	A	2870	C	C5-C4-N4	-6.56	115.61	120.20
23	A	1893	C	C5-C4-N4	-6.53	115.63	120.20
23	A	3046	C	C2-N1-C1'	6.52	125.97	118.80
1	h	842	A	C5'-C4'-O4'	6.50	116.90	109.10
23	A	939	C	C5-C4-N4	-6.47	115.67	120.20
23	A	1272	C	N1-C2-O2	6.47	122.78	118.90
23	A	2223	C	C5-C4-N4	-6.46	115.68	120.20
1	h	734	C	C2-N1-C1'	6.45	125.90	118.80
23	A	2676	C	C5-C4-N4	-6.44	115.69	120.20
23	A	597	C	N3-C4-N4	6.43	122.50	118.00
23	A	1562	C	C6-N1-C2	-6.42	117.73	120.30
38	P	24	ARG	NE-CZ-NH1	6.42	123.51	120.30
23	A	2287	C	C5-C4-N4	-6.40	115.72	120.20
23	A	2288	C	C5-C4-N4	-6.40	115.72	120.20
23	A	1473	G	C2-N3-C4	-6.38	108.71	111.90
23	A	197	C	N1-C2-O2	6.37	122.72	118.90
24	B	87	U	N1-C2-O2	6.37	127.26	122.80
1	h	1299	C	C6-N1-C2	-6.36	117.76	120.30
23	A	2830	C	C5-C4-N4	-6.36	115.75	120.20
23	A	804	A	C5-C6-N1	6.34	120.87	117.70
1	h	1012	U	N1-C2-O2	6.34	127.24	122.80
1	h	1299	C	N3-C2-O2	-6.34	117.47	121.90
23	A	1429	C	C2-N1-C1'	6.33	125.76	118.80
19	8	217	ILE	CG1-CB-CG2	6.33	125.31	111.40
23	A	481	C	N1-C2-O2	6.32	122.69	118.90
1	h	85	C	N3-C2-O2	-6.31	117.48	121.90
1	h	415	C	C6-N1-C2	-6.30	117.78	120.30
19	8	200	ILE	CG1-CB-CG2	6.30	125.26	111.40
23	A	1012	C	C6-N1-C2	-6.30	117.78	120.30
23	A	2915	C	C5-C4-N4	-6.28	115.81	120.20
25	C	221	VAL	C-N-CA	6.28	137.39	121.70
23	A	197	C	N3-C4-N4	6.25	122.38	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1458	G	C4-N9-C1'	6.25	134.63	126.50
1	h	791	C	C5-C4-N4	-6.23	115.84	120.20
23	A	2775	C	N1-C2-O2	6.22	122.63	118.90
1	h	1080	C	C2'-C3'-O3'	6.18	123.59	113.70
23	A	1298	C	N1-C2-O2	6.17	122.61	118.90
54	g	4	GLY	N-CA-C	-6.17	97.68	113.10
23	A	1311	C	C5-C4-N4	-6.16	115.89	120.20
23	A	1874	C	C5-C4-N4	-6.13	115.91	120.20
23	A	29	C	N1-C2-O2	6.11	122.57	118.90
1	h	1081	A	N9-C1'-C2'	6.11	121.94	114.00
1	h	544	C	N1-C2-O2	6.10	122.56	118.90
23	A	1458	G	C8-N9-C1'	-6.10	119.08	127.00
19	8	67	VAL	CG1-CB-CG2	6.09	120.65	110.90
19	8	70	VAL	CG1-CB-CG2	6.09	120.64	110.90
19	8	4	VAL	CG1-CB-CG2	6.07	120.62	110.90
23	A	1992	U	N3-C4-O4	6.07	123.65	119.40
23	A	1428	U	C2-N1-C1'	6.07	124.98	117.70
23	A	853	C	N1-C2-O2	6.06	122.54	118.90
23	A	2870	C	N3-C4-N4	6.06	122.24	118.00
23	A	804	A	C5-C6-N6	-6.05	118.86	123.70
1	h	1012	U	N3-C2-O2	-6.03	117.98	122.20
19	8	187	LEU	CB-CG-CD2	6.02	121.24	111.00
23	A	793	C	N1-C2-O2	6.02	122.51	118.90
23	A	799	G	C2-N3-C4	-6.01	108.89	111.90
23	A	599	G	O4'-C1'-N9	5.99	112.99	108.20
1	h	544	C	C2-N1-C1'	5.98	125.38	118.80
23	A	1234	U	C6-N1-C2	-5.98	117.41	121.00
23	A	848	G	C4-N9-C1'	5.97	134.26	126.50
23	A	2003	A	C5'-C4'-O4'	5.97	116.27	109.10
23	A	1747	C	N1-C2-O2	5.97	122.48	118.90
1	h	1406	G	C4-N9-C1'	5.97	134.26	126.50
23	A	933	G	N1-C2-N2	-5.96	110.83	116.20
1	h	328	U	N1-C2-O2	5.96	126.97	122.80
23	A	1856	C	C5-C4-N4	-5.96	116.03	120.20
23	A	2725	C	N1-C2-O2	5.96	122.48	118.90
23	A	2005	C	C5-C4-N4	-5.96	116.03	120.20
23	A	3074	C	C5-C4-N4	-5.96	116.03	120.20
1	h	1083	C	C5'-C4'-O4'	5.95	116.25	109.10
19	8	100	MET	C-N-CA	5.95	136.57	121.70
23	A	2869	C	C2-N1-C1'	5.95	125.34	118.80
23	A	2870	C	C5-C6-N1	5.95	123.97	121.00
24	B	87	U	C6-N1-C2	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	2004	A	N1-C6-N6	5.94	122.17	118.60
23	A	2556	C	N1-C2-O2	5.94	122.46	118.90
23	A	1492	G	C2-N3-C4	-5.93	108.94	111.90
23	A	2023	C	N1-C2-O2	5.92	122.45	118.90
23	A	2262	C	N1-C2-O2	5.91	122.45	118.90
23	A	556	G	C6-C5-N7	-5.91	126.86	130.40
23	A	1122	C	N1-C2-O2	5.90	122.44	118.90
23	A	1788	G	C8-N9-C1'	5.89	134.65	127.00
1	h	614	C	N3-C2-O2	-5.88	117.78	121.90
23	A	1384	G	C6-C5-N7	-5.88	126.87	130.40
23	A	1843	C	N3-C4-N4	5.88	122.11	118.00
23	A	2235	C	C5-C4-N4	-5.87	116.09	120.20
23	A	2925	C	N1-C2-O2	5.85	122.41	118.90
1	h	544	C	N3-C2-O2	-5.85	117.80	121.90
23	A	848	G	C6-C5-N7	-5.85	126.89	130.40
23	A	174	G	C5-C6-O6	-5.84	125.09	128.60
23	A	848	G	N3-C2-N2	5.83	123.98	119.90
1	h	1482	U	P-O3'-C3'	5.83	126.69	119.70
51	d	9	GLN	N-CA-C	-5.82	95.29	111.00
23	A	390	G	N1-C2-N2	-5.81	110.97	116.20
23	A	1124	C	C5-C4-N4	-5.80	116.14	120.20
1	h	895	A	P-O3'-C3'	5.80	126.66	119.70
1	h	1395	C	C5-C4-N4	-5.80	116.14	120.20
23	A	799	G	N3-C4-C5	5.80	131.50	128.60
1	h	942	U	C2-N1-C1'	5.80	124.66	117.70
23	A	556	G	C4-C5-N7	5.80	113.12	110.80
23	A	2749	G	N3-C4-N9	-5.79	122.53	126.00
23	A	2047	C	N3-C4-N4	5.79	122.05	118.00
23	A	2734	C	C5-C4-N4	-5.79	116.15	120.20
23	A	812	C	C5-C4-N4	-5.78	116.15	120.20
23	A	2874	C	C5-C4-N4	-5.78	116.16	120.20
23	A	851	C	N1-C2-O2	5.76	122.35	118.90
23	A	1234	U	N3-C2-O2	-5.75	118.17	122.20
23	A	1571	C	N1-C2-O2	-5.75	115.45	118.90
23	A	912	C	N1-C2-O2	5.75	122.35	118.90
23	A	1298	C	C2-N1-C1'	5.74	125.11	118.80
19	8	159	SER	C-N-CA	5.74	136.04	121.70
23	A	2749	G	N3-C4-C5	5.72	131.46	128.60
1	h	614	C	N1-C2-O2	5.71	122.33	118.90
23	A	1788	G	C4-N9-C1'	-5.71	119.08	126.50
23	A	2047	C	C5-C4-N4	-5.70	116.21	120.20
23	A	197	C	C2-N1-C1'	5.69	125.06	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	328	U	N3-C2-O2	-5.68	118.22	122.20
23	A	1092	G	O4'-C1'-N9	5.67	112.74	108.20
23	A	2818	C	N1-C2-O2	5.67	122.30	118.90
23	A	2841	C	C5-C4-N4	-5.67	116.23	120.20
23	A	2004	A	C5-C6-N6	-5.67	119.16	123.70
23	A	848	G	C2-N3-C4	-5.67	109.06	111.90
23	A	386	C	C5-C4-N4	-5.66	116.24	120.20
23	A	1260	C	C2-N1-C1'	5.66	125.03	118.80
23	A	2181	C	C5-C4-N4	-5.66	116.24	120.20
23	A	2274	C	N3-C2-O2	-5.66	117.94	121.90
23	A	2723	C	C5-C4-N4	-5.65	116.24	120.20
1	h	1406	G	C8-N9-C1'	-5.65	119.65	127.00
23	A	1409	C	N3-C4-N4	5.63	121.94	118.00
23	A	1302	G	N1-C6-O6	5.62	123.27	119.90
23	A	1089	C	N1-C2-O2	5.61	122.26	118.90
23	A	472	C	C6-N1-C2	-5.60	118.06	120.30
23	A	2508	C	N1-C2-O2	5.60	122.26	118.90
23	A	2766	A	C5-C6-N1	5.59	120.50	117.70
1	h	749	G	N1-C2-N2	-5.59	111.17	116.20
23	A	1968	U	C5-C4-O4	-5.58	122.55	125.90
23	A	1830	C	C5-C4-N4	-5.57	116.30	120.20
1	h	422	C	P-O3'-C3'	5.57	126.38	119.70
23	A	932	C	N1-C2-O2	5.57	122.24	118.90
23	A	2626	U	C2-N1-C1'	5.57	124.38	117.70
23	A	2725	C	N3-C2-O2	-5.56	118.01	121.90
23	A	2218	C	C5-C4-N4	-5.56	116.31	120.20
23	A	1119	A	N1-C6-N6	-5.54	115.27	118.60
23	A	2230	C	C5-C4-N4	-5.54	116.32	120.20
23	A	852	C	C5-C4-N4	-5.53	116.33	120.20
23	A	657	C	C5-C4-N4	-5.53	116.33	120.20
25	C	213	ARG	NE-CZ-NH1	5.53	123.06	120.30
23	A	848	G	C8-N9-C1'	-5.52	119.82	127.00
23	A	1472	C	N1-C2-O2	5.52	122.21	118.90
23	A	1486	G	C2-N3-C4	-5.52	109.14	111.90
23	A	2198	C	C5-C4-N4	-5.52	116.34	120.20
1	h	623	C	N3-C2-O2	-5.52	118.04	121.90
23	A	898	A	C4-N9-C1'	5.52	136.23	126.30
1	h	439	U	C6-N1-C2	-5.50	117.70	121.00
23	A	726	A	N1-C6-N6	5.50	121.90	118.60
1	h	1494	C	N1-C2-O2	5.50	122.20	118.90
23	A	336	C	C6-N1-C2	-5.49	118.10	120.30
1	h	749	G	N3-C2-N2	5.48	123.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1120	G	C4-C5-N7	5.47	112.99	110.80
23	A	1273	G	C2-N3-C4	-5.47	109.16	111.90
1	h	1243	U	N3-C2-O2	-5.46	118.38	122.20
1	h	925	C	N1-C2-O2	5.46	122.18	118.90
23	A	2419	C	C6-N1-C2	-5.46	118.11	120.30
23	A	2004	A	C4-C5-N7	5.46	113.43	110.70
23	A	3046	C	N3-C2-O2	-5.46	118.08	121.90
1	h	885	G	C4-N9-C1'	5.45	133.59	126.50
1	h	942	U	N3-C2-O2	-5.45	118.38	122.20
23	A	472	C	C2-N1-C1'	5.45	124.79	118.80
23	A	2004	A	N9-C4-C5	-5.45	103.62	105.80
23	A	2124	A	N1-C6-N6	5.45	121.87	118.60
23	A	2610	C	N1-C2-O2	5.45	122.17	118.90
23	A	2848	C	C5-C4-N4	-5.44	116.39	120.20
1	h	1383	C	N3-C2-O2	-5.44	118.09	121.90
23	A	1384	G	N7-C8-N9	5.44	115.82	113.10
23	A	2005	C	N3-C4-N4	5.44	121.81	118.00
1	h	1152	C	C6-N1-C2	-5.44	118.12	120.30
1	h	1395	C	N3-C4-N4	5.43	121.80	118.00
23	A	1104	C	N1-C2-O2	5.43	122.16	118.90
23	A	501	C	C5-C4-N4	-5.43	116.40	120.20
23	A	2290	C	N1-C2-O2	5.42	122.16	118.90
23	A	546	G	O4'-C1'-N9	5.42	112.54	108.20
23	A	467	C	C5-C4-N4	-5.42	116.41	120.20
23	A	2260	C	N3-C4-N4	5.42	121.79	118.00
23	A	2249	G	N7-C8-N9	5.42	115.81	113.10
23	A	3045	C	N3-C4-N4	5.42	121.79	118.00
23	A	2605	C	C5-C4-N4	-5.41	116.41	120.20
23	A	2185	C	N3-C4-N4	5.41	121.79	118.00
23	A	974	G	P-O3'-C3'	5.41	126.19	119.70
23	A	1311	C	N3-C4-N4	5.41	121.79	118.00
23	A	2184	A	N9-C4-C5	-5.41	103.64	105.80
29	G	65	LEU	CA-CB-CG	5.41	127.74	115.30
1	h	558	C	C5-C4-N4	-5.41	116.42	120.20
23	A	191	G	C4-N9-C1'	5.41	133.53	126.50
1	h	791	C	N3-C4-N4	5.40	121.78	118.00
19	8	8	GLN	CA-CB-CG	5.40	125.29	113.40
23	A	1123	C	C6-N1-C2	-5.40	118.14	120.30
23	A	2296	C	N1-C2-O2	5.40	122.14	118.90
1	h	1237	C	N3-C2-O2	-5.40	118.12	121.90
1	h	1117	U	P-O3'-C3'	5.40	126.18	119.70
55	y	29	ASP	C-N-CD	5.40	139.73	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	726	A	C4-C5-N7	5.39	113.40	110.70
23	A	860	G	N1-C2-N2	-5.39	111.35	116.20
23	A	1303	U	C5-C4-O4	-5.39	122.66	125.90
23	A	1413	C	C2-N1-C1'	5.39	124.73	118.80
19	8	207	ILE	CG1-CB-CG2	5.39	123.25	111.40
23	A	726	A	N9-C4-C5	-5.39	103.64	105.80
23	A	2419	C	C2-N1-C1'	5.39	124.73	118.80
1	h	828	G	C6-C5-N7	-5.38	127.17	130.40
25	C	222	ARG	NE-CZ-NH1	5.38	122.99	120.30
23	A	851	C	C5-C4-N4	-5.38	116.43	120.20
23	A	1901	C	C5-C4-N4	-5.38	116.43	120.20
23	A	2203	C	N1-C2-O2	5.38	122.13	118.90
23	A	1035	G	C2-N3-C4	-5.37	109.22	111.90
1	h	415	C	C2-N1-C1'	5.36	124.70	118.80
23	A	2249	G	C6-C5-N7	-5.36	127.19	130.40
47	Z	51	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	h	942	U	N1-C2-O2	5.35	126.54	122.80
1	h	975	G	C8-N9-C1'	-5.34	120.05	127.00
23	A	2016	G	C2-N3-C4	-5.34	109.23	111.90
23	A	1561	C	C6-N1-C2	-5.34	118.17	120.30
23	A	1902	C	C5-C4-N4	-5.33	116.47	120.20
23	A	1823	C	N1-C2-O2	5.33	122.10	118.90
1	h	85	C	C6-N1-C1'	-5.33	114.41	120.80
23	A	799	G	N3-C4-N9	-5.33	122.80	126.00
23	A	2521	C	C2-N1-C1'	5.33	124.66	118.80
23	A	2339	G	O4'-C1'-N9	-5.32	103.94	108.20
23	A	2561	G	N1-C6-O6	5.32	123.09	119.90
23	A	896	A	C5'-C4'-O4'	5.32	115.48	109.10
23	A	1012	C	C5-C6-N1	5.32	123.66	121.00
23	A	534	G	C2-N3-C4	-5.31	109.24	111.90
23	A	1436	C	C6-N1-C2	-5.31	118.17	120.30
12	u	7	LEU	CB-CG-CD2	5.31	120.02	111.00
23	A	1027	C	N1-C2-O2	5.31	122.08	118.90
23	A	1638	C	C5-C4-N4	-5.30	116.49	120.20
51	d	9	GLN	C-N-CD	5.29	139.52	128.40
23	A	43	C	C5-C4-N4	-5.29	116.50	120.20
23	A	1030	C	N3-C4-N4	5.29	121.70	118.00
23	A	1509	U	O4'-C1'-N1	-5.29	103.97	108.20
1	h	788	C	N3-C2-O2	-5.28	118.20	121.90
23	A	1413	C	N1-C2-O2	5.28	122.07	118.90
23	A	2230	C	C6-N1-C2	-5.27	118.19	120.30
19	8	228	ARG	N-CA-C	5.27	125.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1298	C	N3-C2-O2	-5.26	118.22	121.90
23	A	1775	C	N1-C2-O2	5.26	122.05	118.90
23	A	2169	G	C5-C6-O6	-5.25	125.45	128.60
19	8	87	VAL	CG1-CB-CG2	5.25	119.29	110.90
23	A	617	U	C2-N1-C1'	5.24	123.98	117.70
23	A	2398	C	N1-C2-O2	-5.24	115.76	118.90
23	A	2510	A	N1-C6-N6	5.24	121.74	118.60
23	A	390	G	N3-C2-N2	5.23	123.56	119.90
23	A	2818	C	C5-C4-N4	-5.23	116.54	120.20
23	A	667	A	C5-C6-N1	5.22	120.31	117.70
23	A	1378	U	C5-C4-O4	-5.22	122.77	125.90
23	A	1788	G	N3-C4-N9	-5.22	122.87	126.00
23	A	81	A	C5'-C4'-O4'	5.22	115.36	109.10
23	A	1409	C	C6-N1-C2	-5.22	118.21	120.30
23	A	939	C	N3-C4-N4	5.21	121.65	118.00
23	A	436	C	N3-C2-O2	-5.21	118.25	121.90
23	A	2730	U	N3-C2-O2	-5.20	118.56	122.20
23	A	2248	C	C2-N1-C1'	5.20	124.52	118.80
23	A	1022	C	N1-C2-O2	5.20	122.02	118.90
23	A	1276	G	C4-N9-C1'	5.20	133.26	126.50
23	A	2841	C	N3-C4-N4	5.20	121.64	118.00
23	A	631	C	N1-C2-O2	5.20	122.02	118.90
23	A	1082	C	C5-C4-N4	-5.20	116.56	120.20
23	A	2900	C	N3-C2-O2	-5.20	118.26	121.90
1	h	886	C	C5-C4-N4	-5.19	116.56	120.20
1	h	419	C	N1-C2-O2	-5.19	115.79	118.90
23	A	1874	C	N3-C4-N4	5.19	121.63	118.00
23	A	202	C	C5-C4-N4	-5.19	116.57	120.20
1	h	1326	C	N1-C2-O2	5.18	122.01	118.90
23	A	617	U	N1-C2-O2	5.18	126.43	122.80
23	A	1251	A	O4'-C1'-N9	5.18	112.35	108.20
23	A	2249	G	C4-C5-N7	5.18	112.87	110.80
23	A	2005	C	C5'-C4'-O4'	5.18	115.32	109.10
23	A	2260	C	C5-C6-N1	5.18	123.59	121.00
23	A	2574	C	C5-C4-N4	-5.18	116.57	120.20
23	A	1458	G	C6-C5-N7	-5.18	127.29	130.40
23	A	1570	C	C6-N1-C2	-5.18	118.23	120.30
36	N	45	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	h	975	G	C4-N9-C1'	5.17	133.22	126.50
23	A	974	G	C8-N9-C4	-5.17	104.33	106.40
23	A	357	U	P-O3'-C3'	5.17	125.90	119.70
23	A	2843	C	C5-C4-N4	-5.17	116.58	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1022	C	N3-C2-O2	-5.16	118.29	121.90
1	h	385	C	N1-C2-O2	5.16	122.00	118.90
19	8	214	THR	OG1-CB-CG2	5.16	121.86	110.00
23	A	97	U	P-O3'-C3'	5.16	125.89	119.70
23	A	2775	C	C2-N1-C1'	5.16	124.47	118.80
23	A	734	C	C5-C4-N4	-5.16	116.59	120.20
23	A	1393	C	C5-C4-N4	-5.16	116.59	120.20
23	A	652	C	N3-C4-N4	5.15	121.61	118.00
26	D	160	VAL	N-CA-CB	-5.15	100.16	111.50
23	A	2899	A	C5-C6-N6	-5.14	119.58	123.70
23	A	902	C	N1-C2-O2	5.14	121.98	118.90
23	A	73	C	C5-C4-N4	-5.13	116.61	120.20
23	A	962	U	C6-N1-C1'	-5.13	114.02	121.20
23	A	1752	C	C5-C4-N4	-5.13	116.61	120.20
23	A	1171	C	C5-C4-N4	-5.13	116.61	120.20
24	B	85	C	C5-C4-N4	-5.13	116.61	120.20
24	B	87	U	C5-C6-N1	5.12	125.26	122.70
23	A	1793	G	C6-C5-N7	-5.12	127.33	130.40
1	h	1139	C	C6-N1-C1'	-5.11	114.66	120.80
23	A	853	C	C2-N1-C1'	5.11	124.42	118.80
23	A	2665	C	C5-C4-N4	-5.11	116.62	120.20
1	h	975	G	C5-C6-O6	-5.11	125.53	128.60
19	8	225	LEU	CB-CG-CD2	5.10	119.68	111.00
50	c	30	ASP	C-N-CD	5.10	139.12	128.40
23	A	174	G	N1-C6-O6	5.10	122.96	119.90
23	A	2230	C	C5-C6-N1	5.10	123.55	121.00
1	h	367	U	C5-C6-N1	5.10	125.25	122.70
23	A	174	G	C4-C5-N7	5.10	112.84	110.80
19	8	170	HIS	C-N-CA	5.09	134.44	121.70
49	b	3	VAL	C-N-CD	5.09	139.10	128.40
1	h	885	G	C8-N9-C1'	-5.09	120.38	127.00
23	A	115	A	C8-N9-C4	-5.09	103.77	105.80
23	A	869	U	C5-C4-O4	-5.08	122.85	125.90
23	A	2561	G	C5-C6-O6	-5.08	125.55	128.60
23	A	1091	A	C5-C6-N1	5.08	120.24	117.70
54	g	90	ARG	N-CA-C	-5.08	97.28	111.00
23	A	161	U	N1-C2-O2	5.08	126.36	122.80
23	A	340	A	N9-C4-C5	-5.08	103.77	105.80
23	A	872	G	N3-C4-C5	5.08	131.14	128.60
1	h	623	C	N1-C2-O2	5.07	121.94	118.90
23	A	139	U	C2-N1-C1'	5.07	123.78	117.70
23	A	946	G	N1-C2-N2	-5.07	111.64	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	113	C	N1-C2-O2	5.07	121.94	118.90
27	E	101	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	h	273	A	C4-C5-N7	5.05	113.23	110.70
1	h	1117	U	OP1-P-O3'	5.05	116.32	105.20
23	A	1638	C	N3-C4-N4	5.05	121.54	118.00
23	A	357	U	OP2-P-O3'	5.05	116.31	105.20
23	A	501	C	N3-C4-N4	5.05	121.53	118.00
23	A	2626	U	N1-C2-O2	5.05	126.33	122.80
1	h	1383	C	C6-N1-C1'	-5.05	114.74	120.80
23	A	957	C	N1-C2-O2	5.05	121.93	118.90
23	A	1894	A	C5-N7-C8	-5.04	101.38	103.90
23	A	1971	C	C5-C4-N4	-5.04	116.67	120.20
23	A	1384	G	C4-N9-C1'	5.04	133.05	126.50
12	u	9	ARG	NE-CZ-NH1	5.04	122.82	120.30
23	A	2610	C	C2-N1-C1'	5.03	124.34	118.80
36	N	10	ARG	NE-CZ-NH1	5.03	122.81	120.30
23	A	1410	C	C6-N1-C2	-5.03	118.29	120.30
23	A	2249	G	C5-N7-C8	-5.03	101.79	104.30
35	M	21	ARG	NE-CZ-NH1	5.03	122.81	120.30
23	A	150	C	C5-C4-N4	-5.02	116.68	120.20
1	h	930	C	N1-C2-O2	5.02	121.91	118.90
23	A	2003	A	C5'-C4'-C3'	5.02	124.03	116.00
23	A	191	G	C8-N9-C1'	-5.01	120.48	127.00
23	A	197	C	C5-C4-N4	-5.01	116.69	120.20
23	A	1473	G	N1-C2-N2	-5.01	111.69	116.20
23	A	303	G	N3-C2-N2	-5.01	116.39	119.90
23	A	709	U	N1-C2-O2	5.01	126.31	122.80
23	A	1234	U	C2-N1-C1'	5.01	123.71	117.70
25	C	218	ARG	NE-CZ-NH2	-5.01	117.80	120.30
8	q	42	ARG	NE-CZ-NH1	5.01	122.80	120.30
23	A	895	G	C2-N3-C4	-5.01	109.40	111.90
1	h	469	G	N3-C4-N9	5.00	129.00	126.00
23	A	898	A	N7-C8-N9	5.00	116.30	113.80
23	A	726	A	C5-N7-C8	-5.00	101.40	103.90
23	A	1102	G	N7-C8-N9	5.00	115.60	113.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	8	159	SER	Peptide
19	8	160	ALA	Peptide

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Mol	Chain	Res	Type	Group
19	8	181	ILE	Peptide
19	8	192	ASP	Peptide
19	8	193	PRO	Peptide
19	8	24	ASN	Peptide
19	8	34	ASP	Peptide
19	8	4	VAL	Peptide
19	8	5	THR	Peptide
19	8	8	GLN	Peptide
26	D	147	ARG	Peptide
32	J	21	ASN	Peptide
45	W	153	ALA	Peptide
4	l	189	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	j	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	k	206/208 (99%)	182 (88%)	24 (12%)	0	100	100
4	l	198/200 (99%)	178 (90%)	19 (10%)	1 (0%)	29	66
5	m	178/180 (99%)	154 (86%)	22 (12%)	2 (1%)	14	50
6	n	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
7	p	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
8	q	129/131 (98%)	113 (88%)	16 (12%)	0	100	100
9	4	124/126 (98%)	111 (90%)	12 (10%)	1 (1%)	19	57
10	s	97/99 (98%)	89 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	t	113/115 (98%)	100 (88%)	13 (12%)	0	100	100
12	u	120/122 (98%)	102 (85%)	18 (15%)	0	100	100
13	v	114/116 (98%)	100 (88%)	14 (12%)	0	100	100
14	x	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	z	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
16	5	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
17	6	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
18	7	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
19	8	226/228 (99%)	196 (87%)	23 (10%)	7 (3%)	4	29
20	r	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
21	Y	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
22	9	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
25	C	273/275 (99%)	232 (85%)	41 (15%)	0	100	100
26	D	212/214 (99%)	182 (86%)	28 (13%)	2 (1%)	17	54
27	E	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
28	F	180/182 (99%)	165 (92%)	14 (8%)	1 (1%)	25	62
29	G	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
30	H	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
31	I	124/126 (98%)	117 (94%)	6 (5%)	1 (1%)	19	57
32	J	131/133 (98%)	116 (88%)	15 (12%)	0	100	100
33	K	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
34	L	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
35	M	143/145 (99%)	120 (84%)	21 (15%)	2 (1%)	11	44
36	N	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
37	O	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
38	P	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
39	Q	111/113 (98%)	94 (85%)	15 (14%)	2 (2%)	8	39
40	R	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
41	S	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
42	T	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
43	U	95/97 (98%)	81 (85%)	14 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	V	93/105 (89%)	87 (94%)	6 (6%)	0	100	100
45	W	190/192 (99%)	169 (89%)	20 (10%)	1 (0%)	29	66
46	X	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
47	Z	62/64 (97%)	62 (100%)	0	0	100	100
48	a	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
49	b	52/54 (96%)	47 (90%)	4 (8%)	1 (2%)	8	38
50	c	51/53 (96%)	26 (51%)	15 (29%)	10 (20%)	0	1
51	d	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	e	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
53	f	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
54	g	71/82 (87%)	50 (70%)	16 (22%)	5 (7%)	1	11
55	y	75/77 (97%)	56 (75%)	8 (11%)	11 (15%)	0	2
56	3	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
All	All	6173/6298 (98%)	5524 (90%)	602 (10%)	47 (1%)	24	57

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	m	103	GLY
19	8	16	PHE
19	8	25	PRO
19	8	161	VAL
26	D	156	THR
28	F	131	GLY
49	b	9	SER
50	c	10	LYS
50	c	12	ARG
50	c	33	ARG
50	c	34	ILE
50	c	36	LEU
54	g	3	PRO
55	y	16	SER
55	y	24	THR
55	y	27	ARG
55	y	31	ASN
9	4	147	TYR
19	8	15	HIS

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Mol	Chain	Res	Type
50	c	32	ASP
50	c	37	ARG
50	c	46	HIS
55	y	23	ARG
55	y	30	PRO
19	8	18	HIS
19	8	193	PRO
31	I	125	ASP
54	g	47	PRO
55	y	14	GLY
55	y	15	ASN
5	m	104	SER
35	M	45	ASN
50	c	43	LEU
54	g	30	THR
26	D	162	LYS
35	M	70	ARG
39	Q	93	ARG
50	c	35	VAL
55	y	4	CYS
55	y	26	ARG
55	y	29	ASP
19	8	21	ARG
39	Q	3	THR
54	g	5	ILE
4	l	189	PRO
45	W	154	GLY
54	g	11	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	j	30/30 (100%)	30 (100%)	0	100 100
3	k	170/170 (100%)	168 (99%)	2 (1%)	71 87
4	l	175/175 (100%)	175 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	m	127/127 (100%)	126 (99%)	1 (1%)	81	92
6	n	85/85 (100%)	83 (98%)	2 (2%)	49	76
7	p	131/131 (100%)	130 (99%)	1 (1%)	81	92
8	q	107/107 (100%)	106 (99%)	1 (1%)	78	91
9	4	102/102 (100%)	99 (97%)	3 (3%)	42	71
10	s	89/89 (100%)	89 (100%)	0	100	100
11	t	89/89 (100%)	88 (99%)	1 (1%)	73	88
12	u	103/103 (100%)	102 (99%)	1 (1%)	76	89
13	v	99/99 (100%)	99 (100%)	0	100	100
14	x	76/76 (100%)	75 (99%)	1 (1%)	69	86
15	z	92/92 (100%)	92 (100%)	0	100	100
16	5	80/80 (100%)	77 (96%)	3 (4%)	33	64
17	6	73/73 (100%)	73 (100%)	0	100	100
18	7	69/69 (100%)	65 (94%)	4 (6%)	20	52
19	8	191/191 (100%)	185 (97%)	6 (3%)	40	70
20	r	70/70 (100%)	70 (100%)	0	100	100
21	Y	91/91 (100%)	91 (100%)	0	100	100
22	9	85/85 (100%)	85 (100%)	0	100	100
25	C	215/215 (100%)	215 (100%)	0	100	100
26	D	160/160 (100%)	159 (99%)	1 (1%)	86	95
27	E	169/169 (100%)	168 (99%)	1 (1%)	86	95
28	F	151/151 (100%)	149 (99%)	2 (1%)	69	86
29	G	148/148 (100%)	148 (100%)	0	100	100
30	H	116/116 (100%)	115 (99%)	1 (1%)	78	91
31	I	89/89 (100%)	89 (100%)	0	100	100
32	J	102/102 (100%)	101 (99%)	1 (1%)	76	89
33	K	119/119 (100%)	119 (100%)	0	100	100
34	L	100/100 (100%)	100 (100%)	0	100	100
35	M	112/112 (100%)	112 (100%)	0	100	100
36	N	114/114 (100%)	113 (99%)	1 (1%)	78	91
37	O	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	P	93/93 (100%)	92 (99%)	1 (1%)	73	88
39	Q	100/100 (100%)	99 (99%)	1 (1%)	76	89
40	R	97/97 (100%)	97 (100%)	0	100	100
41	S	81/81 (100%)	80 (99%)	1 (1%)	71	87
42	T	90/90 (100%)	87 (97%)	3 (3%)	38	68
43	U	83/83 (100%)	83 (100%)	0	100	100
44	V	81/86 (94%)	80 (99%)	1 (1%)	71	87
45	W	155/155 (100%)	155 (100%)	0	100	100
46	X	58/58 (100%)	56 (97%)	2 (3%)	37	67
47	Z	58/58 (100%)	58 (100%)	0	100	100
48	a	52/52 (100%)	52 (100%)	0	100	100
49	b	43/43 (100%)	42 (98%)	1 (2%)	50	76
50	c	49/49 (100%)	48 (98%)	1 (2%)	55	79
51	d	35/35 (100%)	35 (100%)	0	100	100
52	e	53/53 (100%)	53 (100%)	0	100	100
53	f	35/35 (100%)	35 (100%)	0	100	100
54	g	64/70 (91%)	63 (98%)	1 (2%)	62	83
55	y	64/64 (100%)	61 (95%)	3 (5%)	26	59
56	3	18/18 (100%)	18 (100%)	0	100	100
All	All	5135/5146 (100%)	5087 (99%)	48 (1%)	79	91

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	k	169	ARG
3	k	179	ARG
5	m	101	LEU
6	n	47	ARG
6	n	77	ARG
7	p	41	ARG
8	q	78	ARG
9	4	100	ARG
9	4	126	ARG
9	4	133	ARG
11	t	137	ARG

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Mol	Chain	Res	Type
12	u	83	ARG
14	x	88	ARG
16	5	17	ARG
16	5	54	ARG
16	5	89	ARG
18	7	18	ARG
18	7	20	ARG
18	7	33	ARG
18	7	56	ARG
19	8	16	PHE
19	8	18	HIS
19	8	19	GLN
19	8	177	ARG
19	8	212	LEU
19	8	213	LEU
26	D	201	ARG
27	E	46	ARG
28	F	78	ARG
28	F	95	ARG
30	H	57	LYS
32	J	52	ARG
36	N	10	ARG
38	P	26	ARG
39	Q	38	ARG
41	S	81	LYS
42	T	90	LYS
42	T	93	ARG
42	T	104	ARG
44	V	1	MET
46	X	14	ARG
46	X	85	ARG
49	b	6	ARG
50	c	12	ARG
54	g	64	SER
55	y	26	ARG
55	y	45	ARG
55	y	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
10	s	70	HIS

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Mol	Chain	Res	Type
14	x	28	GLN
17	6	29	GLN
21	Y	50	ASN
25	C	53	HIS
25	C	91	ASN
27	E	182	GLN
28	F	31	ASN
30	H	46	GLN
38	P	41	ASN
54	g	58	HIS
55	y	19	HIS
55	y	21	HIS
55	y	33	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	h	1510/1511 (99%)	391 (25%)	0
23	A	3118/3119 (99%)	771 (24%)	32 (1%)
24	B	117/118 (99%)	23 (19%)	1 (0%)
All	All	4745/4748 (99%)	1185 (24%)	33 (0%)

All (1185) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	h	9	U
1	h	10	G
1	h	11	G
1	h	12	A
1	h	13	G
1	h	18	U
1	h	26	G
1	h	36	A
1	h	43	G
1	h	51	C
1	h	52	U
1	h	54	A
1	h	55	A
1	h	59	A
1	h	70	A
1	h	82	U

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Mol	Chain	Res	Type
1	h	87	G
1	h	89	G
1	h	91	U
1	h	92	A
1	h	93	C
1	h	101	G
1	h	117	C
1	h	118	A
1	h	126	G
1	h	127	A
1	h	128	U
1	h	133	C
1	h	136	G
1	h	160	C
1	h	174	G
1	h	179	C
1	h	193	C
1	h	196	G
1	h	200	U
1	h	201	G
1	h	207	G
1	h	211	A
1	h	213	C
1	h	214	U
1	h	215	U
1	h	217	U
1	h	218	G
1	h	219	C
1	h	220	G
1	h	231	G
1	h	240	C
1	h	243	A
1	h	245	C
1	h	247	G
1	h	251	G
1	h	254	G
1	h	258	G
1	h	266	G
1	h	267	C
1	h	268	C
1	h	279	A
1	h	280	C

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Mol	Chain	Res	Type
1	h	281	G
1	h	289	G
1	h	298	A
1	h	300	A
1	h	306	A
1	h	329	A
1	h	330	C
1	h	332	G
1	h	340	U
1	h	345	C
1	h	347	G
1	h	350	G
1	h	351	G
1	h	352	C
1	h	353	A
1	h	359	G
1	h	367	U
1	h	369	G
1	h	372	C
1	h	373	A
1	h	381	C
1	h	382	A
1	h	388	G
1	h	389	A
1	h	390	U
1	h	392	C
1	h	393	A
1	h	397	A
1	h	398	C
1	h	406	G
1	h	412	U
1	h	413	G
1	h	414	A
1	h	421	U
1	h	422	C
1	h	423	G
1	h	424	G
1	h	428	G
1	h	429	U
1	h	430	A
1	h	432	A
1	h	434	C

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Mol	Chain	Res	Type
1	h	438	U
1	h	440	C
1	h	445	C
1	h	449	C
1	h	452	A
1	h	453	G
1	h	456	C
1	h	458	A
1	h	459	G
1	h	461	G
1	h	464	G
1	h	466	U
1	h	469	G
1	h	472	C
1	h	477	G
1	h	478	A
1	h	479	A
1	h	485	G
1	h	486	G
1	h	489	A
1	h	491	C
1	h	492	U
1	h	497	G
1	h	498	C
1	h	499	C
1	h	505	C
1	h	507	G
1	h	509	G
1	h	510	G
1	h	511	U
1	h	512	A
1	h	513	A
1	h	514	U
1	h	516	C
1	h	519	A
1	h	520	G
1	h	525	C
1	h	527	A
1	h	540	A
1	h	542	U
1	h	544	C
1	h	545	U

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Mol	Chain	Res	Type
1	h	552	A
1	h	553	A
1	h	555	G
1	h	556	A
1	h	557	G
1	h	567	G
1	h	576	C
1	h	590	A
1	h	600	U
1	h	603	C
1	h	611	G
1	h	612	U
1	h	629	G
1	h	633	A
1	h	643	A
1	h	645	G
1	h	660	C
1	h	666	U
1	h	668	G
1	h	680	G
1	h	683	G
1	h	694	G
1	h	695	A
1	h	698	A
1	h	701	G
1	h	702	G
1	h	703	U
1	h	711	G
1	h	713	G
1	h	728	A
1	h	729	A
1	h	732	G
1	h	735	G
1	h	739	A
1	h	761	A
1	h	772	A
1	h	773	U
1	h	776	C
1	h	785	C
1	h	790	C
1	h	793	U
1	h	794	A

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Mol	Chain	Res	Type
1	h	797	C
1	h	800	U
1	h	801	G
1	h	808	A
1	h	812	G
1	h	818	U
1	h	821	C
1	h	822	U
1	h	824	C
1	h	826	U
1	h	827	U
1	h	828	G
1	h	840	G
1	h	841	U
1	h	854	A
1	h	855	A
1	h	858	A
1	h	859	C
1	h	867	G
1	h	871	A
1	h	872	G
1	h	882	A
1	h	884	G
1	h	896	A
1	h	908	G
1	h	909	G
1	h	913	C
1	h	914	C
1	h	916	C
1	h	917	A
1	h	921	G
1	h	924	G
1	h	927	G
1	h	930	C
1	h	938	U
1	h	940	A
1	h	942	U
1	h	943	U
1	h	948	G
1	h	950	A
1	h	951	A
1	h	953	G

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Mol	Chain	Res	Type
1	h	956	A
1	h	957	A
1	h	958	G
1	h	959	A
1	h	960	A
1	h	964	U
1	h	965	A
1	h	971	G
1	h	973	U
1	h	974	U
1	h	975	G
1	h	976	A
1	h	982	A
1	h	985	G
1	h	987	A
1	h	988	C
1	h	989	G
1	h	990	C
1	h	992	G
1	h	1003	C
1	h	1008	C
1	h	1009	C
1	h	1010	C
1	h	1012	U
1	h	1014	U
1	h	1019	U
1	h	1021	U
1	h	1024	G
1	h	1025	C
1	h	1026	A
1	h	1027	G
1	h	1030	G
1	h	1033	G
1	h	1034	C
1	h	1036	U
1	h	1045	U
1	h	1047	A
1	h	1048	G
1	h	1054	G
1	h	1059	G
1	h	1074	G
1	h	1075	U

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Mol	Chain	Res	Type
1	h	1079	G
1	h	1080	C
1	h	1081	A
1	h	1084	G
1	h	1089	C
1	h	1092	C
1	h	1104	G
1	h	1106	U
1	h	1107	G
1	h	1112	C
1	h	1113	A
1	h	1115	G
1	h	1117	U
1	h	1118	A
1	h	1120	G
1	h	1121	G
1	h	1124	G
1	h	1125	G
1	h	1126	G
1	h	1129	U
1	h	1133	G
1	h	1136	A
1	h	1138	A
1	h	1139	C
1	h	1140	U
1	h	1148	U
1	h	1149	C
1	h	1150	A
1	h	1151	A
1	h	1155	G
1	h	1160	A
1	h	1162	G
1	h	1163	G
1	h	1165	G
1	h	1168	G
1	h	1177	A
1	h	1178	A
1	h	1182	A
1	h	1193	U
1	h	1194	A
1	h	1200	A
1	h	1206	U

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Mol	Chain	Res	Type
1	h	1218	C
1	h	1219	A
1	h	1220	A
1	h	1221	U
1	h	1222	G
1	h	1234	G
1	h	1237	C
1	h	1238	U
1	h	1239	G
1	h	1241	G
1	h	1244	G
1	h	1248	U
1	h	1249	G
1	h	1255	G
1	h	1258	C
1	h	1259	G
1	h	1261	A
1	h	1265	U
1	h	1266	U
1	h	1267	U
1	h	1268	C
1	h	1270	A
1	h	1279	U
1	h	1280	C
1	h	1282	G
1	h	1283	U
1	h	1284	U
1	h	1287	G
1	h	1299	C
1	h	1300	A
1	h	1301	A
1	h	1304	C
1	h	1313	G
1	h	1320	G
1	h	1322	G
1	h	1326	C
1	h	1327	U
1	h	1328	A
1	h	1329	G
1	h	1332	A
1	h	1343	G
1	h	1345	A

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Mol	Chain	Res	Type
1	h	1346	A
1	h	1348	G
1	h	1353	G
1	h	1357	A
1	h	1360	A
1	h	1361	C
1	h	1362	G
1	h	1364	U
1	h	1381	A
1	h	1382	C
1	h	1383	C
1	h	1405	G
1	h	1407	U
1	h	1409	A
1	h	1423	U
1	h	1425	G
1	h	1426	C
1	h	1429	A
1	h	1433	C
1	h	1434	U
1	h	1435	U
1	h	1436	G
1	h	1438	G
1	h	1451	G
1	h	1477	A
1	h	1478	G
1	h	1481	G
1	h	1483	A
1	h	1486	A
1	h	1487	A
1	h	1488	G
1	h	1490	U
1	h	1491	A
1	h	1501	G
1	h	1502	A
1	h	1503	A
1	h	1504	G
1	h	1513	G
1	h	1514	G
23	A	7	U
23	A	11	A
23	A	19	U

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Mol	Chain	Res	Type
23	A	20	G
23	A	23	G
23	A	25	A
23	A	29	C
23	A	31	U
23	A	32	G
23	A	43	C
23	A	47	U
23	A	60	A
23	A	68	A
23	A	71	A
23	A	72	G
23	A	81	A
23	A	82	G
23	A	85	G
23	A	94	G
23	A	98	U
23	A	99	G
23	A	107	G
23	A	115	A
23	A	117	U
23	A	125	C
23	A	126	C
23	A	128	G
23	A	136	U
23	A	138	A
23	A	148	A
23	A	150	C
23	A	151	A
23	A	159	A
23	A	161	U
23	A	162	A
23	A	180	A
23	A	188	G
23	A	195	A
23	A	198	A
23	A	203	A
23	A	204	G
23	A	212	A
23	A	214	G
23	A	215	A
23	A	220	A

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Mol	Chain	Res	Type
23	A	221	A
23	A	227	A
23	A	229	U
23	A	230	G
23	A	232	G
23	A	233	A
23	A	241	A
23	A	248	G
23	A	265	A
23	A	267	G
23	A	279	U
23	A	282	A
23	A	285	U
23	A	286	G
23	A	287	A
23	A	288	U
23	A	289	A
23	A	290	C
23	A	291	C
23	A	292	G
23	A	298	G
23	A	299	G
23	A	300	G
23	A	301	U
23	A	303	G
23	A	305	G
23	A	315	U
23	A	316	U
23	A	317	G
23	A	318	U
23	A	319	G
23	A	323	C
23	A	324	C
23	A	327	U
23	A	329	U
23	A	330	U
23	A	331	U
23	A	335	G
23	A	336	C
23	A	337	U
23	A	338	C
23	A	340	A

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Mol	Chain	Res	Type
23	A	342	C
23	A	348	G
23	A	351	G
23	A	352	G
23	A	357	U
23	A	358	G
23	A	361	A
23	A	363	A
23	A	369	G
23	A	370	U
23	A	376	G
23	A	383	U
23	A	384	G
23	A	391	G
23	A	393	U
23	A	404	A
23	A	412	A
23	A	413	G
23	A	417	C
23	A	428	A
23	A	433	C
23	A	434	G
23	A	437	G
23	A	441	G
23	A	444	U
23	A	445	U
23	A	446	G
23	A	448	U
23	A	449	G
23	A	450	G
23	A	452	G
23	A	460	G
23	A	467	C
23	A	474	G
23	A	475	U
23	A	482	U
23	A	489	A
23	A	491	U
23	A	493	U
23	A	494	G
23	A	500	A
23	A	505	C

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Mol	Chain	Res	Type
23	A	509	U
23	A	512	G
23	A	514	C
23	A	517	A
23	A	523	U
23	A	531	A
23	A	539	C
23	A	543	U
23	A	544	U
23	A	552	U
23	A	553	G
23	A	556	G
23	A	561	G
23	A	562	G
23	A	563	U
23	A	565	A
23	A	566	A
23	A	567	A
23	A	569	G
23	A	578	G
23	A	585	G
23	A	589	A
23	A	591	G
23	A	592	A
23	A	594	U
23	A	595	A
23	A	596	C
23	A	597	C
23	A	605	G
23	A	614	C
23	A	617	U
23	A	618	C
23	A	619	C
23	A	620	G
23	A	633	A
23	A	634	C
23	A	636	U
23	A	637	G
23	A	638	U
23	A	639	C
23	A	640	G
23	A	642	G

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Mol	Chain	Res	Type
23	A	644	G
23	A	646	U
23	A	648	A
23	A	654	U
23	A	655	G
23	A	661	U
23	A	665	G
23	A	666	A
23	A	667	A
23	A	679	G
23	A	684	G
23	A	685	G
23	A	696	A
23	A	697	G
23	A	706	G
23	A	707	G
23	A	708	G
23	A	714	U
23	A	721	A
23	A	725	A
23	A	731	A
23	A	740	A
23	A	747	A
23	A	756	A
23	A	757	G
23	A	758	A
23	A	760	U
23	A	763	G
23	A	764	U
23	A	766	G
23	A	767	U
23	A	768	G
23	A	784	G
23	A	801	U
23	A	830	A
23	A	832	G
23	A	845	C
23	A	862	U
23	A	863	G
23	A	868	C
23	A	880	G
23	A	890	G

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Mol	Chain	Res	Type
23	A	897	A
23	A	898	A
23	A	899	G
23	A	905	U
23	A	907	A
23	A	909	A
23	A	915	U
23	A	916	G
23	A	920	G
23	A	927	C
23	A	942	U
23	A	943	U
23	A	945	G
23	A	954	U
23	A	960	G
23	A	961	U
23	A	973	G
23	A	974	G
23	A	975	U
23	A	976	A
23	A	981	U
23	A	982	A
23	A	983	C
23	A	995	U
23	A	997	G
23	A	1001	C
23	A	1002	C
23	A	1003	A
23	A	1004	C
23	A	1005	A
23	A	1006	G
23	A	1007	G
23	A	1008	G
23	A	1011	A
23	A	1012	C
23	A	1013	U
23	A	1015	A
23	A	1025	A
23	A	1027	C
23	A	1028	U
23	A	1029	C
23	A	1030	C

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Mol	Chain	Res	Type
23	A	1034	U
23	A	1046	C
23	A	1047	A
23	A	1049	G
23	A	1058	A
23	A	1062	A
23	A	1063	G
23	A	1075	U
23	A	1076	A
23	A	1078	G
23	A	1084	U
23	A	1085	G
23	A	1091	A
23	A	1092	G
23	A	1101	A
23	A	1103	C
23	A	1114	G
23	A	1121	G
23	A	1130	C
23	A	1131	G
23	A	1140	G
23	A	1141	U
23	A	1143	G
23	A	1144	A
23	A	1151	U
23	A	1152	G
23	A	1153	U
23	A	1157	G
23	A	1164	A
23	A	1165	G
23	A	1173	G
23	A	1178	U
23	A	1179	U
23	A	1180	G
23	A	1184	U
23	A	1185	A
23	A	1186	G
23	A	1187	A
23	A	1188	A
23	A	1189	G
23	A	1190	C
23	A	1191	A

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Mol	Chain	Res	Type
23	A	1192	G
23	A	1200	U
23	A	1201	G
23	A	1202	A
23	A	1203	A
23	A	1205	G
23	A	1206	A
23	A	1207	G
23	A	1208	U
23	A	1209	G
23	A	1212	U
23	A	1213	A
23	A	1214	A
23	A	1215	U
23	A	1216	A
23	A	1219	U
23	A	1223	U
23	A	1224	G
23	A	1226	U
23	A	1230	G
23	A	1234	U
23	A	1235	U
23	A	1238	G
23	A	1240	G
23	A	1244	A
23	A	1246	A
23	A	1251	A
23	A	1253	C
23	A	1260	C
23	A	1261	A
23	A	1267	A
23	A	1270	G
23	A	1290	C
23	A	1292	U
23	A	1293	G
23	A	1294	U
23	A	1320	U
23	A	1325	U
23	A	1332	G
23	A	1339	G
23	A	1343	G
23	A	1344	A

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Mol	Chain	Res	Type
23	A	1345	G
23	A	1352	A
23	A	1353	G
23	A	1359	G
23	A	1362	A
23	A	1365	G
23	A	1370	U
23	A	1371	G
23	A	1380	A
23	A	1386	G
23	A	1387	A
23	A	1389	U
23	A	1404	C
23	A	1408	C
23	A	1415	A
23	A	1416	A
23	A	1435	C
23	A	1437	A
23	A	1440	C
23	A	1444	U
23	A	1445	C
23	A	1456	G
23	A	1457	A
23	A	1462	G
23	A	1465	C
23	A	1480	A
23	A	1481	C
23	A	1499	A
23	A	1501	C
23	A	1507	G
23	A	1508	A
23	A	1510	A
23	A	1511	U
23	A	1518	A
23	A	1522	G
23	A	1524	G
23	A	1525	U
23	A	1529	U
23	A	1530	G
23	A	1531	C
23	A	1534	C
23	A	1536	A

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Mol	Chain	Res	Type
23	A	1537	U
23	A	1538	G
23	A	1540	U
23	A	1544	U
23	A	1546	A
23	A	1547	G
23	A	1550	G
23	A	1551	U
23	A	1552	A
23	A	1553	C
23	A	1554	U
23	A	1555	A
23	A	1556	A
23	A	1558	C
23	A	1559	A
23	A	1561	C
23	A	1564	A
23	A	1565	A
23	A	1567	C
23	A	1570	C
23	A	1571	C
23	A	1572	G
23	A	1574	G
23	A	1579	C
23	A	1580	A
23	A	1584	U
23	A	1587	G
23	A	1588	G
23	A	1589	G
23	A	1595	G
23	A	1598	U
23	A	1599	U
23	A	1600	G
23	A	1604	G
23	A	1605	G
23	A	1607	C
23	A	1608	U
23	A	1611	A
23	A	1616	A
23	A	1617	C
23	A	1623	U
23	A	1625	G

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Mol	Chain	Res	Type
23	A	1627	U
23	A	1629	G
23	A	1630	U
23	A	1631	A
23	A	1632	G
23	A	1637	G
23	A	1638	C
23	A	1639	G
23	A	1640	A
23	A	1648	A
23	A	1649	C
23	A	1650	G
23	A	1658	G
23	A	1674	G
23	A	1679	A
23	A	1680	A
23	A	1681	U
23	A	1688	G
23	A	1696	G
23	A	1703	G
23	A	1710	A
23	A	1711	G
23	A	1713	U
23	A	1716	A
23	A	1717	U
23	A	1720	G
23	A	1724	G
23	A	1727	A
23	A	1728	U
23	A	1730	U
23	A	1731	A
23	A	1736	G
23	A	1737	A
23	A	1738	G
23	A	1746	G
23	A	1751	G
23	A	1754	G
23	A	1755	A
23	A	1756	G
23	A	1757	U
23	A	1760	G
23	A	1767	U

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Mol	Chain	Res	Type
23	A	1778	A
23	A	1787	A
23	A	1789	A
23	A	1791	A
23	A	1801	C
23	A	1802	G
23	A	1803	A
23	A	1813	C
23	A	1820	U
23	A	1825	C
23	A	1834	A
23	A	1835	C
23	A	1852	A
23	A	1857	U
23	A	1864	U
23	A	1865	A
23	A	1866	C
23	A	1871	G
23	A	1872	A
23	A	1878	G
23	A	1890	C
23	A	1892	G
23	A	1895	A
23	A	1909	C
23	A	1912	C
23	A	1916	A
23	A	1917	G
23	A	1918	A
23	A	1921	G
23	A	1925	A
23	A	1931	A
23	A	1946	U
23	A	1947	U
23	A	1948	A
23	A	1950	G
23	A	1973	C
23	A	1975	A
23	A	1979	A
23	A	1980	G
23	A	1981	U
23	A	1990	A
23	A	1998	C

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Mol	Chain	Res	Type
23	A	2003	A
23	A	2004	A
23	A	2017	C
23	A	2018	G
23	A	2024	G
23	A	2025	C
23	A	2026	A
23	A	2027	A
23	A	2033	U
23	A	2036	A
23	A	2046	A
23	A	2047	C
23	A	2050	C
23	A	2052	G
23	A	2064	A
23	A	2065	A
23	A	2066	G
23	A	2086	U
23	A	2088	C
23	A	2089	C
23	A	2090	U
23	A	2092	U
23	A	2093	G
23	A	2094	G
23	A	2095	G
23	A	2096	G
23	A	2106	A
23	A	2107	G
23	A	2112	U
23	A	2130	G
23	A	2136	A
23	A	2138	C
23	A	2140	A
23	A	2141	U
23	A	2152	A
23	A	2153	G
23	A	2154	G
23	A	2155	U
23	A	2161	A
23	A	2162	A
23	A	2163	U
23	A	2164	U

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Mol	Chain	Res	Type
23	A	2165	C
23	A	2166	C
23	A	2167	U
23	A	2178	G
23	A	2179	U
23	A	2191	C
23	A	2194	A
23	A	2195	U
23	A	2196	G
23	A	2197	G
23	A	2199	G
23	A	2215	U
23	A	2217	U
23	A	2221	A
23	A	2241	U
23	A	2246	U
23	A	2255	A
23	A	2256	G
23	A	2257	A
23	A	2267	C
23	A	2276	G
23	A	2279	C
23	A	2280	G
23	A	2284	A
23	A	2285	G
23	A	2286	A
23	A	2293	G
23	A	2300	A
23	A	2315	U
23	A	2316	G
23	A	2325	U
23	A	2327	C
23	A	2329	G
23	A	2331	U
23	A	2334	U
23	A	2335	G
23	A	2336	U
23	A	2338	G
23	A	2339	G
23	A	2341	U
23	A	2342	A
23	A	2343	G

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Mol	Chain	Res	Type
23	A	2346	G
23	A	2347	G
23	A	2348	G
23	A	2350	G
23	A	2351	A
23	A	2352	C
23	A	2353	U
23	A	2354	G
23	A	2355	U
23	A	2356	G
23	A	2358	A
23	A	2359	G
23	A	2363	A
23	A	2367	G
23	A	2368	C
23	A	2373	G
23	A	2375	G
23	A	2380	G
23	A	2381	A
23	A	2382	G
23	A	2383	U
23	A	2384	C
23	A	2385	G
23	A	2387	U
23	A	2388	G
23	A	2389	U
23	A	2390	U
23	A	2392	A
23	A	2394	A
23	A	2395	U
23	A	2399	A
23	A	2401	U
23	A	2402	C
23	A	2403	U
23	A	2407	C
23	A	2408	G
23	A	2411	U
23	A	2413	G
23	A	2421	A
23	A	2434	A
23	A	2436	A
23	A	2437	U

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Mol	Chain	Res	Type
23	A	2449	A
23	A	2450	C
23	A	2454	G
23	A	2462	G
23	A	2463	G
23	A	2490	A
23	A	2492	A
23	A	2503	G
23	A	2507	C
23	A	2508	C
23	A	2510	A
23	A	2511	A
23	A	2520	U
23	A	2521	C
23	A	2528	G
23	A	2529	A
23	A	2530	C
23	A	2532	G
23	A	2534	A
23	A	2549	G
23	A	2559	A
23	A	2566	C
23	A	2571	C
23	A	2574	C
23	A	2585	U
23	A	2596	G
23	A	2601	A
23	A	2607	G
23	A	2609	A
23	A	2626	U
23	A	2627	C
23	A	2639	G
23	A	2643	U
23	A	2647	U
23	A	2649	A
23	A	2653	G
23	A	2654	A
23	A	2655	U
23	A	2658	A
23	A	2659	A
23	A	2664	C
23	A	2665	C

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Mol	Chain	Res	Type
23	A	2672	A
23	A	2673	U
23	A	2693	A
23	A	2694	G
23	A	2699	C
23	A	2707	C
23	A	2715	U
23	A	2722	C
23	A	2726	G
23	A	2728	U
23	A	2729	G
23	A	2730	U
23	A	2742	A
23	A	2749	G
23	A	2750	G
23	A	2753	G
23	A	2755	A
23	A	2759	G
23	A	2767	G
23	A	2778	U
23	A	2788	A
23	A	2790	A
23	A	2791	G
23	A	2796	A
23	A	2797	C
23	A	2802	G
23	A	2806	G
23	A	2810	U
23	A	2826	A
23	A	2827	G
23	A	2833	U
23	A	2835	U
23	A	2837	U
23	A	2853	C
23	A	2854	A
23	A	2857	A
23	A	2860	U
23	A	2862	G
23	A	2870	C
23	A	2871	U
23	A	2878	A
23	A	2884	A

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Mol	Chain	Res	Type
23	A	2893	G
23	A	2906	U
23	A	2912	A
23	A	2913	U
23	A	2926	A
23	A	2929	A
23	A	2936	C
23	A	2937	G
23	A	2938	G
23	A	2957	A
23	A	2959	A
23	A	2963	U
23	A	2968	G
23	A	2972	A
23	A	2974	A
23	A	2979	C
23	A	2982	A
23	A	2985	G
23	A	2989	A
23	A	2990	A
23	A	3002	A
23	A	3013	C
23	A	3014	A
23	A	3015	C
23	A	3020	U
23	A	3021	A
23	A	3023	G
23	A	3024	A
23	A	3029	U
23	A	3039	C
23	A	3042	A
23	A	3047	A
23	A	3053	U
23	A	3054	U
23	A	3055	G
23	A	3068	U
23	A	3070	G
23	A	3079	U
23	A	3080	A
23	A	3082	U
23	A	3087	G
23	A	3088	C

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Mol	Chain	Res	Type
23	A	3089	A
23	A	3093	A
23	A	3095	C
23	A	3100	A
23	A	3101	C
23	A	3104	A
23	A	3105	C
23	A	3106	C
23	A	3107	G
23	A	3112	A
23	A	3115	A
23	A	3117	U
24	B	4	A
24	B	5	C
24	B	9	G
24	B	11	U
24	B	12	C
24	B	13	C
24	B	14	A
24	B	26	A
24	B	30	G
24	B	36	U
24	B	37	C
24	B	41	U
24	B	42	C
24	B	43	C
24	B	45	G
24	B	56	C
24	B	67	A
24	B	87	U
24	B	89	C
24	B	90	G
24	B	103	G
24	B	107	A
24	B	114	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	81	A
23	A	97	U
23	A	228	A

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Mol	Chain	Res	Type
23	A	316	U
23	A	336	C
23	A	357	U
23	A	445	U
23	A	552	U
23	A	641	U
23	A	643	G
23	A	899	G
23	A	974	G
23	A	1002	C
23	A	1004	C
23	A	1006	G
23	A	1014	G
23	A	1046	C
23	A	1084	U
23	A	1186	G
23	A	1293	G
23	A	1436	C
23	A	1510	A
23	A	2003	A
23	A	2005	C
23	A	2088	C
23	A	2094	G
23	A	2139	U
23	A	2165	C
23	A	2350	G
23	A	2384	C
23	A	2389	U
23	A	2626	U
24	B	10	G

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)

There are no chain breaks in this entry.

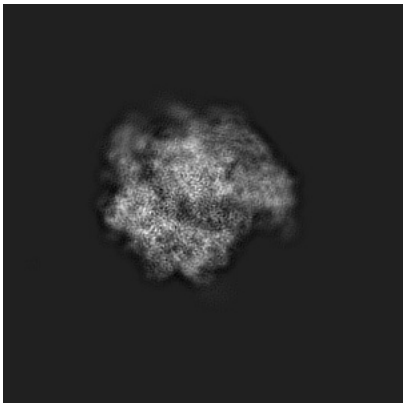
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8932. These allow visual inspection of the internal detail of the map and identification of artifacts.

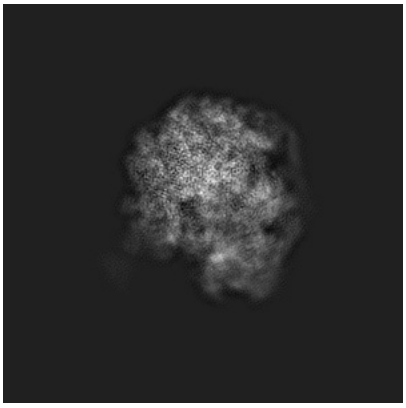
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

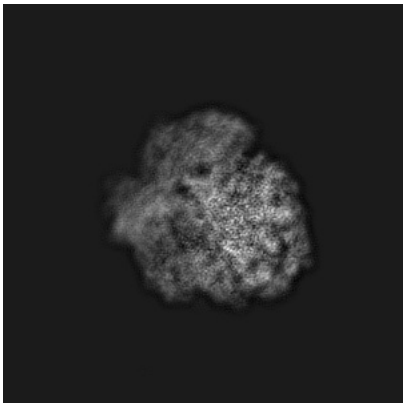
6.1.1 Primary map



X



Y

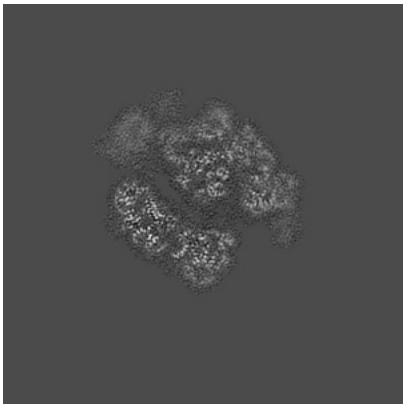


Z

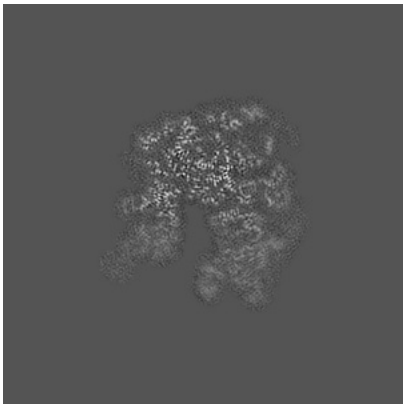
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

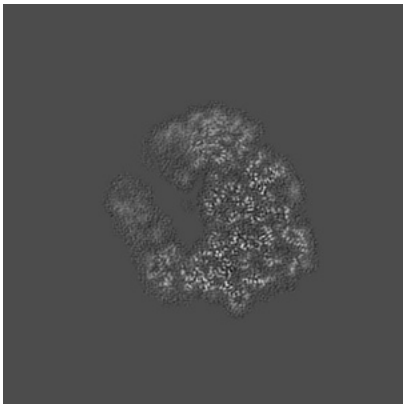
6.2.1 Primary map



X Index: 227



Y Index: 227

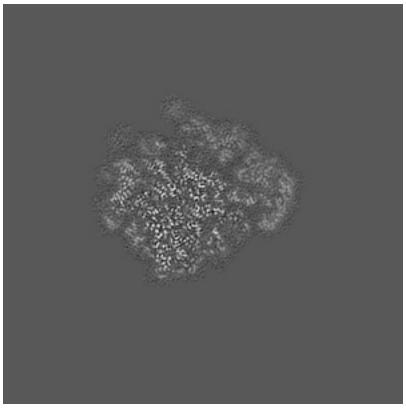


Z Index: 227

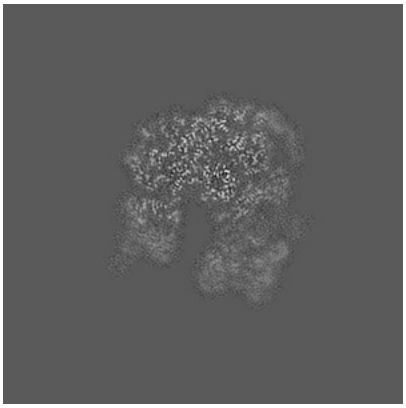
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

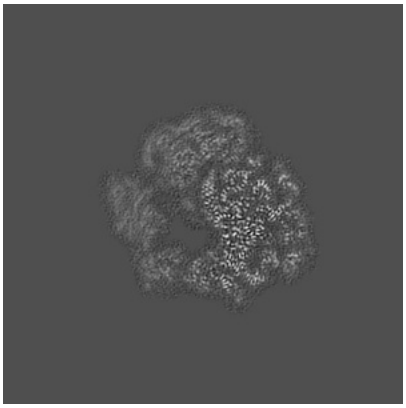
6.3.1 Primary map



X Index: 255



Y Index: 216

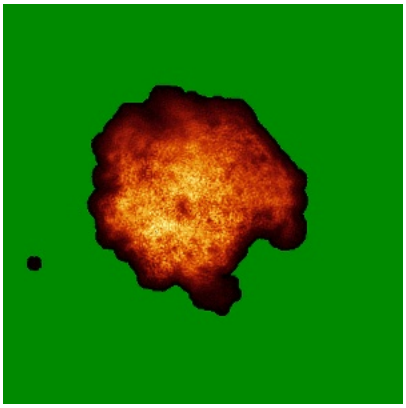


Z Index: 238

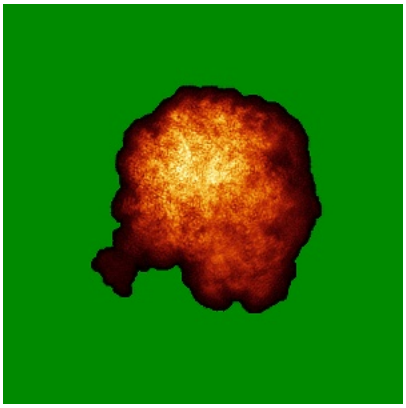
The images above show the largest variance slices of the map in three orthogonal directions.

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

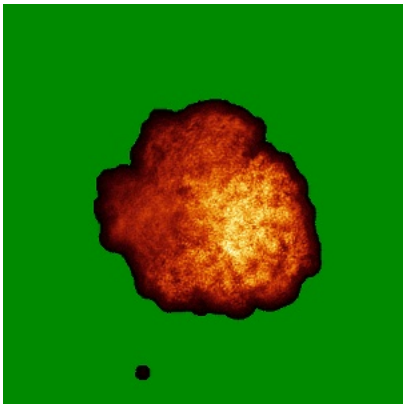
6.4.1 Primary map



X



Y

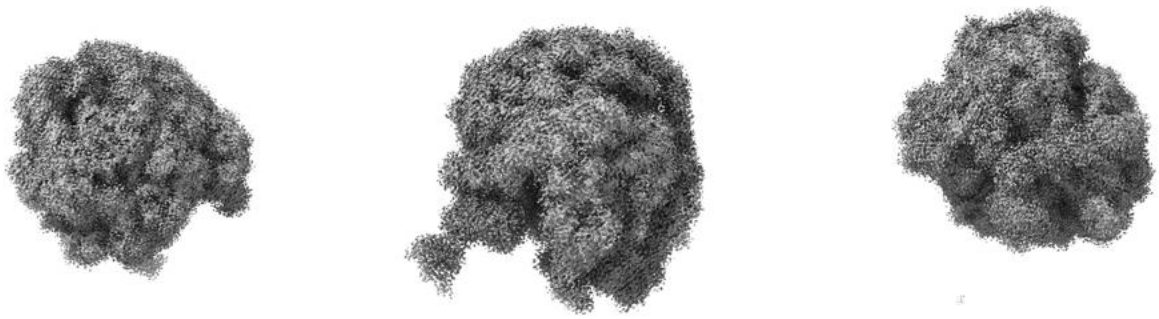


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

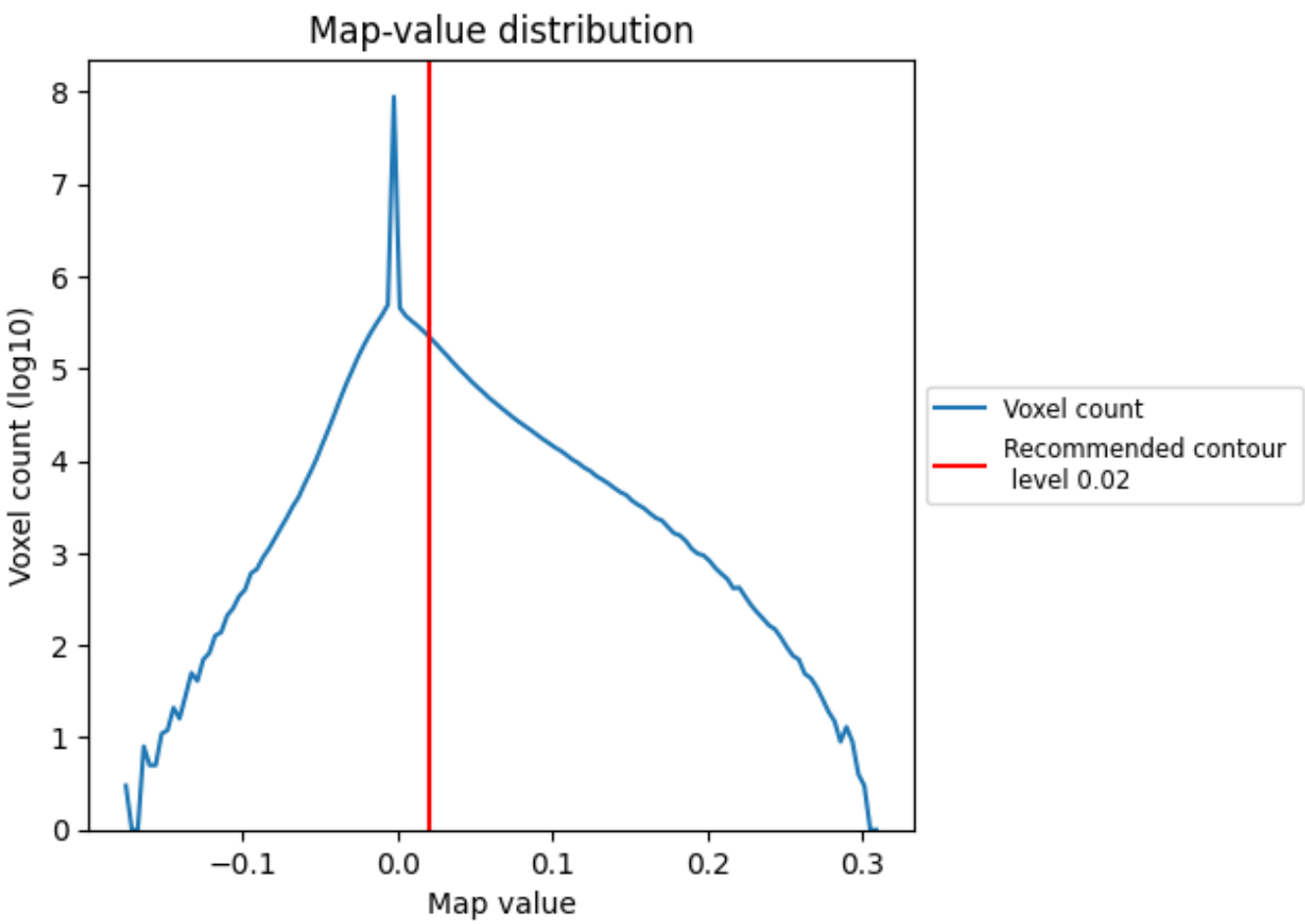
6.6 Mask visualisation (i)

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

7 Map analysis (i)

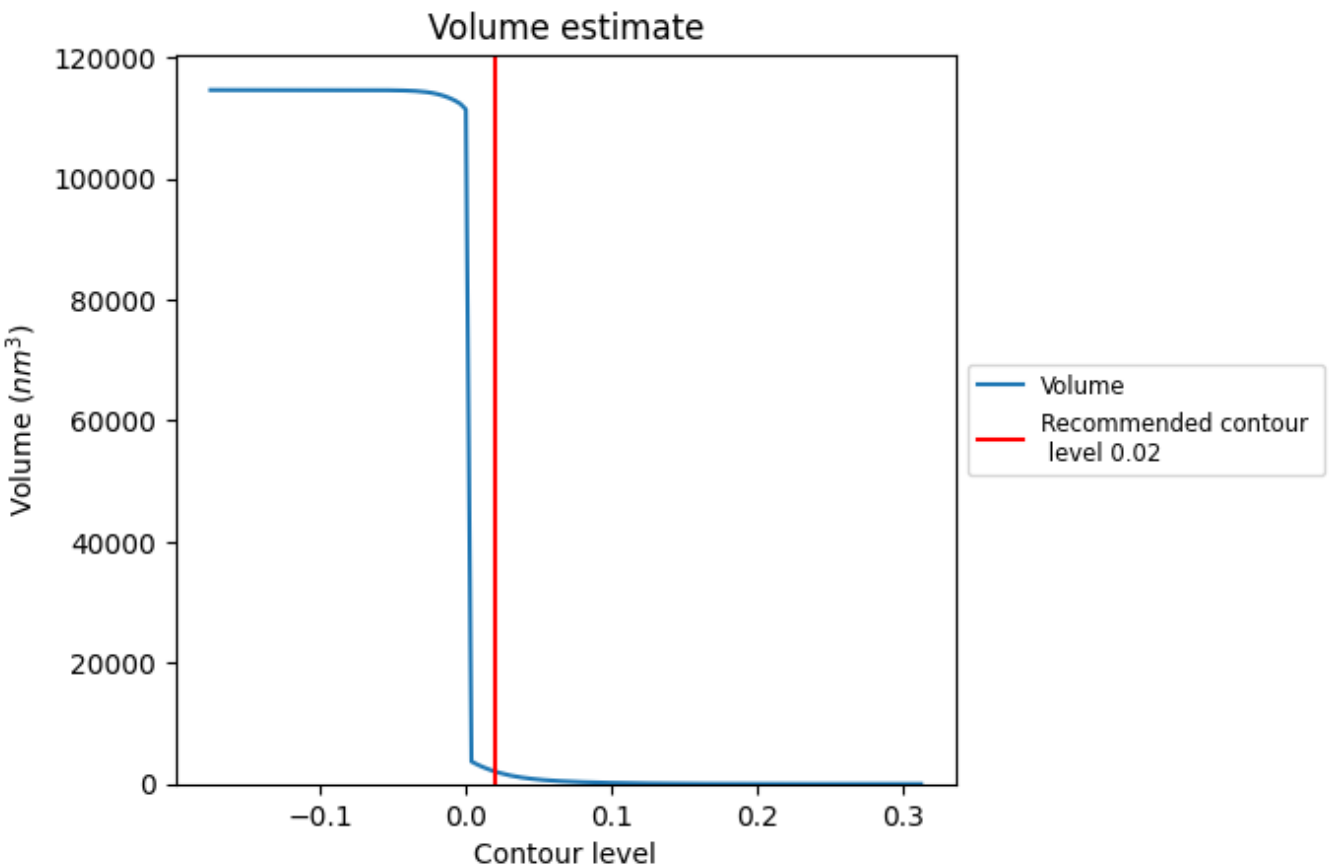
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

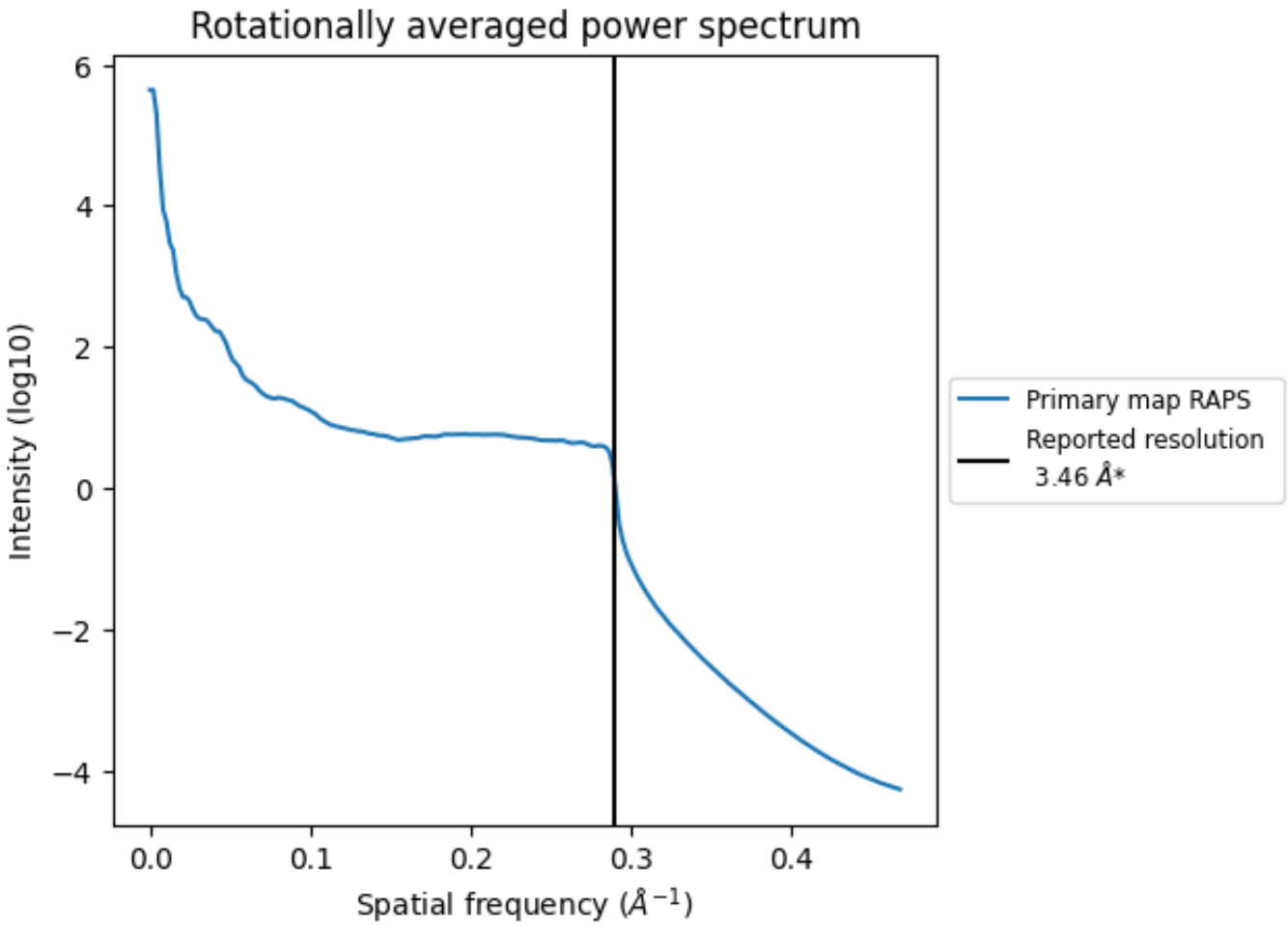
7.2 Volume estimate (i)



The volume at the recommended contour level is 2059 nm^3; this corresponds to an approximate mass of 1860 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)

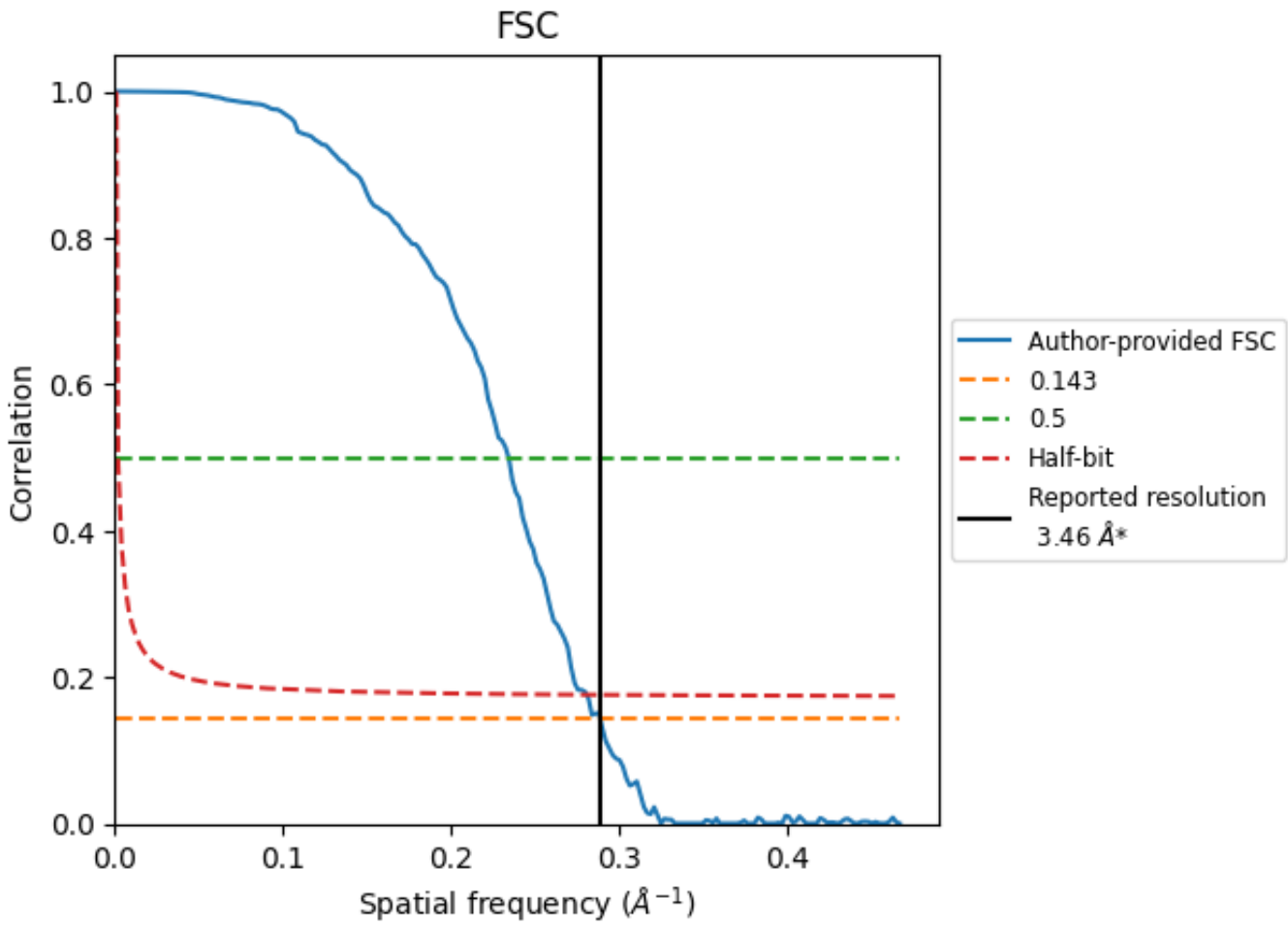


*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8.2 Resolution estimates (i)

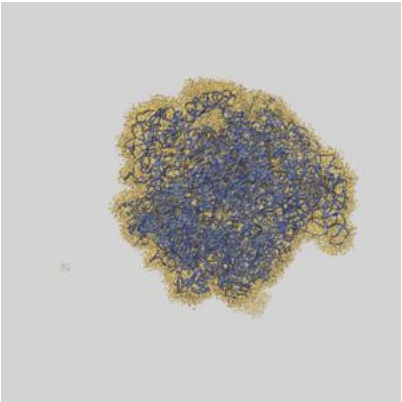
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	4.27	3.56
Unmasked-calculated*	-	-	-

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

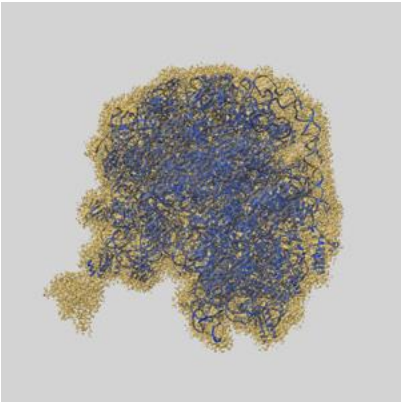
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8932 and PDB model 6DZI. Per-residue inclusion information can be found in section 3 on page 14.

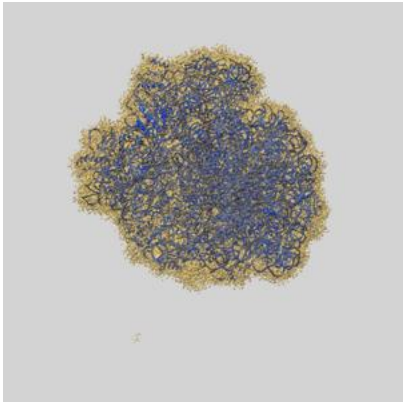
9.1 Map-model overlay (i)



X



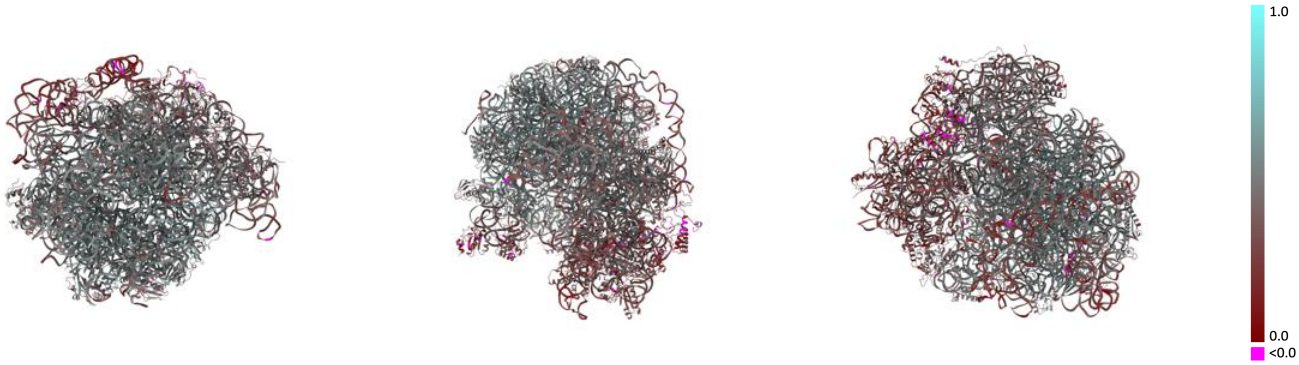
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

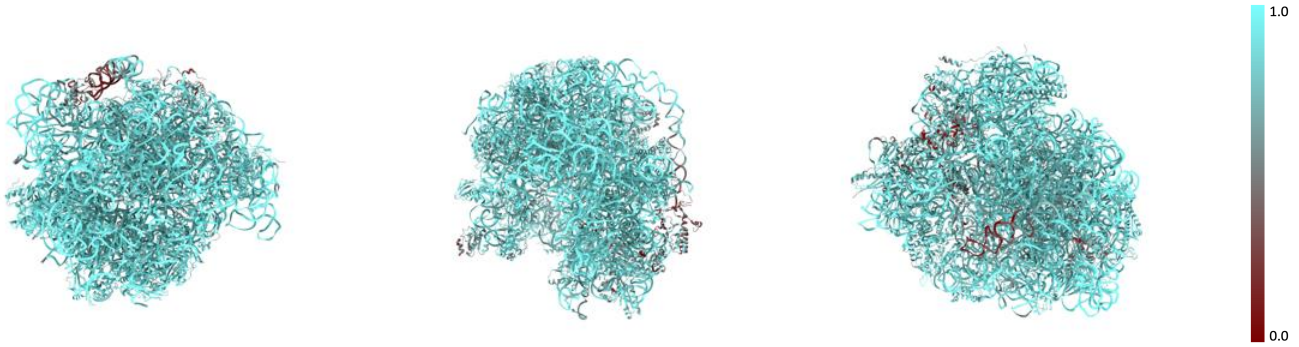
9.2 Q-score mapped to coordinate model (i)



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.

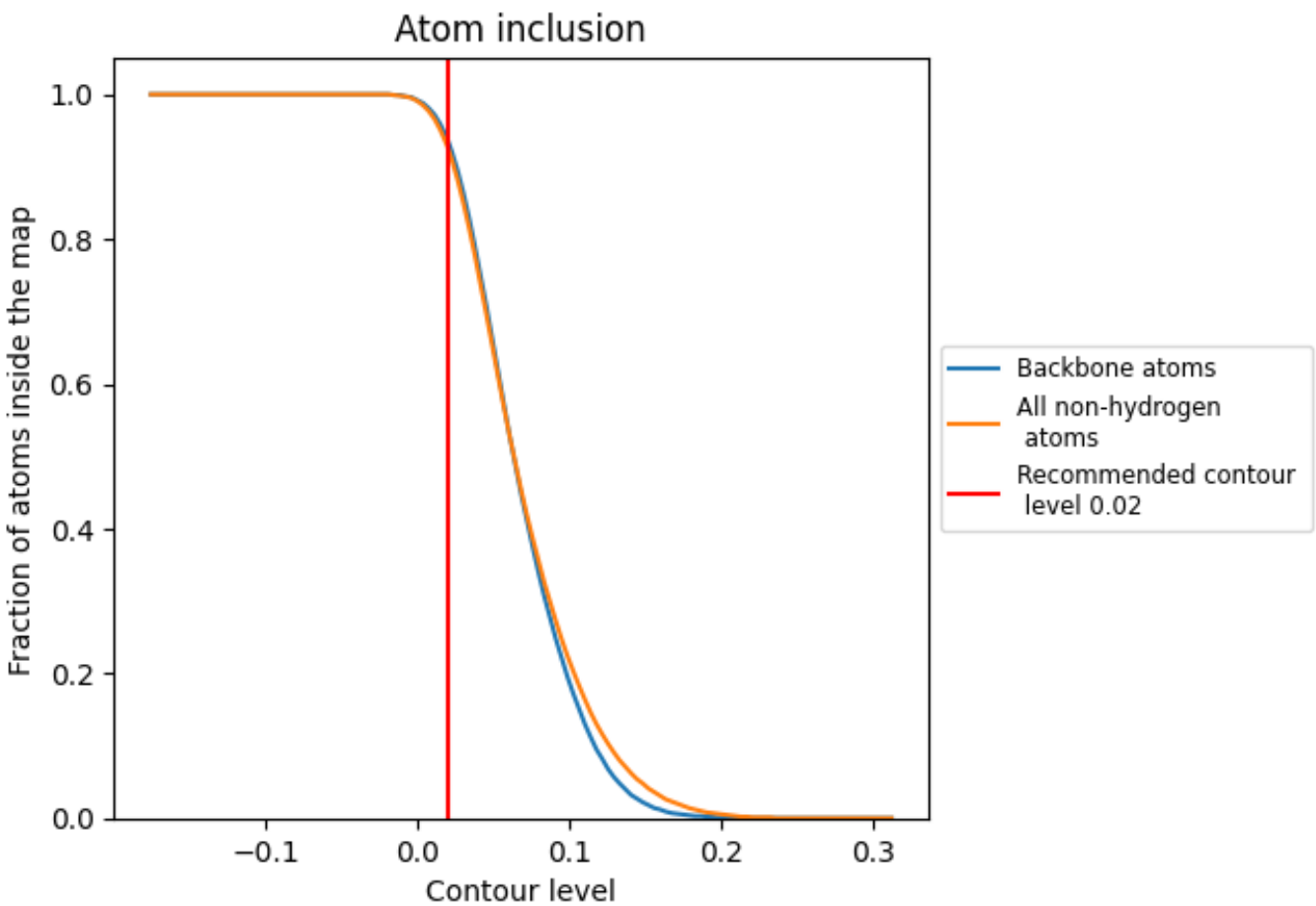
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.4380
3	0.9110	0.5190
4	0.8930	0.3240
5	0.8730	0.4370
6	0.7960	0.3270
7	0.8870	0.3630
8	0.5220	0.1690
9	0.8690	0.3250
A	0.9620	0.4760
B	0.9830	0.4620
C	0.8920	0.5100
D	0.9330	0.5100
E	0.9210	0.4830
F	0.9160	0.4010
G	0.9260	0.4290
H	0.5670	0.2940
I	0.6280	0.2350
J	0.7940	0.2780
K	0.9380	0.5090
L	0.8930	0.5020
M	0.9290	0.4940
N	0.9110	0.5050
O	0.9250	0.5030
P	0.9470	0.4560
Q	0.8920	0.4730
R	0.9120	0.5060
S	0.9500	0.5090
T	0.9110	0.4950
U	0.9110	0.4620
V	0.9030	0.4270
W	0.8950	0.4510
X	0.9330	0.5160
Y	0.5180	0.2720
Z	0.9330	0.4440
a	0.9350	0.4990

Continued on next page...

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Chain	Atom inclusion	Q-score
b	0.9350	0.4940
c	0.7620	0.3500
d	0.9000	0.5200
e	0.9150	0.5140
f	0.9370	0.5230
g	0.8480	0.2800
h	0.9640	0.4050
j	0.7820	0.4360
k	0.8210	0.3330
l	0.8410	0.3100
m	0.8560	0.3790
n	0.8550	0.3930
p	0.8080	0.3130
q	0.9250	0.4160
r	0.7210	0.3310
s	0.8310	0.3250
t	0.8560	0.4150
u	0.8750	0.4180
v	0.8500	0.3210
x	0.8850	0.4130
y	0.8740	0.4340
z	0.8540	0.3830