Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:13 am GMT

PDB ID	:	5LZA
EMDB ID	:	EMD-4121
Title	:	Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC)
Authors	:	Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on	:	2016-09-29
Resolution	:	3.60 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 ⓘ symbol.

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

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

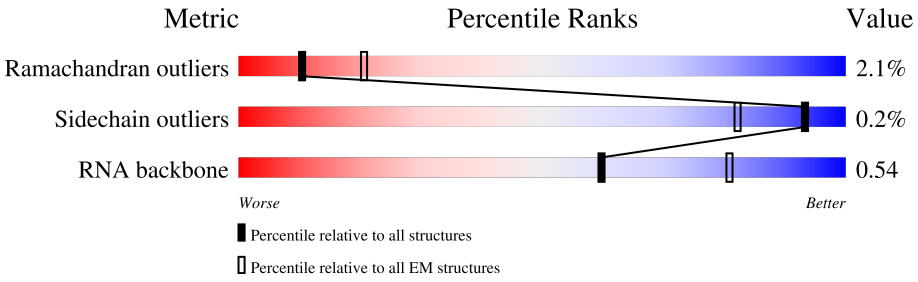
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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.



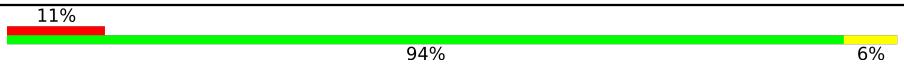
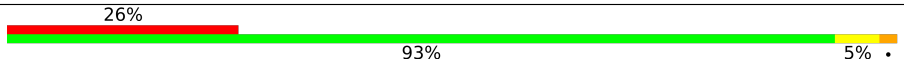
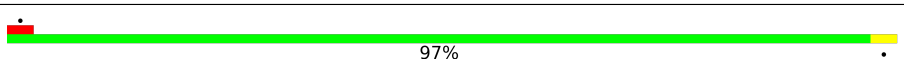
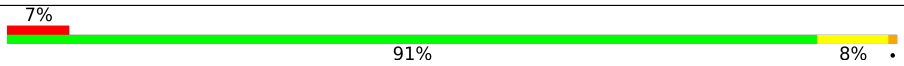
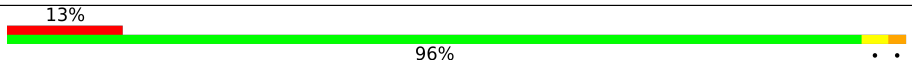
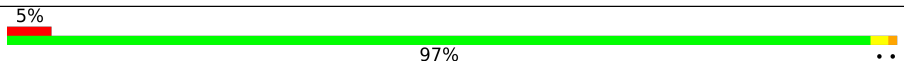
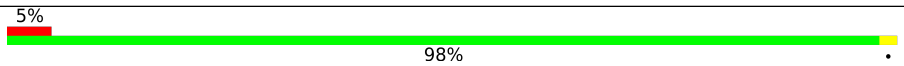
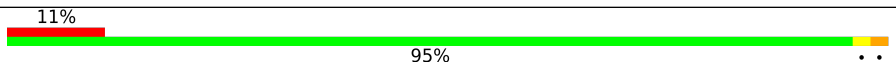
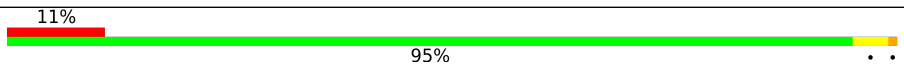
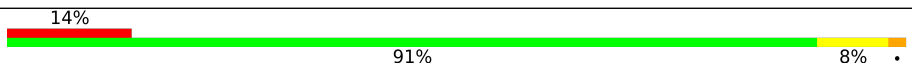
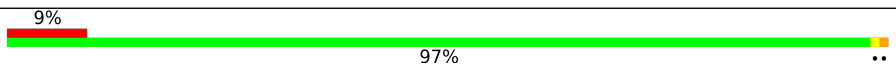
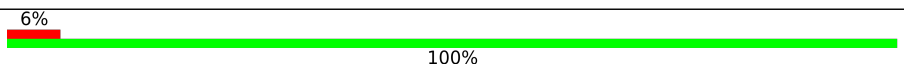
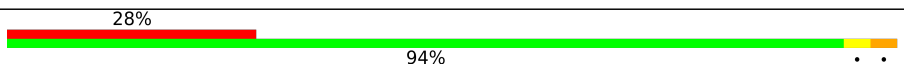
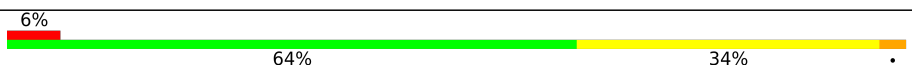
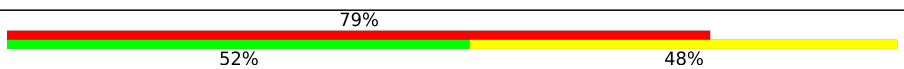
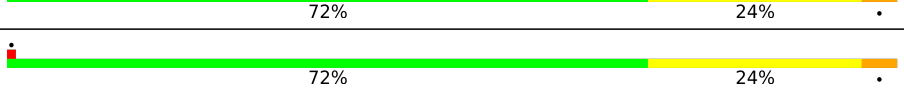
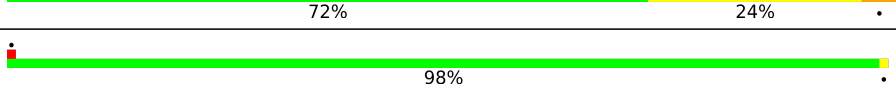
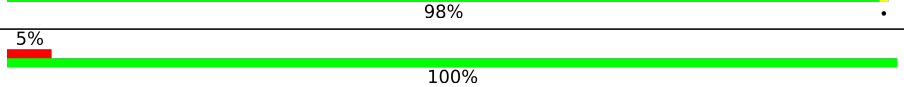
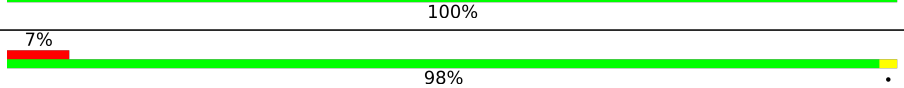
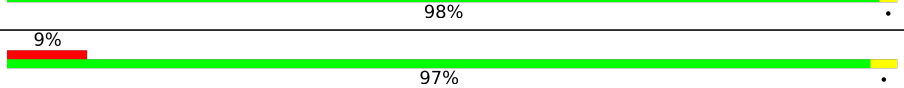
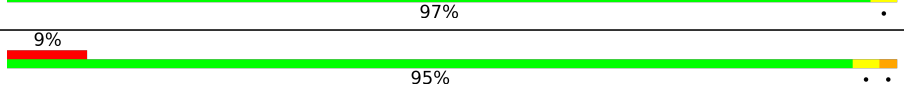
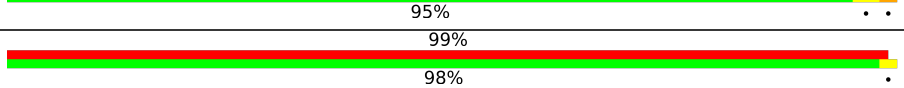
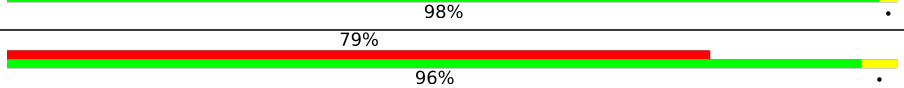
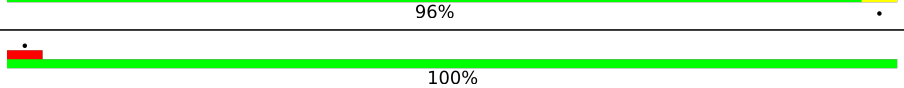
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	a	1539	73% 24%
2	b	218	37% 96%
3	c	206	8% 100%
4	d	205	14% 99%
5	e	157	94%
6	f	100	13% 93% 5%
7	g	151	15% 97%
8	h	129	7% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	100	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	77	
23	x	48	
24	A	2903	
25	B	120	
26	C	271	
27	D	209	
28	E	201	
29	F	177	
30	G	176	
31	I	141	
32	H	149	
33	J	142	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	K	122	93% 6%
35	L	143	95%
36	M	136	97%
37	N	120	100%
38	O	116	6% 98%
39	P	114	7% 99%
40	Q	117	99%
41	R	103	6% 98%
42	S	110	99%
43	T	93	8% 97%
44	U	102	7% 93% 5%
45	V	94	6% 100%
46	W	75	99%
47	X	77	5% 99%
48	Y	63	5% 98%
49	Z	58	5% 100%
50	0	56	9% 96%
51	1	50	16% 94% 6%
52	2	46	98%
53	3	64	97%
54	4	38	95% 5%
55	6	66	38% 98%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
24	G7M	A	2069	X	-	-	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 146037 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33119	14778	6072	10726	1543	4	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1705	1081	305	312	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	206	1625	1028	305	289	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1157	719	218	214	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	100	818	515	148	149	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2900	Total	C	N	O	P	1	0
			62296	27797	11464	20134	2901		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	U	102	Total	C	N	O	0	0
			780	492	146	142		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

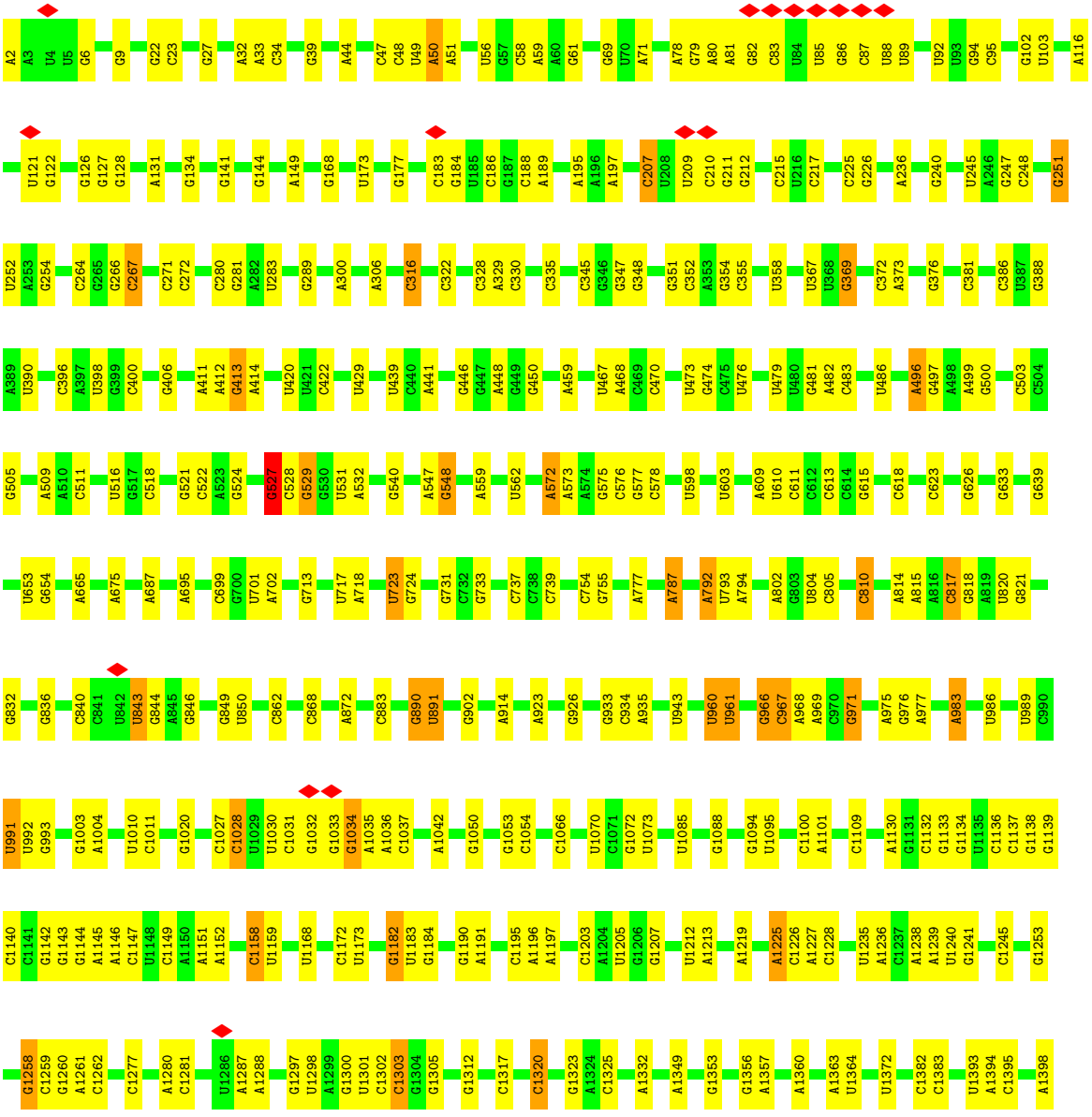
Mol	Chain	Residues	Atoms	AltConf
56	4	1	Total Zn 1 1	0
56	6	1	Total Zn 1 1	0

3 Residue-property plots (i)

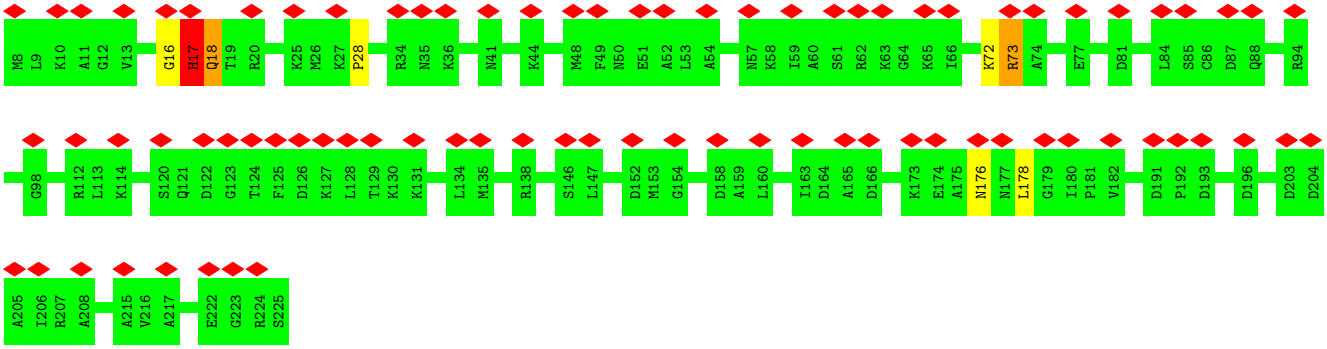
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S ribosomal RNA

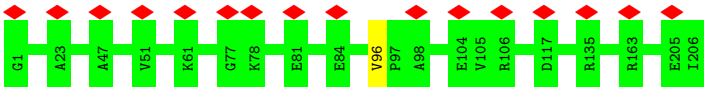
Chain a:



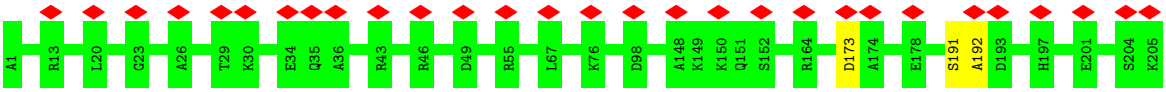
• Molecule 2: 30S ribosomal protein S2



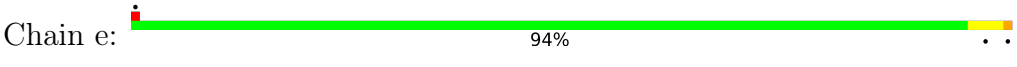
• Molecule 3: 30S ribosomal protein S3

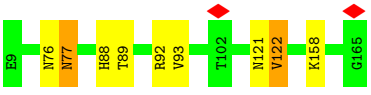


• Molecule 4: 30S ribosomal protein S4

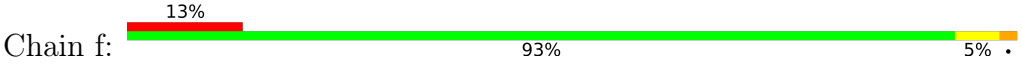


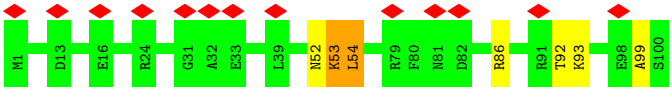
• Molecule 5: 30S ribosomal protein S5



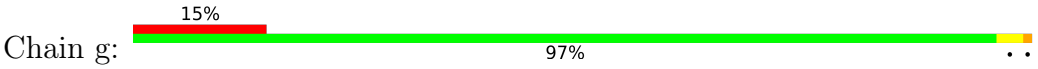


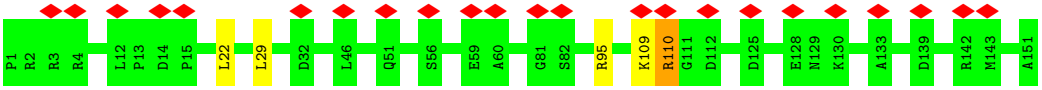
• Molecule 6: 30S ribosomal protein S6



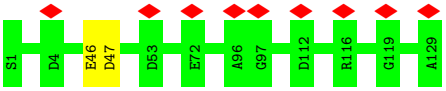


• Molecule 7: 30S ribosomal protein S7

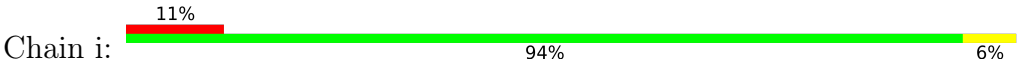


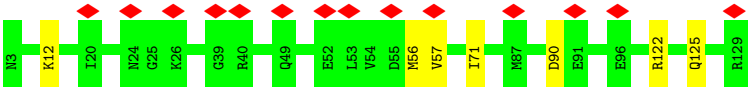


• Molecule 8: 30S ribosomal protein S8

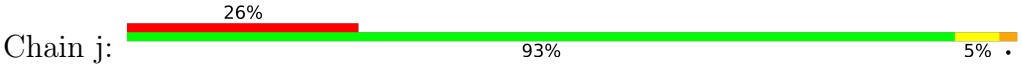


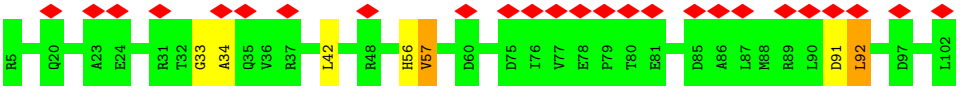
• Molecule 9: 30S ribosomal protein S9



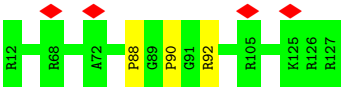


• Molecule 10: 30S ribosomal protein S10

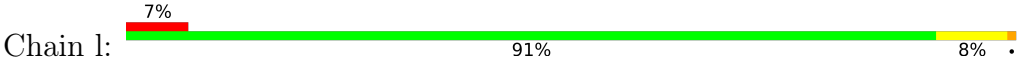


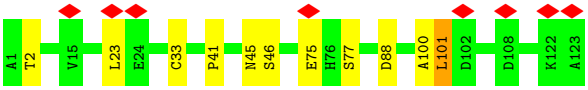


• Molecule 11: 30S ribosomal protein S11



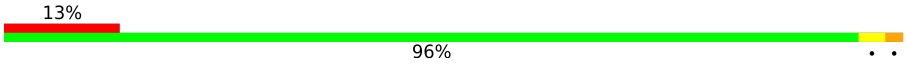
• Molecule 12: 30S ribosomal protein S12

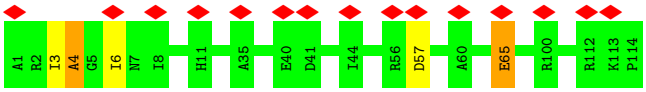




• Molecule 13: 30S ribosomal protein S13

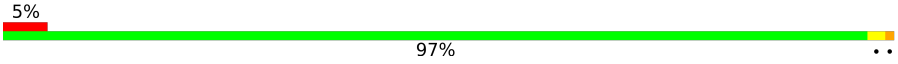
Chain m:

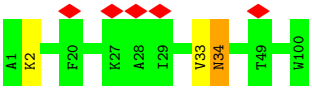




• Molecule 14: 30S ribosomal protein S14

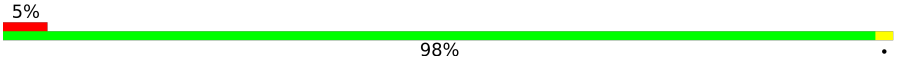
Chain n:

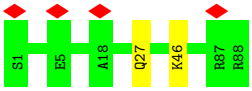




• Molecule 15: 30S ribosomal protein S15

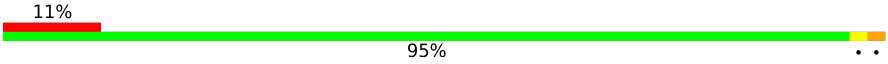
Chain o:

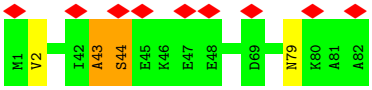




• Molecule 16: 30S ribosomal protein S16

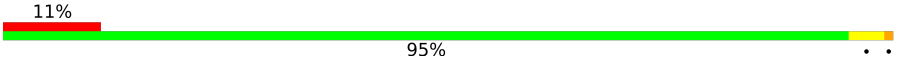
Chain p:

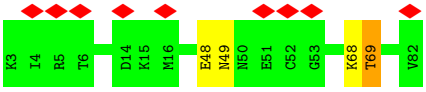




• Molecule 17: 30S ribosomal protein S17

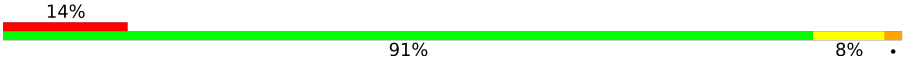
Chain q:

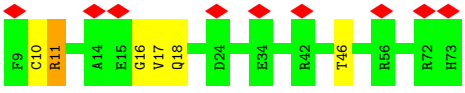




• Molecule 18: 30S ribosomal protein S18

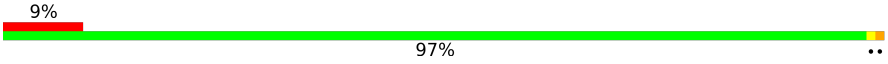
Chain r:

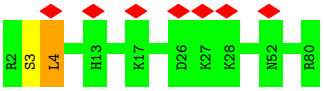




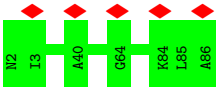
• Molecule 19: 30S ribosomal protein S19

Chain s:

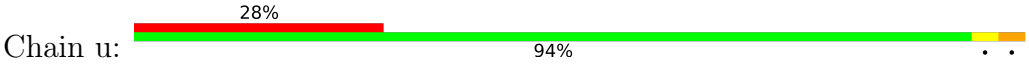


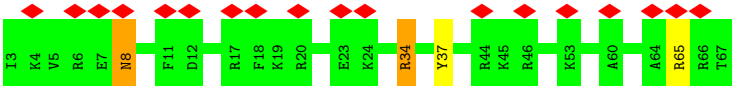


• Molecule 20: 30S ribosomal protein S20

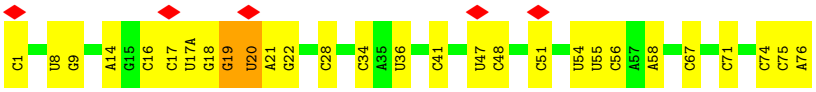


• Molecule 21: 30S ribosomal protein S21

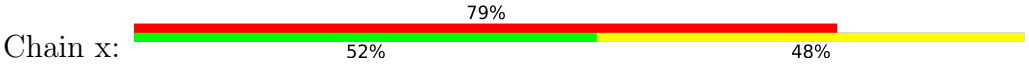


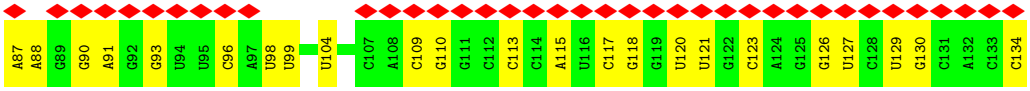


• Molecule 22: fMet-tRNAfMet

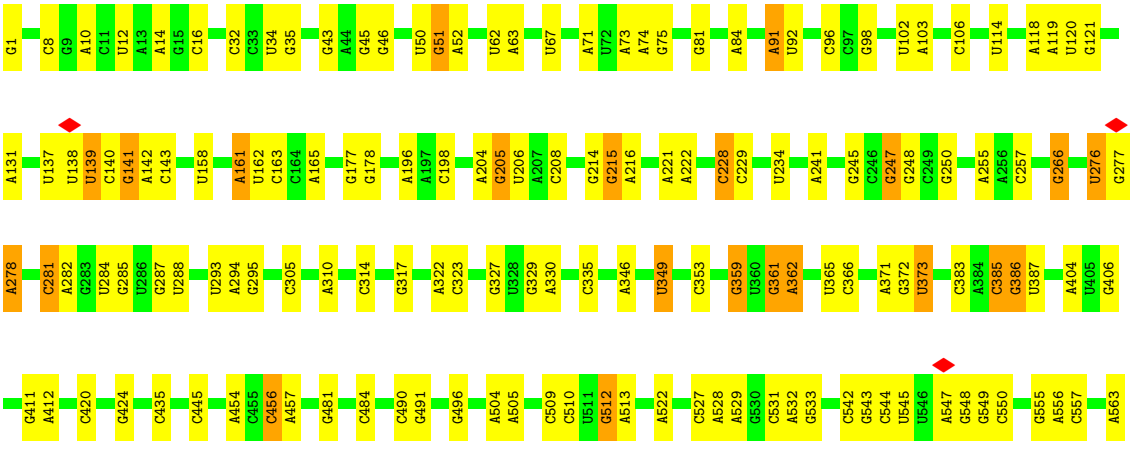


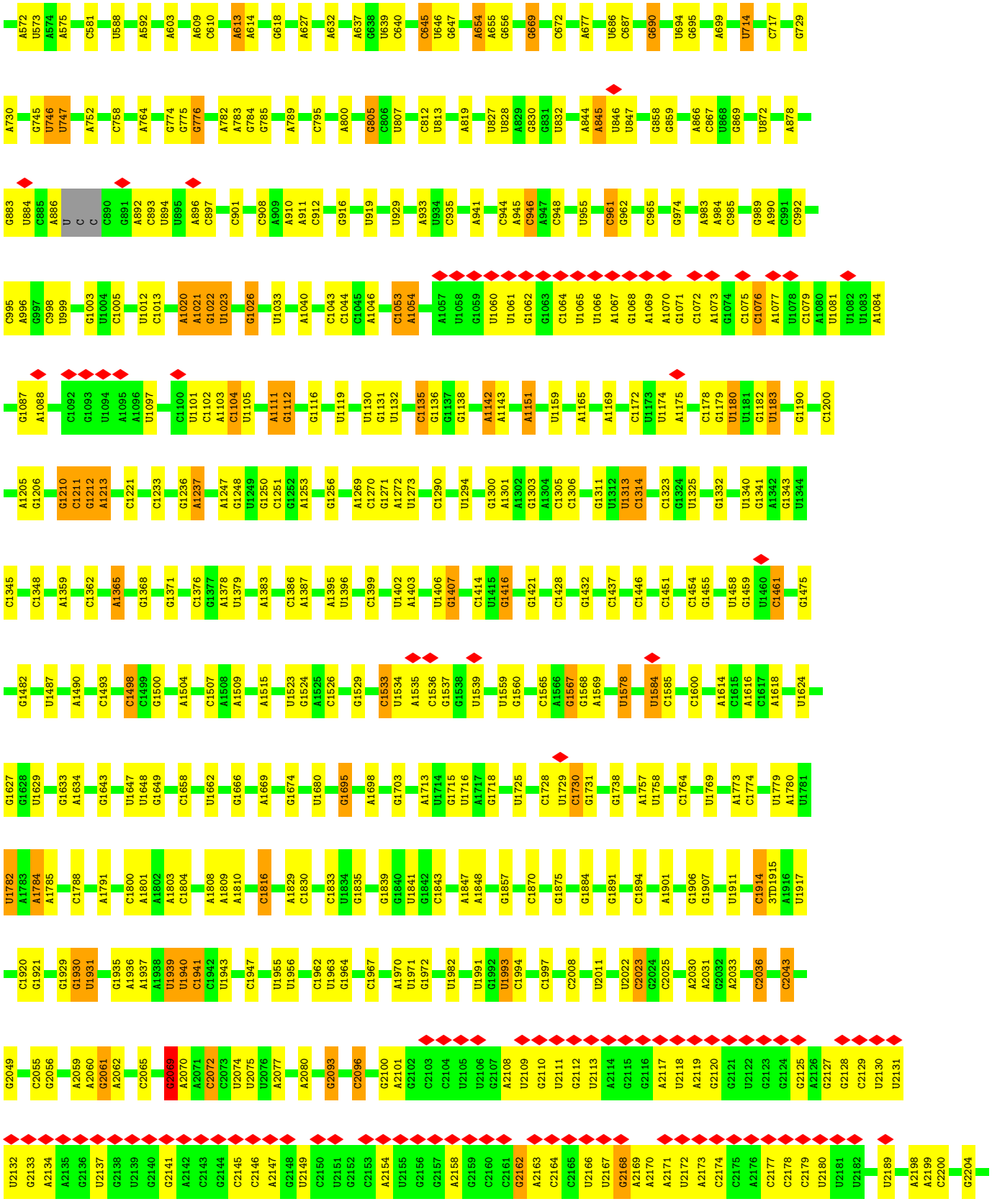
• Molecule 23: SECIS mRNA

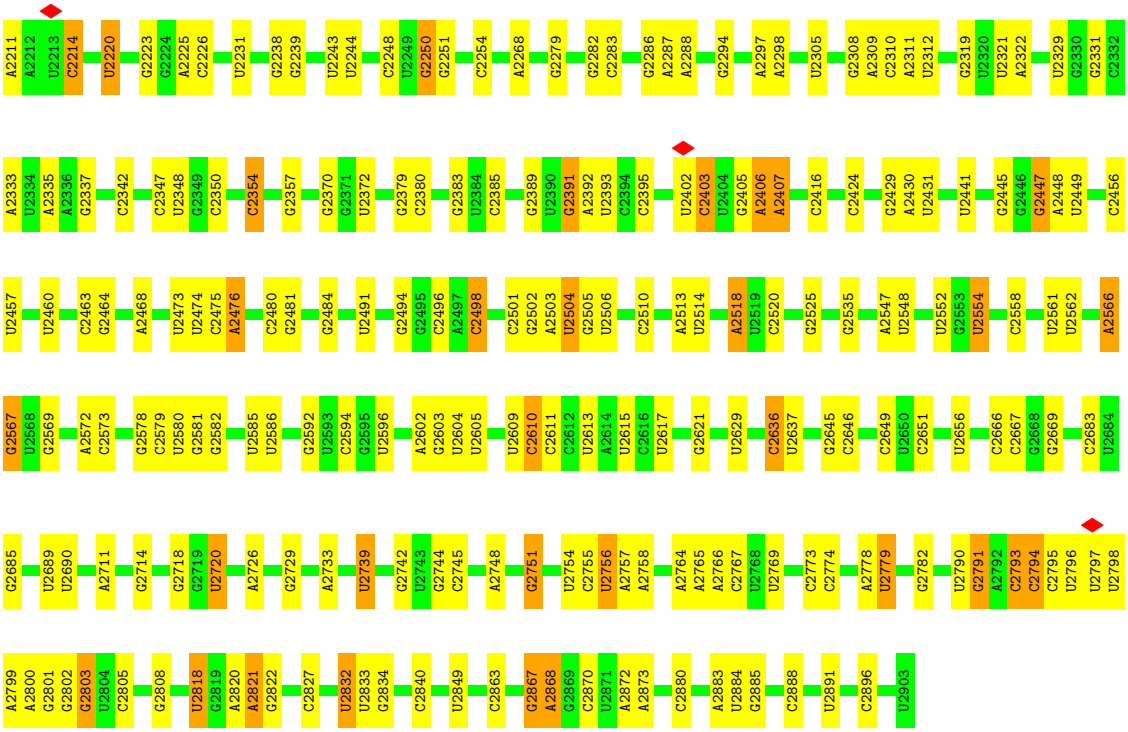




• Molecule 24: 23S ribosomal RNA

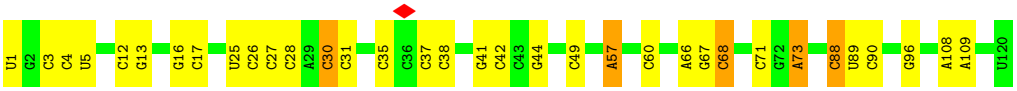



A572 U573 A574 A575 C581 U588 A592 A603 A609 C610 A613 A614 G618 A627 A632 A637 G638 U639 C640 C645 U646 G647 A654 A655 G656 G669 C672 A677 U686 C687 G690 U694 G695 A699 U714 C717 G729
A730 G745 U746 U747 A752 C758 A764 G774 G775 G776 A782 A783 G784 G785 A789 C795 A800 G805 C806 U807 C812 U813 A819 U827 U828 A829 G830 G831 U832 A844 A845 U846 U847 G858 G859 A866 C867 U868 G869 U872 A878
G883 U884 C885 A886 U C C C890 G891 A892 C893 U894 U895 A896 C897 C901 C908 A909 A910 A911 C912 G916 U919 U929 A933 U934 C935 A941 C944 A945 C946 A947 C948 U955 C961 G962 C965 G974 A983 A984 C985 G989 A990 C991 C992
C995 A996 G997 C998 U999 G1003 U1004 C1005 U1012 C1013 A1020 A1021 G1022 U1023 G1026 U1033 A1040 C1043 C1044 C1045 A1046 C1053 A1054 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084
G1087 A1088 C1092 G1093 U1094 A1095 A1096 U1097 C1100 U1101 C1102 A1103 C1104 U1105 A1111 G1112 G1116 U1119 U1130 G1131 U1132 C1135 G1136 G1137 G1138 A1142 A1143 A1151 U1159 A1165 A1169 C1172 U1173 U1174 A1175 C1178 G1179 U1180 U1181 G1182 U1183 G1190 C1200
A1205 C1206 G1210 C1211 G1212 A1213 C1221 C1233 G1236 A1237 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 A1269 C1270 G1271 A1272 U1273 C1290 U1294 G1300 A1301 A1302 G1303 A1304 C1305 C1306 G1311 U1312 U1313 C1314 C1323 G1324 U1325 G1332 U1340 G1341 A1342 G1343 U1344
C1345 C1348 A1359 C1362 A1365 G1368 G1371 C1376 G1377 A1378 U1379 A1383 C1386 A1387 A1395 U1396 C1399 U1402 A1403 U1406 G1407 C1414 U1415 G1416 G1421 C1428 G1432 C1437 C1446 C1451 C1454 G1455 U1458 G1459 U1460 C1461 G1475
G1482 U1487 A1490 C1493 C1498 C1499 G1500 A1504 C1507 A1508 A1509 A1515 U1523 G1524 A1525 C1526 G1529 C1533 U1534 A1535 C1536 G1537 G1538 U1539 U1559 G1560 C1565 A1566 G1567 G1568 A1569 U1578 U1584 C1585 C1600 A1614 C1615 A1616 C1617 A1618 U1624
G1627 G1628 U1629 G1633 A1634 G1643 U1647 U1648 G1649 C1658 U1662 G1666 A1669 G1674 U1680 G1695 A1698 G1703 A1713 U1714 G1715 U1716 A1717 G1718 U1725 C1728 U1729 C1730 G1731 G1738 A1757 U1758 C1764 U1769 A1773 C1774 U1779 A1780 U1781
U1782 A1783 A1784 A1785 C1788 A1791 C1800 A1801 A1802 A1803 C1804 A1808 A1809 A1810 C1816 A1829 C1830 C1833 U1834 G1835 G1839 G1840 U1841 G1842 C1843 A1847 A1848 G1857 C1870 G1875 G1884 G1891 C1894 A1901 G1906 G1907 U1911 C1914 3TD1915 A1916 U1917
C1920 G1921 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 C1947 U1955 U1956 C1962 U1963 G1964 C1967 A1970 U1971 G1972 U1982 U1991 G1992 U1993 C1994 C1997 C2008 U2011 U2022 C2023 G2024 C2025 A2030 A2031 G2032 A2033 C2036 C2043
G2049 C2055 G2056 A2059 A2060 G2061 A2062 C2065 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076 A2077 A2080 G2093 C2096 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131
U2132 G2133 A2134 A2135 A2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 U2189 A2198 A2199 C2200 G2204



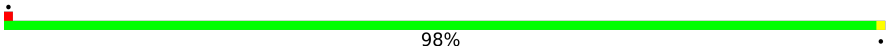
- Molecule 25: 5S ribosomal RNA

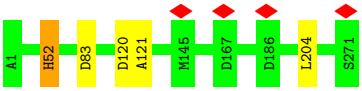
Chain B:



- Molecule 26: 50S ribosomal protein L2

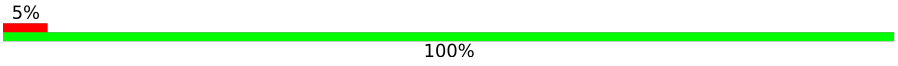
Chain C:

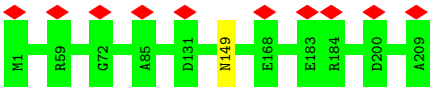




- Molecule 27: 50S ribosomal protein L3

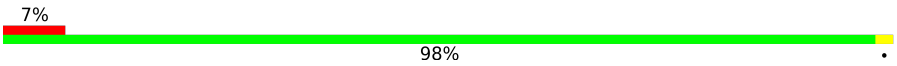
Chain D:

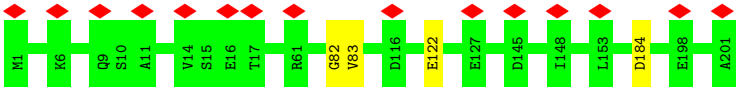




- Molecule 28: 50S ribosomal protein L4

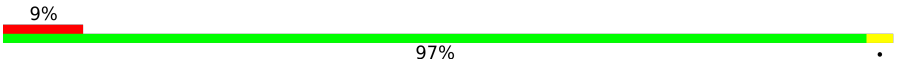
Chain E:

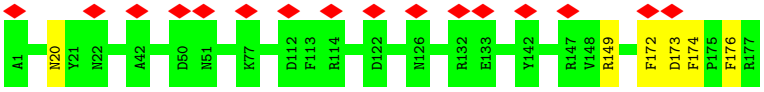




• Molecule 29: 50S ribosomal protein L5

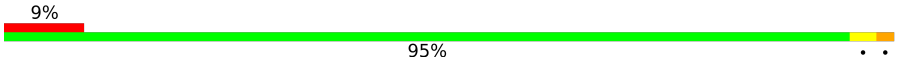
Chain F:

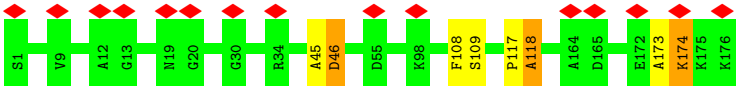




• Molecule 30: 50S ribosomal protein L6

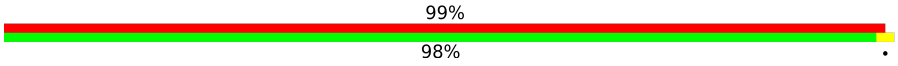
Chain G:

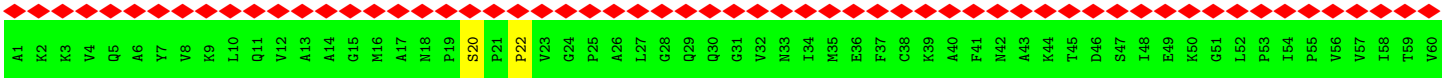


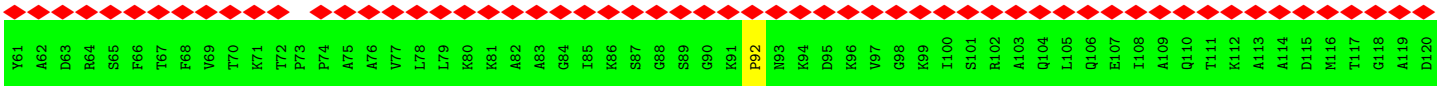


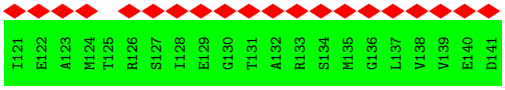
• Molecule 31: 50S ribosomal protein L11

Chain I:



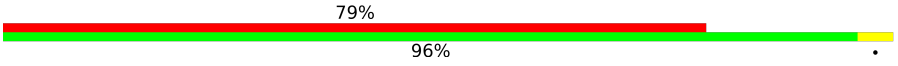


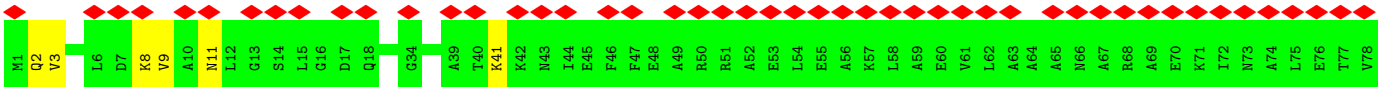


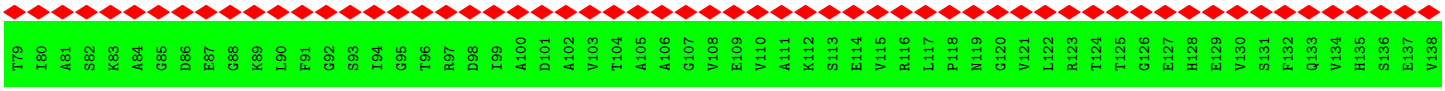


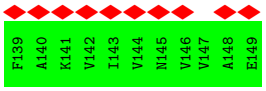
• Molecule 32: 50S ribosomal protein L9

Chain H:



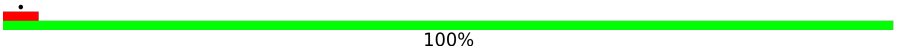


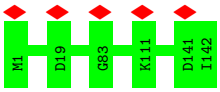




• Molecule 33: 50S ribosomal protein L13

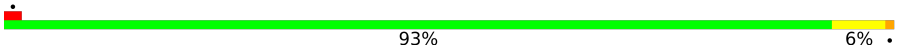
Chain J:

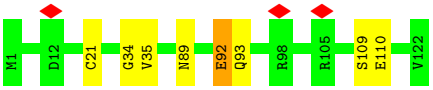




• Molecule 34: 50S ribosomal protein L14

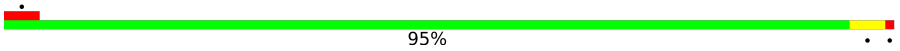
Chain K:

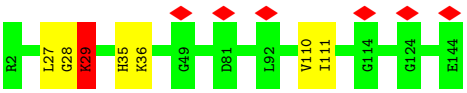




• Molecule 35: 50S ribosomal protein L15

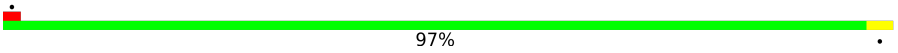
Chain L:

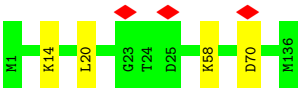




• Molecule 36: 50S ribosomal protein L16

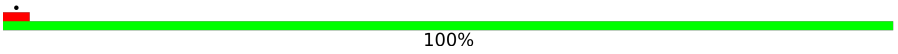
Chain M:

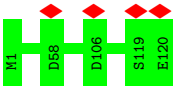




• Molecule 37: 50S ribosomal protein L17

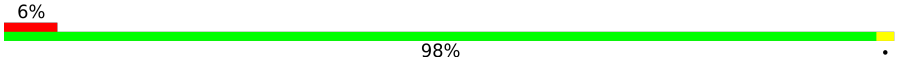
Chain N:

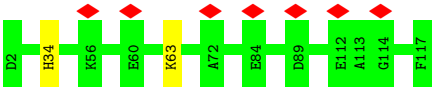




• Molecule 38: 50S ribosomal protein L18

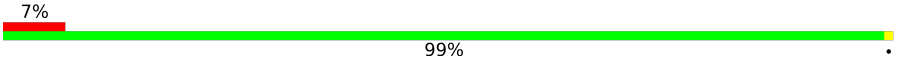
Chain O:

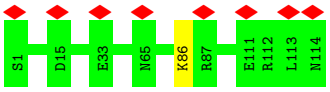




• Molecule 39: 50S ribosomal protein L19

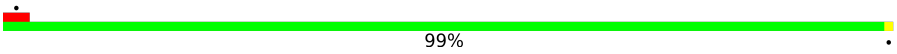
Chain P:

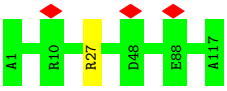




• Molecule 40: 50S ribosomal protein L20

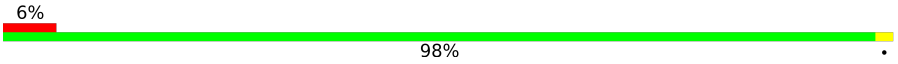
Chain Q:

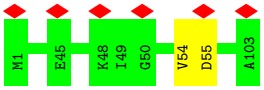




• Molecule 41: 50S ribosomal protein L21

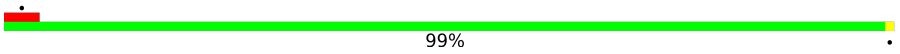
Chain R:

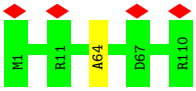




• Molecule 42: 50S ribosomal protein L22

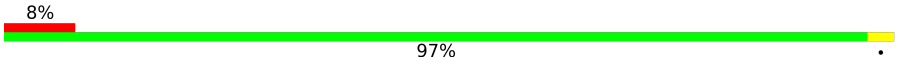
Chain S:

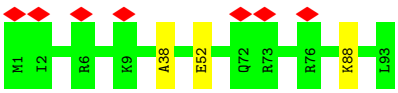




• Molecule 43: 50S ribosomal protein L23

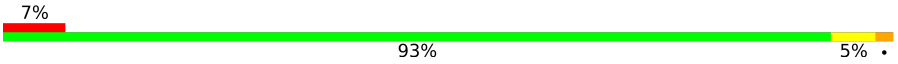
Chain T:

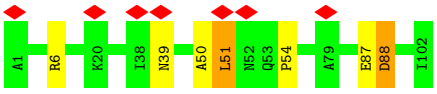




• Molecule 44: 50S ribosomal protein L24

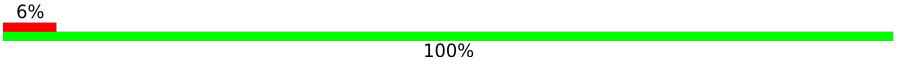
Chain U:

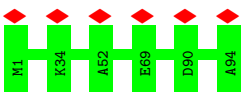




• Molecule 45: 50S ribosomal protein L25

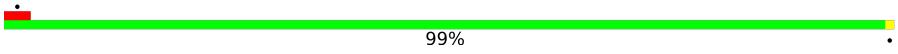
Chain V:

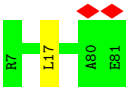




• Molecule 46: 50S ribosomal protein L27

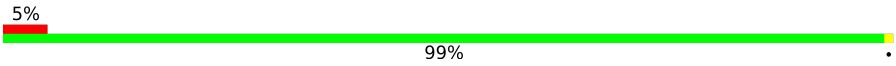
Chain W:

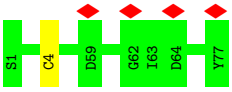




• Molecule 47: 50S ribosomal protein L28

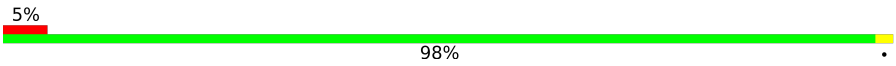
Chain X:

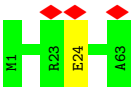




• Molecule 48: 50S ribosomal protein L29

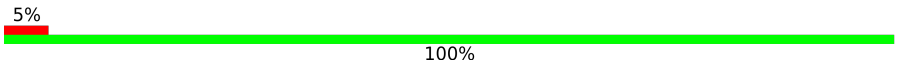
Chain Y:





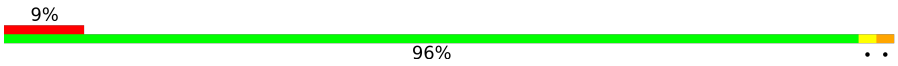
• Molecule 49: 50S ribosomal protein L30

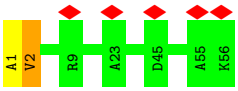
Chain Z:



• Molecule 50: 50S ribosomal protein L32

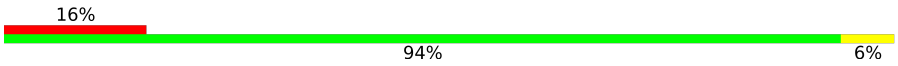
Chain 0:

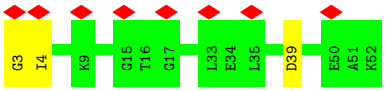




• Molecule 51: 50S ribosomal protein L33

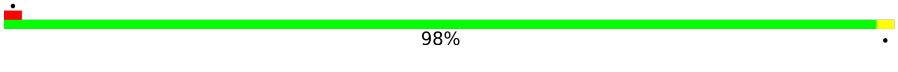
Chain 1:

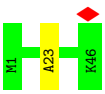




• Molecule 52: 50S ribosomal protein L34

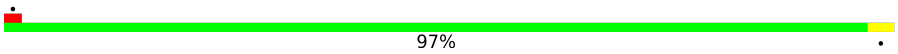
Chain 2:

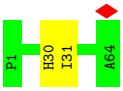




• Molecule 53: 50S ribosomal protein L35

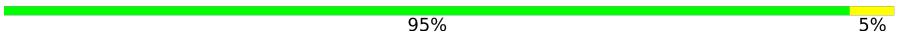
Chain 3:

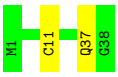




• Molecule 54: 50S ribosomal protein L36

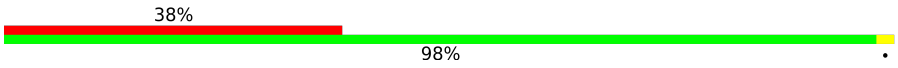
Chain 4:

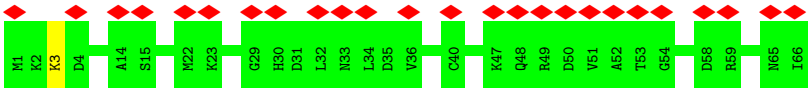




• Molecule 55: 50S ribosomal protein L31

Chain 6:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.934	Depositor
Minimum map value	-2.060	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.265	Depositor
Recommended contour level	0.52	Depositor
Map size (Å)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 2MG, 4SU, 2MA, 5MU, 5MC, ZN, 6MZ, UR3, OMC, 4OC, H2U, PSU, 1MG, OMU, OMG, MA6, 3TD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.61	4/36803 (0.0%)	1.26	322/57406 (0.6%)
2	b	0.43	0/1736	0.66	3/2338 (0.1%)
3	c	0.40	0/1652	0.60	0/2225
4	d	0.43	0/1665	0.62	0/2227
5	e	0.44	0/1170	0.80	2/1573 (0.1%)
6	f	0.49	0/836	0.83	2/1128 (0.2%)
7	g	0.43	0/1196	0.70	3/1602 (0.2%)
8	h	0.42	0/989	0.66	0/1326
9	i	0.41	0/1034	0.69	0/1375
10	j	0.37	0/797	0.74	0/1077
11	k	0.40	0/886	0.71	0/1195
12	l	0.43	0/969	0.82	2/1300 (0.2%)
13	m	0.46	0/893	0.78	3/1193 (0.3%)
14	n	0.45	0/806	0.66	1/1074 (0.1%)
15	o	0.40	0/722	0.61	0/964
16	p	0.45	0/659	0.70	1/884 (0.1%)
17	q	0.45	0/658	0.78	1/881 (0.1%)
18	r	0.42	0/512	0.70	0/689
19	s	0.41	0/653	0.75	1/877 (0.1%)
20	t	0.42	0/671	0.60	0/888
21	u	0.53	0/501	0.84	1/668 (0.1%)
22	v	0.55	1/1747 (0.1%)	1.29	19/2721 (0.7%)
23	x	0.58	1/1145 (0.1%)	1.09	1/1781 (0.1%)
24	A	0.66	9/69196 (0.0%)	1.26	616/107943 (0.6%)
25	B	0.59	1/2873 (0.0%)	1.25	29/4478 (0.6%)
26	C	0.48	0/2122	0.73	1/2852 (0.0%)
27	D	0.44	0/1586	0.67	0/2134
28	E	0.43	0/1571	0.63	0/2113
29	F	0.43	0/1435	0.71	2/1926 (0.1%)
30	G	0.42	0/1343	0.67	4/1816 (0.2%)
31	I	0.38	0/1046	0.61	0/1410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	H	0.38	0/1122	0.63	0/1515
33	J	0.46	0/1152	0.61	0/1551
34	K	0.46	0/948	0.69	0/1268
35	L	0.44	0/1054	0.74	1/1403 (0.1%)
36	M	0.46	0/1093	0.72	1/1460 (0.1%)
37	N	0.44	0/974	0.65	0/1301
38	O	0.42	0/902	0.59	0/1209
39	P	0.45	0/929	0.67	0/1242
40	Q	0.47	0/960	0.60	1/1278 (0.1%)
41	R	0.45	0/829	0.72	0/1107
42	S	0.40	0/864	0.62	0/1156
43	T	0.40	0/745	0.63	0/994
44	U	0.44	0/788	0.78	2/1051 (0.2%)
45	V	0.40	0/766	0.60	0/1025
46	W	0.41	0/582	0.62	0/769
47	X	0.38	0/635	0.59	0/848
48	Y	0.42	0/510	0.64	0/677
49	Z	0.40	0/453	0.60	0/605
50	0	0.41	0/450	0.72	0/599
51	1	0.42	0/417	0.84	1/554 (0.2%)
52	2	0.41	0/380	0.67	0/498
53	3	0.47	0/513	0.65	0/676
54	4	0.67	1/303 (0.3%)	0.78	0/397
55	6	0.42	0/532	0.62	0/709
All	All	0.59	17/157773 (0.0%)	1.14	1020/235956 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
2	b	0	4
5	e	0	4
6	f	0	1
7	g	0	2
8	h	0	1
9	i	0	1
10	j	0	5
12	l	0	1
13	m	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
16	p	0	1
17	q	0	2
18	r	0	3
19	s	0	1
21	u	0	1
24	A	2	0
26	C	0	1
28	E	0	1
30	G	0	3
32	H	0	2
34	K	0	3
35	L	0	4
42	S	0	1
44	U	0	3
48	Y	0	1
50	0	0	2
51	1	0	1
53	3	0	1
All	All	4	51

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	x	87	A	OP3-P	-10.73	1.48	1.61
24	A	1	G	OP3-P	-10.59	1.48	1.61
25	B	1	U	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.52	1.48	1.61
1	a	2	A	OP3-P	-10.51	1.48	1.61
24	A	776	G	N7-C5	-7.66	1.34	1.39
24	A	1784	A	N7-C5	-7.38	1.34	1.39
54	4	11	CYS	CB-SG	-7.14	1.70	1.82
24	A	1779	U	C5-C6	-5.86	1.28	1.34
24	A	800	A	N9-C4	-5.79	1.34	1.37
1	a	89	U	C4-C5	-5.54	1.38	1.43
24	A	1803	A	N9-C4	-5.52	1.34	1.37
24	A	984	A	N9-C4	-5.30	1.34	1.37
24	A	2868	A	N9-C8	-5.26	1.33	1.37
24	A	613	A	N9-C4	5.21	1.41	1.37
1	a	792	A	N7-C5	-5.15	1.36	1.39
1	a	2	A	N7-C5	-5.12	1.36	1.39

All (1020) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1313	U	N3-C2-O2	-14.71	111.90	122.20
24	A	2072	C	C6-N1-C2	-14.04	114.69	120.30
1	a	89	U	C5-C4-O4	-13.94	117.53	125.90
1	a	529	G	C5-C6-O6	-13.71	120.38	128.60
24	A	62	U	N1-C2-O2	13.14	132.00	122.80
24	A	893	C	C6-N1-C2	-13.07	115.07	120.30
24	A	1313	U	N1-C2-O2	12.96	131.87	122.80
24	A	137	U	N3-C2-O2	-12.35	113.56	122.20
24	A	2297	A	C6-N1-C2	12.25	125.95	118.60
24	A	2072	C	C5-C6-N1	12.25	127.12	121.00
24	A	2868	A	N7-C8-N9	12.13	119.86	113.80
24	A	2297	A	N1-C2-N3	-11.50	123.55	129.30
1	a	529	G	N1-C6-O6	11.49	126.80	119.90
24	A	2321	U	C4-C5-C6	11.37	126.52	119.70
24	A	62	U	N3-C2-O2	-11.36	114.25	122.20
24	A	548	G	N7-C8-N9	11.29	118.74	113.10
24	A	1112	G	N3-C2-N2	-11.13	112.11	119.90
19	s	4	LEU	CA-CB-CG	10.99	140.57	115.30
1	a	737	C	C5-C6-N1	10.92	126.46	121.00
1	a	737	C	C6-N1-C2	-10.91	115.94	120.30
1	a	215	C	N1-C2-O2	10.80	125.38	118.90
24	A	548	G	C8-N9-C4	-10.66	102.14	106.40
24	A	1313	U	C2-N1-C1'	10.60	130.42	117.70
5	e	77	ASN	N-CA-CB	-10.46	91.77	110.60
1	a	1027	C	C5-C6-N1	10.40	126.20	121.00
24	A	783	A	C8-N9-C4	-10.22	101.71	105.80
1	a	89	U	N3-C4-O4	10.19	126.53	119.40
24	A	776	G	N3-C4-C5	-10.18	123.51	128.60
24	A	883	G	N1-C6-O6	-9.95	113.93	119.90
24	A	62	U	C2-N1-C1'	9.89	129.56	117.70
1	a	413	G	C5-N7-C8	9.82	109.21	104.30
24	A	1451	C	N1-C2-O2	-9.82	113.01	118.90
24	A	2416	C	C6-N1-C2	-9.77	116.39	120.30
13	m	65	GLU	N-CA-CB	-9.73	93.08	110.60
24	A	1498	C	N1-C2-O2	9.60	124.66	118.90
1	a	503	C	C6-N1-C2	-9.41	116.54	120.30
24	A	2447	G	P-O3'-C3'	9.32	130.89	119.70
24	A	2481	G	C6-N1-C2	9.28	130.67	125.10
24	A	893	C	N3-C2-O2	-9.27	115.41	121.90
24	A	795	C	C5-C6-N1	9.26	125.63	121.00
24	A	783	A	N7-C8-N9	9.23	118.41	113.80
24	A	1314	C	C6-N1-C2	-9.21	116.62	120.30
24	A	2884	U	N3-C2-O2	-9.20	115.76	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	792	A	C5-N7-C8	9.17	108.48	103.90
24	A	1784	A	C5-N7-C8	9.13	108.47	103.90
24	A	2868	A	C8-N9-C4	-9.09	102.17	105.80
24	A	866	A	C5-C6-N6	-9.01	116.49	123.70
24	A	669	G	C2-N3-C4	8.97	116.38	111.90
1	a	1134	G	N3-C2-N2	-8.94	113.64	119.90
1	a	1028	C	C5-C6-N1	8.93	125.47	121.00
1	a	1003	G	N3-C2-N2	-8.88	113.69	119.90
1	a	891	U	C5-C6-N1	8.87	127.13	122.70
22	v	74	C	N1-C2-O2	8.85	124.21	118.90
1	a	1149	C	N1-C2-O2	8.82	124.19	118.90
24	A	2407	A	O5'-P-OP2	-8.81	97.77	105.70
24	A	2226	C	N1-C2-O2	8.76	124.16	118.90
1	a	1027	C	C6-N1-C2	-8.75	116.80	120.30
24	A	581	C	C5-C6-N1	8.71	125.35	121.00
24	A	1081	U	N3-C2-O2	-8.65	116.15	122.20
24	A	613	A	C2-N3-C4	8.64	114.92	110.60
16	p	44	SER	N-CA-CB	-8.62	97.58	110.50
24	A	1362	C	C6-N1-C2	-8.61	116.85	120.30
24	A	385	C	OP2-P-O3'	8.60	124.11	105.20
24	A	1716	U	C5-C6-N1	8.57	126.99	122.70
24	A	278	A	C2-N3-C4	8.51	114.85	110.60
1	a	943	U	N3-C2-O2	-8.45	116.28	122.20
24	A	67	U	C5-C4-O4	-8.45	120.83	125.90
24	A	1105	U	N3-C2-O2	-8.45	116.29	122.20
24	A	1451	C	C2-N3-C4	-8.38	115.71	119.90
25	B	31	C	C6-N1-C2	-8.38	116.95	120.30
24	A	1779	U	C4-C5-C6	8.37	124.72	119.70
24	A	893	C	C5-C6-N1	8.33	125.16	121.00
2	b	73	ARG	N-CA-CB	-8.31	95.64	110.60
1	a	168	G	C5-C6-O6	-8.28	123.63	128.60
24	A	2884	U	N1-C2-O2	8.27	128.59	122.80
24	A	1101	U	N3-C2-O2	-8.24	116.43	122.20
1	a	529	G	C4-C5-N7	8.22	114.09	110.80
24	A	67	U	N3-C4-O4	8.22	125.15	119.40
24	A	484	C	C5-C6-N1	8.18	125.09	121.00
44	U	51	LEU	N-CA-CB	-8.15	94.11	110.40
24	A	687	C	N1-C2-O2	8.13	123.78	118.90
24	A	281	C	C6-N1-C2	-8.09	117.06	120.30
24	A	2406	A	O5'-P-OP2	-8.07	98.44	105.70
24	A	1498	C	C6-N1-C2	-8.07	117.07	120.30
24	A	2473	U	N3-C2-O2	-8.06	116.56	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	34	C	N1-C2-O2	8.05	123.73	118.90
24	A	2226	C	N3-C2-O2	-8.03	116.28	121.90
1	a	522	C	C5-C4-N4	8.01	125.81	120.20
1	a	413	G	N7-C8-N9	-8.01	109.10	113.10
1	a	754	C	C2-N1-C1'	8.01	127.61	118.80
24	A	948	C	C5-C6-N1	8.00	125.00	121.00
24	A	1416	G	N3-C2-N2	-7.99	114.30	119.90
1	a	1158	C	C2-N1-C1'	7.95	127.55	118.80
24	A	1387	A	N7-C8-N9	7.95	117.78	113.80
24	A	1104	C	N1-C2-O2	7.94	123.66	118.90
24	A	1237	A	N7-C8-N9	7.92	117.76	113.80
24	A	1183	U	N3-C2-O2	-7.92	116.66	122.20
24	A	1507	C	C6-N1-C2	-7.89	117.14	120.30
1	a	1427	C	C6-N1-C2	-7.88	117.15	120.30
24	A	137	U	N1-C2-O2	7.87	128.31	122.80
24	A	1941	C	N1-C2-O2	7.86	123.62	118.90
24	A	1005	C	C6-N1-C2	-7.85	117.16	120.30
1	a	923	A	N7-C8-N9	7.83	117.72	113.80
24	A	1498	C	N3-C2-O2	-7.83	116.42	121.90
1	a	413	G	N1-C6-O6	-7.82	115.21	119.90
24	A	2791	G	N3-C2-N2	-7.79	114.44	119.90
24	A	2131	U	N3-C2-O2	-7.79	116.75	122.20
24	A	2069	G7M	P-O3'-C3'	7.78	129.03	119.70
24	A	1461	C	C6-N1-C2	-7.75	117.20	120.30
24	A	1680	U	N3-C2-O2	-7.75	116.78	122.20
24	A	281	C	C5-C6-N1	7.72	124.86	121.00
24	A	912	C	N1-C2-O2	7.71	123.53	118.90
24	A	2473	U	N1-C2-O2	7.71	128.20	122.80
17	q	69	THR	N-CA-CB	-7.70	95.68	110.30
22	v	19	G	N1-C6-O6	-7.69	115.29	119.90
12	l	101	LEU	N-CA-CB	-7.67	95.06	110.40
24	A	948	C	C6-N1-C2	-7.65	117.24	120.30
24	A	2758	A	N1-C6-N6	-7.65	114.01	118.60
7	g	110	ARG	N-CA-CB	-7.64	96.85	110.60
24	A	999	U	N3-C2-O2	-7.62	116.87	122.20
24	A	2868	A	C5-N7-C8	-7.62	100.09	103.90
1	a	413	G	OP2-P-O3'	7.58	121.88	105.20
24	A	795	C	C6-N1-C2	-7.58	117.27	120.30
1	a	87	C	C5-C6-N1	7.58	124.79	121.00
24	A	2424	C	N3-C4-C5	7.57	124.93	121.90
1	a	1028	C	C6-N1-C2	-7.57	117.27	120.30
24	A	141	G	C2-N3-C4	7.57	115.69	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	581	C	C6-N1-C2	-7.57	117.27	120.30
24	A	1843	C	C6-N1-C2	-7.57	117.27	120.30
1	a	1205	U	N3-C2-O2	-7.56	116.91	122.20
24	A	1402	U	N3-C2-O2	-7.55	116.91	122.20
1	a	422	C	N1-C2-O2	7.55	123.43	118.90
24	A	1539	U	C5-C6-N1	7.50	126.45	122.70
24	A	893	C	N1-C2-O2	7.50	123.40	118.90
24	A	2796	U	N3-C2-O2	-7.48	116.96	122.20
24	A	2074	U	N3-C2-O2	-7.48	116.97	122.20
1	a	1158	C	C6-N1-C2	-7.47	117.31	120.30
1	a	87	C	C6-N1-C2	-7.46	117.32	120.30
22	v	56	C	N1-C2-O2	7.46	123.37	118.90
1	a	754	C	N1-C2-O2	7.44	123.36	118.90
24	A	776	G	C4-N9-C1'	7.43	136.16	126.50
1	a	1197	A	O5'-P-OP2	-7.42	99.02	105.70
24	A	1507	C	C5-C6-N1	7.42	124.71	121.00
24	A	373	U	N3-C2-O2	-7.42	117.01	122.20
24	A	654	A	C2-N3-C4	7.41	114.31	110.60
25	B	26	C	N1-C2-O2	7.41	123.35	118.90
24	A	1314	C	C5-C6-N1	7.41	124.70	121.00
24	A	1005	C	N1-C2-O2	7.39	123.34	118.90
25	B	30	C	C6-N1-C2	-7.38	117.35	120.30
24	A	2243	U	O5'-P-OP1	-7.38	99.06	105.70
1	a	868	C	C6-N1-C2	-7.37	117.35	120.30
24	A	1774	C	N3-C2-O2	-7.36	116.75	121.90
1	a	1393	U	N3-C2-O2	-7.35	117.06	122.20
1	a	1497	G	N1-C6-O6	-7.35	115.49	119.90
24	A	2179	C	C5-C6-N1	7.34	124.67	121.00
24	A	198	C	C5-C6-N1	7.34	124.67	121.00
24	A	12	U	N3-C2-O2	-7.33	117.07	122.20
6	f	53	LYS	N-CA-CB	7.32	123.78	110.60
24	A	548	G	C5-N7-C8	-7.32	100.64	104.30
24	A	776	G	N3-C4-N9	7.31	130.39	126.00
1	a	529	G	N9-C4-C5	-7.31	102.48	105.40
1	a	1149	C	N3-C2-O2	-7.31	116.78	121.90
24	A	361	G	C5-C6-O6	-7.30	124.22	128.60
24	A	867	C	N1-C2-O2	7.30	123.28	118.90
24	A	484	C	C6-N1-C2	-7.30	117.38	120.30
1	a	215	C	N3-C4-N4	7.30	123.11	118.00
1	a	623	C	C6-N1-C2	-7.30	117.38	120.30
1	a	1132	C	N3-C2-O2	-7.29	116.80	121.90
24	A	1313	U	C6-N1-C2	-7.28	116.63	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1225	A	C2-N3-C4	7.27	114.24	110.60
30	G	46	ASP	N-CA-CB	-7.27	97.51	110.60
1	a	215	C	N3-C2-O2	-7.24	116.83	121.90
24	A	2827	C	C6-N1-C2	-7.23	117.41	120.30
24	A	1237	A	C8-N9-C4	-7.21	102.92	105.80
24	A	1081	U	N1-C2-O2	7.21	127.84	122.80
24	A	1843	C	C5-C6-N1	7.20	124.60	121.00
1	a	225	C	C6-N1-C2	-7.20	117.42	120.30
26	C	83	ASP	CB-CG-OD1	7.20	124.78	118.30
1	a	1395	C	N1-C2-O2	7.18	123.21	118.90
24	A	139	U	N3-C2-O2	-7.16	117.19	122.20
1	a	522	C	N3-C4-C5	-7.16	119.04	121.90
24	A	2179	C	C6-N1-C2	-7.16	117.44	120.30
25	B	26	C	N3-C2-O2	-7.15	116.89	121.90
24	A	1340	U	N3-C2-O2	-7.13	117.21	122.20
1	a	168	G	N1-C6-O6	7.12	124.17	119.90
24	A	1387	A	C8-N9-C4	-7.10	102.96	105.80
24	A	2250	G	N3-C4-C5	7.09	132.14	128.60
1	a	1277	C	N3-C2-O2	-7.08	116.94	121.90
1	a	225	C	C5-C6-N1	7.07	124.53	121.00
24	A	883	G	C5-C6-O6	7.06	132.84	128.60
1	a	1195	C	N1-C2-O2	7.06	123.14	118.90
24	A	669	G	N3-C4-C5	-7.06	125.07	128.60
24	A	1183	U	N1-C2-O2	7.05	127.74	122.80
24	A	776	G	C4-C5-C6	7.05	123.03	118.80
24	A	2610	C	P-O3'-C3'	7.03	128.14	119.70
1	a	177	G	C2-N3-C4	7.03	115.41	111.90
1	a	264	C	C5-C6-N1	7.03	124.51	121.00
24	A	32	C	C6-N1-C2	-7.02	117.49	120.30
24	A	2476	A	N1-C2-N3	7.02	132.81	129.30
1	a	450	G	N1-C6-O6	-7.00	115.70	119.90
24	A	1848	A	N7-C8-N9	7.00	117.30	113.80
22	v	56	C	N3-C2-O2	-6.98	117.01	121.90
24	A	2840	C	C5-C6-N1	6.98	124.49	121.00
24	A	2821	A	O5'-P-OP1	-6.98	99.42	105.70
24	A	1076	C	C6-N1-C2	-6.97	117.51	120.30
24	A	1841	U	N3-C2-O2	-6.97	117.32	122.20
1	a	739	C	C6-N1-C2	-6.97	117.51	120.30
1	a	1132	C	N1-C2-O2	6.97	123.08	118.90
24	A	1212	G	P-O3'-C3'	6.97	128.06	119.70
1	a	236	A	N7-C8-N9	6.94	117.27	113.80
24	A	1211	C	OP2-P-O3'	6.94	120.47	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1914	C	C4-C5-C6	6.93	120.86	117.40
24	A	645	C	N1-C2-O2	6.90	123.04	118.90
24	A	1044	C	N3-C4-N4	-6.90	113.17	118.00
24	A	2162	G	OP2-P-O3'	6.89	120.36	105.20
24	A	228	C	P-O3'-C3'	6.89	127.97	119.70
29	F	173	ASP	CB-CG-OD1	6.89	124.50	118.30
1	a	623	C	N1-C2-O2	6.88	123.03	118.90
1	a	1412	C	C6-N1-C2	-6.87	117.55	120.30
24	A	2416	C	C5-C6-N1	6.87	124.44	121.00
1	a	1395	C	N3-C2-O2	-6.87	117.09	121.90
1	a	1520	C	C6-N1-C2	-6.87	117.55	120.30
24	A	2822	G	O5'-P-OP1	-6.87	99.52	105.70
24	A	2131	U	N1-C2-O2	6.86	127.60	122.80
1	a	267	C	N1-C2-O2	6.85	123.01	118.90
1	a	78	A	N1-C2-N3	-6.85	125.88	129.30
24	A	2793	C	N3-C4-N4	-6.85	113.21	118.00
24	A	2474	U	N3-C2-O2	-6.84	117.41	122.20
1	a	186	C	C6-N1-C2	-6.83	117.57	120.30
1	a	1455	G	N1-C6-O6	6.83	124.00	119.90
1	a	1173	U	C5-C6-N1	6.82	126.11	122.70
1	a	960	U	P-O3'-C3'	6.81	127.87	119.70
1	a	598	U	N3-C2-O2	-6.80	117.44	122.20
1	a	1433	A	N7-C8-N9	6.80	117.20	113.80
24	A	2888	C	C6-N1-C2	-6.80	117.58	120.30
1	a	527	G7M	P-O3'-C3'	6.80	127.86	119.70
24	A	205	G	O4'-C1'-N9	6.79	113.64	108.20
1	a	1143	G	N3-C2-N2	-6.79	115.15	119.90
24	A	2011	U	N3-C2-O2	-6.79	117.45	122.20
1	a	1297	G	P-O3'-C3'	6.79	127.85	119.70
24	A	1290	C	C5-C6-N1	6.79	124.39	121.00
1	a	960	U	N1-C2-O2	6.78	127.55	122.80
24	A	257	C	N1-C2-O2	6.78	122.97	118.90
24	A	1305	C	C6-N1-C2	-6.78	117.59	120.30
24	A	2248	C	N1-C2-O2	6.78	122.97	118.90
24	A	867	C	N3-C2-O2	-6.77	117.16	121.90
1	a	1496	C	C6-N1-C2	-6.77	117.59	120.30
25	B	68	C	C6-N1-C2	-6.74	117.60	120.30
24	A	1362	C	C5-C6-N1	6.74	124.37	121.00
24	A	1600	C	C6-N1-C2	-6.72	117.61	120.30
1	a	754	C	N3-C2-O2	-6.72	117.20	121.90
24	A	866	A	N1-C6-N6	6.72	122.63	118.60
1	a	422	C	N3-C2-O2	-6.71	117.20	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	755	G	O5'-P-OP2	-6.70	99.67	105.70
24	A	327	G	N3-C2-N2	-6.70	115.21	119.90
24	A	1371	G	N3-C4-N9	-6.70	121.98	126.00
24	A	365	U	C5-C6-N1	6.70	126.05	122.70
1	a	522	C	C6-N1-C2	-6.70	117.62	120.30
24	A	1399	C	C5-C6-N1	6.70	124.35	121.00
24	A	2745	C	N1-C2-O2	6.70	122.92	118.90
24	A	2561	U	N1-C2-N3	6.69	118.92	114.90
24	A	847	U	N3-C2-O2	-6.69	117.52	122.20
24	A	1578	U	N3-C2-O2	-6.69	117.52	122.20
24	A	12	U	N1-C2-O2	6.68	127.48	122.80
24	A	758	C	N3-C2-O2	-6.68	117.22	121.90
24	A	2617	U	N3-C2-O2	-6.68	117.52	122.20
24	A	2554	U	O5'-P-OP1	-6.68	99.69	105.70
24	A	1498	C	C2-N1-C1'	6.68	126.15	118.80
1	a	1455	G	C6-C5-N7	-6.68	126.39	130.40
24	A	912	C	C2-N1-C1'	6.67	126.14	118.80
1	a	1404	C	C6-N1-C2	-6.67	117.63	120.30
1	a	264	C	C6-N1-C2	-6.66	117.64	120.30
1	a	252	U	N3-C2-O2	-6.65	117.55	122.20
24	A	1624	U	N3-C2-O2	-6.65	117.55	122.20
24	A	1022	G	N3-C2-N2	-6.64	115.25	119.90
1	a	529	G	C6-C5-N7	-6.64	126.42	130.40
1	a	817	C	N1-C2-O2	6.62	122.87	118.90
1	a	623	C	C5-C6-N1	6.61	124.31	121.00
24	A	2649	C	C5-C6-N1	6.61	124.31	121.00
24	A	361	G	N1-C6-O6	6.61	123.87	119.90
24	A	373	U	N1-C2-O2	6.61	127.42	122.80
1	a	386	C	C6-N1-C2	-6.60	117.66	120.30
24	A	2354	C	C6-N1-C2	-6.60	117.66	120.30
24	A	2774	C	C6-N1-C2	-6.60	117.66	120.30
24	A	1365	A	C2-N3-C4	6.59	113.90	110.60
24	A	143	C	C6-N1-C2	-6.59	117.66	120.30
24	A	1005	C	N3-C2-O2	-6.58	117.29	121.90
24	A	2036	C	C6-N1-C2	-6.58	117.67	120.30
24	A	2796	U	N1-C2-N3	6.57	118.84	114.90
24	A	1294	U	N3-C2-O2	-6.57	117.60	122.20
24	A	62	U	C5-C6-N1	6.55	125.98	122.70
1	a	792	A	N7-C8-N9	-6.54	110.53	113.80
1	a	1027	C	C2-N3-C4	6.53	123.16	119.90
24	A	714	U	N3-C2-O2	-6.53	117.63	122.20
24	A	2403	C	C6-N1-C2	-6.52	117.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	783	A	C5-N7-C8	-6.51	100.64	103.90
24	A	528	A	N7-C8-N9	6.51	117.05	113.80
24	A	91	A	P-O3'-C3'	6.51	127.51	119.70
1	a	1372	U	N3-C2-O2	-6.50	117.65	122.20
24	A	687	C	N3-C2-O2	-6.50	117.35	121.90
1	a	400	C	C5-C6-N1	6.49	124.25	121.00
24	A	550	C	C5-C6-N1	6.49	124.25	121.00
1	a	1172	C	C6-N1-C2	-6.48	117.71	120.30
1	a	217	C	C5-C6-N1	6.47	124.23	121.00
24	A	1658	C	C6-N1-C2	-6.47	117.71	120.30
24	A	1947	C	C6-N1-C2	-6.47	117.71	120.30
24	A	758	C	C6-N1-C2	-6.46	117.71	120.30
13	m	4	ALA	N-CA-CB	-6.46	101.05	110.10
25	B	42	C	N1-C2-O2	6.46	122.78	118.90
1	a	1494[A]	G	C8-N9-C4	-6.44	103.82	106.40
1	a	1494[C]	G	C8-N9-C4	-6.44	103.82	106.40
24	A	2561	U	C2-N3-C4	-6.44	123.13	127.00
1	a	983	A	C2-N3-C4	6.44	113.82	110.60
24	A	62	U	C2-N3-C4	6.44	130.86	127.00
1	a	1225	A	N3-C4-N9	6.43	132.54	127.40
24	A	807	U	N3-C2-O2	-6.43	117.70	122.20
24	A	2424	C	C5-C4-N4	-6.43	115.70	120.20
24	A	121	G	N1-C6-O6	6.42	123.75	119.90
24	A	1994	C	N3-C2-O2	-6.41	117.41	121.90
25	B	60	C	C5-C6-N1	6.41	124.21	121.00
24	A	1348	C	N1-C2-O2	6.41	122.75	118.90
24	A	386	G	O5'-P-OP2	-6.41	99.93	105.70
24	A	2321	U	N3-C4-O4	6.41	123.88	119.40
25	B	17	C	N1-C2-O2	6.41	122.74	118.90
2	b	17	HIS	N-CA-CB	-6.40	99.07	110.60
24	A	2870	C	C6-N1-C2	-6.40	117.74	120.30
1	a	610	U	N3-C2-O2	-6.40	117.72	122.20
24	A	2372	U	N3-C2-O2	-6.40	117.72	122.20
24	A	2481	G	C5-C6-N1	-6.40	108.30	111.50
1	a	1205	U	N1-C2-O2	6.39	127.28	122.80
24	A	2312	U	C5-C6-N1	6.39	125.90	122.70
24	A	807	U	N1-C2-O2	6.39	127.27	122.80
22	v	74	C	N3-C2-O2	-6.39	117.43	121.90
1	a	810	C	C5-C6-N1	6.38	124.19	121.00
1	a	923	A	C8-N9-C4	-6.38	103.25	105.80
24	A	919	U	N1-C2-O2	6.37	127.26	122.80
24	A	866	A	C5-C6-N1	6.36	120.88	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1804	C	C6-N1-C2	-6.36	117.76	120.30
24	A	1848	A	C8-N9-C4	-6.35	103.26	105.80
24	A	2168	G	N3-C4-C5	-6.33	125.43	128.60
24	A	999	U	N1-C2-O2	6.33	127.23	122.80
1	a	413	G	C2-N3-C4	6.33	115.06	111.90
22	v	67	C	N1-C2-O2	6.33	122.70	118.90
24	A	2168	G	C2-N3-C4	6.33	115.06	111.90
1	a	207	C	N3-C2-O2	-6.33	117.47	121.90
24	A	894	U	N3-C2-O2	-6.32	117.77	122.20
24	A	512	G	O4'-C1'-N9	6.32	113.25	108.20
24	A	547	A	C2-N3-C4	6.31	113.75	110.60
1	a	618	C	N1-C2-O2	6.31	122.68	118.90
1	a	1011	C	C5-C6-N1	6.31	124.15	121.00
24	A	1669	A	C2-N3-C4	6.31	113.75	110.60
25	B	12	C	N3-C2-O2	-6.31	117.48	121.90
24	A	454	A	OP2-P-O3'	6.30	119.06	105.20
1	a	960	U	N3-C2-O2	-6.29	117.79	122.20
24	A	1314	C	C2-N1-C1'	6.29	125.72	118.80
24	A	1567	G	P-O3'-C3'	6.29	127.25	119.70
24	A	2755	C	N1-C2-O2	6.29	122.67	118.90
1	a	413	G	C4-C5-N7	-6.29	108.29	110.80
1	a	483	C	C6-N1-C2	-6.28	117.79	120.30
24	A	2025	C	C6-N1-C2	-6.28	117.79	120.30
24	A	2250	G	N3-C4-N9	-6.28	122.23	126.00
24	A	366	C	C6-N1-C2	-6.28	117.79	120.30
25	B	37	C	N1-C2-O2	6.26	122.66	118.90
1	a	1538	C	C6-N1-C2	-6.26	117.80	120.30
24	A	2220	U	C5-C6-N1	6.26	125.83	122.70
1	a	1258	G	N1-C6-O6	-6.25	116.15	119.90
24	A	1784	A	N7-C8-N9	-6.24	110.68	113.80
1	a	33	A	N7-C8-N9	6.24	116.92	113.80
24	A	314	C	C6-N1-C2	-6.24	117.80	120.30
1	a	1011	C	C6-N1-C2	-6.24	117.81	120.30
1	a	80	A	N1-C2-N3	6.24	132.42	129.30
1	a	369	G	C6-C5-N7	-6.21	126.67	130.40
1	a	186	C	N1-C2-O2	6.21	122.62	118.90
25	B	37	C	N3-C2-O2	-6.20	117.56	121.90
24	A	16	C	C6-N1-C2	-6.20	117.82	120.30
24	A	205	G	OP2-P-O3'	6.20	118.83	105.20
24	A	581	C	O5'-P-OP1	-6.19	100.13	105.70
1	a	500	G	N1-C6-O6	6.19	123.61	119.90
24	A	1920	C	C6-N1-C2	-6.18	117.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	276	U	N1-C2-O2	6.17	127.12	122.80
24	A	287	G	C6-N1-C2	-6.17	121.40	125.10
24	A	1081	U	N3-C4-C5	6.17	118.30	114.60
24	A	2794	C	C6-N1-C2	-6.17	117.83	120.30
1	a	810	C	C6-N1-C2	-6.17	117.83	120.30
1	a	1320	C	N1-C2-O2	6.17	122.60	118.90
24	A	1399	C	C6-N1-C2	-6.17	117.83	120.30
24	A	2782	G	C6-C5-N7	-6.17	126.70	130.40
1	a	207	C	N1-C2-O2	6.16	122.60	118.90
22	v	56	C	C6-N1-C2	-6.16	117.83	120.30
24	A	2561	U	N3-C2-O2	-6.16	117.89	122.20
24	A	1044	C	C5-C4-N4	6.16	124.51	120.20
24	A	2405	G	OP2-P-O3'	6.16	118.75	105.20
1	a	1432	G	P-O3'-C3'	6.15	127.08	119.70
24	A	198	C	N1-C2-O2	6.15	122.59	118.90
1	a	316	C	N1-C2-O2	6.14	122.59	118.90
1	a	754	C	OP1-P-O3'	6.14	118.72	105.20
1	a	1134	G	C6-N1-C2	-6.14	121.41	125.10
24	A	805	G	N9-C4-C5	-6.14	102.94	105.40
25	B	68	C	C5-C6-N1	6.14	124.07	121.00
1	a	1383	C	N1-C2-O2	6.13	122.58	118.90
24	A	2742	G	C4-C5-N7	6.13	113.25	110.80
1	a	1301	U	P-O3'-C3'	6.12	127.05	119.70
24	A	106	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1497	G	N3-C2-N2	-6.12	115.62	119.90
1	a	961	U	N3-C2-O2	-6.12	117.92	122.20
24	A	512	G	OP2-P-O3'	6.11	118.63	105.20
1	a	890	G	P-O3'-C3'	6.10	127.02	119.70
1	a	1262	C	N1-C2-O2	6.10	122.56	118.90
24	A	832	U	N1-C2-N3	6.10	118.56	114.90
25	B	38	C	C5-C4-N4	-6.10	115.93	120.20
24	A	1584	U	C5-C6-N1	6.10	125.75	122.70
24	A	1716	U	C2-N1-C1'	6.10	125.02	117.70
25	B	28	C	C6-N1-C2	-6.09	117.86	120.30
1	a	1277	C	C6-N1-C2	-6.09	117.86	120.30
24	A	2566	A	P-O3'-C3'	6.09	127.00	119.70
24	A	2683	C	N3-C2-O2	-6.08	117.64	121.90
1	a	840	C	N3-C4-N4	-6.08	113.74	118.00
1	a	272	C	C6-N1-C2	-6.07	117.87	120.30
1	a	578	C	C6-N1-C2	-6.07	117.87	120.30
24	A	353	C	C6-N1-C2	-6.07	117.87	120.30
1	a	548	G	N1-C6-O6	6.06	123.54	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	847	U	N1-C2-O2	6.06	127.04	122.80
1	a	1357	A	N7-C8-N9	6.05	116.83	113.80
1	a	991	U	N1-C2-O2	6.05	127.04	122.80
1	a	1303	C	N1-C2-O2	6.05	122.53	118.90
24	A	1994	C	C6-N1-C2	-6.05	117.88	120.30
24	A	2074	U	N1-C2-O2	6.04	127.03	122.80
24	A	385	C	P-O3'-C3'	6.04	126.95	119.70
1	a	503	C	C5-C6-N1	6.04	124.02	121.00
24	A	349	U	N1-C2-O2	6.03	127.02	122.80
24	A	2244	U	C5-C4-O4	-6.03	122.28	125.90
24	A	2141	G	N7-C8-N9	6.03	116.12	113.10
25	B	27	C	N1-C2-O2	6.03	122.52	118.90
1	a	883	C	N1-C2-O2	6.02	122.51	118.90
24	A	214	G	N3-C4-C5	-6.02	125.59	128.60
40	Q	27	ARG	NE-CZ-NH1	-6.02	117.29	120.30
5	e	122	VAL	N-CA-CB	-6.02	98.26	111.50
24	A	935	C	C6-N1-C2	-6.02	117.89	120.30
1	a	215	C	C2-N1-C1'	6.01	125.42	118.80
24	A	672	C	C6-N1-C2	-6.01	117.89	120.30
24	A	1894	C	N1-C2-O2	6.01	122.51	118.90
24	A	2061	G	P-O3'-C3'	6.01	126.92	119.70
1	a	626	G	C6-C5-N7	-6.01	126.79	130.40
24	A	2496	C	N1-C2-O2	6.01	122.50	118.90
1	a	1494[A]	G	N7-C8-N9	6.00	116.10	113.10
1	a	1494[C]	G	N7-C8-N9	6.00	116.10	113.10
24	A	1340	U	N1-C2-O2	6.00	127.00	122.80
24	A	2720	U	N3-C2-O2	-6.00	118.00	122.20
24	A	1784	A	C4-C5-C6	6.00	120.00	117.00
24	A	2558	C	C5-C6-N1	6.00	124.00	121.00
24	A	366	C	C5-C6-N1	5.99	124.00	121.00
1	a	248	C	C6-N1-C2	-5.99	117.90	120.30
24	A	2379	G	N1-C6-O6	5.99	123.49	119.90
24	A	543	G	N1-C6-O6	5.99	123.49	119.90
24	A	284	U	N3-C2-O2	-5.99	118.01	122.20
24	A	284	U	N1-C2-O2	5.98	126.99	122.80
24	A	528	A	C5-N7-C8	-5.98	100.91	103.90
24	A	1023	U	N1-C2-O2	5.98	126.99	122.80
24	A	62	U	C6-N1-C1'	-5.98	112.83	121.20
24	A	528	A	C8-N9-C4	-5.98	103.41	105.80
1	a	1147	C	N1-C2-O2	5.97	122.48	118.90
24	A	2463	C	C5-C6-N1	5.97	123.99	121.00
1	a	50	A	C2-N3-C4	5.97	113.58	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1578	U	N1-C2-O2	5.97	126.98	122.80
24	A	2711	A	O5'-P-OP2	5.97	117.86	110.70
24	A	1313	U	C6-N1-C1'	-5.97	112.85	121.20
1	a	943	U	N1-C2-O2	5.96	126.97	122.80
24	A	2329	U	C5-C6-N1	5.96	125.68	122.70
29	F	172	PHE	C-N-CA	5.96	136.59	121.70
1	a	1140	C	N1-C2-O2	5.96	122.47	118.90
1	a	626	G	N3-C4-N9	5.94	129.56	126.00
24	A	2518	A	C2-N3-C4	5.94	113.57	110.60
22	v	36	U	N3-C2-O2	-5.94	118.04	122.20
24	A	919	U	N3-C2-O2	-5.94	118.04	122.20
24	A	2254	C	N1-C2-O2	5.94	122.46	118.90
30	G	174	LYS	N-CA-CB	5.94	121.29	110.60
24	A	81	G	N3-C2-N2	-5.93	115.75	119.90
24	A	866	A	N9-C4-C5	-5.93	103.43	105.80
1	a	1037	C	C6-N1-C2	-5.92	117.93	120.30
1	a	1455	G	N3-C4-N9	5.92	129.56	126.00
24	A	62	U	C6-N1-C2	-5.92	117.45	121.00
1	a	56	U	C5-C4-O4	-5.92	122.35	125.90
1	a	1228	C	C6-N1-C2	-5.91	117.94	120.30
24	A	1782	U	O5'-P-OP1	-5.91	100.38	105.70
24	A	456	C	O5'-P-OP2	-5.90	100.39	105.70
1	a	1109	C	C6-N1-C2	-5.90	117.94	120.30
24	A	1020	A	P-O3'-C3'	5.90	126.78	119.70
24	A	1112	G	N3-C4-N9	-5.90	122.46	126.00
24	A	140	C	C6-N1-C2	-5.90	117.94	120.30
25	B	49	C	C6-N1-C2	-5.89	117.94	120.30
1	a	322	C	C5-C6-N1	5.89	123.95	121.00
24	A	51	G	P-O3'-C3'	5.89	126.77	119.70
1	a	369	G	N1-C6-O6	5.89	123.43	119.90
24	A	758	C	N1-C2-O2	5.89	122.43	118.90
24	A	1020	A	OP2-P-O3'	5.89	118.16	105.20
1	a	217	C	C6-N1-C2	-5.88	117.95	120.30
24	A	1994	C	N1-C2-O2	5.88	122.42	118.90
25	B	42	C	N3-C2-O2	-5.87	117.79	121.90
24	A	141	G	N3-C4-C5	-5.87	125.67	128.60
25	B	12	C	N1-C2-O2	5.87	122.42	118.90
25	B	38	C	N3-C4-N4	5.87	122.11	118.00
24	A	1830	C	N1-C2-O2	5.87	122.42	118.90
1	a	1535	C	C5-C6-N1	5.87	123.93	121.00
24	A	435	C	C6-N1-C2	-5.86	117.95	120.30
24	A	1054	A	N1-C2-N3	-5.86	126.37	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2782	G	N3-C4-N9	5.86	129.52	126.00
24	A	1810	A	C8-N9-C4	-5.85	103.46	105.80
24	A	2036	C	C5-C6-N1	5.85	123.93	121.00
24	A	2867	G	N9-C4-C5	-5.85	103.06	105.40
24	A	2282	G	N1-C6-O6	-5.85	116.39	119.90
24	A	2794	C	C2-N1-C1'	5.84	125.23	118.80
25	B	5	U	N3-C2-O2	-5.84	118.11	122.20
1	a	723	U	C5-C6-N1	5.84	125.62	122.70
24	A	1455	G	N3-C4-N9	5.84	129.50	126.00
1	a	1433	A	C8-N9-C4	-5.83	103.47	105.80
24	A	288	U	C5-C6-N1	5.83	125.62	122.70
24	A	2354	C	C5-C6-N1	5.83	123.92	121.00
24	A	776	G	C8-N9-C1'	-5.82	119.43	127.00
24	A	2096	C	O5'-P-OP2	-5.82	100.46	105.70
24	A	2773	C	C6-N1-C2	-5.82	117.97	120.30
1	a	850	U	C5-C6-N1	5.81	125.61	122.70
24	A	2683	C	N1-C2-O2	5.81	122.39	118.90
24	A	2581	G	N3-C4-N9	5.81	129.49	126.00
24	A	805	G	N3-C4-N9	5.80	129.48	126.00
25	B	12	C	C6-N1-C2	-5.80	117.98	120.30
24	A	965	C	C6-N1-C2	-5.80	117.98	120.30
24	A	305	C	C5-C6-N1	5.80	123.90	121.00
24	A	2180	U	C2-N3-C4	5.79	130.48	127.00
24	A	1135	C	OP1-P-O3'	5.79	117.93	105.20
1	a	1190	G	P-O3'-C3'	5.78	126.64	119.70
22	v	34	C	C5-C4-N4	-5.78	116.16	120.20
1	a	1245	C	C5-C6-N1	5.78	123.89	121.00
25	B	31	C	N3-C2-O2	-5.78	117.86	121.90
24	A	866	A	C4-C5-N7	5.77	113.58	110.70
1	a	1538	C	C5-C6-N1	5.76	123.88	121.00
24	A	2072	C	C2-N1-C1'	5.76	125.14	118.80
24	A	714	U	N1-C2-O2	5.76	126.83	122.80
24	A	893	C	N3-C4-C5	-5.76	119.60	121.90
24	A	2739	U	N1-C2-O2	5.76	126.83	122.80
24	A	1180	U	C5-C4-O4	-5.75	122.45	125.90
1	a	188	C	N1-C2-O2	5.75	122.35	118.90
13	m	57	ASP	CB-CG-OD1	5.75	123.48	118.30
24	A	1105	U	C2-N3-C4	-5.75	123.55	127.00
24	A	1213	A	C2-N3-C4	5.75	113.48	110.60
24	A	1769	U	N3-C2-O2	-5.75	118.17	122.20
24	A	1305	C	C5-C6-N1	5.75	123.88	121.00
1	a	316	C	N3-C2-O2	-5.75	117.88	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1539	U	C2-N3-C4	5.74	130.45	127.00
24	A	8	C	C5-C6-N1	5.74	123.87	121.00
24	A	984	A	C2-N3-C4	-5.74	107.73	110.60
1	a	186	C	C5-C6-N1	5.74	123.87	121.00
24	A	1159	U	N1-C2-O2	5.74	126.81	122.80
24	A	2370	G	C6-N1-C2	-5.74	121.66	125.10
30	G	174	LYS	N-CA-C	-5.73	95.52	111.00
24	A	1930	G	O4'-C1'-N9	5.73	112.79	108.20
24	A	91	A	OP2-P-O3'	5.73	117.81	105.20
24	A	2803	G	C6-C5-N7	-5.73	126.96	130.40
24	A	1940	U	P-O3'-C3'	5.73	126.57	119.70
24	A	1416	G	C6-N1-C2	-5.73	121.67	125.10
24	A	1920	C	C5-C6-N1	5.73	123.86	121.00
1	a	215	C	C5-C4-N4	-5.72	116.19	120.20
1	a	1182	G	P-O3'-C3'	5.72	126.57	119.70
24	A	383	C	N1-C2-O2	5.72	122.33	118.90
24	A	1159	U	N3-C2-O2	-5.72	118.20	122.20
24	A	1303	G	N1-C6-O6	5.72	123.33	119.90
1	a	611	C	N1-C2-O2	5.72	122.33	118.90
1	a	623	C	N3-C4-N4	5.72	122.00	118.00
1	a	1320	C	N3-C2-O2	-5.72	117.90	121.90
22	v	34	C	C2-N1-C1'	5.71	125.08	118.80
24	A	1728	C	N1-C2-O2	-5.71	115.47	118.90
24	A	205	G	C8-N9-C4	5.71	108.68	106.40
24	A	2649	C	C6-N1-C2	-5.71	118.02	120.30
24	A	2321	U	N3-C4-C5	-5.70	111.18	114.60
24	A	2594	C	C6-N1-C2	-5.70	118.02	120.30
24	A	1533	C	N3-C4-N4	-5.70	114.01	118.00
24	A	1461	C	C5-C6-N1	5.70	123.85	121.00
24	A	2226	C	C6-N1-C2	-5.70	118.02	120.30
24	A	2827	C	C5-C6-N1	5.70	123.85	121.00
24	A	2370	G	N3-C4-C5	-5.70	125.75	128.60
24	A	640	C	C6-N1-C2	-5.69	118.02	120.30
24	A	2403	C	N1-C2-O2	5.69	122.31	118.90
24	A	2405	G	P-O3'-C3'	5.69	126.53	119.70
24	A	557	C	N1-C2-O2	5.69	122.31	118.90
1	a	572	A	P-O3'-C3'	5.68	126.52	119.70
24	A	2867	G	C8-N9-C4	5.68	108.67	106.40
1	a	369	G	N3-C4-N9	5.68	129.41	126.00
1	a	470	C	C6-N1-C2	-5.68	118.03	120.30
24	A	1730	C	C6-N1-C2	-5.67	118.03	120.30
7	g	22	LEU	CA-CB-CG	5.67	128.34	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	101	LEU	CA-CB-CG	5.67	128.33	115.30
1	a	1034	G	N1-C6-O6	-5.67	116.50	119.90
1	a	717	U	N1-C2-O2	5.66	126.76	122.80
1	a	891	U	C6-N1-C2	-5.66	117.60	121.00
24	A	1021	A	C2-N3-C4	5.66	113.43	110.60
1	a	1158	C	N3-C2-O2	-5.66	117.94	121.90
24	A	2174	C	N1-C2-O2	5.65	122.29	118.90
1	a	883	C	C6-N1-C2	-5.65	118.04	120.30
22	v	34	C	N3-C4-N4	5.65	121.95	118.00
24	A	1314	C	N1-C2-O2	5.65	122.29	118.90
35	L	29	LYS	N-CA-CB	-5.65	100.43	110.60
24	A	349	U	N3-C2-O2	-5.64	118.25	122.20
24	A	1662	U	N3-C2-O2	-5.64	118.25	122.20
1	a	348	G	N1-C6-O6	5.64	123.28	119.90
1	a	1356	G	N3-C2-N2	5.64	123.85	119.90
24	A	961	C	C6-N1-C2	-5.64	118.04	120.30
24	A	1043	C	C6-N1-C2	-5.64	118.04	120.30
24	A	2884	U	C2-N1-C1'	5.64	124.47	117.70
24	A	645	C	N3-C2-O2	-5.64	117.95	121.90
24	A	1816	C	N1-C2-O2	5.64	122.28	118.90
1	a	613	C	C6-N1-C2	-5.64	118.05	120.30
24	A	2244	U	N3-C4-O4	5.64	123.35	119.40
1	a	754	C	C6-N1-C1'	-5.63	114.04	120.80
24	A	1142	A	C2-N3-C4	-5.63	107.78	110.60
1	a	1303	C	N3-C2-O2	-5.63	117.96	121.90
1	a	1455	G	C5-C6-O6	-5.63	125.22	128.60
24	A	1963	U	C5-C6-N1	5.63	125.51	122.70
24	A	2162	G	OP1-P-OP2	-5.63	111.16	119.60
24	A	1290	C	C6-N1-C2	-5.63	118.05	120.30
24	A	805	G	C4-C5-N7	5.62	113.05	110.80
24	A	1680	U	N1-C2-O2	5.62	126.74	122.80
1	a	1382	C	N1-C2-O2	5.62	122.27	118.90
24	A	484	C	N1-C2-O2	5.62	122.27	118.90
24	A	1585	C	N1-C2-O2	5.62	122.27	118.90
24	A	2474	U	N1-C2-O2	5.62	126.73	122.80
24	A	2795	C	C6-N1-C2	-5.62	118.05	120.30
1	a	961	U	N1-C2-O2	5.62	126.73	122.80
24	A	542	C	N3-C4-N4	-5.61	114.07	118.00
24	A	901	C	N1-C2-O2	5.61	122.27	118.90
1	a	413	G	C8-N9-C4	5.61	108.64	106.40
1	a	1149	C	C6-N1-C2	-5.61	118.06	120.30
24	A	1323	C	N3-C2-O2	-5.60	117.98	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	348	G	C6-C5-N7	-5.59	127.05	130.40
24	A	2496	C	N3-C2-O2	-5.59	117.99	121.90
24	A	2796	U	C2-N3-C4	-5.59	123.65	127.00
1	a	413	G	N3-C4-N9	5.59	129.35	126.00
1	a	251	G	O4'-C1'-N9	-5.58	103.73	108.20
1	a	1173	U	C5-C4-O4	-5.58	122.55	125.90
22	v	71	C	C6-N1-C2	-5.58	118.07	120.30
24	A	1839	G	C2-N3-C4	5.58	114.69	111.90
24	A	1105	U	N1-C2-O2	5.58	126.70	122.80
24	A	872	U	C5-C6-N1	5.58	125.49	122.70
24	A	912	C	N3-C2-O2	-5.58	118.00	121.90
24	A	1526	C	C6-N1-C2	-5.58	118.07	120.30
24	A	1104	C	N3-C4-N4	5.57	121.90	118.00
30	G	46	ASP	N-CA-C	5.57	126.04	111.00
24	A	1269	A	N1-C2-N3	-5.57	126.52	129.30
24	A	1407	G	C4-C5-N7	5.57	113.03	110.80
24	A	1371	G	N3-C4-C5	5.56	131.38	128.60
24	A	2312	U	C6-N1-C2	-5.56	117.66	121.00
24	A	1081	U	C2-N3-C4	-5.56	123.67	127.00
1	a	316	C	C2-N1-C1'	5.56	124.91	118.80
1	a	986	U	C5-C6-N1	5.56	125.48	122.70
24	A	2562	U	N3-C2-O2	-5.56	118.31	122.20
1	a	1261	A	C2-N3-C4	5.55	113.38	110.60
24	A	1005	C	C2-N1-C1'	5.55	124.91	118.80
24	A	1500	G	N1-C6-O6	5.55	123.23	119.90
24	A	198	C	C6-N1-C2	-5.55	118.08	120.30
24	A	1402	U	N1-C2-O2	5.55	126.69	122.80
24	A	2562	U	N1-C2-O2	5.55	126.69	122.80
24	A	205	G	P-O3'-C3'	5.55	126.36	119.70
1	a	814	A	C2-N3-C4	5.55	113.37	110.60
1	a	1003	G	N1-C2-N2	5.55	121.19	116.20
1	a	1277	C	N1-C2-O2	5.55	122.23	118.90
24	A	2782	G	N1-C6-O6	5.55	123.23	119.90
24	A	2863	C	C6-N1-C2	-5.54	118.08	120.30
24	A	1731	G	C8-N9-C4	-5.54	104.18	106.40
24	A	2818	U	N1-C2-O2	5.54	126.68	122.80
1	a	843	U	C5-C6-N1	5.54	125.47	122.70
24	A	2739	U	N3-C2-O2	-5.54	118.32	122.20
1	a	322	C	C6-N1-C2	-5.54	118.09	120.30
24	A	1102	C	N3-C2-O2	-5.54	118.03	121.90
24	A	1941	C	N3-C2-O2	-5.54	118.03	121.90
24	A	1930	G	P-O3'-C3'	5.53	126.34	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	935	C	C5-C6-N1	5.53	123.76	121.00
1	a	991	U	N3-C2-O2	-5.53	118.33	122.20
44	U	88	ASP	N-CA-CB	-5.52	100.66	110.60
24	A	2751	G	O5'-P-OP2	5.52	117.33	110.70
1	a	1195	C	N3-C2-O2	-5.52	118.04	121.90
1	a	737	C	C2-N3-C4	5.52	122.66	119.90
24	A	1138	G	N1-C6-O6	-5.51	116.59	119.90
24	A	2456	C	C6-N1-C2	-5.51	118.10	120.30
24	A	257	C	N3-C2-O2	-5.51	118.05	121.90
24	A	1111	A	P-O3'-C3'	5.50	126.30	119.70
1	a	1486	G	N3-C4-C5	-5.50	125.85	128.60
1	a	102	G	N1-C6-O6	-5.50	116.60	119.90
1	a	717	U	N3-C2-O2	-5.50	118.35	122.20
24	A	2168	G	N3-C4-N9	5.50	129.30	126.00
1	a	618	C	N3-C2-O2	-5.50	118.05	121.90
24	A	776	G	C8-N9-C4	-5.50	104.20	106.40
24	A	845	A	N1-C2-N3	-5.50	126.55	129.30
24	A	933	A	C2-N3-C4	5.50	113.35	110.60
1	a	34	C	C5-C6-N1	5.49	123.75	121.00
1	a	804	U	N3-C2-O2	-5.49	118.36	122.20
24	A	1210	G	C2-N3-C4	5.49	114.65	111.90
24	A	2782	G	N9-C4-C5	-5.49	103.20	105.40
1	a	168	G	N3-C4-N9	5.49	129.29	126.00
1	a	1288	A	N7-C8-N9	5.49	116.55	113.80
24	A	1982	U	N1-C2-O2	5.49	126.64	122.80
24	A	916	G	C4-C5-N7	5.49	112.99	110.80
24	A	1498	C	C5-C6-N1	5.49	123.74	121.00
1	a	1372	U	N1-C2-O2	5.48	126.64	122.80
24	A	2023	C	N1-C2-O2	5.48	122.19	118.90
22	v	71	C	N3-C2-O2	-5.47	118.07	121.90
24	A	208	C	C6-N1-C2	-5.47	118.11	120.30
25	B	88	C	N1-C2-O2	5.47	122.18	118.90
1	a	1452	C	C6-N1-C2	-5.46	118.11	120.30
14	n	33	VAL	C-N-CA	5.46	135.36	121.70
24	A	314	C	C5-C6-N1	5.46	123.73	121.00
1	a	1088	G	N9-C4-C5	-5.46	103.22	105.40
24	A	2514	U	C5-C6-N1	5.46	125.43	122.70
1	a	1010	U	N3-C2-O2	-5.46	118.38	122.20
24	A	2867	G	P-O3'-C3'	5.46	126.25	119.70
1	a	1034	G	C5-C6-N1	5.45	114.22	111.50
1	a	1173	U	N3-C4-O4	5.45	123.22	119.40
24	A	789	A	OP2-P-O3'	5.45	117.18	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	613	A	N3-C4-C5	-5.45	122.99	126.80
1	a	1297	G	O5'-P-OP2	-5.44	100.80	105.70
24	A	383	C	N3-C2-O2	-5.44	118.09	121.90
1	a	1134	G	N1-C2-N2	5.44	121.10	116.20
1	a	188	C	C6-N1-C2	-5.44	118.12	120.30
24	A	1343	G	C4-N9-C1'	5.44	133.57	126.50
24	A	2510	C	C6-N1-C2	-5.44	118.13	120.30
1	a	890	G	OP2-P-O3'	5.43	117.16	105.20
24	A	1839	G	N3-C4-C5	-5.43	125.89	128.60
24	A	690	G	C4-N9-C1'	5.43	133.55	126.50
1	a	609	A	C2-N3-C4	5.42	113.31	110.60
24	A	215	G	OP1-P-O3'	5.42	117.13	105.20
24	A	435	C	N1-C2-O2	5.42	122.16	118.90
24	A	894	U	N1-C2-O2	5.42	126.60	122.80
24	A	2567	G	C4-N9-C1'	5.42	133.54	126.50
1	a	358	U	N3-C2-O2	-5.42	118.41	122.20
24	A	161	A	OP1-P-O3'	5.41	117.11	105.20
24	A	813	U	N3-C2-O2	-5.41	118.41	122.20
1	a	413	G	N3-C4-C5	-5.41	125.90	128.60
24	A	177	G	C4-N9-C1'	5.41	133.53	126.50
24	A	2754	U	N1-C2-O2	5.41	126.58	122.80
51	1	39	ASP	CB-CG-OD1	5.41	123.17	118.30
24	A	2793	C	N3-C2-O2	-5.40	118.12	121.90
24	A	609	A	C8-N9-C4	-5.40	103.64	105.80
1	a	1219	A	N7-C8-N9	5.40	116.50	113.80
1	a	1493[A]	A	P-O3'-C3'	5.40	126.18	119.70
1	a	1493[C]	A	P-O3'-C3'	5.40	126.18	119.70
1	a	335	C	C6-N1-C2	-5.40	118.14	120.30
24	A	32	C	C5-C6-N1	5.40	123.70	121.00
24	A	1875	G	OP2-P-O3'	5.40	117.07	105.20
24	A	2008	C	C6-N1-C2	-5.40	118.14	120.30
24	A	1112	G	C5-C6-O6	5.39	131.84	128.60
24	A	2581	G	C2-N3-C4	5.39	114.60	111.90
1	a	355	C	C6-N1-C2	-5.39	118.14	120.30
24	A	276	U	N3-C2-O2	-5.39	118.43	122.20
24	A	287	G	N3-C2-N2	-5.39	116.13	119.90
24	A	669	G	C4-N9-C1'	5.39	133.50	126.50
24	A	278	A	N3-C4-C5	-5.39	123.03	126.80
24	A	137	U	N1-C2-N3	5.38	118.13	114.90
1	a	1182	G	OP2-P-O3'	5.38	117.03	105.20
1	a	787	A	C2-N3-C4	5.38	113.29	110.60
1	a	58	C	N3-C4-N4	-5.38	114.24	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	623	C	C2-N1-C1'	5.38	124.71	118.80
1	a	1383	C	N3-C2-O2	-5.38	118.14	121.90
1	a	891	U	C2-N1-C1'	5.37	124.15	117.70
24	A	1104	C	C2-N1-C1'	5.37	124.71	118.80
24	A	2896	C	C5-C6-N1	5.37	123.69	121.00
24	A	1993	U	N1-C2-O2	5.37	126.56	122.80
1	a	500	G	C6-C5-N7	-5.37	127.18	130.40
1	a	1225	A	N1-C2-N3	-5.37	126.62	129.30
1	a	1432	G	OP2-P-O3'	5.37	117.01	105.20
1	a	603	U	C5-C6-N1	5.36	125.38	122.70
1	a	1399	C	N1-C2-O2	-5.36	115.68	118.90
24	A	2460	U	N1-C2-O2	5.36	126.56	122.80
24	A	672	C	C5-C6-N1	5.36	123.68	121.00
24	A	1956	U	N3-C2-O2	-5.35	118.45	122.20
24	A	2372	U	N1-C2-O2	5.35	126.55	122.80
24	A	2109	U	C5-C6-N1	5.35	125.38	122.70
24	A	2666	C	N1-C2-O2	5.35	122.11	118.90
24	A	2311	A	C5-N7-C8	5.35	106.57	103.90
1	a	1073	U	N3-C2-O2	-5.34	118.46	122.20
24	A	1407	G	C6-C5-N7	-5.34	127.19	130.40
24	A	1993	U	N3-C2-O2	-5.34	118.46	122.20
24	A	445	C	C6-N1-C2	-5.34	118.16	120.30
24	A	1026	G	C2-N3-C4	5.33	114.57	111.90
1	a	390	U	N3-C4-O4	5.33	123.13	119.40
24	A	2025	C	N1-C2-O2	5.33	122.10	118.90
24	A	456	C	C6-N1-C2	-5.33	118.17	120.30
24	A	335	C	C6-N1-C2	-5.33	118.17	120.30
24	A	1982	U	N3-C2-O2	-5.33	118.47	122.20
1	a	983	A	N3-C4-C5	-5.33	123.07	126.80
24	A	1102	C	N1-C2-O2	5.33	122.09	118.90
1	a	805	C	N1-C2-O2	5.32	122.09	118.90
1	a	1460	C	N1-C2-O2	5.32	122.09	118.90
24	A	1104	C	C2-N3-C4	5.32	122.56	119.90
1	a	23	C	C6-N1-C2	-5.32	118.17	120.30
1	a	1527	U	O5'-P-OP2	-5.32	100.92	105.70
24	A	2669	G	N1-C6-O6	-5.32	116.71	119.90
24	A	639	U	N3-C2-O2	-5.31	118.48	122.20
1	a	56	U	C5-C6-N1	5.31	125.36	122.70
1	a	540	G	C8-N9-C4	-5.31	104.28	106.40
1	a	1262	C	N3-C2-O2	-5.31	118.19	121.90
1	a	983	A	N3-C4-N9	5.31	131.65	127.40
1	a	883	C	N3-C2-O2	-5.30	118.19	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1371	G	C4-N9-C1'	-5.30	119.61	126.50
24	A	2220	U	N1-C2-O2	5.30	126.51	122.80
24	A	2794	C	C5-C6-N1	5.30	123.65	121.00
25	B	26	C	C6-N1-C2	-5.30	118.18	120.30
1	a	470	C	C5-C6-N1	5.29	123.64	121.00
1	a	529	G	OP2-P-O3'	5.29	116.84	105.20
24	A	1658	C	C5-C6-N1	5.29	123.65	121.00
1	a	1184	G	N3-C4-C5	-5.29	125.95	128.60
24	A	929	U	N3-C2-O2	-5.29	118.50	122.20
1	a	575	G	N3-C2-N2	-5.29	116.20	119.90
1	a	675	A	N7-C8-N9	5.29	116.44	113.80
22	v	41	C	C6-N1-C2	-5.29	118.19	120.30
24	A	1406	U	C5-C6-N1	5.29	125.34	122.70
24	A	1212	G	OP2-P-O3'	5.28	116.82	105.20
1	a	473	U	N3-C2-O2	-5.28	118.50	122.20
24	A	121	G	C6-C5-N7	-5.28	127.23	130.40
24	A	2075	U	C5-C6-N1	5.28	125.34	122.70
24	A	143	C	N1-C2-O2	5.28	122.07	118.90
1	a	78	A	N9-C4-C5	-5.28	103.69	105.80
24	A	327	G	C6-N1-C2	-5.28	121.93	125.10
24	A	2832	U	P-O3'-C3'	5.28	126.03	119.70
24	A	2337	G	N3-C4-C5	-5.28	125.96	128.60
1	a	27	G	C5-C6-O6	-5.27	125.44	128.60
7	g	110	ARG	N-CA-C	5.27	125.24	111.00
24	A	362	A	C2-N3-C4	5.27	113.24	110.60
1	a	188	C	N3-C2-O2	-5.27	118.21	121.90
24	A	2888	C	N3-C2-O2	-5.26	118.22	121.90
1	a	450	G	N3-C2-N2	-5.26	116.22	119.90
24	A	366	C	N1-C2-O2	5.25	122.05	118.90
24	A	998	C	C5-C6-N1	5.25	123.63	121.00
1	a	862	C	C6-N1-C2	-5.25	118.20	120.30
24	A	1830	C	C6-N1-C2	-5.25	118.20	120.30
24	A	2581	G	N3-C4-C5	-5.25	125.98	128.60
25	B	31	C	C2-N1-C1'	5.25	124.57	118.80
24	A	2645	G	C4-N9-C1'	5.25	133.32	126.50
25	B	73	A	C2-N3-C4	5.25	113.22	110.60
24	A	445	C	N3-C2-O2	-5.25	118.23	121.90
24	A	776	G	C6-C5-N7	-5.25	127.25	130.40
24	A	1894	C	N3-C2-O2	-5.24	118.23	121.90
1	a	971	G	C8-N9-C4	5.24	108.50	106.40
24	A	2093	G	C5-N7-C8	5.24	106.92	104.30
24	A	1921	G	N1-C6-O6	5.24	123.05	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	420	U	C5-C6-N1	5.24	125.32	122.70
24	A	2254	C	N3-C2-O2	-5.23	118.24	121.90
24	A	1200	C	C6-N1-C2	-5.23	118.21	120.30
24	A	1043	C	C5-C6-N1	5.22	123.61	121.00
24	A	1716	U	C6-N1-C2	-5.22	117.86	121.00
25	B	27	C	N3-C2-O2	-5.22	118.24	121.90
24	A	1782	U	C5-C6-N1	5.22	125.31	122.70
24	A	1151	A	N1-C2-N3	-5.22	126.69	129.30
1	a	810	C	C2-N1-C1'	5.22	124.54	118.80
24	A	1666	G	N1-C6-O6	-5.22	116.77	119.90
1	a	923	A	C5-N7-C8	-5.21	101.29	103.90
24	A	1788	C	C6-N1-C2	-5.21	118.21	120.30
24	A	2380	C	C6-N1-C2	-5.21	118.22	120.30
24	A	2395	C	C5-C6-N1	5.21	123.61	121.00
24	A	2558	C	C6-N1-C2	-5.21	118.21	120.30
24	A	1180	U	C2-N1-C1'	5.21	123.96	117.70
24	A	2592	G	C6-C5-N7	-5.21	127.27	130.40
6	f	54	LEU	CB-CG-CD1	5.21	119.85	111.00
24	A	2321	U	C5-C6-N1	-5.21	120.10	122.70
24	A	2818	U	N3-C2-O2	-5.21	118.56	122.20
24	A	2248	C	C5-C6-N1	5.20	123.60	121.00
1	a	236	A	C8-N9-C4	-5.20	103.72	105.80
1	a	496	A	C2-N3-C4	5.20	113.20	110.60
25	B	57	A	C8-N9-C4	-5.20	103.72	105.80
1	a	1349	A	O5'-P-OP1	-5.20	101.03	105.70
24	A	2200	C	N1-C2-O2	5.20	122.02	118.90
24	A	992	C	C6-N1-C2	-5.19	118.22	120.30
24	A	2870	C	C5-C6-N1	5.19	123.60	121.00
24	A	2779	U	O5'-P-OP2	-5.19	101.03	105.70
1	a	1245	C	C6-N1-C2	-5.19	118.22	120.30
1	a	1142	G	N3-C2-N2	5.19	123.53	119.90
24	A	139	U	C6-N1-C2	-5.19	117.89	121.00
24	A	1725	U	N3-C2-O2	-5.19	118.57	122.20
24	A	2348	U	N3-C2-O2	-5.19	118.57	122.20
24	A	2128	G	N1-C6-O6	5.18	123.01	119.90
1	a	1497	G	C6-C5-N7	5.18	133.51	130.40
22	v	51	C	C6-N1-C2	-5.18	118.23	120.30
24	A	121	G	N9-C4-C5	-5.18	103.33	105.40
24	A	1023	U	N3-C2-O2	-5.18	118.58	122.20
24	A	1103	A	OP1-P-O3'	5.18	116.59	105.20
1	a	1190	G	OP2-P-O3'	5.17	116.58	105.20
24	A	247	G	C5-N7-C8	5.17	106.89	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	27	G	N1-C6-O6	5.17	123.00	119.90
1	a	1142	G	C6-C5-N7	-5.17	127.30	130.40
1	a	1144	G	C8-N9-C4	-5.17	104.33	106.40
24	A	543	G	C5-C6-O6	-5.17	125.50	128.60
1	a	610	U	N1-C2-O2	5.17	126.42	122.80
1	a	1203	C	O5'-P-OP2	-5.17	101.05	105.70
24	A	435	C	N3-C2-O2	-5.17	118.28	121.90
24	A	2214	C	C6-N1-C2	-5.17	118.23	120.30
2	b	18	GLN	N-CA-CB	-5.17	101.30	110.60
24	A	1455	G	C6-C5-N7	-5.16	127.30	130.40
24	A	2101	A	N7-C8-N9	5.16	116.38	113.80
24	A	1461	C	N1-C2-O2	5.16	122.00	118.90
24	A	1935	G	OP2-P-O3'	5.16	116.55	105.20
1	a	1474	U	C5-C6-N1	5.16	125.28	122.70
25	B	71	C	C6-N1-C2	-5.16	118.24	120.30
1	a	1228	C	C5-C6-N1	5.15	123.58	121.00
24	A	293	U	N3-C2-O2	-5.15	118.59	122.20
24	A	2805	C	C6-N1-C2	-5.15	118.24	120.30
24	A	2636	C	N1-C2-O2	5.15	121.99	118.90
24	A	2669	G	N3-C2-N2	-5.15	116.29	119.90
24	A	1303	G	C6-C5-N7	-5.15	127.31	130.40
1	a	1147	C	N3-C2-O2	-5.15	118.30	121.90
24	A	2297	A	C2-N3-C4	5.15	113.17	110.60
24	A	2596	U	N3-C2-O2	-5.15	118.60	122.20
24	A	908	C	C6-N1-C2	-5.14	118.24	120.30
24	A	1487	U	N3-C2-O2	-5.14	118.60	122.20
24	A	2141	G	C8-N9-C4	-5.14	104.34	106.40
24	A	2231	U	C5-C6-N1	5.14	125.27	122.70
24	A	2667	C	N1-C2-O2	5.14	121.99	118.90
22	v	56	C	C2-N1-C1'	5.14	124.45	118.80
24	A	1233	C	C6-N1-C2	-5.14	118.24	120.30
24	A	543	G	C6-C5-N7	-5.14	127.32	130.40
1	a	1486	G	N3-C4-N9	5.14	129.08	126.00
24	A	2214	C	N1-C2-O2	5.14	121.98	118.90
24	A	2720	U	N1-C2-O2	5.13	126.39	122.80
1	a	381	C	C6-N1-C2	-5.13	118.25	120.30
1	a	450	G	N9-C4-C5	5.13	107.45	105.40
24	A	1236	G	P-O3'-C3'	5.13	125.86	119.70
1	a	476	U	N3-C2-O2	-5.13	118.61	122.20
1	a	737	C	N3-C4-N4	5.13	121.59	118.00
23	x	123	C	N1-C2-O2	5.13	121.98	118.90
24	A	639	U	N1-C2-O2	5.13	126.39	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1325	C	C6-N1-C2	-5.12	118.25	120.30
24	A	51	G	C8-N9-C4	-5.12	104.35	106.40
1	a	355	C	N1-C2-O2	5.12	121.97	118.90
1	a	524	G	C6-C5-N7	-5.12	127.33	130.40
24	A	1022	G	N3-C4-N9	-5.12	122.93	126.00
24	A	1348	C	N3-C2-O2	-5.12	118.31	121.90
1	a	1382	C	N3-C2-O2	-5.12	118.31	121.90
1	a	1521	C	C6-N1-C2	-5.12	118.25	120.30
24	A	2802	G	C6-N1-C2	-5.12	122.03	125.10
24	A	1323	C	C6-N1-C2	-5.12	118.25	120.30
24	A	610	C	N1-C2-O2	5.11	121.97	118.90
24	A	2025	C	C5-C6-N1	5.11	123.56	121.00
24	A	2867	G	OP2-P-O3'	5.11	116.45	105.20
24	A	420	C	C6-N1-C2	-5.11	118.26	120.30
1	a	1259	C	N1-C2-O2	5.11	121.97	118.90
24	A	2342	C	C5-C6-N1	5.11	123.55	121.00
1	a	316	C	C6-N1-C2	-5.10	118.26	120.30
1	a	386	C	N3-C2-O2	-5.10	118.33	121.90
24	A	1695	G	N3-C4-N9	5.10	129.06	126.00
1	a	1003	G	C6-N1-C2	-5.10	122.04	125.10
22	v	51	C	N1-C2-O2	5.10	121.96	118.90
24	A	1303	G	N3-C4-N9	5.10	129.06	126.00
24	A	2065	C	C5-C6-N1	5.10	123.55	121.00
24	A	484	C	C2-N3-C4	5.09	122.45	119.90
24	A	2395	C	C6-N1-C2	-5.09	118.26	120.30
24	A	266	G	N3-C4-N9	5.09	129.06	126.00
24	A	1446	C	C6-N1-C2	-5.09	118.26	120.30
1	a	390	U	C5-C4-O4	-5.09	122.85	125.90
24	A	1053	C	C5-C6-N1	5.09	123.55	121.00
24	A	2637	U	N1-C2-O2	5.09	126.36	122.80
24	A	1376	C	N1-C2-O2	5.09	121.95	118.90
1	a	1493[A]	A	OP2-P-O3'	5.08	116.39	105.20
1	a	1493[C]	A	OP2-P-O3'	5.08	116.39	105.20
24	A	669	G	C8-N9-C4	-5.08	104.37	106.40
1	a	413	G	C6-C5-N7	5.08	133.45	130.40
1	a	1225	A	N3-C4-C5	-5.08	123.24	126.80
24	A	2774	C	N1-C2-O2	5.08	121.95	118.90
1	a	396	C	C6-N1-C2	-5.07	118.27	120.30
1	a	1235	U	C5-C4-O4	-5.07	122.86	125.90
24	A	2782	G	C4-C5-N7	5.07	112.83	110.80
24	A	1627	G	N3-C4-N9	5.07	129.04	126.00
24	A	2043	C	C6-N1-C2	-5.07	118.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1134	G	C5-C6-O6	-5.07	125.56	128.60
24	A	911	A	N7-C8-N9	5.07	116.33	113.80
22	v	28	C	N1-C2-O2	5.06	121.94	118.90
24	A	234	U	N3-C2-O2	-5.06	118.66	122.20
24	A	1629	U	N1-C2-N3	5.06	117.94	114.90
24	A	2651	C	C6-N1-C2	-5.06	118.28	120.30
24	A	717	C	C6-N1-C2	-5.06	118.28	120.30
24	A	1313	U	C5-C6-N1	5.06	125.23	122.70
1	a	496	A	C8-N9-C4	-5.06	103.78	105.80
24	A	946	C	N1-C2-O2	5.05	121.93	118.90
24	A	2755	C	N3-C2-O2	-5.05	118.36	121.90
24	A	2756	U	OP1-P-O3'	5.05	116.31	105.20
1	a	459	A	N1-C2-N3	-5.05	126.78	129.30
1	a	699	C	C6-N1-C2	-5.05	118.28	120.30
24	A	2456	C	C5-C6-N1	5.05	123.52	121.00
24	A	1931	U	C2-N1-C1'	5.05	123.75	117.70
1	a	89	U	C2-N1-C1'	5.04	123.75	117.70
1	a	1072	G	N3-C2-N2	5.04	123.43	119.90
1	a	87	C	C2-N3-C4	5.04	122.42	119.90
1	a	1473	G	N1-C6-O6	-5.04	116.88	119.90
24	A	2888	C	N1-C2-O2	5.04	121.92	118.90
36	M	20	LEU	CA-CB-CG	5.04	126.89	115.30
24	A	177	G	C8-N9-C4	-5.04	104.38	106.40
24	A	158	U	N1-C2-O2	5.04	126.33	122.80
24	A	2149	U	N1-C2-O2	5.04	126.33	122.80
24	A	2297	A	C5-C6-N1	-5.03	115.18	117.70
1	a	254	G	O5'-P-OP1	-5.03	101.17	105.70
1	a	1144	G	N7-C8-N9	5.03	115.61	113.10
24	A	512	G	O5'-P-OP2	-5.03	101.17	105.70
24	A	1314	C	N3-C4-N4	5.03	121.52	118.00
24	A	2579	C	C5-C6-N1	5.03	123.52	121.00
24	A	2782	G	C5-C6-O6	-5.03	125.58	128.60
24	A	618	G	N3-C4-C5	-5.03	126.08	128.60
24	A	2074	U	C6-N1-C2	-5.03	117.98	121.00
24	A	2177	C	C5-C6-N1	5.03	123.51	121.00
1	a	103	U	N3-C2-O2	-5.03	118.68	122.20
21	u	34	ARG	NE-CZ-NH1	5.03	122.81	120.30
24	A	2180	U	C5-C6-N1	5.02	125.21	122.70
1	a	283	U	N1-C2-O2	5.02	126.31	122.80
1	a	1184	G	C2-N3-C4	5.02	114.41	111.90
1	a	271	C	C5-C6-N1	5.02	123.51	121.00
24	A	359	G	N3-C2-N2	-5.02	116.39	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2129	C	C6-N1-C2	-5.02	118.29	120.30
24	A	1774	C	C6-N1-C2	-5.02	118.29	120.30
24	A	2745	C	N3-C2-O2	-5.02	118.39	121.90
24	A	1169	A	C5-C6-N1	5.01	120.21	117.70
24	A	2767	C	N1-C2-O2	5.01	121.91	118.90
1	a	754	C	C6-N1-C2	-5.01	118.30	120.30
24	A	2393	U	N3-C2-O2	-5.01	118.69	122.20
24	A	2645	G	O4'-C1'-N9	5.00	112.20	108.20
24	A	2391	G	P-O3'-C3'	5.00	125.70	119.70
1	a	1356	G	N9-C4-C5	-5.00	103.40	105.40
24	A	640	C	C5-C6-N1	5.00	123.50	121.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
24	A	2069	G7M	C4',C3'

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	0	1	ALA	Mainchain,Peptide
51	1	3	GLY	Mainchain
53	3	30	HIS	Peptide
26	C	120	ASP	Peptide
28	E	82	GLY	Peptide
30	G	117	PRO	Mainchain
30	G	118	ALA	Mainchain
30	G	173	ALA	Mainchain
32	H	2	GLN	Peptide
32	H	8	LYS	Peptide
34	K	34	GLY	Peptide
34	K	89	ASN	Mainchain
34	K	92	GLU	Mainchain
35	L	110	VAL	Mainchain
35	L	28	GLY	Mainchain
35	L	29	LYS	Mainchain
35	L	35	HIS	Mainchain
42	S	64	ALA	Mainchain
44	U	50	ALA	Peptide
44	U	87	GLU	Mainchain,Peptide
48	Y	24	GLU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain,Peptide
2	b	72	LYS	Peptide
5	e	121	ASN	Peptide
5	e	76	ASN	Peptide
5	e	88	HIS	Peptide
5	e	92	ARG	Peptide
6	f	52	ASN	Mainchain
7	g	109	LYS	Mainchain,Peptide
8	h	46	GLU	Mainchain
9	i	56	MET	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Mainchain
10	j	57	VAL	Mainchain
10	j	91	ASP	Mainchain
10	j	92	LEU	Mainchain
12	l	100	ALA	Peptide
13	m	3	ILE	Peptide
16	p	43	ALA	Peptide
17	q	48	GLU	Mainchain
17	q	68	LYS	Peptide
18	r	10	CYS	Peptide
18	r	11	ARG	Mainchain
18	r	16	GLY	Peptide
19	s	3	SER	Peptide
21	u	8	ASN	Mainchain

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	b	216/218 (99%)	189 (88%)	23 (11%)	4 (2%)	8 42
3	c	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	29 68
4	d	203/205 (99%)	187 (92%)	14 (7%)	2 (1%)	15 55
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	4 31
6	f	98/100 (98%)	82 (84%)	10 (10%)	6 (6%)	1 17
7	g	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	7 41
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19 59
9	i	125/127 (98%)	104 (83%)	15 (12%)	6 (5%)	2 22
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3 25
11	k	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	5 35
12	l	121/123 (98%)	98 (81%)	14 (12%)	9 (7%)	1 13
13	m	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5 35
14	n	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	7 41
15	o	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	6 38
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	3 27
17	q	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	5 35
18	r	63/65 (97%)	57 (90%)	2 (3%)	4 (6%)	1 17
19	s	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12 50
20	t	83/85 (98%)	77 (93%)	6 (7%)	0	100 100
21	u	63/65 (97%)	50 (79%)	9 (14%)	4 (6%)	1 17
26	C	269/271 (99%)	246 (91%)	20 (7%)	3 (1%)	14 53
27	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	29 68
28	E	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	10 47
29	F	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	6 38
30	G	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	3 31
31	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6 39
32	H	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	5 35
33	J	140/142 (99%)	136 (97%)	4 (3%)	0	100 100
34	K	120/122 (98%)	105 (88%)	10 (8%)	5 (4%)	3 25
35	L	141/143 (99%)	129 (92%)	9 (6%)	3 (2%)	7 40
36	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6 39
37	N	118/120 (98%)	106 (90%)	12 (10%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	O	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	8 43
39	P	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	17 57
40	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100 100
41	R	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	7 41
42	S	108/110 (98%)	102 (94%)	6 (6%)	0	100 100
43	T	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	4 31
44	U	100/102 (98%)	89 (89%)	6 (6%)	5 (5%)	2 21
45	V	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
46	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	11 48
47	X	75/77 (97%)	71 (95%)	4 (5%)	0	100 100
48	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
49	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100 100
50	0	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	8 42
51	1	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7 40
52	2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 38
53	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9 46
54	4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5 34
55	6	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	9 46
All	All	5717/5817 (98%)	5150 (90%)	447 (8%)	120 (2%)	10 40

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	73	ARG
4	d	192	ALA
5	e	77	ASN
5	e	89	THR
5	e	122	VAL
5	e	158	LYS
6	f	53	LYS
6	f	54	LEU
6	f	86	ARG
7	g	110	ARG
8	h	47	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	90	ASP
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	65	GLU
15	o	46	LYS
16	p	44	SER
16	p	79	ASN
17	q	49	ASN
17	q	69	THR
18	r	11	ARG
18	r	17	VAL
19	s	4	LEU
21	u	8	ASN
21	u	34	ARG
21	u	37	TYR
26	C	121	ALA
26	C	204	LEU
28	E	83	VAL
29	F	174	PHE
30	G	46	ASP
30	G	108	PHE
30	G	118	ALA
30	G	174	LYS
32	H	9	VAL
34	K	92	GLU
35	L	29	LYS
35	L	36	LYS
35	L	111	ILE
38	O	63	LYS
44	U	6	ARG
44	U	51	LEU
44	U	88	ASP
50	0	2	VAL
51	1	4	ILE
53	3	31	ILE
5	e	93	VAL
7	g	29	LEU
7	g	95	ARG
9	i	57	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	125	GLN
10	j	42	LEU
11	k	88	PRO
12	l	75	GLU
13	m	4	ALA
13	m	6	ILE
14	n	2	LYS
29	F	20	ASN
30	G	45	ALA
32	H	3	VAL
32	H	11	ASN
32	H	41	LYS
34	K	35	VAL
34	K	110	GLU
36	M	58	LYS
36	M	70	ASP
41	R	54	VAL
41	R	55	ASP
43	T	38	ALA
43	T	52	GLU
55	6	3	LYS
9	i	12	LYS
9	i	122	ARG
14	n	34	ASN
16	p	43	ALA
18	r	18	GLN
26	C	52	HIS
27	D	149	ASN
28	E	184	ASP
31	I	22	PRO
36	M	14	LYS
43	T	88	LYS
44	U	39	ASN
46	W	17	LEU
54	4	37	GLN
3	c	96	VAL
4	d	191	SER
6	f	92	THR
6	f	99	ALA
12	l	2	THR
12	l	23	LEU
12	l	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	l	46	SER
12	l	77	SER
12	l	88	ASP
15	o	27	GLN
18	r	46	THR
21	u	65	ARG
29	F	149	ARG
29	F	176	PHE
34	K	109	SER
6	f	93	LYS
28	E	122	GLU
30	G	109	SER
31	I	20	SER
38	O	34	HIS
39	P	86	LYS
52	2	23	ALA
34	K	93	GLN
9	i	71	ILE
44	U	54	PRO
11	k	90	PRO
12	l	41	PRO
2	b	28	PRO
31	I	92	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	b	180/180 (100%)	178 (99%)	2 (1%)	73 88
3	c	170/170 (100%)	170 (100%)	0	100 100
4	d	172/172 (100%)	171 (99%)	1 (1%)	86 94
5	e	119/119 (100%)	119 (100%)	0	100 100
6	f	87/87 (100%)	87 (100%)	0	100 100
7	g	124/124 (100%)	124 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	88
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	78 (99%)	1 (1%)	69	86
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	64 (98%)	1 (2%)	65	84
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
26	C	216/216 (100%)	215 (100%)	1 (0%)	88	95
27	D	164/164 (100%)	164 (100%)	0	100	100
28	E	165/165 (100%)	165 (100%)	0	100	100
29	F	148/148 (100%)	148 (100%)	0	100	100
30	G	137/137 (100%)	137 (100%)	0	100	100
31	I	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	J	116/116 (100%)	116 (100%)	0	100	100
34	K	103/103 (100%)	102 (99%)	1 (1%)	76	88
35	L	102/102 (100%)	101 (99%)	1 (1%)	76	88
36	M	109/109 (100%)	109 (100%)	0	100	100
37	N	100/100 (100%)	100 (100%)	0	100	100
38	O	86/86 (100%)	86 (100%)	0	100	100
39	P	99/99 (100%)	99 (100%)	0	100	100
40	Q	89/89 (100%)	89 (100%)	0	100	100
41	R	84/84 (100%)	84 (100%)	0	100	100
42	S	93/93 (100%)	93 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	T	80/80 (100%)	80 (100%)	0	100 100
44	U	83/83 (100%)	83 (100%)	0	100 100
45	V	78/78 (100%)	78 (100%)	0	100 100
46	W	57/57 (100%)	57 (100%)	0	100 100
47	X	67/67 (100%)	66 (98%)	1 (2%)	65 84
48	Y	55/55 (100%)	55 (100%)	0	100 100
49	Z	48/48 (100%)	48 (100%)	0	100 100
50	0	47/47 (100%)	46 (98%)	1 (2%)	53 78
51	1	45/45 (100%)	45 (100%)	0	100 100
52	2	38/38 (100%)	38 (100%)	0	100 100
53	3	51/51 (100%)	51 (100%)	0	100 100
54	4	34/34 (100%)	34 (100%)	0	100 100
55	6	59/59 (100%)	59 (100%)	0	100 100
All	All	4728/4751 (100%)	4717 (100%)	11 (0%)	93 98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	176	ASN
2	b	178	LEU
4	d	173	ASP
12	l	33	CYS
14	n	34	ASN
16	p	2	VAL
26	C	52	HIS
34	K	21	CYS
35	L	27	LEU
47	X	4	CYS
50	0	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	40	GLN
3	c	122	GLN
8	h	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	31	GLN
12	l	72	ASN
16	p	26	ASN
20	t	12	GLN
26	C	44	ASN
27	D	49	GLN
30	G	21	GLN
35	L	38	GLN
35	L	99	ASN
37	N	62	ASN
37	N	81	ASN
44	U	39	ASN
54	4	35	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1531/1539 (99%)	260 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	21 (44%)	0
24	A	2893/2903 (99%)	540 (18%)	34 (1%)
25	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4666/4687 (99%)	853 (18%)	37 (0%)

All (853) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	59	A
1	a	61	G
1	a	69	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	85	U
1	a	86	G
1	a	88	U
1	a	92	U
1	a	94	G
1	a	95	C
1	a	116	A
1	a	121	U
1	a	122	G
1	a	126	G
1	a	127	G
1	a	128	G
1	a	131	A
1	a	134	G
1	a	141	G
1	a	144	G
1	a	149	A
1	a	173	U
1	a	183	C
1	a	184	G
1	a	189	A
1	a	195	A
1	a	197	A
1	a	207	C
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	280	C
1	a	281	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	289	G
1	a	300	A
1	a	306	A
1	a	316	C
1	a	328	C
1	a	329	A
1	a	330	C
1	a	345	C
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	376	G
1	a	388	G
1	a	398	U
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	429	U
1	a	439	U
1	a	441	A
1	a	446	G
1	a	448	A
1	a	467	U
1	a	468	A
1	a	474	G
1	a	479	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A
1	a	497	G
1	a	499	A
1	a	505	G
1	a	509	A
1	a	511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	528	C
1	a	529	G
1	a	531	U
1	a	532	A
1	a	547	A
1	a	548	G
1	a	559	A
1	a	562	U
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	615	G
1	a	633	G
1	a	639	G
1	a	653	U
1	a	654	G
1	a	665	A
1	a	687	A
1	a	695	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	777	A
1	a	787	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	810	C
1	a	815	A
1	a	817	C
1	a	818	G
1	a	820	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	821	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	849	G
1	a	872	A
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	933	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	983	A
1	a	989	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1036	A
1	a	1042	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1050	G
1	a	1053	G
1	a	1054	C
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1100	C
1	a	1101	A
1	a	1130	A
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1145	A
1	a	1146	A
1	a	1151	A
1	a	1152	A
1	a	1158	C
1	a	1159	U
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1196	A
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1239	A
1	a	1240	U
1	a	1241	G
1	a	1253	G
1	a	1258	G
1	a	1260	G
1	a	1280	A
1	a	1281	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1287	A
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1303	C
1	a	1305	G
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1353	G
1	a	1360	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1398	A
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1440	U
1	a	1441	A
1	a	1446	A
1	a	1452	C
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1537	U
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	17(A)	U
22	v	18	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	v	19	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	47	U
22	v	48	C
22	v	58	A
22	v	75	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	91	A
23	x	93	G
23	x	96	C
23	x	98	U
23	x	99	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	115	A
23	x	117	C
23	x	118	G
23	x	120	U
23	x	121	U
23	x	126	G
23	x	127	U
23	x	129	U
23	x	130	G
23	x	134	C
24	A	10	A
24	A	14	A
24	A	34	U
24	A	35	G
24	A	43	G
24	A	45	G
24	A	46	G
24	A	50	U
24	A	51	G
24	A	52	A
24	A	63	A
24	A	71	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	73	A
24	A	74	A
24	A	75	G
24	A	84	A
24	A	92	U
24	A	96	C
24	A	98	G
24	A	102	U
24	A	103	A
24	A	114	U
24	A	118	A
24	A	119	A
24	A	120	U
24	A	131	A
24	A	138	U
24	A	139	U
24	A	141	G
24	A	142	A
24	A	161	A
24	A	162	U
24	A	163	C
24	A	165	A
24	A	178	G
24	A	196	A
24	A	204	A
24	A	205	G
24	A	206	U
24	A	215	G
24	A	216	A
24	A	221	A
24	A	222	A
24	A	228	C
24	A	229	C
24	A	241	A
24	A	245	G
24	A	247	G
24	A	248	G
24	A	250	G
24	A	255	A
24	A	266	G
24	A	276	U
24	A	277	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	278	A
24	A	281	C
24	A	282	A
24	A	285	G
24	A	294	A
24	A	295	G
24	A	310	A
24	A	317	G
24	A	322	A
24	A	323	C
24	A	329	G
24	A	330	A
24	A	346	A
24	A	349	U
24	A	359	G
24	A	361	G
24	A	362	A
24	A	371	A
24	A	372	G
24	A	373	U
24	A	386	G
24	A	387	U
24	A	404	A
24	A	406	G
24	A	411	G
24	A	412	A
24	A	424	G
24	A	456	C
24	A	457	A
24	A	481	G
24	A	490	C
24	A	491	G
24	A	496	G
24	A	504	A
24	A	505	A
24	A	509	C
24	A	510	C
24	A	513	A
24	A	522	A
24	A	527	C
24	A	529	A
24	A	531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	532	A
24	A	533	G
24	A	544	C
24	A	545	U
24	A	549	G
24	A	556	A
24	A	563	A
24	A	573	U
24	A	575	A
24	A	588	U
24	A	592	A
24	A	603	A
24	A	613	A
24	A	614	A
24	A	627	A
24	A	632	A
24	A	637	A
24	A	645	C
24	A	646	U
24	A	647	G
24	A	654	A
24	A	655	A
24	A	656	G
24	A	669	G
24	A	677	A
24	A	686	U
24	A	690	G
24	A	694	U
24	A	695	G
24	A	699	A
24	A	714	U
24	A	729	G
24	A	730	A
24	A	746	PSU
24	A	747	5MU
24	A	752	A
24	A	764	A
24	A	774	G
24	A	775	G
24	A	776	G
24	A	782	A
24	A	784	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	785	G
24	A	805	G
24	A	812	C
24	A	819	A
24	A	827	U
24	A	828	U
24	A	844	A
24	A	845	A
24	A	846	U
24	A	858	G
24	A	859	G
24	A	869	G
24	A	878	A
24	A	884	U
24	A	886	A
24	A	892	A
24	A	896	A
24	A	897	C
24	A	910	A
24	A	941	A
24	A	944	C
24	A	945	A
24	A	946	C
24	A	961	C
24	A	962	G
24	A	974	G
24	A	983	A
24	A	985	C
24	A	990	A
24	A	995	C
24	A	996	A
24	A	1003	G
24	A	1012	U
24	A	1013	C
24	A	1021	A
24	A	1022	G
24	A	1023	U
24	A	1026	G
24	A	1033	U
24	A	1040	A
24	A	1046	A
24	A	1053	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	1054	A
24	A	1060	U
24	A	1061	U
24	A	1062	G
24	A	1064	C
24	A	1065	U
24	A	1066	U
24	A	1067	A
24	A	1068	G
24	A	1069	A
24	A	1070	A
24	A	1071	G
24	A	1072	C
24	A	1073	A
24	A	1075	C
24	A	1076	C
24	A	1077	A
24	A	1079	C
24	A	1084	A
24	A	1087	G
24	A	1088	A
24	A	1097	U
24	A	1104	C
24	A	1111	A
24	A	1112	G
24	A	1116	G
24	A	1119	U
24	A	1130	U
24	A	1131	G
24	A	1132	U
24	A	1135	C
24	A	1136	G
24	A	1142	A
24	A	1143	A
24	A	1151	A
24	A	1165	A
24	A	1172	C
24	A	1174	U
24	A	1175	A
24	A	1178	C
24	A	1179	G
24	A	1180	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	1183	U
24	A	1205	A
24	A	1206	G
24	A	1210	G
24	A	1212	G
24	A	1213	A
24	A	1221	C
24	A	1237	A
24	A	1247	A
24	A	1248	G
24	A	1250	G
24	A	1251	C
24	A	1253	A
24	A	1256	G
24	A	1270	C
24	A	1271	G
24	A	1272	A
24	A	1273	U
24	A	1300	G
24	A	1301	A
24	A	1306	C
24	A	1311	G
24	A	1313	U
24	A	1314	C
24	A	1325	U
24	A	1332	G
24	A	1341	G
24	A	1345	C
24	A	1359	A
24	A	1365	A
24	A	1368	G
24	A	1378	A
24	A	1379	U
24	A	1383	A
24	A	1386	C
24	A	1395	A
24	A	1396	U
24	A	1403	A
24	A	1407	G
24	A	1414	C
24	A	1416	G
24	A	1421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	1428	C
24	A	1437	C
24	A	1454	C
24	A	1458	U
24	A	1459	G
24	A	1461	C
24	A	1475	G
24	A	1482	G
24	A	1490	A
24	A	1493	C
24	A	1498	C
24	A	1504	A
24	A	1509	A
24	A	1515	A
24	A	1523	U
24	A	1524	G
24	A	1529	G
24	A	1533	C
24	A	1534	U
24	A	1535	A
24	A	1536	C
24	A	1537	G
24	A	1559	U
24	A	1560	G
24	A	1565	C
24	A	1568	G
24	A	1569	A
24	A	1578	U
24	A	1584	U
24	A	1614	A
24	A	1616	A
24	A	1633	G
24	A	1634	A
24	A	1643	G
24	A	1647	U
24	A	1648	U
24	A	1649	G
24	A	1674	G
24	A	1695	G
24	A	1698	A
24	A	1703	G
24	A	1713	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	1715	G
24	A	1718	G
24	A	1729	U
24	A	1730	C
24	A	1738	G
24	A	1757	A
24	A	1758	U
24	A	1764	C
24	A	1773	A
24	A	1780	A
24	A	1782	U
24	A	1784	A
24	A	1785	A
24	A	1791	A
24	A	1800	C
24	A	1801	A
24	A	1808	A
24	A	1809	A
24	A	1816	C
24	A	1829	A
24	A	1833	C
24	A	1847	A
24	A	1857	G
24	A	1870	C
24	A	1884	G
24	A	1891	G
24	A	1901	A
24	A	1906	G
24	A	1907	G
24	A	1914	C
24	A	1929	G
24	A	1930	G
24	A	1931	U
24	A	1936	A
24	A	1937	A
24	A	1939	5MU
24	A	1940	U
24	A	1941	C
24	A	1943	U
24	A	1955	U
24	A	1964	G
24	A	1967	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	1970	A
24	A	1971	U
24	A	1972	G
24	A	1991	U
24	A	1993	U
24	A	1997	C
24	A	2022	U
24	A	2023	C
24	A	2031	A
24	A	2033	A
24	A	2036	C
24	A	2043	C
24	A	2049	G
24	A	2055	C
24	A	2056	G
24	A	2059	A
24	A	2060	A
24	A	2061	G
24	A	2062	A
24	A	2069	G7M
24	A	2070	A
24	A	2072	C
24	A	2077	A
24	A	2080	A
24	A	2093	G
24	A	2096	C
24	A	2100	G
24	A	2108	A
24	A	2110	G
24	A	2111	U
24	A	2112	G
24	A	2113	U
24	A	2117	A
24	A	2118	U
24	A	2119	A
24	A	2120	G
24	A	2125	G
24	A	2127	G
24	A	2130	U
24	A	2132	U
24	A	2133	G
24	A	2134	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	2137	U
24	A	2145	C
24	A	2146	C
24	A	2147	A
24	A	2154	A
24	A	2158	A
24	A	2162	G
24	A	2163	A
24	A	2164	C
24	A	2166	U
24	A	2167	U
24	A	2168	G
24	A	2169	A
24	A	2170	A
24	A	2171	A
24	A	2172	U
24	A	2173	A
24	A	2178	C
24	A	2189	U
24	A	2198	A
24	A	2199	A
24	A	2204	G
24	A	2211	A
24	A	2214	C
24	A	2220	U
24	A	2223	G
24	A	2225	A
24	A	2238	G
24	A	2239	G
24	A	2250	G
24	A	2268	A
24	A	2279	G
24	A	2283	C
24	A	2286	G
24	A	2287	A
24	A	2288	A
24	A	2294	G
24	A	2298	A
24	A	2305	U
24	A	2309	A
24	A	2310	C
24	A	2319	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	2322	A
24	A	2331	G
24	A	2333	A
24	A	2335	A
24	A	2347	C
24	A	2350	C
24	A	2354	C
24	A	2357	G
24	A	2383	G
24	A	2385	C
24	A	2389	G
24	A	2392	A
24	A	2402	U
24	A	2403	C
24	A	2406	A
24	A	2407	A
24	A	2429	G
24	A	2430	A
24	A	2431	U
24	A	2441	U
24	A	2448	A
24	A	2464	G
24	A	2468	A
24	A	2475	C
24	A	2476	A
24	A	2480	C
24	A	2484	G
24	A	2491	U
24	A	2494	G
24	A	2498	OMC
24	A	2501	C
24	A	2502	G
24	A	2504	PSU
24	A	2505	G
24	A	2506	U
24	A	2513	A
24	A	2518	A
24	A	2520	C
24	A	2525	G
24	A	2535	G
24	A	2547	A
24	A	2548	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	2554	U
24	A	2567	G
24	A	2569	G
24	A	2572	A
24	A	2573	C
24	A	2578	G
24	A	2582	G
24	A	2585	U
24	A	2586	U
24	A	2602	A
24	A	2603	G
24	A	2609	U
24	A	2610	C
24	A	2611	C
24	A	2613	U
24	A	2615	U
24	A	2621	G
24	A	2629	U
24	A	2636	C
24	A	2646	C
24	A	2656	U
24	A	2685	G
24	A	2689	U
24	A	2690	U
24	A	2714	G
24	A	2718	G
24	A	2720	U
24	A	2726	A
24	A	2729	G
24	A	2733	A
24	A	2739	U
24	A	2744	G
24	A	2748	A
24	A	2751	G
24	A	2757	A
24	A	2764	A
24	A	2765	A
24	A	2766	A
24	A	2769	U
24	A	2778	A
24	A	2779	U
24	A	2790	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	A	2791	G
24	A	2793	C
24	A	2794	C
24	A	2797	U
24	A	2798	U
24	A	2799	A
24	A	2800	A
24	A	2801	G
24	A	2803	G
24	A	2808	G
24	A	2818	U
24	A	2820	A
24	A	2821	A
24	A	2833	U
24	A	2834	G
24	A	2849	U
24	A	2867	G
24	A	2868	A
24	A	2872	A
24	A	2873	A
24	A	2880	C
24	A	2883	A
24	A	2885	G
24	A	2891	U
25	B	4	C
25	B	13	G
25	B	16	G
25	B	25	U
25	B	30	C
25	B	35	C
25	B	41	G
25	B	44	G
25	B	57	A
25	B	67	G
25	B	68	C
25	B	73	A
25	B	89	U
25	B	90	C
25	B	96	G
25	B	108	A
25	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	51	G
24	A	91	A
24	A	205	G
24	A	228	C
24	A	385	C
24	A	512	G
24	A	555	G
24	A	572	A
24	A	774	G
24	A	830	G
24	A	989	G
24	A	1020	A
24	A	1070	A
24	A	1111	A
24	A	1182	G
24	A	1190	G
24	A	1211	C
24	A	1212	G
24	A	1251	C
24	A	1432	G
24	A	1458	U
24	A	1567	G
24	A	1930	G
24	A	1940	U
24	A	2061	G
24	A	2308	G
24	A	2391	G
24	A	2447	G
24	A	2566	A
24	A	2610	C
24	A	2756	U
24	A	2820	A
24	A	2832	U
24	A	2867	G
25	B	3	C
25	B	66	A
25	B	88	C

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

39 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	OMU	A	2552	24	19,22,23	1.23	2 (10%)	26,31,34	1.94	7 (26%)
24	PSU	A	746	24	18,21,22	1.34	2 (11%)	22,30,33	1.74	4 (18%)
24	PSU	A	2504	24	18,21,22	1.44	3 (16%)	22,30,33	1.84	3 (13%)
24	3TD	A	1915	24	18,22,23	4.06	7 (38%)	22,32,35	1.79	3 (13%)
24	2MA	A	2503	24	17,25,26	1.00	1 (5%)	17,37,40	0.96	2 (11%)
1	5MC	a	967	1	18,22,23	0.92	2 (11%)	26,32,35	1.10	3 (11%)
24	OMG	A	2251	22,24	18,26,27	1.01	1 (5%)	19,38,41	1.19	2 (10%)
22	4SU	v	8	22	18,21,22	1.80	4 (22%)	26,30,33	2.35	5 (19%)
22	5MU	v	54	22	19,22,23	1.40	6 (31%)	28,32,35	2.05	6 (21%)
24	PSU	A	955	24	18,21,22	1.42	4 (22%)	22,30,33	1.94	3 (13%)
1	MA6	a	1519	1	19,26,27	0.93	1 (5%)	18,38,41	1.89	4 (22%)
1	MA6	a	1518	1	19,26,27	0.99	1 (5%)	18,38,41	1.74	4 (22%)
24	PSU	A	2580	24	18,21,22	1.51	3 (16%)	22,30,33	1.94	3 (13%)
1	2MG	a	1207	1	18,26,27	1.02	1 (5%)	16,38,41	1.04	2 (12%)
24	PSU	A	2604	24	18,21,22	1.48	3 (16%)	22,30,33	1.84	4 (18%)
24	5MU	A	1939	24	19,22,23	1.45	4 (21%)	28,32,35	2.18	5 (17%)
24	OMC	A	2498	24	19,22,23	0.88	1 (5%)	26,31,34	1.13	2 (7%)
1	UR3	a	1498	1	19,22,23	1.13	2 (10%)	26,32,35	2.06	5 (19%)
24	2MG	A	2445	24	18,26,27	0.98	1 (5%)	16,38,41	1.19	3 (18%)
24	6MZ	A	1618	24	18,25,26	0.94	1 (5%)	16,36,39	2.35	4 (25%)
24	5MC	A	1962	24	18,22,23	1.00	1 (5%)	26,32,35	1.49	3 (11%)
24	1MG	A	745	24	18,26,27	0.81	1 (5%)	19,39,42	1.07	2 (10%)
22	PSU	v	55	22	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
24	6MZ	A	2030	24	18,25,26	0.95	1 (5%)	16,36,39	2.69	4 (25%)
24	PSU	A	2605	24	18,21,22	1.40	3 (16%)	22,30,33	1.90	4 (18%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	0.98	2 (7%)
24	PSU	A	1911	24	18,21,22	1.38	3 (16%)	22,30,33	1.94	3 (13%)
1	2MG	a	1516	1	18,26,27	0.89	1 (5%)	16,38,41	1.15	2 (12%)
1	5MC	a	1407	1	18,22,23	0.89	2 (11%)	26,32,35	1.19	3 (11%)
24	H2U	A	2449	24	18,21,22	1.05	2 (11%)	21,30,33	1.76	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	G7M	a	527	1	20,26,27	1.74	5 (25%)	17,39,42	1.94	6 (35%)
1	PSU	a	516	1	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
24	2MG	A	1835	24	18,26,27	0.91	1 (5%)	16,38,41	1.22	3 (18%)
1	2MG	a	966	1	18,26,27	0.91	1 (5%)	16,38,41	1.22	2 (12%)
24	G7M	A	2069	24	20,26,27	1.41	3 (15%)	17,39,42	1.59	2 (11%)
22	H2U	v	20	22	18,21,22	0.94	2 (11%)	21,30,33	1.26	3 (14%)
24	5MU	A	747	24	19,22,23	1.42	5 (26%)	28,32,35	2.06	8 (28%)
24	PSU	A	2457	24	18,21,22	1.55	4 (22%)	22,30,33	2.11	5 (22%)
24	PSU	A	1917	24	18,21,22	1.42	3 (16%)	22,30,33	1.93	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMU	A	2552	24	-	2/9/27/28	0/2/2/2
24	PSU	A	746	24	-	2/7/25/26	0/2/2/2
24	PSU	A	2504	24	-	2/7/25/26	0/2/2/2
24	3TD	A	1915	24	-	5/7/25/26	0/2/2/2
24	2MA	A	2503	24	-	2/3/25/26	0/3/3/3
1	5MC	a	967	1	-	2/7/25/26	0/2/2/2
24	OMG	A	2251	22,24	-	3/5/27/28	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/7/29/30	0/3/3/3
24	PSU	A	955	24	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	3/7/29/30	0/3/3/3
24	PSU	A	2580	24	-	2/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
24	PSU	A	2604	24	-	1/7/25/26	0/2/2/2
24	5MU	A	1939	24	-	2/7/25/26	0/2/2/2
24	OMC	A	2498	24	-	2/9/27/28	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
24	2MG	A	2445	24	-	3/5/27/28	0/3/3/3
24	6MZ	A	1618	24	-	0/5/27/28	0/3/3/3
24	5MC	A	1962	24	-	4/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	A	745	24	-	0/3/25/26	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
24	6MZ	A	2030	24	-	3/5/27/28	0/3/3/3
24	PSU	A	2605	24	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
24	PSU	A	1911	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
24	H2U	A	2449	24	-	0/7/38/39	0/2/2/2
1	G7M	a	527	1	2/2/5/5	1/3/25/26	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
24	2MG	A	1835	24	-	2/5/27/28	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
24	G7M	A	2069	24	2/2/5/5	2/3/25/26	0/3/3/3
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
24	5MU	A	747	24	-	1/7/25/26	0/2/2/2
24	PSU	A	2457	24	-	2/7/25/26	0/2/2/2
24	PSU	A	1917	24	-	0/7/25/26	0/2/2/2

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1915	3TD	C6-C5	11.98	1.49	1.35
24	A	1915	3TD	C2-N1	8.97	1.48	1.37
24	A	1915	3TD	C6-N1	5.66	1.45	1.36
1	a	527	G7M	C5-C4	4.81	1.48	1.39
22	v	8	4SU	C4-S4	-4.62	1.59	1.68
24	A	2069	G7M	C5-C4	3.67	1.46	1.39
24	A	1915	3TD	C2-N3	3.50	1.46	1.38
24	A	2504	PSU	C6-C5	3.37	1.39	1.35
24	A	2457	PSU	C4-N3	-3.29	1.32	1.38
24	A	1917	PSU	C6-C5	3.28	1.39	1.35
22	v	8	4SU	C4-N3	-3.19	1.34	1.37
24	A	746	PSU	C6-C5	3.19	1.39	1.35
24	A	2580	PSU	C4-N3	-3.17	1.33	1.38
22	v	55	PSU	C6-C5	3.16	1.39	1.35
24	A	2604	PSU	C4-N3	-3.10	1.33	1.38
24	A	2605	PSU	C6-C5	3.09	1.38	1.35
24	A	955	PSU	C4-N3	-3.04	1.33	1.38
24	A	1962	5MC	C6-C5	3.04	1.39	1.34
24	A	747	5MU	C4-N3	-3.03	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1939	5MU	C4-N3	-3.02	1.33	1.38
24	A	2457	PSU	C6-C5	3.00	1.38	1.35
24	A	2580	PSU	C6-C5	2.99	1.38	1.35
24	A	2030	6MZ	C5-C4	2.99	1.48	1.40
22	v	8	4SU	C5-C4	-2.98	1.38	1.42
24	A	1911	PSU	C4-N3	-2.95	1.33	1.38
1	a	1498	UR3	C2-N1	2.94	1.42	1.38
1	a	527	G7M	O6-C6	2.94	1.29	1.23
24	A	2251	OMG	C6-N1	-2.93	1.33	1.37
22	v	55	PSU	C4-N3	-2.91	1.33	1.38
1	a	516	PSU	C6-C5	2.91	1.38	1.35
24	A	2605	PSU	C4-N3	-2.90	1.33	1.38
24	A	1618	6MZ	C5-C4	2.90	1.48	1.40
24	A	2504	PSU	C4-N3	-2.87	1.33	1.38
1	a	1207	2MG	C6-N1	-2.86	1.33	1.37
24	A	2445	2MG	C6-N1	-2.85	1.33	1.37
24	A	1915	3TD	C4-N3	2.83	1.46	1.40
1	a	516	PSU	C4-N3	-2.83	1.33	1.38
24	A	747	5MU	C6-C5	2.78	1.39	1.34
22	v	54	5MU	C4-N3	-2.77	1.33	1.38
24	A	2604	PSU	C6-C5	2.76	1.38	1.35
24	A	1917	PSU	C4-N3	-2.68	1.33	1.38
1	a	527	G7M	C6-N1	-2.68	1.33	1.37
24	A	2449	H2U	C2-N3	-2.67	1.33	1.38
1	a	1518	MA6	C5-C4	2.67	1.48	1.40
1	a	967	5MC	C6-C5	2.63	1.38	1.34
24	A	2552	OMU	C4-N3	-2.63	1.33	1.38
24	A	2069	G7M	C6-N1	-2.62	1.34	1.37
24	A	2449	H2U	C4-N3	-2.62	1.33	1.37
1	a	966	2MG	C6-N1	-2.61	1.34	1.37
22	v	54	5MU	C6-C5	2.60	1.38	1.34
24	A	2604	PSU	C2-N3	-2.58	1.33	1.37
24	A	746	PSU	C4-N3	-2.58	1.34	1.38
24	A	1835	2MG	C6-N1	-2.56	1.34	1.37
24	A	1911	PSU	C6-C5	2.55	1.38	1.35
24	A	1939	5MU	C6-N1	-2.55	1.33	1.38
1	a	1516	2MG	C6-N1	-2.53	1.34	1.37
1	a	527	G7M	C5-C6	2.49	1.51	1.45
24	A	1939	5MU	C2-N3	-2.48	1.33	1.38
24	A	1915	3TD	O2-C2	-2.47	1.18	1.23
22	v	20	H2U	C2-N3	-2.44	1.33	1.38
1	a	1519	MA6	C5-C4	2.40	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	54	5MU	C6-N1	-2.38	1.34	1.38
24	A	1915	3TD	O4-C4	-2.37	1.18	1.23
24	A	1939	5MU	C6-C5	2.36	1.38	1.34
22	v	8	4SU	C2-N1	2.35	1.42	1.38
24	A	747	5MU	C2-N1	2.31	1.42	1.38
1	a	967	5MC	C6-N1	-2.31	1.34	1.38
24	A	2605	PSU	C2-N3	-2.28	1.33	1.37
24	A	955	PSU	C6-C5	2.27	1.38	1.35
24	A	2457	PSU	C2-N3	-2.26	1.33	1.37
24	A	2552	OMU	C2-N3	-2.26	1.33	1.38
1	a	1407	5MC	C6-N1	-2.25	1.34	1.38
24	A	1911	PSU	C2-N3	-2.25	1.33	1.37
24	A	2069	G7M	O2'-C2'	-2.24	1.37	1.43
22	v	54	5MU	C2-N1	2.21	1.42	1.38
22	v	55	PSU	C2-N3	-2.21	1.33	1.37
24	A	747	5MU	C6-N1	-2.18	1.34	1.38
24	A	745	1MG	C5-C4	2.18	1.48	1.43
24	A	747	5MU	C2-N3	-2.17	1.34	1.38
1	a	1407	5MC	C6-C5	2.16	1.38	1.34
22	v	54	5MU	C4-C5	2.14	1.48	1.44
1	a	516	PSU	C2-N3	-2.13	1.33	1.37
24	A	2580	PSU	C2-N3	-2.12	1.33	1.37
24	A	2503	2MA	C2-N3	2.12	1.35	1.31
24	A	955	PSU	C2-N1	-2.11	1.33	1.36
1	a	527	G7M	O2'-C2'	-2.08	1.38	1.43
22	v	54	5MU	C2-N3	-2.07	1.34	1.38
22	v	20	H2U	C4-N3	-2.07	1.34	1.37
24	A	2457	PSU	C2-N1	-2.05	1.34	1.36
24	A	2504	PSU	C2-N3	-2.03	1.34	1.37
24	A	955	PSU	C2-N3	-2.02	1.34	1.37
24	A	2498	OMC	C6-C5	2.01	1.39	1.35
24	A	1917	PSU	C2-N1	-2.01	1.34	1.36
1	a	1498	UR3	C5-C4	-2.00	1.38	1.43

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2030	6MZ	C9-N6-C6	-7.16	116.71	122.87
24	A	2457	PSU	N1-C2-N3	6.97	123.03	115.13
22	v	8	4SU	C4-N3-C2	-6.82	120.71	127.34
24	A	1618	6MZ	C2-N1-C6	6.65	122.29	116.59
24	A	2449	H2U	C4-N3-C2	-6.55	120.36	125.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2580	PSU	N1-C2-N3	6.55	122.55	115.13
24	A	2030	6MZ	C2-N1-C6	6.41	122.09	116.59
24	A	955	PSU	N1-C2-N3	6.14	122.09	115.13
22	v	8	4SU	C5-C4-N3	6.14	120.39	114.69
24	A	1911	PSU	N1-C2-N3	6.05	121.99	115.13
24	A	1917	PSU	N1-C2-N3	6.02	121.95	115.13
1	a	516	PSU	N1-C2-N3	5.97	121.89	115.13
24	A	2504	PSU	N1-C2-N3	5.96	121.89	115.13
24	A	1915	3TD	N1-C2-N3	5.81	120.72	116.14
24	A	2604	PSU	N1-C2-N3	5.74	121.64	115.13
1	a	1498	UR3	C1'-N1-C2	5.70	126.61	116.99
22	v	55	PSU	N1-C2-N3	5.65	121.53	115.13
24	A	747	5MU	N3-C2-N1	5.53	122.23	114.89
24	A	2605	PSU	N1-C2-N3	5.45	121.31	115.13
24	A	1939	5MU	C4-N3-C2	-5.42	120.33	127.35
24	A	1939	5MU	C5-C4-N3	5.15	119.70	115.31
22	v	54	5MU	C4-N3-C2	-5.05	120.82	127.35
1	a	1498	UR3	C4-N3-C2	-5.03	119.83	124.56
22	v	54	5MU	N3-C2-N1	4.91	121.41	114.89
24	A	747	5MU	C4-N3-C2	-4.89	121.03	127.35
1	a	1519	MA6	C4-C5-N7	-4.85	104.34	109.40
24	A	746	PSU	N1-C2-N3	4.84	120.61	115.13
22	v	8	4SU	C5-C4-S4	-4.79	118.29	124.47
24	A	1939	5MU	N3-C2-N1	4.75	121.19	114.89
1	a	1498	UR3	O2-C2-N3	-4.55	114.92	121.34
24	A	2552	OMU	N3-C2-N1	4.49	120.86	114.89
24	A	1618	6MZ	C9-N6-C6	-4.44	119.05	122.87
22	v	54	5MU	C5-C4-N3	4.40	119.07	115.31
1	a	1518	MA6	C4-C5-N7	-4.38	104.83	109.40
24	A	1962	5MC	C5-C6-N1	-4.28	118.94	123.34
24	A	2457	PSU	C4-N3-C2	-4.24	120.23	126.34
24	A	1917	PSU	O2-C2-N1	-4.22	118.14	122.79
24	A	1939	5MU	O4-C4-C5	-4.22	120.01	124.90
24	A	1939	5MU	C5-C6-N1	-4.21	119.00	123.34
24	A	2552	OMU	C4-N3-C2	-4.21	121.03	126.58
24	A	2552	OMU	C1'-N1-C2	4.16	125.10	117.57
24	A	2605	PSU	C4-N3-C2	-4.15	120.35	126.34
22	v	54	5MU	O4-C4-C5	-4.03	120.23	124.90
24	A	2069	G7M	O3'-C3'-C4'	4.00	122.61	111.05
24	A	955	PSU	O2-C2-N1	-3.97	118.42	122.79
24	A	747	5MU	O4-C4-C5	-3.92	120.35	124.90
22	v	8	4SU	N3-C2-N1	3.91	120.08	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1915	3TD	C4-N3-C2	-3.91	120.37	124.61
24	A	2498	OMC	O2-C2-N3	-3.89	116.01	122.33
24	A	955	PSU	C4-N3-C2	-3.88	120.74	126.34
24	A	1962	5MC	O2-C2-N3	-3.88	116.02	122.33
24	A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
1	a	516	PSU	C4-N3-C2	-3.82	120.83	126.34
22	v	55	PSU	C4-N3-C2	-3.80	120.87	126.34
24	A	747	5MU	C5-C4-N3	3.79	118.55	115.31
24	A	1911	PSU	O2-C2-N1	-3.75	118.67	122.79
24	A	1917	PSU	C4-N3-C2	-3.74	120.95	126.34
24	A	2504	PSU	C4-N3-C2	-3.71	120.99	126.34
22	v	20	H2U	C4-N3-C2	-3.61	122.79	125.79
1	a	1519	MA6	C10-N6-C6	-3.61	108.58	119.51
24	A	2604	PSU	C4-N3-C2	-3.57	121.19	126.34
24	A	746	PSU	C4-N3-C2	-3.56	121.21	126.34
24	A	2580	PSU	C4-N3-C2	-3.56	121.21	126.34
1	a	527	G7M	O3'-C3'-C4'	3.53	121.25	111.05
1	a	1519	MA6	N3-C2-N1	-3.51	123.19	128.68
1	a	967	5MC	C5-C6-N1	-3.51	119.73	123.34
24	A	2552	OMU	C5-C4-N3	3.49	120.07	114.84
1	a	527	G7M	O6-C6-N1	-3.47	116.56	120.65
1	a	1518	MA6	N3-C2-N1	-3.33	123.47	128.68
1	a	527	G7M	O3'-C3'-C2'	3.30	122.51	111.82
24	A	2457	PSU	O2-C2-N1	-3.30	119.15	122.79
1	a	1498	UR3	C6-N1-C2	-3.30	118.83	121.79
22	v	54	5MU	C5-C6-N1	-3.29	119.96	123.34
24	A	1618	6MZ	C4-C5-N7	-3.23	106.03	109.40
24	A	2030	6MZ	C4-C5-N7	-3.15	106.11	109.40
24	A	2580	PSU	O2-C2-N1	-3.11	119.36	122.79
1	a	516	PSU	O2-C2-N1	-3.11	119.37	122.79
24	A	2552	OMU	O2-C2-N3	-3.08	115.76	121.50
24	A	2030	6MZ	N3-C2-N1	-3.02	123.95	128.68
1	a	1518	MA6	C9-N6-C6	-3.02	110.38	119.51
1	a	1407	5MC	C5-C6-N1	-3.01	120.25	123.34
24	A	747	5MU	C5-C6-N1	-2.99	120.27	123.34
22	v	8	4SU	C1'-N1-C2	2.97	122.95	117.57
1	a	1407	5MC	O2-C2-N3	-2.95	117.53	122.33
1	a	1519	MA6	C10-N6-C9	-2.95	106.61	116.12
24	A	2605	PSU	C6-C5-C4	-2.94	116.14	118.20
1	a	1498	UR3	C1'-N1-C6	-2.88	114.55	120.84
24	A	1618	6MZ	N3-C2-N1	-2.87	124.20	128.68
24	A	746	PSU	C6-C5-C4	-2.80	116.24	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1835	2MG	C5-C6-N1	2.76	118.83	113.95
24	A	746	PSU	O2-C2-N1	-2.75	119.76	122.79
1	a	1402	4OC	O2-C2-N3	-2.66	118.00	122.33
24	A	1962	5MC	C5-C4-N3	-2.64	118.82	121.67
1	a	1518	MA6	C10-N6-C9	-2.64	107.62	116.12
24	A	2504	PSU	O2-C2-N1	-2.63	119.89	122.79
22	v	55	PSU	C6-C5-C4	-2.62	116.36	118.20
1	a	966	2MG	C5-C6-N1	2.62	118.58	113.95
24	A	2605	PSU	O2-C2-N1	-2.55	119.98	122.79
22	v	55	PSU	O2-C2-N1	-2.55	119.98	122.79
24	A	2449	H2U	C5-C6-N1	-2.55	103.21	111.61
24	A	2552	OMU	O4-C4-C5	-2.52	120.73	125.16
24	A	2503	2MA	C5-C6-N1	2.51	118.35	114.02
24	A	2604	PSU	O2-C2-N1	-2.49	120.05	122.79
24	A	745	1MG	C8-N7-C5	2.49	107.73	102.99
24	A	2445	2MG	CM2-N2-C2	-2.45	118.45	123.86
1	a	527	G7M	C5'-C4'-C3'	2.43	124.30	115.18
24	A	2069	G7M	C3'-C2'-C1'	2.43	104.63	100.98
1	a	1516	2MG	C5-C6-N1	2.43	118.24	113.95
24	A	745	1MG	C5-C6-N1	2.42	117.55	113.90
24	A	2251	OMG	C5-C6-N1	2.41	118.20	113.95
1	a	966	2MG	C8-N7-C5	2.41	107.58	102.99
1	a	1207	2MG	C5-C6-N1	2.40	118.20	113.95
1	a	967	5MC	C5-C4-N3	-2.40	119.08	121.67
24	A	747	5MU	O2-C2-N3	-2.39	117.05	121.50
24	A	2604	PSU	C6-C5-C4	-2.37	116.54	118.20
24	A	2445	2MG	C5-C6-N1	2.30	118.01	113.95
24	A	747	5MU	C6-N1-C2	-2.29	118.97	121.30
24	A	2445	2MG	C8-N7-C5	2.29	107.35	102.99
24	A	1835	2MG	CM2-N2-C2	-2.29	118.81	123.86
24	A	1835	2MG	C8-N7-C5	2.27	107.32	102.99
24	A	747	5MU	C1'-N1-C2	2.26	121.67	117.57
24	A	2251	OMG	C8-N7-C5	2.26	107.29	102.99
1	a	1516	2MG	C8-N7-C5	2.25	107.28	102.99
24	A	2449	H2U	O4-C4-N3	2.25	123.84	120.28
24	A	2457	PSU	C5-C6-N1	-2.19	118.83	122.11
24	A	2552	OMU	C6-N1-C2	-2.17	118.21	120.99
22	v	20	H2U	C5-C6-N1	-2.16	104.50	111.61
22	v	20	H2U	C5-C4-N3	2.15	119.06	116.65
1	a	1407	5MC	C5-C4-N3	-2.14	119.36	121.67
24	A	1915	3TD	O4-C4-N3	-2.14	116.38	120.30
24	A	2457	PSU	O2-C2-N3	-2.13	117.80	121.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	54	5MU	O2-C2-N1	-2.13	119.96	122.79
1	a	527	G7M	C3'-C2'-C1'	2.13	104.18	100.98
24	A	2503	2MA	C8-N7-C5	2.12	107.03	102.99
24	A	2498	OMC	O2-C2-N1	2.07	123.18	118.89
1	a	516	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	a	1402	4OC	CM4-N4-C4	-2.05	118.44	122.45
1	a	527	G7M	O2'-C2'-C3'	2.02	118.37	111.82
1	a	1207	2MG	C8-N7-C5	2.00	106.81	102.99
1	a	967	5MC	O2-C2-N3	-2.00	119.08	122.33

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
24	A	2069	G7M	C4'
24	A	2069	G7M	C3'

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	967	5MC	O4'-C4'-C5'-O5'
1	a	967	5MC	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C10
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	A	1915	3TD	O4'-C1'-C5-C4
24	A	1915	3TD	O4'-C1'-C5-C6
24	A	1915	3TD	C3'-C4'-C5'-O5'
24	A	1915	3TD	O4'-C4'-C5'-O5'
24	A	1962	5MC	C2'-C1'-N1-C2
24	A	1962	5MC	C2'-C1'-N1-C6
24	A	2445	2MG	O4'-C4'-C5'-O5'
24	A	2445	2MG	C3'-C4'-C5'-O5'
24	A	2504	PSU	C3'-C4'-C5'-O5'
24	A	2504	PSU	O4'-C4'-C5'-O5'
24	A	2552	OMU	O4'-C1'-N1-C2
24	A	746	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	746	PSU	O4'-C4'-C5'-O5'
24	A	2030	6MZ	C3'-C4'-C5'-O5'
24	A	2498	OMC	C3'-C4'-C5'-O5'
24	A	2498	OMC	O4'-C4'-C5'-O5'
24	A	2457	PSU	O4'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	N1-C6-N6-C10
24	A	2552	OMU	O4'-C1'-N1-C6
24	A	2069	G7M	O4'-C4'-C5'-O5'
24	A	2069	G7M	C3'-C4'-C5'-O5'
24	A	2580	PSU	O4'-C4'-C5'-O5'
24	A	2030	6MZ	O4'-C4'-C5'-O5'
24	A	2251	OMG	O4'-C4'-C5'-O5'
24	A	1915	3TD	C4'-C5'-O5'-P
24	A	1962	5MC	O4'-C1'-N1-C6
24	A	1835	2MG	O4'-C4'-C5'-O5'
24	A	2030	6MZ	C4'-C5'-O5'-P
24	A	2251	OMG	C4'-C5'-O5'-P
24	A	1939	5MU	C3'-C4'-C5'-O5'
1	a	527	G7M	C4'-C5'-O5'-P
24	A	1962	5MC	O4'-C1'-N1-C2
24	A	2503	2MA	C4'-C5'-O5'-P
24	A	1835	2MG	C3'-C4'-C5'-O5'
24	A	747	5MU	C3'-C4'-C5'-O5'
24	A	2457	PSU	C3'-C4'-C5'-O5'
24	A	2580	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'
24	A	2604	PSU	O4'-C4'-C5'-O5'
24	A	2445	2MG	C4'-C5'-O5'-P
24	A	1939	5MU	O4'-C4'-C5'-O5'
24	A	2251	OMG	C3'-C4'-C5'-O5'
24	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

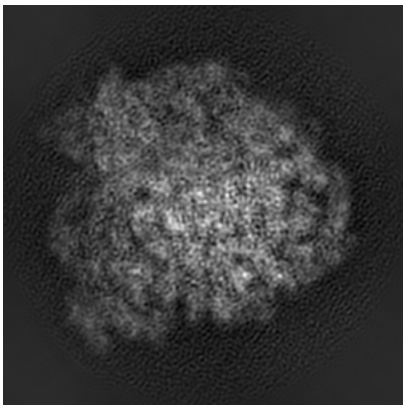
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4121. These allow visual inspection of the internal detail of the map and identification of artifacts.

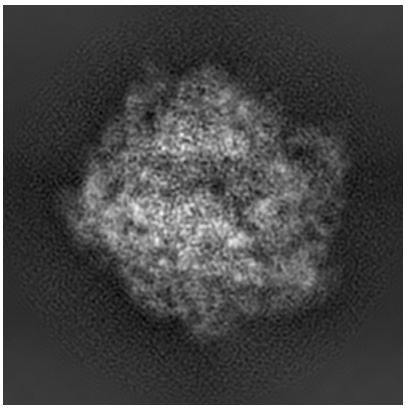
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

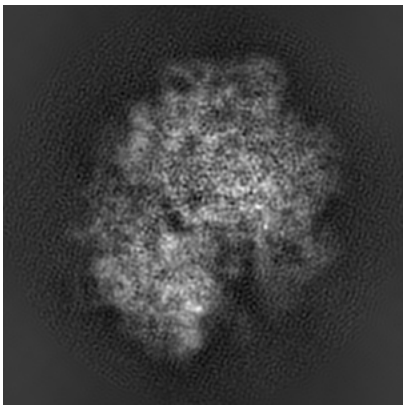
6.1.1 Primary map



X

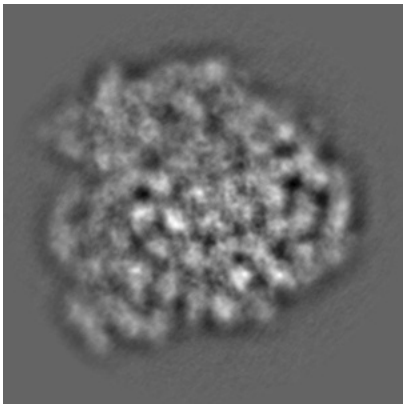


Y

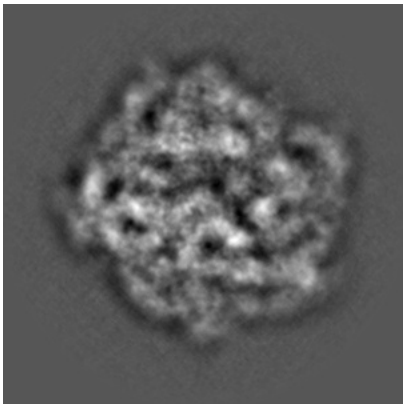


Z

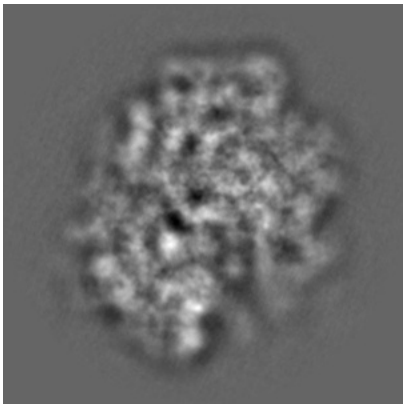
6.1.2 Raw map



X



Y

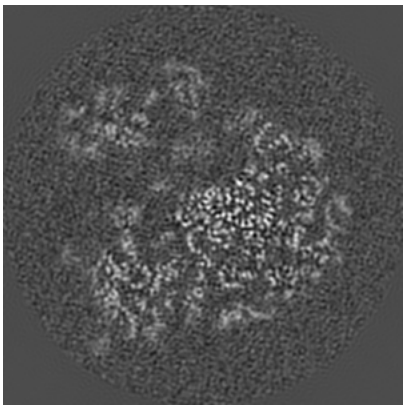


Z

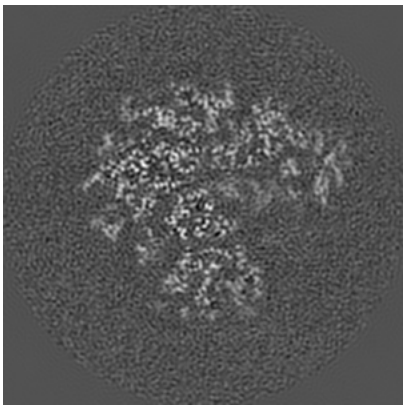
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

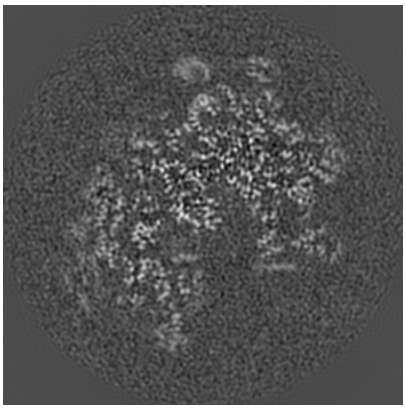
6.2.1 Primary map



X Index: 136

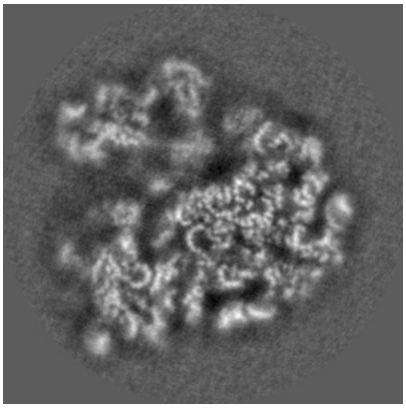


Y Index: 136

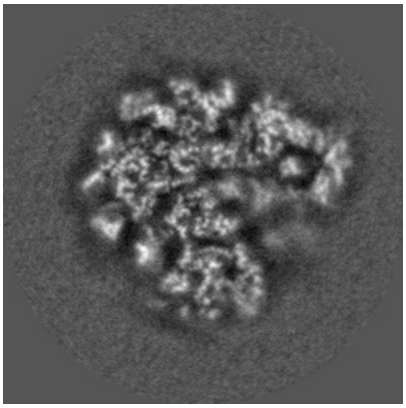


Z Index: 136

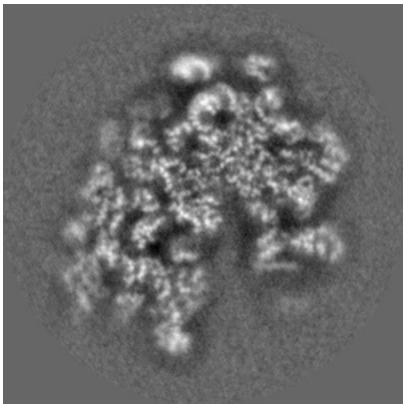
6.2.2 Raw map



X Index: 136



Y Index: 136

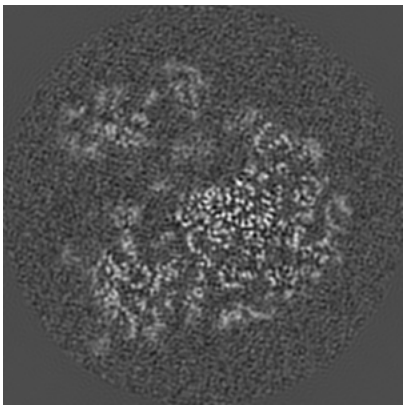


Z Index: 136

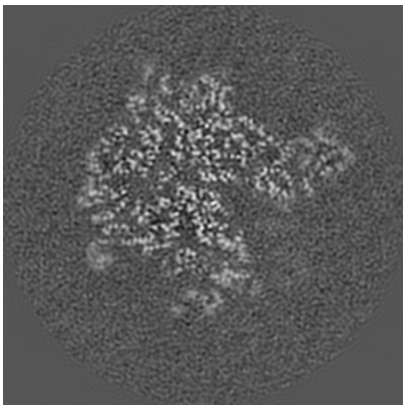
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

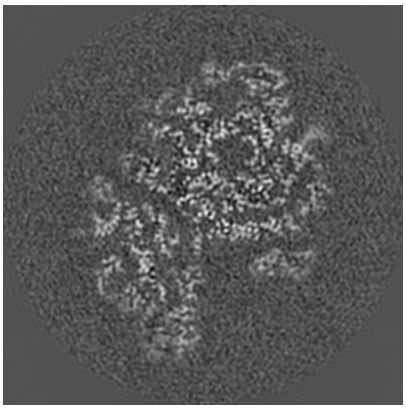
6.3.1 Primary map



X Index: 136

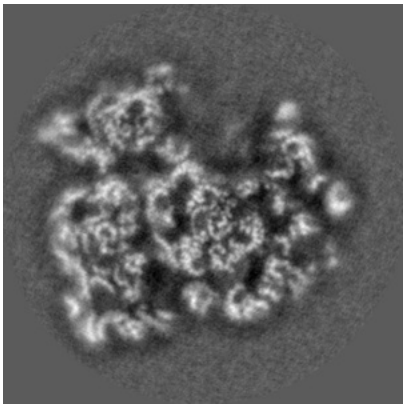


Y Index: 152

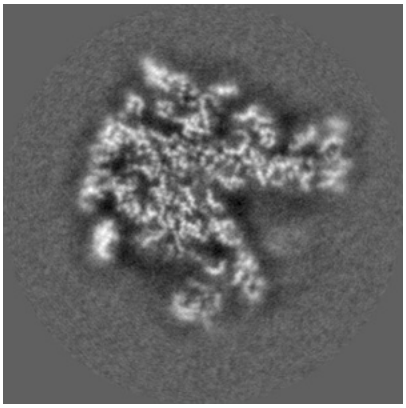


Z Index: 119

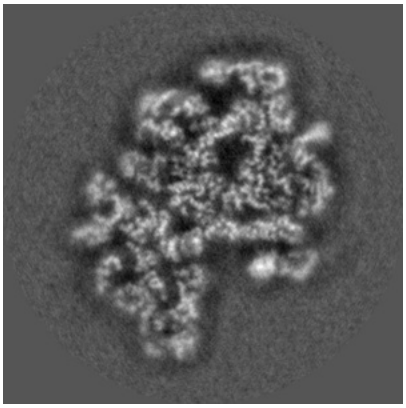
6.3.2 Raw map



X Index: 125



Y Index: 146

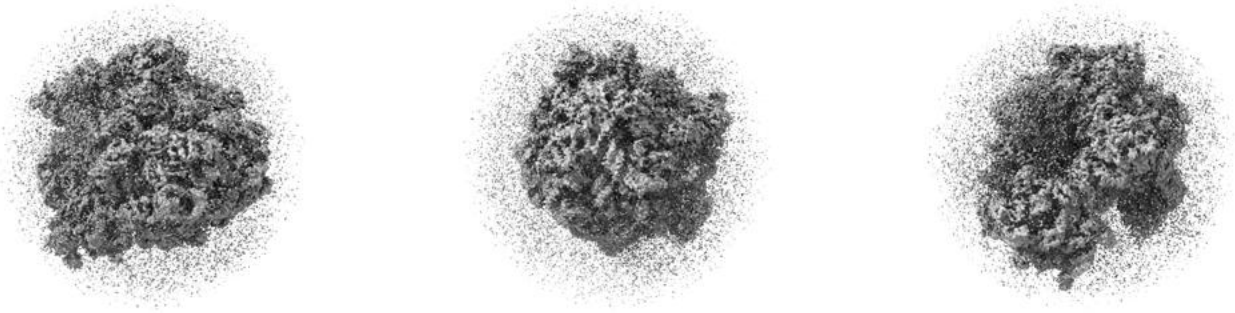


Z Index: 121

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

6.4 Orthogonal surface views (i)

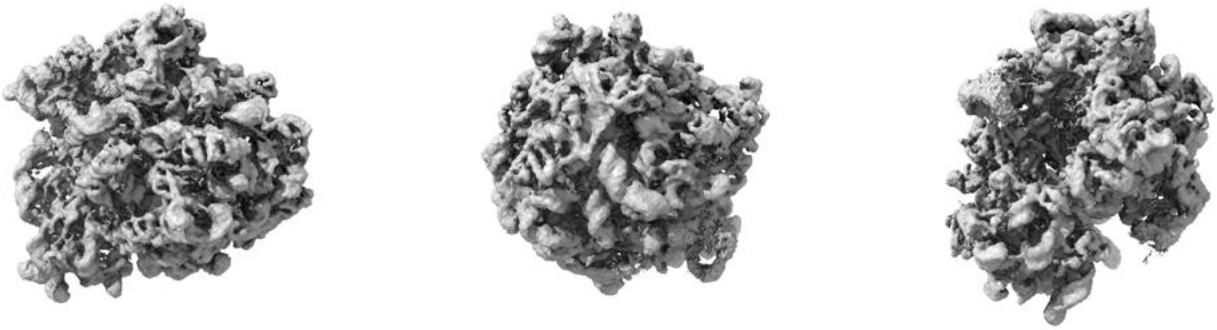
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

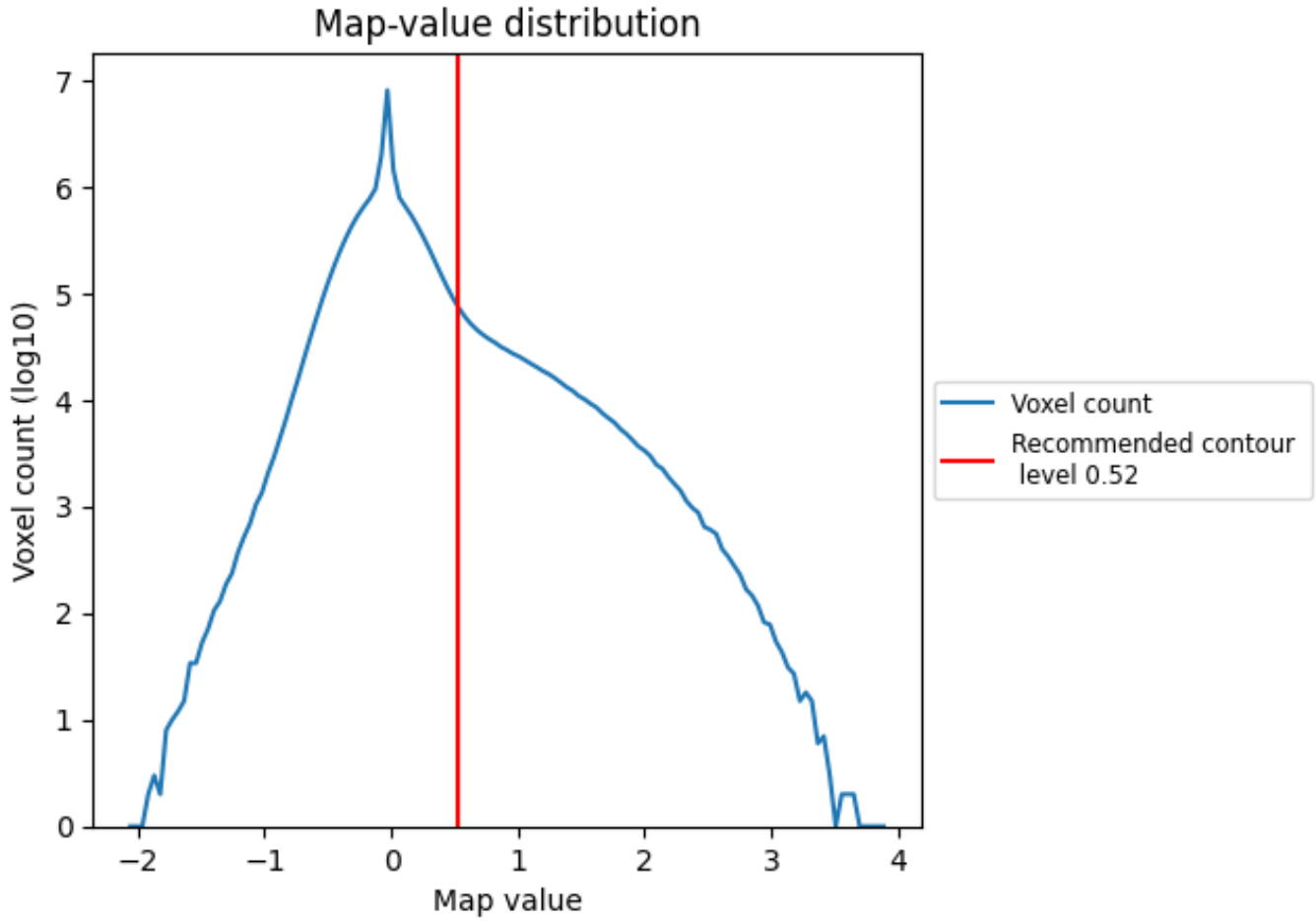
6.5 Mask visualisation (i)

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

7 Map analysis

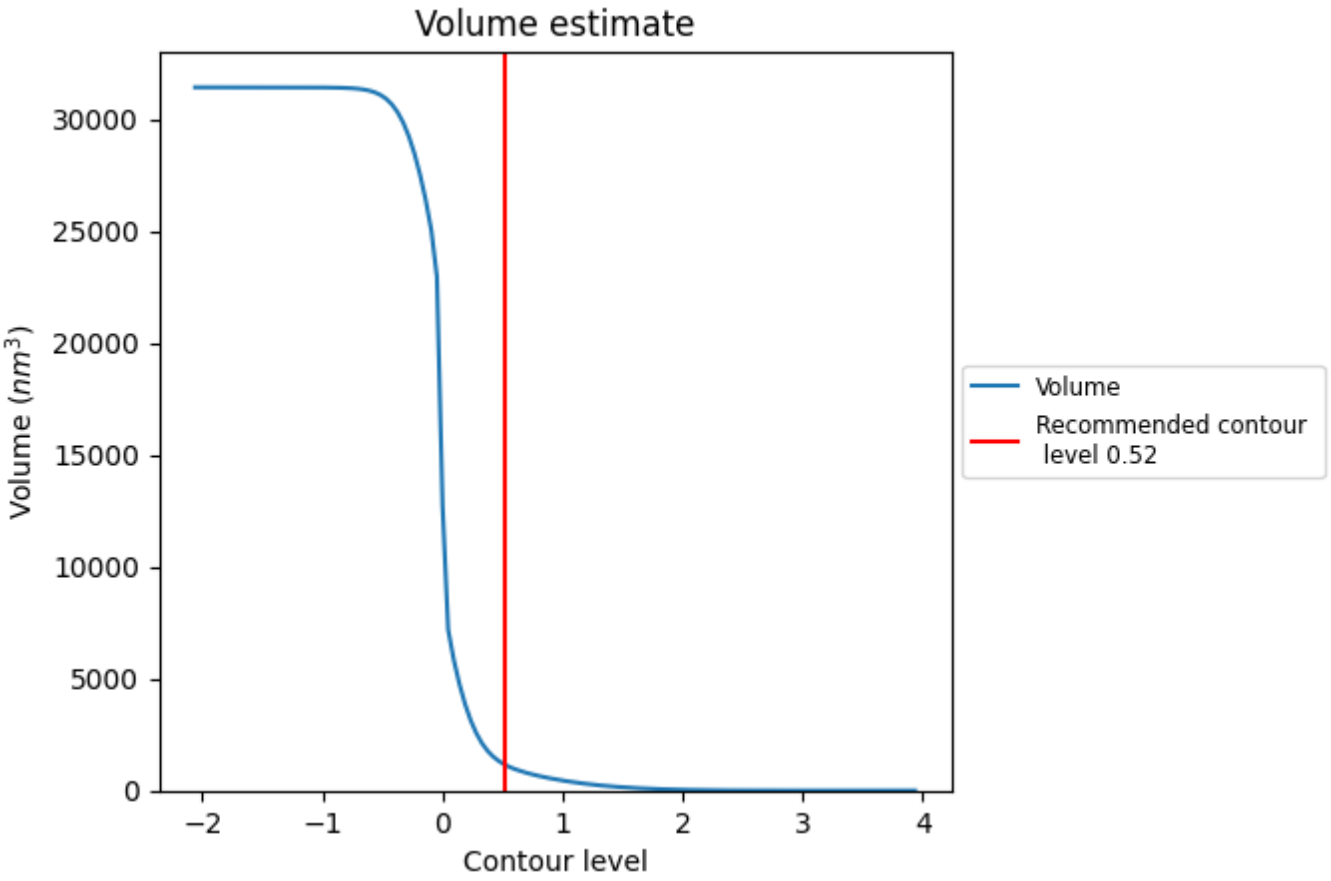
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

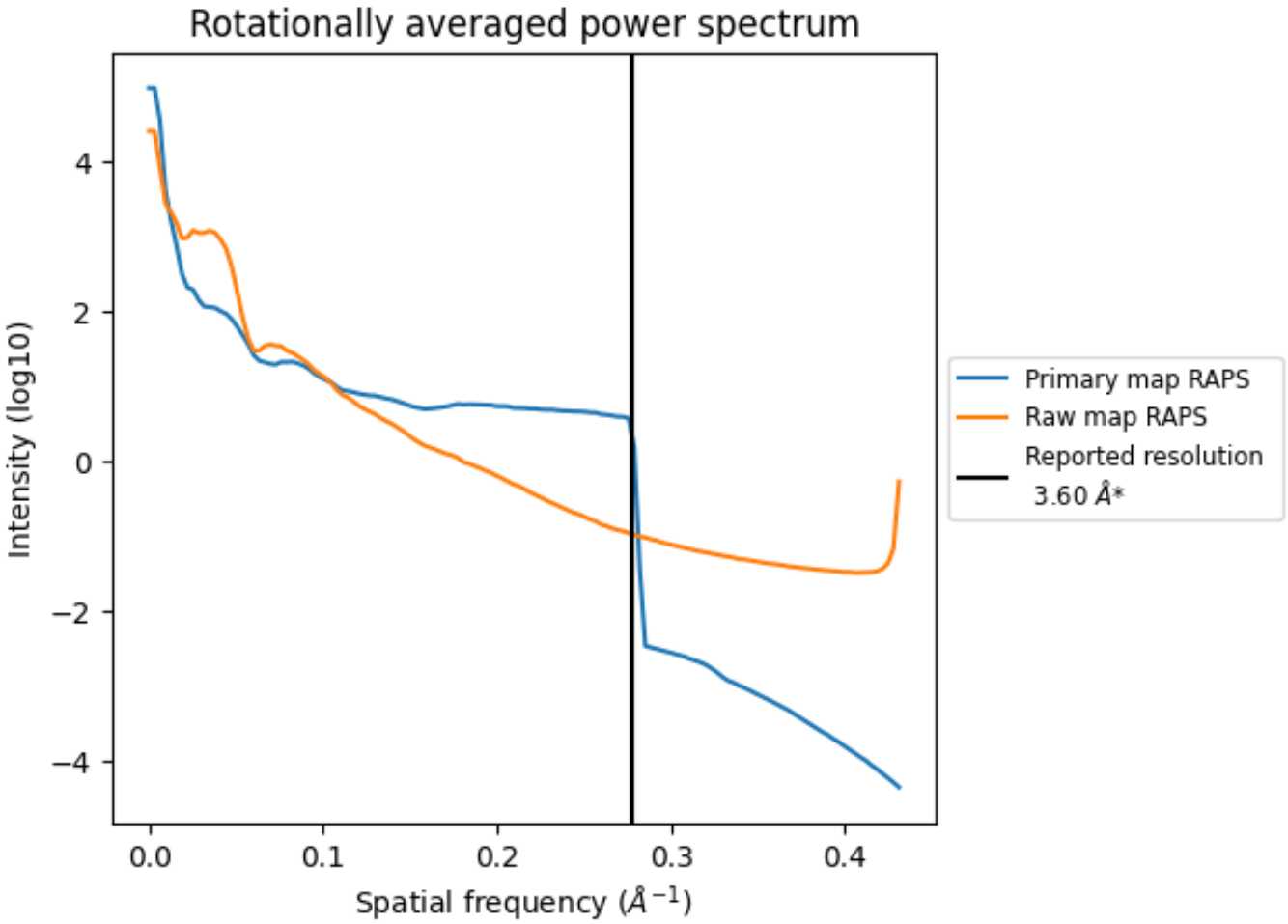
7.2 Volume estimate



The volume at the recommended contour level is 1155 nm^3; this corresponds to an approximate mass of 1043 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)

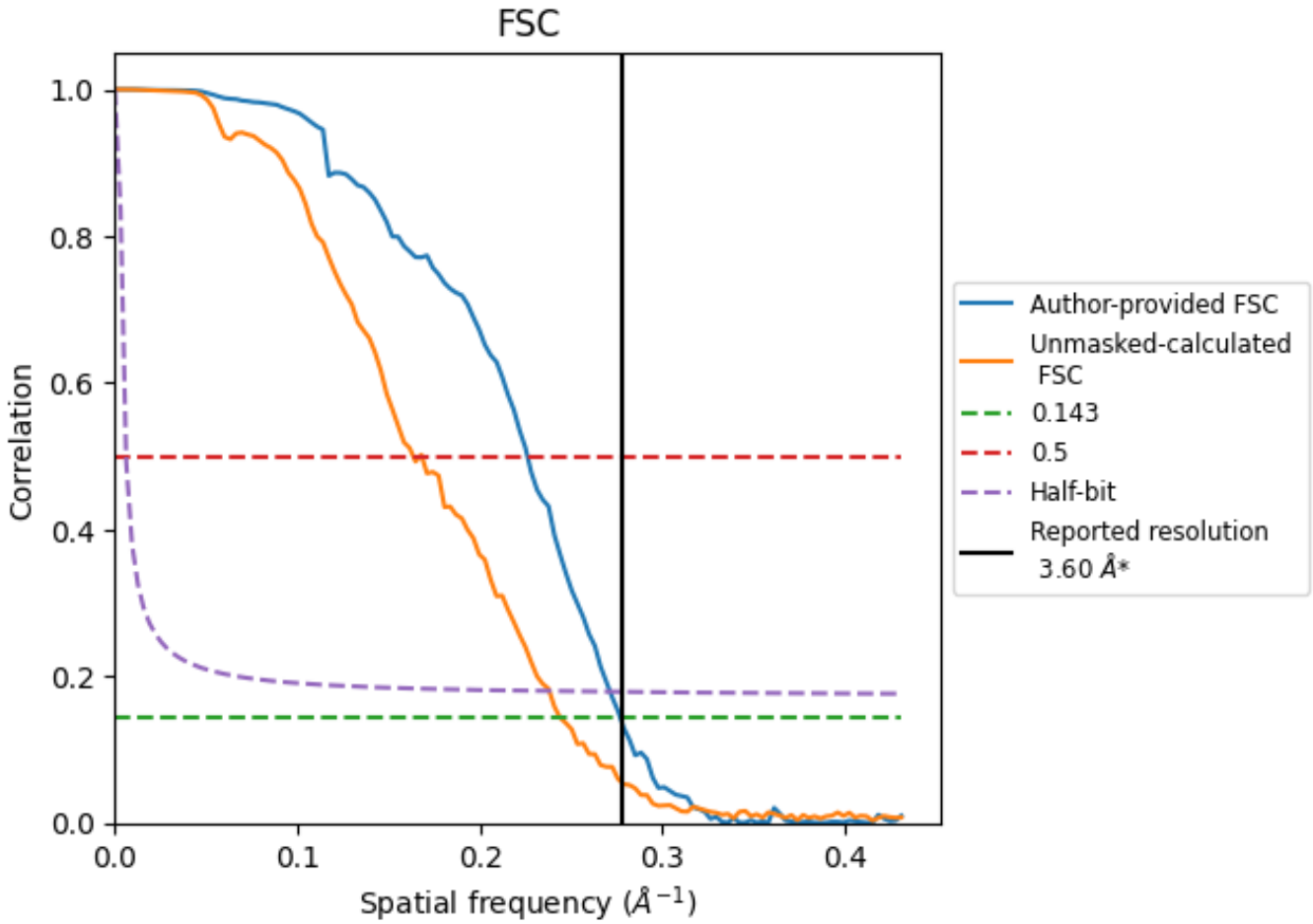


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

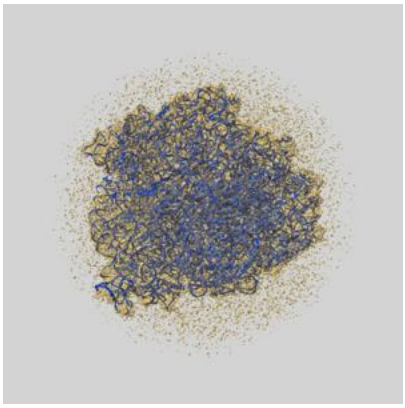
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.42	3.68
Unmasked-calculated*	4.10	6.12	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 3.6 by more than 10 %

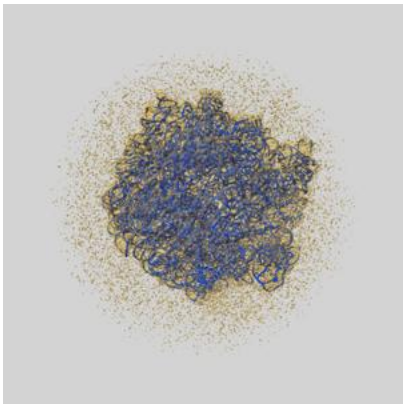
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4121 and PDB model 5LZA. Per-residue inclusion information can be found in section 3 on page 15.

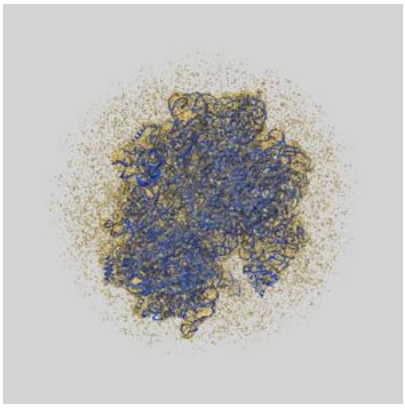
9.1 Map-model overlay



X



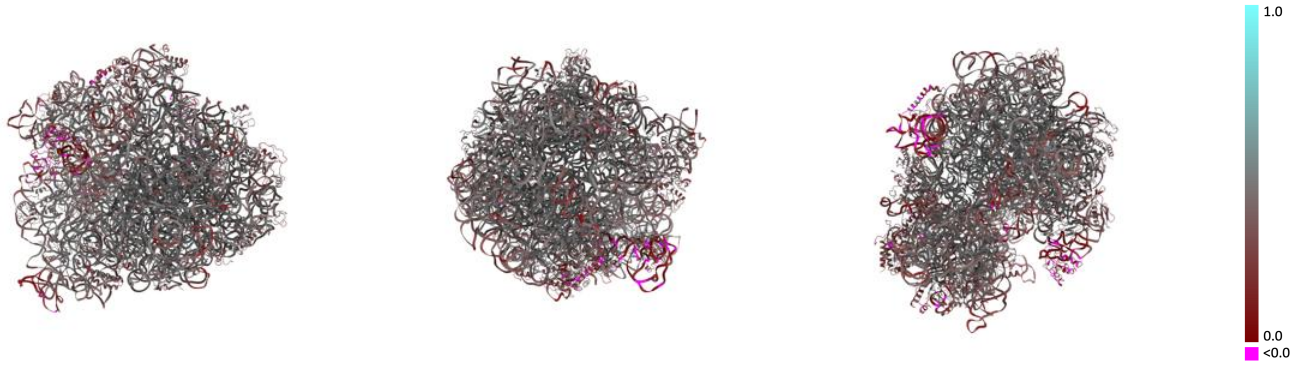
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.52 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.

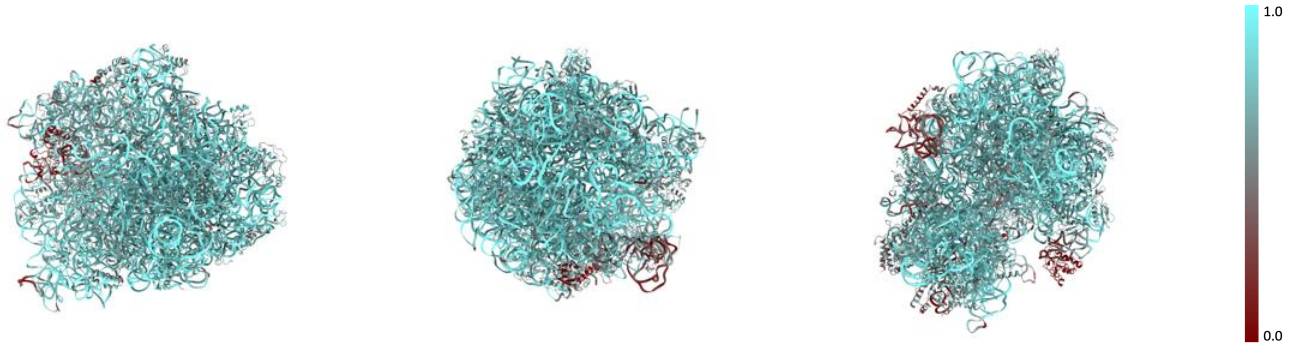
9.2 Q-score mapped to coordinate model (i)



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.

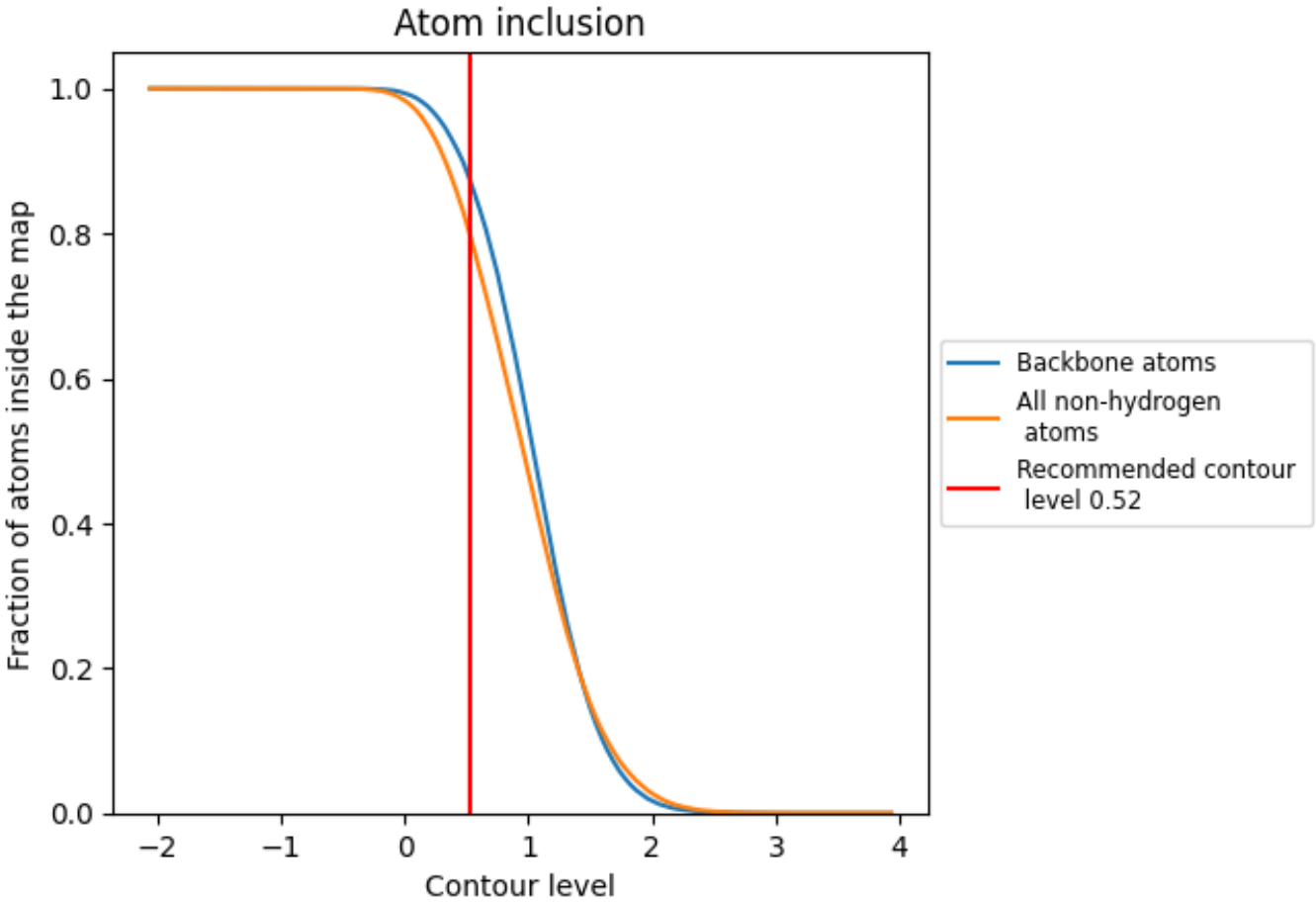
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.52).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8022	0.4070
0	0.7313	0.4610
1	0.6119	0.3830
2	0.7944	0.4860
3	0.7637	0.4790
4	0.7270	0.4640
6	0.5107	0.2440
A	0.8745	0.4260
B	0.8942	0.4000
C	0.7714	0.4680
D	0.7256	0.4450
E	0.6776	0.3990
F	0.6638	0.3560
G	0.6685	0.3660
H	0.2190	0.2180
I	0.0499	0.0810
J	0.7218	0.4380
K	0.7177	0.4370
L	0.7323	0.4350
M	0.7418	0.4440
N	0.7411	0.4440
O	0.6674	0.3800
P	0.7140	0.4120
Q	0.7335	0.4480
R	0.7189	0.4200
S	0.7045	0.4270
T	0.6722	0.3980
U	0.6628	0.3880
V	0.6911	0.3840
W	0.7335	0.4540
X	0.7171	0.4400
Y	0.6660	0.3720
Z	0.7048	0.4150
a	0.8815	0.4160
b	0.4785	0.3010

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.6523	0.3940
d	0.6126	0.3520
e	0.6960	0.4120
f	0.6863	0.3480
g	0.6341	0.3380
h	0.6896	0.4030
i	0.6118	0.3400
j	0.5486	0.3390
k	0.7104	0.3950
l	0.7242	0.4100
m	0.6643	0.3530
n	0.6920	0.3970
o	0.7246	0.4000
p	0.6746	0.4080
q	0.6540	0.3540
r	0.6975	0.4040
s	0.6576	0.3670
t	0.6831	0.3690
u	0.5199	0.2610
v	0.7141	0.3550
x	0.1990	0.1580