Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 07:27 am GMT

PDB ID	:	6HA1
EMDB ID	:	EMD-0176
Title	:	Cryo-EM structure of a 70S Bacillus subtilis ribosome translating the ErmD leader peptide in complex with telithromycin
Authors	:	Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wilson, D.N.
Deposited on	:	2018-08-07
Resolution	:	3.10 Å(reported)
Based on initial model	:	3J9W

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

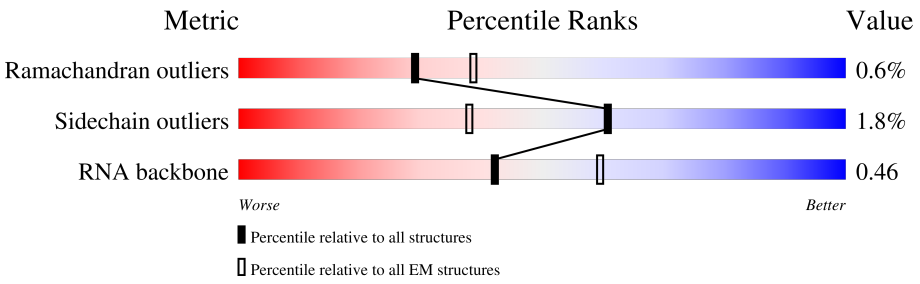
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2928	64% 31%
2	B	112	59% 35% 6%
3	C	277	97%
4	D	209	98%
5	E	207	96%
6	F	179	91% 7%
7	G	179	13% 98%
8	J	145	94%

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Mol	Chain	Length	Quality of chain
9	K	122	98%
10	L	146	97%
11	M	144	94% 6%
12	N	120	98%
13	O	120	97%
14	P	115	97%
15	Q	119	93%
16	R	102	94%
17	S	113	93%
18	T	95	93% 5%
19	U	103	98%
20	W	94	84% 13%
21	X	62	5% 87% 6% 6%
22	Y	66	98%
23	Z	59	97%
24	0	59	85% 8%
25	1	49	98%
26	2	44	98%
27	3	66	94%
28	4	37	100%
29	6	63	17% 97%
30	7	3	100%
31	a	1554	65% 30%
32	b	246	49% 83% 5% 11%
33	c	218	5% 94% 6%

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Mol	Chain	Length	Quality of chain
34	d	200	5% 92%
35	e	166	96%
36	f	95	6% 95%
37	g	156	92%
38	h	132	95% 5%
39	i	130	92% 5%
40	j	102	8% 92% 7%
41	k	131	86% 13%
42	l	138	96%
43	m	121	85% 11%
44	n	61	95%
45	o	89	91%
46	p	90	92%
47	q	87	5% 94%
48	r	79	76% 5% 19%
49	s	92	84% 15%
50	t	88	91% 6%
51	x	87	16% 68% 28% 5%

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
52	TEL	A	3001	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 140824 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2887	61997	27661	11460	19992	2884	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2392	1068	435	778	111	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	272	2083	1296	408	373	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	206	1569	985	289	290	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	176	1386	882	241	256	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

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

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	135	1076	690	205	176	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	P	115	944	600	185	158	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	90	725	452	134	136	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	101	762	478	142	138	4	0	0

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

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	0	54	426	262	86	71	7	0	0

- Molecule 25 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1	48	401	244	80	73	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	2	44	367	222	89	54	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	3	64	512	321	107	82	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	4	37	296	186	60	45	5	0	0

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	6	63	499	312	91	91	5	0	0

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	7	3	60	27	7	23	3	0	0

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	a	1533	32891	14667	6034	10657	1533	0	0

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	218	1757	1119	309	323	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	206	1619	1011	304	301	3	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	195	1568	991	291	284	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	164	1218	767	225	224	2	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	92	755	476	132	146	1	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	149	1181	740	220	215	6	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	131	1036	655	191	187	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	125	966	599	191	175	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	95	761	479	139	141	2	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	114	838	516	164	156	2	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l	136	1052	653	211	186	2	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	m	108	868	534	176	158	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	60	497	317	98	77	5	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	85	710	436	144	129	1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	88	695	441	128	124	2	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	84	691	435	128	126	2	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	r	64	518	332	96	88	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	78	633	409	112	110	2	0	0

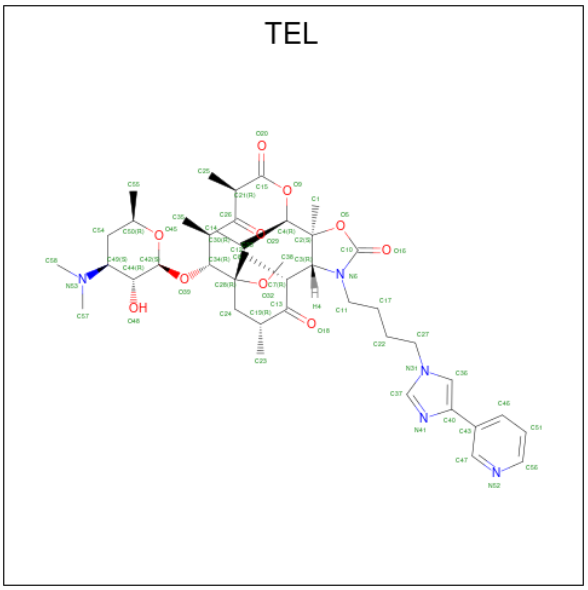
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t	83	637	390	130	116	1	0	0

- Molecule 51 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	x	87	1861	829	333	612	87	0	0

- Molecule 52 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



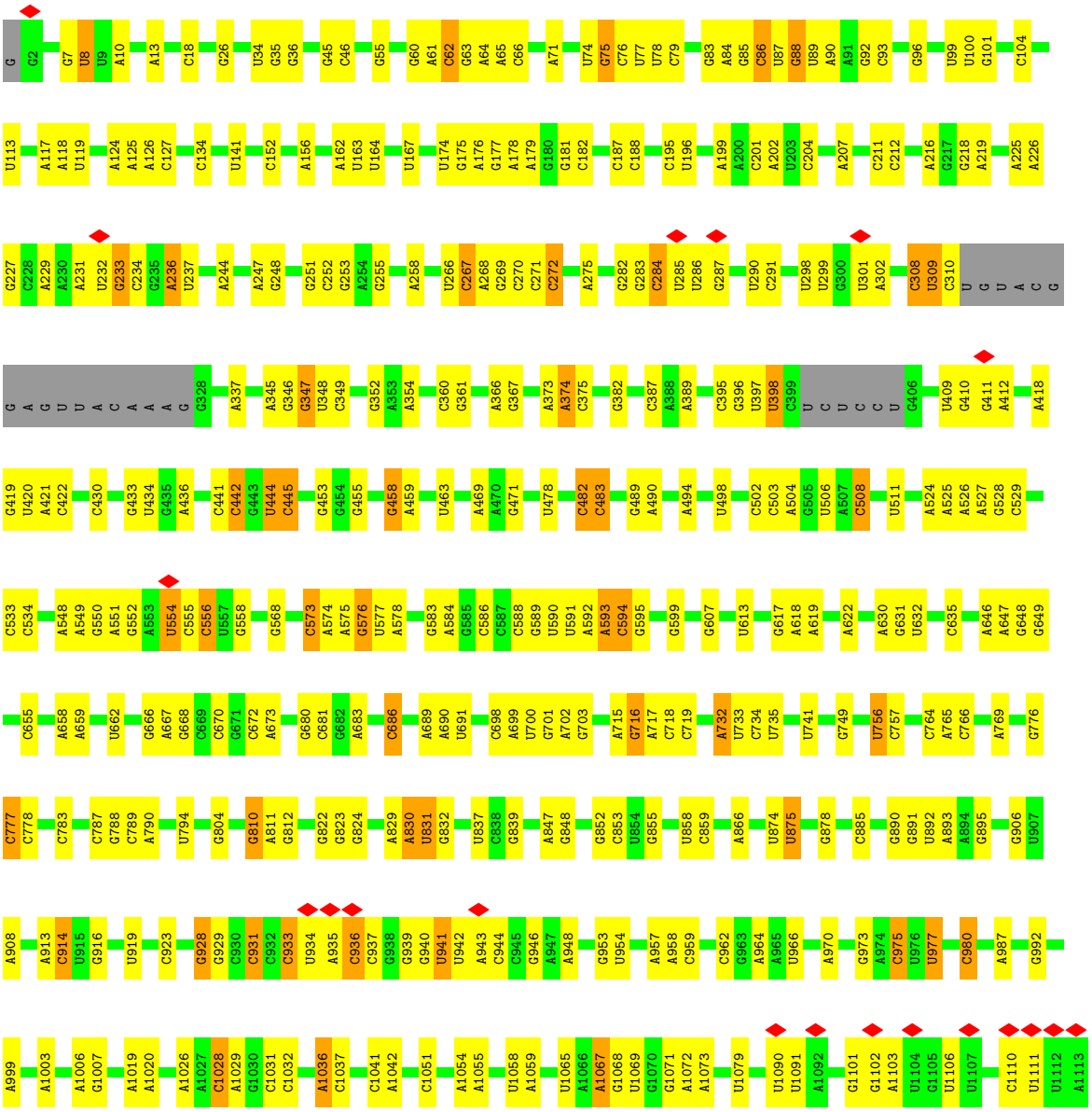
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
52	A	1	58	43	5	10	0

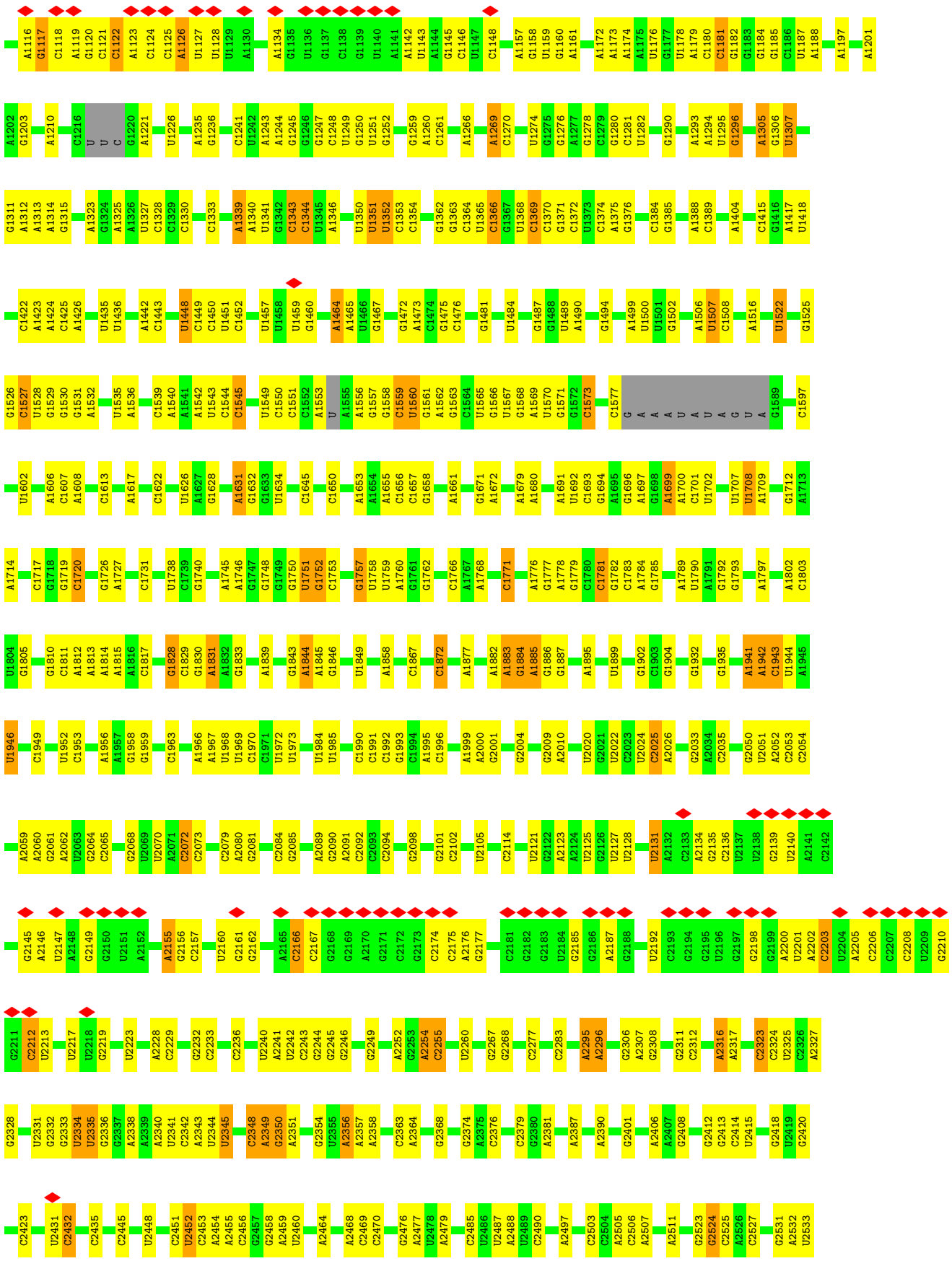
3 Residue-property plots (i)

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: 23S ribosomal RNA

Chain A: 64% 31%




A1116 G1117 C1118 A1119 G1120 C1121 C1122 A1123 C1124 C1125 A1126 U1127 U1128 U1129 A1130 A1134 G1135 U1136 G1137 C1138 G1139 U1140 A1141 A1142 U1143 A1144 G1145 C1146 U1147 C1148 A1157 G1158 U1159 G1160 A1161 A1172 A1173 A1174 A1175 U1176 G1177 U1178 A1179 C1180 C1181 G1182 G1183 G1184 G1185 C1186 U1187 A1188 A1197 A1201
A1202 G1203 A1210 C1216 U U C G1220 A1221 U1226 A1235 G1236 C1241 U1242 A1243 A1244 G1245 G1246 A1247 C1248 U1249 G1250 U1251 G1252 G1259 A1260 C1261 A1266 A1269 C1270 U1274 G1275 G1276 A1277 G1278 C1279 G1280 C1281 U1282 G1290 A1293 A1294 U1295 G1296 A1305 G1306 U1307
G1311 A1312 A1313 A1314 G1315 A1323 G1324 A1325 A1326 U1327 C1328 C1329 C1330 C1333 A1339 A1340 U1341 G1342 C1343 C1344 U1345 A1346 U1350 U1351 U1352 C1353 C1354 G1362 G1363 C1364 U1365 C1366 G1367 U1368 C1369 C1370 G1371 C1372 U1373 C1374 A1375 G1376 C1384 G1385 A1388 C1389 A1404 C1415 G1416 A1417 U1418
C1422 A1423 A1424 C1425 A1426 U1435 U1436 A1442 C1443 U1448 C1449 C1450 U1451 C1452 U1457 U1458 U1459 G1460 A1464 A1465 U1466 G1467 G1472 A1473 C1474 G1475 C1476 G1481 U1484 G1487 G1488 U1489 A1490 G1494 A1499 U1500 U1501 G1502 A1506 U1507 C1508 A1516 U1522 G1525
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A1714 C1717 G1718 G1719 C1720 G1726 A1727 C1731 U1738 C1739 G1740 A1745 A1746 G1747 G1748 G1749 G1750 U1751 G1752 C1753 G1757 U1758 U1759 A1760 G1761 G1762 C1766 A1767 A1768 C1771 A1776 G1777 A1778 G1779 C1780 C1781 G1782 C1783 A1784 G1785 A1789 U1790 A1791 G1792 G1793 A1797 A1802 C1803
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U1946 C1949 U1952 C1953 A1956 A1957 G1958 G1959 C1963 A1966 A1967 U1968 U1969 C1970 C1971 U1972 U1973 U1984 U1985 C1990 C1991 C1992 G1993 C1994 A1995 C1996 A1999 A2000 G2001 G2004 G2009 A2010 U2020 G2021 U2022 C2023 U2024 C2025 A2026 G2033 A2034 C2035 G2050 U2051 A2052 C2053 C2054
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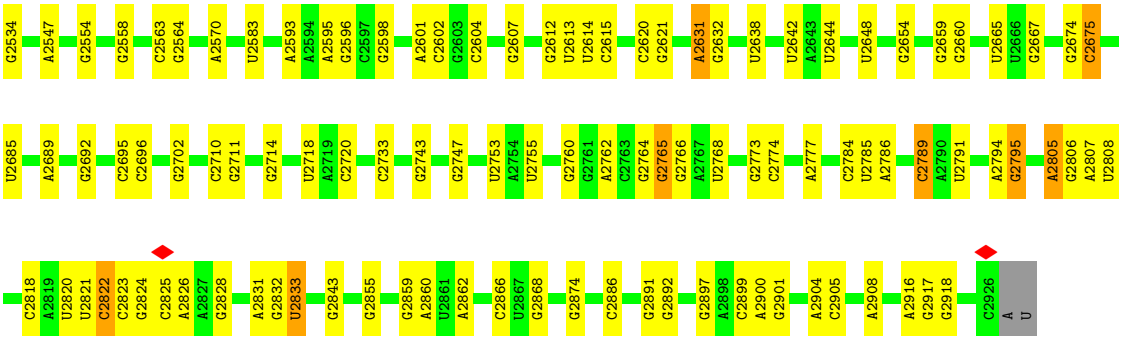
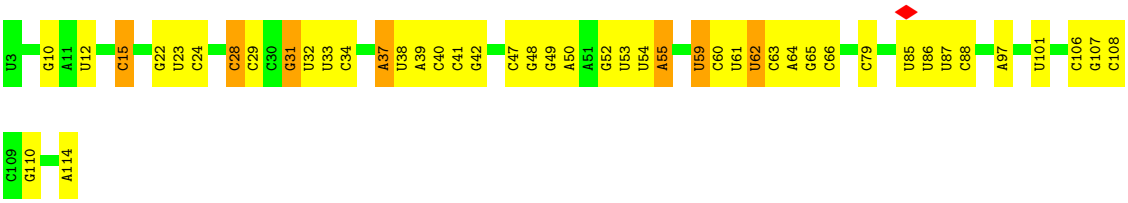
G2145 A2146 U2147 A2148 G2149 G2150 U2151 A2152 A2155 G2156 C2157 U2160 G2161 G2162 A2165 C2166 C2167 G2168 G2169 A2170 G2171 C2172 G2173 C2174 C2175 A2176 G2177 C2181 G2182 G2183 U2184 G2185 G2186 A2187 G2188 U2192 C2193 G2194 G2195 U2196 G2197 G2198 G2199 A2200 U2201 A2202 C2203 U2204 A2205 C2206 C2207 C2208 U2209 G2210
G2211 C2212 U2213 U2217 U2218 G2219 U2223 A2228 C2229 G2232 C2233 C2236 U2240 A2241 U2242 C2243 G2244 G2245 G2246 G2249 A2252 G2253 A2254 C2255 U2260 G2267 G2268 C2277 C2283 A2295 A2296 G2306 A2307 G2308 G2311 C2312 A2316 A2317 C2323 C2324 U2325 C2326 A2327
G2328 U2331 G2332 G2333 U2334 U2335 G2336 C2337 A2338 A2339 A2340 U2341 C2342 A2343 U2344 U2345 C2348 A2349 G2350 A2351 C2354 U2355 A2356 A2357 A2358 C2363 A2364 G2368 G2374 A2375 C2376 C2379 G2380 A2381 A2387 A2390 G2401 A2406 A2407 G2408 G2412 G2413 C2414 U2415 G2418 U2419 G2420
C2423 U2431 C2432 C2435 C2445 U2448 C2451 U2452 C2453 A2454 A2455 C2456 G2457 G2458 A2459 U2460 A2464 A2468 C2469 C2470 G2476 A2477 U2478 A2479 C2485 U2486 U2487 A2488 U2489 C2490 A2497 C2503 C2504 A2505 C2506 A2507 A2511 G2523 G2524 C2525 A2526 C2527 G2531 A2532 U2533



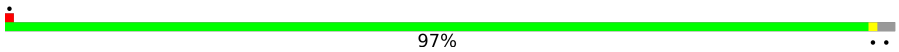
- Molecule 2: 5S ribosomal RNA

Chain B:



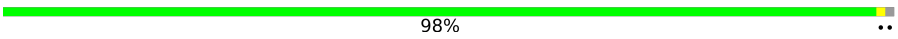
- Molecule 3: 50S ribosomal protein L2

Chain C:



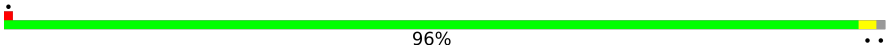
- Molecule 4: 50S ribosomal protein L3

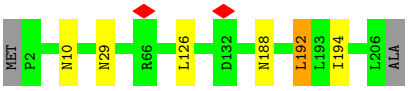
Chain D:



- Molecule 5: 50S ribosomal protein L4

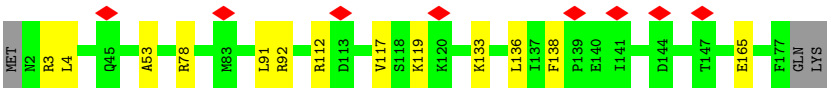
Chain E:





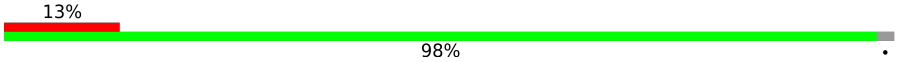
- Molecule 6: 50S ribosomal protein L5

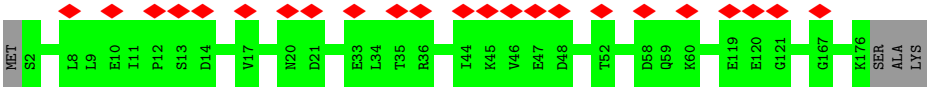
Chain F:



- Molecule 7: 50S ribosomal protein L6

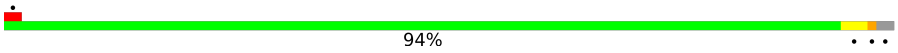
Chain G:





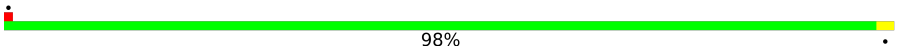
- Molecule 8: 50S ribosomal protein L13

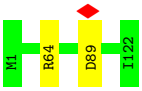
Chain J:



- Molecule 9: 50S ribosomal protein L14

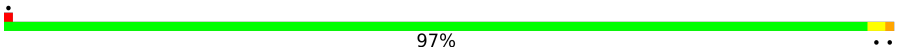
Chain K:

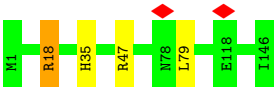




- Molecule 10: 50S ribosomal protein L15

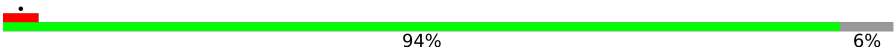
Chain L:

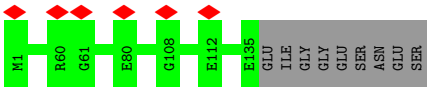




- Molecule 11: 50S ribosomal protein L16

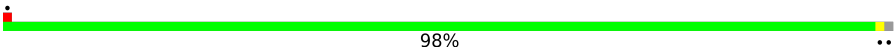
Chain M:

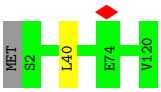




- Molecule 12: 50S ribosomal protein L17

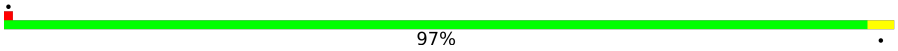
Chain N:

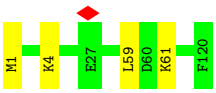




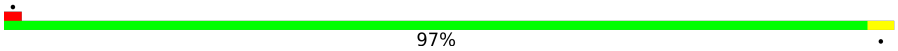
- Molecule 13: 50S ribosomal protein L18

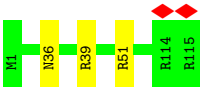
Chain O:



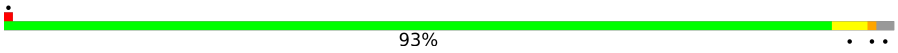


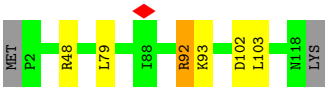
• Molecule 14: 50S ribosomal protein L19

Chain P: 

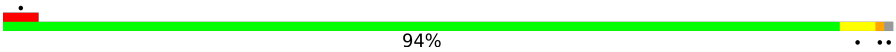


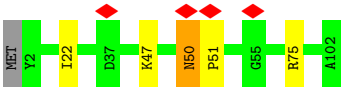
• Molecule 15: 50S ribosomal protein L20

Chain Q: 

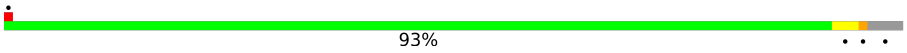


• Molecule 16: 50S ribosomal protein L21

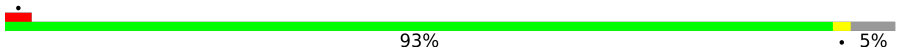
Chain R: 

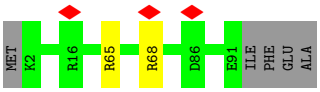


• Molecule 17: 50S ribosomal protein L22

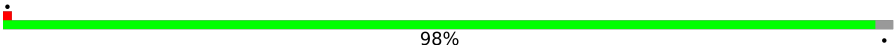
Chain S: 

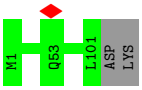
• Molecule 18: 50S ribosomal protein L23

Chain T: 



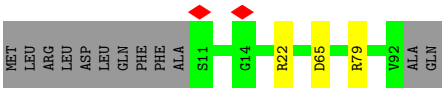
• Molecule 19: 50S ribosomal protein L24

Chain U: 



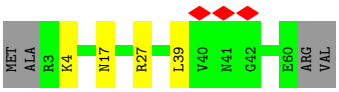
• Molecule 20: 50S ribosomal protein L27

Chain W: 84% 13%



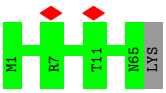
• Molecule 21: 50S ribosomal protein L28

Chain X: 5% 87% 6% 6%



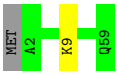
• Molecule 22: 50S ribosomal protein L29

Chain Y: 98%



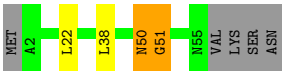
• Molecule 23: 50S ribosomal protein L30

Chain Z: 97%



• Molecule 24: 50S ribosomal protein L32

Chain 0: 85% 8%



• Molecule 25: 50S ribosomal protein L33 1

Chain 1: 98%

• Molecule 26: 50S ribosomal protein L34

Chain 2: 98%

• Molecule 27: 50S ribosomal protein L35

Chain 3: 94%

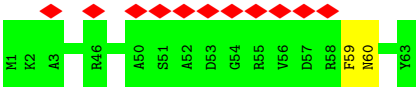
• Molecule 28: 50S ribosomal protein L36

Chain 4: 100%

There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L31

Chain 6: 17% 97%



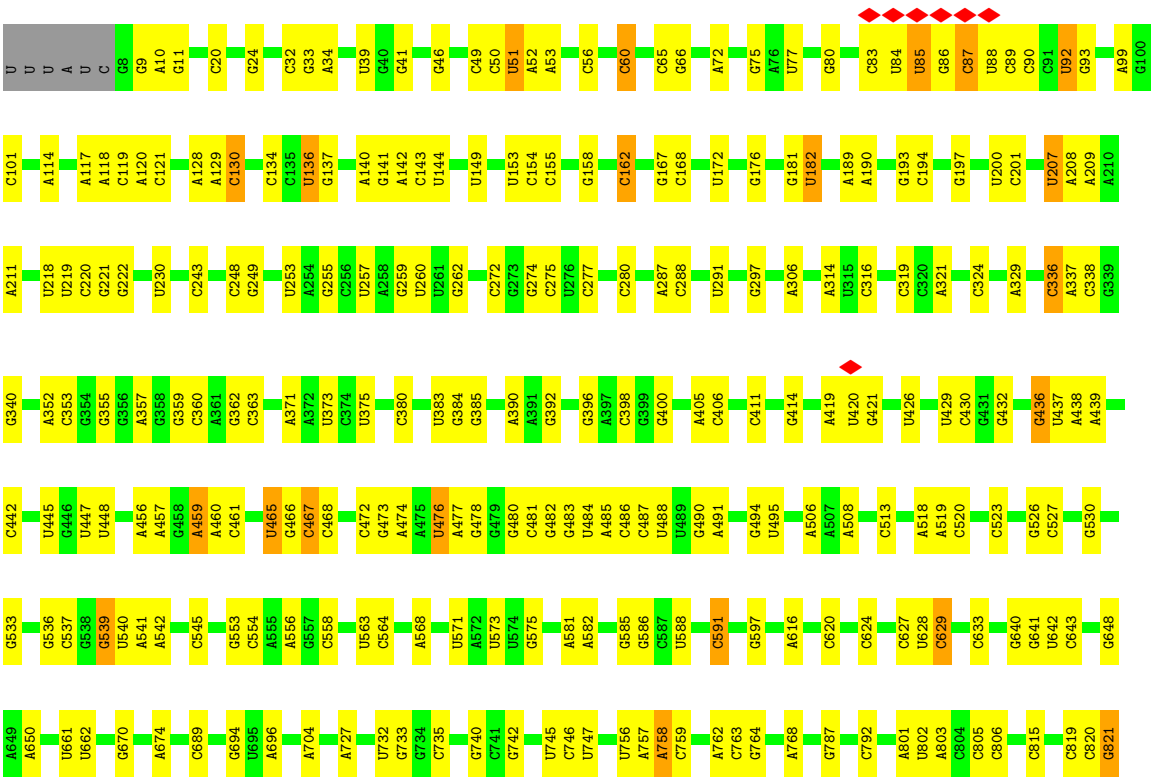
• Molecule 30: mRNA

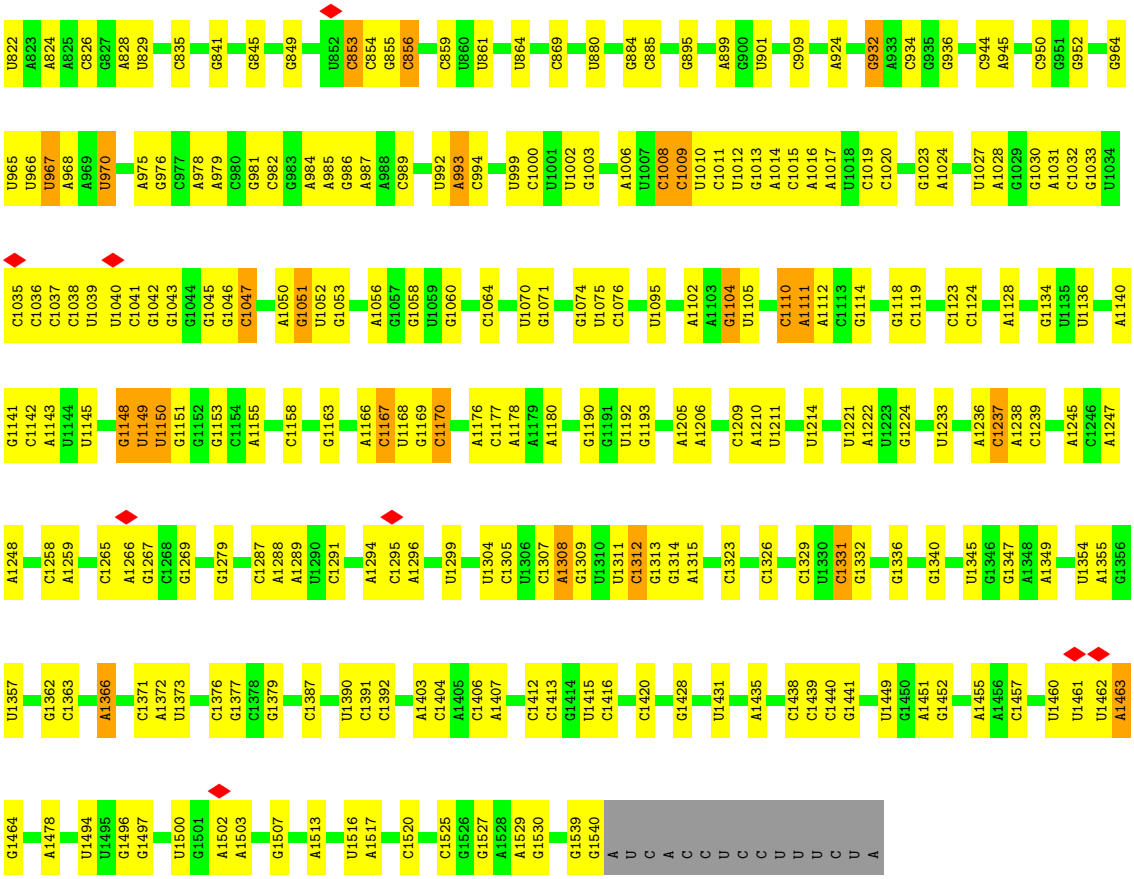
Chain 7: 100%

There are no outlier residues recorded for this chain.

• Molecule 31: 16S ribosomal RNA

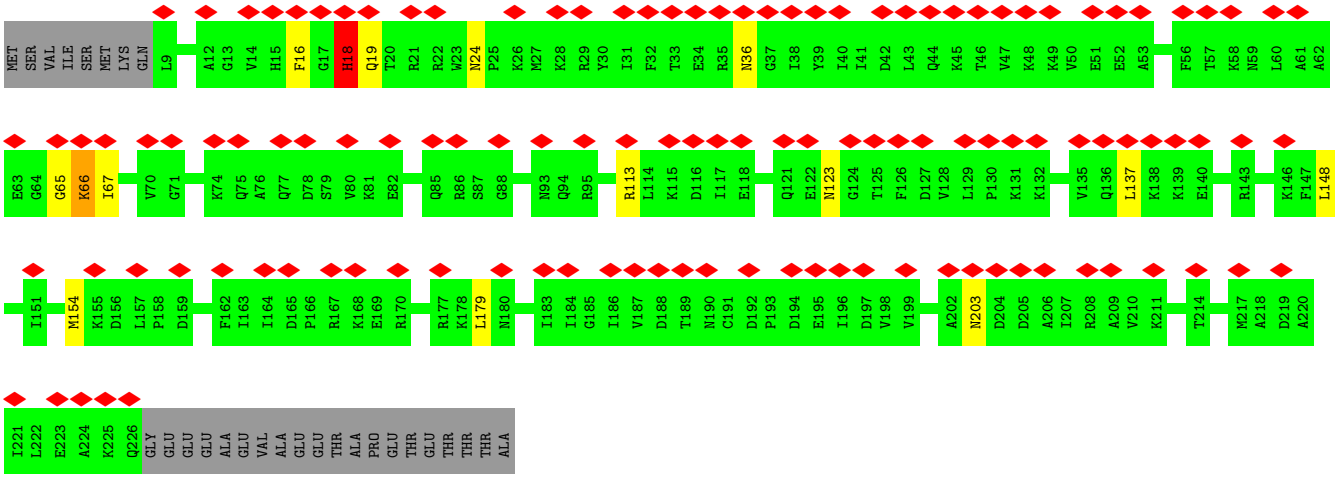
Chain a: 65% 30%





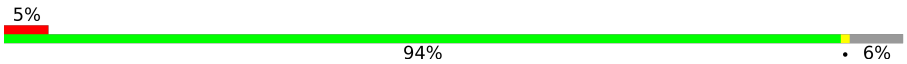
- Molecule 32: 30S ribosomal protein S2

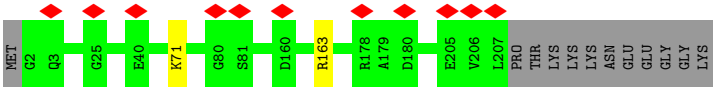
Chain b:



- Molecule 33: 30S ribosomal protein S3

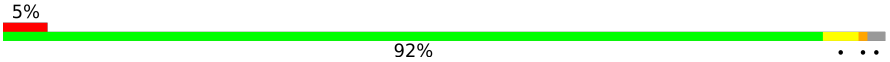
Chain c:

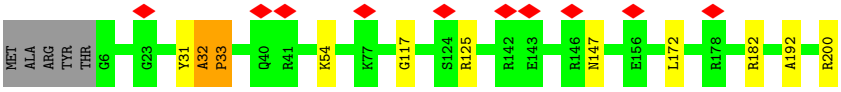




• Molecule 34: 30S ribosomal protein S4

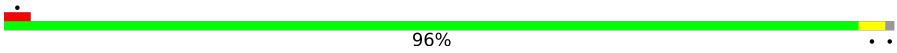
Chain d:

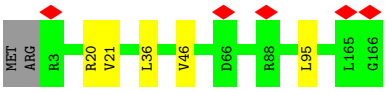




• Molecule 35: 30S ribosomal protein S5

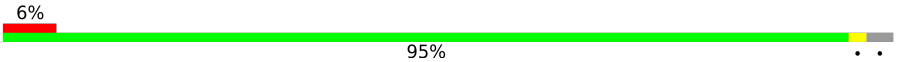
Chain e:

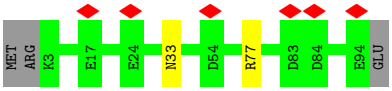




• Molecule 36: 30S ribosomal protein S6

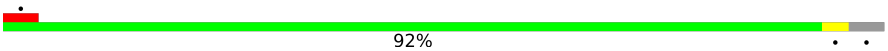
Chain f:

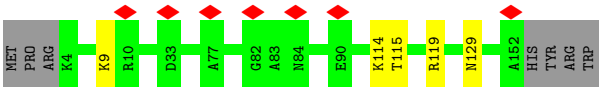




• Molecule 37: 30S ribosomal protein S7

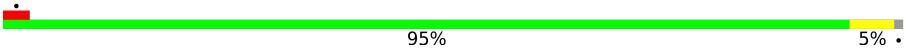
Chain g:

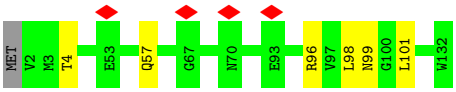




• Molecule 38: 30S ribosomal protein S8

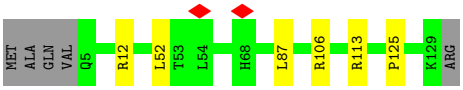
Chain h:





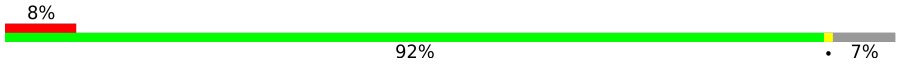
• Molecule 39: 30S ribosomal protein S9

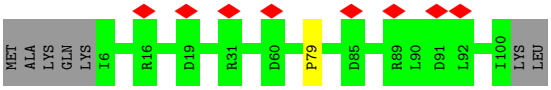
Chain i:



• Molecule 40: 30S ribosomal protein S10

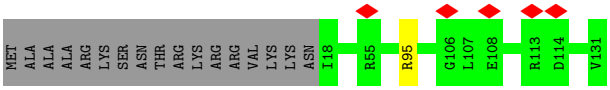
Chain j:





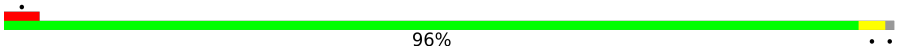
- Molecule 41: 30S ribosomal protein S11

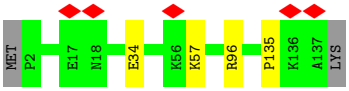
Chain k:



- Molecule 42: 30S ribosomal protein S12

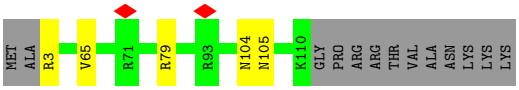
Chain l:





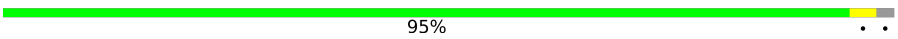
- Molecule 43: 30S ribosomal protein S13

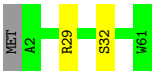
Chain m:



- Molecule 44: 30S ribosomal protein S14

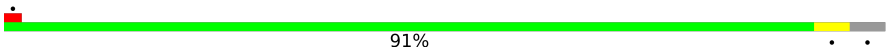
Chain n:

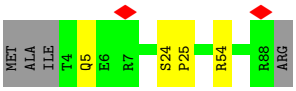




- Molecule 45: 30S ribosomal protein S15

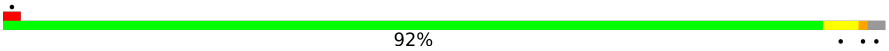
Chain o:

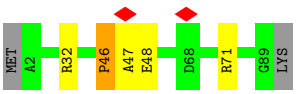




- Molecule 46: 30S ribosomal protein S16

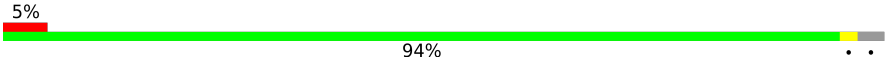
Chain p:





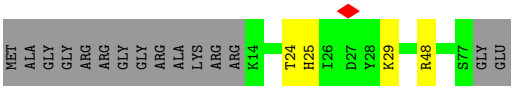
• Molecule 47: 30S ribosomal protein S17

Chain q:



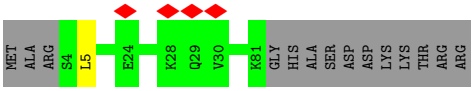
• Molecule 48: 30S ribosomal protein S18

Chain r:



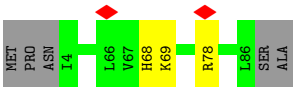
• Molecule 49: 30S ribosomal protein S19

Chain s:



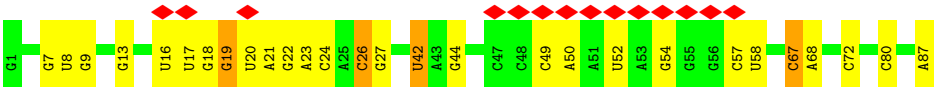
• Molecule 50: 30S ribosomal protein S20

Chain t:



• Molecule 51: P-tRNA

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.425	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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: TEL

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	0.69	2/69438 (0.0%)	1.17	488/108311 (0.5%)
2	B	0.54	0/2675	1.24	33/4170 (0.8%)
3	C	0.43	0/2120	0.65	0/2845
4	D	0.44	0/1591	0.65	0/2132
5	E	0.43	0/1580	0.67	2/2132 (0.1%)
6	F	0.38	0/1405	0.69	1/1887 (0.1%)
7	G	0.32	0/1360	0.59	0/1832
8	J	0.42	0/1146	0.71	1/1542 (0.1%)
9	K	0.44	0/927	0.73	1/1245 (0.1%)
10	L	0.42	0/1093	0.66	1/1457 (0.1%)
11	M	0.40	0/1099	0.60	0/1468
12	N	0.44	0/960	0.68	1/1284 (0.1%)
13	O	0.38	0/921	0.71	1/1236 (0.1%)
14	P	0.39	0/957	0.65	0/1279
15	Q	0.47	0/952	0.76	3/1266 (0.2%)
16	R	0.46	0/797	0.75	3/1070 (0.3%)
17	S	0.42	0/851	0.72	1/1146 (0.1%)
18	T	0.36	0/731	0.57	0/974
19	U	0.40	0/772	0.67	0/1032
20	W	0.44	0/638	0.73	1/847 (0.1%)
21	X	0.34	0/448	0.72	1/596 (0.2%)
22	Y	0.34	0/531	0.61	0/707
23	Z	0.36	0/457	0.68	0/613
24	0	0.42	0/433	0.73	0/574
25	1	0.42	0/406	0.62	0/540
26	2	0.41	0/370	0.60	0/483
27	3	0.40	0/519	0.59	0/680
28	4	0.40	0/299	0.59	0/393
29	6	0.33	0/509	0.58	0/678
30	7	0.52	0/65	1.28	0/98
31	a	0.82	0/36826	1.20	272/57450 (0.5%)
32	b	0.37	0/1782	0.69	2/2392 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.44	0/1641	0.65	0/2208
34	d	0.44	0/1598	0.72	1/2147 (0.0%)
35	e	0.47	1/1230 (0.1%)	0.73	0/1655
36	f	0.43	0/766	0.61	0/1031
37	g	0.40	0/1196	0.70	0/1604
38	h	0.47	0/1048	0.77	1/1407 (0.1%)
39	i	0.41	0/979	0.75	2/1315 (0.2%)
40	j	0.46	0/773	0.69	0/1044
41	k	0.37	0/852	0.62	0/1153
42	l	0.45	0/1069	0.72	0/1435
43	m	0.43	0/873	0.76	0/1166
44	n	0.49	0/507	0.80	0/672
45	o	0.41	0/718	0.63	0/960
46	p	0.47	0/708	0.75	1/950 (0.1%)
47	q	0.44	0/699	0.70	0/933
48	r	0.40	0/526	0.64	0/705
49	s	0.37	0/649	0.66	0/872
50	t	0.39	0/639	0.62	0/852
51	x	0.66	0/2080	1.22	11/3242 (0.3%)
All	All	0.66	3/153209 (0.0%)	1.08	828/229710 (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
3	C	0	1
4	D	0	1
6	F	0	3
8	J	0	1
10	L	0	2
13	O	0	1
15	Q	0	1
16	R	0	2
17	S	0	1
24	0	0	2
29	6	0	1
32	b	0	5
34	d	0	5
35	e	0	1
36	f	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	g	0	2
38	h	0	1
42	l	0	2
43	m	0	3
45	o	0	2
48	r	0	2
All	All	0	40

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	21	VAL	CB-CG1	-5.79	1.40	1.52
1	A	574	A	N9-C4	-5.57	1.34	1.37
1	A	631	G	N9-C4	-5.42	1.33	1.38

All (828) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2243	C	N1-C2-O2	10.80	125.38	118.90
1	A	756	U	N3-C2-O2	-10.77	114.66	122.20
31	a	1009	C	C2-N1-C1'	10.53	130.38	118.80
31	a	60	C	C6-N1-C2	-10.45	116.12	120.30
1	A	589	G	N1-C6-O6	-10.38	113.67	119.90
31	a	60	C	C5-C6-N1	10.24	126.12	121.00
31	a	989	C	C6-N1-C2	-10.13	116.25	120.30
31	a	1009	C	N1-C2-O2	10.08	124.95	118.90
1	A	589	G	C5-C6-O6	10.00	134.60	128.60
31	a	143	C	N1-C2-O2	9.99	124.89	118.90
31	a	747	U	C5-C6-N1	9.94	127.67	122.70
1	A	631	G	N3-C4-N9	-9.89	120.06	126.00
2	B	24	C	N1-C2-O2	9.85	124.81	118.90
1	A	589	G	N3-C4-N9	-9.72	120.17	126.00
31	a	1076	C	C2-N1-C1'	9.66	129.43	118.80
1	A	442	C	C5-C6-N1	9.44	125.72	121.00
1	A	1527	C	C2-N1-C1'	9.34	129.07	118.80
1	A	1028	C	N1-C2-O2	9.23	124.44	118.90
31	a	1331	C	C2-N1-C1'	9.17	128.89	118.80
1	A	2243	C	N3-C2-O2	-9.15	115.49	121.90
1	A	1527	C	N1-C2-O2	9.15	124.39	118.90
1	A	2054	C	C5-C6-N1	9.13	125.56	121.00
1	A	1476	C	C5-C6-N1	9.10	125.55	121.00
31	a	1076	C	C5-C6-N1	8.95	125.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1985	U	N3-C2-O2	-8.88	115.99	122.20
1	A	1366	C	C6-N1-C2	-8.86	116.76	120.30
31	a	1076	C	C6-N1-C2	-8.80	116.78	120.30
31	a	746	C	C6-N1-C2	-8.77	116.79	120.30
31	a	1305	C	N3-C2-O2	-8.77	115.76	121.90
1	A	442	C	C6-N1-C2	-8.76	116.80	120.30
1	A	2323	C	N1-C2-O2	8.72	124.14	118.90
31	a	143	C	N3-C2-O2	-8.69	115.82	121.90
31	a	1331	C	N1-C2-O2	8.69	124.11	118.90
1	A	2105	U	C2-N1-C1'	8.64	128.06	117.70
1	A	631	G	C4-N9-C1'	-8.63	115.28	126.50
1	A	1028	C	N3-C2-O2	-8.63	115.86	121.90
31	a	1305	C	N1-C2-O2	8.62	124.07	118.90
31	a	1076	C	N1-C2-O2	8.59	124.05	118.90
2	B	24	C	C2-N1-C1'	8.51	128.16	118.80
31	a	989	C	N3-C2-O2	-8.49	115.95	121.90
1	A	1353	C	C2-N1-C1'	8.44	128.08	118.80
1	A	2157	C	N1-C2-O2	8.39	123.94	118.90
1	A	769	A	N1-C6-N6	-8.38	113.57	118.60
1	A	2025	C	N1-C2-O2	8.35	123.91	118.90
1	A	573	C	N1-C2-O2	8.34	123.90	118.90
1	A	1817	C	C6-N1-C2	-8.31	116.97	120.30
1	A	508	C	C2-N1-C1'	8.30	127.93	118.80
1	A	2918	G	C4-N9-C1'	8.28	137.27	126.50
1	A	1943	C	N1-C2-O2	8.28	123.87	118.90
1	A	631	G	N3-C4-C5	8.27	132.73	128.60
31	a	537	C	N1-C2-O2	8.26	123.86	118.90
1	A	1872	C	C2-N1-C1'	8.21	127.83	118.80
1	A	2822	C	C2-N1-C1'	8.20	127.82	118.80
1	A	588	C	N1-C2-O2	8.19	123.81	118.90
1	A	2695	C	N1-C2-O2	8.18	123.81	118.90
2	B	62	U	N1-C2-O2	8.16	128.51	122.80
1	A	631	G	C8-N9-C1'	8.16	137.60	127.00
31	a	1009	C	C6-N1-C1'	-8.15	111.02	120.80
1	A	1985	U	N1-C2-O2	8.12	128.48	122.80
1	A	2485	C	C5-C6-N1	8.03	125.01	121.00
1	A	2092	C	C6-N1-C2	-8.02	117.09	120.30
1	A	875	U	C2-N1-C1'	7.95	127.24	117.70
2	B	24	C	N3-C2-O2	-7.95	116.33	121.90
2	B	62	U	N3-C2-O2	-7.94	116.64	122.20
51	x	49	C	N3-C2-O2	-7.94	116.34	121.90
31	a	853	C	N1-C2-O2	7.86	123.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	39	U	N3-C2-O2	-7.85	116.70	122.20
1	A	1476	C	C6-N1-C2	-7.85	117.16	120.30
1	A	272	C	N1-C2-O2	7.84	123.61	118.90
31	a	1331	C	N3-C2-O2	-7.79	116.44	121.90
2	B	62	U	C2-N1-C1'	7.79	127.05	117.70
1	A	1366	C	N1-C2-O2	7.74	123.55	118.90
1	A	211	C	C6-N1-C2	-7.72	117.21	120.30
1	A	2025	C	C2-N1-C1'	7.72	127.29	118.80
31	a	758	A	N7-C8-N9	7.71	117.65	113.80
2	B	79	C	N1-C2-O2	7.70	123.52	118.90
1	A	589	G	N9-C4-C5	7.67	108.47	105.40
1	A	422	C	C2-N1-C1'	7.66	127.22	118.80
31	a	481	C	C6-N1-C2	-7.62	117.25	120.30
1	A	2025	C	N3-C2-O2	-7.59	116.58	121.90
31	a	465	U	C2-N1-C1'	7.59	126.80	117.70
1	A	2054	C	C6-N1-C2	-7.58	117.27	120.30
1	A	2695	C	N3-C2-O2	-7.56	116.61	121.90
31	a	1149	U	N1-C2-O2	7.55	128.08	122.80
31	a	1149	U	N3-C2-O2	-7.54	116.92	122.20
1	A	589	G	C6-C5-N7	7.54	134.92	130.40
1	A	1369	C	C2-N1-C1'	7.50	127.06	118.80
1	A	719	C	C5-C6-N1	7.50	124.75	121.00
1	A	284	C	C6-N1-C2	-7.48	117.31	120.30
2	B	59	U	C2-N1-C1'	7.45	126.64	117.70
1	A	588	C	C2-N1-C1'	7.42	126.97	118.80
1	A	284	C	N3-C2-O2	-7.41	116.72	121.90
1	A	1831	A	N7-C8-N9	7.39	117.50	113.80
1	A	1353	C	C6-N1-C2	-7.39	117.34	120.30
1	A	397	U	N1-C2-O2	7.38	127.97	122.80
31	a	1441	G	O5'-P-OP1	-7.37	99.07	105.70
2	B	24	C	C6-N1-C2	-7.36	117.36	120.30
1	A	2323	C	C2-N1-C1'	7.34	126.88	118.80
1	A	769	A	N1-C2-N3	-7.34	125.63	129.30
1	A	1476	C	C2-N1-C1'	7.34	126.87	118.80
1	A	2774	C	C2-N1-C1'	7.33	126.86	118.80
31	a	486	C	C2-N1-C1'	7.30	126.84	118.80
1	A	1872	C	C5-C6-N1	7.26	124.63	121.00
1	A	1366	C	N3-C2-O2	-7.26	116.82	121.90
31	a	465	U	N1-C2-O2	7.25	127.88	122.80
1	A	1817	C	C5-C6-N1	7.25	124.62	121.00
31	a	60	C	C2-N1-C1'	7.24	126.77	118.80
31	a	1391	C	C6-N1-C2	-7.24	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2620	C	C6-N1-C2	-7.23	117.41	120.30
1	A	830	A	N7-C8-N9	7.22	117.41	113.80
51	x	49	C	N1-C2-O2	7.21	123.22	118.90
1	A	1366	C	C5-C6-N1	7.19	124.60	121.00
31	a	1331	C	C6-N1-C1'	-7.18	112.19	120.80
1	A	1817	C	C2-N1-C1'	7.17	126.69	118.80
1	A	1872	C	C6-N1-C2	-7.17	117.43	120.30
1	A	508	C	C5-C6-N1	7.16	124.58	121.00
31	a	101	C	N3-C2-O2	-7.15	116.89	121.90
1	A	1949	C	C5-C6-N1	7.14	124.57	121.00
1	A	2485	C	C6-N1-C2	-7.14	117.45	120.30
1	A	1949	C	C6-N1-C2	-7.13	117.45	120.30
1	A	397	U	N3-C2-O2	-7.10	117.23	122.20
31	a	136	U	C2-N1-C1'	7.08	126.19	117.70
1	A	1374	C	N1-C2-O2	7.06	123.14	118.90
31	a	1009	C	N3-C2-O2	-7.06	116.96	121.90
1	A	756	U	N1-C2-O2	7.06	127.74	122.80
13	O	59	LEU	CA-CB-CG	7.03	131.47	115.30
31	a	993	A	C2-N3-C4	7.02	114.11	110.60
1	A	1559	C	N1-C2-O2	7.02	123.11	118.90
31	a	746	C	C5-C6-N1	7.00	124.50	121.00
1	A	1352	U	C2-N1-C1'	6.98	126.08	117.70
1	A	2114	C	C2-N1-C1'	6.97	126.47	118.80
31	a	143	C	C2-N1-C1'	6.96	126.45	118.80
1	A	1527	C	C6-N1-C1'	-6.95	112.47	120.80
31	a	363	C	C6-N1-C2	-6.94	117.52	120.30
1	A	1327	U	N1-C2-O2	6.94	127.66	122.80
1	A	1450	C	C2-N1-C1'	6.94	126.43	118.80
31	a	101	C	N1-C2-O2	6.92	123.05	118.90
1	A	1527	C	N3-C2-O2	-6.92	117.06	121.90
1	A	1122	C	N1-C2-O2	6.90	123.04	118.90
1	A	885	C	N1-C2-O2	6.88	123.03	118.90
31	a	1047	C	C6-N1-C2	-6.88	117.55	120.30
1	A	2054	C	C2-N1-C1'	6.85	126.33	118.80
31	a	993	A	N3-C4-N9	6.83	132.87	127.40
1	A	1327	U	N3-C2-O2	-6.83	117.42	122.20
31	a	620	C	N1-C2-O2	6.83	123.00	118.90
1	A	831	U	N3-C2-O2	-6.79	117.45	122.20
31	a	1110	C	C6-N1-C2	-6.78	117.59	120.30
1	A	716	G	C4-N9-C1'	6.77	135.30	126.50
31	a	1149	U	C2-N1-C1'	6.77	125.82	117.70
31	a	982	C	C6-N1-C2	-6.76	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1707	U	N3-C2-O2	-6.76	117.47	122.20
1	A	2335	U	C6-N1-C2	-6.75	116.95	121.00
31	a	1167	C	C2-N1-C1'	6.74	126.21	118.80
31	a	629	C	N1-C2-O2	6.73	122.94	118.90
31	a	1391	C	N1-C2-O2	6.72	122.94	118.90
31	a	1438	C	C6-N1-C2	-6.72	117.61	120.30
1	A	1720	C	N1-C2-O2	6.71	122.93	118.90
1	A	1352	U	N1-C2-O2	6.67	127.47	122.80
1	A	777	C	C5-C6-N1	6.66	124.33	121.00
1	A	980	C	N1-C2-O2	6.66	122.89	118.90
51	x	42	U	N3-C2-O2	-6.65	117.54	122.20
1	A	1941	A	N7-C8-N9	6.65	117.12	113.80
1	A	2695	C	C2-N1-C1'	6.65	126.11	118.80
31	a	467	C	C2-N1-C1'	6.65	126.11	118.80
1	A	272	C	N3-C2-O2	-6.64	117.25	121.90
1	A	1943	C	N3-C2-O2	-6.64	117.25	121.90
1	A	309	U	C2-N1-C1'	6.63	125.66	117.70
1	A	2072	C	C5-C6-N1	6.62	124.31	121.00
1	A	2092	C	N3-C2-O2	-6.61	117.27	121.90
1	A	2918	G	C8-N9-C1'	-6.61	118.41	127.00
2	B	28	C	C6-N1-C2	-6.60	117.66	120.30
1	A	397	U	C2-N1-C1'	6.59	125.61	117.70
1	A	875	U	N1-C2-O2	6.58	127.40	122.80
1	A	1545	C	C2-N1-C1'	6.57	126.03	118.80
1	A	1247	G	O4'-C1'-N9	6.57	113.45	108.20
1	A	2157	C	C2-N1-C1'	6.57	126.03	118.80
31	a	1305	C	C6-N1-C2	-6.57	117.67	120.30
1	A	573	C	N3-C2-O2	-6.57	117.30	121.90
31	a	83	C	N1-C2-O2	6.57	122.84	118.90
1	A	508	C	C6-N1-C2	-6.57	117.67	120.30
10	L	79	LEU	CA-CB-CG	6.57	130.40	115.30
31	a	1366	A	N7-C8-N9	6.56	117.08	113.80
31	a	735	C	C6-N1-C2	-6.55	117.68	120.30
31	a	759	C	C6-N1-C2	-6.54	117.68	120.30
1	A	2157	C	N3-C2-O2	-6.52	117.33	121.90
1	A	2685	U	N3-C2-O2	-6.52	117.63	122.20
31	a	1449	U	N1-C2-O2	6.51	127.36	122.80
31	a	476	U	N1-C2-O2	6.51	127.36	122.80
1	A	830	A	C5-N7-C8	-6.50	100.65	103.90
31	a	1390	U	N3-C2-O2	-6.50	117.65	122.20
1	A	631	G	C6-C5-N7	6.50	134.30	130.40
31	a	1076	C	N3-C2-O2	-6.49	117.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	822	U	N1-C2-O2	6.49	127.34	122.80
51	x	49	C	C6-N1-C2	-6.49	117.70	120.30
1	A	1352	U	N3-C2-O2	-6.47	117.67	122.20
2	B	61	U	C2-N1-C1'	6.47	125.47	117.70
31	a	821	G	O4'-C1'-N9	6.46	113.37	108.20
1	A	1328	C	N1-C2-O2	6.46	122.78	118.90
31	a	476	U	C2-N1-C1'	6.46	125.45	117.70
31	a	155	C	C5-C6-N1	6.46	124.23	121.00
31	a	1439	C	N1-C2-O2	6.45	122.77	118.90
1	A	2503	C	N1-C2-O2	6.45	122.77	118.90
1	A	2487	U	N3-C2-O2	-6.44	117.69	122.20
1	A	769	A	C5-C6-N6	6.44	128.85	123.70
1	A	1567	U	OP1-P-O3'	6.44	119.37	105.20
1	A	573	C	C2-N1-C1'	6.44	125.88	118.80
31	a	465	U	N3-C2-O2	-6.43	117.70	122.20
31	a	336	C	N1-C2-O2	6.43	122.76	118.90
31	a	472	C	C6-N1-C2	-6.43	117.73	120.30
31	a	1460	U	N1-C2-O2	6.43	127.30	122.80
1	A	2323	C	C5-C6-N1	6.42	124.21	121.00
1	A	533	C	C6-N1-C2	-6.42	117.73	120.30
1	A	1353	C	C5-C6-N1	6.42	124.21	121.00
1	A	211	C	C5-C6-N1	6.42	124.21	121.00
1	A	1559	C	N3-C2-O2	-6.41	117.41	121.90
31	a	319	C	C6-N1-C2	-6.41	117.73	120.30
1	A	1327	U	C2-N1-C1'	6.41	125.39	117.70
1	A	483	C	C5-C6-N1	6.41	124.20	121.00
2	B	28	C	C5-C6-N1	6.39	124.20	121.00
1	A	8	U	C2-N1-C1'	6.39	125.36	117.70
2	B	79	C	N3-C2-O2	-6.38	117.43	121.90
31	a	1008	C	C6-N1-C2	-6.38	117.75	120.30
1	A	1757	G	O4'-C1'-N9	6.38	113.30	108.20
31	a	155	C	C2-N1-C1'	6.38	125.82	118.80
31	a	405	A	C2-N3-C4	6.37	113.78	110.60
31	a	1123	C	N1-C2-O2	6.35	122.71	118.90
1	A	2283	C	N1-C2-O2	6.35	122.71	118.90
1	A	977	U	C5-C6-N1	6.34	125.87	122.70
31	a	143	C	C6-N1-C2	-6.34	117.76	120.30
31	a	792	C	C6-N1-C2	-6.34	117.77	120.30
31	a	1440	C	C5-C6-N1	6.33	124.17	121.00
1	A	2665	U	C2-N1-C1'	6.33	125.29	117.70
1	A	2685	U	N1-C2-O2	6.32	127.22	122.80
31	a	1312	C	C6-N1-C2	-6.32	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1307	U	N3-C2-O2	-6.31	117.78	122.20
31	a	853	C	N3-C2-O2	-6.31	117.48	121.90
31	a	537	C	N3-C2-O2	-6.30	117.49	121.90
1	A	308	C	C2-N1-C1'	6.29	125.72	118.80
1	A	75	G	O4'-C1'-N9	6.29	113.23	108.20
1	A	2166	C	N1-C2-O2	6.28	122.67	118.90
1	A	2503	C	N3-C2-O2	-6.28	117.51	121.90
31	a	1158	C	C6-N1-C2	-6.27	117.79	120.30
1	A	2072	C	C6-N1-C2	-6.27	117.79	120.30
31	a	260	U	N3-C2-O2	-6.27	117.81	122.20
31	a	1390	U	N1-C2-O2	6.26	127.18	122.80
1	A	113	U	C2-N1-C1'	6.26	125.21	117.70
1	A	2073	C	C6-N1-C2	-6.26	117.80	120.30
31	a	763	C	C2-N1-C1'	6.26	125.69	118.80
1	A	1803	C	C6-N1-C2	-6.26	117.80	120.30
31	a	970	U	C2-N1-C1'	6.26	125.21	117.70
51	x	19	G	P-O3'-C3'	6.26	127.21	119.70
1	A	1946	U	C5-C6-N1	6.26	125.83	122.70
1	A	589	G	C4-C5-N7	-6.25	108.30	110.80
1	A	789	C	C6-N1-C2	-6.25	117.80	120.30
1	A	1731	C	N1-C2-O2	6.25	122.65	118.90
31	a	1051	G	N3-C4-N9	6.25	129.75	126.00
1	A	2105	U	N1-C2-O2	6.24	127.17	122.80
31	a	1111	A	P-O3'-C3'	6.24	127.19	119.70
9	K	89	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	670	C	C6-N1-C2	-6.23	117.81	120.30
1	A	1577	C	C6-N1-C2	-6.22	117.81	120.30
31	a	1008	C	N1-C2-O2	6.22	122.63	118.90
1	A	681	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2349	A	C2-N3-C4	6.22	113.71	110.60
1	A	716	G	C8-N9-C1'	-6.22	118.92	127.00
1	A	2105	U	N3-C2-O2	-6.21	117.85	122.20
1	A	719	C	C6-N1-C2	-6.21	117.81	120.30
31	a	1415	U	N3-C2-O2	-6.21	117.85	122.20
1	A	588	C	N3-C2-O2	-6.21	117.56	121.90
1	A	936	C	N1-C2-O2	6.21	122.62	118.90
1	A	2296	A	O5'-P-OP1	-6.20	100.12	105.70
31	a	56	C	N1-C2-O2	6.20	122.62	118.90
1	A	422	C	C6-N1-C2	-6.19	117.82	120.30
31	a	1032	C	C6-N1-C2	-6.19	117.83	120.30
31	a	467	C	C5-C6-N1	6.19	124.09	121.00
31	a	1416	C	N3-C2-O2	-6.18	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1119	C	C6-N1-C2	-6.18	117.83	120.30
31	a	1460	U	N3-C2-O2	-6.18	117.87	122.20
1	A	1476	C	N1-C2-O2	6.18	122.61	118.90
1	A	895	G	N3-C4-N9	6.18	129.71	126.00
1	A	445	C	C5-C6-N1	6.17	124.09	121.00
31	a	1357	U	N1-C2-O2	6.17	127.12	122.80
1	A	2094	C	C5-C6-N1	6.17	124.09	121.00
1	A	936	C	C2-N1-C1'	6.17	125.59	118.80
1	A	482	C	O4'-C1'-N1	6.16	113.13	108.20
31	a	495	U	N1-C2-O2	6.16	127.11	122.80
1	A	2255	C	N1-C2-O2	6.16	122.59	118.90
31	a	1016	A	P-O3'-C3'	6.16	127.09	119.70
31	a	1037	C	N1-C2-O2	6.16	122.59	118.90
1	A	1781	C	C6-N1-C2	-6.15	117.84	120.30
31	a	136	U	N1-C2-O2	6.15	127.11	122.80
31	a	545	C	C6-N1-C2	-6.15	117.84	120.30
1	A	810	G	OP1-P-O3'	6.15	118.73	105.20
1	A	1028	C	C6-N1-C2	-6.14	117.84	120.30
1	A	1036	A	C8-N9-C4	-6.14	103.34	105.80
31	a	822	U	N3-C2-O2	-6.14	117.90	122.20
2	B	28	C	N1-C2-O2	6.14	122.58	118.90
32	b	18	HIS	C-N-CA	6.14	137.06	121.70
31	a	136	U	C5-C6-N1	6.13	125.77	122.70
1	A	593	A	C2-N3-C4	6.13	113.66	110.60
1	A	769	A	C6-N1-C2	6.12	122.27	118.60
31	a	989	C	N1-C2-O2	6.12	122.57	118.90
31	a	1391	C	N3-C2-O2	-6.12	117.62	121.90
2	B	108	C	C5-C6-N1	6.11	124.06	121.00
31	a	448	U	N1-C2-O2	6.11	127.08	122.80
1	A	483	C	C6-N1-C2	-6.11	117.86	120.30
1	A	589	G	C8-N9-C1'	6.10	134.93	127.00
1	A	2243	C	C2-N1-C1'	6.09	125.50	118.80
31	a	523	C	C5-C6-N1	6.09	124.04	121.00
1	A	1028	C	C2-N1-C1'	6.07	125.48	118.80
31	a	1392	C	C6-N1-C2	-6.07	117.87	120.30
1	A	2820	U	C2-N1-C1'	6.07	124.98	117.70
1	A	1122	C	C6-N1-C2	-6.06	117.88	120.30
1	A	1353	C	N1-C2-O2	6.06	122.54	118.90
1	A	2789	C	C6-N1-C2	-6.06	117.88	120.30
1	A	1634	U	N3-C2-O2	-6.06	117.96	122.20
31	a	1366	A	C8-N9-C4	-6.06	103.38	105.80
21	X	39	LEU	CA-CB-CG	6.06	129.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1941	A	C8-N9-C4	-6.05	103.38	105.80
31	a	854	C	N1-C2-O2	6.05	122.53	118.90
1	A	783	C	C6-N1-C2	-6.04	117.88	120.30
31	a	1070	U	C5-C6-N1	6.04	125.72	122.70
31	a	820	C	N1-C2-O2	6.04	122.52	118.90
31	a	1008	C	C2-N1-C1'	6.04	125.44	118.80
31	a	1457	C	C2-N1-C1'	6.03	125.43	118.80
31	a	1438	C	N3-C2-O2	-6.02	117.68	121.90
1	A	2695	C	C6-N1-C2	-6.02	117.89	120.30
2	B	24	C	C5-C6-N1	6.02	124.01	121.00
1	A	1631	A	P-O3'-C3'	6.02	126.92	119.70
1	A	2203	C	C5-C6-N1	6.01	124.01	121.00
1	A	2774	C	N1-C2-O2	6.01	122.50	118.90
1	A	1307	U	N1-C2-O2	6.00	127.00	122.80
1	A	2073	C	C5-C6-N1	6.00	124.00	121.00
1	A	933	C	P-O3'-C3'	6.00	126.89	119.70
2	B	15	C	N1-C2-O2	5.99	122.50	118.90
31	a	513	C	C5-C6-N1	5.99	124.00	121.00
1	A	201	C	C6-N1-C2	-5.98	117.91	120.30
1	A	1577	C	C2-N1-C1'	5.98	125.38	118.80
31	a	989	C	C2-N1-C1'	5.98	125.38	118.80
2	B	59	U	N1-C2-O2	5.97	126.98	122.80
31	a	85	U	C2-N1-C1'	5.97	124.87	117.70
31	a	970	U	N1-C2-O2	5.97	126.98	122.80
31	a	1038	C	C5-C6-N1	5.97	123.99	121.00
1	A	1450	C	C6-N1-C2	-5.97	117.91	120.30
1	A	2614	U	N1-C2-O2	5.97	126.98	122.80
1	A	422	C	C5-C6-N1	5.96	123.98	121.00
31	a	1076	C	C6-N1-C1'	-5.95	113.66	120.80
1	A	734	C	N1-C2-O2	5.95	122.47	118.90
31	a	363	C	C5-C6-N1	5.95	123.97	121.00
1	A	831	U	N1-C2-O2	5.94	126.96	122.80
31	a	130	C	N1-C2-O2	5.94	122.47	118.90
31	a	272	C	C6-N1-C2	-5.93	117.93	120.30
1	A	2131	U	N1-C2-O2	5.93	126.95	122.80
31	a	476	U	N3-C2-O2	-5.92	118.05	122.20
1	A	830	A	C8-N9-C4	-5.92	103.43	105.80
2	B	31	G	C4-N9-C1'	5.92	134.19	126.50
31	a	468	C	C6-N1-C2	-5.91	117.94	120.30
1	A	1656	C	N1-C2-O2	5.91	122.44	118.90
1	A	1699	A	O4'-C1'-N9	5.91	112.93	108.20
1	A	2733	C	C5-C6-N1	5.90	123.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2774	C	C6-N1-C2	-5.90	117.94	120.30
1	A	1872	C	N1-C2-O2	5.89	122.44	118.90
31	a	1438	C	N1-C2-O2	5.89	122.44	118.90
1	A	1339	A	P-O3'-C3'	5.89	126.76	119.70
31	a	970	U	N3-C2-O2	-5.89	118.08	122.20
1	A	975	C	C2-N1-C1'	5.88	125.27	118.80
1	A	875	U	N3-C2-O2	-5.88	118.08	122.20
1	A	2822	C	C6-N1-C2	-5.87	117.95	120.30
1	A	2345	U	C2-N1-C1'	5.87	124.74	117.70
31	a	1287	C	N1-C2-O2	5.87	122.42	118.90
1	A	398	U	N3-C2-O2	-5.86	118.09	122.20
1	A	2203	C	C2-N1-C1'	5.86	125.24	118.80
1	A	2350	G	N3-C4-N9	5.86	129.51	126.00
31	a	1439	C	N3-C2-O2	-5.86	117.80	121.90
1	A	2025	C	C6-N1-C1'	-5.85	113.78	120.80
1	A	2614	U	N3-C2-O2	-5.85	118.11	122.20
1	A	589	G	C4-N9-C1'	-5.84	118.90	126.50
31	a	336	C	N3-C2-O2	-5.84	117.81	121.90
32	b	137	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	1452	C	C6-N1-C2	-5.84	117.96	120.30
1	A	2102	C	N1-C2-O2	5.84	122.40	118.90
2	B	15	C	C2-N1-C1'	5.84	125.22	118.80
31	a	248	C	O4'-C1'-N1	5.84	112.87	108.20
1	A	1702	U	O5'-P-OP1	-5.83	100.45	105.70
1	A	272	C	C2-N1-C1'	5.83	125.21	118.80
31	a	486	C	N1-C2-O2	5.83	122.40	118.90
1	A	2295	A	O4'-C1'-N9	-5.83	103.54	108.20
1	A	1522	U	N1-C2-O2	5.82	126.88	122.80
1	A	201	C	C5-C6-N1	5.82	123.91	121.00
1	A	2795	G	C4-N9-C1'	5.82	134.06	126.50
31	a	411	C	C5-C6-N1	5.82	123.91	121.00
1	A	895	G	N3-C4-C5	-5.81	125.69	128.60
1	A	2335	U	C5-C6-N1	5.81	125.61	122.70
1	A	686	C	C5-C6-N1	5.81	123.91	121.00
31	a	1170	C	N3-C2-O2	-5.81	117.83	121.90
2	B	31	G	C8-N9-C1'	-5.80	119.46	127.00
1	A	2822	C	C5-C6-N1	5.80	123.90	121.00
1	A	1634	U	N1-C2-O2	5.80	126.86	122.80
1	A	1374	C	N3-C2-O2	-5.80	117.84	121.90
1	A	1720	C	N3-C2-O2	-5.80	117.84	121.90
31	a	398	C	C6-N1-C2	-5.80	117.98	120.30
1	A	2155	A	P-O3'-C3'	5.79	126.65	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1817	C	N1-C2-O2	5.79	122.37	118.90
31	a	1045	G	N9-C4-C5	-5.79	103.08	105.40
1	A	271	C	C6-N1-C2	-5.78	117.99	120.30
1	A	2631	A	P-O3'-C3'	5.78	126.64	119.70
51	x	57	C	C5-C6-N1	5.78	123.89	121.00
1	A	1122	C	N3-C2-O2	-5.78	117.86	121.90
31	a	1404	C	N1-C2-O2	5.78	122.36	118.90
1	A	445	C	C6-N1-C2	-5.77	117.99	120.30
1	A	1771	C	C2-N1-C1'	5.77	125.15	118.80
31	a	136	U	N3-C2-O2	-5.77	118.16	122.20
1	A	1708	U	N1-C2-O2	5.77	126.84	122.80
1	A	778	C	C6-N1-C2	-5.77	117.99	120.30
31	a	155	C	N1-C2-O2	5.77	122.36	118.90
1	A	1343	C	C2-N1-C1'	5.77	125.14	118.80
6	F	91	LEU	CA-CB-CG	5.76	128.56	115.30
31	a	467	C	C6-N1-C2	-5.76	117.99	120.30
1	A	2254	A	P-O3'-C3'	5.76	126.61	119.70
15	Q	103	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	586	C	N3-C2-O2	-5.76	117.87	121.90
1	A	2105	U	C6-N1-C1'	-5.76	113.14	121.20
31	a	1449	U	N3-C2-O2	-5.75	118.17	122.20
31	a	1391	C	C2-N1-C1'	5.75	125.13	118.80
51	x	26	C	C2-N1-C1'	5.75	125.13	118.80
1	A	2479	A	N1-C2-N3	-5.75	126.43	129.30
1	A	586	C	N1-C2-O2	5.74	122.34	118.90
1	A	1831	A	C5-N7-C8	-5.74	101.03	103.90
1	A	1065	U	N3-C2-O2	-5.73	118.19	122.20
2	B	29	C	C6-N1-C2	-5.73	118.01	120.30
31	a	1404	C	N3-C2-O2	-5.73	117.89	121.90
1	A	1415	C	N1-C2-O2	5.73	122.34	118.90
1	A	445	C	N1-C2-O2	5.73	122.34	118.90
1	A	757	C	C5-C6-N1	5.72	123.86	121.00
1	A	2092	C	C2-N1-C1'	5.71	125.08	118.80
1	A	2334	U	N1-C2-O2	5.71	126.80	122.80
1	A	789	C	C5-C6-N1	5.70	123.85	121.00
1	A	2485	C	C2-N1-C1'	5.70	125.07	118.80
31	a	869	C	N1-C2-O2	5.70	122.32	118.90
1	A	1781	C	C5-C6-N1	5.69	123.85	121.00
31	a	1438	C	C2-N1-C1'	5.69	125.06	118.80
31	a	993	A	N3-C4-C5	-5.69	122.82	126.80
1	A	1036	A	N7-C8-N9	5.68	116.64	113.80
31	a	1363	C	C6-N1-C2	-5.68	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1831	A	C8-N9-C4	-5.68	103.53	105.80
1	A	2789	C	C5-C6-N1	5.67	123.83	121.00
31	a	967	U	C2-N1-C1'	5.67	124.51	117.70
31	a	1051	G	C4-N9-C1'	5.67	133.87	126.50
1	A	931	C	C2-N1-C1'	5.67	125.03	118.80
1	A	1731	C	N3-C2-O2	-5.66	117.94	121.90
1	A	2765	G	C4-N9-C1'	5.66	133.86	126.50
1	A	2452	U	N3-C2-O2	-5.66	118.24	122.20
1	A	1577	C	C5-C6-N1	5.66	123.83	121.00
1	A	2768	U	N1-C2-O2	5.66	126.76	122.80
1	A	1803	C	N3-C2-O2	-5.66	117.94	121.90
1	A	2503	C	C6-N1-C2	-5.66	118.04	120.30
2	B	29	C	C2-N1-C1'	5.65	125.02	118.80
1	A	885	C	N3-C2-O2	-5.65	117.95	121.90
31	a	1308	A	N3-C4-N9	5.65	131.92	127.40
31	a	1416	C	N1-C2-O2	5.65	122.29	118.90
31	a	523	C	C6-N1-C2	-5.64	118.04	120.30
31	a	864	U	N3-C2-O2	-5.64	118.25	122.20
31	a	994	C	C6-N1-C2	-5.64	118.04	120.30
1	A	104	C	N3-C2-O2	-5.64	117.95	121.90
1	A	875	U	C6-N1-C1'	-5.64	113.31	121.20
1	A	2323	C	C6-N1-C2	-5.63	118.05	120.30
31	a	1412	C	C5-C6-N1	5.63	123.82	121.00
31	a	1525	C	C5-C6-N1	5.63	123.82	121.00
31	a	436	G	O4'-C1'-N9	5.63	112.70	108.20
1	A	670	C	C5-C6-N1	5.62	123.81	121.00
31	a	1123	C	N3-C2-O2	-5.62	117.97	121.90
31	a	747	U	C6-N1-C2	-5.61	117.63	121.00
31	a	130	C	C6-N1-C2	-5.61	118.06	120.30
31	a	207	U	C5-C6-N1	5.61	125.50	122.70
1	A	2918	G	N3-C4-C5	-5.61	125.80	128.60
1	A	1184	G	N1-C6-O6	-5.60	116.54	119.90
1	A	398	U	N1-C2-O2	5.60	126.72	122.80
31	a	633	C	N3-C2-O2	-5.60	117.98	121.90
1	A	980	C	N3-C2-O2	-5.59	117.98	121.90
1	A	2822	C	C6-N1-C1'	-5.59	114.09	120.80
31	a	1315	A	N7-C8-N9	5.59	116.60	113.80
1	A	1527	C	C5-C6-N1	5.59	123.79	121.00
1	A	1366	C	C2-N1-C1'	5.58	124.94	118.80
1	A	287	G	C6-N1-C2	-5.58	121.75	125.10
1	A	556	C	C2-N1-C1'	5.58	124.94	118.80
1	A	1805	G	C4-N9-C1'	5.58	133.75	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	C	C6-N1-C2	-5.58	118.07	120.30
1	A	735	U	C5-C6-N1	5.58	125.49	122.70
1	A	2334	U	C2-N1-C1'	5.58	124.39	117.70
1	A	387	C	C5-C6-N1	5.57	123.78	121.00
1	A	113	U	C5-C6-N1	5.57	125.48	122.70
1	A	2768	U	N3-C2-O2	-5.57	118.30	122.20
1	A	2452	U	N1-C2-O2	5.56	126.69	122.80
1	A	2791	U	C2-N1-C1'	5.56	124.37	117.70
1	A	8	U	C5-C6-N1	5.55	125.48	122.70
1	A	1963	C	C6-N1-C2	-5.55	118.08	120.30
1	A	2695	C	O4'-C1'-N1	5.55	112.64	108.20
31	a	155	C	C6-N1-C2	-5.55	118.08	120.30
1	A	719	C	C2-N1-C1'	5.55	124.91	118.80
1	A	2255	C	C6-N1-C2	-5.55	118.08	120.30
1	A	1374	C	C2-N1-C1'	5.55	124.91	118.80
1	A	2094	C	C6-N1-C2	-5.55	118.08	120.30
1	A	88	G	P-O3'-C3'	5.55	126.36	119.70
1	A	2316	A	P-O3'-C3'	5.55	126.36	119.70
2	B	61	U	N1-C2-O2	5.54	126.68	122.80
31	a	819	C	C6-N1-C2	-5.54	118.08	120.30
1	A	1296	G	C4-N9-C1'	5.54	133.70	126.50
1	A	732	A	P-O3'-C3'	5.53	126.34	119.70
1	A	1369	C	C6-N1-C1'	-5.53	114.16	120.80
31	a	162	C	N1-C2-O2	5.53	122.22	118.90
31	a	486	C	C6-N1-C2	-5.53	118.09	120.30
1	A	783	C	C5-C6-N1	5.52	123.76	121.00
1	A	777	C	C6-N1-C2	-5.52	118.09	120.30
31	a	1210	A	P-O3'-C3'	5.52	126.33	119.70
1	A	1990	C	N1-C2-O2	5.52	122.21	118.90
31	a	994	C	C5-C6-N1	5.51	123.76	121.00
31	a	1045	G	C4-C5-N7	5.51	113.01	110.80
1	A	309	U	OP1-P-O3'	5.51	117.33	105.20
1	A	589	G	N3-C4-C5	5.51	131.35	128.60
31	a	1520	C	C6-N1-C2	-5.51	118.10	120.30
31	a	1037	C	C6-N1-C2	-5.50	118.10	120.30
31	a	1237	C	N3-C2-O2	-5.50	118.05	121.90
1	A	2665	U	N1-C2-O2	5.50	126.65	122.80
31	a	633	C	N1-C2-O2	5.50	122.20	118.90
1	A	2452	U	C2-N1-C1'	5.50	124.30	117.70
39	i	52	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	2277	C	C6-N1-C2	-5.49	118.10	120.30
1	A	2092	C	N1-C2-O2	5.49	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2833	U	N3-C2-O2	-5.49	118.36	122.20
1	A	576	G	P-O3'-C3'	5.49	126.29	119.70
1	A	1351	U	P-O3'-C3'	5.49	126.28	119.70
31	a	448	U	N3-C2-O2	-5.49	118.36	122.20
1	A	594	C	C5-C6-N1	5.49	123.74	121.00
1	A	1631	A	OP1-P-O3'	5.49	117.27	105.20
2	B	15	C	C5-C6-N1	5.47	123.74	121.00
31	a	629	C	N3-C2-O2	-5.47	118.07	121.90
1	A	2445	C	C6-N1-C2	-5.47	118.11	120.30
1	A	594	C	C6-N1-C2	-5.47	118.11	120.30
1	A	204	C	C6-N1-C2	-5.47	118.11	120.30
1	A	1714	A	C2-N3-C4	5.47	113.33	110.60
5	E	192	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	A	672	C	C6-N1-C2	-5.47	118.11	120.30
31	a	967	U	N1-C2-O2	5.47	126.63	122.80
31	a	1357	U	N3-C2-O2	-5.46	118.38	122.20
31	a	56	C	N3-C2-O2	-5.46	118.08	121.90
1	A	631	G	N3-C2-N2	-5.46	116.08	119.90
38	h	101	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	2805	A	P-O3'-C3'	5.46	126.25	119.70
1	A	2833	U	N1-C2-O2	5.46	126.62	122.80
31	a	467	C	N1-C2-O2	5.46	122.17	118.90
31	a	758	A	C8-N9-C4	-5.46	103.62	105.80
1	A	810	G	C4-N9-C1'	5.45	133.59	126.50
12	N	40	LEU	CB-CG-CD1	-5.45	101.73	111.00
2	B	59	U	C5-C6-N1	5.45	125.42	122.70
1	A	2072	C	C2-N1-C1'	5.45	124.79	118.80
31	a	495	U	C2-N3-C4	5.45	130.27	127.00
1	A	2255	C	C5-C6-N1	5.44	123.72	121.00
1	A	1484	U	C5-C6-N1	5.44	125.42	122.70
1	A	442	C	C2-N3-C4	5.43	122.62	119.90
1	A	1296	G	C8-N9-C1'	-5.43	119.94	127.00
31	a	291	U	N1-C2-O2	5.43	126.60	122.80
1	A	1752	G	N3-C4-N9	5.43	129.26	126.00
31	a	1008	C	N3-C2-O2	-5.43	118.10	121.90
17	S	38	LEU	C-N-CA	5.43	135.27	121.70
1	A	1274	U	N1-C2-O2	5.43	126.60	122.80
1	A	508	C	C6-N1-C1'	-5.42	114.29	120.80
1	A	2348	C	C2-N1-C1'	5.42	124.77	118.80
31	a	805	C	N1-C2-O2	5.42	122.15	118.90
1	A	478	U	N3-C2-O2	-5.42	118.40	122.20
1	A	631	G	N1-C2-N2	5.42	121.08	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	168	C	N1-C2-O2	5.42	122.15	118.90
1	A	1883	A	N7-C8-N9	5.42	116.51	113.80
1	A	2348	C	N1-C2-O2	5.42	122.15	118.90
31	a	932	G	N1-C6-O6	-5.42	116.65	119.90
1	A	2685	U	C2-N1-C1'	5.42	124.20	117.70
1	A	2423	C	C5-C6-N1	5.41	123.71	121.00
1	A	1597	C	N1-C2-O2	5.41	122.15	118.90
31	a	130	C	N3-C2-O2	-5.41	118.11	121.90
1	A	2223	U	N1-C2-O2	5.41	126.59	122.80
1	A	534	C	N1-C2-O2	5.41	122.14	118.90
1	A	1328	C	N3-C2-O2	-5.41	118.11	121.90
31	a	620	C	N3-C2-O2	-5.41	118.11	121.90
1	A	914	C	N1-C2-O2	5.41	122.14	118.90
31	a	967	U	N3-C2-O2	-5.41	118.42	122.20
51	x	67	C	C5-C6-N1	5.40	123.70	121.00
1	A	62	C	P-O3'-C3'	5.40	126.18	119.70
1	A	1241	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1559	C	C2-N1-C1'	5.39	124.73	118.80
1	A	2295	A	P-O3'-C3'	5.39	126.17	119.70
1	A	2825	C	C5-C6-N1	5.39	123.69	121.00
1	A	2349	A	N3-C4-N9	5.39	131.71	127.40
1	A	2323	C	N3-C2-O2	-5.39	118.13	121.90
1	A	2114	C	C6-N1-C2	-5.38	118.15	120.30
1	A	2131	U	C2-N1-C1'	5.38	124.16	117.70
31	a	1037	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1844	A	OP1-P-O3'	5.37	117.01	105.20
1	A	1148	C	N1-C2-O2	5.37	122.12	118.90
1	A	1344	C	C6-N1-C2	-5.36	118.16	120.30
16	R	75	ARG	NE-CZ-NH2	5.36	122.98	120.30
31	a	982	C	N3-C2-O2	-5.36	118.15	121.90
1	A	2223	U	C2-N1-C1'	5.35	124.12	117.70
31	a	1150	U	C2-N1-C1'	5.35	124.12	117.70
1	A	1067	A	C5-N7-C8	-5.35	101.22	103.90
1	A	2733	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2114	C	C5-C6-N1	5.35	123.67	121.00
31	a	243	C	N1-C2-O2	5.35	122.11	118.90
31	a	445	U	C5-C6-N1	5.35	125.37	122.70
31	a	1308	A	C2-N3-C4	5.35	113.27	110.60
1	A	735	U	C5-C4-O4	-5.34	122.69	125.90
5	E	126	LEU	CB-CG-CD1	-5.34	101.91	111.00
31	a	1038	C	C6-N1-C2	-5.34	118.16	120.30
2	B	59	U	N3-C2-O2	-5.34	118.47	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	486	C	C5-C6-N1	5.34	123.67	121.00
31	a	1104	G	O4'-C1'-N9	5.33	112.47	108.20
1	A	1369	C	N1-C2-O2	5.33	122.10	118.90
1	A	2358	A	C5-N7-C8	-5.33	101.23	103.90
1	A	1567	U	P-O3'-C3'	5.33	126.10	119.70
1	A	2604	C	C6-N1-C2	-5.33	118.17	120.30
31	a	319	C	C5-C6-N1	5.33	123.67	121.00
1	A	2229	C	C6-N1-C2	-5.33	118.17	120.30
31	a	689	C	N3-C2-O2	-5.33	118.17	121.90
1	A	588	C	C6-N1-C1'	-5.32	114.41	120.80
1	A	1883	A	C8-N9-C4	-5.32	103.67	105.80
1	A	2822	C	N1-C2-O2	5.32	122.09	118.90
31	a	1237	C	N1-C2-O2	5.32	122.09	118.90
1	A	8	U	N1-C2-O2	5.31	126.52	122.80
1	A	1573	C	C6-N1-C2	-5.31	118.17	120.30
1	A	2114	C	N1-C2-O2	5.31	122.09	118.90
2	B	24	C	C6-N1-C1'	-5.31	114.43	120.80
1	A	2918	G	C8-N9-C4	-5.31	104.28	106.40
31	a	448	U	C5-C6-N1	5.31	125.35	122.70
1	A	2356	A	N7-C8-N9	5.30	116.45	113.80
31	a	1463	A	P-O3'-C3'	5.30	126.07	119.70
1	A	267	C	N1-C2-O2	5.30	122.08	118.90
31	a	545	C	N3-C2-O2	-5.30	118.19	121.90
31	a	481	C	C2-N1-C1'	5.30	124.63	118.80
1	A	1577	C	N1-C2-O2	5.30	122.08	118.90
1	A	1771	C	N1-C2-O2	5.30	122.08	118.90
31	a	558	C	N1-C2-O2	5.30	122.08	118.90
1	A	152	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1353	C	C6-N1-C1'	-5.29	114.45	120.80
31	a	1308	A	C4-N9-C1'	5.29	135.82	126.30
1	A	556	C	N1-C2-O2	5.29	122.07	118.90
1	A	2024	U	N3-C2-O2	-5.29	118.50	122.20
1	A	1067	A	N7-C8-N9	5.29	116.44	113.80
1	A	2490	C	C6-N1-C2	-5.28	118.19	120.30
1	A	2524	G	N3-C4-N9	5.28	129.17	126.00
31	a	835	C	N1-C2-O2	5.28	122.07	118.90
1	A	1828	G	P-O3'-C3'	5.28	126.04	119.70
31	a	1170	C	C6-N1-C2	-5.28	118.19	120.30
1	A	1990	C	N3-C2-O2	-5.28	118.20	121.90
1	A	1884	G	P-O3'-C3'	5.28	126.03	119.70
1	A	2236	C	C6-N1-C2	-5.28	118.19	120.30
1	A	2648	U	N1-C2-O2	5.28	126.49	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	C	N1-C2-O2	5.28	122.07	118.90
46	p	46	PRO	C-N-CA	5.28	134.89	121.70
1	A	1701	C	C6-N1-C2	-5.27	118.19	120.30
31	a	92	U	P-O3'-C3'	5.27	126.03	119.70
31	a	901	U	N1-C2-O2	5.27	126.49	122.80
1	A	86	C	O4'-C1'-N1	5.27	112.42	108.20
1	A	554	U	P-O3'-C3'	5.27	126.02	119.70
1	A	2334	U	N3-C2-O2	-5.27	118.51	122.20
31	a	934	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1752	G	N3-C4-C5	-5.26	125.97	128.60
31	a	121	C	C6-N1-C2	-5.25	118.20	120.30
1	A	2166	C	N3-C2-O2	-5.25	118.22	121.90
31	a	87	C	N1-C2-O2	5.25	122.05	118.90
31	a	1032	C	C5-C6-N1	5.25	123.62	121.00
1	A	2035	C	N1-C2-O2	5.24	122.04	118.90
1	A	2131	U	N3-C2-O2	-5.24	118.53	122.20
31	a	759	C	C2-N1-C1'	5.24	124.56	118.80
1	A	1872	C	C6-N1-C1'	-5.24	114.51	120.80
1	A	2345	U	C5-C6-N1	5.24	125.32	122.70
1	A	463	U	C5-C6-N1	5.24	125.32	122.70
31	a	1391	C	C5-C6-N1	5.23	123.61	121.00
31	a	1110	C	C5-C6-N1	5.23	123.61	121.00
31	a	1287	C	C2-N1-C1'	5.23	124.55	118.80
1	A	309	U	P-O3'-C3'	5.23	125.97	119.70
1	A	941	U	C2-N1-C1'	5.23	123.97	117.70
31	a	1287	C	N3-C2-O2	-5.23	118.24	121.90
1	A	1117	G	N3-C4-C5	-5.22	125.99	128.60
1	A	2665	U	N3-C2-O2	-5.22	118.54	122.20
31	a	859	C	C6-N1-C2	-5.22	118.21	120.30
1	A	810	G	P-O3'-C3'	5.22	125.97	119.70
1	A	2415	U	C5-C6-N1	5.22	125.31	122.70
1	A	1707	U	C2-N1-C1'	5.22	123.96	117.70
1	A	1941	A	C4-N9-C1'	5.22	135.69	126.30
1	A	1305	A	P-O3'-C3'	5.21	125.95	119.70
31	a	20	C	C5-C6-N1	5.21	123.60	121.00
31	a	411	C	C6-N1-C2	-5.21	118.22	120.30
31	a	1170	C	N1-C2-O2	5.21	122.02	118.90
1	A	1752	G	C4-N9-C1'	5.20	133.26	126.50
1	A	2212	C	C6-N1-C2	-5.20	118.22	120.30
1	A	458	G	P-O3'-C3'	5.20	125.94	119.70
1	A	1527	C	C6-N1-C2	-5.20	118.22	120.30
1	A	2277	C	C2-N1-C1'	5.19	124.51	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1448	U	OP1-P-O3'	5.19	116.63	105.20
1	A	1560	U	N1-C2-O2	5.19	126.44	122.80
2	B	79	C	C6-N1-C2	-5.19	118.22	120.30
1	A	236	A	C3'-C2'-C1'	5.19	105.65	101.50
1	A	387	C	C6-N1-C2	-5.19	118.22	120.30
31	a	257	U	N3-C2-O2	-5.19	118.57	122.20
31	a	182	U	N1-C2-O2	5.18	126.43	122.80
1	A	2620	C	C5-C6-N1	5.18	123.59	121.00
1	A	1771	C	C6-N1-C2	-5.18	118.23	120.30
31	a	869	C	N3-C2-O2	-5.18	118.28	121.90
15	Q	79	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	A	1507	U	P-O3'-C3'	5.17	125.90	119.70
1	A	635	C	C6-N1-C2	-5.17	118.23	120.30
31	a	758	A	C5-N7-C8	-5.17	101.32	103.90
1	A	1117	G	N3-C4-N9	5.16	129.10	126.00
1	A	374	A	C2-N3-C4	-5.16	108.02	110.60
1	A	2487	U	N1-C2-O2	5.16	126.41	122.80
1	A	2791	U	N1-C2-O2	5.16	126.41	122.80
31	a	384	G	C4-N9-C1'	5.16	133.20	126.50
31	a	1431	U	N3-C2-O2	-5.16	118.59	122.20
1	A	2918	G	N3-C4-N9	5.15	129.09	126.00
15	Q	92	ARG	CA-CB-CG	5.15	124.74	113.40
1	A	1942	A	C4-N9-C1'	5.15	135.57	126.30
1	A	2243	C	C6-N1-C2	-5.15	118.24	120.30
1	A	2105	U	O4'-C1'-N1	5.15	112.32	108.20
31	a	459	A	P-O3'-C3'	5.15	125.88	119.70
31	a	1420	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1545	C	C6-N1-C2	-5.14	118.24	120.30
31	a	1404	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1181	C	N1-C2-O2	5.14	121.98	118.90
31	a	201	C	N1-C2-O2	5.14	121.98	118.90
31	a	1312	C	C2-N1-C1'	5.14	124.45	118.80
1	A	2432	C	C6-N1-C2	-5.14	118.25	120.30
31	a	200	U	N3-C2-O2	-5.13	118.61	122.20
1	A	2675	C	N1-C2-O2	5.13	121.98	118.90
31	a	336	C	C6-N1-C2	-5.13	118.25	120.30
1	A	2306	G	N3-C2-N2	-5.13	116.31	119.90
31	a	1530	G	C4-C5-N7	5.13	112.85	110.80
34	d	200	ARG	NE-CZ-NH2	-5.13	117.74	120.30
31	a	591	C	N1-C2-O2	5.13	121.98	118.90
31	a	230	U	N3-C2-O2	-5.12	118.61	122.20
1	A	1831	A	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	51	U	C5-C4-O4	5.12	128.97	125.90
1	A	2621	G	C4-N9-C1'	5.12	133.15	126.50
1	A	444	U	C5-C6-N1	5.11	125.26	122.70
31	a	1304	U	N3-C2-O2	-5.11	118.62	122.20
1	A	212	C	C5-C6-N1	5.11	123.56	121.00
31	a	1148	G	P-O3'-C3'	5.11	125.83	119.70
1	A	233	G	O4'-C1'-N9	5.11	112.29	108.20
16	R	75	ARG	NE-CZ-NH1	-5.11	117.75	120.30
31	a	1376	C	N3-C2-O2	-5.11	118.33	121.90
2	B	55	A	C2-N3-C4	5.11	113.15	110.60
2	B	62	U	C6-N1-C1'	-5.11	114.05	121.20
31	a	85	U	N1-C2-O2	5.10	126.37	122.80
1	A	776	G	C4-N9-C1'	5.10	133.13	126.50
1	A	1559	C	C6-N1-C2	-5.10	118.26	120.30
1	A	1885	A	O5'-P-OP1	5.10	116.82	110.70
31	a	624	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2621	G	N3-C4-N9	5.10	129.06	126.00
31	a	200	U	N1-C2-O2	5.10	126.37	122.80
2	B	108	C	C6-N1-C2	-5.09	118.26	120.30
31	a	1457	C	N1-C2-O2	5.09	121.96	118.90
1	A	1448	U	P-O3'-C3'	5.09	125.81	119.70
1	A	941	U	N1-C2-O2	5.09	126.36	122.80
1	A	2192	U	N1-C2-O2	5.09	126.36	122.80
1	A	1126	A	O4'-C1'-N9	5.09	112.27	108.20
31	a	1051	G	N7-C8-N9	5.08	115.64	113.10
31	a	134	C	C6-N1-C2	-5.08	118.27	120.30
1	A	1269	A	P-O3'-C3'	5.08	125.80	119.70
31	a	801	A	O4'-C1'-N9	5.08	112.26	108.20
1	A	2795	G	C8-N9-C1'	-5.08	120.40	127.00
1	A	830	A	C4-C5-N7	5.08	113.24	110.70
31	a	950	C	C6-N1-C2	-5.08	118.27	120.30
1	A	1751	U	N3-C2-O2	-5.07	118.65	122.20
1	A	885	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1350	U	N3-C2-O2	-5.07	118.65	122.20
51	x	26	C	C6-N1-C2	-5.07	118.27	120.30
1	A	931	C	N1-C2-O2	5.06	121.94	118.90
1	A	2918	G	N7-C8-N9	5.06	115.63	113.10
1	A	347	G	P-O3'-C3'	5.06	125.77	119.70
1	A	2102	C	N3-C2-O2	-5.06	118.36	121.90
1	A	966	U	N1-C2-O2	5.05	126.34	122.80
1	A	2825	C	C6-N1-C2	-5.05	118.28	120.30
8	J	80	GLN	C-N-CA	5.05	134.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1883	A	P-O3'-C3'	5.05	125.76	119.70
1	A	1953	C	C2-N1-C1'	5.05	124.35	118.80
1	A	2166	C	C6-N1-C2	-5.05	118.28	120.30
31	a	60	C	C2-N3-C4	5.05	122.42	119.90
31	a	1110	C	N1-C2-O2	5.05	121.93	118.90
31	a	856	C	C5-C6-N1	5.05	123.52	121.00
1	A	556	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1464	A	P-O3'-C3'	5.05	125.76	119.70
31	a	482	G	P-O3'-C3'	5.05	125.75	119.70
31	a	1416	C	C6-N1-C2	-5.05	118.28	120.30
39	i	87	LEU	CA-CB-CG	5.05	126.91	115.30
20	W	65	ASP	CB-CG-OD1	5.04	122.84	118.30
31	a	149	U	C5-C6-N1	5.04	125.22	122.70
1	A	1527	C	OP1-P-O3'	5.04	116.29	105.20
1	A	2223	U	N3-C2-O2	-5.04	118.67	122.20
1	A	776	G	C6-C5-N7	-5.04	127.38	130.40
1	A	1650	C	N3-C2-O2	-5.04	118.37	121.90
31	a	965	U	P-O3'-C3'	5.04	125.75	119.70
31	a	405	A	N3-C4-N9	5.04	131.43	127.40
1	A	2335	U	C2-N1-C1'	5.03	123.74	117.70
1	A	1344	C	N1-C2-O2	5.03	121.92	118.90
2	B	37	A	P-O3'-C3'	5.03	125.74	119.70
31	a	539	G	C4-N9-C1'	5.03	133.04	126.50
31	a	640	G	C8-N9-C4	-5.03	104.39	106.40
31	a	1051	G	N3-C2-N2	5.03	123.42	119.90
31	a	201	C	N3-C2-O2	-5.02	118.38	121.90
1	A	1415	C	C2-N1-C1'	5.02	124.33	118.80
1	A	1122	C	C5-C6-N1	5.02	123.51	121.00
1	A	928	G	C4-N9-C1'	5.02	133.02	126.50
1	A	2356	A	C3'-C2'-C1'	5.02	105.52	101.50
1	A	2648	U	C2-N1-C1'	5.02	123.72	117.70
31	a	324	C	C6-N1-C2	-5.02	118.29	120.30
1	A	1803	C	N1-C2-O2	5.01	121.91	118.90
1	A	2035	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1339	A	OP2-P-O3'	5.01	116.23	105.20
31	a	1051	G	N3-C4-C5	-5.01	126.09	128.60
1	A	936	C	N3-C2-O2	-5.01	118.39	121.90
1	A	946	G	C4-N9-C1'	5.01	133.01	126.50
1	A	1650	C	C6-N1-C2	-5.01	118.30	120.30
1	A	2295	A	OP2-P-O3'	5.01	116.22	105.20
51	x	57	C	C6-N1-C2	-5.01	118.30	120.30
51	x	80	C	C5-C6-N1	5.01	123.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1167	C	C6-N1-C1'	-5.00	114.79	120.80
1	A	1803	C	C5-C6-N1	5.00	123.50	121.00
1	A	2167	C	N1-C2-O2	5.00	121.90	118.90
1	A	2356	A	C8-N9-C4	-5.00	103.80	105.80
16	R	22	ILE	CG1-CB-CG2	-5.00	100.40	111.40
31	a	101	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	0	50	ASN	Peptide
24	0	51	GLY	Peptide
29	6	59	PHE	Peptide
3	C	153	GLN	Peptide
4	D	53	PHE	Peptide
6	F	117	VAL	Peptide
6	F	138	PHE	Peptide
6	F	53	ALA	Peptide
8	J	132	PRO	Peptide
10	L	18	ARG	Peptide
10	L	35	HIS	Peptide
13	O	1	MET	Peptide
15	Q	102	ASP	Peptide
16	R	50	ASN	Peptide
16	R	51	PRO	Peptide
17	S	39	THR	Peptide
32	b	148	LEU	Peptide
32	b	16	PHE	Peptide
32	b	18	HIS	Peptide
32	b	65	GLY	Peptide
32	b	66	LYS	Peptide
34	d	117	GLY	Peptide
34	d	192	ALA	Peptide
34	d	31	TYR	Peptide
34	d	32	ALA	Peptide
34	d	33	PRO	Peptide
35	e	20	ARG	Peptide
36	f	33	ASN	Peptide
37	g	114	LYS	Peptide
37	g	129	ASN	Peptide
38	h	98	LEU	Peptide

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Mol	Chain	Res	Type	Group
42	l	34	GLU	Peptide
42	l	57	LYS	Peptide
43	m	104	ASN	Peptide
43	m	3	ARG	Peptide
43	m	65	VAL	Peptide
45	o	24	SER	Peptide
45	o	5	GLN	Peptide
48	r	24	THR	Peptide
48	r	25	HIS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	270/277 (98%)	253 (94%)	17 (6%)	0	100	100
4	D	204/209 (98%)	194 (95%)	10 (5%)	0	100	100
5	E	203/207 (98%)	187 (92%)	16 (8%)	0	100	100
6	F	174/179 (97%)	158 (91%)	16 (9%)	0	100	100
7	G	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	11	40
9	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	L	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
11	M	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
12	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
13	O	118/120 (98%)	107 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
15	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	9	36
16	R	99/102 (97%)	83 (84%)	15 (15%)	1 (1%)	15	49
17	S	107/113 (95%)	91 (85%)	14 (13%)	2 (2%)	8	33
18	T	88/95 (93%)	83 (94%)	5 (6%)	0	100	100
19	U	99/103 (96%)	86 (87%)	13 (13%)	0	100	100
20	W	80/94 (85%)	70 (88%)	10 (12%)	0	100	100
21	X	56/62 (90%)	46 (82%)	10 (18%)	0	100	100
22	Y	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
23	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
24	0	52/59 (88%)	50 (96%)	1 (2%)	1 (2%)	8	33
25	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
26	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
27	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
28	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
29	6	61/63 (97%)	51 (84%)	9 (15%)	1 (2%)	9	37
32	b	216/246 (88%)	185 (86%)	27 (12%)	4 (2%)	8	33
33	c	204/218 (94%)	185 (91%)	19 (9%)	0	100	100
34	d	193/200 (96%)	173 (90%)	18 (9%)	2 (1%)	15	49
35	e	162/166 (98%)	152 (94%)	10 (6%)	0	100	100
36	f	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
37	g	147/156 (94%)	134 (91%)	12 (8%)	1 (1%)	22	57
38	h	129/132 (98%)	108 (84%)	19 (15%)	2 (2%)	9	37
39	i	123/130 (95%)	104 (85%)	18 (15%)	1 (1%)	19	54
40	j	93/102 (91%)	83 (89%)	9 (10%)	1 (1%)	14	46
41	k	112/131 (86%)	102 (91%)	10 (9%)	0	100	100
42	l	134/138 (97%)	115 (86%)	18 (13%)	1 (1%)	22	57
43	m	106/121 (88%)	93 (88%)	12 (11%)	1 (1%)	17	52
44	n	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	9	36
45	o	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	13	44
46	p	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
48	r	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
49	s	76/92 (83%)	66 (87%)	10 (13%)	0	100	100
50	t	81/88 (92%)	76 (94%)	3 (4%)	2 (2%)	5	27
All	All	5207/5515 (94%)	4721 (91%)	457 (9%)	29 (1%)	29	59

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	133	HIS
15	Q	93	LYS
17	S	40	PRO
32	b	18	HIS
32	b	19	GLN
34	d	32	ALA
38	h	99	ASN
46	p	47	ALA
50	t	69	LYS
8	J	132	PRO
15	Q	92	ARG
34	d	33	PRO
38	h	4	THR
44	n	32	SER
29	6	60	ASN
32	b	67	ILE
43	m	105	ASN
46	p	48	GLU
17	S	39	THR
24	0	51	GLY
32	b	66	LYS
37	g	115	THR
42	l	135	PRO
50	t	68	HIS
46	p	46	PRO
16	R	50	ASN
45	o	25	PRO
39	i	125	PRO
40	j	79	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	
3	C	220/225 (98%)	218 (99%)	2 (1%)	78	91
4	D	167/170 (98%)	166 (99%)	1 (1%)	86	94
5	E	169/170 (99%)	164 (97%)	5 (3%)	41	71
6	F	151/154 (98%)	142 (94%)	9 (6%)	19	49
7	G	148/151 (98%)	148 (100%)	0	100	100
8	J	120/123 (98%)	118 (98%)	2 (2%)	60	83
9	K	101/101 (100%)	100 (99%)	1 (1%)	76	90
10	L	110/110 (100%)	108 (98%)	2 (2%)	59	82
11	M	109/116 (94%)	109 (100%)	0	100	100
12	N	99/100 (99%)	99 (100%)	0	100	100
13	O	93/93 (100%)	91 (98%)	2 (2%)	52	78
14	P	100/100 (100%)	97 (97%)	3 (3%)	41	71
15	Q	96/98 (98%)	95 (99%)	1 (1%)	76	90
16	R	83/84 (99%)	82 (99%)	1 (1%)	71	88
17	S	90/93 (97%)	89 (99%)	1 (1%)	73	89
18	T	81/85 (95%)	79 (98%)	2 (2%)	47	75
19	U	85/87 (98%)	85 (100%)	0	100	100
20	W	64/74 (86%)	62 (97%)	2 (3%)	40	70
21	X	47/50 (94%)	44 (94%)	3 (6%)	17	48
22	Y	56/57 (98%)	56 (100%)	0	100	100
23	Z	52/53 (98%)	51 (98%)	1 (2%)	57	81
24	0	48/53 (91%)	45 (94%)	3 (6%)	18	48
25	1	46/47 (98%)	46 (100%)	0	100	100
26	2	39/39 (100%)	38 (97%)	1 (3%)	46	74
27	3	54/56 (96%)	52 (96%)	2 (4%)	34	66
28	4	35/35 (100%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	6	53/53 (100%)	53 (100%)	0	100	100
32	b	189/212 (89%)	182 (96%)	7 (4%)	34	66
33	c	168/178 (94%)	166 (99%)	2 (1%)	71	88
34	d	169/173 (98%)	164 (97%)	5 (3%)	41	71
35	e	128/130 (98%)	125 (98%)	3 (2%)	50	77
36	f	81/84 (96%)	80 (99%)	1 (1%)	71	88
37	g	125/132 (95%)	123 (98%)	2 (2%)	62	84
38	h	111/112 (99%)	109 (98%)	2 (2%)	59	82
39	i	98/102 (96%)	95 (97%)	3 (3%)	40	70
40	j	86/92 (94%)	86 (100%)	0	100	100
41	k	86/100 (86%)	85 (99%)	1 (1%)	71	88
42	l	114/116 (98%)	113 (99%)	1 (1%)	78	91
43	m	94/104 (90%)	93 (99%)	1 (1%)	73	89
44	n	53/54 (98%)	52 (98%)	1 (2%)	57	81
45	o	80/83 (96%)	79 (99%)	1 (1%)	69	87
46	p	74/76 (97%)	72 (97%)	2 (3%)	44	74
47	q	77/80 (96%)	75 (97%)	2 (3%)	46	74
48	r	56/64 (88%)	54 (96%)	2 (4%)	35	67
49	s	70/81 (86%)	69 (99%)	1 (1%)	67	86
50	t	66/70 (94%)	65 (98%)	1 (2%)	65	85
All	All	4441/4620 (96%)	4359 (98%)	82 (2%)	61	82

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	221	ARG
3	C	273	ARG
4	D	199	LEU
5	E	10	ASN
5	E	29	ASN
5	E	188	ASN
5	E	192	LEU
5	E	194	ILE
6	F	3	ARG
6	F	4	LEU

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Mol	Chain	Res	Type
6	F	78	ARG
6	F	92	ARG
6	F	112	ARG
6	F	119	LYS
6	F	133	LYS
6	F	136	LEU
6	F	165	GLU
8	J	26	LEU
8	J	123	LEU
9	K	64	ARG
10	L	18	ARG
10	L	47	ARG
13	O	4	LYS
13	O	61	LYS
14	P	36	ASN
14	P	39	ARG
14	P	51	ARG
15	Q	48	ARG
16	R	47	LYS
17	S	104	THR
18	T	65	ARG
18	T	68	ARG
20	W	22	ARG
20	W	79	ARG
21	X	4	LYS
21	X	17	ASN
21	X	27	ARG
23	Z	9	LYS
24	0	22	LEU
24	0	38	LEU
24	0	50	ASN
26	2	28	ARG
27	3	32	LEU
27	3	62	LEU
32	b	24	ASN
32	b	36	ASN
32	b	113	ARG
32	b	123	ASN
32	b	154	MET
32	b	179	LEU
32	b	203	ASN
33	c	71	LYS

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Mol	Chain	Res	Type
33	c	163	ARG
34	d	54	LYS
34	d	125	ARG
34	d	147	ASN
34	d	172	LEU
34	d	182	ARG
35	e	36	LEU
35	e	46	VAL
35	e	95	LEU
36	f	77	ARG
37	g	9	LYS
37	g	119	ARG
38	h	57	GLN
38	h	96	ARG
39	i	12	ARG
39	i	106	ARG
39	i	113	ARG
41	k	95	ARG
42	l	96	ARG
43	m	79	ARG
44	n	29	ARG
45	o	54	ARG
46	p	32	ARG
46	p	71	ARG
47	q	32	LYS
47	q	67	ARG
48	r	29	LYS
48	r	48	ARG
49	s	5	LEU
50	t	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	86	ASN
3	C	177	ASN
3	C	230	HIS
3	C	232	HIS
4	D	33	ASN
5	E	10	ASN
5	E	29	ASN
5	E	67	GLN

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Mol	Chain	Res	Type
5	E	75	GLN
5	E	188	ASN
6	F	27	GLN
6	F	135	GLN
7	G	66	HIS
7	G	148	ASN
10	L	27	ASN
10	L	126	ASN
12	N	57	HIS
12	N	61	GLN
13	O	15	HIS
14	P	36	ASN
15	Q	29	HIS
15	Q	37	GLN
15	Q	66	ASN
15	Q	107	ASN
17	S	102	HIS
18	T	55	ASN
19	U	64	HIS
20	W	37	GLN
21	X	17	ASN
21	X	23	ASN
24	0	40	HIS
24	0	50	ASN
25	1	22	ASN
25	1	26	ASN
32	b	18	HIS
32	b	24	ASN
32	b	36	ASN
32	b	123	ASN
32	b	203	ASN
34	d	59	HIS
34	d	96	ASN
35	e	45	HIS
35	e	83	HIS
36	f	33	ASN
36	f	61	GLN
37	g	142	HIS
38	h	57	GLN
39	i	81	HIS
39	i	126	GLN
41	k	121	ASN

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Mol	Chain	Res	Type
42	l	85	HIS
42	l	109	HIS
44	n	10	GLN
45	o	5	GLN
45	o	28	GLN
45	o	37	ASN
45	o	42	HIS
45	o	46	HIS
45	o	51	HIS
46	p	88	GLN
50	t	68	HIS
50	t	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2876/2928 (98%)	859 (29%)	89 (3%)
2	B	111/112 (99%)	40 (36%)	3 (2%)
30	7	2/3 (66%)	0	0
31	a	1532/1554 (98%)	411 (26%)	0
51	x	86/87 (98%)	25 (29%)	0
All	All	4607/4684 (98%)	1335 (28%)	92 (1%)

All (1335) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	U
1	A	10	A
1	A	13	A
1	A	18	C
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	C
1	A	55	G
1	A	60	G
1	A	61	A
1	A	62	C

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Mol	Chain	Res	Type
1	A	63	G
1	A	64	A
1	A	65	A
1	A	66	C
1	A	71	A
1	A	74	U
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C
1	A	83	G
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	99	U
1	A	100	U
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	126	A
1	A	127	C
1	A	134	C
1	A	141	U
1	A	156	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	167	U
1	A	174	U
1	A	175	G
1	A	176	A
1	A	177	G

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Mol	Chain	Res	Type
1	A	178	A
1	A	179	A
1	A	182	C
1	A	187	C
1	A	188	C
1	A	196	U
1	A	199	A
1	A	202	A
1	A	207	A
1	A	216	A
1	A	218	G
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	234	C
1	A	236	A
1	A	237	U
1	A	244	A
1	A	247	A
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	255	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	275	A
1	A	282	G
1	A	283	G
1	A	284	C
1	A	285	U
1	A	286	U

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Mol	Chain	Res	Type
1	A	290	U
1	A	291	C
1	A	298	U
1	A	299	U
1	A	301	U
1	A	302	A
1	A	308	C
1	A	309	U
1	A	310	C
1	A	337	A
1	A	345	A
1	A	346	G
1	A	348	U
1	A	349	C
1	A	352	G
1	A	354	A
1	A	360	C
1	A	361	G
1	A	366	A
1	A	367	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	382	G
1	A	389	A
1	A	395	C
1	A	396	G
1	A	398	U
1	A	409	U
1	A	411	G
1	A	412	A
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	430	C
1	A	433	G
1	A	434	U
1	A	436	A
1	A	442	C
1	A	444	U
1	A	445	C

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Mol	Chain	Res	Type
1	A	453	G
1	A	458	G
1	A	459	A
1	A	469	A
1	A	471	G
1	A	482	C
1	A	483	C
1	A	489	G
1	A	490	A
1	A	494	A
1	A	498	U
1	A	502	C
1	A	503	C
1	A	504	A
1	A	506	U
1	A	508	C
1	A	511	U
1	A	524	A
1	A	526	A
1	A	527	A
1	A	528	G
1	A	529	C
1	A	548	A
1	A	550	G
1	A	551	A
1	A	552	G
1	A	554	U
1	A	555	C
1	A	556	C
1	A	558	G
1	A	568	G
1	A	573	C
1	A	575	A
1	A	577	U
1	A	578	A
1	A	583	G
1	A	584	A
1	A	590	U
1	A	591	U
1	A	592	A
1	A	593	A
1	A	595	G

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Mol	Chain	Res	Type
1	A	599	G
1	A	607	G
1	A	613	U
1	A	617	G
1	A	618	A
1	A	619	A
1	A	622	A
1	A	630	A
1	A	632	U
1	A	646	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	655	C
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	668	G
1	A	673	A
1	A	680	G
1	A	683	A
1	A	686	C
1	A	689	A
1	A	690	A
1	A	691	U
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	703	G
1	A	715	A
1	A	716	G
1	A	717	A
1	A	718	C
1	A	733	U
1	A	741	U
1	A	749	G
1	A	764	C
1	A	765	A
1	A	766	C
1	A	777	C

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Mol	Chain	Res	Type
1	A	787	C
1	A	788	G
1	A	790	A
1	A	794	U
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	837	U
1	A	839	G
1	A	847	A
1	A	852	G
1	A	853	C
1	A	858	U
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	878	G
1	A	890	G
1	A	891	G
1	A	892	U
1	A	893	A
1	A	906	G
1	A	908	A
1	A	913	A
1	A	914	C
1	A	916	G
1	A	919	U
1	A	923	C
1	A	928	G
1	A	929	G
1	A	931	C
1	A	933	C
1	A	934	U

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Mol	Chain	Res	Type
1	A	935	A
1	A	936	C
1	A	937	C
1	A	939	G
1	A	940	G
1	A	941	U
1	A	942	U
1	A	943	A
1	A	944	C
1	A	948	A
1	A	953	G
1	A	954	U
1	A	957	A
1	A	958	A
1	A	959	C
1	A	962	C
1	A	964	A
1	A	970	A
1	A	973	G
1	A	975	C
1	A	977	U
1	A	980	C
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1006	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1026	A
1	A	1029	A
1	A	1031	C
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1058	U
1	A	1059	A
1	A	1067	A

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Mol	Chain	Res	Type
1	A	1068	G
1	A	1069	U
1	A	1071	G
1	A	1072	A
1	A	1073	A
1	A	1079	U
1	A	1090	U
1	A	1091	U
1	A	1101	G
1	A	1102	G
1	A	1103	A
1	A	1106	U
1	A	1110	C
1	A	1111	U
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1119	A
1	A	1120	G
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1125	C
1	A	1126	A
1	A	1127	U
1	A	1128	U
1	A	1134	A
1	A	1142	A
1	A	1143	U
1	A	1145	G
1	A	1146	C
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A
1	A	1173	A
1	A	1174	A
1	A	1176	U
1	A	1178	U
1	A	1179	A

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Mol	Chain	Res	Type
1	A	1180	C
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1210	A
1	A	1221	A
1	A	1235	A
1	A	1236	G
1	A	1244	A
1	A	1245	G
1	A	1248	C
1	A	1249	U
1	A	1250	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1261	C
1	A	1270	C
1	A	1276	G
1	A	1278	G
1	A	1280	G
1	A	1281	C
1	A	1282	U
1	A	1290	G
1	A	1293	A
1	A	1294	A
1	A	1295	U
1	A	1296	G
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1323	A
1	A	1325	A

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Mol	Chain	Res	Type
1	A	1330	C
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C
1	A	1344	C
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1354	C
1	A	1362	G
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1369	C
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1422	C
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1443	C
1	A	1448	U
1	A	1449	C
1	A	1451	U

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Mol	Chain	Res	Type
1	A	1457	U
1	A	1459	U
1	A	1460	G
1	A	1465	A
1	A	1467	G
1	A	1472	G
1	A	1473	A
1	A	1475	G
1	A	1481	G
1	A	1487	G
1	A	1489	U
1	A	1490	A
1	A	1494	G
1	A	1499	A
1	A	1500	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1522	U
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1544	C
1	A	1545	C
1	A	1549	U
1	A	1550	C
1	A	1551	C
1	A	1553	A
1	A	1556	A
1	A	1557	G

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Mol	Chain	Res	Type
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1562	A
1	A	1563	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1573	C
1	A	1602	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1613	C
1	A	1617	A
1	A	1622	C
1	A	1626	U
1	A	1628	G
1	A	1631	A
1	A	1632	G
1	A	1645	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1661	A
1	A	1672	A
1	A	1679	A
1	A	1680	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1694	G
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1708	U
1	A	1709	A

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Mol	Chain	Res	Type
1	A	1712	G
1	A	1717	C
1	A	1719	G
1	A	1720	C
1	A	1727	A
1	A	1738	U
1	A	1740	G
1	A	1745	A
1	A	1746	A
1	A	1748	G
1	A	1750	G
1	A	1752	G
1	A	1753	C
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1762	G
1	A	1766	C
1	A	1768	A
1	A	1771	C
1	A	1776	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1781	C
1	A	1782	G
1	A	1783	C
1	A	1785	G
1	A	1789	A
1	A	1790	U
1	A	1792	G
1	A	1793	G
1	A	1797	A
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1812	A
1	A	1813	A
1	A	1814	A
1	A	1815	A
1	A	1829	C

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Mol	Chain	Res	Type
1	A	1830	G
1	A	1831	A
1	A	1833	G
1	A	1839	A
1	A	1843	G
1	A	1845	A
1	A	1846	G
1	A	1849	U
1	A	1858	A
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1895	A
1	A	1899	U
1	A	1902	G
1	A	1904	G
1	A	1932	G
1	A	1935	G
1	A	1941	A
1	A	1942	A
1	A	1943	C
1	A	1944	U
1	A	1946	U
1	A	1952	U
1	A	1956	A
1	A	1958	G
1	A	1959	G
1	A	1966	A
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1970	C
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1992	C
1	A	1993	G

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Mol	Chain	Res	Type
1	A	1995	A
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2004	G
1	A	2010	A
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2033	G
1	A	2050	G
1	A	2051	U
1	A	2052	A
1	A	2053	C
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2065	C
1	A	2068	G
1	A	2070	U
1	A	2072	C
1	A	2079	C
1	A	2080	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2098	G
1	A	2101	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2131	U
1	A	2134	A
1	A	2135	G

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Mol	Chain	Res	Type
1	A	2136	C
1	A	2139	G
1	A	2140	U
1	A	2145	G
1	A	2146	A
1	A	2147	U
1	A	2149	G
1	A	2156	G
1	A	2160	U
1	A	2161	G
1	A	2162	G
1	A	2166	C
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2177	G
1	A	2185	G
1	A	2187	A
1	A	2198	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2208	C
1	A	2210	G
1	A	2212	C
1	A	2213	U
1	A	2217	U
1	A	2219	G
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2241	A
1	A	2242	U
1	A	2244	G
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A

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Mol	Chain	Res	Type
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2267	G
1	A	2268	G
1	A	2295	A
1	A	2296	A
1	A	2307	A
1	A	2308	G
1	A	2311	G
1	A	2312	C
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2324	C
1	A	2325	U
1	A	2327	A
1	A	2328	G
1	A	2331	U
1	A	2332	G
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2340	A
1	A	2341	U
1	A	2342	C
1	A	2343	A
1	A	2344	U
1	A	2345	U
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2354	G
1	A	2356	A
1	A	2357	A
1	A	2363	C
1	A	2364	A
1	A	2368	G
1	A	2374	G

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Mol	Chain	Res	Type
1	A	2376	C
1	A	2379	C
1	A	2381	A
1	A	2387	A
1	A	2390	A
1	A	2401	G
1	A	2406	A
1	A	2408	G
1	A	2412	G
1	A	2413	G
1	A	2414	C
1	A	2418	G
1	A	2420	G
1	A	2431	U
1	A	2432	C
1	A	2435	C
1	A	2448	U
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2497	A
1	A	2505	A
1	A	2506	C
1	A	2507	A
1	A	2511	A
1	A	2523	G
1	A	2524	G
1	A	2525	C
1	A	2527	C
1	A	2531	G

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Mol	Chain	Res	Type
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2547	A
1	A	2554	G
1	A	2558	G
1	A	2563	C
1	A	2564	G
1	A	2570	A
1	A	2583	U
1	A	2593	A
1	A	2595	A
1	A	2596	G
1	A	2598	G
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2612	G
1	A	2613	U
1	A	2615	C
1	A	2631	A
1	A	2632	G
1	A	2638	U
1	A	2642	U
1	A	2644	U
1	A	2654	G
1	A	2659	G
1	A	2660	G
1	A	2667	G
1	A	2674	G
1	A	2675	C
1	A	2689	A
1	A	2692	G
1	A	2696	C
1	A	2702	G
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2747	G
1	A	2753	U

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Mol	Chain	Res	Type
1	A	2755	U
1	A	2760	G
1	A	2762	A
1	A	2764	G
1	A	2765	G
1	A	2766	G
1	A	2773	G
1	A	2777	A
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2789	C
1	A	2794	A
1	A	2795	G
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2821	U
1	A	2822	C
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2828	G
1	A	2831	A
1	A	2832	G
1	A	2833	U
1	A	2843	G
1	A	2855	G
1	A	2859	G
1	A	2860	A
1	A	2862	A
1	A	2866	C
1	A	2868	G
1	A	2874	G
1	A	2886	C
1	A	2891	G
1	A	2892	G
1	A	2897	G
1	A	2899	C
1	A	2900	A
1	A	2901	G

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Mol	Chain	Res	Type
1	A	2905	C
1	A	2908	A
1	A	2916	A
1	A	2917	G
2	B	10	G
2	B	12	U
2	B	15	C
2	B	22	G
2	B	23	U
2	B	28	C
2	B	31	G
2	B	32	U
2	B	33	U
2	B	34	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	47	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	62	U
2	B	63	C
2	B	64	A
2	B	65	G
2	B	66	C
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A
2	B	101	U
2	B	106	C
2	B	107	G

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Mol	Chain	Res	Type
2	B	110	G
2	B	114	A
31	a	9	G
31	a	10	A
31	a	11	G
31	a	24	G
31	a	32	C
31	a	33	G
31	a	34	A
31	a	41	G
31	a	46	G
31	a	49	C
31	a	50	C
31	a	51	U
31	a	52	A
31	a	53	A
31	a	60	C
31	a	65	C
31	a	66	G
31	a	72	A
31	a	75	G
31	a	77	U
31	a	80	G
31	a	84	U
31	a	85	U
31	a	86	G
31	a	87	C
31	a	88	U
31	a	89	C
31	a	90	C
31	a	92	U
31	a	93	G
31	a	99	A
31	a	114	A
31	a	117	A
31	a	118	A
31	a	119	C
31	a	120	A
31	a	128	A
31	a	129	A
31	a	130	C
31	a	136	U

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Mol	Chain	Res	Type
31	a	137	G
31	a	140	A
31	a	141	G
31	a	142	A
31	a	144	U
31	a	153	U
31	a	154	C
31	a	158	G
31	a	162	C
31	a	167	G
31	a	172	U
31	a	176	G
31	a	181	G
31	a	182	U
31	a	189	A
31	a	190	A
31	a	193	G
31	a	194	C
31	a	197	G
31	a	207	U
31	a	208	A
31	a	209	A
31	a	211	A
31	a	218	U
31	a	219	U
31	a	220	C
31	a	221	G
31	a	222	G
31	a	249	G
31	a	253	U
31	a	255	G
31	a	259	G
31	a	262	G
31	a	274	G
31	a	275	C
31	a	277	C
31	a	280	C
31	a	287	A
31	a	288	C
31	a	297	G
31	a	306	A
31	a	314	A

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Mol	Chain	Res	Type
31	a	316	C
31	a	321	A
31	a	329	A
31	a	336	C
31	a	337	A
31	a	338	C
31	a	340	G
31	a	352	A
31	a	353	C
31	a	355	G
31	a	357	A
31	a	359	G
31	a	360	C
31	a	362	G
31	a	371	A
31	a	373	U
31	a	375	U
31	a	380	C
31	a	383	U
31	a	385	G
31	a	390	A
31	a	392	G
31	a	396	G
31	a	400	G
31	a	406	C
31	a	414	G
31	a	419	A
31	a	420	U
31	a	421	G
31	a	426	U
31	a	429	U
31	a	430	C
31	a	432	G
31	a	436	G
31	a	437	U
31	a	438	A
31	a	439	A
31	a	442	C
31	a	447	U
31	a	456	A
31	a	457	A
31	a	459	A

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Mol	Chain	Res	Type
31	a	460	A
31	a	461	C
31	a	465	U
31	a	466	G
31	a	467	C
31	a	473	G
31	a	474	A
31	a	476	U
31	a	477	A
31	a	478	G
31	a	480	G
31	a	483	G
31	a	484	U
31	a	485	A
31	a	487	C
31	a	488	U
31	a	490	G
31	a	491	A
31	a	494	G
31	a	506	A
31	a	508	A
31	a	518	A
31	a	519	A
31	a	520	C
31	a	526	G
31	a	527	C
31	a	530	G
31	a	533	G
31	a	536	G
31	a	539	G
31	a	540	U
31	a	541	A
31	a	542	A
31	a	553	G
31	a	554	C
31	a	556	A
31	a	563	U
31	a	564	C
31	a	568	A
31	a	571	U
31	a	573	U
31	a	575	G

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Mol	Chain	Res	Type
31	a	581	A
31	a	582	A
31	a	585	G
31	a	586	G
31	a	588	U
31	a	591	C
31	a	597	G
31	a	616	A
31	a	627	C
31	a	628	U
31	a	629	C
31	a	641	G
31	a	642	U
31	a	643	C
31	a	648	G
31	a	650	A
31	a	661	U
31	a	662	U
31	a	670	G
31	a	674	A
31	a	694	G
31	a	696	A
31	a	704	A
31	a	727	A
31	a	732	U
31	a	733	G
31	a	740	G
31	a	742	G
31	a	745	U
31	a	756	U
31	a	757	A
31	a	758	A
31	a	762	A
31	a	764	G
31	a	768	A
31	a	787	G
31	a	802	U
31	a	803	A
31	a	806	C
31	a	815	C
31	a	821	G
31	a	824	A

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Mol	Chain	Res	Type
31	a	826	C
31	a	828	A
31	a	829	U
31	a	841	G
31	a	845	G
31	a	849	G
31	a	853	C
31	a	855	G
31	a	856	C
31	a	861	U
31	a	880	U
31	a	884	G
31	a	885	C
31	a	895	G
31	a	899	A
31	a	909	C
31	a	924	A
31	a	932	G
31	a	936	G
31	a	944	C
31	a	945	A
31	a	952	G
31	a	964	G
31	a	966	U
31	a	967	U
31	a	968	A
31	a	970	U
31	a	975	A
31	a	976	G
31	a	978	A
31	a	979	A
31	a	981	G
31	a	984	A
31	a	985	A
31	a	986	G
31	a	987	A
31	a	992	U
31	a	993	A
31	a	999	U
31	a	1000	C
31	a	1002	U
31	a	1003	G

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Mol	Chain	Res	Type
31	a	1006	A
31	a	1008	C
31	a	1009	C
31	a	1010	U
31	a	1011	C
31	a	1012	U
31	a	1013	G
31	a	1014	A
31	a	1015	C
31	a	1017	A
31	a	1019	C
31	a	1020	C
31	a	1023	G
31	a	1024	A
31	a	1027	U
31	a	1028	A
31	a	1030	G
31	a	1031	A
31	a	1033	G
31	a	1035	C
31	a	1036	C
31	a	1039	U
31	a	1040	U
31	a	1041	C
31	a	1042	G
31	a	1043	G
31	a	1046	G
31	a	1047	C
31	a	1050	A
31	a	1051	G
31	a	1052	U
31	a	1053	G
31	a	1056	A
31	a	1058	G
31	a	1060	G
31	a	1064	C
31	a	1071	G
31	a	1074	G
31	a	1075	U
31	a	1095	U
31	a	1102	A
31	a	1104	G

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Mol	Chain	Res	Type
31	a	1105	U
31	a	1110	C
31	a	1111	A
31	a	1112	A
31	a	1114	G
31	a	1118	G
31	a	1124	C
31	a	1128	A
31	a	1134	G
31	a	1136	U
31	a	1140	A
31	a	1141	G
31	a	1142	C
31	a	1143	A
31	a	1145	U
31	a	1148	G
31	a	1149	U
31	a	1150	U
31	a	1151	G
31	a	1153	G
31	a	1155	A
31	a	1163	G
31	a	1166	A
31	a	1167	C
31	a	1168	U
31	a	1169	G
31	a	1170	C
31	a	1176	A
31	a	1177	C
31	a	1178	A
31	a	1180	A
31	a	1190	G
31	a	1192	U
31	a	1193	G
31	a	1205	A
31	a	1206	A
31	a	1209	C
31	a	1211	U
31	a	1214	U
31	a	1221	U
31	a	1222	A
31	a	1224	G

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Mol	Chain	Res	Type
31	a	1233	U
31	a	1236	A
31	a	1237	C
31	a	1238	A
31	a	1239	C
31	a	1245	A
31	a	1247	A
31	a	1248	A
31	a	1258	C
31	a	1259	A
31	a	1265	C
31	a	1266	A
31	a	1267	G
31	a	1269	G
31	a	1279	G
31	a	1288	A
31	a	1289	A
31	a	1291	C
31	a	1294	A
31	a	1295	C
31	a	1296	A
31	a	1299	U
31	a	1307	C
31	a	1308	A
31	a	1309	G
31	a	1311	U
31	a	1312	C
31	a	1313	G
31	a	1314	G
31	a	1323	C
31	a	1326	C
31	a	1329	C
31	a	1331	C
31	a	1332	G
31	a	1336	G
31	a	1340	G
31	a	1345	U
31	a	1347	G
31	a	1349	A
31	a	1354	U
31	a	1355	A
31	a	1362	G

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Mol	Chain	Res	Type
31	a	1366	A
31	a	1371	C
31	a	1372	A
31	a	1373	U
31	a	1377	G
31	a	1379	G
31	a	1387	C
31	a	1403	A
31	a	1406	C
31	a	1407	A
31	a	1413	C
31	a	1428	G
31	a	1435	A
31	a	1451	A
31	a	1452	G
31	a	1455	A
31	a	1461	U
31	a	1462	U
31	a	1463	A
31	a	1464	G
31	a	1478	A
31	a	1494	U
31	a	1496	G
31	a	1497	G
31	a	1500	U
31	a	1502	A
31	a	1503	A
31	a	1507	G
31	a	1513	A
31	a	1516	U
31	a	1517	A
31	a	1527	G
31	a	1529	A
31	a	1539	G
31	a	1540	G
51	x	7	G
51	x	8	U
51	x	9	G
51	x	13	G
51	x	16	U
51	x	17	U
51	x	18	G

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Mol	Chain	Res	Type
51	x	19	G
51	x	20	U
51	x	21	A
51	x	22	G
51	x	23	A
51	x	24	C
51	x	26	C
51	x	27	G
51	x	42	U
51	x	44	G
51	x	50	A
51	x	52	U
51	x	54	G
51	x	58	U
51	x	67	C
51	x	68	A
51	x	72	C
51	x	87	A

All (92) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	C
1	A	88	G
1	A	92	G
1	A	118	A
1	A	163	U
1	A	181	G
1	A	199	A
1	A	236	A
1	A	252	C
1	A	347	G
1	A	410	G
1	A	411	G
1	A	441	C
1	A	455	G
1	A	458	G
1	A	459	A
1	A	482	C
1	A	490	A
1	A	525	A
1	A	549	A

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Mol	Chain	Res	Type
1	A	554	U
1	A	576	G
1	A	594	C
1	A	666	G
1	A	689	A
1	A	702	A
1	A	732	A
1	A	756	U
1	A	810	G
1	A	831	U
1	A	848	G
1	A	855	G
1	A	933	C
1	A	1028	C
1	A	1032	C
1	A	1036	A
1	A	1041	C
1	A	1172	A
1	A	1187	U
1	A	1210	A
1	A	1226	U
1	A	1243	A
1	A	1250	G
1	A	1260	A
1	A	1266	A
1	A	1269	A
1	A	1294	A
1	A	1305	A
1	A	1325	A
1	A	1339	A
1	A	1351	U
1	A	1448	U
1	A	1464	A
1	A	1507	U
1	A	1525	G
1	A	1529	G
1	A	1530	G
1	A	1535	U
1	A	1543	U
1	A	1565	U
1	A	1570	U
1	A	1631	A

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Mol	Chain	Res	Type
1	A	1671	G
1	A	1726	G
1	A	1751	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1844	A
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1991	C
1	A	2009	G
1	A	2127	U
1	A	2139	G
1	A	2155	A
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2356	A
1	A	2454	A
1	A	2456	C
1	A	2468	A
1	A	2531	G
1	A	2631	A
1	A	2710	C
1	A	2805	A
1	A	2904	A
2	B	37	A
2	B	48	G
2	B	49	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
52	TEL	A	3001	-	59,62,62	1.29	4 (6%)	77,92,92	1.97	13 (16%)

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
52	TEL	A	3001	-	1/1/19/19	14/73/108/108	0/4/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	3001	TEL	O5-C10	5.85	1.45	1.35
52	A	3001	TEL	O9-C15	4.93	1.45	1.34
52	A	3001	TEL	C36-N31	-2.79	1.34	1.38
52	A	3001	TEL	O5-C2	-2.72	1.43	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A	3001	TEL	O9-C15-C21	9.23	120.25	110.88
52	A	3001	TEL	C11-N6-C10	6.84	130.89	122.25
52	A	3001	TEL	C17-C11-N6	-5.41	104.95	113.31
52	A	3001	TEL	C1-C2-C3	-4.59	111.17	116.69
52	A	3001	TEL	C4-O9-C15	-3.68	111.64	118.18
52	A	3001	TEL	O20-C15-C21	-3.19	120.57	124.77
52	A	3001	TEL	C8-C4-C2	-3.12	110.94	115.23
52	A	3001	TEL	C28-C24-C19	-2.96	111.08	116.11
52	A	3001	TEL	O9-C15-O20	-2.55	119.18	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A	3001	TEL	C56-N52-C47	2.50	121.18	116.85
52	A	3001	TEL	C42-O39-C34	-2.38	112.12	116.25
52	A	3001	TEL	C24-C19-C13	-2.30	109.37	113.32
52	A	3001	TEL	C54-C49-N53	-2.20	109.45	115.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	A	3001	TEL	C21

All (14) torsion outliers are listed below:

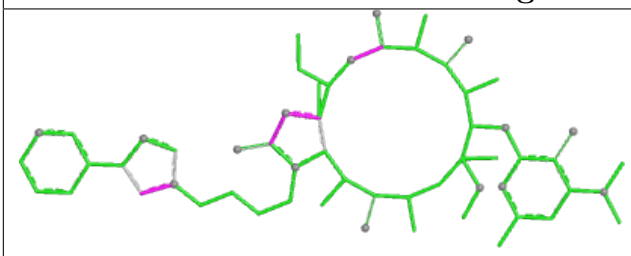
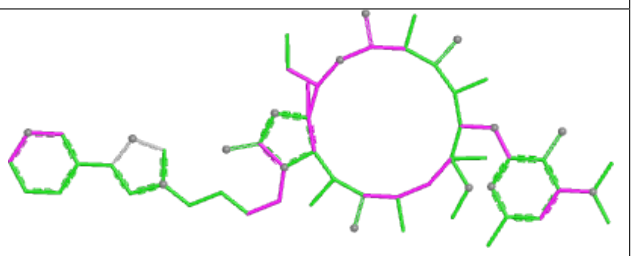
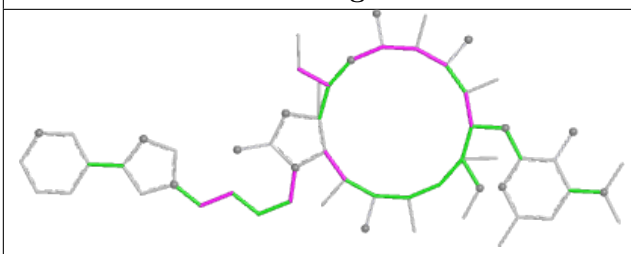
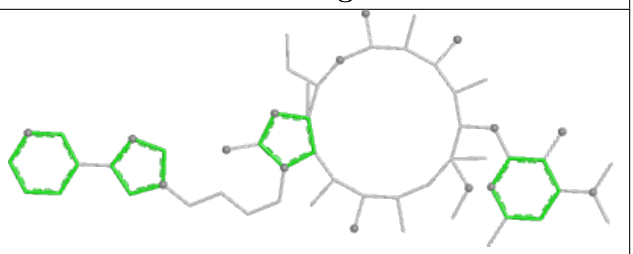
Mol	Chain	Res	Type	Atoms
52	A	3001	TEL	C15-C21-C26-O29
52	A	3001	TEL	C15-C21-C26-C30
52	A	3001	TEL	C21-C15-O9-C4
52	A	3001	TEL	O20-C15-O9-C4
52	A	3001	TEL	O9-C4-C8-C14
52	A	3001	TEL	N6-C3-C7-C12
52	A	3001	TEL	C17-C22-C27-N31
52	A	3001	TEL	C17-C11-N6-C10
52	A	3001	TEL	O20-C15-C21-C25
52	A	3001	TEL	O9-C15-C21-C25
52	A	3001	TEL	C35-C30-C34-C28
52	A	3001	TEL	C2-C4-C8-C14
52	A	3001	TEL	O20-C15-C21-C26
52	A	3001	TEL	C26-C30-C34-C28

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand TEL A 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	182:C	O3'	183:A	P	6.67
1	A	1449:C	O3'	1450:C	P	4.07
1	A	1451:U	O3'	1452:C	P	3.36
1	A	1452:C	O3'	1453:A	P	3.32
1	A	183:A	O3'	184:G	P	3.31

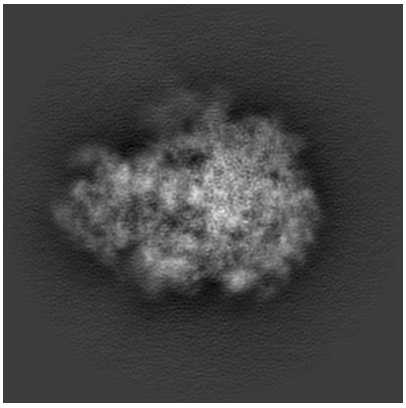
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0176. These allow visual inspection of the internal detail of the map and identification of artifacts.

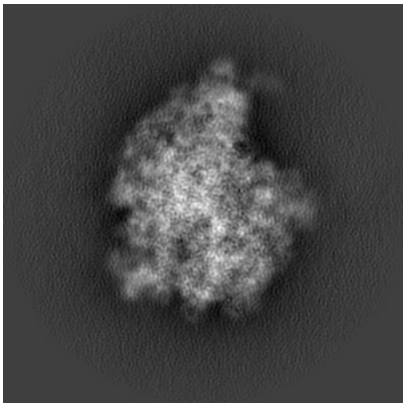
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

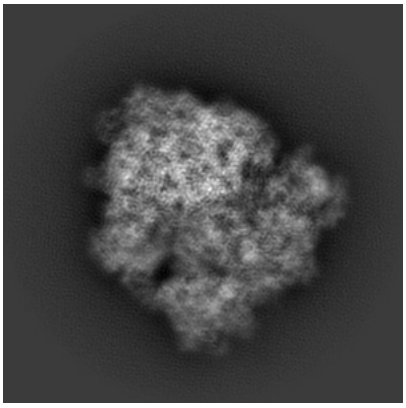
6.1.1 Primary map



X



Y

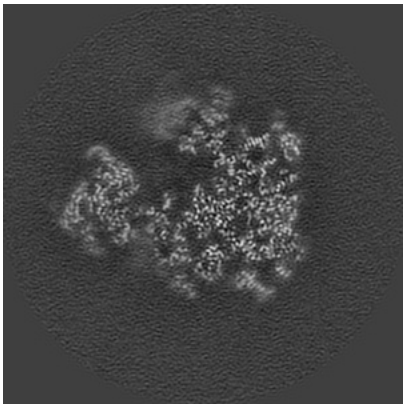


Z

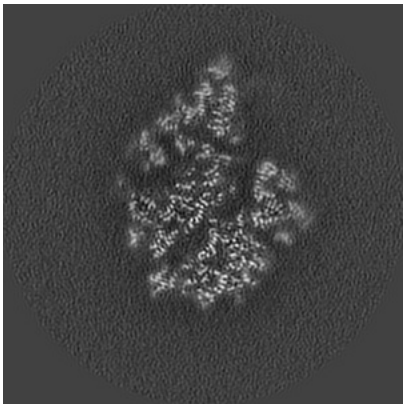
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

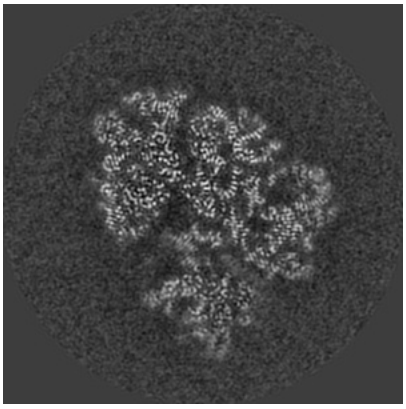
6.2.1 Primary map



X Index: 180



Y Index: 180

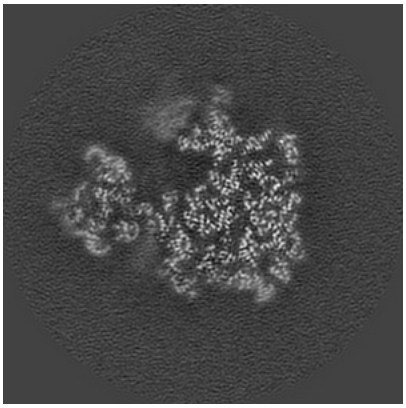


Z Index: 180

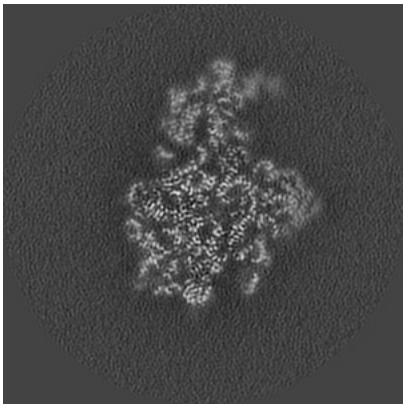
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

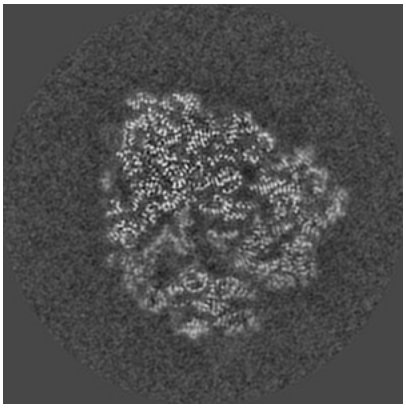
6.3.1 Primary map



X Index: 184



Y Index: 190



Z Index: 190

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

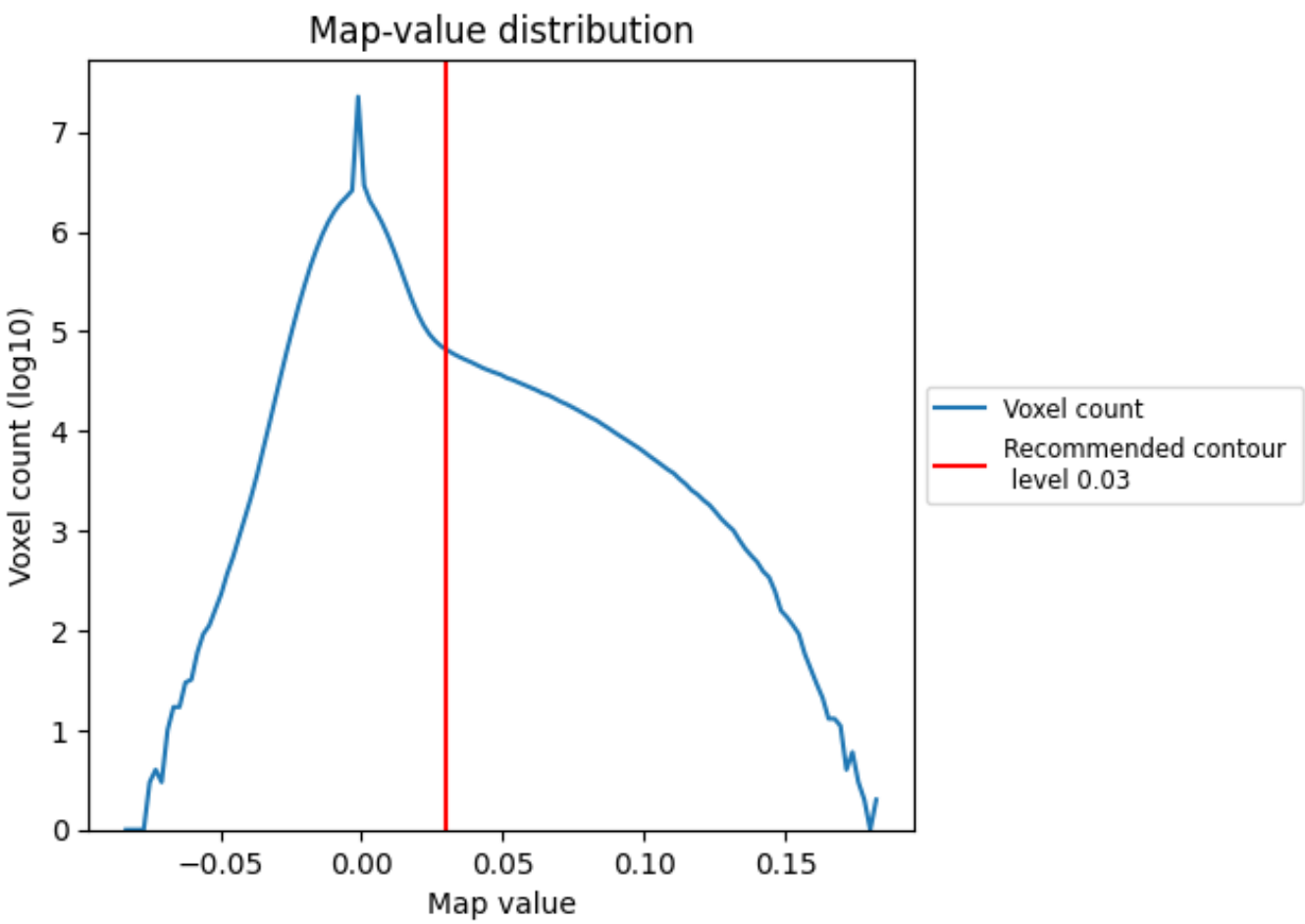
6.5 Mask visualisation (i)

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

7 Map analysis (i)

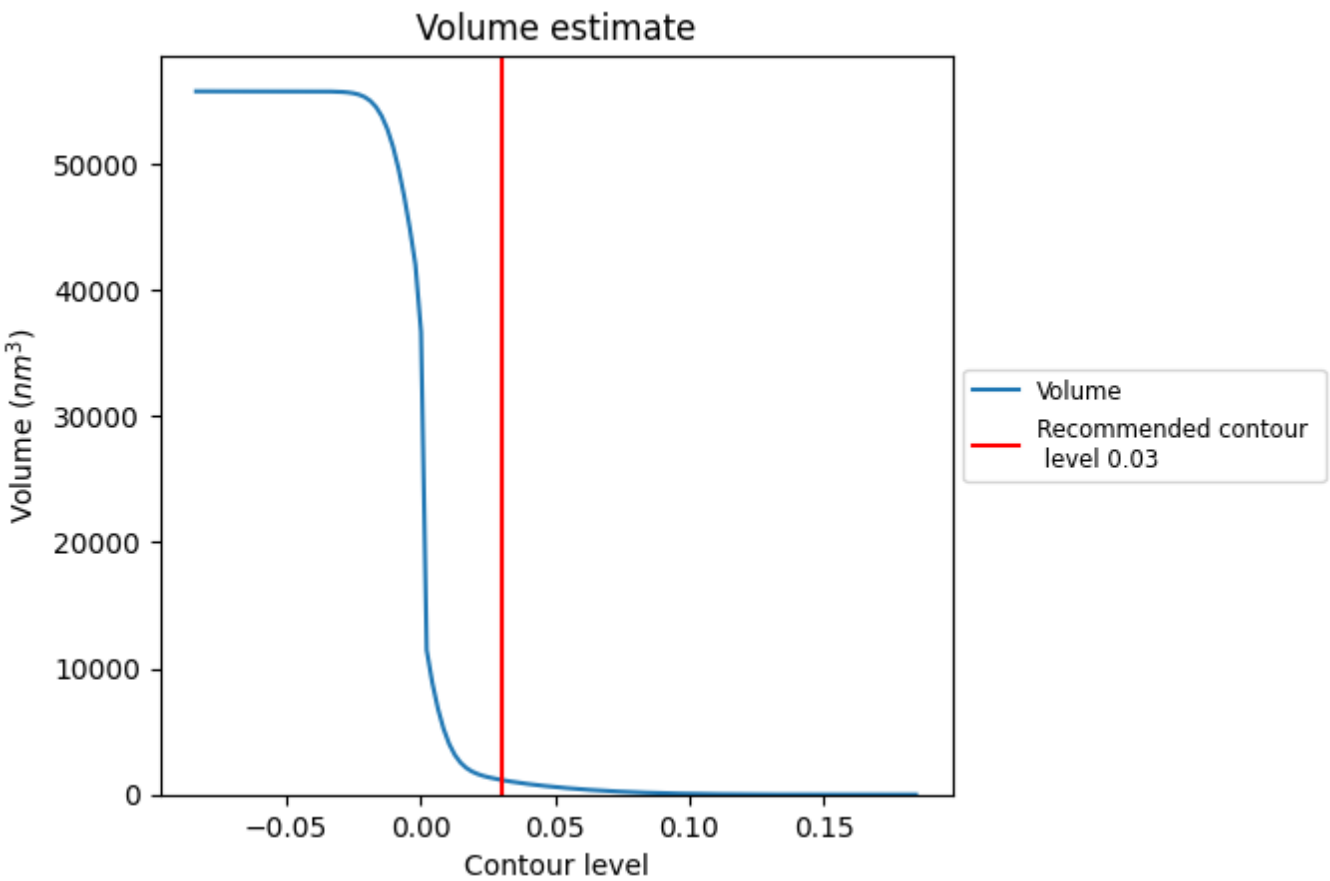
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

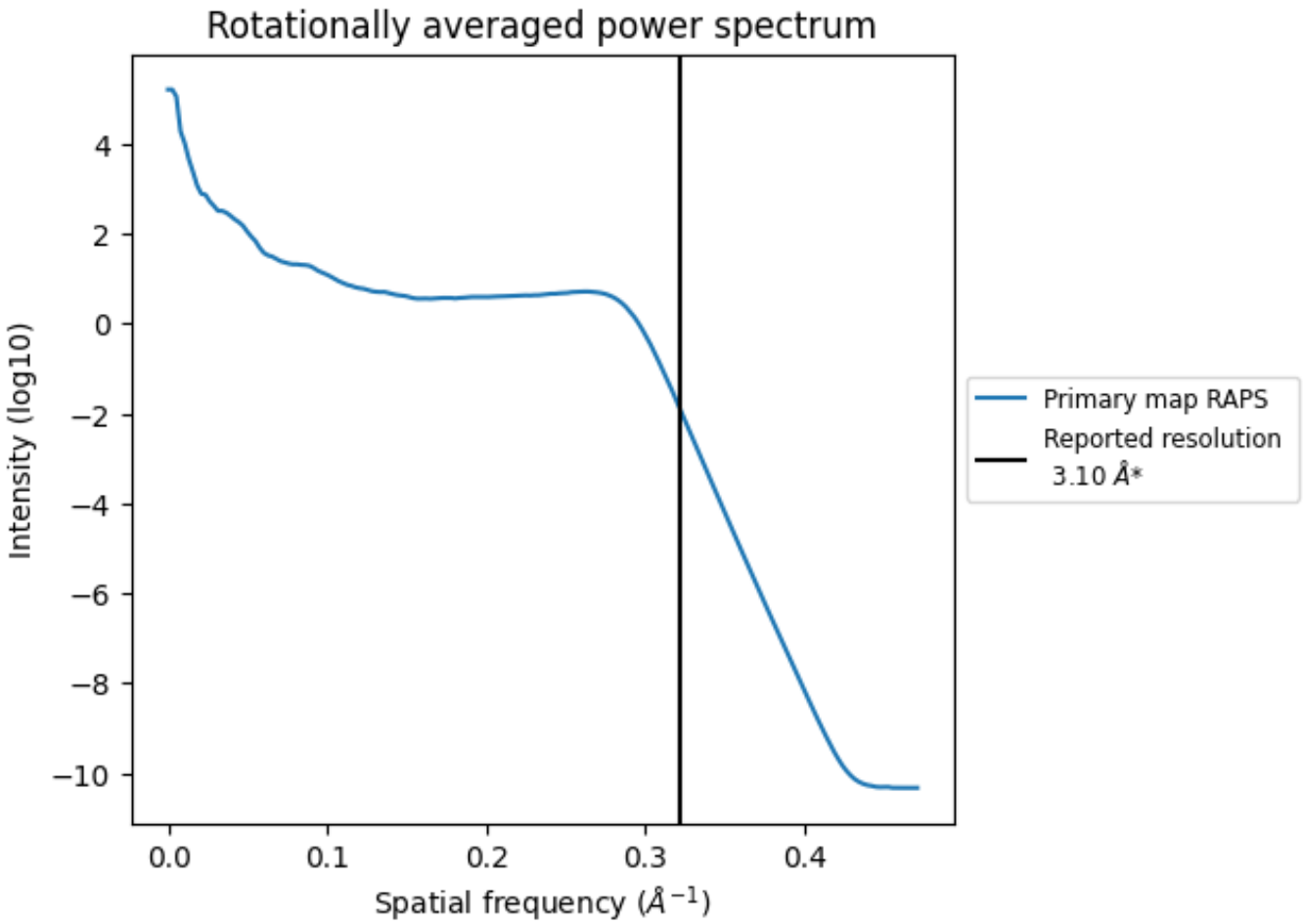
7.2 Volume estimate (i)



The volume at the recommended contour level is 1164 nm^3; this corresponds to an approximate mass of 1051 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

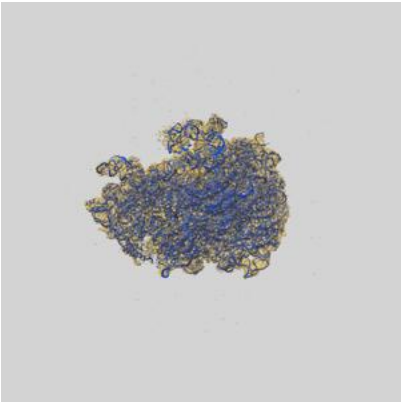
8 Fourier-Shell correlation (i)

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

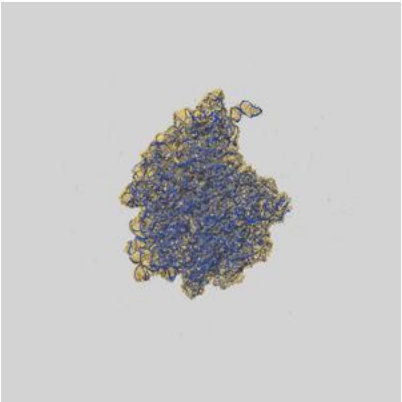
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0176 and PDB model 6HA1. Per-residue inclusion information can be found in section 3 on page 13.

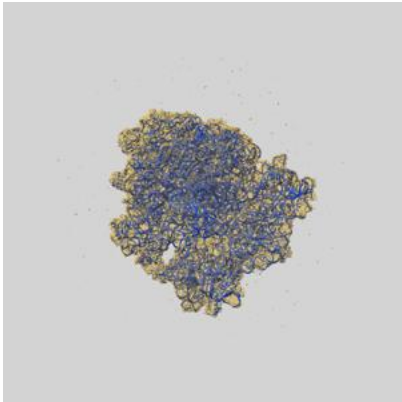
9.1 Map-model overlay (i)



X



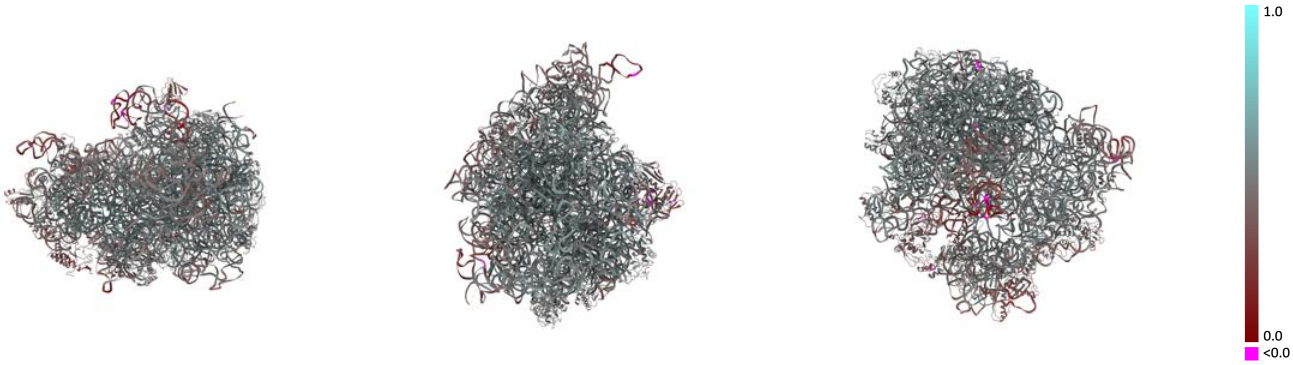
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

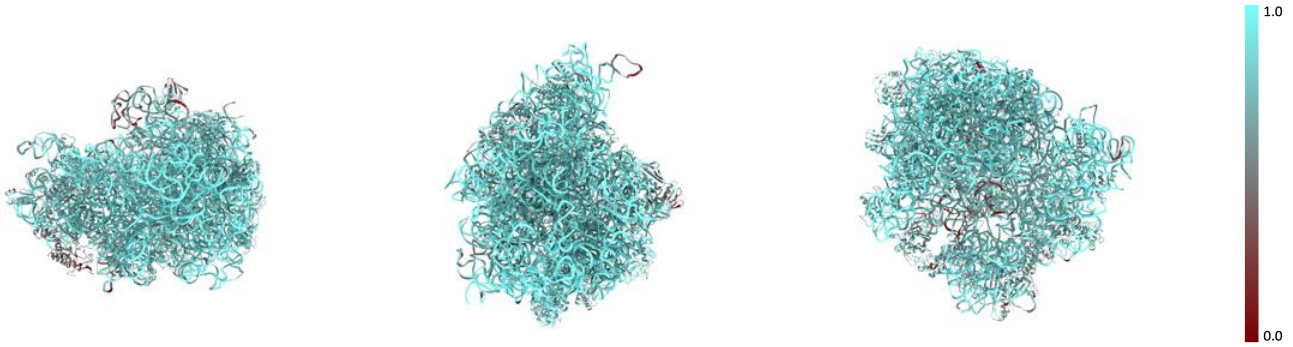
9.2 Q-score mapped to coordinate model (i)



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.

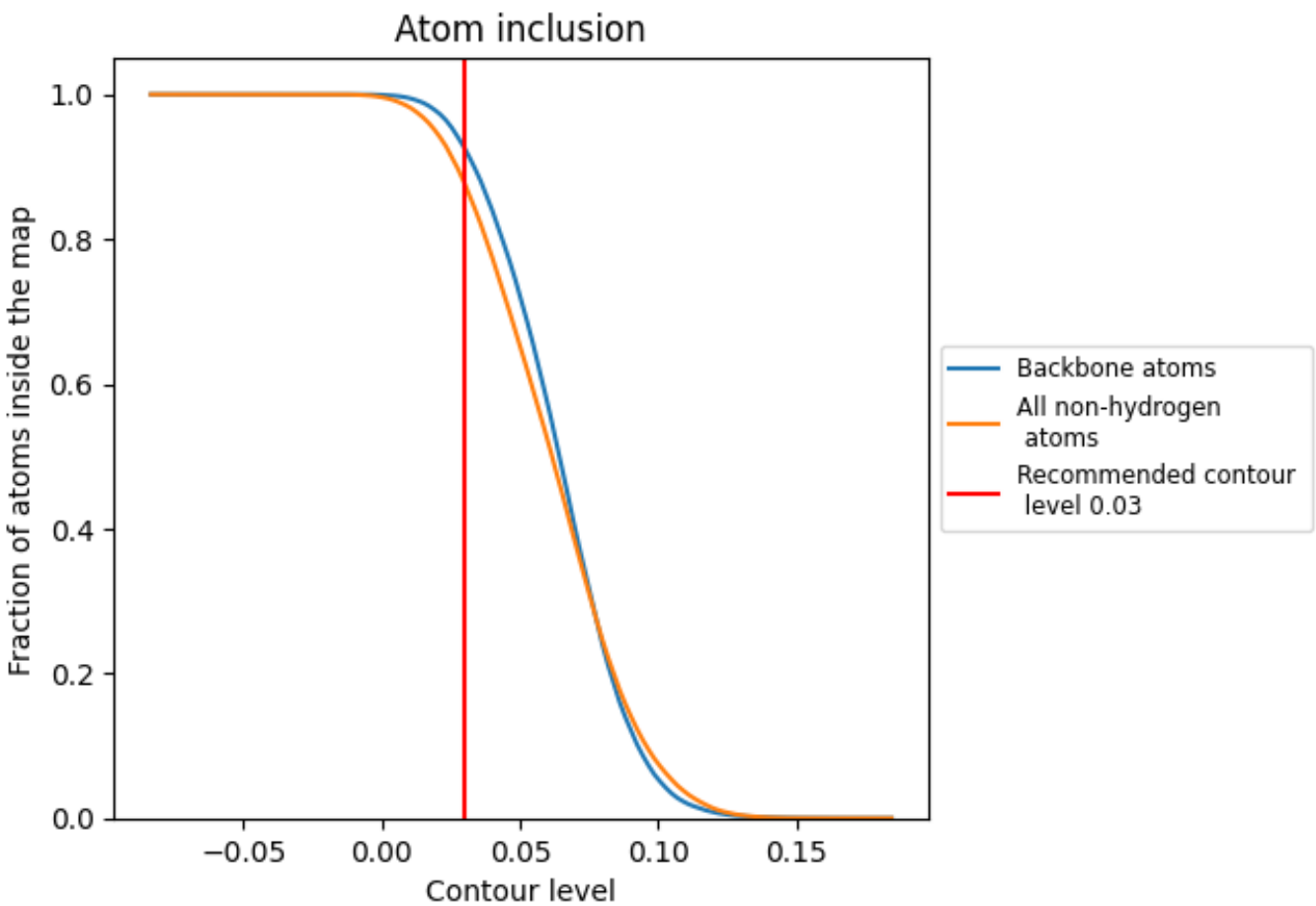
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8768	0.4800
0	0.8475	0.5250
1	0.8165	0.4980
2	0.8609	0.5440
3	0.8277	0.5380
4	0.7862	0.5210
6	0.6483	0.3300
7	0.9667	0.5420
A	0.9242	0.4910
B	0.9569	0.4680
C	0.8043	0.5220
D	0.8184	0.5140
E	0.8240	0.5020
F	0.7207	0.4040
G	0.6646	0.3860
J	0.8097	0.4980
K	0.7692	0.5100
L	0.8267	0.5080
M	0.7937	0.5120
N	0.8462	0.5170
O	0.7982	0.4590
P	0.7881	0.5040
Q	0.8460	0.4980
R	0.8119	0.4890
S	0.8095	0.5200
T	0.7827	0.4850
U	0.8066	0.4710
W	0.8309	0.5160
X	0.6505	0.4710
Y	0.7704	0.4290
Z	0.8090	0.4840
a	0.9387	0.4790
b	0.3770	0.3560
c	0.6987	0.4430
d	0.7434	0.4310

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Chain	Atom inclusion	Q-score
e	0.7647	0.4990
f	0.7378	0.4540
g	0.7017	0.4240
h	0.7669	0.4780
i	0.7508	0.4310
j	0.7176	0.4350
k	0.7466	0.4570
l	0.7483	0.4780
m	0.7572	0.4310
n	0.7521	0.4880
o	0.8052	0.4490
p	0.7566	0.4670
q	0.7236	0.4650
r	0.7430	0.4400
s	0.7669	0.4320
t	0.7524	0.4500
x	0.7453	0.4170