Full wwPDB EM Validation Report ⓘ

Dec 14, 2023 – 05:11 pm GMT

PDB ID	:	8P5D
EMDB ID	:	EMD-17448
Title	:	Spraguea lophii ribosome in the closed conformation by cryo sub tomogram averaging
Authors	:	Gil Diez, P.; McLaren, M.; Isupov, M.N.; Daum, B.; Conners, R.; Williams, B.
Deposited on	:	2023-05-23
Resolution	:	10.80 Å(reported)

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

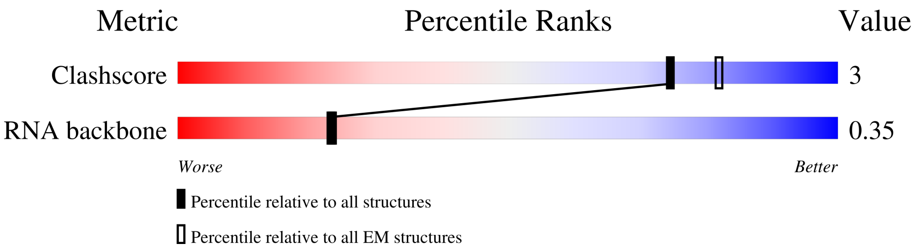
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

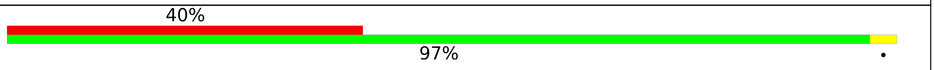
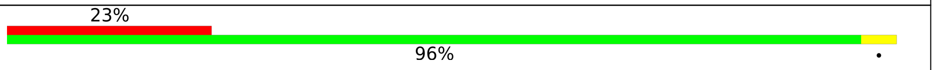
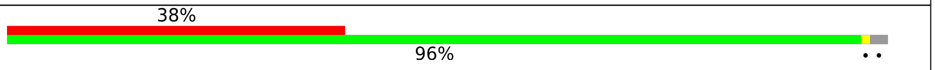
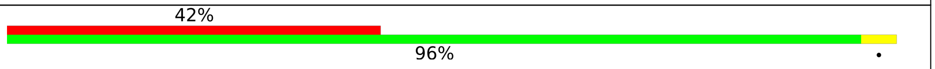
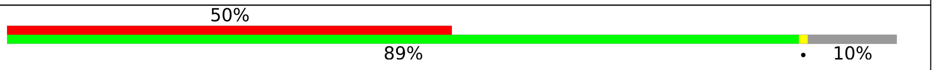
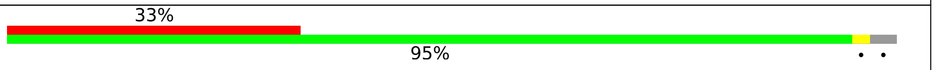
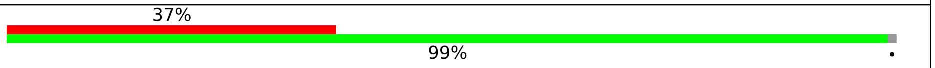
The reported resolution of this entry is 10.80 Å.

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.



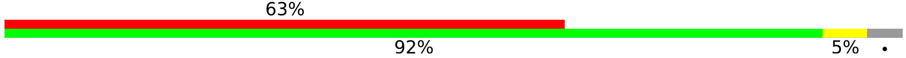
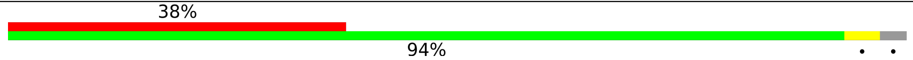
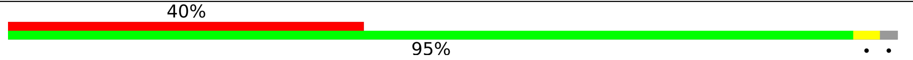
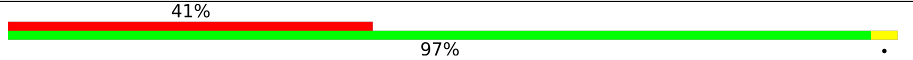
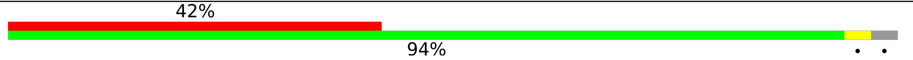
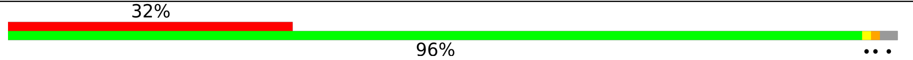
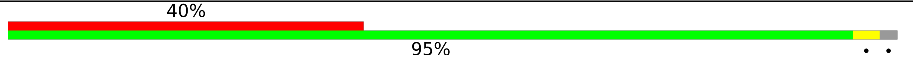
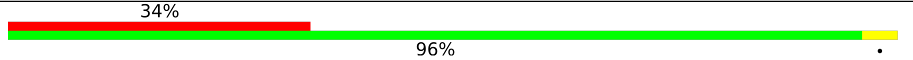
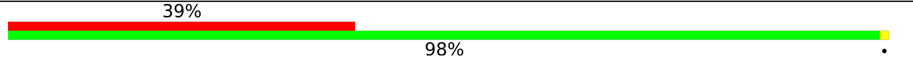
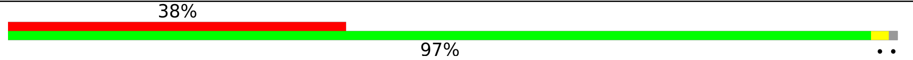
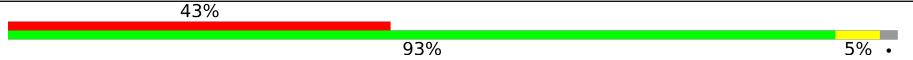
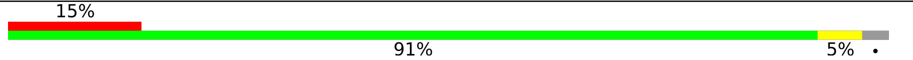
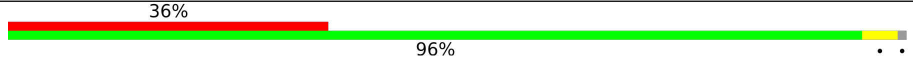
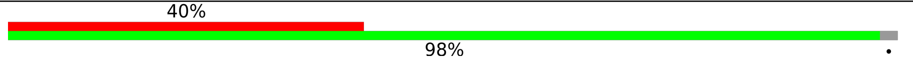
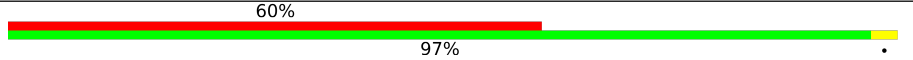
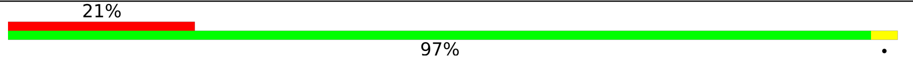
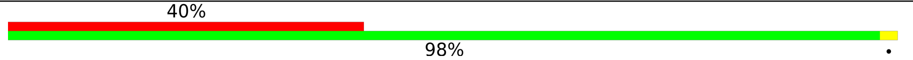
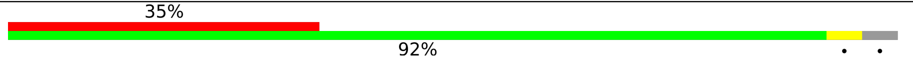
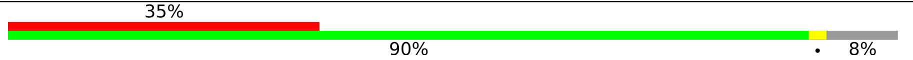
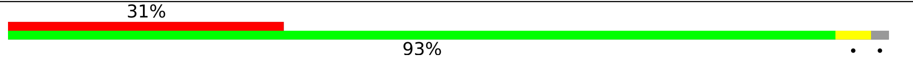
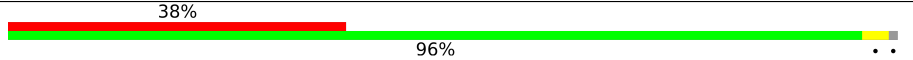
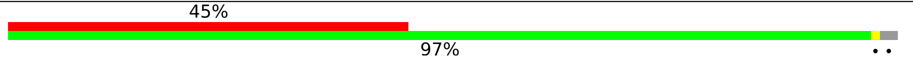
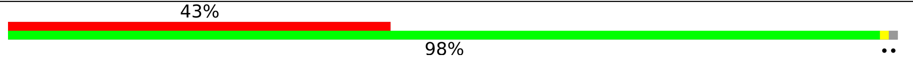
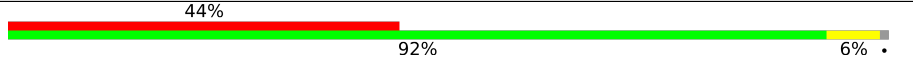
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
RNA backbone	4643	859

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	L50	2618	
2	L70	119	
3	LA0	246	
4	LAA	147	
5	LB0	392	
6	LC0	328	
7	LCC	110	
8	LD0	291	
9	LDD	110	

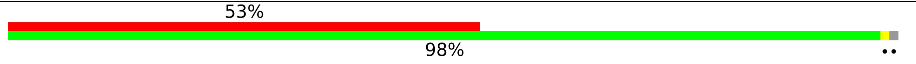
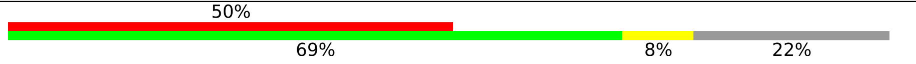
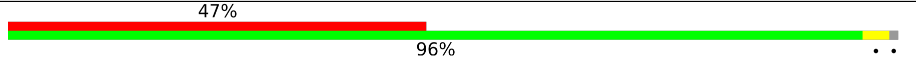
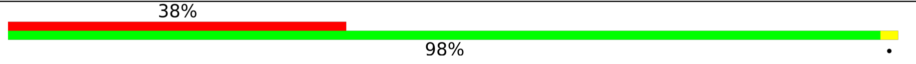
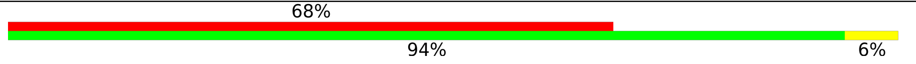
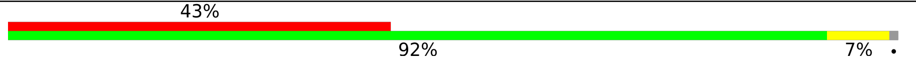
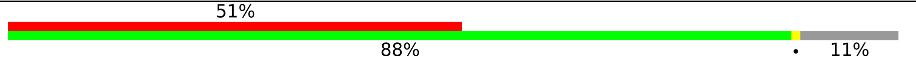
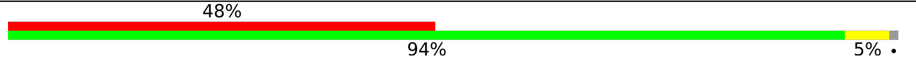
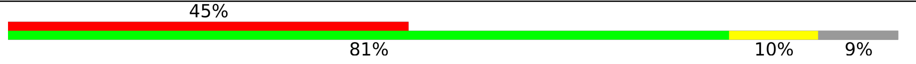
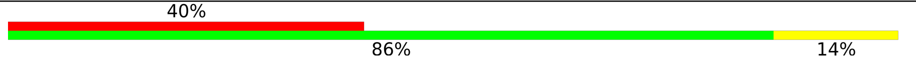
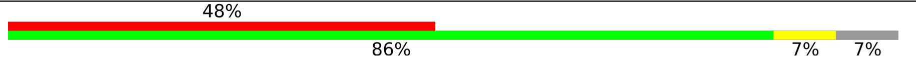
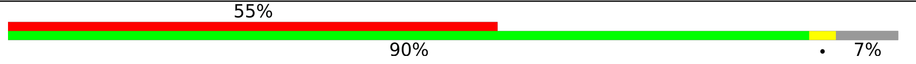
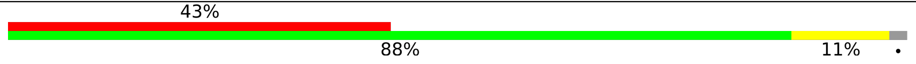
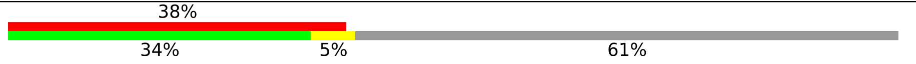
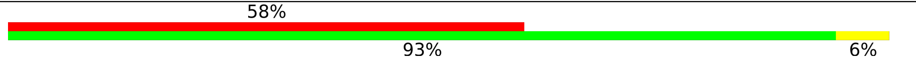
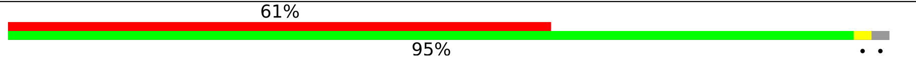
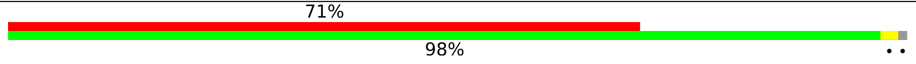
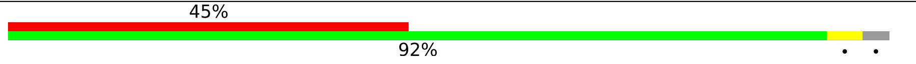
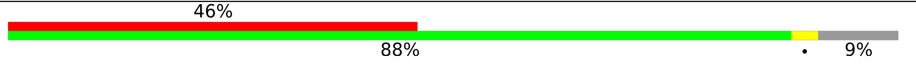
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	LE0	171	
11	LEE	139	
12	LF0	235	
13	LFF	111	
14	LG0	206	
15	LGG	106	
16	LH0	187	
17	LHH	119	
18	LI0	218	
19	LII	98	
20	LJ0	171	
21	LJJ	92	
22	LL0	165	
23	LLL	52	
24	LM0	115	
25	LMM	127	
26	LN0	204	
27	LO0	198	
28	LOO	104	
29	LP0	167	
30	LPP	89	
31	LQ0	183	
32	LR0	168	
33	LS0	171	
34	LT0	158	

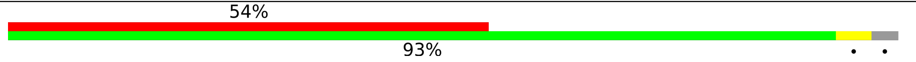
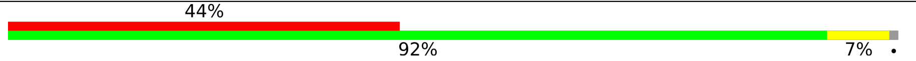
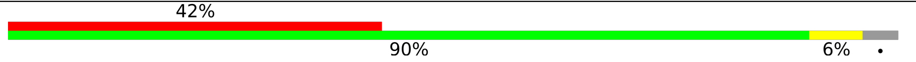
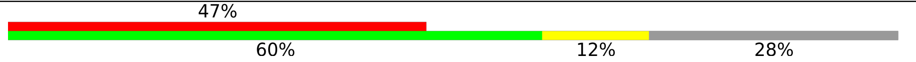
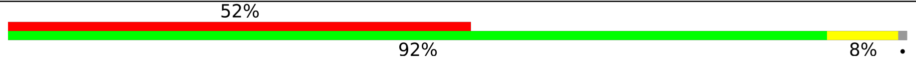
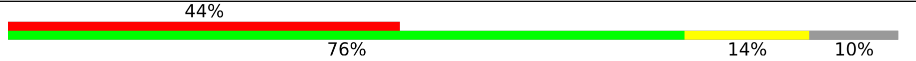
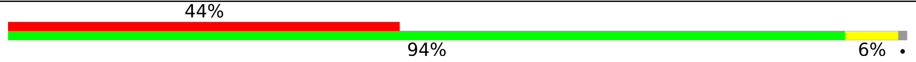
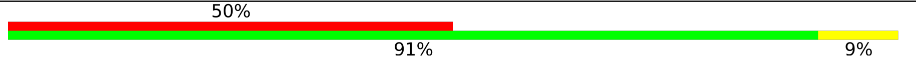
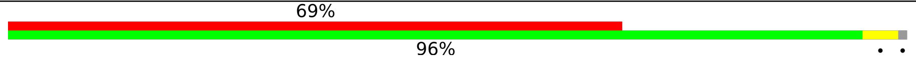
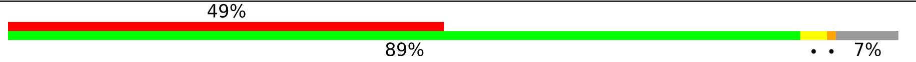
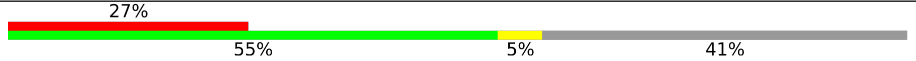
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	LU0	113	
36	LV0	142	
37	LW0	131	
38	LX0	113	
39	LY0	131	
40	LZ0	153	
41	MD1	151	
42	S60	1368	
43	SA0	233	
44	SAA	102	
45	SB0	230	
46	SBB	82	
47	SC0	248	
48	SCC	65	
49	SD0	242	
50	SDD	65	
51	SE0	280	
52	SEE	60	
53	SF0	195	
54	SFF	150	
55	SG0	230	
56	SGG	326	
57	SH0	164	
58	SI0	173	
59	SJ0	184	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
60	SK0	107	
61	SL0	155	
62	SM0	130	
63	SN0	143	
64	SO0	135	
65	SP0	163	
66	SQ0	143	
67	SR0	120	
68	SS0	160	
69	ST0	143	
70	SU0	119	
71	SV0	67	
72	SW0	128	
73	SX0	141	
74	SY0	146	
75	SZ0	128	

2 Entry composition (i)

There are 76 unique types of molecules in this entry. The entry contains 171817 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 RNA 28S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L50	2499	53655	23950	9876	17330	2499	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L70	119	2542	1136	459	828	119	0	0

- Molecule 3 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	LA0	245	1889	1189	361	334	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA0	206	ASN	THR	conflict	UNP S7W736

- Molecule 4 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LAA	147	1167	738	229	194	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB0	383	3039	1926	559	543	11	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC0	327	2604	1629	478	485	12	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LCC	99	781	504	126	148	3	0	0

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LD0	281	2298	1451	410	426	11	0	0

- Molecule 9 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LDD	109	895	575	163	154	3	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LE0	165	1371	879	227	262	3	0	0

- Molecule 11 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LEE	135	1090	697	205	182	6	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LF0	231	1933	1234	342	350	7	0	0

- Molecule 13 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LFF	111	893	567	159	162	5	0	0

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LG0	199	1590	1015	275	290	10	0	0

- Molecule 15 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LGG	104	819	504	169	139	7	0	0

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LH0	183	1477	951	252	266	8	0	0

- Molecule 17 is a protein called Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LHH	119	992	626	188	175	3	0	0

- Molecule 18 is a protein called S60 ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LI0	217	1750	1096	333	308	13	0	0

- Molecule 19 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LII	97	784	496	146	136	6	0	0

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ0	167	Total 1332	C 847	N 242	O 236	S 7	0	0

- Molecule 21 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJJ	89	Total 701	C 427	N 146	O 118	S 10	0	0

- Molecule 22 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL0	164	Total 1353	C 857	N 252	O 232	S 12	0	0

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LLL	51	Total 427	C 272	N 87	O 65	S 3	0	0

- Molecule 24 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LM0	115	Total 927	C 588	N 151	O 183	S 5	0	0

- Molecule 25 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LMM	52	Total 427	C 264	N 89	O 70	S 4	0	0

- Molecule 26 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LN0	203	Total 1688	C 1055	N 346	O 276	S 11	0	0

- Molecule 27 is a protein called Ribosomal protein L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LO0	198	1598	1018	286	280	14	0	0

- Molecule 28 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LOO	100	801	504	163	130	4	0	0

- Molecule 29 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LP0	154	1238	794	225	213	6	0	0

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LPP	87	684	427	131	116	10	0	0

- Molecule 31 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LQ0	182	1491	950	270	266	5	0	0

- Molecule 32 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LR0	164	1336	832	261	236	7	0	0

- Molecule 33 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LS0	170	1400	898	241	256	5	0	0

- Molecule 34 is a protein called 60s ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LT0	156	1270	808	233	224	5	0	0

- Molecule 35 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LU0	100	810	526	135	147	2	0	0

- Molecule 36 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LV0	141	1057	663	200	189	5	0	0

- Molecule 37 is a protein called Ribosomal protein L24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LW0	102	832	539	143	147	3	0	0

- Molecule 38 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LX0	112	874	562	156	155	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LY0	131	1048	658	197	186	7	0	0

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LZ0	118	963	618	172	169	4	0	0

- Molecule 41 is a protein called DNL-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	MD1	151	Total 1229	C 776	N 201	O 241	S 11	0	0

- Molecule 42 is a RNA chain called RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S60	1354	Total 29181	C 13024	N 5463	O 9340	P 1354	0	0

- Molecule 43 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SA0	220	Total 1725	C 1091	N 292	O 328	S 14	0	0

- Molecule 44 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SAA	101	Total 827	C 513	N 163	O 145	S 6	0	0

- Molecule 45 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SB0	204	Total 1609	C 1018	N 286	O 298	S 7	0	0

- Molecule 46 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SBB	81	Total 627	C 394	N 108	O 116	S 9	0	0

- Molecule 47 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC0	226	Total 1727	C 1099	N 300	O 321	S 7	0	0

- Molecule 48 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	SCC	62	476	295	86	91	4	0	0

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SD0	216	1700	1085	300	307	8	0	0

- Molecule 50 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SDD	65	550	345	102	96	7	0	0

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SE0	260	2044	1297	361	379	7	0	0

- Molecule 52 is a protein called eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	SEE	56	447	284	89	74	0	0

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SF0	192	1509	953	275	275	6	0	0

- Molecule 54 is a protein called Ubiquitin/40s ribosomal protein S27a fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SFF	58	422	261	77	79	5	0	0

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SG0	229	1836	1179	325	328	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SG0	171	ALA	GLY	conflict	UNP S7WDE5
SG0	173	GLY	ASP	conflict	UNP S7WDE5

- Molecule 56 is a protein called Guanine nucleotide binding protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SGG	319	2478	1558	411	494	15	0	0

- Molecule 57 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SH0	163	1335	855	219	255	6	0	0

- Molecule 58 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SI0	167	1347	834	266	240	7	0	0

- Molecule 59 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SJ0	168	1379	880	252	243	4	0	0

- Molecule 60 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SK0	88	737	472	127	135	3	0	0

- Molecule 61 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SL0	150	1229	790	217	216	6	0	0

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SM0	113	876	553	156	162	5	0	0

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SN0	142	1130	728	196	202	4	0	0

- Molecule 64 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	SO0	129	983	606	191	183	3	0	0

- Molecule 65 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	SP0	117	950	598	172	173	7	0	0

- Molecule 66 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SQ0	142	1143	726	204	207	6	0	0

- Molecule 67 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	SR0	119	974	613	172	186	3	0	0

- Molecule 68 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	SS0	144	1150	720	220	207	3	0	0

- Molecule 69 is a protein called 40S Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	ST0	142	1161	741	208	211	1	0	0

- Molecule 70 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SU0	100	809	515	144	143	7	0	0

- Molecule 71 is a protein called Ribosomal protein S21E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SV0	65	521	319	96	101	5	0	0

- Molecule 72 is a protein called 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	SW0	128	1022	639	195	180	8	0	0

- Molecule 73 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	SX0	140	1098	692	216	186	4	0	0

- Molecule 74 is a protein called 40s ribosomal protein s24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	SY0	136	1118	693	215	204	6	0	0

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	SZ0	76	633	403	116	113	1	0	0

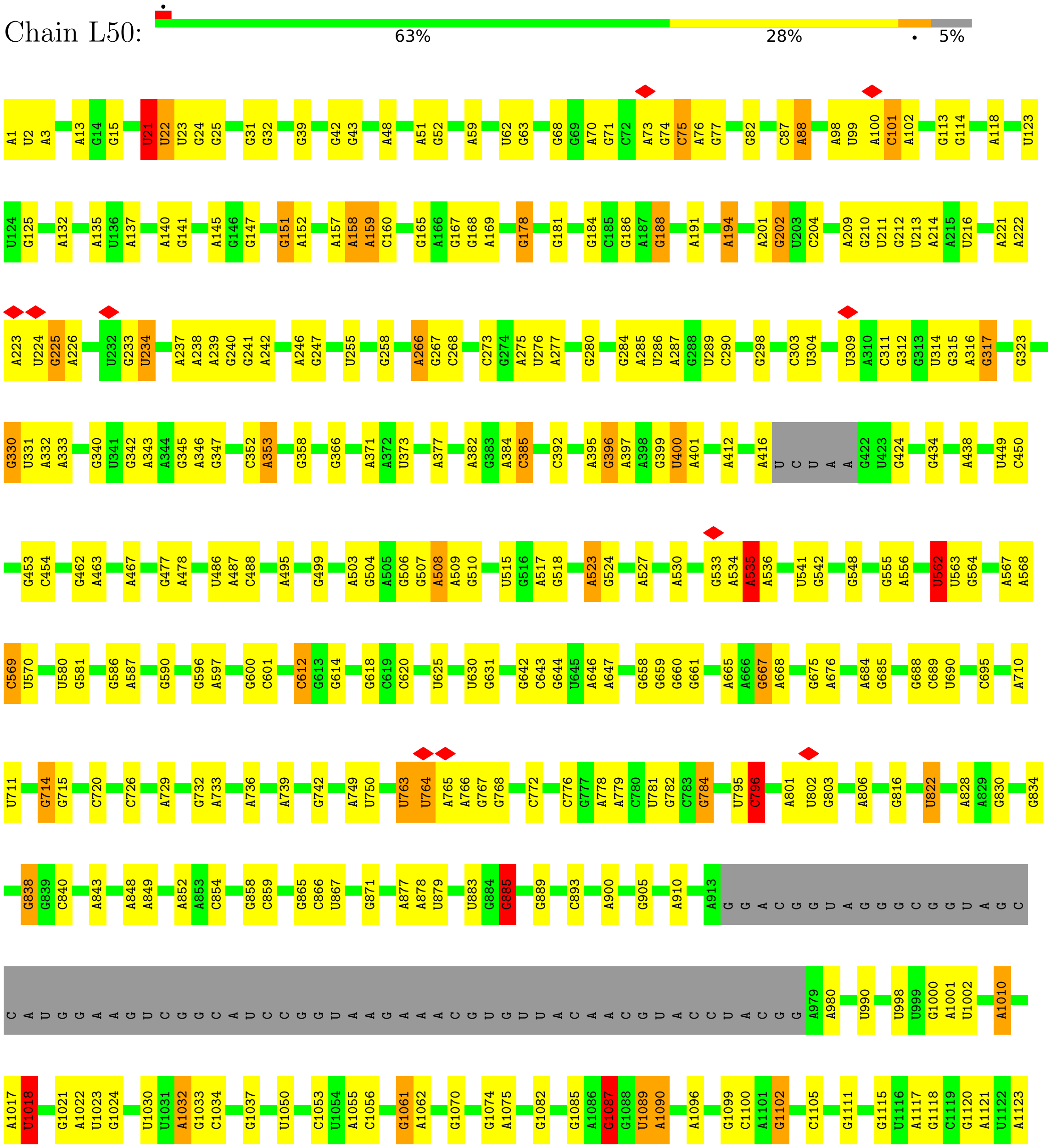
- Molecule 76 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

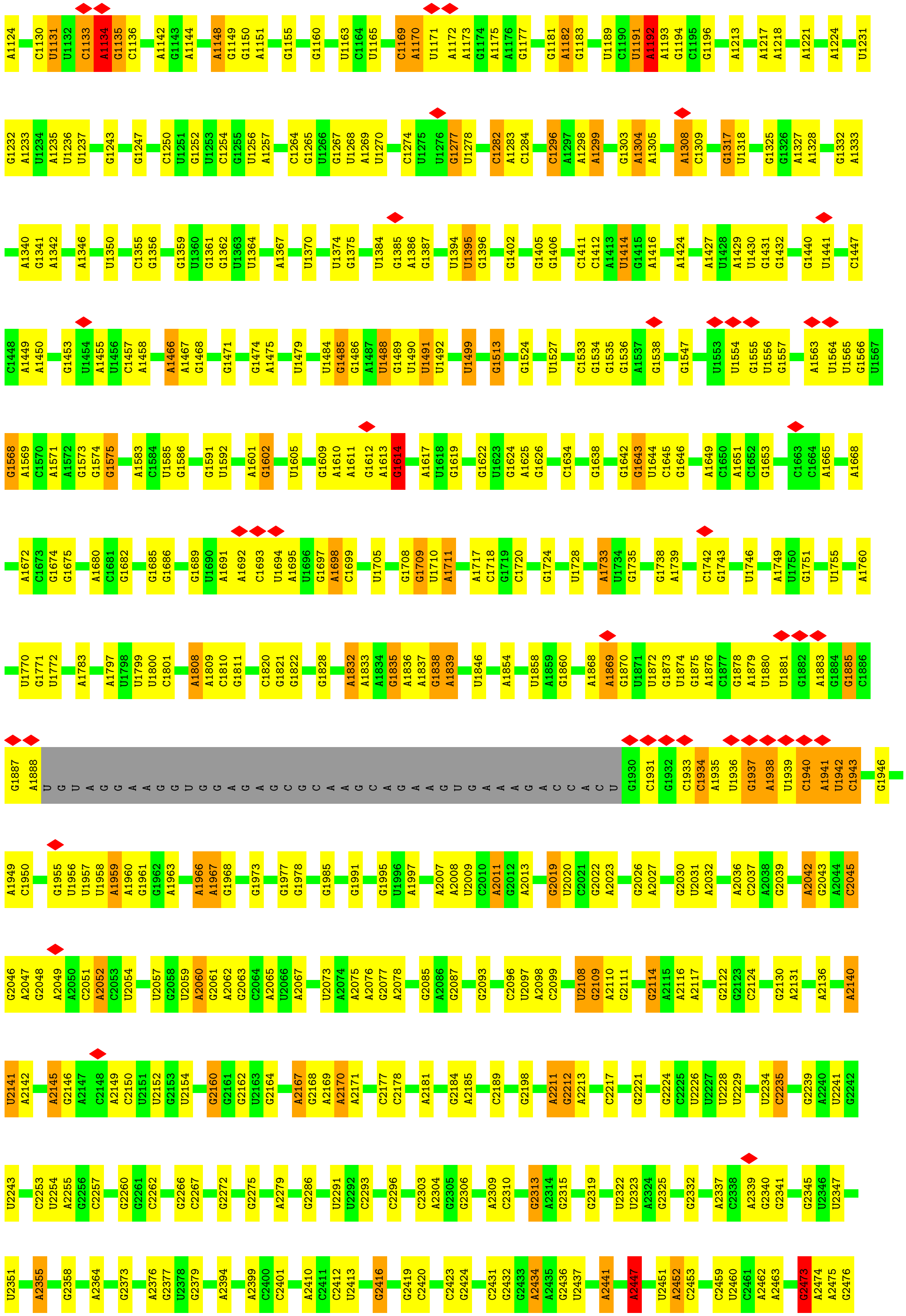
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
76	LGG	1	1	1	0
76	LJJ	1	1	1	0
76	LMM	1	1	1	0
76	LOO	1	1	1	0
76	LPP	1	1	1	0
76	SAA	1	1	1	0
76	SBB	1	1	1	0
76	SDD	1	1	1	0
76	SFF	1	1	1	0

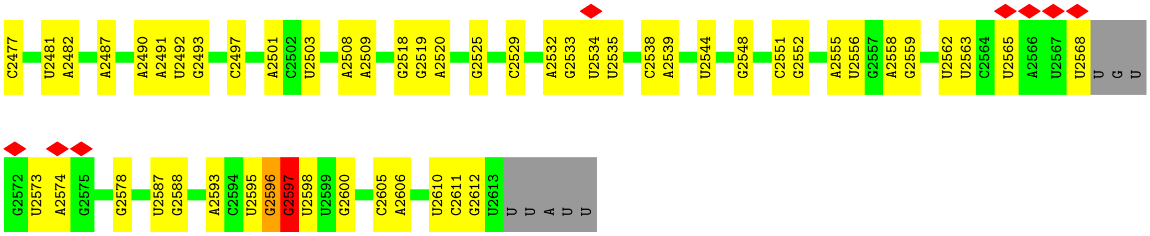
3 Residue-property plots ⓘ

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

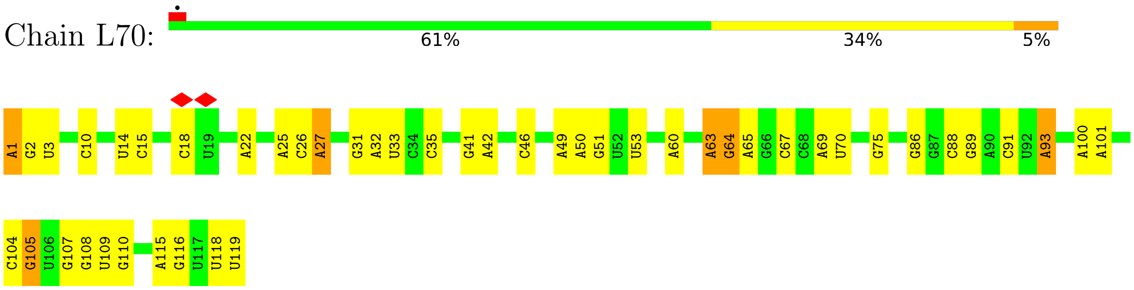
- Molecule 1: RNA 28S



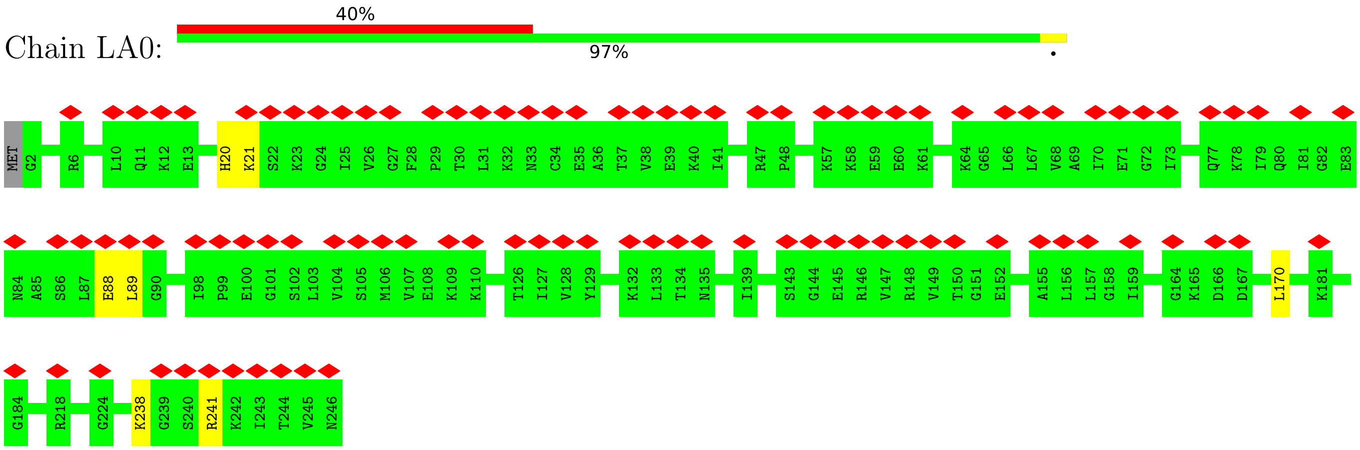

A1124 C1130 U1131 U1132 C1133 A1134 G1135 C1136 A1142 G1143 A1144 A1148 G1149 G1150 A1151 G1155 G1160 U1163 C1164 U1165 C1169 A1170 U1171 A1172 A1173 G1174 A1175 A1176 G1177 G1181 A1182 G1183 U1189 C1190 U1191 A1192 A1193 G1194 C1195 G1196 A1213 A1217 A1218 A1221 A1224 U1231
G1232 A1233 U1234 A1235 U1236 U1237 G1243 G1247 C1250 U1251 G1252 U1253 C1254 G1255 U1256 A1257 C1264 G1265 U1266 G1267 U1268 A1269 U1270 C1274 U1275 U1276 G1277 U1278 C1282 A1283 C1284 C1296 A1297 A1298 A1299 G1303 A1304 A1305 A1308 C1309 G1317 U1318 G1325 G1326 A1327 A1328 G1332 A1333
A1340 G1341 A1342 A1346 U1350 C1355 G1356 G1359 U1360 G1361 G1362 U1363 U1364 A1367 U1370 U1374 G1375 U1384 G1385 A1386 G1387 U1394 U1395 G1396 G1402 G1405 G1406 C1411 C1412 A1413 U1414 G1415 A1416 A1424 A1427 U1428 A1429 U1430 G1431 G1432 G1440 U1441 C1447
C1448 A1449 A1450 G1453 U1454 A1455 U1456 C1457 A1458 A1466 A1467 G1468 G1471 G1474 A1475 U1479 U1484 G1485 G1486 A1487 U1488 G1489 U1490 U1491 U1492 U1499 G1513 G1524 U1527 C1533 G1534 G1535 G1536 A1537 G1538 G1547 U1553 U1554 G1555 U1556 G1557 A1563 U1564 U1565 G1566 U1567
G1568 A1569 C1570 A1571 A1572 G1573 G1574 G1575 A1583 C1584 U1585 G1586 G1591 U1592 A1601 G1602 U1605 G1609 A1610 A1611 G1612 A1613 G1614 A1617 U1618 G1619 G1622 U1623 G1624 A1625 G1626 C1634 G1638 G1642 G1643 U1644 C1645 G1646 A1649 C1650 A1651 C1652 G1653 C1663 C1664 A1665 A1668
A1672 C1673 G1674 G1675 A1680 C1681 G1682 G1685 G1686 G1689 U1690 A1691 A1692 C1693 U1694 A1695 U1696 G1697 A1698 C1699 U1705 G1708 G1709 U1710 A1711 A1717 C1718 G1719 C1720 G1724 U1728 A1733 U1734 G1735 G1738 A1739 C1742 G1743 U1746 A1749 U1750 G1751 U1755 A1760
U1770 G1771 U1772 A1783 A1797 U1798 U1799 U1800 C1801 A1808 A1809 C1810 G1811 C1820 G1821 G1822 G1828 A1832 A1833 A1834 G1835 A1836 A1837 G1838 A1839 U1846 A1854 U1858 A1859 G1860 A1868 A1869 G1870 U1871 U1872 G1873 U1874 G1875 A1876 C1877 G1878 A1879 U1880 U1881 G1882 A1883 G1884 G1885 C1886
G1887 A1888 U G U A G G A A G G U G G A G A G C G C A A G C A G A A G U G A A A G A C C A C U G1930 C1931 G1932 C1933 C1934 A1935 U1936 G1937 A1938 U1939 C1940 A1941 U1942 C1943 G1946
A1949 C1950 G1955 U1956 U1957 U1958 A1959 A1960 G1961 G1962 A1963 A1966 A1967 G1968 G1973 G1977 G1978 G1985 G1991 G1995 U1996 A1997 A2007 A2008 U2009 C2010 A2011 G2012 A2013 G2019 U2020 C2021 G2022 A2023 G2026 A2027 G2030 U2031 A2032 A2036 C2037 A2038 G2039 A2042 G2043 A2044 C2045
G2046 A2047 G2048 A2049 A2050 C2051 A2052 C2053 U2054 U2057 G2058 U2059 A2060 G2061 A2062 G2063 C2064 A2065 U2066 A2067 U2073 A2074 A2075 A2076 G2077 A2078 G2085 A2086 G2087 G2093 C2096 U2097 A2098 C2099 U2108 G2109 A2110 G2111 C2114 A2115 A2116 A2117 G2122 G2123 C2124 G2130 A2131 A2136 A2140
U2141 A2142 A2145 G2146 A2147 C2148 A2149 C2150 U2151 C2152 G2153 U2154 G2160 G2161 C2162 U2163 G2164 A2167 C2168 A2169 A2170 A2171 C2177 C2178 A2181 G2184 A2185 C2189 G2198 A2211 G2212 A2213 C2217 G2221 G2224 C2225 U2226 U2227 U2228 U2229 U2234 C2235 G2239 A2240 U2241 G2242
U2243 C2253 U2254 A2255 G2256 C2257 G2260 G2261 C2262 G2266 C2267 G2272 G2275 A2279 G2286 U2291 U2292 C2293 C2296 C2303 A2304 G2305 G2306 A2309 C2310 G2313 A2314 G2315 G2319 U2322 U2323 A2324 G2325 G2332 A2337 C2338 A2339 G2340 G2341 G2345 U2346 U2347
U2351 A2355 G2358 A2364 G2373 A2376 G2377 U2378 G2379 A2394 A2399 C2400 C2401 A2410 C2411 C2412 U2413 G2416 G2419 C2420 C2423 G2424 C2431 G2432 G2433 A2434 A2435 G2436 U2437 A2441 A2447 U2451 A2452 C2453 C2459 U2460 C2461 A2462 A2463 G2473 A2474 A2475 G2476



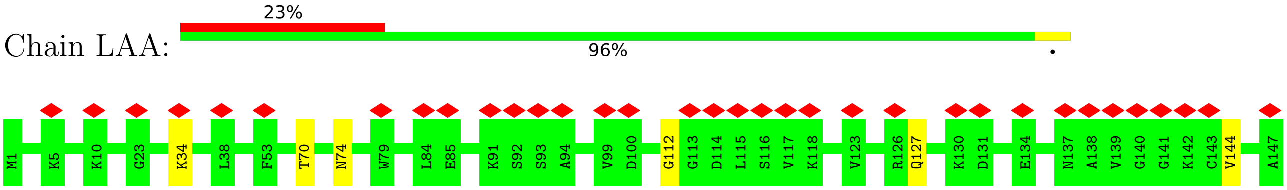
- Molecule 2: RNA 5S



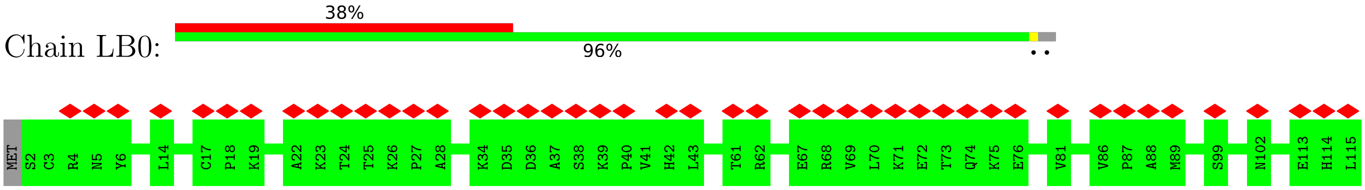
- Molecule 3: 60S ribosomal protein L8

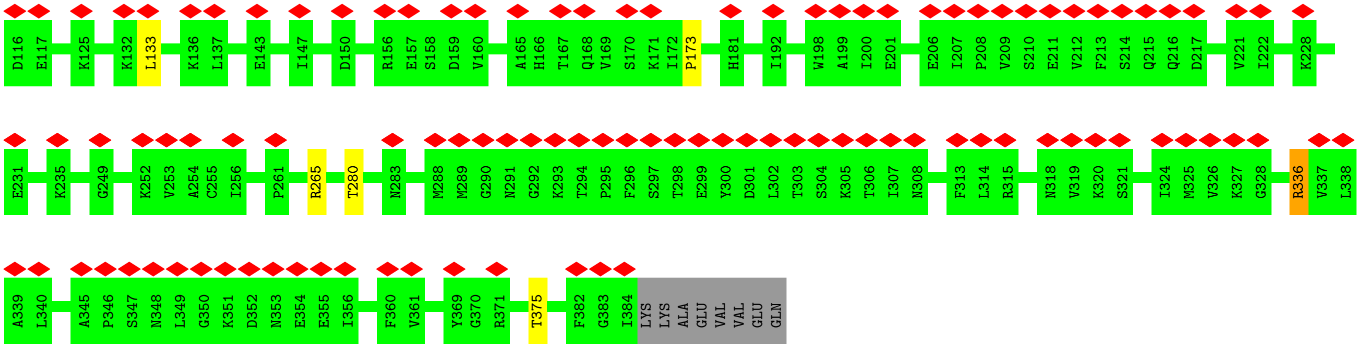


- Molecule 4: uL15



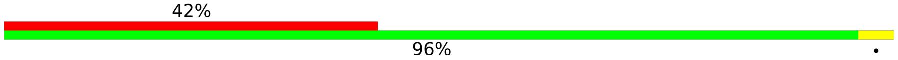
- Molecule 5: 60S ribosomal protein L3

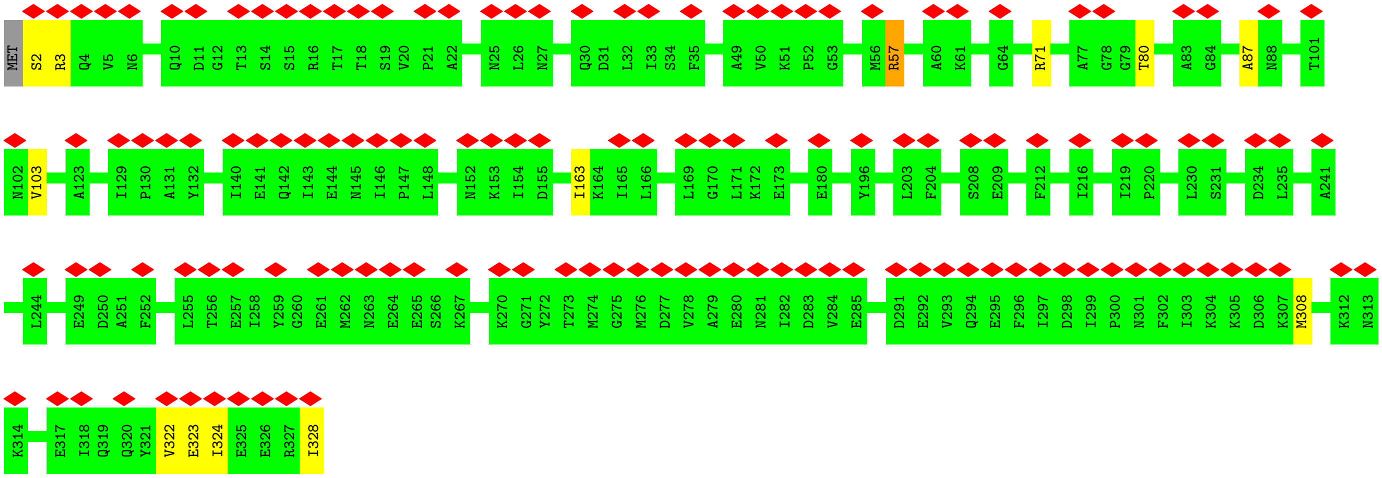




- Molecule 6: 60S ribosomal protein L4

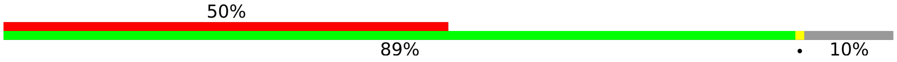
Chain LC0:

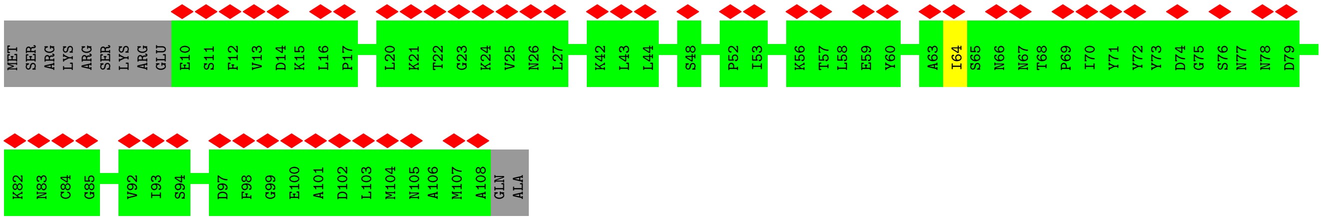




- Molecule 7: 60S ribosomal protein L3

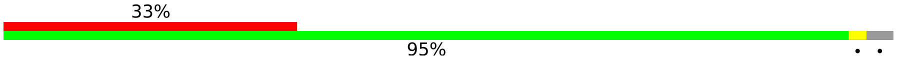
Chain LCC:

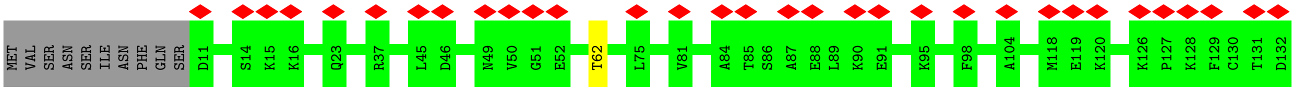


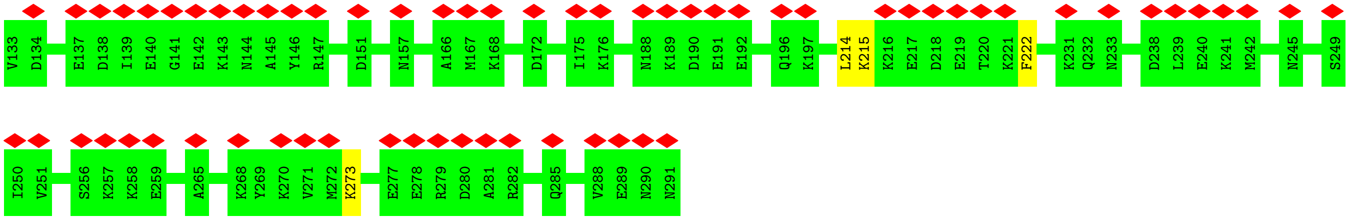


- Molecule 8: 60S ribosomal protein L5

Chain LD0:

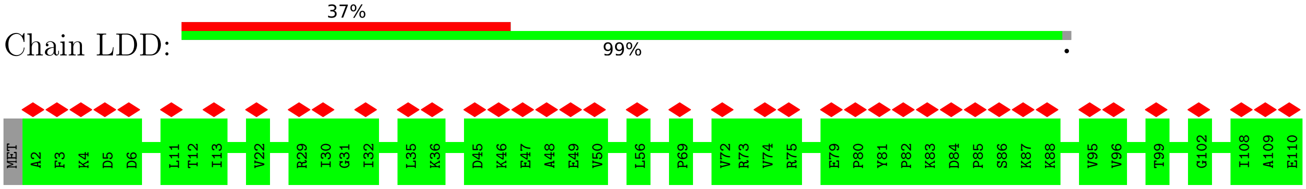






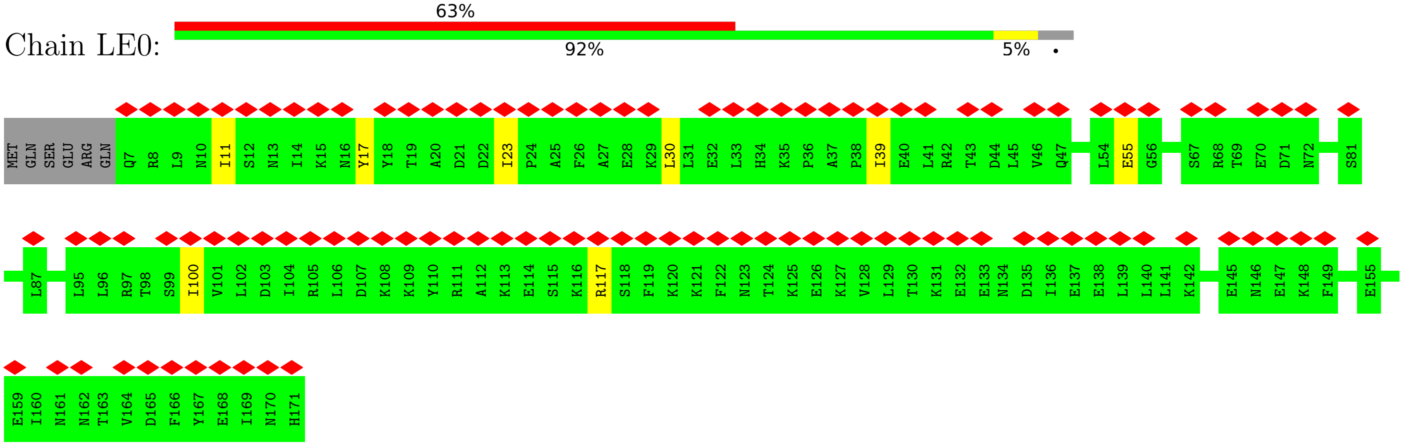
- Molecule 9: 60S ribosomal protein L31

Chain LDD:



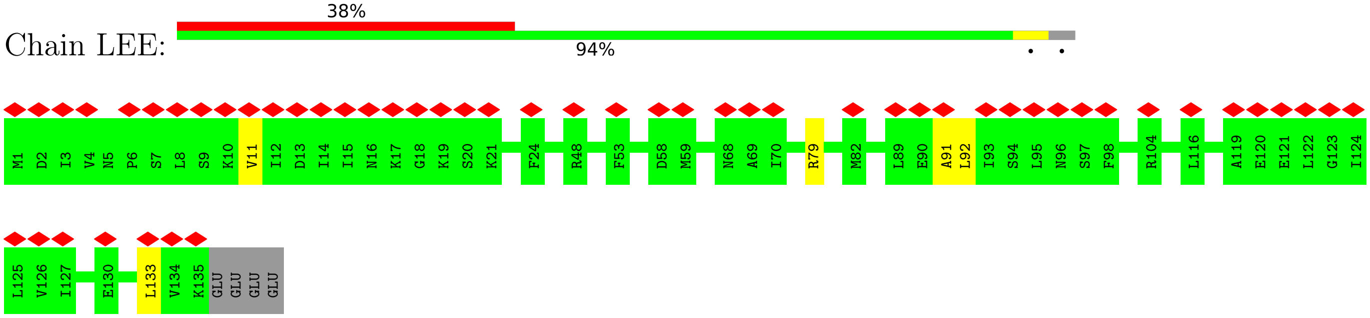
- Molecule 10: 60S ribosomal protein L6

Chain LE0:



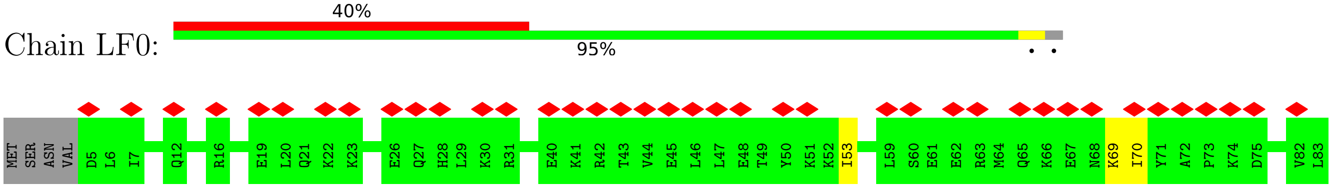
- Molecule 11: 60S ribosomal protein L32

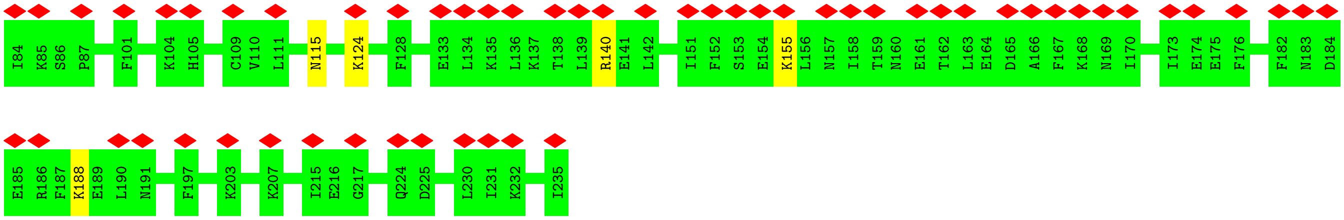
Chain LEE:



- Molecule 12: 60S ribosomal protein L7

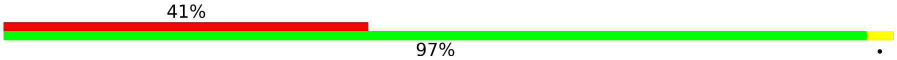
Chain LF0:

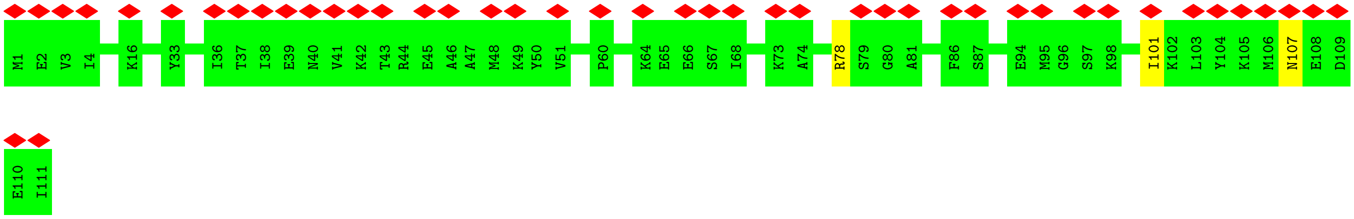




- Molecule 13: 60S ribosomal protein L35a

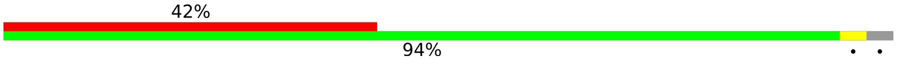
Chain LFF:

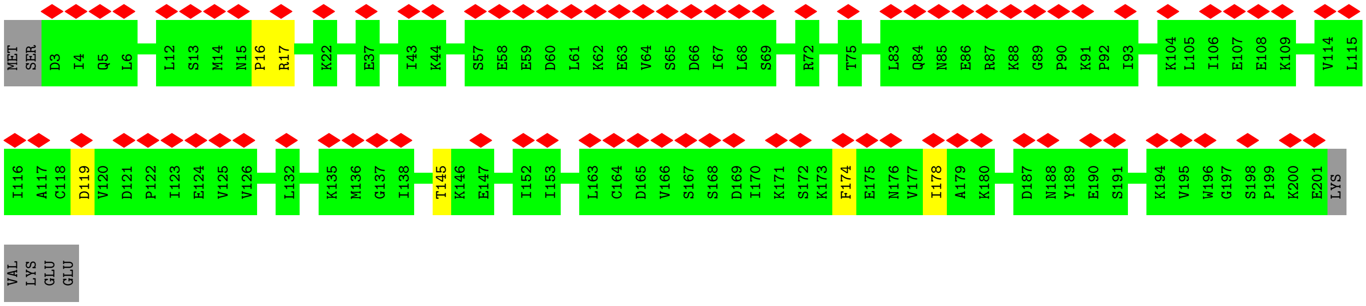




- Molecule 14: 60S ribosomal protein L8

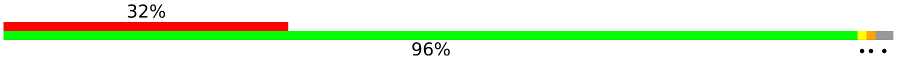
Chain LG0:

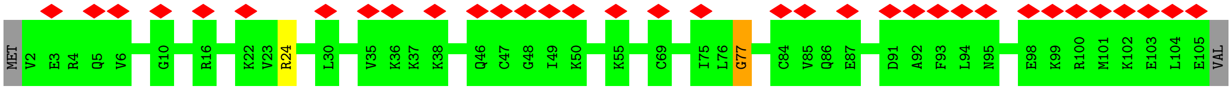




- Molecule 15: Ribosomal protein L34

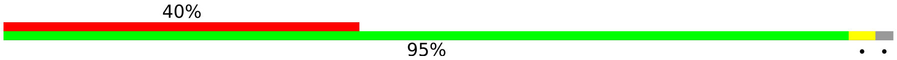
Chain LGG:

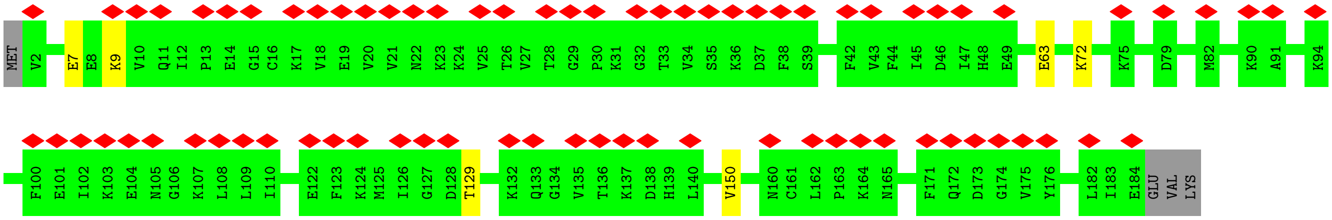




- Molecule 16: 60S ribosomal protein L9

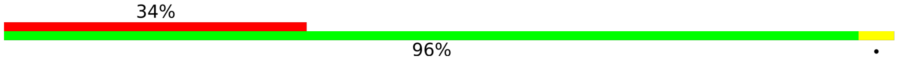
Chain LH0:

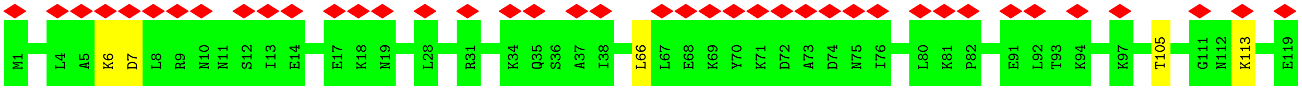




- Molecule 17: Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein

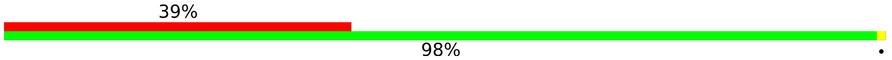
Chain LHH:

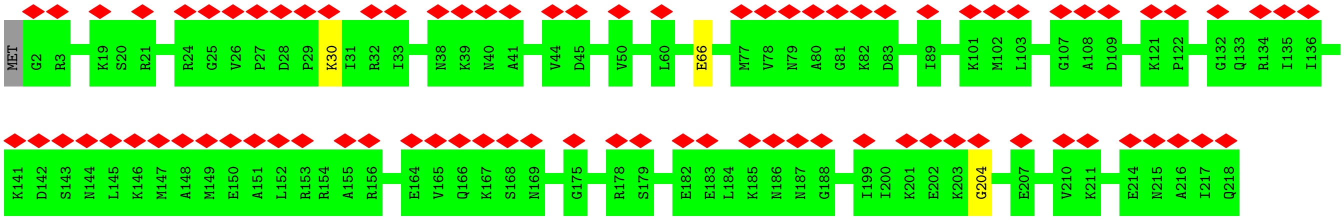




- Molecule 18: S60 ribosomal protein L10

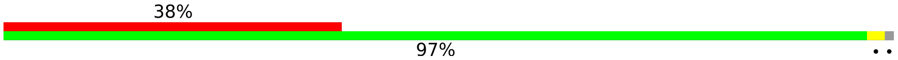
Chain LI0:

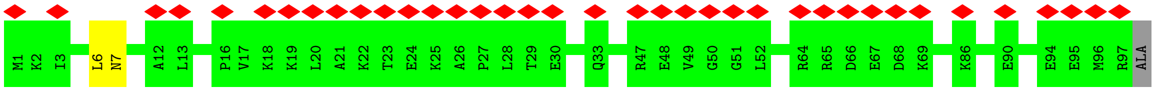




- Molecule 19: 60S ribosomal protein L36

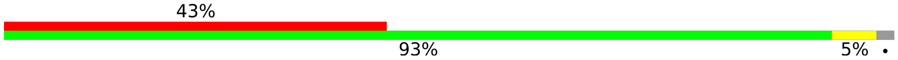
Chain LII:

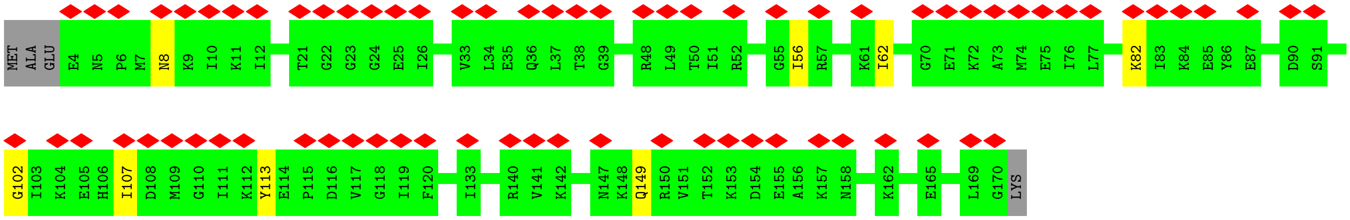




- Molecule 20: 60S ribosomal protein L11

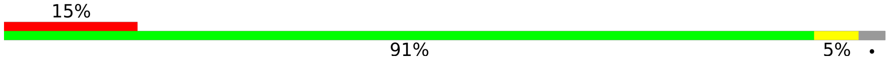
Chain LJ0:

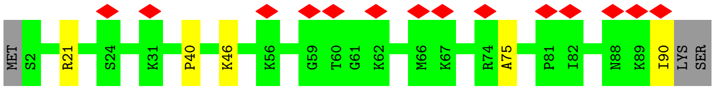




- Molecule 21: eL37

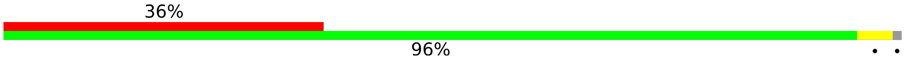
Chain LJJ:

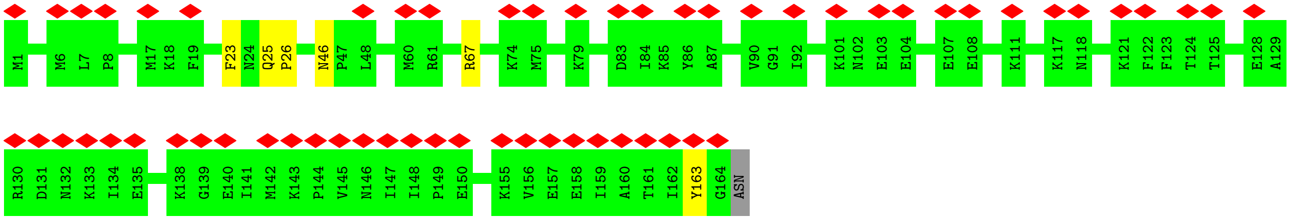




- Molecule 22: 60S ribosomal protein L13

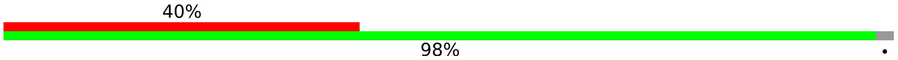
Chain LL0:

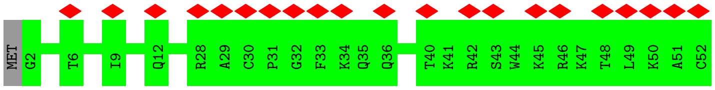




- Molecule 23: 60S ribosomal protein L39

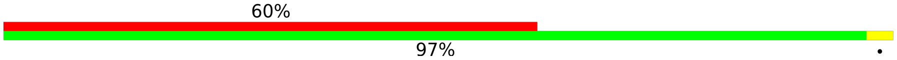
Chain LLL:

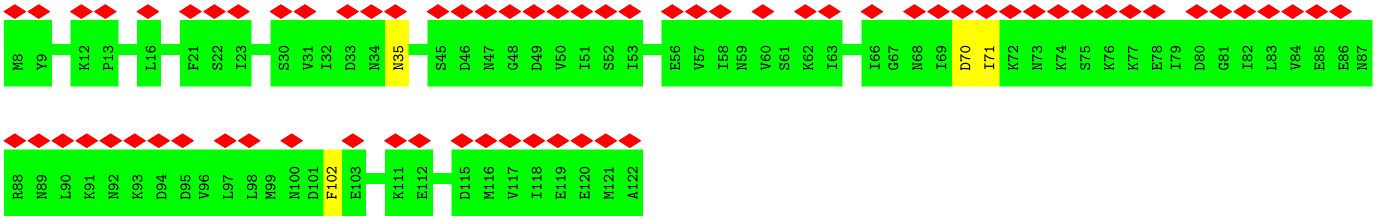




- Molecule 24: Transposase

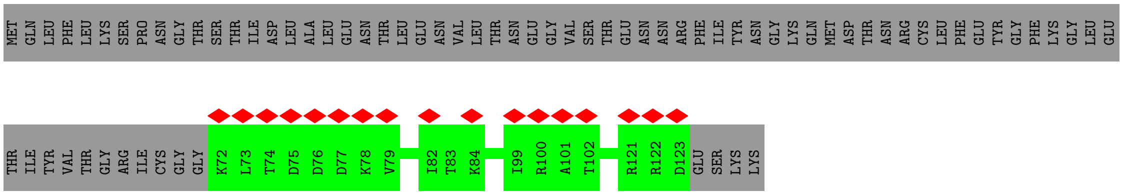
Chain LM0:





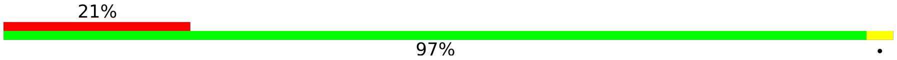
- Molecule 25: Ubiquitin

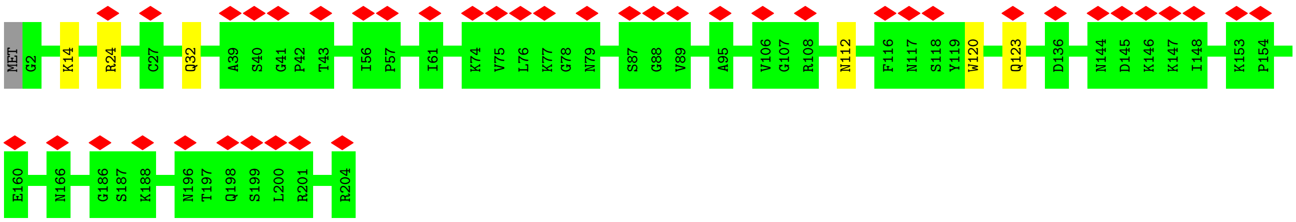
Chain LMM:



- Molecule 26: Ribosomal protein L15

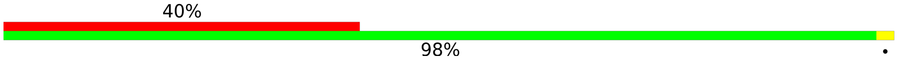
Chain LN0:

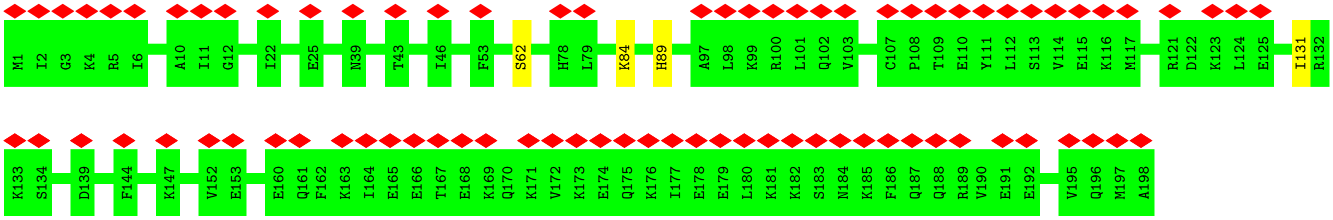




- Molecule 27: Ribosomal protein L13A

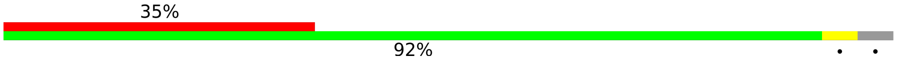
Chain LO0:

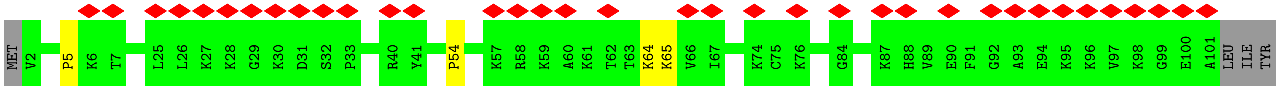




- Molecule 28: 60S ribosomal protein L44

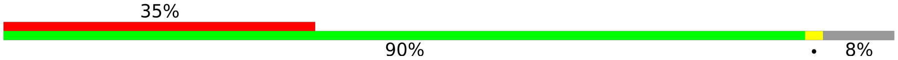
Chain LOO:

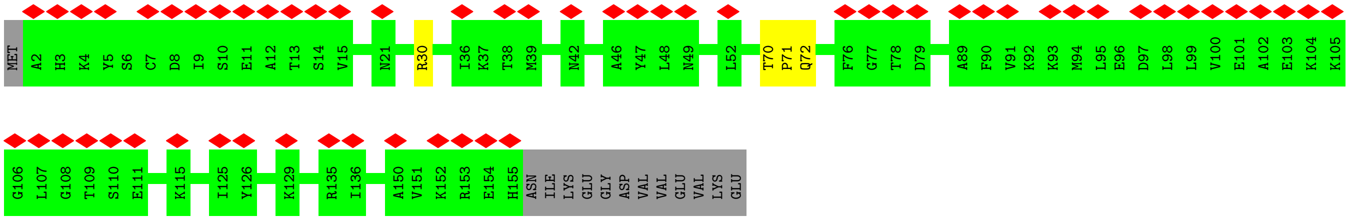




- Molecule 29: 60S ribosomal protein L17

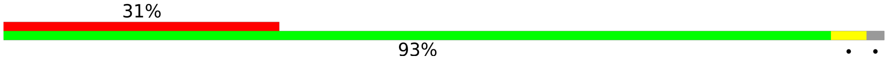
Chain LP0:

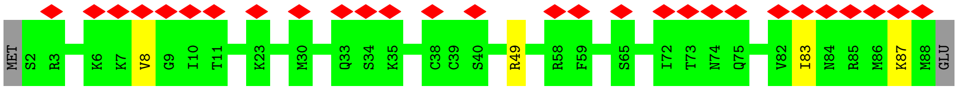




- Molecule 30: 60S ribosomal protein L37a

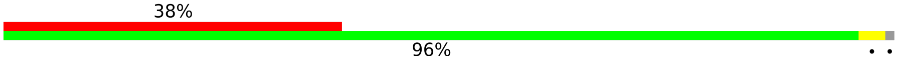
Chain LPP:

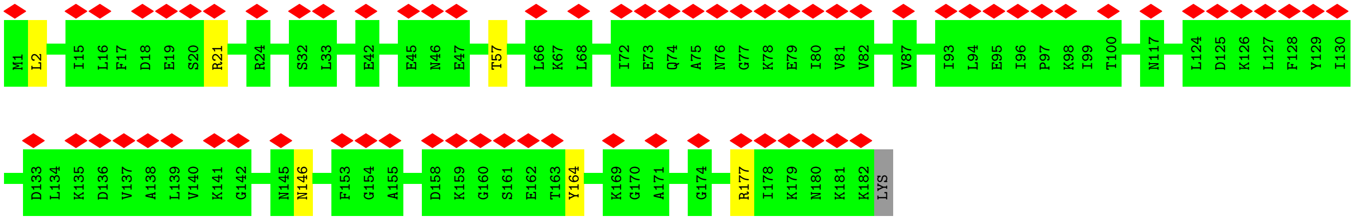




- Molecule 31: 60S ribosomal protein L18

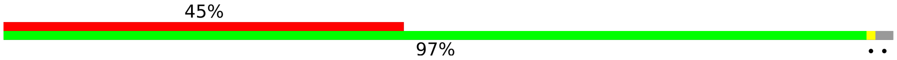
Chain LQ0:

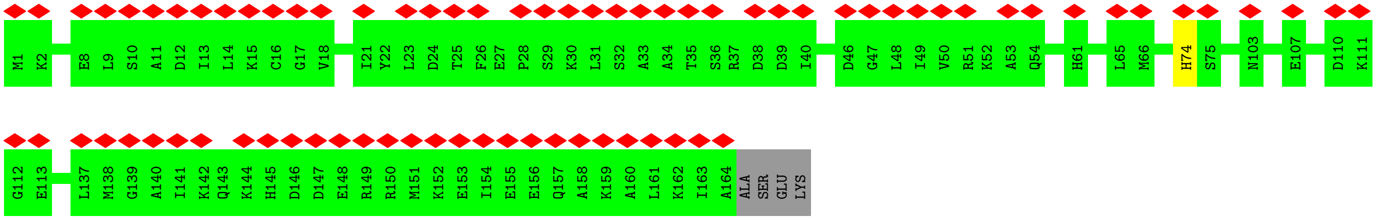




- Molecule 32: 60S ribosomal protein L19

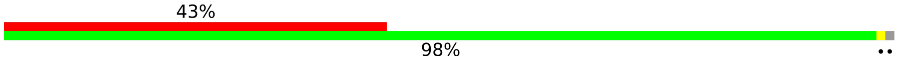
Chain LR0:

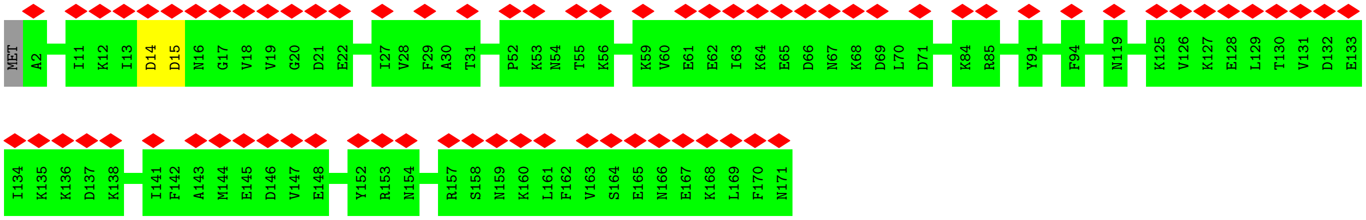




- Molecule 33: 60S ribosomal protein L20

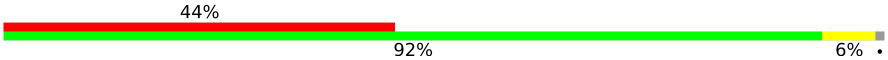
Chain LS0:

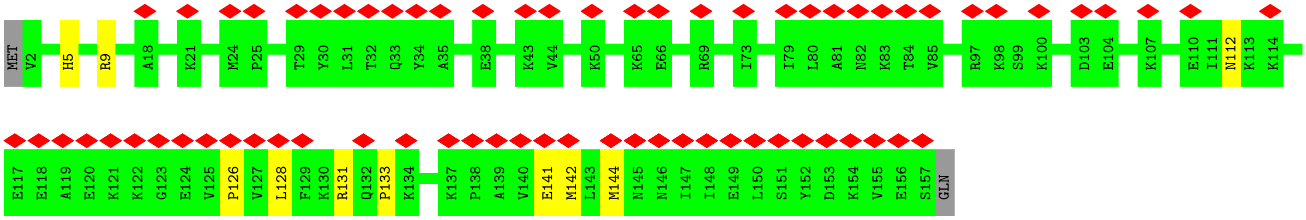




- Molecule 34: 60s ribosomal protein L21

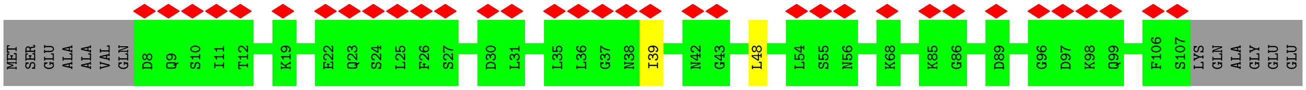
Chain LT0:





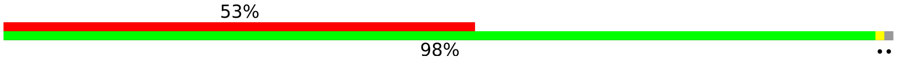
- Molecule 35: 60S ribosomal protein L22

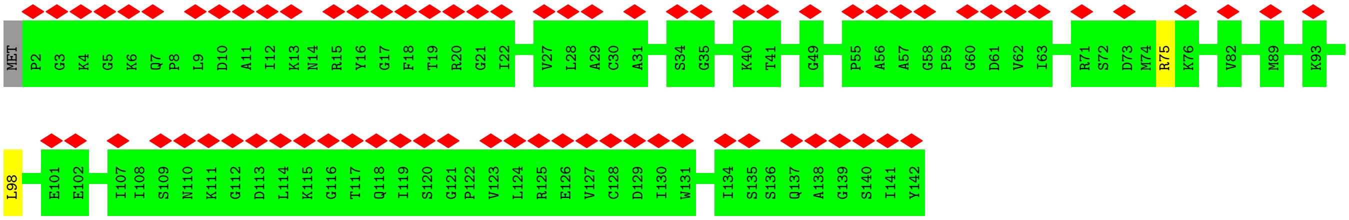
Chain LU0:



- Molecule 36: Ribosomal protein L23

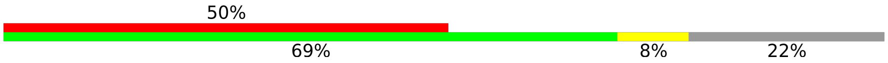
Chain LV0:

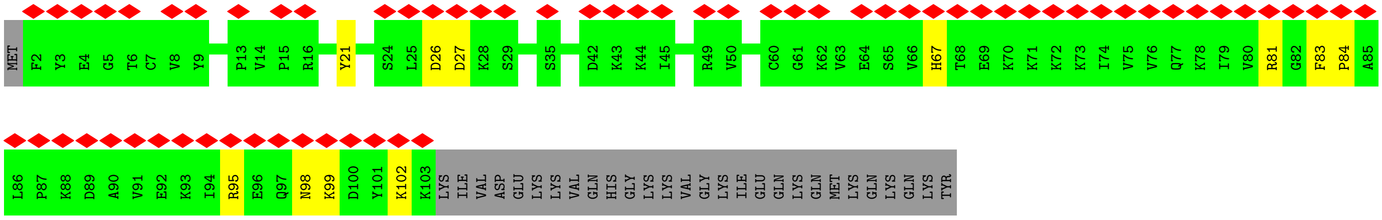




- Molecule 37: Ribosomal protein L24E

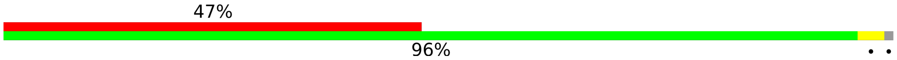
Chain LW0:

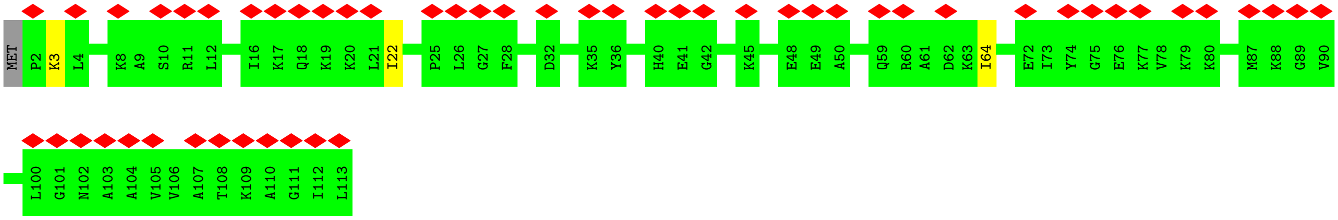




- Molecule 38: 60S ribosomal protein L23a

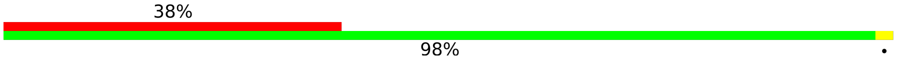
Chain LX0:

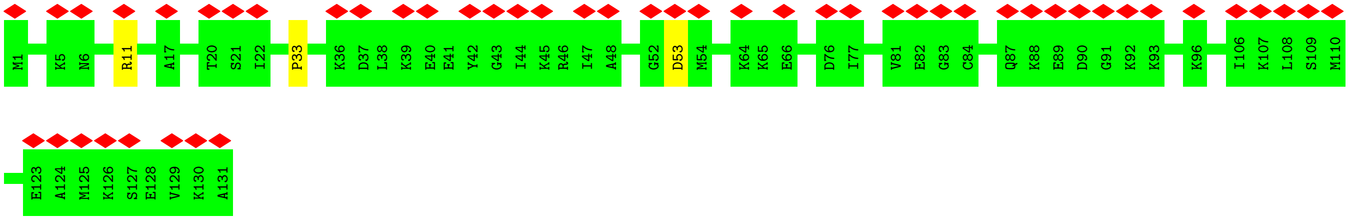




- Molecule 39: 60S ribosomal protein L26

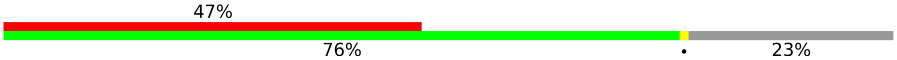
Chain LY0:

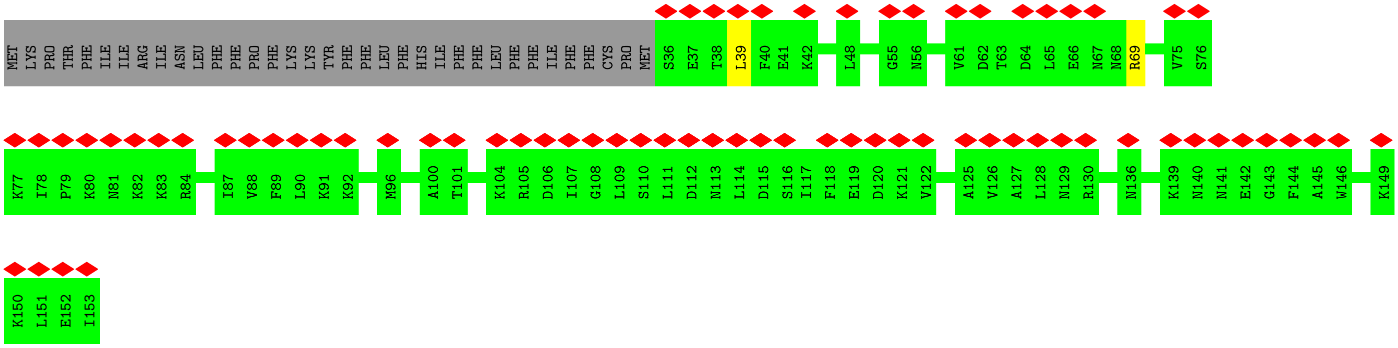




- Molecule 40: 60S ribosomal protein L27

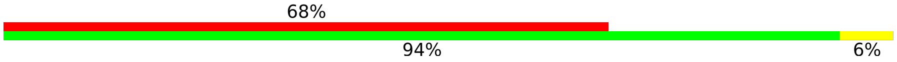
Chain LZ0:

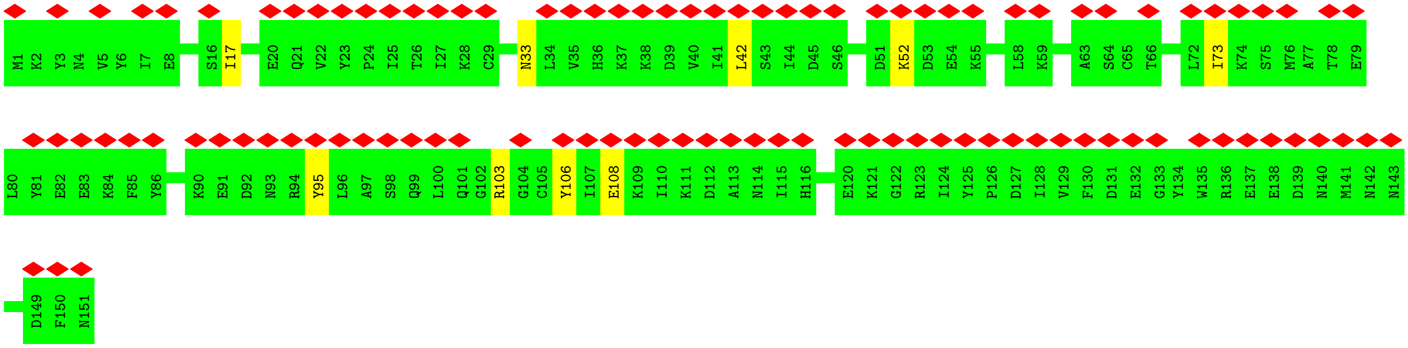




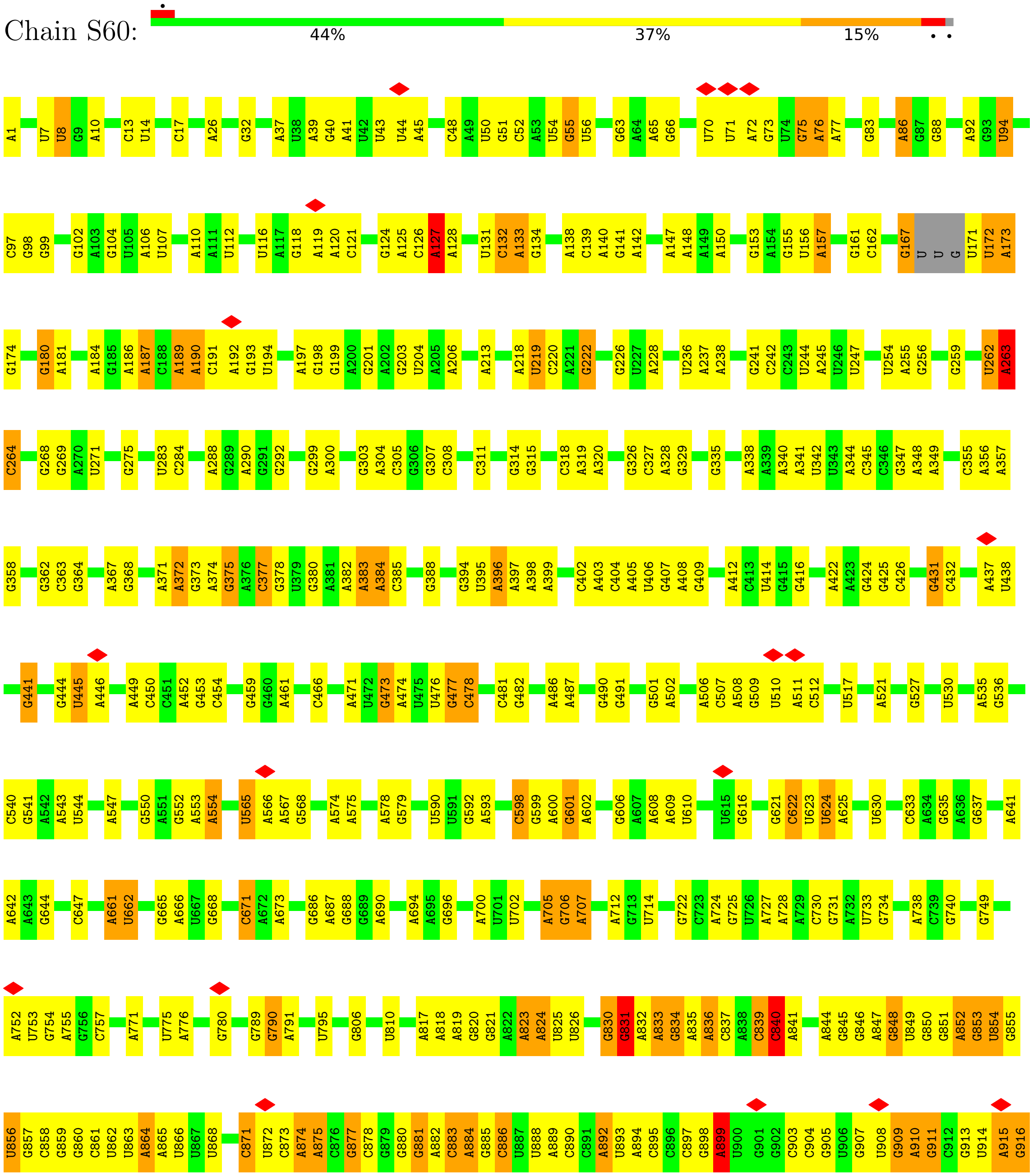
- Molecule 41: DNL-type domain-containing protein

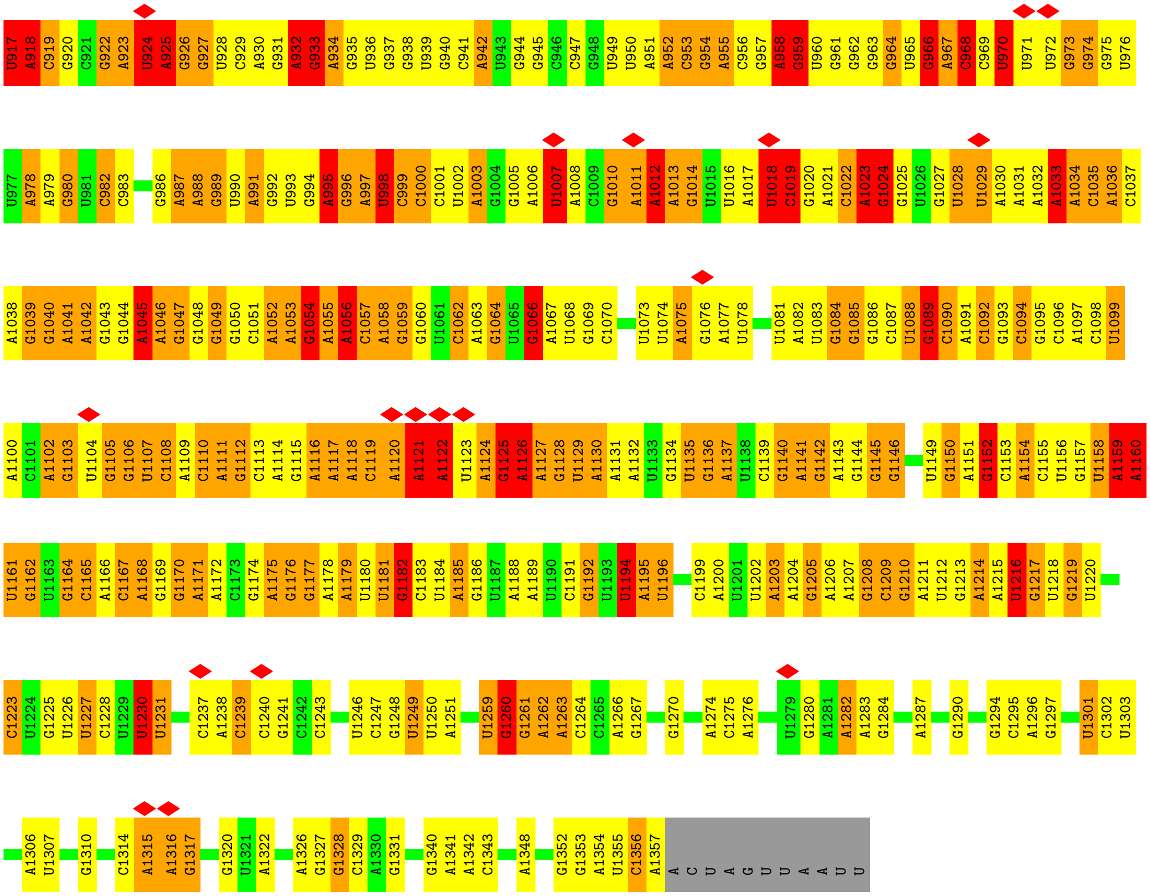
Chain MD1:





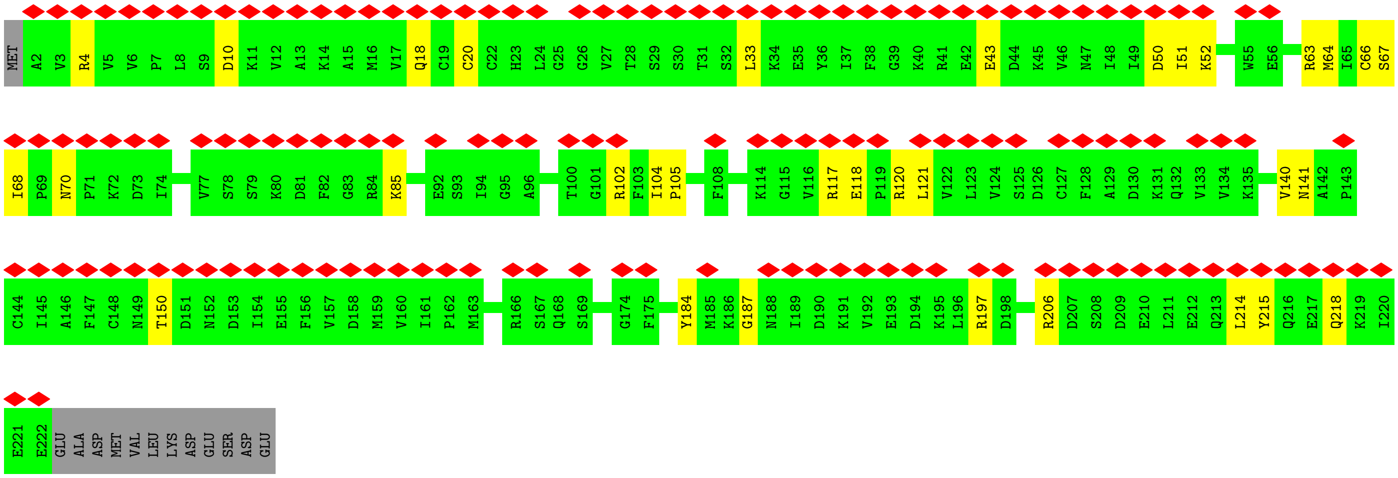
- Molecule 42: RNA 16S





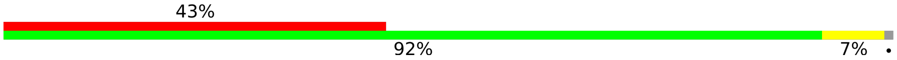
- Molecule 43: 40S ribosomal protein S0

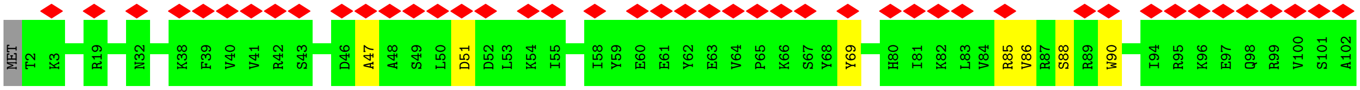
Chain SA0:



- Molecule 44: 40S ribosomal protein S26

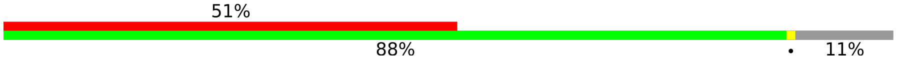
Chain SAA:

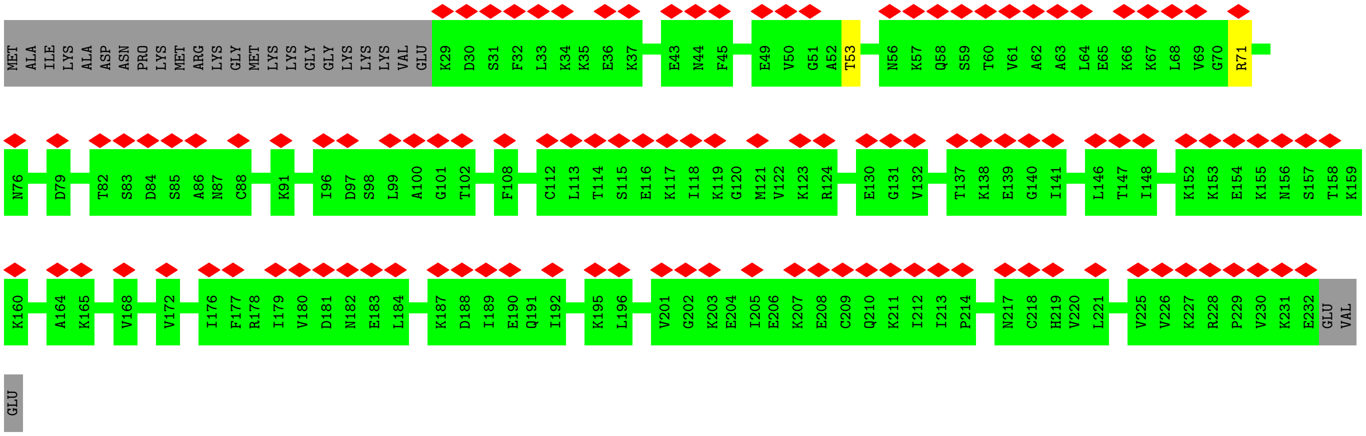




- Molecule 45: eS1

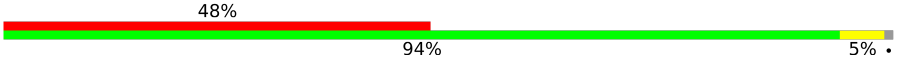
Chain SB0:

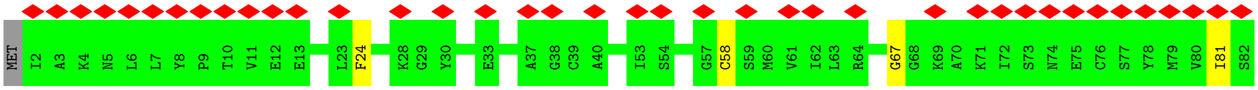




- Molecule 46: eS27

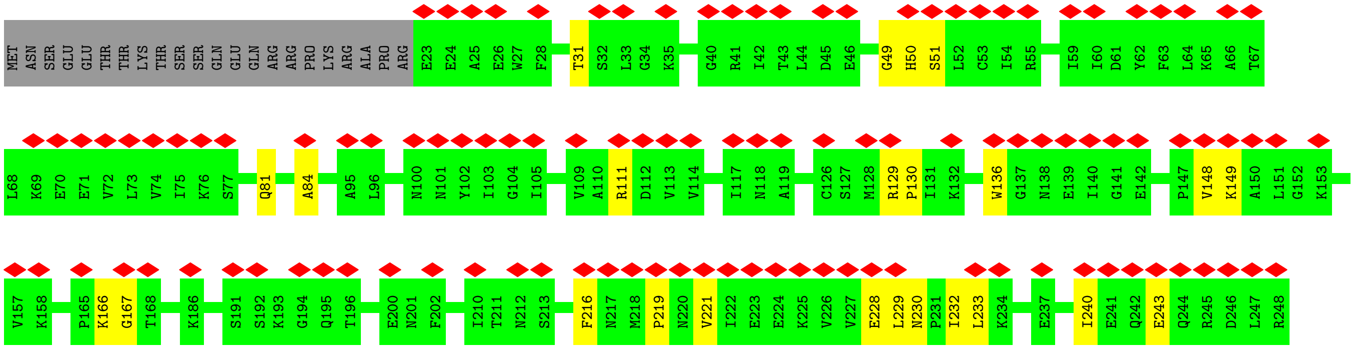
Chain SBB:





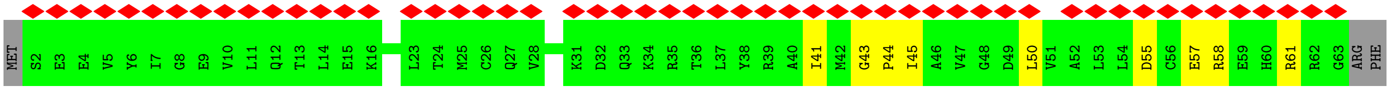
- Molecule 47: 40S ribosomal protein S2

Chain SC0:



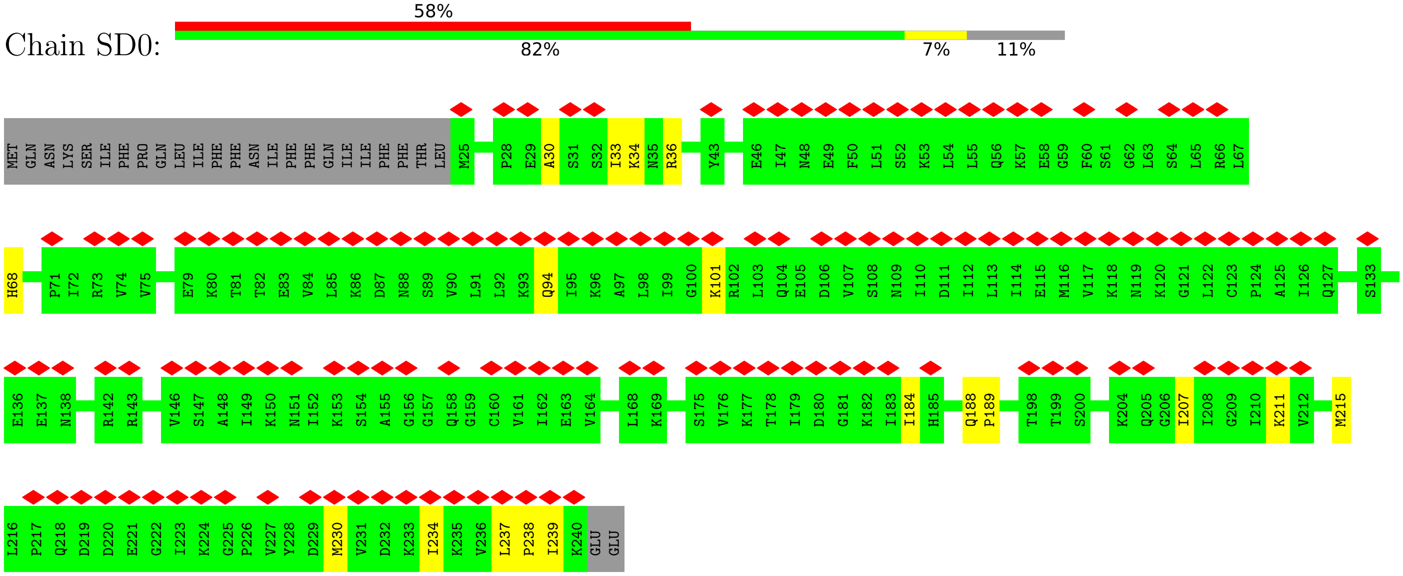
- Molecule 48: eS28

Chain SCC:



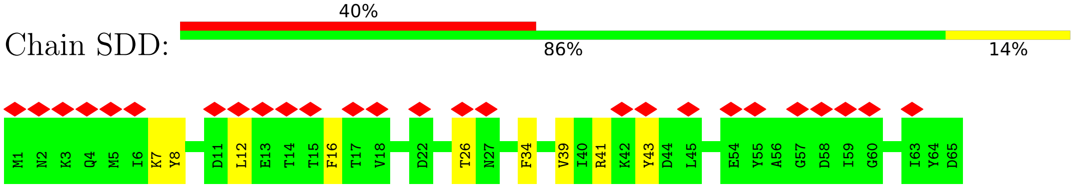
- Molecule 49: 40S ribosomal protein S3

Chain SD0:



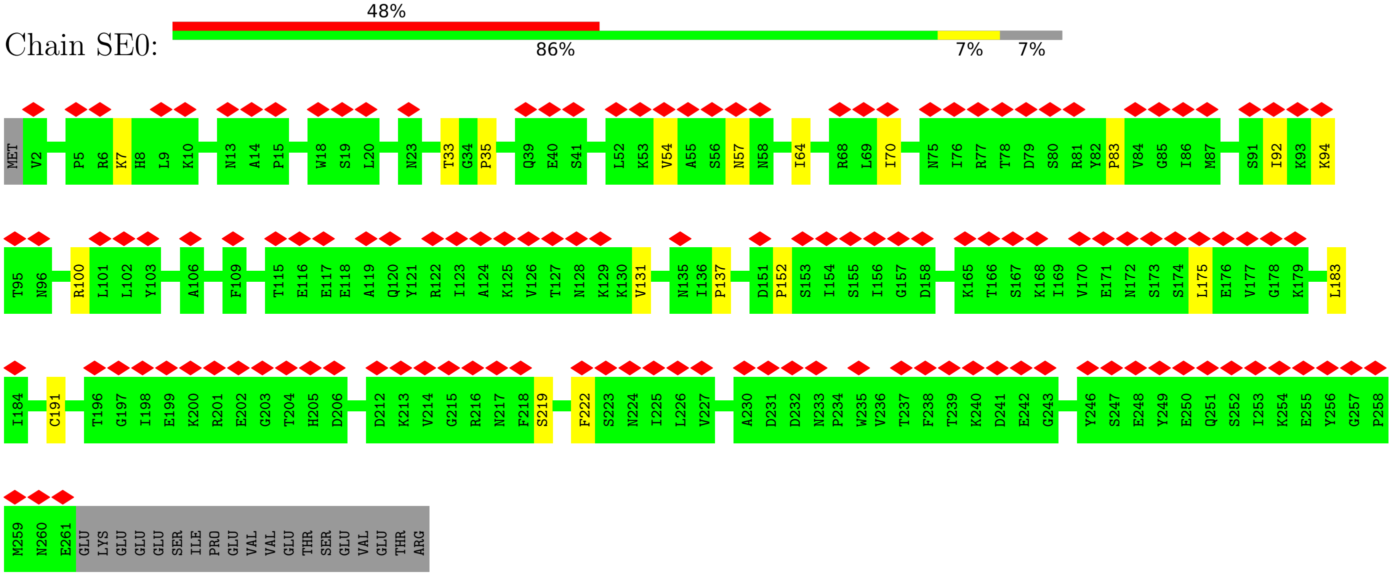
- Molecule 50: 40S ribosomal protein S29

Chain SDD:



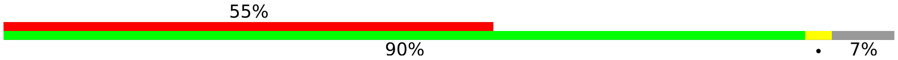
- Molecule 51: 40S ribosomal protein S4

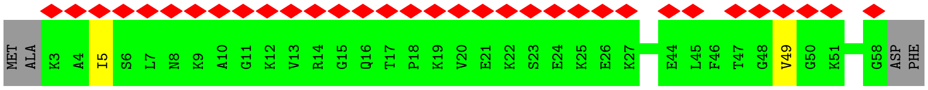
Chain SE0:



- Molecule 52: eS30

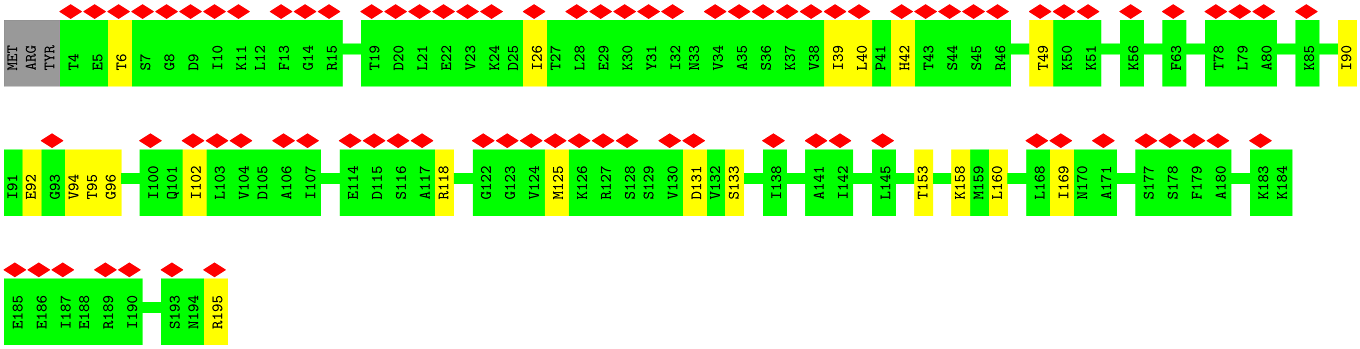
Chain SEE:





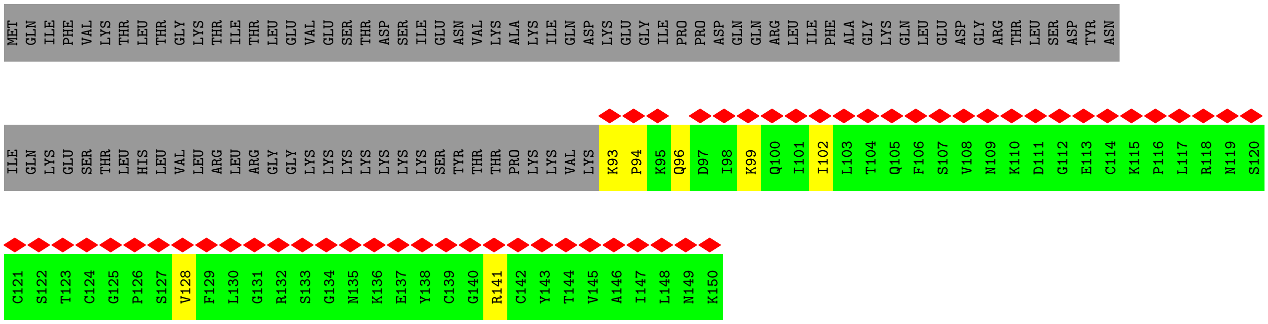
- Molecule 53: 40S ribosomal protein S5

Chain SF0:



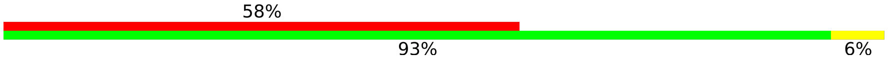
- Molecule 54: Ubiquitin/40s ribosomal protein S27a fusion

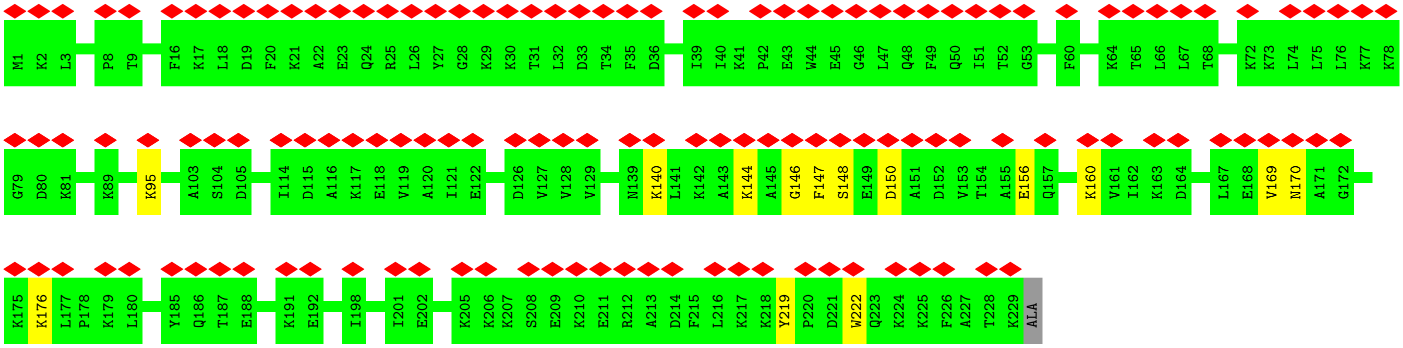
Chain SFF:



- Molecule 55: 40S ribosomal protein S6

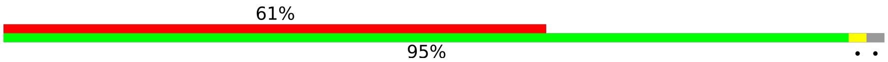
Chain SG0:

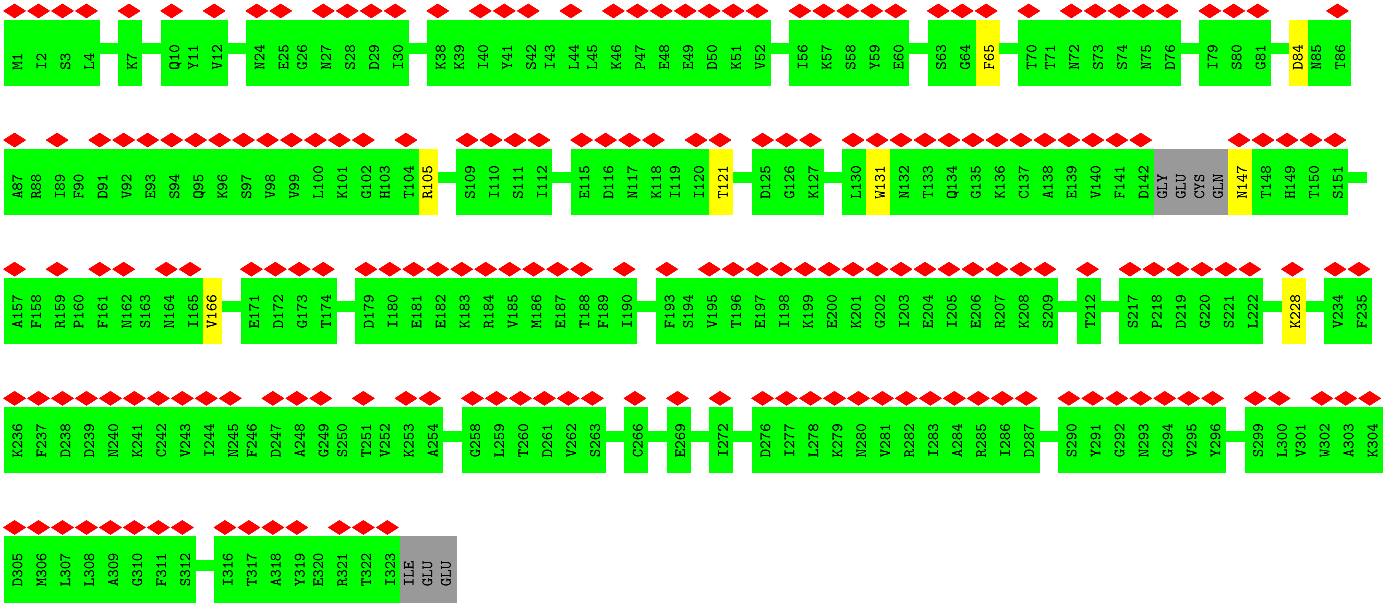




- Molecule 56: Guanine nucleotide binding protein beta subunit

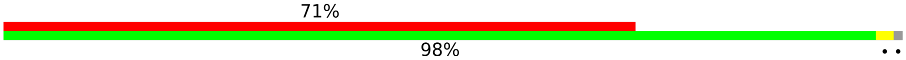
Chain SGG:

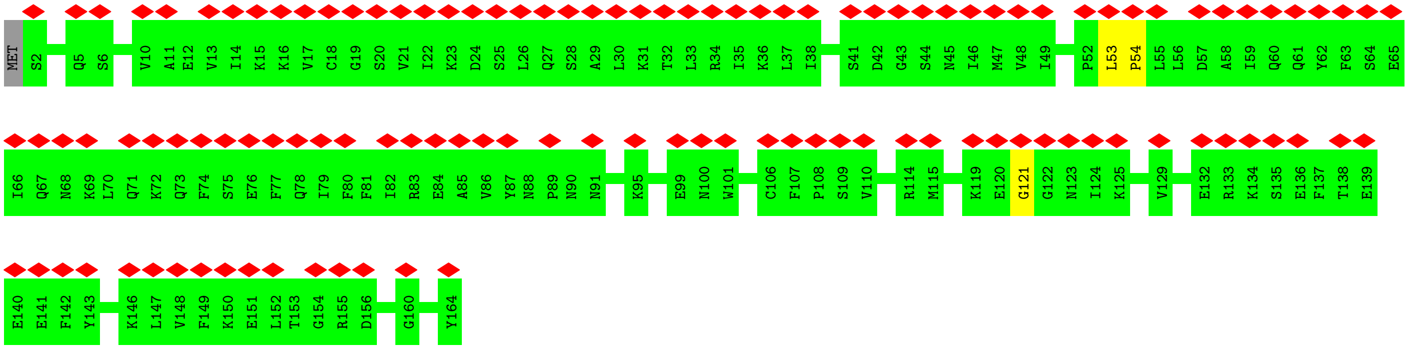




- Molecule 57: 40S ribosomal protein S7

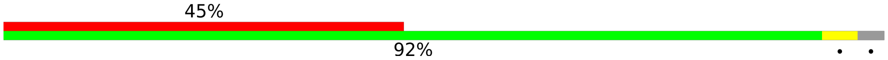
Chain SH0:

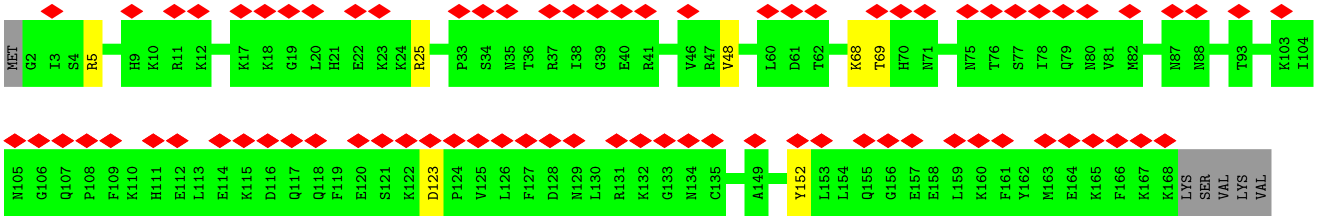




- Molecule 58: 40S ribosomal protein S8

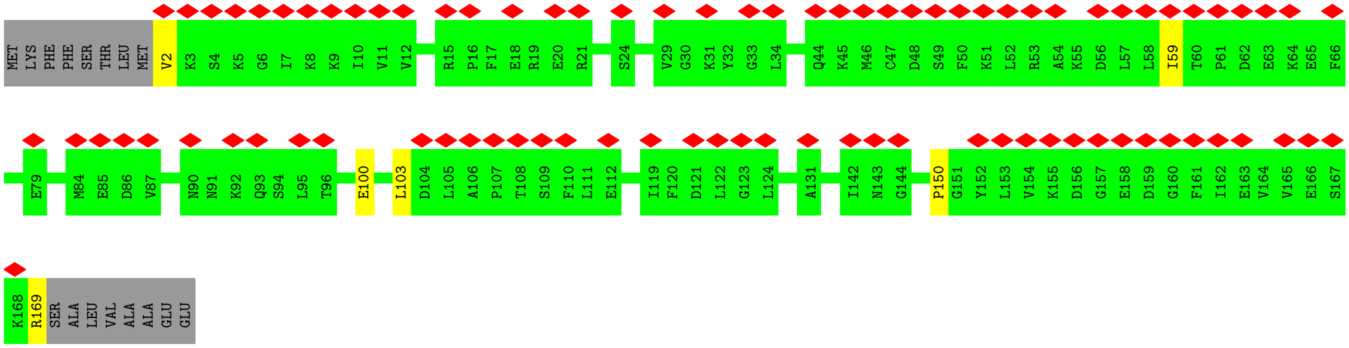
Chain SI0:





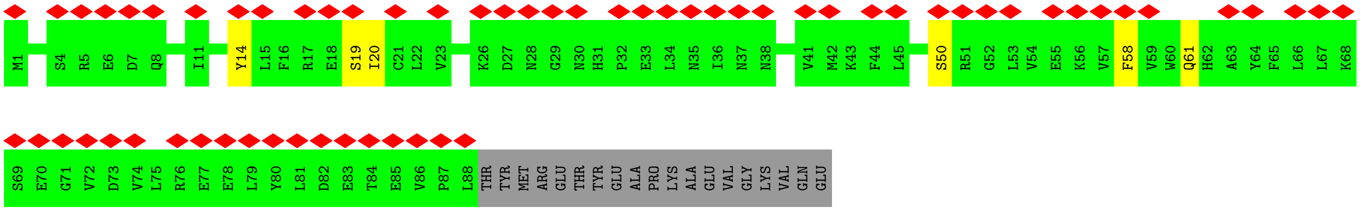
- Molecule 59: 40S ribosomal protein S9

Chain SJ0:



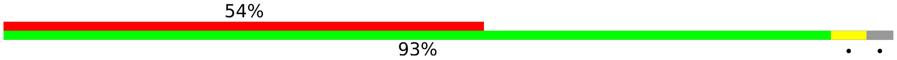
- Molecule 60: 40S ribosomal protein S10

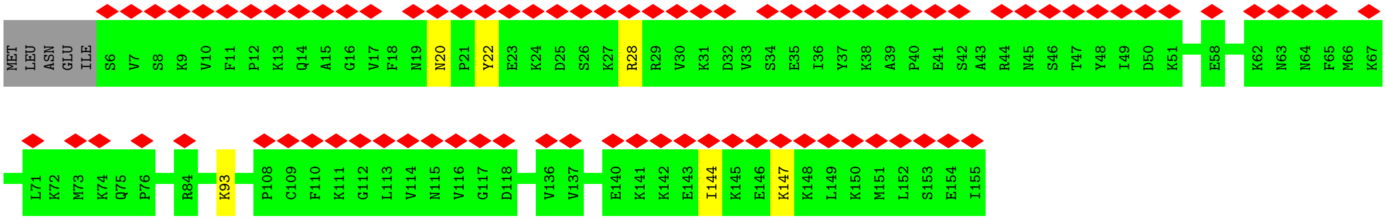
Chain SK0:



- Molecule 61: 40S ribosomal protein S11

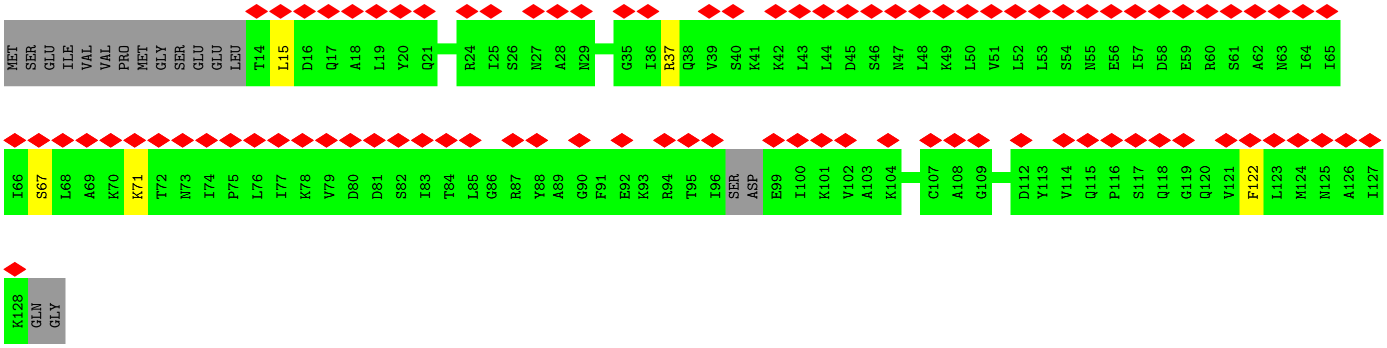
Chain SL0:





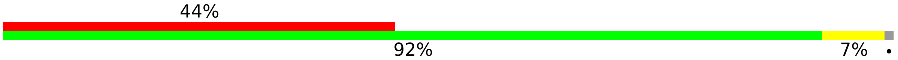
- Molecule 62: 40S ribosomal protein S12

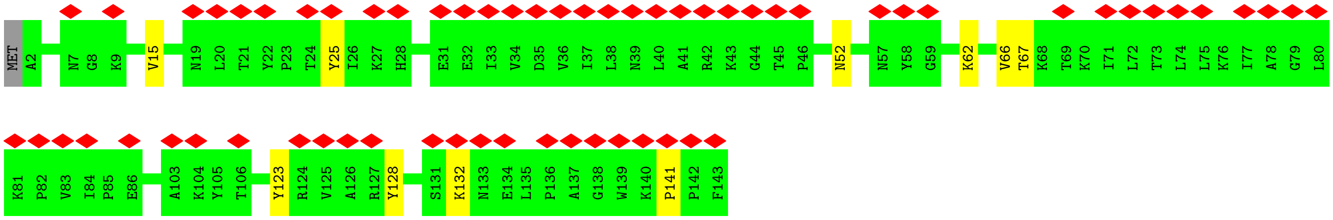
Chain SM0:



- Molecule 63: 40S ribosomal protein S13

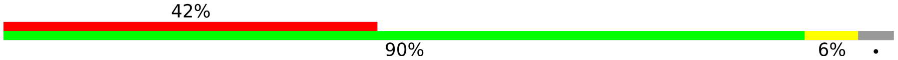
Chain SN0:

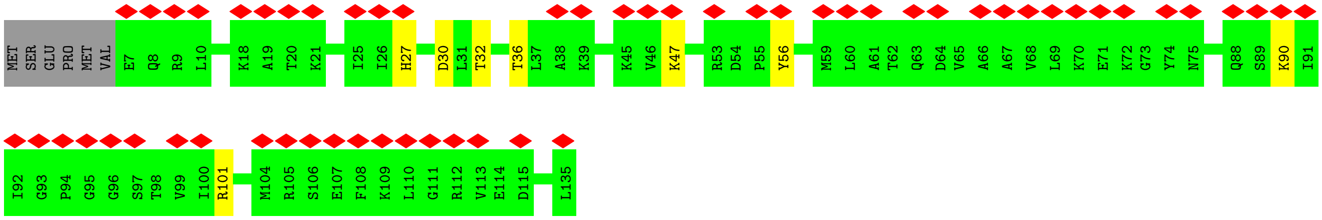




- Molecule 64: 40S ribosomal protein S14

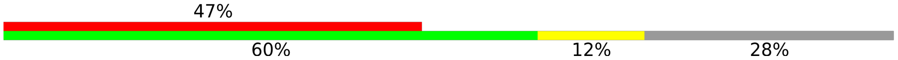
Chain SO0:

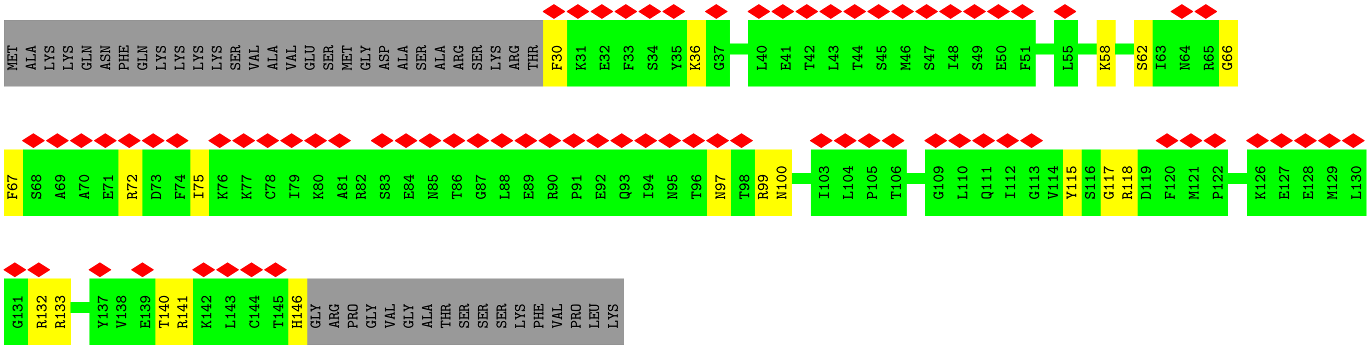




- Molecule 65: Ribosomal protein S19

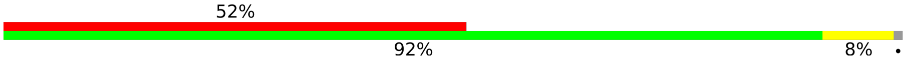
Chain SP0:

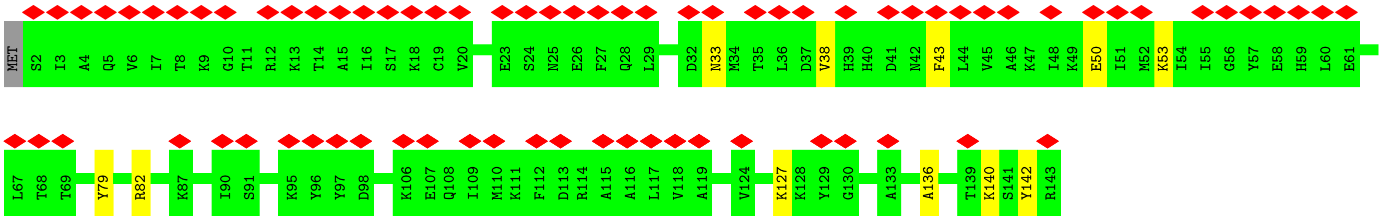




- Molecule 66: 40S ribosomal protein S16

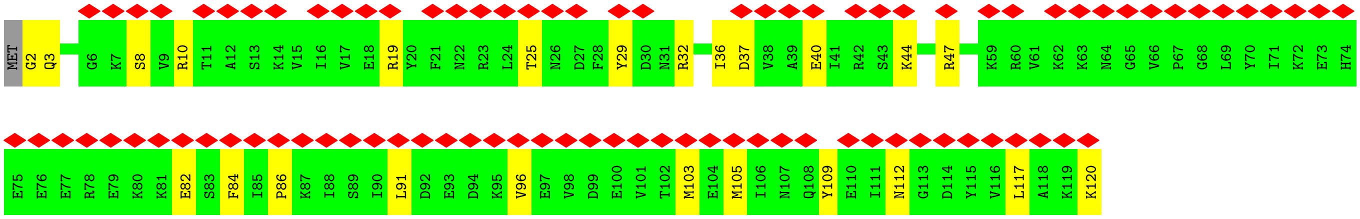
Chain SQ0:





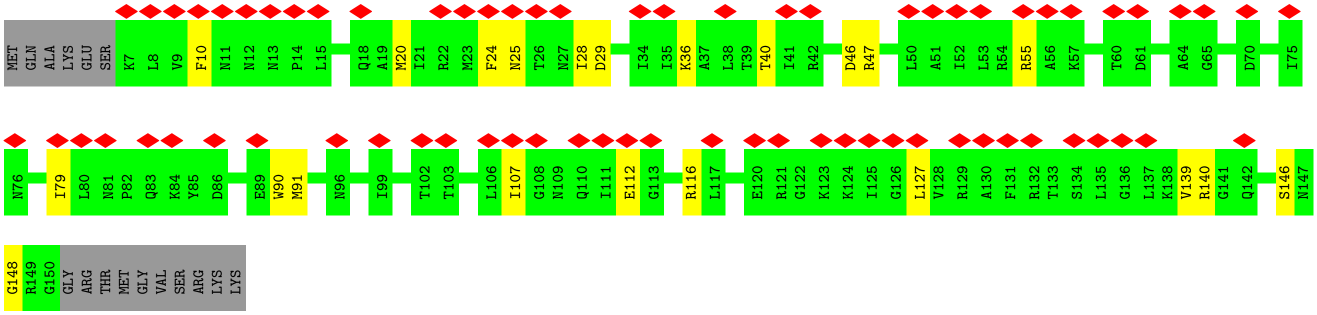
- Molecule 67: eS17

Chain SR0:



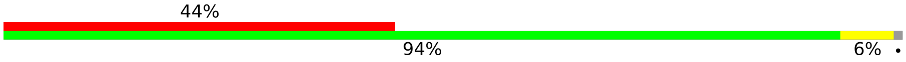
- Molecule 68: 40S ribosomal protein S18

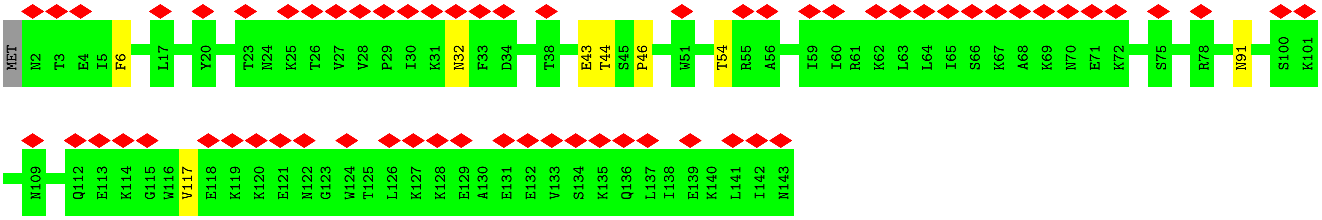
Chain SS0:



- Molecule 69: 40S Ribosomal protein S19

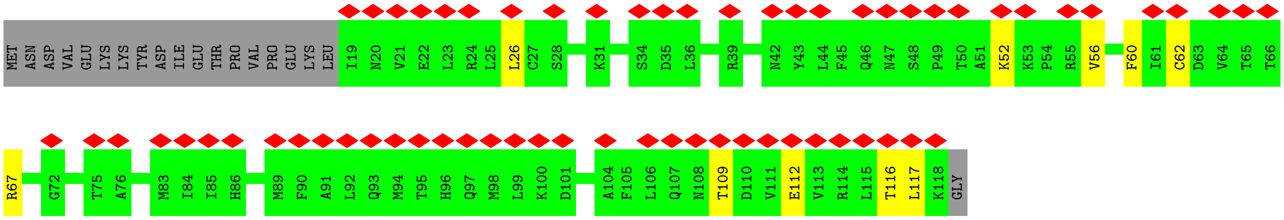
Chain ST0:





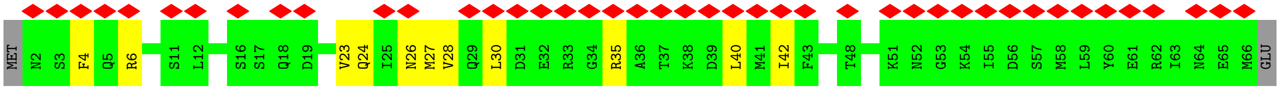
- Molecule 70: 40S ribosomal protein S20

Chain SU0:



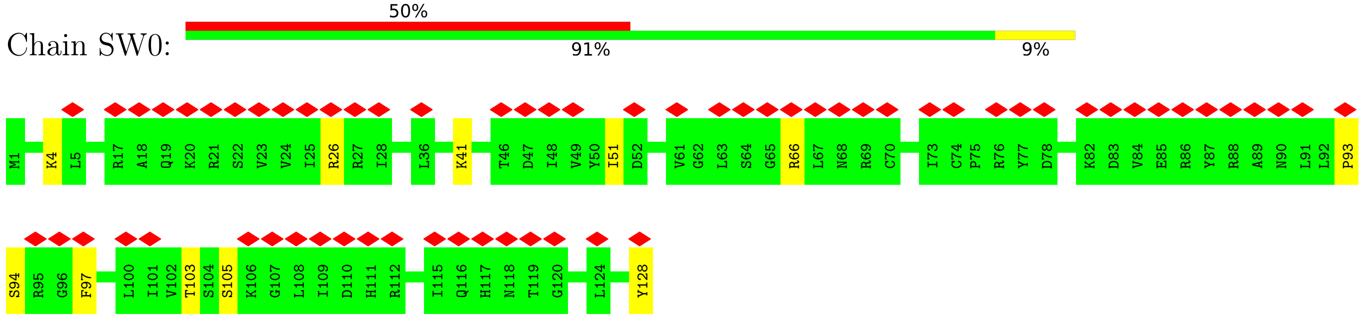
- Molecule 71: Ribosomal protein S21E

Chain SV0:



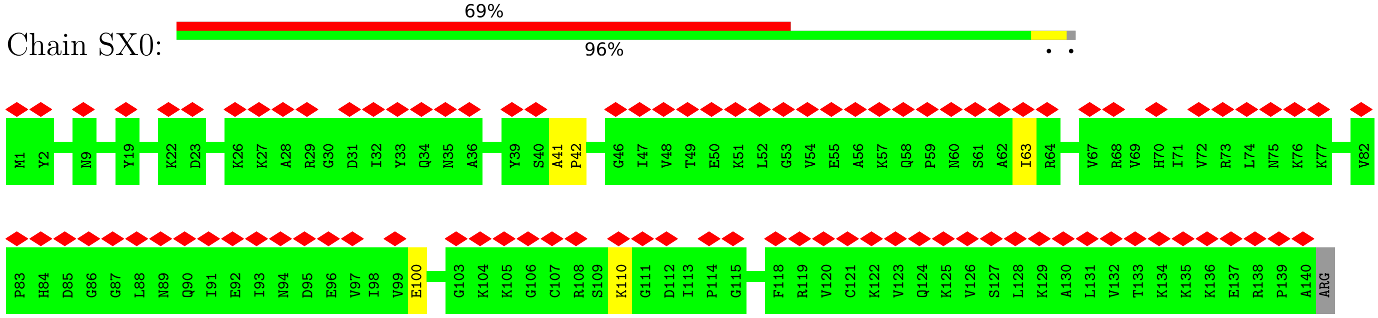
- Molecule 72: 40S ribosomal protein S15A

Chain SW0:



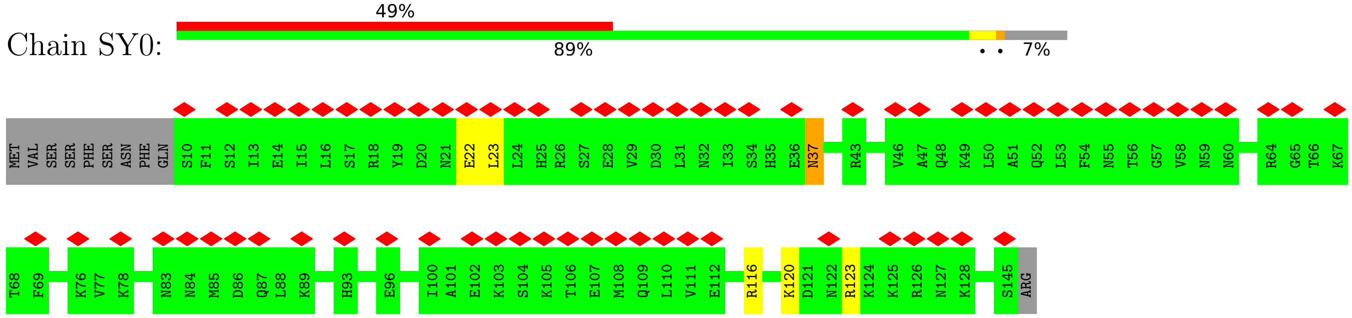
- Molecule 73: uS12

Chain SX0:



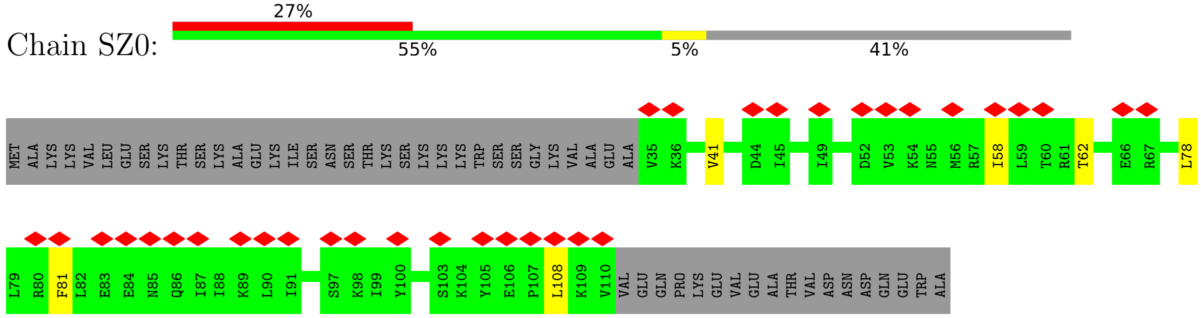
- Molecule 74: 40s ribosomal protein s24

Chain SY0:



- Molecule 75: 40S ribosomal protein S25

Chain SZ0:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	1344	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 $(e^-/\text{Å}^2)$	120, 120	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.622	Depositor
Minimum map value	-0.859	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.39	Depositor
Map size (Å)	453.00003, 453.00003, 453.00003	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.53, 4.53, 4.53	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	L50	0.75	1/60107 (0.0%)	1.19	161/93753 (0.2%)
2	L70	0.75	1/2844 (0.0%)	1.11	6/4429 (0.1%)
3	LA0	0.32	0/1926	0.74	0/2590
4	LAA	0.34	0/1191	0.66	0/1586
5	LB0	0.32	0/3092	0.70	1/4144 (0.0%)
6	LC0	0.33	0/2646	0.75	1/3555 (0.0%)
7	LCC	0.32	0/794	0.62	0/1067
8	LD0	0.29	0/2328	0.67	0/3098
9	LDD	0.30	0/913	0.66	0/1223
10	LE0	0.28	0/1394	0.65	0/1875
11	LEE	0.32	0/1108	0.69	0/1477
12	LF0	0.30	0/1963	0.68	0/2618
13	LFF	0.33	0/906	0.70	0/1207
14	LG0	0.28	0/1612	0.63	0/2163
15	LGG	0.34	0/825	0.78	1/1090 (0.1%)
16	LH0	0.30	0/1503	0.66	0/2018
17	LHH	0.28	0/999	0.66	0/1324
18	LI0	0.32	0/1781	0.69	0/2382
19	LII	0.30	0/790	0.59	0/1041
20	LJ0	0.30	0/1350	0.66	0/1797
21	LJJ	0.40	0/710	0.83	2/932 (0.2%)
22	LL0	0.30	0/1374	0.76	1/1827 (0.1%)
23	LLL	0.34	0/435	0.72	0/576
24	LM0	0.32	0/935	0.65	0/1251
25	LMM	0.41	0/431	0.68	0/568
26	LN0	0.35	0/1722	0.74	1/2297 (0.0%)
27	LO0	0.30	0/1626	0.65	0/2168
28	LOO	0.34	0/811	0.70	0/1071
29	LP0	0.32	0/1262	0.77	0/1689
30	LPP	0.40	0/693	0.78	2/918 (0.2%)
31	LQ0	0.30	0/1512	0.64	0/2014
32	LR0	0.31	0/1352	0.65	1/1790 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
33	LS0	0.30	0/1422	0.67	0/1898
34	LT0	0.31	0/1294	0.68	0/1736
35	LU0	0.30	0/826	0.67	0/1104
36	LV0	0.31	0/1068	0.70	0/1429
37	LW0	0.43	0/849	0.72	0/1129
38	LX0	0.28	0/883	0.67	0/1175
39	LY0	0.29	0/1058	0.69	1/1399 (0.1%)
40	LZ0	0.29	0/976	0.73	1/1302 (0.1%)
41	MD1	0.66	0/1249	0.87	1/1677 (0.1%)
42	S60	1.41	352/32725 (1.1%)	1.41	375/51066 (0.7%)
43	SA0	0.36	1/1751 (0.1%)	0.64	0/2358
44	SAA	0.38	0/839	0.73	0/1120
45	SB0	0.29	0/1623	0.67	0/2169
46	SBB	0.47	1/634 (0.2%)	0.65	0/844
47	SC0	0.31	0/1751	0.69	2/2359 (0.1%)
48	SCC	0.33	0/480	0.73	0/644
49	SD0	0.30	0/1721	0.66	0/2304
50	SDD	0.40	0/559	0.75	1/742 (0.1%)
51	SE0	0.32	0/2080	0.72	2/2804 (0.1%)
52	SEE	0.36	0/453	0.74	1/596 (0.2%)
53	SF0	0.31	0/1527	0.68	0/2045
54	SFF	0.43	0/427	0.68	0/573
55	SG0	0.29	0/1864	0.68	0/2485
56	SGG	0.34	0/2517	0.71	1/3397 (0.0%)
57	SH0	0.31	0/1356	0.66	0/1820
58	SI0	0.33	0/1369	0.68	0/1825
59	SJ0	0.33	0/1403	0.68	0/1880
60	SK0	0.29	0/750	0.71	0/1009
61	SL0	0.32	0/1252	0.72	2/1672 (0.1%)
62	SM0	0.32	0/881	0.71	0/1182
63	SN0	0.38	0/1154	0.78	0/1557
64	SO0	0.33	0/993	0.72	0/1326
65	SP0	0.33	0/964	0.71	0/1289
66	SQ0	0.33	0/1163	0.74	3/1556 (0.2%)
67	SR0	0.64	0/985	0.96	2/1315 (0.2%)
68	SS0	0.34	0/1165	0.74	0/1566
69	ST0	0.34	0/1181	0.75	1/1585 (0.1%)
70	SU0	0.33	0/824	0.74	2/1110 (0.2%)
71	SV0	0.33	0/525	0.66	0/700
72	SW0	0.32	0/1037	0.71	0/1389
73	SX0	0.31	0/1113	0.70	0/1486
74	SY0	0.30	0/1131	0.72	1/1503 (0.1%)
75	SZ0	0.33	0/640	0.75	0/855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.78	356/183397 (0.2%)	1.06	573/266518 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LC0	0	1
13	LFF	0	1
15	LGG	0	1
All	All	0	3

All (356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	934	A	P-O5'	10.34	1.70	1.59
42	S60	988	A	N9-C4	-8.57	1.32	1.37
43	SA0	20	CYS	C-N	8.40	1.53	1.34
1	L50	1	A	OP3-P	-8.36	1.51	1.61
42	S60	1049	G	N7-C5	-8.34	1.34	1.39
42	S60	1052	A	N9-C4	-8.30	1.32	1.37
42	S60	968	C	N1-C6	-8.24	1.32	1.37
42	S60	835	A	N7-C5	-7.93	1.34	1.39
42	S60	989	G	N7-C5	-7.77	1.34	1.39
42	S60	979	A	N7-C5	-7.70	1.34	1.39
42	S60	1011	A	N7-C5	-7.57	1.34	1.39
42	S60	1178	A	N9-C4	-7.56	1.33	1.37
42	S60	1045	A	N3-C4	-7.50	1.30	1.34
42	S60	1	A	OP3-P	-7.50	1.52	1.61
2	L70	1	A	OP3-P	-7.40	1.52	1.61
42	S60	952	A	N9-C4	-7.34	1.33	1.37
42	S60	978	A	N9-C4	-7.34	1.33	1.37
42	S60	1089	G	C8-N7	7.28	1.35	1.30
42	S60	849	U	C2-N3	-7.28	1.32	1.37
42	S60	1045	A	N7-C5	-7.24	1.34	1.39
42	S60	847	A	N3-C4	-7.22	1.30	1.34
42	S60	835	A	N3-C4	-7.21	1.30	1.34
42	S60	1084	G	C8-N7	7.21	1.35	1.30
42	S60	951	A	N9-C4	-7.16	1.33	1.37
42	S60	885	G	N9-C8	-7.13	1.32	1.37
42	S60	1058	A	N9-C4	-7.12	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	987	A	N9-C4	-7.11	1.33	1.37
42	S60	1036	A	C5-C4	-7.09	1.33	1.38
42	S60	989	G	C6-N1	-7.05	1.34	1.39
42	S60	963	G	C5-C4	-6.98	1.33	1.38
42	S60	1164	G	N7-C5	6.96	1.43	1.39
42	S60	836	A	N3-C4	-6.92	1.30	1.34
42	S60	1228	C	C4-C5	-6.90	1.37	1.43
42	S60	848	G	N9-C8	-6.87	1.33	1.37
42	S60	1028	U	C2-N3	-6.87	1.32	1.37
42	S60	979	A	N3-C4	-6.87	1.30	1.34
42	S60	1181	U	C2-N3	-6.86	1.32	1.37
42	S60	1014	G	N7-C5	-6.86	1.35	1.39
42	S60	1176	G	N7-C5	6.84	1.43	1.39
42	S60	851	G	N7-C5	6.84	1.43	1.39
42	S60	1121	A	N9-C4	6.83	1.42	1.37
42	S60	1038	A	N9-C4	-6.80	1.33	1.37
42	S60	1027	G	C5-C4	-6.80	1.33	1.38
42	S60	1053	A	N3-C4	6.78	1.39	1.34
42	S60	1154	A	N9-C4	6.77	1.42	1.37
42	S60	994	G	N7-C5	-6.77	1.35	1.39
42	S60	877	G	N9-C8	-6.77	1.33	1.37
42	S60	1182	G	C8-N7	-6.76	1.26	1.30
42	S60	1086	G	P-O5'	6.72	1.66	1.59
42	S60	1066	G	N9-C8	-6.71	1.33	1.37
42	S60	1095	G	C8-N7	6.70	1.34	1.30
42	S60	884	A	N9-C4	6.69	1.41	1.37
42	S60	1022	C	P-O5'	6.65	1.66	1.59
42	S60	877	G	P-O5'	6.64	1.66	1.59
42	S60	1114	A	P-O5'	6.62	1.66	1.59
42	S60	871	C	N1-C6	-6.61	1.33	1.37
42	S60	1162	G	C8-N7	6.61	1.34	1.30
42	S60	1032	A	C8-N7	-6.57	1.26	1.31
42	S60	1120	A	N3-C4	6.55	1.38	1.34
42	S60	1102	A	N9-C4	6.54	1.41	1.37
42	S60	1036	A	C6-N6	-6.54	1.28	1.33
42	S60	859	G	C8-N7	6.53	1.34	1.30
42	S60	856	U	P-O5'	6.52	1.66	1.59
42	S60	1067	A	N7-C5	6.52	1.43	1.39
42	S60	1183	C	C4-C5	-6.50	1.37	1.43
42	S60	839	C	C4-C5	-6.49	1.37	1.43
42	S60	1053	A	N7-C5	6.49	1.43	1.39
42	S60	1110	C	C4-C5	6.47	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1159	A	N9-C4	6.47	1.41	1.37
42	S60	1179	A	N3-C4	-6.44	1.30	1.34
42	S60	885	G	C6-N1	-6.43	1.35	1.39
42	S60	970	U	C2-N3	-6.42	1.33	1.37
42	S60	978	A	N7-C5	-6.41	1.35	1.39
42	S60	1050	G	N9-C8	-6.40	1.33	1.37
42	S60	1174	G	C2-N3	6.40	1.37	1.32
42	S60	954	G	N7-C5	-6.39	1.35	1.39
42	S60	1140	G	N7-C5	6.39	1.43	1.39
42	S60	1116	A	N3-C4	6.37	1.38	1.34
42	S60	1003	A	C5-C4	-6.37	1.34	1.38
42	S60	983	C	N1-C6	-6.34	1.33	1.37
42	S60	989	G	N3-C4	-6.34	1.31	1.35
42	S60	892	A	N3-C4	6.32	1.38	1.34
42	S60	1111	A	P-O5’	6.29	1.66	1.59
42	S60	1062	C	N1-C6	-6.28	1.33	1.37
42	S60	850	G	N9-C4	-6.27	1.32	1.38
42	S60	1106	G	N7-C5	6.27	1.43	1.39
42	S60	847	A	N7-C5	-6.25	1.35	1.39
42	S60	1171	A	N3-C4	6.25	1.38	1.34
42	S60	892	A	P-O5’	6.24	1.66	1.59
42	S60	1111	A	N9-C4	6.22	1.41	1.37
42	S60	1112	G	P-O5’	6.22	1.66	1.59
42	S60	1058	A	N7-C5	-6.22	1.35	1.39
42	S60	885	G	N3-C4	-6.19	1.31	1.35
42	S60	1219	G	C5-C4	-6.19	1.34	1.38
42	S60	1136	G	P-O5’	6.19	1.66	1.59
42	S60	1113	C	P-O5’	6.19	1.66	1.59
42	S60	1046	A	C5-C4	-6.17	1.34	1.38
42	S60	835	A	C6-N1	-6.17	1.31	1.35
42	S60	1155	C	P-O5’	6.17	1.66	1.59
42	S60	877	G	N3-C4	-6.15	1.31	1.35
42	S60	1064	G	C8-N7	6.15	1.34	1.30
42	S60	1046	A	C6-N6	-6.13	1.29	1.33
42	S60	877	G	C6-N1	-6.12	1.35	1.39
42	S60	877	G	C8-N7	6.12	1.34	1.30
42	S60	1045	A	C6-N1	-6.11	1.31	1.35
42	S60	1053	A	C6-N1	6.11	1.39	1.35
42	S60	1177	G	C8-N7	-6.10	1.27	1.30
42	S60	886	C	C4-N4	-6.10	1.28	1.33
42	S60	865	A	N9-C4	6.08	1.41	1.37
42	S60	915	A	N9-C4	6.08	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1030	A	N7-C5	-6.08	1.35	1.39
42	S60	1018	U	C2-N3	-6.08	1.33	1.37
42	S60	1003	A	N9-C4	6.07	1.41	1.37
42	S60	847	A	C6-N1	-6.06	1.31	1.35
42	S60	857	G	P-O5'	6.06	1.65	1.59
42	S60	913	G	C6-N1	6.05	1.43	1.39
42	S60	875	A	C5-C4	-6.05	1.34	1.38
42	S60	939	U	P-O5'	6.05	1.65	1.59
42	S60	1067	A	N3-C4	6.05	1.38	1.34
42	S60	1116	A	C6-N1	6.03	1.39	1.35
42	S60	938	G	P-O5'	6.02	1.65	1.59
42	S60	1049	G	C6-N1	-6.02	1.35	1.39
42	S60	1161	U	C2-N3	-6.02	1.33	1.37
42	S60	1120	A	C6-N1	6.00	1.39	1.35
42	S60	1129	U	C2-N3	-5.99	1.33	1.37
42	S60	1048	G	N9-C4	-5.99	1.33	1.38
42	S60	1086	G	C6-N1	5.99	1.43	1.39
42	S60	1092	C	N3-C4	5.99	1.38	1.33
42	S60	1103	G	N3-C4	5.98	1.39	1.35
42	S60	861	C	P-O5'	5.97	1.65	1.59
42	S60	995	A	C5-C4	-5.97	1.34	1.38
42	S60	1152	G	C8-N7	5.96	1.34	1.30
42	S60	1086	G	N3-C4	5.94	1.39	1.35
42	S60	1092	C	P-O5'	5.93	1.65	1.59
42	S60	988	A	N7-C5	-5.92	1.35	1.39
42	S60	1046	A	N7-C5	5.92	1.42	1.39
42	S60	1156	U	P-O5'	5.92	1.65	1.59
42	S60	1165	C	N3-C4	5.92	1.38	1.33
42	S60	932	A	N7-C5	5.91	1.42	1.39
42	S60	863	U	C2-N3	5.91	1.41	1.37
42	S60	1171	A	C6-N1	5.91	1.39	1.35
42	S60	1174	G	C8-N7	5.90	1.34	1.30
42	S60	1086	G	N7-C5	5.89	1.42	1.39
42	S60	1154	A	P-O5'	5.89	1.65	1.59
42	S60	1066	G	C5-C4	-5.89	1.34	1.38
42	S60	885	G	N7-C5	-5.87	1.35	1.39
42	S60	935	G	C8-N7	5.87	1.34	1.30
42	S60	938	G	N7-C5	5.86	1.42	1.39
42	S60	1051	C	C4-N4	-5.86	1.28	1.33
42	S60	1067	A	C6-N1	5.84	1.39	1.35
42	S60	892	A	C6-N1	5.83	1.39	1.35
42	S60	1084	G	C2-N3	5.80	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1180	U	C2-N3	-5.80	1.33	1.37
42	S60	899	A	N9-C4	5.80	1.41	1.37
42	S60	848	G	C6-N1	-5.80	1.35	1.39
42	S60	1117	A	N7-C5	5.79	1.42	1.39
42	S60	1088	U	P-O5'	5.79	1.65	1.59
42	S60	889	A	P-O5'	5.79	1.65	1.59
42	S60	913	G	N3-C4	5.79	1.39	1.35
42	S60	1134	G	N7-C5	5.78	1.42	1.39
42	S60	973	G	P-O5'	5.77	1.65	1.59
42	S60	932	A	N9-C4	5.77	1.41	1.37
42	S60	1122	A	N9-C4	5.76	1.41	1.37
42	S60	1207	A	N9-C4	5.76	1.41	1.37
42	S60	989	G	N9-C8	-5.76	1.33	1.37
42	S60	1050	G	C5-C4	-5.75	1.34	1.38
42	S60	836	A	N7-C5	-5.74	1.35	1.39
42	S60	1117	A	N3-C4	5.74	1.38	1.34
42	S60	1027	G	N1-C2	-5.74	1.33	1.37
42	S60	1040	G	C5-C4	-5.74	1.34	1.38
42	S60	1030	A	N3-C4	-5.73	1.31	1.34
42	S60	991	A	C5-C4	-5.73	1.34	1.38
42	S60	860	G	C2-N3	5.72	1.37	1.32
42	S60	844	A	N9-C4	-5.71	1.34	1.37
42	S60	969	C	C4-N4	-5.71	1.28	1.33
42	S60	1117	A	N9-C4	5.71	1.41	1.37
42	S60	1209	C	N1-C6	5.70	1.40	1.37
42	S60	1092	C	N1-C6	5.70	1.40	1.37
42	S60	1141	A	N7-C5	5.70	1.42	1.39
42	S60	920	G	C8-N7	5.69	1.34	1.30
42	S60	952	A	C5-C6	-5.69	1.35	1.41
42	S60	1203	A	P-O5'	5.69	1.65	1.59
42	S60	1087	C	N3-C4	5.68	1.38	1.33
42	S60	1141	A	N3-C4	5.66	1.38	1.34
42	S60	1031	A	C5-C4	-5.66	1.34	1.38
42	S60	852	A	N3-C4	5.65	1.38	1.34
42	S60	1051	C	C2-N3	-5.65	1.31	1.35
42	S60	1052	A	N7-C5	-5.64	1.35	1.39
42	S60	1206	A	N3-C4	-5.64	1.31	1.34
42	S60	864	A	N3-C4	-5.64	1.31	1.34
42	S60	954	G	P-O5'	5.61	1.65	1.59
42	S60	1129	U	P-O5'	5.60	1.65	1.59
42	S60	1073	U	P-O5'	5.60	1.65	1.59
42	S60	1186	G	C2'-C1'	-5.58	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1051	C	C5-C6	-5.58	1.29	1.34
42	S60	1185	A	C8-N7	-5.57	1.27	1.31
42	S60	875	A	C6-N6	-5.56	1.29	1.33
42	S60	907	G	N7-C5	5.56	1.42	1.39
42	S60	1047	G	P-O5’	5.55	1.65	1.59
42	S60	1055	A	N7-C5	-5.55	1.35	1.39
42	S60	1164	G	C6-N1	5.54	1.43	1.39
42	S60	1200	A	P-O5’	5.54	1.65	1.59
42	S60	1195	A	C8-N7	5.54	1.35	1.31
42	S60	1016	U	C2-N3	-5.53	1.33	1.37
42	S60	852	A	P-O5’	5.53	1.65	1.59
42	S60	1160	A	N9-C4	5.53	1.41	1.37
42	S60	1002	U	N1-C6	-5.53	1.32	1.38
42	S60	1230	U	N1-C6	-5.53	1.32	1.38
42	S60	1059	G	N7-C5	5.52	1.42	1.39
42	S60	1165	C	N1-C6	5.52	1.40	1.37
42	S60	1174	G	N9-C4	5.52	1.42	1.38
42	S60	877	G	C2-N3	5.52	1.37	1.32
42	S60	1047	G	C8-N7	-5.51	1.27	1.30
42	S60	1039	G	N7-C5	-5.51	1.35	1.39
42	S60	1037	C	C4-N4	-5.50	1.28	1.33
42	S60	1075	A	P-O5’	5.50	1.65	1.59
42	S60	1029	U	C2-N3	-5.50	1.33	1.37
42	S60	995	A	N3-C4	-5.49	1.31	1.34
42	S60	1098	C	P-O5’	5.49	1.65	1.59
42	S60	1049	G	N3-C4	-5.49	1.31	1.35
42	S60	991	A	N9-C8	-5.48	1.33	1.37
42	S60	1106	G	P-O5’	5.48	1.65	1.59
42	S60	990	U	N1-C6	-5.47	1.33	1.38
42	S60	1087	C	N1-C6	5.47	1.40	1.37
42	S60	1145	G	C2’-C1’	-5.47	1.47	1.53
42	S60	944	G	C2-N3	5.47	1.37	1.32
42	S60	886	C	C5-C6	-5.46	1.29	1.34
42	S60	969	C	C5-C6	-5.44	1.29	1.34
42	S60	833	A	N9-C4	-5.43	1.34	1.37
42	S60	992	G	C5-C4	-5.42	1.34	1.38
42	S60	1209	C	N3-C4	5.42	1.37	1.33
42	S60	953	C	P-O5’	5.42	1.65	1.59
42	S60	1192	G	C8-N7	5.42	1.34	1.30
42	S60	1121	A	N7-C5	5.42	1.42	1.39
42	S60	1176	G	C2-N3	5.42	1.37	1.32
42	S60	968	C	N3-C4	-5.40	1.30	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1137	A	C5-C4	5.40	1.42	1.38
42	S60	974	G	C5-C4	-5.39	1.34	1.38
42	S60	857	G	N3-C4	5.39	1.39	1.35
42	S60	1028	U	C4-O4	-5.39	1.19	1.23
42	S60	864	A	N7-C5	-5.38	1.36	1.39
42	S60	1115	G	C8-N7	5.38	1.34	1.30
42	S60	1132	A	C6-N1	5.38	1.39	1.35
42	S60	1093	G	P-O5'	5.37	1.65	1.59
42	S60	1220	U	C2-N3	-5.37	1.33	1.37
42	S60	1117	A	C6-N1	5.37	1.39	1.35
42	S60	913	G	P-O5'	5.37	1.65	1.59
42	S60	987	A	C5-C6	-5.37	1.36	1.41
42	S60	1113	C	N3-C4	5.37	1.37	1.33
42	S60	1010	G	N9-C4	-5.36	1.33	1.38
42	S60	1194	U	N1-C2	5.36	1.43	1.38
42	S60	975	G	C8-N7	-5.36	1.27	1.30
42	S60	1097	A	N7-C5	5.35	1.42	1.39
42	S60	995	A	N9-C8	-5.35	1.33	1.37
42	S60	1164	G	P-O5'	5.34	1.65	1.59
42	S60	950	U	P-O5'	5.34	1.65	1.59
42	S60	836	A	N9-C8	-5.33	1.33	1.37
42	S60	1206	A	N7-C5	-5.33	1.36	1.39
42	S60	969	C	C2-N3	-5.32	1.31	1.35
42	S60	840	C	N1-C6	5.32	1.40	1.37
42	S60	1036	A	N1-C2	-5.31	1.29	1.34
42	S60	1047	G	N3-C4	5.31	1.39	1.35
42	S60	1000	C	C4-C5	-5.31	1.38	1.43
42	S60	1054	G	N9-C8	5.30	1.41	1.37
42	S60	1209	C	P-O5'	5.30	1.65	1.59
42	S60	1161	U	C4-O4	-5.29	1.19	1.23
42	S60	1165	C	P-O5'	5.29	1.65	1.59
42	S60	1074	U	C2-N3	5.29	1.41	1.37
42	S60	1176	G	N9-C4	5.28	1.42	1.38
42	S60	979	A	C6-N1	-5.28	1.31	1.35
42	S60	1066	G	C2-N3	5.28	1.36	1.32
42	S60	1179	A	N7-C5	-5.28	1.36	1.39
42	S60	1131	A	N3-C4	5.27	1.38	1.34
42	S60	1059	G	N3-C4	5.27	1.39	1.35
42	S60	857	G	C6-N1	5.27	1.43	1.39
42	S60	837	C	N1-C6	-5.26	1.33	1.37
42	S60	1127	A	C5-C4	-5.26	1.35	1.38
42	S60	1182	G	C5-C4	-5.25	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1120	A	N7-C5	5.25	1.42	1.39
42	S60	1140	G	C6-N1	5.25	1.43	1.39
42	S60	1118	A	C5-C4	5.25	1.42	1.38
42	S60	952	A	C2-N3	-5.25	1.28	1.33
42	S60	1018	U	C4-O4	-5.25	1.19	1.23
42	S60	1172	A	P-O5’	5.24	1.65	1.59
42	S60	886	C	C2-N3	-5.24	1.31	1.35
42	S60	935	G	C2-N3	5.23	1.36	1.32
42	S60	855	G	C2-N3	5.23	1.36	1.32
42	S60	847	A	N9-C8	-5.22	1.33	1.37
42	S60	1085	G	N7-C5	5.21	1.42	1.39
42	S60	970	U	C4-O4	-5.21	1.19	1.23
46	SBB	58	CYS	CB-SG	-5.21	1.73	1.81
42	S60	884	A	N7-C5	5.20	1.42	1.39
42	S60	1141	A	C6-N1	5.20	1.39	1.35
42	S60	1085	G	C2-N3	5.18	1.36	1.32
42	S60	1226	U	C2-N3	-5.18	1.34	1.37
42	S60	1081	U	P-O5’	5.18	1.65	1.59
42	S60	955	A	N9-C4	-5.18	1.34	1.37
42	S60	1142	G	C2-N3	5.17	1.36	1.32
42	S60	1164	G	N3-C4	5.17	1.39	1.35
42	S60	853	G	C8-N7	5.16	1.34	1.30
42	S60	1207	A	C5-C4	-5.16	1.35	1.38
42	S60	1185	A	C5-C4	-5.16	1.35	1.38
42	S60	963	G	N1-C2	-5.16	1.33	1.37
42	S60	839	C	P-O5’	5.16	1.65	1.59
42	S60	1175	A	C5-C4	5.16	1.42	1.38
42	S60	1116	A	N7-C5	5.15	1.42	1.39
42	S60	931	G	N7-C5	5.15	1.42	1.39
42	S60	963	G	N9-C8	-5.15	1.34	1.37
42	S60	1227	U	C2-N3	-5.14	1.34	1.37
42	S60	932	A	N3-C4	5.14	1.38	1.34
42	S60	1176	G	N3-C4	5.14	1.39	1.35
42	S60	1130	A	N9-C4	5.13	1.41	1.37
42	S60	836	A	C6-N1	-5.13	1.31	1.35
42	S60	849	U	C4-O4	-5.13	1.19	1.23
42	S60	862	U	P-O5’	5.12	1.64	1.59
42	S60	892	A	N7-C5	5.12	1.42	1.39
42	S60	979	A	N9-C8	-5.12	1.33	1.37
42	S60	1126	A	N9-C4	5.12	1.41	1.37
42	S60	1223	C	P-O5’	5.12	1.64	1.59
42	S60	955	A	N7-C5	-5.11	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S60	1018	U	P-O5’	5.11	1.64	1.59
42	S60	1011	A	N3-C4	-5.11	1.31	1.34
42	S60	1095	G	N7-C5	-5.11	1.36	1.39
42	S60	938	G	N3-C4	5.10	1.39	1.35
42	S60	853	G	C5-C4	5.10	1.42	1.38
42	S60	1137	A	P-O5’	5.10	1.64	1.59
42	S60	1162	G	C2-N3	5.10	1.36	1.32
42	S60	1152	G	C5-C4	5.09	1.42	1.38
42	S60	1157	G	C5-C4	5.08	1.42	1.38
42	S60	1002	U	N3-C4	-5.08	1.33	1.38
42	S60	1127	A	C6-N6	-5.07	1.29	1.33
42	S60	855	G	N9-C4	5.07	1.42	1.38
42	S60	1057	C	N1-C6	-5.07	1.34	1.37
42	S60	1120	A	N9-C8	5.06	1.41	1.37
42	S60	1122	A	C8-N7	5.06	1.35	1.31
42	S60	1178	A	N7-C5	-5.06	1.36	1.39
42	S60	990	U	N3-C4	-5.06	1.33	1.38
42	S60	840	C	N3-C4	5.05	1.37	1.33
42	S60	1106	G	N3-C4	5.05	1.39	1.35
42	S60	1206	A	C6-N1	-5.05	1.32	1.35
42	S60	951	A	P-O5’	5.05	1.64	1.59
42	S60	1186	G	P-O5’	5.05	1.64	1.59
42	S60	1059	G	C6-N1	5.05	1.43	1.39
42	S60	1132	A	N3-C4	5.04	1.37	1.34
42	S60	1186	G	N7-C5	-5.04	1.36	1.39
42	S60	953	C	C4-N4	-5.04	1.29	1.33
42	S60	937	G	N9-C4	5.03	1.42	1.38
42	S60	1096	C	N1-C6	-5.03	1.34	1.37
42	S60	931	G	C2-N3	5.03	1.36	1.32
42	S60	1047	G	C6-N1	5.03	1.43	1.39
42	S60	1129	U	O3’-P	-5.03	1.55	1.61
42	S60	1103	G	N9-C8	5.03	1.41	1.37
42	S60	949	U	P-O5’	5.02	1.64	1.59
42	S60	1160	A	N7-C5	5.01	1.42	1.39
42	S60	1055	A	N3-C4	-5.00	1.31	1.34
42	S60	982	C	C4-C5	-5.00	1.39	1.43

All (573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	1356	C	O5’-P-OP1	-18.09	89.00	110.70
42	S60	910	A	P-O3’-C3’	-11.68	105.69	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	850	G	C5-N7-C8	-11.31	98.65	104.30
42	S60	1034	A	P-O3'-C3'	-11.29	106.16	119.70
42	S60	904	C	P-O3'-C3'	-10.87	106.66	119.70
1	L50	330	G	C2'-C3'-O3'	10.38	132.33	109.50
42	S60	917	U	P-O3'-C3'	-10.32	107.31	119.70
42	S60	1108	C	P-O3'-C3'	-10.24	107.42	119.70
42	S60	996	G	P-O3'-C3'	-10.14	107.53	119.70
42	S60	1261	G	P-O3'-C3'	-9.97	107.73	119.70
42	S60	1033	A	P-O3'-C3'	-9.95	107.76	119.70
42	S60	958	A	P-O3'-C3'	-9.82	107.91	119.70
1	L50	1265	G	OP1-P-OP2	-9.81	104.88	119.60
42	S60	965	U	P-O3'-C3'	-9.81	107.93	119.70
42	S60	964	G	P-O3'-C3'	-9.54	108.25	119.70
1	L50	535	A	P-O3'-C3'	9.48	131.08	119.70
42	S60	956	C	P-O3'-C3'	-9.37	108.46	119.70
42	S60	877	G	N9-C4-C5	9.31	109.12	105.40
42	S60	845	G	P-O3'-C3'	-9.28	108.57	119.70
42	S60	995	A	P-O3'-C3'	-9.07	108.81	119.70
1	L50	1395	U	C2'-C3'-O3'	9.06	129.43	109.50
42	S60	1170	G	C1'-O4'-C4'	-9.04	102.67	109.90
42	S60	1260	G	P-O3'-C3'	-9.02	108.87	119.70
42	S60	998	U	P-O3'-C3'	-8.98	108.93	119.70
42	S60	850	G	C4-C5-N7	8.96	114.38	110.80
42	S60	923	A	P-O3'-C3'	-8.91	109.01	119.70
1	L50	1282	C	N1-C2-O2	8.89	124.23	118.90
42	S60	877	G	C4-C5-N7	-8.86	107.25	110.80
1	L50	1959	A	C2'-C3'-O3'	8.84	128.94	109.50
42	S60	824	A	P-O3'-C3'	-8.81	109.12	119.70
1	L50	1585	U	P-O3'-C3'	-8.79	109.15	119.70
1	L50	1148	A	C4'-C3'-O3'	8.77	130.55	113.00
42	S60	961	G	P-O3'-C3'	-8.71	109.25	119.70
42	S60	1135	U	C3'-C2'-C1'	-8.64	94.58	101.50
42	S60	1125	G	C3'-C2'-C1'	-8.48	94.72	101.50
42	S60	394	G	O5'-P-OP1	-8.45	98.09	105.70
69	ST0	117	VAL	CA-CB-CG1	8.36	123.44	110.90
42	S60	831	G	P-O3'-C3'	-8.27	109.78	119.70
42	S60	997	A	P-O3'-C3'	-8.25	109.80	119.70
1	L50	1709	G	C1'-O4'-C4'	-8.20	103.34	109.90
42	S60	1107	U	P-O3'-C3'	-8.19	109.88	119.70
1	L50	424	G	O4'-C1'-N9	8.17	114.74	108.20
1	L50	141	G	O4'-C1'-N9	8.17	114.74	108.20
42	S60	850	G	N7-C8-N9	8.12	117.16	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	919	C	N3-C4-C5	-8.12	118.65	121.90
42	S60	1150	G	P-O3'-C3'	-8.10	109.98	119.70
1	L50	2431	C	O5'-P-OP1	-8.06	98.44	105.70
42	S60	848	G	OP2-P-O3'	8.06	122.94	105.20
1	L50	1000	G	C1'-O4'-C4'	-8.05	103.46	109.90
42	S60	1168	A	P-O3'-C3'	-8.05	110.04	119.70
42	S60	1046	A	C8-N9-C4	8.04	109.02	105.80
42	S60	1167	C	P-O3'-C3'	-8.04	110.06	119.70
1	L50	2597	G	C2'-C3'-O3'	8.02	127.13	109.50
42	S60	1174	G	C3'-C2'-C1'	8.01	107.91	101.50
42	S60	1231	U	P-O3'-C3'	-7.94	110.18	119.70
42	S60	933	G	O3'-P-O5'	7.93	119.06	104.00
1	L50	600	G	O4'-C1'-N9	7.90	114.52	108.20
21	LJJ	21	ARG	NE-CZ-NH2	7.90	124.25	120.30
42	S60	262	U	C2'-C3'-O3'	7.89	126.85	109.50
42	S60	989	G	N9-C4-C5	7.88	108.55	105.40
1	L50	1277	G	C2'-C3'-O3'	7.88	126.84	109.50
42	S60	473	G	C2'-C3'-O3'	7.82	126.70	109.50
42	S60	1066	G	N3-C4-C5	-7.76	124.72	128.60
1	L50	1192	A	C2'-C3'-O3'	7.74	126.52	109.50
42	S60	1023	A	P-O3'-C3'	-7.71	110.45	119.70
42	S60	127	A	C2'-C3'-O3'	7.70	126.45	109.50
42	S60	383	A	C2'-C3'-O3'	7.66	126.34	109.50
42	S60	1111	A	N7-C8-N9	-7.63	109.99	113.80
1	L50	796	C	O4'-C1'-N1	7.59	114.28	108.20
42	S60	264	C	O5'-P-OP1	7.59	119.81	110.70
42	S60	1049	G	C8-N9-C4	-7.59	103.36	106.40
42	S60	1001	C	N3-C4-C5	-7.58	118.87	121.90
42	S60	180	G	C4'-C3'-O3'	7.58	128.15	113.00
42	S60	1043	G	P-O3'-C3'	-7.57	110.61	119.70
1	L50	385	C	O5'-P-OP1	-7.57	98.89	105.70
42	S60	1095	G	N9-C4-C5	7.57	108.43	105.40
42	S60	1041	A	P-O3'-C3'	-7.56	110.63	119.70
42	S60	819	A	P-O3'-C3'	7.55	128.76	119.70
1	L50	1838	G	O4'-C1'-C2'	-7.54	98.26	105.80
42	S60	1216	U	P-O3'-C3'	-7.52	110.67	119.70
56	SGG	166	VAL	CA-CB-CG1	7.48	122.13	110.90
1	L50	1966	A	C2'-C3'-O3'	7.48	125.95	109.50
42	S60	1003	A	C5-N7-C8	7.46	107.63	103.90
74	SY0	37	ASN	CB-CA-C	7.46	125.31	110.40
1	L50	463	A	OP1-P-OP2	-7.45	108.43	119.60
42	S60	1186	G	C3'-C2'-C1'	-7.40	95.58	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	1046	A	C2-N3-C4	7.39	114.30	110.60
1	L50	159	A	OP1-P-OP2	-7.38	108.53	119.60
42	S60	994	G	C4'-C3'-C2'	-7.37	95.23	102.60
42	S60	1192	G	C8-N9-C4	-7.36	103.46	106.40
50	SDD	39	VAL	CA-CB-CG1	7.36	121.94	110.90
42	S60	598	C	C2'-C3'-O3'	7.34	125.66	109.50
42	S60	944	G	P-O3'-C3'	-7.34	110.89	119.70
42	S60	960	U	P-O3'-C3'	-7.33	110.90	119.70
1	L50	1967	A	C2'-C3'-O3'	7.32	125.60	109.50
42	S60	847	A	N9-C4-C5	7.30	108.72	105.80
42	S60	1066	G	C4-C5-N7	-7.30	107.88	110.80
42	S60	848	G	C4-C5-N7	-7.26	107.89	110.80
42	S60	966	G	P-O3'-C3'	-7.24	111.01	119.70
1	L50	644	G	O5'-P-OP1	7.23	119.37	110.70
42	S60	1089	G	N9-C4-C5	7.18	108.27	105.40
1	L50	1394	U	C2'-C3'-O3'	7.18	125.30	109.50
42	S60	1055	A	N9-C4-C5	7.18	108.67	105.80
1	L50	586	G	O4'-C1'-N9	7.17	113.94	108.20
42	S60	1230	U	P-O3'-C3'	-7.17	111.10	119.70
42	S60	1195	A	N9-C4-C5	7.14	108.66	105.80
42	S60	933	G	C4'-C3'-O3'	7.12	127.23	113.00
42	S60	1095	G	C8-N9-C4	-7.08	103.57	106.40
1	L50	353	A	O5'-P-OP1	-7.08	99.33	105.70
1	L50	21	U	C2'-C3'-O3'	7.05	125.01	109.50
42	S60	830	G	P-O3'-C3'	-7.03	111.27	119.70
52	SEE	49	VAL	CA-CB-CG1	7.03	121.44	110.90
1	L50	1182	A	P-O3'-C3'	6.97	128.07	119.70
42	S60	864	A	N9-C4-C5	6.97	108.59	105.80
42	S60	1206	A	N9-C4-C5	6.93	108.57	105.80
42	S60	1048	G	C4'-C3'-C2'	-6.91	95.69	102.60
42	S60	1003	A	C2-N3-C4	6.91	114.05	110.60
42	S60	883	C	C6-N1-C2	6.90	123.06	120.30
42	S60	1051	C	C6-N1-C2	6.89	123.06	120.30
42	S60	894	A	P-O3'-C3'	-6.88	111.44	119.70
42	S60	859	G	C8-N9-C4	-6.88	103.65	106.40
42	S60	1094	C	N3-C4-C5	-6.88	119.15	121.90
42	S60	1062	C	N3-C4-C5	-6.85	119.16	121.90
42	S60	1111	A	C5-N7-C8	6.85	107.32	103.90
42	S60	1046	A	N7-C8-N9	-6.84	110.38	113.80
42	S60	1049	G	N9-C4-C5	6.84	108.14	105.40
42	S60	1134	G	P-O3'-C3'	-6.83	111.50	119.70
42	S60	1070	C	N3-C4-C5	-6.82	119.17	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L50	562	U	P-O5'-C5'	-6.81	110.00	120.90
42	S60	918	A	P-O3'-C3'	-6.81	111.53	119.70
42	S60	1192	G	N9-C4-C5	6.78	108.11	105.40
1	L50	147	G	P-O3'-C3'	-6.75	111.59	119.70
42	S60	1182	G	N9-C4-C5	-6.75	102.70	105.40
67	SR0	47	ARG	NE-CZ-NH2	6.74	123.67	120.30
42	S60	565	U	C2'-C3'-O3'	6.74	124.48	113.70
42	S60	1011	A	C8-N9-C4	-6.74	103.10	105.80
42	S60	1207	A	C5-N7-C8	6.74	107.27	103.90
42	S60	919	C	C6-N1-C2	-6.73	117.61	120.30
42	S60	13	C	OP1-P-OP2	-6.73	109.51	119.60
42	S60	963	G	P-O3'-C3'	-6.73	111.63	119.70
1	L50	1808	A	C4'-C3'-O3'	6.71	126.42	113.00
42	S60	1014	G	C8-N9-C4	-6.71	103.72	106.40
42	S60	1014	G	N9-C4-C5	6.69	108.08	105.40
42	S60	1207	A	N7-C8-N9	-6.68	110.46	113.80
1	L50	1488	U	O4'-C1'-N1	6.67	113.54	108.20
1	L50	1317	G	P-O3'-C3'	-6.67	111.70	119.70
1	L50	600	G	O4'-C1'-C2'	-6.66	99.14	105.80
1	L50	1771	G	P-O3'-C3'	6.64	127.67	119.70
42	S60	1185	A	C8-N9-C4	6.64	108.46	105.80
1	L50	1134	A	C2'-C3'-O3'	6.64	124.32	113.70
42	S60	848	G	N3-C4-C5	-6.64	125.28	128.60
42	S60	1053	A	C8-N9-C4	6.60	108.44	105.80
1	L50	667	G	P-O3'-C3'	6.59	127.61	119.70
42	S60	954	G	C8-N9-C4	-6.58	103.77	106.40
42	S60	875	A	C2-N3-C4	6.57	113.88	110.60
42	S60	1003	A	N7-C8-N9	-6.57	110.52	113.80
42	S60	854	U	P-O3'-C3'	-6.56	111.83	119.70
42	S60	1356	C	OP1-P-OP2	6.56	129.44	119.60
42	S60	1179	A	N9-C4-C5	6.55	108.42	105.80
1	L50	1783	A	P-O3'-C3'	-6.55	111.84	119.70
42	S60	877	G	N3-C4-C5	-6.54	125.33	128.60
42	S60	1212	U	O4'-C1'-N1	6.54	113.43	108.20
42	S60	213	A	P-O3'-C3'	-6.53	111.86	119.70
42	S60	874	A	N9-C4-C5	6.53	108.41	105.80
42	S60	1001	C	C6-N1-C2	-6.53	117.69	120.30
42	S60	671	C	O5'-P-OP1	6.52	118.52	110.70
42	S60	857	G	C4-C5-N7	6.51	113.41	110.80
41	MD1	103	ARG	NE-CZ-NH2	6.50	123.55	120.30
42	S60	1153	C	P-O3'-C3'	-6.50	111.90	119.70
42	S60	1038	A	C4'-C3'-C2'	-6.49	96.11	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	2355	A	OP1-P-OP2	-6.48	109.88	119.60
42	S60	1205	G	C8-N9-C4	-6.46	103.82	106.40
42	S60	982	C	N3-C4-C5	-6.45	119.32	121.90
47	SC0	221	VAL	CA-CB-CG1	6.45	120.57	110.90
2	L70	46	C	P-O3'-C3'	-6.43	111.98	119.70
42	S60	903	C	P-O3'-C3'	-6.40	112.02	119.70
22	LL0	67	ARG	CG-CD-NE	6.37	125.17	111.80
1	L50	2114	G	C4'-C3'-C2'	-6.37	96.23	102.60
1	L50	548	G	OP1-P-OP2	-6.36	110.07	119.60
42	S60	1066	G	C5-N7-C8	6.36	107.48	104.30
1	L50	400	U	O5'-P-OP2	-6.35	99.99	105.70
42	S60	1052	A	C5-N7-C8	-6.31	100.75	103.90
42	S60	1053	A	N9-C4-C5	-6.30	103.28	105.80
6	LC0	57	ARG	CG-CD-NE	-6.29	98.59	111.80
42	S60	1177	G	C4-C5-N7	6.27	113.31	110.80
1	L50	371	A	N7-C8-N9	-6.26	110.67	113.80
5	LB0	336	ARG	CG-CD-NE	6.25	124.92	111.80
26	LN0	123	GLN	CB-CA-C	-6.25	97.91	110.40
1	L50	342	G	P-O3'-C3'	-6.24	112.21	119.70
1	L50	1102	G	O4'-C1'-C2'	-6.24	99.56	105.80
1	L50	1277	G	C4'-C3'-O3'	6.24	125.47	113.00
1	L50	412	A	OP1-P-OP2	-6.22	110.27	119.60
42	S60	1047	G	N9-C4-C5	-6.22	102.91	105.40
42	S60	1127	A	C8-N9-C4	6.22	108.29	105.80
42	S60	1055	A	C8-N9-C4	-6.21	103.31	105.80
1	L50	2481	U	P-O3'-C3'	6.19	127.13	119.70
42	S60	201	G	P-O3'-C3'	-6.18	112.28	119.70
42	S60	1182	G	C8-N9-C4	6.18	108.87	106.40
42	S60	1195	A	C8-N9-C4	-6.17	103.33	105.80
42	S60	1093	G	C4-C5-N7	6.16	113.26	110.80
42	S60	989	G	C8-N9-C4	-6.15	103.94	106.40
42	S60	1089	G	C8-N9-C4	-6.15	103.94	106.40
42	S60	1047	G	C4-C5-N7	6.15	113.26	110.80
42	S60	1048	G	C5-N7-C8	-6.15	101.22	104.30
42	S60	973	G	N9-C4-C5	6.15	107.86	105.40
1	L50	462	G	OP1-P-OP2	-6.15	110.38	119.60
42	S60	987	A	C5-N7-C8	-6.14	100.83	103.90
42	S60	1103	G	O4'-C1'-C2'	-6.14	99.66	105.80
1	L50	125	G	OP1-P-OP2	-6.13	110.41	119.60
70	SU0	67	ARG	CG-CD-NE	6.12	124.64	111.80
42	S60	1050	G	C4-C5-N7	-6.11	108.36	110.80
42	S60	885	G	N9-C4-C5	6.10	107.84	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	877	G	C8-N9-C4	-6.09	103.97	106.40
47	SC0	129	ARG	CB-CA-C	-6.09	98.23	110.40
42	S60	954	G	N7-C8-N9	6.08	116.14	113.10
1	L50	562	U	C5'-C4'-C3'	-6.07	106.29	116.00
42	S60	920	G	N9-C4-C5	6.07	107.83	105.40
42	S60	835	A	C8-N9-C4	-6.04	103.39	105.80
42	S60	895	C	P-O3'-C3'	-6.03	112.46	119.70
42	S60	1119	C	C2-N3-C4	6.03	122.92	119.90
42	S60	858	C	C2-N3-C4	6.03	122.92	119.90
42	S60	262	U	C4'-C3'-O3'	6.03	125.05	113.00
1	L50	1835	G	C3'-C2'-C1'	6.02	106.32	101.50
42	S60	1046	A	C5-C6-N1	6.02	120.71	117.70
1	L50	477	G	P-O3'-C3'	6.02	126.92	119.70
1	L50	140	A	P-O3'-C3'	6.01	126.92	119.70
42	S60	953	C	C6-N1-C2	6.01	122.70	120.30
1	L50	1061	G	O4'-C1'-N9	6.00	113.00	108.20
42	S60	859	G	N9-C4-C5	5.99	107.80	105.40
42	S60	933	G	C3'-C2'-C1'	-5.99	96.70	101.50
42	S60	952	A	C4-C5-N7	5.98	113.69	110.70
42	S60	847	A	C4-C5-C6	5.97	119.98	117.00
42	S60	1019	C	C3'-C2'-C1'	5.96	106.27	101.50
42	S60	885	G	C4-C5-N7	-5.96	108.42	110.80
21	LJJ	21	ARG	NE-CZ-NH1	-5.95	117.32	120.30
42	S60	1056	A	N9-C4-C5	5.95	108.18	105.80
42	S60	1066	G	C2-N3-C4	5.94	114.87	111.90
42	S60	1067	A	C8-N9-C4	5.94	108.17	105.80
42	S60	180	G	P-O3'-C3'	5.94	126.82	119.70
42	S60	924	U	P-O3'-C3'	-5.94	112.58	119.70
42	S60	884	A	C3'-C2'-C1'	5.93	106.24	101.50
2	L70	31	G	P-O3'-C3'	-5.92	112.59	119.70
42	S60	853	G	C8-N9-C4	-5.91	104.03	106.40
42	S60	1054	G	C4-C5-N7	5.91	113.16	110.80
42	S60	875	A	N7-C8-N9	-5.90	110.85	113.80
15	LGG	24	ARG	CG-CD-NE	-5.89	99.42	111.80
42	S60	1182	G	C2-N3-C4	5.89	114.84	111.90
1	L50	1277	G	C3'-C2'-C1'	-5.89	96.79	101.50
42	S60	1053	A	N1-C2-N3	-5.89	126.36	129.30
42	S60	1208	G	C2-N3-C4	5.88	114.84	111.90
42	S60	848	G	N9-C4-C5	5.88	107.75	105.40
42	S60	1128	G	C4-C5-N7	5.87	113.15	110.80
42	S60	1176	G	C2-N3-C4	5.87	114.83	111.90
42	S60	874	A	C4-C5-N7	-5.84	107.78	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	1011	A	C5-C6-N1	-5.84	114.78	117.70
42	S60	1182	G	C5-C6-O6	-5.84	125.10	128.60
42	S60	959	G	P-O3'-C3'	-5.83	112.70	119.70
42	S60	969	C	C6-N1-C2	5.83	122.63	120.30
1	L50	317	G	C3'-C2'-C1'	-5.83	96.83	101.50
1	L50	523	A	C1'-C2'-O2'	-5.83	93.11	110.60
42	S60	952	A	N1-C6-N6	5.83	122.10	118.60
42	S60	1058	A	C1'-O4'-C4'	-5.83	105.23	109.90
42	S60	1186	G	O4'-C1'-N9	5.82	112.86	108.20
42	S60	1215	A	C8-N9-C4	5.82	108.13	105.80
1	L50	2235	C	O5'-P-OP2	-5.82	100.46	105.70
42	S60	865	A	C5-N7-C8	5.82	106.81	103.90
42	S60	1010	G	C1'-O4'-C4'	-5.82	105.25	109.90
42	S60	942	A	C8-N9-C4	-5.81	103.47	105.80
42	S60	1064	G	N9-C4-C5	5.81	107.72	105.40
42	S60	897	C	P-O3'-C3'	-5.81	112.73	119.70
61	SL0	28	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	L50	1491	U	P-O3'-C3'	5.80	126.66	119.70
1	L50	225	G	C2'-C3'-O3'	5.80	122.98	113.70
30	LPP	8	VAL	CA-CB-CG1	5.79	119.59	110.90
42	S60	864	A	C8-N9-C4	-5.79	103.48	105.80
42	S60	954	G	C2-N3-C4	-5.79	109.00	111.90
42	S60	947	C	P-O3'-C3'	-5.79	112.75	119.70
42	S60	1024	G	P-O3'-C3'	-5.78	112.76	119.70
1	L50	395	A	C4'-C3'-O3'	-5.77	97.27	109.40
42	S60	1177	G	N9-C4-C5	-5.77	103.09	105.40
51	SE0	100	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	L50	1838	G	O5'-P-OP2	-5.77	100.51	105.70
1	L50	280	G	C4'-C3'-C2'	-5.76	96.84	102.60
42	S60	888	U	C3'-C2'-C1'	-5.76	96.89	101.50
66	SQ0	38	VAL	CA-CB-CG1	5.76	119.54	110.90
1	L50	1835	G	P-O5'-C5'	-5.76	111.69	120.90
70	SU0	56	VAL	CA-CB-CG1	5.75	119.53	110.90
1	L50	234	U	O5'-P-OP2	-5.75	100.53	105.70
42	S60	1203	A	C5-N7-C8	5.74	106.77	103.90
42	S60	875	A	C8-N9-C4	5.74	108.09	105.80
1	L50	1102	G	O5'-P-OP1	5.73	117.58	110.70
30	LPP	49	ARG	CG-CD-NE	5.73	123.83	111.80
1	L50	2373	G	C4'-C3'-C2'	-5.73	96.87	102.60
42	S60	952	A	N9-C4-C5	-5.72	103.51	105.80
42	S60	955	A	C4'-C3'-C2'	-5.72	96.88	102.60
42	S60	1106	G	P-O3'-C3'	-5.71	112.84	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	1176	G	O4'-C4'-C3'	5.71	110.67	106.10
42	S60	222	G	C4'-C3'-C2'	-5.71	96.89	102.60
42	S60	262	U	O4'-C4'-C3'	-5.71	98.29	104.00
1	L50	1303	G	C4'-C3'-C2'	-5.71	96.89	102.60
42	S60	871	C	N3-C4-C5	-5.71	119.62	121.90
42	S60	960	U	C4'-C3'-C2'	-5.71	96.89	102.60
61	SL0	28	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	L50	2452	A	C4'-C3'-O3'	5.70	124.39	113.00
42	S60	1185	A	N9-C4-C5	-5.70	103.52	105.80
1	L50	822	U	P-O3'-C3'	-5.68	112.88	119.70
1	L50	1733	A	C4'-C3'-O3'	-5.68	97.47	109.40
42	S60	1184	U	C3'-C2'-C1'	-5.68	96.96	101.50
42	S60	915	A	P-O3'-C3'	-5.68	112.89	119.70
32	LR0	74	HIS	CB-CA-C	5.67	121.74	110.40
42	S60	1045	A	N9-C4-C5	5.67	108.07	105.80
42	S60	1048	G	C6-C5-N7	-5.67	127.00	130.40
42	S60	1062	C	C4-C5-C6	5.67	120.23	117.40
42	S60	963	G	C2-N3-C4	5.66	114.73	111.90
42	S60	1146	G	C3'-C2'-C1'	-5.66	96.97	101.50
42	S60	840	C	P-O3'-C3'	-5.66	112.91	119.70
42	S60	848	G	C5-N7-C8	5.66	107.13	104.30
1	L50	1304	A	P-O3'-C3'	-5.65	112.92	119.70
42	S60	1207	A	C2-N3-C4	5.65	113.43	110.60
42	S60	1125	G	C2'-C3'-O3'	5.65	122.74	113.70
1	L50	1277	G	C4'-C3'-C2'	-5.64	96.96	102.60
42	S60	922	G	P-O3'-C3'	-5.64	112.94	119.70
42	S60	1093	G	C5-N7-C8	-5.64	101.48	104.30
1	L50	600	G	N9-C1'-C2'	-5.63	105.81	112.00
42	S60	920	G	C4-C5-N7	-5.62	108.55	110.80
42	S60	1127	A	C2-N3-C4	5.62	113.41	110.60
42	S60	1259	U	P-O3'-C3'	-5.62	112.96	119.70
42	S60	919	C	C2-N3-C4	5.61	122.70	119.90
42	S60	1005	G	C4'-C3'-C2'	-5.60	97.00	102.60
42	S60	1094	C	C2-N3-C4	5.59	122.70	119.90
42	S60	1035	C	P-O3'-C3'	-5.58	113.00	119.70
2	L70	64	G	OP1-P-OP2	-5.58	111.24	119.60
1	L50	2587	U	C3'-C2'-C1'	-5.57	97.05	101.50
1	L50	1832	A	O5'-P-OP2	-5.57	100.69	105.70
42	S60	835	A	N9-C4-C5	5.57	108.03	105.80
42	S60	982	C	C6-N1-C2	-5.56	118.08	120.30
42	S60	856	U	C3'-C2'-C1'	-5.55	97.06	101.50
40	LZ0	69	ARG	CB-CG-CD	5.55	126.03	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	944	G	C4-C5-N7	-5.54	108.58	110.80
42	S60	1067	A	N9-C4-C5	-5.54	103.58	105.80
1	L50	1282	C	C2-N3-C4	5.54	122.67	119.90
42	S60	973	G	C4-C5-N7	-5.54	108.58	110.80
42	S60	1206	A	C8-N9-C4	-5.54	103.58	105.80
1	L50	1471	G	OP1-P-OP2	-5.53	111.31	119.60
51	SE0	100	ARG	NE-CZ-NH2	5.53	123.06	120.30
42	S60	886	C	C6-N1-C2	5.53	122.51	120.30
42	S60	839	C	C2-N3-C4	5.53	122.66	119.90
42	S60	1007	U	O4'-C1'-N1	5.53	112.62	108.20
1	L50	1485	G	O4'-C1'-N9	5.52	112.62	108.20
42	S60	951	A	C5-N7-C8	-5.52	101.14	103.90
42	S60	871	C	C4-C5-C6	5.52	120.16	117.40
42	S60	1089	G	C4-C5-N7	-5.52	108.59	110.80
42	S60	1106	G	C8-N9-C4	5.51	108.61	106.40
42	S60	1003	A	C4-C5-N7	-5.51	107.94	110.70
1	L50	667	G	OP1-P-OP2	-5.51	111.34	119.60
42	S60	1183	C	C2-N3-C4	5.51	122.65	119.90
42	S60	1195	A	C4-C5-C6	5.51	119.75	117.00
42	S60	1239	C	O5'-P-OP2	-5.51	100.74	105.70
42	S60	622	C	P-O3'-C3'	-5.50	113.09	119.70
42	S60	1052	A	N7-C8-N9	5.50	116.55	113.80
42	S60	1127	A	N7-C8-N9	-5.50	111.05	113.80
1	L50	178	G	C5-C6-O6	5.50	131.90	128.60
1	L50	714	G	O5'-P-OP1	5.50	117.30	110.70
42	S60	986	G	C3'-C2'-C1'	5.50	105.90	101.50
42	S60	968	C	O5'-P-OP2	-5.50	100.75	105.70
42	S60	865	A	C4-C5-N7	-5.49	107.95	110.70
42	S60	1228	C	C2-N3-C4	5.49	122.64	119.90
42	S60	877	G	C4-C5-C6	5.48	122.09	118.80
42	S60	1182	G	N1-C2-N3	-5.47	120.62	123.90
1	L50	1711	A	O5'-P-OP2	-5.47	100.78	105.70
42	S60	839	C	C5-C6-N1	5.46	123.73	121.00
42	S60	1055	A	C4-C5-C6	5.46	119.73	117.00
2	L70	86	G	C4'-C3'-C2'	-5.46	97.14	102.60
42	S60	1084	G	N9-C4-C5	5.45	107.58	105.40
1	L50	1614	G	O4'-C1'-N9	5.45	112.56	108.20
2	L70	75	G	C3'-C2'-C1'	-5.45	97.14	101.50
42	S60	1056	A	C4-C5-N7	-5.45	107.98	110.70
1	L50	838	G	OP1-P-OP2	-5.44	111.44	119.60
1	L50	2441	A	P-O3'-C3'	-5.44	113.17	119.70
42	S60	1094	C	C6-N1-C2	-5.43	118.13	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	269	G	OP1-P-OP2	-5.43	111.45	119.60
42	S60	1049	G	C4-C5-C6	5.43	122.06	118.80
1	L50	330	G	C8-N9-C4	-5.42	104.23	106.40
1	L50	1074	G	C2'-C3'-O3'	5.42	122.37	113.70
42	S60	944	G	C5-N7-C8	5.42	107.01	104.30
42	S60	836	A	N9-C4-C5	5.42	107.97	105.80
67	SR0	32	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	L50	2473	G	OP1-P-OP2	-5.42	111.48	119.60
42	S60	1205	G	N7-C8-N9	5.41	115.81	113.10
42	S60	1054	G	C1'-O4'-C4'	-5.40	105.58	109.90
42	S60	1328	G	C3'-C2'-C1'	5.39	105.81	101.50
42	S60	1032	A	N9-C4-C5	-5.39	103.64	105.80
1	L50	1808	A	P-O3'-C3'	5.39	126.16	119.70
1	L50	1634	C	C1'-O4'-C4'	-5.38	105.60	109.90
42	S60	10	A	P-O3'-C3'	-5.38	113.24	119.70
1	L50	141	G	C1'-O4'-C4'	-5.37	105.60	109.90
1	L50	42	G	C4'-C3'-C2'	-5.37	97.23	102.60
1	L50	1282	C	N3-C2-O2	-5.36	118.15	121.90
1	L50	141	G	O4'-C1'-C2'	-5.35	100.45	105.80
1	L50	518	G	OP1-P-OP2	-5.35	111.57	119.60
42	S60	477	G	C3'-C2'-C1'	5.35	105.78	101.50
42	S60	860	G	N3-C4-C5	-5.35	125.93	128.60
42	S60	860	G	C4-C5-N7	-5.34	108.67	110.80
42	S60	952	A	C5-N7-C8	-5.33	101.23	103.90
1	L50	1466	A	C3'-C2'-C1'	5.33	105.76	101.50
42	S60	864	A	C4-C5-C6	5.33	119.67	117.00
42	S60	1206	A	C4-C5-C6	5.33	119.66	117.00
42	S60	873	C	C5-C6-N1	-5.32	118.34	121.00
42	S60	888	U	OP1-P-OP2	-5.32	111.62	119.60
42	S60	954	G	C5-C6-N1	-5.32	108.84	111.50
42	S60	1213	G	C8-N9-C4	5.32	108.53	106.40
42	S60	925	A	P-O3'-C3'	-5.32	113.32	119.70
42	S60	1118	A	C5-C6-N1	-5.31	115.05	117.70
42	S60	1010	G	C4-C5-N7	5.30	112.92	110.80
42	S60	10	A	O5'-P-OP2	5.30	117.06	110.70
42	S60	979	A	N9-C4-C5	5.30	107.92	105.80
42	S60	1089	G	C3'-C2'-C1'	5.30	105.74	101.50
1	L50	2332	G	C4'-C3'-C2'	-5.29	97.31	102.60
42	S60	847	A	C4-C5-N7	-5.29	108.05	110.70
42	S60	849	U	O5'-P-OP2	-5.29	100.94	105.70
42	S60	893	U	P-O3'-C3'	-5.29	113.35	119.70
42	S60	851	G	C5-C6-O6	-5.29	125.43	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	1128	G	N9-C4-C5	-5.29	103.29	105.40
42	S60	1154	A	P-O3'-C3'	-5.29	113.36	119.70
42	S60	1052	A	C5-C6-N1	-5.28	115.06	117.70
42	S60	1208	G	C5-C6-N1	5.28	114.14	111.50
42	S60	601	G	C4'-C3'-C2'	-5.28	97.32	102.60
42	S60	1010	G	C5-N7-C8	-5.27	101.66	104.30
1	L50	2184	G	P-O3'-C3'	5.27	126.03	119.70
42	S60	954	G	C6-C5-N7	-5.27	127.24	130.40
42	S60	947	C	N3-C4-C5	-5.27	119.79	121.90
42	S60	1003	A	C5-C6-N1	5.27	120.33	117.70
42	S60	1051	C	N3-C4-C5	5.27	124.01	121.90
42	S60	1054	G	C5-N7-C8	-5.26	101.67	104.30
42	S60	834	G	P-O3'-C3'	-5.25	113.40	119.70
42	S60	954	G	C5-N7-C8	-5.25	101.68	104.30
42	S60	1097	A	C8-N9-C4	5.25	107.90	105.80
66	SQ0	82	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	L50	885	G	P-O3'-C3'	-5.25	113.41	119.70
1	L50	1605	U	P-O3'-C3'	-5.24	113.41	119.70
42	S60	1003	A	C6-N1-C2	-5.24	115.46	118.60
1	L50	141	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	L50	1010	A	O5'-P-OP2	-5.24	100.99	105.70
42	S60	850	G	C4'-C3'-C2'	-5.23	97.37	102.60
42	S60	994	G	C8-N9-C4	-5.23	104.31	106.40
1	L50	1839	A	P-O3'-C3'	-5.23	113.43	119.70
42	S60	993	U	P-O3'-C3'	-5.23	113.43	119.70
42	S60	1194	U	C5-C6-N1	-5.23	120.09	122.70
1	L50	2447	A	P-O5'-C5'	-5.23	112.54	120.90
42	S60	1012	A	C4'-C3'-C2'	-5.22	97.38	102.60
42	S60	1218	U	C3'-C2'-C1'	5.22	105.68	101.50
1	L50	515	U	P-O3'-C3'	-5.22	113.44	119.70
1	L50	1575	G	C4'-C3'-C2'	-5.22	97.38	102.60
1	L50	323	G	C4'-C3'-C2'	-5.21	97.39	102.60
1	L50	371	A	C5-N7-C8	5.21	106.51	103.90
42	S60	275	G	C4'-C3'-C2'	-5.21	97.39	102.60
42	S60	1161	U	C6-N1-C2	5.21	124.13	121.00
42	S60	1053	A	C3'-C2'-C1'	-5.21	97.33	101.50
42	S60	918	A	C3'-C2'-C1'	-5.21	97.34	101.50
1	L50	1513	G	P-O3'-C3'	5.20	125.94	119.70
1	L50	2181	A	O5'-P-OP1	-5.20	101.02	105.70
42	S60	1018	U	N3-C4-C5	5.20	117.72	114.60
1	L50	1499	U	C2'-C3'-O3'	5.19	122.01	113.70
42	S60	1039	G	C8-N9-C4	-5.19	104.33	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	1000	G	C1'-C2'-O2'	-5.18	95.05	110.60
42	S60	934	A	P-O3'-C3'	-5.18	113.49	119.70
42	S60	1203	A	C2-N3-C4	5.18	113.19	110.60
42	S60	963	G	C4-C5-N7	-5.17	108.73	110.80
42	S60	1018	U	C6-N1-C2	5.17	124.11	121.00
1	L50	1160	G	O4'-C1'-N9	5.17	112.34	108.20
1	L50	2447	A	O4'-C1'-N9	5.17	112.34	108.20
1	L50	596	G	C4'-C3'-C2'	-5.17	97.43	102.60
1	L50	1165	U	P-O3'-C3'	-5.17	113.50	119.70
42	S60	861	C	C6-N1-C2	5.17	122.37	120.30
42	S60	1097	A	C2-N3-C4	5.17	113.19	110.60
42	S60	441	G	C4'-C3'-C2'	-5.17	97.44	102.60
42	S60	1189	A	N7-C8-N9	-5.17	111.22	113.80
1	L50	1586	G	OP1-P-OP2	-5.16	111.85	119.60
42	S60	1069	G	C5-N7-C8	-5.16	101.72	104.30
42	S60	1208	G	C5-N7-C8	5.16	106.88	104.30
1	L50	462	G	OP1-P-O3'	5.16	116.55	105.20
1	L50	690	U	C4'-C3'-C2'	-5.16	97.44	102.60
1	L50	1364	U	P-O3'-C3'	-5.16	113.51	119.70
1	L50	1602	G	C4'-C3'-C2'	-5.16	97.44	102.60
42	S60	1179	A	C4-C5-N7	-5.16	108.12	110.70
1	L50	541	U	P-O3'-C3'	-5.16	113.51	119.70
42	S60	989	G	C4-C5-N7	-5.16	108.74	110.80
1	L50	2315	G	C4'-C3'-C2'	-5.15	97.45	102.60
42	S60	459	G	C4'-C3'-C2'	-5.15	97.45	102.60
42	S60	1094	C	C5-C6-N1	5.15	123.58	121.00
42	S60	1001	C	C2-N3-C4	5.15	122.47	119.90
1	L50	2009	U	O5'-P-OP2	-5.14	101.07	105.70
2	L70	93	A	P-O3'-C3'	-5.14	113.53	119.70
42	S60	1052	A	C2-N3-C4	-5.14	108.03	110.60
42	S60	1118	A	C8-N9-C4	-5.14	103.75	105.80
39	LY0	53	ASP	CB-CA-C	5.13	120.67	110.40
42	S60	1176	G	C5-C6-N1	5.13	114.07	111.50
42	S60	1050	G	N3-C4-C5	-5.13	126.04	128.60
1	L50	194	A	OP1-P-OP2	-5.13	111.91	119.60
1	L50	1192	A	OP1-P-OP2	-5.12	111.91	119.60
42	S60	952	A	C6-N1-C2	5.12	121.67	118.60
42	S60	1088	U	C5-C6-N1	-5.12	120.14	122.70
1	L50	2452	A	P-O3'-C3'	5.12	125.84	119.70
1	L50	614	G	N3-C4-C5	-5.12	126.04	128.60
1	L50	330	G	P-O3'-C3'	5.12	125.84	119.70
42	S60	995	A	C5-N7-C8	5.11	106.46	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	S60	858	C	C5-C6-N1	5.11	123.56	121.00
42	S60	263	A	C5'-C4'-C3'	-5.11	107.83	116.00
1	L50	590	G	N3-C4-C5	-5.10	126.05	128.60
42	S60	1062	C	C6-N1-C2	-5.10	118.26	120.30
42	S60	857	G	N9-C4-C5	-5.10	103.36	105.40
66	SQ0	82	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	L50	2341	G	C4'-C3'-C2'	-5.09	97.51	102.60
42	S60	883	C	N3-C4-C5	5.09	123.94	121.90
42	S60	1095	G	C4-C5-C6	5.09	121.85	118.80
1	L50	690	U	OP1-P-O3'	5.09	116.39	105.20
42	S60	987	A	C4-C5-N7	5.09	113.24	110.70
42	S60	1208	G	N7-C8-N9	-5.09	110.56	113.10
1	L50	569	C	O5'-P-OP2	-5.08	101.13	105.70
1	L50	1018	U	C1'-C2'-O2'	-5.08	95.35	110.60
1	L50	1622	G	C4'-C3'-C2'	-5.08	97.52	102.60
42	S60	1059	G	N9-C4-C5	-5.08	103.37	105.40
1	L50	2011	A	P-O3'-C3'	-5.08	113.61	119.70
1	L50	1182	A	O5'-P-OP2	5.07	116.79	110.70
42	S60	835	A	C4-C5-C6	5.07	119.54	117.00
1	L50	2145	A	O5'-P-OP1	-5.07	101.14	105.70
42	S60	1000	C	C2-N3-C4	5.07	122.44	119.90
42	S60	881	G	OP1-P-OP2	-5.07	112.00	119.60
42	S60	1064	G	OP1-P-OP2	-5.07	112.00	119.60
42	S60	844	A	P-O3'-C3'	-5.07	113.62	119.70
1	L50	1614	G	C1'-O4'-C4'	-5.07	105.85	109.90
1	L50	2313	G	O5'-P-OP1	-5.07	101.14	105.70
42	S60	162	C	P-O3'-C3'	-5.07	113.62	119.70
42	S60	1228	C	C5-C6-N1	5.07	123.53	121.00
1	L50	1625	A	O5'-P-OP2	-5.07	101.14	105.70
1	L50	2167	A	C3'-C2'-C1'	5.07	105.55	101.50
42	S60	975	G	C4-C5-N7	5.07	112.83	110.80
42	S60	1214	A	P-O3'-C3'	-5.07	113.62	119.70
1	L50	266	A	O5'-P-OP1	-5.06	101.14	105.70
42	S60	951	A	C4-C5-N7	5.06	113.23	110.70
42	S60	989	G	C4-C5-C6	5.06	121.83	118.80
42	S60	308	C	P-O3'-C3'	-5.06	113.63	119.70
42	S60	1209	C	C6-N1-C2	5.06	122.32	120.30
1	L50	612	C	OP1-P-OP2	-5.05	112.02	119.60
42	S60	8	U	O5'-P-OP2	-5.05	101.15	105.70
42	S60	1111	A	C8-N9-C4	5.05	107.82	105.80
42	S60	859	G	C4-C5-C6	5.05	121.83	118.80
42	S60	1011	A	N9-C4-C5	5.05	107.82	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S60	1161	U	N3-C4-C5	5.05	117.63	114.60
42	S60	1053	A	C4-C5-C6	-5.04	114.48	117.00
42	S60	1086	G	C3'-C2'-C1'	-5.04	97.47	101.50
42	S60	1048	G	N7-C8-N9	5.04	115.62	113.10
42	S60	1011	A	C4-C5-C6	5.04	119.52	117.00
42	S60	1048	G	C5-C6-N1	-5.04	108.98	111.50
42	S60	875	A	C5-N7-C8	5.04	106.42	103.90
42	S60	885	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	L50	2556	U	P-O3'-C3'	-5.03	113.67	119.70
1	L50	1087	G	C4'-C3'-C2'	-5.03	97.57	102.60
1	L50	1484	U	O5'-P-OP2	5.03	116.73	110.70
1	L50	75	C	C2'-C3'-O3'	5.02	121.74	113.70
1	L50	2019	G	C4'-C3'-C2'	-5.02	97.58	102.60
42	S60	833	A	P-O3'-C3'	-5.02	113.67	119.70
1	L50	1115	G	C3'-C2'-C1'	-5.02	97.49	101.50
42	S60	624	U	P-O3'-C3'	-5.01	113.68	119.70
1	L50	784	G	P-O3'-C3'	-5.01	113.69	119.70
1	L50	1018	U	C1'-O4'-C4'	-5.01	105.89	109.90
1	L50	1568	G	OP1-P-OP2	-5.01	112.09	119.60
1	L50	1414	U	P-O5'-C5'	-5.01	112.89	120.90
1	L50	2154	U	P-O3'-C3'	-5.01	113.69	119.70
42	S60	987	A	N1-C6-N6	5.01	121.61	118.60
1	L50	151	G	P-O3'-C3'	5.01	125.71	119.70
1	L50	1182	A	OP1-P-OP2	-5.00	112.09	119.60
42	S60	882	A	C5-N7-C8	5.00	106.40	103.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LC0	87	ALA	Peptide
13	LFF	101	ILE	Peptide
15	LGG	77	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L50	53655	0	26955	118	0
2	L70	2542	0	1282	8	0
3	LA0	1889	0	1985	12	0
4	LAA	1167	0	1214	5	0
5	LB0	3039	0	3183	6	0
6	LC0	2604	0	2638	12	0
7	LCC	781	0	803	2	0
8	LD0	2298	0	2384	6	0
9	LDD	895	0	948	0	0
10	LE0	1371	0	1389	13	0
11	LEE	1090	0	1173	10	0
12	LF0	1933	0	2011	11	0
13	LFF	893	0	945	2	0
14	LG0	1590	0	1709	4	0
15	LGG	819	0	882	1	0
16	LH0	1477	0	1528	4	0
17	LHH	992	0	1097	5	0
18	LI0	1750	0	1797	2	0
19	LII	784	0	874	2	0
20	LJ0	1332	0	1411	12	0
21	LJJ	701	0	753	4	0
22	LL0	1353	0	1433	4	0
23	LLL	427	0	468	0	0
24	LM0	927	0	961	5	0
25	LMM	427	0	461	0	0
26	LN0	1688	0	1752	5	0
27	LO0	1598	0	1681	3	0
28	LOO	801	0	886	4	0
29	LP0	1238	0	1304	3	0
30	LPP	684	0	720	2	0
31	LQ0	1491	0	1587	6	0
32	LR0	1336	0	1430	0	0
33	LS0	1400	0	1450	1	0
34	LT0	1270	0	1321	15	0
35	LU0	810	0	834	1	0
36	LV0	1057	0	1139	2	0
37	LW0	832	0	873	45	0
38	LX0	874	0	956	5	0
39	LY0	1048	0	1135	2	0
40	LZ0	963	0	1022	2	0
41	MD1	1229	0	1216	10	0
42	S60	29181	0	14605	315	0
43	SA0	1725	0	1750	137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SAA	827	0	859	18	0
45	SB0	1609	0	1728	6	0
46	SBB	627	0	651	3	0
47	SC0	1727	0	1802	90	0
48	SCC	476	0	488	18	0
49	SD0	1700	0	1815	33	0
50	SDD	550	0	542	29	0
51	SE0	2044	0	2116	26	0
52	SEE	447	0	483	1	0
53	SF0	1509	0	1604	39	0
54	SFF	422	0	412	6	0
55	SG0	1836	0	1972	38	0
56	SGG	2478	0	2458	22	0
57	SH0	1335	0	1356	2	0
58	SI0	1347	0	1379	9	0
59	SJ0	1379	0	1436	15	0
60	SK0	737	0	746	17	0
61	SL0	1229	0	1302	5	0
62	SM0	876	0	937	6	0
63	SN0	1130	0	1189	10	0
64	SO0	983	0	1028	14	0
65	SP0	950	0	984	58	0
66	SQ0	1143	0	1171	19	0
67	SR0	974	0	1003	99	0
68	SS0	1150	0	1207	32	0
69	ST0	1161	0	1219	9	0
70	SU0	809	0	838	14	0
71	SV0	521	0	525	72	0
72	SW0	1022	0	1052	18	0
73	SX0	1098	0	1183	4	0
74	SY0	1118	0	1166	12	0
75	SZ0	633	0	678	13	0
76	LGG	1	0	0	0	0
76	LJJ	1	0	0	0	0
76	LMM	1	0	0	0	0
76	LOO	1	0	0	0	0
76	LPP	1	0	0	0	0
76	SAA	1	0	0	0	0
76	SBB	1	0	0	0	0
76	SDD	1	0	0	0	0
76	SFF	1	0	0	0	0
All	All	171817	0	133274	959	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (959) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA0:70:ASN:HB2	47:SC0:240:ILE:CD1	1.35	1.56
47:SC0:51:SER:HB2	71:SV0:6:ARG:NH2	1.30	1.44
49:SD0:238:PRO:C	67:SR0:19:ARG:HH12	1.27	1.36
43:SA0:70:ASN:HB2	47:SC0:240:ILE:CG1	1.56	1.35
20:LJ0:82:LYS:HB3	65:SP0:30:PHE:CE2	1.62	1.34
43:SA0:70:ASN:CB	47:SC0:240:ILE:HD11	1.59	1.30
43:SA0:141:ASN:O	71:SV0:23:VAL:HG23	1.21	1.26
49:SD0:239:ILE:N	67:SR0:19:ARG:HH12	1.35	1.24
3:LA0:241:ARG:NH1	42:S60:592:G:H4'	1.51	1.22
50:SDD:8:TYR:CE2	65:SP0:72:ARG:HD2	1.75	1.21
49:SD0:238:PRO:C	67:SR0:19:ARG:NH1	1.98	1.17
43:SA0:63:ARG:CZ	71:SV0:30:LEU:HG	1.75	1.16
47:SC0:51:SER:CB	71:SV0:6:ARG:HH21	1.60	1.14
43:SA0:70:ASN:CB	47:SC0:240:ILE:CD1	2.22	1.12
47:SC0:51:SER:CB	71:SV0:6:ARG:NH2	2.11	1.11
37:LW0:99:LYS:HA	37:LW0:102:LYS:HE2	1.30	1.09
20:LJ0:82:LYS:CB	65:SP0:30:PHE:HE2	1.65	1.09
43:SA0:63:ARG:HG2	71:SV0:30:LEU:HD21	1.31	1.08
43:SA0:70:ASN:CG	47:SC0:240:ILE:HG12	1.73	1.08
1:L50:1691:A:N6	42:S60:1248:G:H4'	1.68	1.08
43:SA0:63:ARG:O	71:SV0:28:VAL:HG22	1.55	1.07
47:SC0:219:PRO:HB3	72:SW0:66:ARG:NH2	1.68	1.07
74:SY0:22:GLU:O	74:SY0:23:LEU:HG	1.53	1.06
3:LA0:241:ARG:HH12	42:S60:592:G:C4'	1.69	1.06
1:L50:535:A:O2'	31:LQ0:146:ASN:HB3	1.55	1.05
43:SA0:187:GLY:HA2	71:SV0:35:ARG:NH2	1.71	1.05
43:SA0:64:MET:HB3	71:SV0:27:MET:HG2	1.38	1.05
43:SA0:141:ASN:C	71:SV0:23:VAL:HG23	1.76	1.05
37:LW0:83:PHE:CD1	55:SG0:144:LYS:HG2	1.92	1.05
34:LT0:126:PRO:HB2	34:LT0:128:LEU:HG	1.34	1.04
1:L50:1695:A:N1	42:S60:1249:U:C5'	2.20	1.04
43:SA0:70:ASN:CB	47:SC0:240:ILE:CG1	2.35	1.04
43:SA0:141:ASN:O	71:SV0:23:VAL:CG2	2.05	1.04
50:SDD:12:LEU:HD21	65:SP0:67:PHE:CD2	1.92	1.03
47:SC0:136:TRP:HH2	59:SJ0:59:ILE:CG2	1.71	1.03
43:SA0:215:TYR:CD1	67:SR0:84:PHE:CE2	2.46	1.03
55:SG0:140:LYS:O	55:SG0:144:LYS:HD3	1.58	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LW0:83:PHE:CD1	55:SG0:144:LYS:CG	2.41	1.02
49:SD0:239:ILE:N	67:SR0:19:ARG:NH1	2.05	1.02
50:SDD:12:LEU:CD1	65:SP0:75:ILE:HG21	1.90	1.02
37:LW0:83:PHE:CD1	37:LW0:84:PRO:HD2	1.93	1.02
43:SA0:63:ARG:CG	71:SV0:30:LEU:HD21	1.90	1.02
10:LE0:55:GLU:OE2	10:LE0:117:ARG:HG3	1.59	1.01
55:SG0:147:PHE:HZ	55:SG0:160:LYS:HE2	1.22	1.01
43:SA0:117:ARG:HH12	47:SC0:243:GLU:CD	1.64	1.00
1:L50:1695:A:N1	42:S60:1249:U:H5’	1.76	1.00
1:L50:1695:A:C2	42:S60:1249:U:H5”	1.97	0.98
44:SAA:47:ALA:CB	48:SCC:61:ARG:HE	1.78	0.97
47:SC0:230:ASN:N	71:SV0:24:GLN:HE22	1.61	0.97
3:LA0:241:ARG:HH12	42:S60:592:G:H4’	1.13	0.96
43:SA0:215:TYR:HA	67:SR0:84:PHE:CD2	2.01	0.96
47:SC0:51:SER:HB2	71:SV0:6:ARG:HH22	1.15	0.96
37:LW0:98:ASN:ND2	55:SG0:147:PHE:HA	1.81	0.95
42:S60:973:G:H1	44:SAA:90:TRP:HZ2	1.09	0.95
43:SA0:70:ASN:HB2	47:SC0:240:ILE:HD11	0.95	0.95
43:SA0:63:ARG:NE	71:SV0:30:LEU:HG	1.81	0.94
56:SGG:65:PHE:CE2	67:SR0:29:TYR:CE2	2.55	0.94
43:SA0:51:ILE:HG13	67:SR0:105:MET:SD	2.09	0.93
20:LJ0:82:LYS:HB3	65:SP0:30:PHE:CD2	2.03	0.93
42:S60:554:A:N3	72:SW0:103:THR:HG22	1.83	0.93
1:L50:1691:A:N6	42:S60:1248:G:C4’	2.32	0.93
43:SA0:184:TYR:CD1	71:SV0:35:ARG:NH1	2.36	0.92
50:SDD:8:TYR:O	65:SP0:67:PHE:N	2.01	0.92
43:SA0:120:ARG:HE	47:SC0:232:ILE:HG21	1.35	0.92
43:SA0:70:ASN:CA	47:SC0:240:ILE:HD11	1.98	0.92
43:SA0:4:ARG:O	71:SV0:30:LEU:HD12	1.69	0.92
10:LE0:100:ILE:HD11	24:LM0:102:PHE:HB2	1.49	0.91
50:SDD:8:TYR:CE2	65:SP0:72:ARG:CD	2.54	0.91
37:LW0:99:LYS:CA	37:LW0:102:LYS:HE2	2.00	0.91
43:SA0:70:ASN:CB	47:SC0:240:ILE:HG12	1.99	0.91
42:S60:973:G:N1	44:SAA:90:TRP:CZ2	2.39	0.90
47:SC0:136:TRP:CH2	59:SJ0:59:ILE:CG2	2.54	0.90
42:S60:958:A:H3’	42:S60:959:G:H21	1.37	0.90
43:SA0:184:TYR:O	71:SV0:35:ARG:HD2	1.72	0.90
43:SA0:63:ARG:HD3	71:SV0:30:LEU:HD23	1.52	0.90
47:SC0:130:PRO:HB2	71:SV0:4:PHE:CZ	2.07	0.90
48:SCC:58:ARG:HH12	64:SO0:101:ARG:HH22	1.19	0.90
20:LJ0:82:LYS:CB	65:SP0:30:PHE:CE2	2.44	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC0:230:ASN:H	71:SV0:24:GLN:HE22	0.91	0.89
43:SA0:70:ASN:ND2	47:SC0:240:ILE:HG12	1.88	0.89
43:SA0:63:ARG:HD3	71:SV0:30:LEU:CD2	2.03	0.89
43:SA0:67:SER:OG	71:SV0:40:LEU:CD2	2.21	0.89
42:S60:203:G:N3	51:SE0:33:THR:HG21	1.88	0.88
43:SA0:51:ILE:HD12	67:SR0:105:MET:HG2	1.53	0.88
1:L50:1695:A:N1	42:S60:1249:U:H5”	1.85	0.88
37:LW0:99:LYS:HA	37:LW0:102:LYS:CE	2.03	0.88
43:SA0:117:ARG:NH1	47:SC0:243:GLU:OE2	2.06	0.88
50:SDD:8:TYR:CD2	65:SP0:72:ARG:HD2	2.08	0.87
43:SA0:120:ARG:HE	47:SC0:232:ILE:CG2	1.88	0.86
47:SC0:219:PRO:HB3	72:SW0:66:ARG:HH22	1.39	0.86
47:SC0:230:ASN:HB2	71:SV0:24:GLN:CD	1.95	0.86
50:SDD:12:LEU:CD2	65:SP0:67:PHE:CD2	2.57	0.86
42:S60:973:G:N1	44:SAA:90:TRP:HZ2	1.72	0.86
50:SDD:8:TYR:CZ	65:SP0:72:ARG:HD2	2.09	0.86
37:LW0:26:ASP:O	37:LW0:27:ASP:OD1	1.94	0.86
47:SC0:230:ASN:H	71:SV0:24:GLN:NE2	1.73	0.86
20:LJ0:82:LYS:HB3	65:SP0:30:PHE:HE2	1.06	0.86
42:S60:1084:G:N2	65:SP0:117:GLY:O	2.09	0.85
43:SA0:67:SER:OG	71:SV0:40:LEU:HD22	1.75	0.85
42:S60:995:A:H3’	42:S60:996:G:H8	1.42	0.85
53:SF0:118:ARG:HD2	53:SF0:125:MET:HB3	1.58	0.85
42:S60:1149:U:OP1	68:SS0:139:VAL:N	2.10	0.84
42:S60:826:U:O2’	47:SC0:81:GLN:O	1.94	0.84
42:S60:705:A:N3	42:S60:706:G:C6	2.46	0.84
42:S60:706:G:N3	42:S60:706:G:H2’	1.92	0.83
41:MD1:52:LYS:HG3	42:S60:606:G:N2	1.93	0.83
50:SDD:12:LEU:HD11	65:SP0:75:ILE:HG21	1.59	0.83
3:LA0:241:ARG:NH1	42:S60:592:G:C4’	2.33	0.82
43:SA0:63:ARG:CD	71:SV0:30:LEU:CD2	2.57	0.82
42:S60:914:U:H3	42:S60:918:A:H61	1.23	0.82
43:SA0:215:TYR:O	67:SR0:84:PHE:HE2	1.62	0.82
42:S60:1159:A:O2’	65:SP0:100:ASN:ND2	2.11	0.82
42:S60:923:A:H4’	42:S60:924:U:H2’	1.61	0.81
53:SF0:39:ILE:HG21	66:SQ0:50:GLU:HB2	1.62	0.81
55:SG0:147:PHE:CZ	55:SG0:160:LYS:HE2	2.13	0.81
42:S60:173:A:C8	51:SE0:131:VAL:CG1	2.64	0.81
43:SA0:63:ARG:HG2	71:SV0:30:LEU:CD2	2.11	0.81
49:SD0:234:ILE:HD12	67:SR0:8:SER:HB2	1.62	0.81
43:SA0:215:TYR:HA	67:SR0:84:PHE:CE2	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SFF:93:LYS:HB3	54:SFF:94:PRO:HD2	1.63	0.81
1:L50:1728:U:HO2'	42:S60:1259:U:HO2'	1.05	0.81
1:L50:1691:A:C6	42:S60:1248:G:O4'	2.34	0.81
56:SGG:65:PHE:CZ	67:SR0:29:TYR:CE2	2.69	0.81
42:S60:1055:A:O3'	47:SC0:84:ALA:HB2	1.81	0.80
49:SD0:101:LYS:NZ	60:SK0:14:TYR:OH	2.13	0.80
47:SC0:136:TRP:HH2	59:SJ0:59:ILE:HG21	1.46	0.80
47:SC0:230:ASN:HB2	71:SV0:24:GLN:OE1	1.80	0.80
66:SQ0:33:ASN:ND2	69:ST0:6:PHE:CD2	2.50	0.80
10:LE0:23:ILE:HD11	11:LEE:79:ARG:HH12	1.46	0.80
54:SFF:99:LYS:HE2	54:SFF:102:ILE:HG12	1.64	0.80
56:SGG:65:PHE:HE2	67:SR0:29:TYR:CE2	1.96	0.79
53:SF0:96:GLY:O	75:SZ0:108:LEU:CD2	2.31	0.79
37:LW0:83:PHE:CE1	55:SG0:144:LYS:HG2	2.17	0.79
43:SA0:67:SER:CA	71:SV0:28:VAL:HG13	2.13	0.79
50:SDD:8:TYR:N	65:SP0:67:PHE:O	2.14	0.79
42:S60:973:G:H22	44:SAA:90:TRP:HH2	1.27	0.79
37:LW0:83:PHE:CD1	55:SG0:144:LYS:HG3	2.17	0.79
42:S60:988:A:O2'	43:SA0:105:PRO:O	2.00	0.79
43:SA0:215:TYR:HA	67:SR0:84:PHE:HD2	1.48	0.79
47:SC0:166:LYS:HD2	59:SJ0:100:GLU:OE2	1.83	0.78
34:LT0:126:PRO:HB2	34:LT0:128:LEU:CG	2.13	0.78
43:SA0:52:LYS:HB2	67:SR0:109:TYR:CZ	2.19	0.78
37:LW0:83:PHE:CG	37:LW0:84:PRO:HD2	2.18	0.78
53:SF0:39:ILE:CG2	66:SQ0:50:GLU:HB2	2.11	0.78
50:SDD:12:LEU:CD1	65:SP0:75:ILE:CG2	2.62	0.78
42:S60:1188:A:H5”	66:SQ0:136:ALA:HB2	1.65	0.77
42:S60:1045:A:OP2	67:SR0:2:GLY:N	2.17	0.77
43:SA0:63:ARG:O	71:SV0:28:VAL:CG2	2.32	0.77
43:SA0:206:ARG:NE	67:SR0:86:PRO:HG2	1.99	0.77
42:S60:1055:A:O3'	47:SC0:84:ALA:CB	2.33	0.77
43:SA0:118:GLU:OE2	47:SC0:31:THR:HA	1.84	0.77
43:SA0:187:GLY:HA2	71:SV0:35:ARG:CZ	2.14	0.77
1:L50:796:C:H5”	34:LT0:131:ARG:H	1.48	0.77
3:LA0:241:ARG:CZ	42:S60:592:G:H4'	2.15	0.77
53:SF0:6:THR:HG23	66:SQ0:53:LYS:NZ	2.00	0.77
55:SG0:169:VAL:CG1	55:SG0:176:LYS:HE2	2.14	0.77
53:SF0:40:LEU:HD23	66:SQ0:43:PHE:CE1	2.20	0.77
43:SA0:102:ARG:H	43:SA0:102:ARG:HD2	1.49	0.76
43:SA0:215:TYR:HD1	67:SR0:84:PHE:CD2	2.03	0.76
1:L50:2497:C:H5”	5:LB0:280:THR:HG21	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
43:SA0:67:SER:HA	71:SV0:28:VAL:HG13	1.66	0.76
48:SCC:58:ARG:HH12	64:SO0:101:ARG:NH2	1.82	0.76
55:SG0:170:ASN:HD21	55:SG0:176:LYS:HD3	1.50	0.76
1:L50:1695:A:C2	42:S60:1249:U:C5'	2.66	0.76
44:SAA:47:ALA:HB1	48:SCC:61:ARG:HE	1.49	0.76
50:SDD:12:LEU:CD2	65:SP0:67:PHE:HD2	1.98	0.76
1:L50:883:U:H5"	24:LM0:35:ASN:ND2	2.01	0.76
43:SA0:70:ASN:N	47:SC0:240:ILE:HD11	2.00	0.76
42:S60:982:C:H4'	67:SR0:10:ARG:NH1	2.01	0.75
43:SA0:52:LYS:HB2	67:SR0:109:TYR:CE1	2.21	0.75
43:SA0:120:ARG:NE	47:SC0:232:ILE:HG21	2.02	0.75
49:SD0:238:PRO:CA	67:SR0:19:ARG:HH12	1.98	0.75
43:SA0:64:MET:CB	71:SV0:27:MET:HG2	2.17	0.74
37:LW0:98:ASN:ND2	55:SG0:147:PHE:CA	2.48	0.74
37:LW0:98:ASN:HD22	55:SG0:147:PHE:HA	1.52	0.74
42:S60:982:C:O3'	67:SR0:10:ARG:NH1	2.21	0.74
56:SGG:228:LYS:NZ	67:SR0:25:THR:HG22	2.02	0.74
42:S60:840:C:H4'	42:S60:1182:G:H5"	1.68	0.74
44:SAA:51:ASP:OD2	48:SCC:57:GLU:O	2.06	0.74
1:L50:883:U:H5"	24:LM0:35:ASN:HD21	1.51	0.74
43:SA0:52:LYS:CB	67:SR0:109:TYR:CZ	2.70	0.74
56:SGG:228:LYS:HZ2	67:SR0:25:THR:HG22	1.51	0.74
5:LB0:336:ARG:HG3	5:LB0:336:ARG:HH11	1.51	0.74
45:SB0:53:THR:HG22	64:SO0:30:ASP:OD2	1.88	0.73
53:SF0:96:GLY:O	75:SZ0:108:LEU:HD21	1.88	0.73
1:L50:2052:A:H5'	20:LJ0:62:ILE:HD11	1.69	0.73
42:S60:173:A:H8	51:SE0:131:VAL:HG12	1.50	0.73
37:LW0:99:LYS:CB	37:LW0:102:LYS:HE2	2.18	0.73
2:L70:27:A:OP2	8:LD0:62:THR:HG23	1.88	0.73
43:SA0:141:ASN:C	71:SV0:23:VAL:CG2	2.55	0.73
43:SA0:184:TYR:CE2	71:SV0:35:ARG:HD3	2.24	0.73
42:S60:173:A:C8	51:SE0:131:VAL:HG12	2.23	0.72
43:SA0:215:TYR:CD1	67:SR0:84:PHE:CD2	2.76	0.72
49:SD0:36:ARG:NH1	70:SU0:112:GLU:OE2	2.21	0.72
42:S60:203:G:N3	51:SE0:33:THR:CG2	2.51	0.72
2:L70:3:U:H3	2:L70:116:G:H1	1.37	0.72
68:SS0:20:MET:HG2	68:SS0:29:ASP:HA	1.71	0.72
43:SA0:184:TYR:O	71:SV0:35:ARG:CD	2.36	0.72
41:MD1:106:TYR:CE1	64:SO0:47:LYS:NZ	2.54	0.72
1:L50:1691:A:N1	42:S60:1248:G:O4'	2.23	0.71
7:LCC:64:ILE:HG22	40:LZ0:39:LEU:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:705:A:C2	42:S60:706:G:O6	2.43	0.71
43:SA0:52:LYS:HD2	67:SR0:109:TYR:CE1	2.25	0.71
42:S60:995:A:H3'	42:S60:996:G:C8	2.24	0.71
42:S60:1034:A:H2'	42:S60:1035:C:C6	2.26	0.71
42:S60:237:A:H5'	58:SI0:48:VAL:CG1	2.21	0.71
53:SF0:40:LEU:CD2	66:SQ0:43:PHE:CD1	2.74	0.71
2:L70:63:A:H2'	18:LI0:204:GLY:O	1.91	0.70
53:SF0:95:THR:HG21	53:SF0:102:ILE:HG12	1.72	0.70
42:S60:1315:A:H2'	42:S60:1316:A:H8	1.54	0.70
48:SCC:41:ILE:HG23	53:SF0:131:ASP:O	1.90	0.70
53:SF0:6:THR:HG23	66:SQ0:53:LYS:HZ1	1.54	0.70
42:S60:982:C:O2'	67:SR0:10:ARG:NH1	2.22	0.70
42:S60:1040:G:N2	42:S60:1042:A:H3'	2.06	0.70
42:S60:438:U:H4'	73:SX0:110:LYS:HD2	1.72	0.70
47:SC0:136:TRP:CH2	59:SJ0:59:ILE:HG21	2.23	0.70
42:S60:237:A:H5'	58:SI0:48:VAL:HG13	1.74	0.69
42:S60:1158:U:O2'	50:SDD:7:LYS:NZ	2.18	0.69
45:SB0:53:THR:HG21	64:SO0:32:THR:OG1	1.92	0.69
68:SS0:24:PHE:CZ	68:SS0:107:ILE:HG21	2.27	0.69
42:S60:854:U:OP2	68:SS0:148:GLY:N	2.24	0.69
47:SC0:49:GLY:O	71:SV0:6:ARG:HB2	1.92	0.69
1:L50:796:C:H5"	34:LT0:131:ARG:N	2.06	0.69
53:SF0:92:GLU:HG3	75:SZ0:108:LEU:HD12	1.73	0.69
14:LG0:119:ASP:OD1	14:LG0:145:THR:HA	1.92	0.69
26:LN0:112:ASN:HD22	26:LN0:112:ASN:H	1.40	0.69
43:SA0:120:ARG:HH11	47:SC0:232:ILE:HG21	1.57	0.69
42:S60:666:A:OP1	63:SN0:132:LYS:NZ	2.25	0.69
47:SC0:219:PRO:CB	72:SW0:66:ARG:NH2	2.51	0.69
52:SEE:5:ILE:HD12	73:SX0:63:ILE:HD12	1.74	0.68
43:SA0:67:SER:HA	71:SV0:28:VAL:CG1	2.22	0.68
10:LE0:55:GLU:CD	10:LE0:117:ARG:HG3	2.14	0.68
42:S60:1056:A:OP1	47:SC0:84:ALA:HB1	1.93	0.68
42:S60:1035:C:H2'	42:S60:1036:A:C8	2.29	0.68
51:SE0:64:ILE:HD12	74:SY0:23:LEU:HD13	1.75	0.68
53:SF0:42:HIS:HD1	66:SQ0:79:TYR:HH	1.41	0.68
42:S60:1315:A:H2'	42:S60:1316:A:C8	2.28	0.68
37:LW0:98:ASN:ND2	55:SG0:147:PHE:N	2.43	0.67
42:S60:173:A:H8	51:SE0:131:VAL:CG1	2.04	0.67
49:SD0:94:GLN:HE21	60:SK0:19:SER:HB3	1.59	0.67
36:LV0:98:LEU:HD23	37:LW0:21:TYR:HB2	1.75	0.67
42:S60:705:A:C2	42:S60:706:G:C6	2.82	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA0:51:ILE:CG1	67:SR0:105:MET:SD	2.82	0.67
43:SA0:67:SER:CB	71:SV0:28:VAL:HG13	2.24	0.67
50:SDD:12:LEU:HD23	65:SP0:67:PHE:HD2	1.59	0.67
56:SGG:65:PHE:HZ	67:SR0:29:TYR:OH	1.77	0.67
43:SA0:118:GLU:CD	47:SC0:31:THR:HG1	1.98	0.67
56:SGG:65:PHE:CZ	67:SR0:29:TYR:CZ	2.83	0.67
47:SC0:130:PRO:HB2	71:SV0:4:PHE:CE1	2.29	0.67
67:SR0:103:MET:CE	67:SR0:117:LEU:HG	2.25	0.67
1:L50:2045:C:H5’	20:LJ0:102:GLY:HA3	1.77	0.66
20:LJ0:107:ILE:HD11	20:LJ0:113:TYR:HD1	1.60	0.66
42:S60:1066:G:C5	60:SK0:58:PHE:CD1	2.83	0.66
43:SA0:63:ARG:CD	71:SV0:30:LEU:HD21	2.24	0.66
45:SB0:71:ARG:HD3	64:SO0:32:THR:HG21	1.78	0.66
47:SC0:166:LYS:CD	59:SJ0:100:GLU:OE2	2.43	0.66
42:S60:826:U:O2	47:SC0:81:GLN:HB3	1.96	0.66
42:S60:958:A:OP1	47:SC0:111:ARG:NH2	2.28	0.66
1:L50:535:A:O2’	31:LQ0:146:ASN:CB	2.38	0.65
1:L50:535:A:HO2’	31:LQ0:146:ASN:HB3	1.61	0.65
1:L50:1191:U:H2’	1:L50:1192:A:H5”	1.77	0.65
42:S60:823:A:H2’	42:S60:824:A:C8	2.31	0.65
1:L50:2109:G:H5”	1:L50:2109:G:H8	1.59	0.65
10:LE0:30:LEU:HD22	11:LEE:11:VAL:CG1	2.26	0.65
42:S60:914:U:H3	42:S60:918:A:N6	1.94	0.65
48:SCC:55:ASP:OD2	53:SF0:195:ARG:HD3	1.96	0.65
1:L50:1018:U:O2’	13:LFF:78:ARG:HD2	1.97	0.65
42:S60:1230:U:O2’	44:SAA:88:SER:HB3	1.96	0.65
42:S60:982:C:H4’	67:SR0:10:ARG:HH11	1.62	0.65
42:S60:1144:G:C2’	42:S60:1145:G:H5’	2.27	0.64
42:S60:661:A:H4’	63:SN0:62:LYS:HE2	1.78	0.64
42:S60:840:C:O2’	42:S60:1182:G:OP1	2.14	0.64
47:SC0:136:TRP:HH2	59:SJ0:59:ILE:HG23	1.60	0.64
42:S60:892:A:N3	65:SP0:115:TYR:OH	2.29	0.64
42:S60:910:A:H62	42:S60:922:G:H21	1.44	0.64
55:SG0:169:VAL:HG11	55:SG0:176:LYS:HE2	1.79	0.64
56:SGG:105:ARG:HH22	67:SR0:37:ASP:CA	2.11	0.64
68:SS0:139:VAL:O	68:SS0:139:VAL:HG12	1.96	0.64
51:SE0:137:PRO:HG3	55:SG0:222:TRP:HE1	1.63	0.64
55:SG0:147:PHE:HZ	55:SG0:160:LYS:CE	2.02	0.64
37:LW0:99:LYS:HG2	37:LW0:102:LYS:NZ	2.13	0.64
42:S60:1066:G:C6	60:SK0:58:PHE:CZ	2.84	0.64
42:S60:1091:A:O4’	65:SP0:146:HIS:HD2	1.81	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SGG:65:PHE:HZ	67:SR0:29:TYR:HH	1.42	0.64
34:LT0:5:HIS:HA	34:LT0:9:ARG:HD2	1.80	0.64
1:L50:1691:A:C6	42:S60:1248:G:C4’	2.80	0.64
68:SS0:24:PHE:O	68:SS0:25:ASN:OD1	2.15	0.64
48:SCC:50:LEU:CD1	53:SF0:26:ILE:HD12	2.28	0.63
48:SCC:50:LEU:HD13	53:SF0:26:ILE:HD12	1.80	0.63
53:SF0:96:GLY:O	75:SZ0:108:LEU:HD23	1.97	0.63
20:LJ0:107:ILE:HD11	20:LJ0:113:TYR:CD1	2.33	0.63
37:LW0:99:LYS:HG2	37:LW0:102:LYS:HE2	1.80	0.63
41:MD1:52:LYS:HG3	42:S60:606:G:C2	2.32	0.63
1:L50:1694:U:O4	42:S60:1249:U:H4’	1.98	0.63
43:SA0:140:VAL:O	43:SA0:141:ASN:OD1	2.17	0.63
49:SD0:184:ILE:HD11	49:SD0:230:MET:SD	2.39	0.63
43:SA0:70:ASN:ND2	47:SC0:240:ILE:CG1	2.61	0.63
43:SA0:206:ARG:NE	67:SR0:86:PRO:CG	2.62	0.63
68:SS0:24:PHE:CE1	68:SS0:107:ILE:HG21	2.34	0.63
42:S60:1085:G:H5”	65:SP0:140:THR:HG21	1.81	0.63
49:SD0:33:ILE:HG21	70:SU0:26:LEU:HD21	1.79	0.63
37:LW0:99:LYS:HA	37:LW0:102:LYS:CD	2.27	0.63
42:S60:1105:G:H5”	42:S60:1105:G:C8	2.34	0.63
56:SGG:65:PHE:HZ	67:SR0:29:TYR:CZ	2.17	0.62
42:S60:1158:U:H4’	50:SDD:7:LYS:HE3	1.81	0.62
67:SR0:3:GLN:HG3	67:SR0:3:GLN:O	1.99	0.62
37:LW0:99:LYS:O	37:LW0:102:LYS:HG2	1.97	0.62
42:S60:1160:A:H2’	65:SP0:58:LYS:HD3	1.80	0.62
42:S60:1181:U:OP1	66:SQ0:142:TYR:HE2	1.82	0.61
37:LW0:83:PHE:CE1	37:LW0:84:PRO:HD2	2.34	0.61
42:S60:982:C:C3’	67:SR0:10:ARG:NH1	2.63	0.61
43:SA0:184:TYR:CE1	71:SV0:35:ARG:NH1	2.69	0.61
47:SC0:49:GLY:O	71:SV0:6:ARG:HD2	1.99	0.61
49:SD0:94:GLN:HE21	60:SK0:19:SER:CB	2.11	0.61
2:L70:26:C:OP1	8:LD0:62:THR:HG21	2.01	0.61
55:SG0:169:VAL:HG12	55:SG0:176:LYS:HE2	1.82	0.61
42:S60:1099:U:H1’	69:ST0:91:ASN:OD1	2.01	0.61
43:SA0:4:ARG:O	71:SV0:30:LEU:CD1	2.47	0.61
42:S60:924:U:H1’	42:S60:925:A:N7	2.16	0.61
43:SA0:52:LYS:HB3	67:SR0:109:TYR:CZ	2.35	0.61
48:SCC:58:ARG:NH1	64:SO0:101:ARG:NH2	2.49	0.61
42:S60:1166:A:O2’	68:SS0:90:TRP:O	2.19	0.61
43:SA0:118:GLU:OE2	47:SC0:31:THR:OG1	2.18	0.61
53:SF0:40:LEU:O	53:SF0:42:HIS:N	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:1143:A:H5’	68:SS0:36:LYS:HE3	1.84	0.60
43:SA0:52:LYS:CB	67:SR0:109:TYR:CE1	2.84	0.60
43:SA0:120:ARG:NH1	47:SC0:232:ILE:HG21	2.15	0.60
53:SF0:40:LEU:CD2	66:SQ0:43:PHE:HD1	2.12	0.60
62:SM0:67:SER:O	62:SM0:71:LYS:HG2	2.01	0.60
42:S60:856:U:O4	68:SS0:146:SER:HB3	2.02	0.60
42:S60:1034:A:H2’	42:S60:1035:C:H6	1.63	0.60
1:L50:2042:A:H61	1:L50:2054:U:H3	1.48	0.60
12:LF0:115:ASN:HD21	34:LT0:133:PRO:HB2	1.66	0.60
21:LJJ:90:ILE:HG22	21:LJJ:90:ILE:O	2.02	0.60
42:S60:705:A:N3	42:S60:706:G:O6	2.35	0.60
53:SF0:90:ILE:HG23	75:SZ0:58:ILE:CD1	2.32	0.60
62:SM0:15:LEU:HB3	62:SM0:122:PHE:HE2	1.67	0.60
42:S60:918:A:C8	42:S60:919:C:C5	2.90	0.59
43:SA0:102:ARG:H	43:SA0:102:ARG:CD	2.15	0.59
42:S60:988:A:H4’	43:SA0:105:PRO:HG2	1.83	0.59
43:SA0:51:ILE:HG13	67:SR0:105:MET:CE	2.30	0.59
43:SA0:215:TYR:O	67:SR0:84:PHE:CE2	2.51	0.59
68:SS0:24:PHE:O	68:SS0:25:ASN:CG	2.41	0.59
42:S60:924:U:H1’	42:S60:925:A:C5	2.36	0.59
42:S60:1144:G:H2’	42:S60:1145:G:H5’	1.84	0.59
49:SD0:94:GLN:HG2	60:SK0:20:ILE:HG23	1.84	0.59
50:SDD:12:LEU:HD11	65:SP0:75:ILE:HD13	1.84	0.59
10:LE0:23:ILE:CD1	11:LEE:79:ARG:HH12	2.16	0.59
42:S60:999:C:H2’	42:S60:1000:C:C6	2.37	0.59
43:SA0:18:GLN:HE22	67:SR0:96:VAL:HB	1.67	0.59
49:SD0:238:PRO:CA	67:SR0:19:ARG:NH1	2.63	0.59
37:LW0:99:LYS:HG2	37:LW0:102:LYS:CE	2.33	0.59
50:SDD:34:PHE:CE1	60:SK0:61:GLN:NE2	2.70	0.59
1:L50:733:A:O3’	12:LF0:124:LYS:NZ	2.35	0.59
43:SA0:67:SER:OG	71:SV0:40:LEU:HD21	2.01	0.59
42:S60:403:A:H2’	42:S60:404:C:C6	2.37	0.59
47:SC0:148:VAL:CG2	72:SW0:97:PHE:HE1	2.15	0.59
54:SFF:96:GLN:O	54:SFF:96:GLN:HG2	2.02	0.59
42:S60:405:A:H2’	42:S60:406:U:C6	2.38	0.59
47:SC0:148:VAL:CG2	72:SW0:97:PHE:CE1	2.86	0.59
50:SDD:8:TYR:CZ	65:SP0:72:ARG:CD	2.84	0.59
10:LE0:30:LEU:CD2	11:LEE:11:VAL:HG13	2.33	0.58
7:LCC:64:ILE:CG2	40:LZ0:39:LEU:HD11	2.32	0.58
37:LW0:83:PHE:CD1	37:LW0:84:PRO:CD	2.81	0.58
43:SA0:63:ARG:NH1	71:SV0:30:LEU:HG	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA0:70:ASN:CA	47:SC0:240:ILE:CD1	2.68	0.58
51:SE0:64:ILE:CD1	74:SY0:23:LEU:HD13	2.33	0.58
55:SG0:170:ASN:HD21	55:SG0:176:LYS:CD	2.15	0.58
42:S60:203:G:C2	51:SE0:33:THR:HG21	2.38	0.58
42:S60:945:G:OP1	49:SD0:211:LYS:HE3	2.03	0.58
12:LF0:188:LYS:HE3	31:LQ0:2:LEU:HD23	1.85	0.58
42:S60:999:C:H42	42:S60:1049:G:H1	1.52	0.58
42:S60:1007:U:C4	56:SGG:84:ASP:OD2	2.56	0.58
42:S60:187:A:H62	42:S60:194:U:H3	1.51	0.58
37:LW0:99:LYS:HA	37:LW0:102:LYS:HG2	1.85	0.58
42:S60:554:A:N3	72:SW0:103:THR:CG2	2.62	0.58
43:SA0:63:ARG:NH1	71:SV0:30:LEU:H	2.01	0.58
53:SF0:90:ILE:HG23	75:SZ0:58:ILE:HD13	1.86	0.58
37:LW0:99:LYS:CG	37:LW0:102:LYS:HE2	2.34	0.57
43:SA0:206:ARG:CZ	67:SR0:86:PRO:HG2	2.34	0.57
53:SF0:40:LEU:HD23	66:SQ0:43:PHE:CD1	2.38	0.57
68:SS0:55:ARG:HH22	69:ST0:32:ASN:HD22	1.51	0.57
42:S60:1107:U:H5”	69:ST0:43:GLU:HG2	1.86	0.57
42:S60:1125:G:H2’	42:S60:1126:A:O4’	2.03	0.57
43:SA0:102:ARG:HD2	43:SA0:102:ARG:N	2.16	0.57
43:SA0:120:ARG:NH1	47:SC0:232:ILE:HD13	2.19	0.57
51:SE0:152:PRO:HD2	55:SG0:219:TYR:CE1	2.40	0.57
44:SAA:69:TYR:HE2	64:SO0:90:LYS:O	1.86	0.57
37:LW0:95:ARG:HG2	37:LW0:99:LYS:HE3	1.85	0.57
43:SA0:197:ARG:HB3	67:SR0:91:LEU:CB	2.34	0.57
42:S60:1091:A:O4’	65:SP0:146:HIS:CD2	2.57	0.57
43:SA0:66:CYS:HB2	71:SV0:28:VAL:HG21	1.86	0.57
42:S60:1160:A:H5’	65:SP0:133:ARG:NH2	2.20	0.56
42:S60:203:G:H21	51:SE0:33:THR:HG21	1.70	0.56
1:L50:2596:G:O2’	5:LB0:173:PRO:HG2	2.04	0.56
42:S60:1108:C:H5”	69:ST0:44:THR:O	2.05	0.56
42:S60:1230:U:H4’	44:SAA:88:SER:HB3	1.88	0.56
43:SA0:51:ILE:N	67:SR0:105:MET:SD	2.77	0.56
42:S60:864:A:N7	65:SP0:118:ARG:NH2	2.53	0.56
42:S60:923:A:H5’	42:S60:924:U:C4	2.40	0.56
42:S60:982:C:C4’	67:SR0:10:ARG:NH1	2.68	0.56
1:L50:1405:G:H2’	1:L50:1406:G:C8	2.39	0.56
37:LW0:98:ASN:HD22	55:SG0:146:GLY:C	2.08	0.56
49:SD0:237:LEU:O	67:SR0:19:ARG:CZ	2.53	0.56
1:L50:1691:A:C6	42:S60:1248:G:C1’	2.87	0.56
42:S60:1290:G:H8	42:S60:1290:G:H5”	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA0:52:LYS:CD	67:SR0:109:TYR:CE1	2.87	0.56
43:SA0:63:ARG:NE	71:SV0:30:LEU:CG	2.64	0.56
43:SA0:206:ARG:CD	67:SR0:86:PRO:HG2	2.35	0.56
53:SF0:118:ARG:HD2	53:SF0:125:MET:CB	2.34	0.56
41:MD1:106:TYR:CE2	41:MD1:108:GLU:HA	2.41	0.56
42:S60:1007:U:O4	56:SGG:84:ASP:OD2	2.23	0.56
43:SA0:215:TYR:CA	67:SR0:84:PHE:CE2	2.87	0.56
50:SDD:12:LEU:HD21	65:SP0:67:PHE:CE2	2.41	0.56
42:S60:1066:G:C6	60:SK0:58:PHE:CE1	2.94	0.56
42:S60:852:A:H2'	42:S60:853:G:C8	2.41	0.55
55:SG0:170:ASN:HD21	55:SG0:176:LYS:CE	2.19	0.55
1:L50:796:C:H5'	34:LT0:131:ARG:HE	1.70	0.55
42:S60:171:U:H5'	42:S60:172:U:H2'	1.88	0.55
43:SA0:70:ASN:HB2	47:SC0:240:ILE:HG13	1.76	0.55
42:S60:856:U:O4	68:SS0:146:SER:CB	2.54	0.55
42:S60:1066:G:C5	60:SK0:58:PHE:CE1	2.95	0.55
42:S60:1055:A:O3'	47:SC0:84:ALA:HB1	2.07	0.55
42:S60:1160:A:OP1	65:SP0:133:ARG:NH1	2.39	0.55
47:SC0:230:ASN:HB2	71:SV0:24:GLN:NE2	2.20	0.55
42:S60:932:A:H2'	42:S60:933:G:C8	2.42	0.55
42:S60:1084:G:O3'	65:SP0:99:ARG:HD3	2.06	0.55
50:SDD:12:LEU:HD12	65:SP0:75:ILE:HG21	1.86	0.55
42:S60:958:A:H3'	42:S60:959:G:N2	2.16	0.55
42:S60:1089:G:O4'	65:SP0:141:ARG:HD3	2.06	0.55
43:SA0:67:SER:HB2	71:SV0:28:VAL:HG13	1.88	0.55
51:SE0:54:VAL:HG22	74:SY0:23:LEU:HD11	1.88	0.55
42:S60:1150:G:H2'	42:S60:1151:A:C8	2.42	0.55
43:SA0:68:ILE:HD12	43:SA0:121:LEU:HD22	1.89	0.55
47:SC0:130:PRO:HG2	71:SV0:4:PHE:CE1	2.42	0.55
47:SC0:229:LEU:HD12	71:SV0:42:ILE:HG12	1.89	0.55
37:LW0:83:PHE:CG	55:SG0:144:LYS:HG3	2.42	0.54
43:SA0:10:ASP:CG	67:SR0:112:ASN:HD21	2.10	0.54
48:SCC:44:PRO:O	53:SF0:133:SER:CB	2.55	0.54
50:SDD:7:LYS:HA	65:SP0:67:PHE:O	2.07	0.54
4:LAA:70:THR:HG21	19:LII:6:LEU:HG	1.88	0.54
43:SA0:197:ARG:CB	67:SR0:91:LEU:CB	2.86	0.54
53:SF0:153:THR:HG21	53:SF0:160:LEU:HD13	1.88	0.54
42:S60:1181:U:OP1	66:SQ0:142:TYR:CE2	2.61	0.54
1:L50:1940:C:H2'	1:L50:1941:A:C8	2.42	0.54
2:L70:60:A:H5'	8:LD0:273:LYS:HG2	1.88	0.54
43:SA0:67:SER:HG	71:SV0:40:LEU:HD22	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:275:A:N6	6:LC0:163:ILE:CD1	2.71	0.54
37:LW0:83:PHE:CG	55:SG0:144:LYS:HB3	2.43	0.54
42:S60:1056:A:H5’	47:SC0:84:ALA:HA	1.89	0.54
42:S60:1208:G:OP2	66:SQ0:127:LYS:HE3	2.07	0.54
10:LE0:30:LEU:HD22	11:LEE:11:VAL:HG13	1.89	0.54
42:S60:932:A:H3’	42:S60:933:G:H8	1.73	0.54
50:SDD:34:PHE:CZ	60:SK0:61:GLN:HG2	2.43	0.54
63:SN0:123:TYR:OH	63:SN0:141:PRO:HG2	2.07	0.54
68:SS0:24:PHE:CZ	68:SS0:107:ILE:HG12	2.42	0.54
42:S60:288:A:H5”	58:SI0:25:ARG:NH2	2.23	0.54
43:SA0:117:ARG:NH1	47:SC0:243:GLU:CD	2.48	0.54
67:SR0:103:MET:HE1	67:SR0:117:LEU:HG	1.90	0.54
42:S60:1066:G:N7	60:SK0:58:PHE:CG	2.76	0.54
44:SAA:47:ALA:CB	48:SCC:61:ARG:NE	2.61	0.54
49:SD0:188:GLN:N	49:SD0:189:PRO:HD2	2.23	0.54
42:S60:982:C:C3’	67:SR0:10:ARG:HH11	2.22	0.53
37:LW0:83:PHE:CG	55:SG0:144:LYS:CG	2.90	0.53
42:S60:982:C:C4’	67:SR0:10:ARG:HH11	2.21	0.53
42:S60:1010:G:OP1	70:SU0:52:LYS:NZ	2.39	0.53
49:SD0:237:LEU:HD21	67:SR0:40:GLU:OE2	2.08	0.53
49:SD0:36:ARG:NH1	70:SU0:112:GLU:CD	2.62	0.53
49:SD0:94:GLN:NE2	60:SK0:19:SER:OG	2.42	0.53
24:LM0:70:ASP:O	24:LM0:71:ILE:HG12	2.09	0.53
43:SA0:51:ILE:HG13	67:SR0:105:MET:HE3	1.91	0.53
47:SC0:130:PRO:HG2	71:SV0:4:PHE:HE1	1.74	0.53
74:SY0:116:ARG:NH2	74:SY0:120:LYS:HZ1	2.06	0.53
42:S60:1007:U:C5	56:SGG:84:ASP:OD2	2.62	0.53
68:SS0:28:ILE:CD1	68:SS0:40:THR:HB	2.39	0.53
1:L50:2198:G:H1	1:L50:2226:U:H3	1.54	0.53
37:LW0:98:ASN:HD22	55:SG0:147:PHE:CA	2.15	0.53
1:L50:22:U:OP2	39:LY0:11:ARG:NH1	2.39	0.53
1:L50:1738:G:N3	42:S60:1306:A:H2	2.06	0.53
1:L50:1880:U:H3	1:L50:1938:A:H61	1.56	0.53
42:S60:132:C:H3’	42:S60:133:A:H8	1.72	0.53
20:LJ0:82:LYS:HB2	65:SP0:30:PHE:HE2	1.65	0.53
37:LW0:83:PHE:CD2	55:SG0:144:LYS:HB3	2.44	0.53
42:S60:918:A:N7	42:S60:919:C:C4	2.77	0.53
42:S60:1023:A:P	67:SR0:3:GLN:CD	2.87	0.53
42:S60:1023:A:H5”	67:SR0:3:GLN:HG2	1.90	0.53
43:SA0:51:ILE:HD12	67:SR0:105:MET:CG	2.32	0.53
42:S60:1108:C:H4’	69:ST0:46:PRO:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
56:SGG:105:ARG:HH21	67:SR0:36:ILE:HG22	1.73	0.53
1:L50:1169:C:H1’	1:L50:1170:A:H8	1.73	0.52
42:S60:1090:C:O2	65:SP0:146:HIS:CE1	2.62	0.52
42:S60:1160:A:OP1	65:SP0:62:SER:OG	2.22	0.52
42:S60:1167:C:H2’	42:S60:1168:A:O4’	2.08	0.52
43:SA0:120:ARG:CZ	47:SC0:232:ILE:HG21	2.39	0.52
42:S60:372:A:C4	59:SJ0:2:VAL:HG21	2.45	0.52
48:SCC:43:GLY:HA3	53:SF0:133:SER:OG	2.09	0.52
1:L50:796:C:H4’	34:LT0:131:ARG:O	2.10	0.52
37:LW0:98:ASN:ND2	55:SG0:146:GLY:C	2.63	0.52
42:S60:167:G:H21	42:S60:173:A:H2	1.55	0.52
42:S60:244:U:H2’	42:S60:245:A:C8	2.44	0.52
42:S60:932:A:H3’	42:S60:933:G:C8	2.44	0.52
42:S60:886:C:O2’	50:SDD:26:THR:HB	2.08	0.52
51:SE0:137:PRO:HG3	55:SG0:222:TRP:NE1	2.23	0.52
68:SS0:24:PHE:CE1	68:SS0:107:ILE:CG2	2.92	0.52
10:LE0:11:ILE:HD11	11:LEE:92:LEU:HD23	1.90	0.52
42:S60:203:G:N2	51:SE0:33:THR:HG21	2.25	0.52
48:SCC:44:PRO:O	53:SF0:133:SER:HB2	2.09	0.52
53:SF0:40:LEU:HD23	66:SQ0:43:PHE:HE1	1.73	0.52
55:SG0:176:LYS:HD2	55:SG0:176:LYS:N	2.25	0.52
68:SS0:139:VAL:O	68:SS0:139:VAL:CG1	2.57	0.52
12:LF0:69:LYS:HD3	34:LT0:141:GLU:HG2	1.91	0.52
42:S60:864:A:C8	65:SP0:118:ARG:NH2	2.77	0.52
12:LF0:70:ILE:HG12	34:LT0:144:MET:HG3	1.92	0.52
37:LW0:81:ARG:HH12	55:SG0:148:SER:HB2	1.74	0.52
42:S60:1181:U:H4’	66:SQ0:140:LYS:O	2.09	0.52
53:SF0:92:GLU:HG3	75:SZ0:108:LEU:CD1	2.40	0.52
64:SO0:27:HIS:CE1	64:SO0:36:THR:HG23	2.45	0.52
3:LA0:89:LEU:HD13	30:LPP:83:ILE:CD1	2.39	0.52
37:LW0:83:PHE:CG	37:LW0:84:PRO:CD	2.92	0.52
42:S60:1056:A:P	47:SC0:84:ALA:HB1	2.49	0.52
37:LW0:99:LYS:C	37:LW0:102:LYS:HG2	2.30	0.52
43:SA0:184:TYR:CZ	71:SV0:35:ARG:HD3	2.44	0.52
1:L50:290:C:O3’	39:LY0:33:PRO:HG3	2.09	0.52
1:L50:401:A:N1	6:LC0:80:THR:HG22	2.24	0.52
2:L70:27:A:OP2	8:LD0:62:THR:CG2	2.57	0.52
1:L50:2596:G:H5’	1:L50:2597:G:H5”	1.92	0.51
12:LF0:115:ASN:ND2	34:LT0:133:PRO:HB2	2.24	0.51
1:L50:555:G:H1’	6:LC0:71:ARG:HH11	1.75	0.51
43:SA0:18:GLN:HE22	67:SR0:96:VAL:CB	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SA0:63:ARG:CD	71:SV0:30:LEU:HG	2.39	0.51
50:SDD:12:LEU:HD13	65:SP0:75:ILE:CG2	2.41	0.51
59:SJ0:100:GLU:OE1	59:SJ0:103:LEU:HD12	2.11	0.51
43:SA0:215:TYR:C	67:SR0:84:PHE:HE2	2.14	0.51
53:SF0:40:LEU:HD21	66:SQ0:43:PHE:HD1	1.76	0.51
1:L50:1942:U:H2'	1:L50:1943:C:C5	2.46	0.51
34:LT0:112:ASN:C	34:LT0:112:ASN:HD22	2.12	0.51
42:S60:823:A:H2'	42:S60:824:A:H8	1.73	0.51
1:L50:1131:U:H3	1:L50:1135:G:H1	1.57	0.51
37:LW0:99:LYS:HA	37:LW0:102:LYS:CG	2.40	0.51
41:MD1:42:LEU:HG	41:MD1:73:ILE:HD11	1.91	0.51
42:S60:1143:A:C4	68:SS0:36:LYS:HB2	2.46	0.51
42:S60:1152:G:OP1	65:SP0:36:LYS:NZ	2.37	0.51
1:L50:2544:U:OP1	5:LB0:375:THR:HG22	2.11	0.51
4:LAA:74:ASN:HD22	4:LAA:112:GLY:H	1.59	0.51
42:S60:966:G:H2'	42:S60:967:A:C8	2.46	0.51
33:LS0:14:ASP:CG	33:LS0:15:ASP:H	2.15	0.50
41:MD1:33:ASN:ND2	64:SO0:56:TYR:CE2	2.80	0.50
42:S60:995:A:H2'	42:S60:996:G:O4'	2.10	0.50
42:S60:1315:A:C2	42:S60:1316:A:N6	2.79	0.50
43:SA0:51:ILE:CD1	67:SR0:105:MET:CE	2.89	0.50
45:SB0:53:THR:CG2	64:SO0:32:THR:OG1	2.58	0.50
56:SGG:65:PHE:CE2	67:SR0:29:TYR:CZ	2.99	0.50
1:L50:1328:A:H62	1:L50:1367:A:H61	1.59	0.50
53:SF0:92:GLU:CG	75:SZ0:108:LEU:HD12	2.41	0.50
56:SGG:105:ARG:HH22	67:SR0:37:ASP:CB	2.24	0.50
1:L50:396:G:N3	1:L50:396:G:H5"	2.26	0.50
42:S60:139:C:O3'	55:SG0:95:LYS:NZ	2.45	0.50
42:S60:1066:G:N7	60:SK0:58:PHE:CD1	2.79	0.50
51:SE0:70:ILE:HD13	51:SE0:92:ILE:HG12	1.92	0.50
1:L50:562:U:H5"	1:L50:562:U:H6	1.76	0.50
42:S60:834:G:H5'	44:SAA:85:ARG:HD2	1.93	0.50
47:SC0:216:PHE:HZ	72:SW0:128:TYR:HD1	1.59	0.50
68:SS0:10:PHE:HD1	75:SZ0:81:PHE:CD2	2.30	0.50
45:SB0:71:ARG:HB3	64:SO0:32:THR:HG21	1.93	0.50
1:L50:1089:U:H2'	1:L50:1090:A:C8	2.47	0.50
42:S60:923:A:H5'	42:S60:924:U:N3	2.27	0.50
42:S60:926:G:H2'	42:S60:927:G:N7	2.26	0.50
42:S60:1167:C:H4'	68:SS0:91:MET:O	2.12	0.50
43:SA0:52:LYS:HD2	67:SR0:109:TYR:CD1	2.47	0.50
3:LA0:88:GLU:HG2	30:LPP:87:LYS:HE2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
42:S60:55:G:H5'	74:SY0:123:ARG:HH11	1.77	0.50
42:S60:832:A:H2'	42:S60:833:A:C8	2.47	0.50
55:SG0:170:ASN:ND2	55:SG0:176:LYS:HD3	2.22	0.50
56:SGG:65:PHE:HE2	67:SR0:29:TYR:CD2	2.29	0.50
1:L50:1601:A:H4'	3:LA0:170:LEU:O	2.11	0.49
37:LW0:99:LYS:CA	37:LW0:102:LYS:HG2	2.42	0.49
42:S60:1149:U:C5	68:SS0:140:ARG:NH2	2.79	0.49
42:S60:1216:U:H2'	42:S60:1217:G:C8	2.47	0.49
42:S60:1019:C:H2'	42:S60:1020:G:C8	2.47	0.49
47:SC0:229:LEU:HB2	71:SV0:42:ILE:HD11	1.94	0.49
10:LE0:23:ILE:HD11	11:LEE:79:ARG:NH1	2.21	0.49
53:SF0:90:ILE:O	53:SF0:94:VAL:HG23	2.12	0.49
1:L50:2473:G:OP1	16:LH0:72:LYS:HG3	2.12	0.49
42:S60:1124:A:H2'	42:S60:1125:G:C8	2.46	0.49
42:S60:1160:A:C2'	65:SP0:58:LYS:HD3	2.41	0.49
1:L50:1441:U:H4'	38:LX0:64:ILE:HD11	1.95	0.49
1:L50:2051:C:C6	20:LJ0:56:ILE:HD11	2.48	0.49
67:SR0:36:ILE:HD11	67:SR0:44:LYS:NZ	2.27	0.49
70:SU0:116:THR:C	70:SU0:117:LEU:HG	2.32	0.49
49:SD0:34:LYS:HE3	70:SU0:60:PHE:HB3	1.93	0.49
42:S60:1083:U:O2'	65:SP0:97:ASN:ND2	2.46	0.49
49:SD0:237:LEU:O	67:SR0:19:ARG:NH1	2.45	0.49
53:SF0:6:THR:CG2	66:SQ0:53:LYS:HZ1	2.23	0.49
53:SF0:158:LYS:HA	75:SZ0:62:THR:HG21	1.95	0.49
1:L50:2108:U:H6	1:L50:2108:U:H5"	1.78	0.49
42:S60:917:U:H5'	42:S60:918:A:N3	2.27	0.49
42:S60:1066:G:O6	60:SK0:58:PHE:CE2	2.66	0.49
54:SFF:99:LYS:HE2	54:SFF:102:ILE:CG1	2.40	0.49
56:SGG:105:ARG:HH22	67:SR0:37:ASP:HB2	1.78	0.49
56:SGG:121:THR:HG21	56:SGG:131:TRP:CH2	2.47	0.49
42:S60:999:C:H2'	42:S60:1000:C:H6	1.76	0.49
16:LH0:63:GLU:OE2	27:LO0:131:ILE:HG21	2.13	0.49
1:L50:2447:A:H5"	1:L50:2447:A:H8	1.78	0.48
42:S60:65:A:H62	42:S60:75:G:H21	1.60	0.48
42:S60:377:C:OP1	59:SJ0:150:PRO:HD2	2.13	0.48
42:S60:995:A:C2'	42:S60:996:G:H5'	2.43	0.48
42:S60:1126:A:H8	42:S60:1164:G:H21	1.61	0.48
56:SGG:105:ARG:NH2	67:SR0:36:ILE:HG22	2.28	0.48
1:L50:399:G:O6	6:LC0:57:ARG:NH1	2.46	0.48
1:L50:486:U:H2'	1:L50:487:A:C8	2.48	0.48
14:LG0:17:ARG:NH1	26:LN0:32:GLN:HE22	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:237:A:C5'	58:SI0:48:VAL:HG13	2.43	0.48
42:S60:899:A:O2'	60:SK0:50:SER:OG	2.18	0.48
45:SB0:71:ARG:HB3	64:SO0:32:THR:CG2	2.43	0.48
47:SC0:166:LYS:CE	59:SJ0:100:GLU:OE2	2.61	0.48
51:SE0:92:ILE:HG22	51:SE0:94:LYS:O	2.13	0.48
75:SZ0:41:VAL:HG21	75:SZ0:78:LEU:HD22	1.93	0.48
1:L50:1691:A:C2	42:S60:1317:G:N2	2.81	0.48
3:LA0:238:LYS:HZ3	42:S60:714:U:P	2.37	0.48
42:S60:126:C:H2'	42:S60:127:A:C8	2.48	0.48
42:S60:236:U:O2	58:SI0:5:ARG:NH1	2.46	0.48
42:S60:1091:A:C8	65:SP0:146:HIS:CD2	3.01	0.48
1:L50:1424:A:H5'	15:LGG:77:GLY:HA3	1.94	0.48
53:SF0:96:GLY:C	75:SZ0:108:LEU:HD21	2.34	0.48
1:L50:1643:G:H1	1:L50:1672:A:H61	1.61	0.48
42:S60:1208:G:C2'	42:S60:1209:C:H5'	2.44	0.48
42:S60:404:C:H4'	74:SY0:37:ASN:HA	1.95	0.48
44:SAA:47:ALA:HB2	48:SCC:61:ARG:HE	1.71	0.48
16:LH0:7:GLU:OE2	16:LH0:9:LYS:HE3	2.13	0.48
42:S60:1209:C:H2'	42:S60:1210:G:C8	2.49	0.48
42:S60:1262:A:H3'	42:S60:1263:A:H8	1.79	0.48
68:SS0:46:ASP:OD1	68:SS0:47:ARG:N	2.43	0.48
42:S60:1165:C:H2'	42:S60:1166:A:C8	2.48	0.48
53:SF0:6:THR:CG2	66:SQ0:53:LYS:NZ	2.74	0.48
42:S60:125:A:H2'	42:S60:126:C:C6	2.49	0.48
42:S60:662:U:H1'	63:SN0:52:ASN:ND2	2.29	0.48
42:S60:1260:G:H1	42:S60:1303:U:H3	1.61	0.48
1:L50:1325:G:H22	1:L50:1370:U:H3	1.62	0.47
41:MD1:52:LYS:HG3	42:S60:606:G:H22	1.78	0.47
42:S60:911:G:H8	42:S60:911:G:OP2	1.97	0.47
50:SDD:8:TYR:CE2	65:SP0:72:ARG:NE	2.82	0.47
42:S60:1068:U:H5'	49:SD0:207:ILE:HD11	1.96	0.47
43:SA0:215:TYR:CA	67:SR0:84:PHE:HE2	2.26	0.47
47:SC0:230:ASN:N	71:SV0:24:GLN:NE2	2.45	0.47
1:L50:1609:G:N2	1:L50:1614:G:O2'	2.47	0.47
42:S60:1151:A:C2	42:S60:1152:G:H1'	2.49	0.47
43:SA0:52:LYS:HB2	67:SR0:109:TYR:CE2	2.49	0.47
49:SD0:68:HIS:NE2	70:SU0:109:THR:O	2.47	0.47
50:SDD:43:TYR:CE2	70:SU0:62:CYS:HB2	2.49	0.47
42:S60:999:C:H2'	42:S60:1000:C:O4'	2.14	0.47
1:L50:1878:G:H2'	1:L50:1879:A:C8	2.50	0.47
42:S60:997:A:H3'	42:S60:998:U:C5	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD0:215:LYS:HE2	8:LD0:222:PHE:CE2	2.49	0.47
42:S60:1140:G:H5'	42:S60:1143:A:N7	2.29	0.47
43:SA0:215:TYR:CD1	67:SR0:84:PHE:CZ	3.01	0.47
47:SC0:216:PHE:HZ	72:SW0:128:TYR:CD1	2.33	0.47
47:SC0:233:LEU:HD13	71:SV0:26:ASN:ND2	2.30	0.47
55:SG0:144:LYS:N	55:SG0:144:LYS:HD2	2.30	0.47
68:SS0:112:GLU:O	68:SS0:116:ARG:HG2	2.15	0.47
1:L50:2060:A:N3	1:L50:2060:A:H2'	2.30	0.47
1:L50:2116:A:H2'	1:L50:2117:A:C8	2.49	0.47
42:S60:932:A:C6	42:S60:933:G:C6	3.03	0.47
43:SA0:10:ASP:CB	67:SR0:112:ASN:HD21	2.28	0.47
43:SA0:118:GLU:CD	47:SC0:31:THR:OG1	2.51	0.47
47:SC0:50:HIS:O	71:SV0:6:ARG:NH2	2.48	0.47
1:L50:1869:A:H5'	26:LN0:24:ARG:HD2	1.96	0.47
1:L50:2109:G:H5"	1:L50:2109:G:C8	2.45	0.47
3:LA0:238:LYS:HD3	42:S60:714:U:H5'	1.96	0.47
20:LJ0:8:ASN:HD22	20:LJ0:149:GLN:HE22	1.61	0.47
42:S60:916:G:H5'	42:S60:916:G:H8	1.80	0.47
42:S60:967:A:O5'	42:S60:967:A:H8	1.97	0.47
42:S60:1168:A:H3'	42:S60:1169:G:H8	1.79	0.47
37:LW0:95:ARG:O	37:LW0:99:LYS:HG3	2.14	0.47
42:S60:1110:C:H5'	69:ST0:54:THR:HG22	1.97	0.47
46:SBB:24:PHE:CZ	72:SW0:51:ILE:HG23	2.49	0.47
68:SS0:10:PHE:CD1	75:SZ0:81:PHE:CD2	3.03	0.47
42:S60:349:A:OP1	51:SE0:57:ASN:ND2	2.48	0.46
42:S60:384:A:C2	59:SJ0:169:ARG:HB2	2.50	0.46
42:S60:910:A:H62	42:S60:922:G:N2	2.11	0.46
49:SD0:36:ARG:NH1	70:SU0:112:GLU:OE1	2.48	0.46
37:LW0:98:ASN:CG	55:SG0:147:PHE:HA	2.35	0.46
42:S60:909:G:O6	62:SM0:37:ARG:HB3	2.15	0.46
42:S60:1018:U:H4'	42:S60:1019:C:OP2	2.15	0.46
1:L50:303:C:H2'	1:L50:304:U:C6	2.51	0.46
42:S60:995:A:C8	42:S60:996:G:C8	3.03	0.46
42:S60:1012:A:HO2'	42:S60:1013:A:H8	1.61	0.46
42:S60:1035:C:H2'	42:S60:1036:A:H8	1.74	0.46
43:SA0:120:ARG:HE	47:SC0:232:ILE:HG22	1.75	0.46
47:SC0:233:LEU:HD13	71:SV0:26:ASN:CG	2.35	0.46
31:LQ0:21:ARG:HB3	31:LQ0:57:THR:HG21	1.98	0.46
10:LE0:39:ILE:HG22	13:LFF:107:ASN:ND2	2.30	0.46
42:S60:507:C:H2'	42:S60:508:A:C8	2.50	0.46
42:S60:958:A:OP1	47:SC0:111:ARG:CZ	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:970:U:H5"	42:S60:970:U:H6	1.80	0.46
42:S60:997:A:C2	42:S60:998:U:H1'	2.50	0.46
54:SFF:128:VAL:HG21	54:SFF:141:ARG:HE	1.80	0.46
42:S60:86:A:H1'	51:SE0:7:LYS:HD2	1.97	0.46
42:S60:131:U:H2'	42:S60:132:C:C6	2.51	0.46
1:L50:2140:A:O2'	1:L50:2141:U:H2'	2.15	0.46
42:S60:396:A:H2'	42:S60:397:A:C8	2.51	0.46
42:S60:964:G:N2	42:S60:966:G:H3'	2.31	0.46
42:S60:1085:G:C5'	65:SP0:140:THR:HG21	2.44	0.46
43:SA0:10:ASP:HB3	67:SR0:112:ASN:OD1	2.16	0.46
51:SE0:183:LEU:HD22	51:SE0:191:CYS:HB2	1.98	0.46
57:SH0:121:GLY:HA3	72:SW0:41:LYS:HG3	1.96	0.46
22:LL0:25:GLN:HB3	22:LL0:26:PRO:HD3	1.97	0.46
42:S60:466:C:H4'	73:SX0:100:GLU:HG2	1.97	0.46
42:S60:1194:U:H2'	42:S60:1196:U:C5	2.51	0.46
37:LW0:99:LYS:O	37:LW0:102:LYS:CG	2.64	0.46
41:MD1:52:LYS:CG	42:S60:606:G:N2	2.74	0.46
42:S60:1085:G:H4'	65:SP0:140:THR:CG2	2.46	0.46
42:S60:244:U:H2'	42:S60:245:A:H8	1.81	0.45
42:S60:517:U:H5'	51:SE0:219:SER:O	2.15	0.45
42:S60:989:G:H5'	43:SA0:104:ILE:HG23	1.98	0.45
63:SN0:66:VAL:HG23	63:SN0:67:THR:HG23	1.97	0.45
68:SS0:20:MET:CE	68:SS0:29:ASP:OD1	2.63	0.45
1:L50:1308:A:H61	1:L50:2434:A:H2	1.63	0.45
6:LC0:322:VAL:O	12:LF0:140:ARG:NH2	2.49	0.45
29:LP0:30:ARG:HD3	29:LP0:30:ARG:C	2.36	0.45
42:S60:706:G:N3	42:S60:706:G:C2'	2.74	0.45
42:S60:864:A:N1	65:SP0:118:ARG:HB2	2.31	0.45
42:S60:864:A:C4	65:SP0:118:ARG:HD3	2.52	0.45
43:SA0:63:ARG:CG	71:SV0:30:LEU:CD2	2.67	0.45
68:SS0:24:PHE:CE2	68:SS0:107:ILE:HG12	2.52	0.45
68:SS0:55:ARG:HH22	69:ST0:32:ASN:ND2	2.13	0.45
2:L70:1:A:H61	2:L70:118:U:H3	1.63	0.45
4:LAA:127:GLN:HE22	19:LII:7:ASN:H	1.63	0.45
6:LC0:103:VAL:HG13	22:LL0:23:PHE:CZ	2.52	0.45
10:LE0:11:ILE:HD12	11:LEE:91:ALA:HB1	1.99	0.45
37:LW0:83:PHE:HB2	55:SG0:144:LYS:HG3	1.97	0.45
42:S60:63:G:H2'	42:S60:76:A:C2	2.50	0.45
42:S60:864:A:C2	65:SP0:118:ARG:HB2	2.52	0.45
1:L50:2267:C:O2	1:L50:2267:C:O4'	2.33	0.45
42:S60:705:A:C2	42:S60:706:G:N1	2.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:1109:A:H2'	42:S60:1110:C:C6	2.52	0.45
43:SA0:85:LYS:NZ	67:SR0:82:GLU:OE2	2.48	0.45
49:SD0:239:ILE:CA	67:SR0:19:ARG:NH1	2.77	0.45
1:L50:1691:A:H61	42:S60:1248:G:C4'	2.25	0.45
42:S60:1010:G:OP1	70:SU0:52:LYS:CE	2.65	0.45
43:SA0:197:ARG:HD3	67:SR0:91:LEU:CB	2.46	0.45
42:S60:55:G:H5'	74:SY0:123:ARG:NH1	2.32	0.45
47:SC0:148:VAL:HG21	72:SW0:97:PHE:CE1	2.51	0.45
1:L50:1032:A:H8	1:L50:1032:A:H5"	1.82	0.45
29:LP0:70:THR:HG22	29:LP0:72:GLN:H	1.81	0.45
43:SA0:52:LYS:HB2	67:SR0:109:TYR:CD1	2.51	0.45
54:SFF:96:GLN:N	54:SFF:96:GLN:OE1	2.50	0.45
65:SP0:132:ARG:NH2	68:SS0:127:LEU:HD22	2.32	0.45
42:S60:171:U:H5'	42:S60:172:U:H6	1.82	0.45
42:S60:1121:A:H3'	42:S60:1122:A:H8	1.82	0.45
49:SD0:34:LYS:HD3	70:SU0:62:CYS:HB3	1.98	0.45
1:L50:188:G:OP2	4:LAA:34:LYS:HG2	2.17	0.45
42:S60:661:A:H5'	63:SN0:15:VAL:O	2.17	0.45
43:SA0:64:MET:HB3	71:SV0:27:MET:CG	2.28	0.45
47:SC0:50:HIS:HA	71:SV0:6:ARG:HD2	1.98	0.45
1:L50:202:G:O2'	17:LHH:105:THR:HG22	2.16	0.44
2:L70:70:U:H3	2:L70:105:G:H1	1.65	0.44
34:LT0:126:PRO:HB2	34:LT0:128:LEU:CD2	2.47	0.44
42:S60:1082:A:H2'	42:S60:1083:U:C6	2.52	0.44
43:SA0:218:GLN:HB3	67:SR0:84:PHE:CE2	2.51	0.44
48:SCC:45:ILE:HG12	53:SF0:133:SER:HB3	1.99	0.44
51:SE0:175:LEU:HD22	51:SE0:222:PHE:CD1	2.52	0.44
42:S60:478:C:O2	61:SL0:93:LYS:HE2	2.17	0.44
43:SA0:117:ARG:CZ	47:SC0:243:GLU:OE2	2.65	0.44
74:SY0:116:ARG:CZ	74:SY0:120:LYS:NZ	2.80	0.44
12:LF0:69:LYS:HG3	34:LT0:142:MET:O	2.17	0.44
24:LM0:71:ILE:O	24:LM0:71:ILE:HG13	2.18	0.44
42:S60:997:A:H3'	42:S60:998:U:C6	2.53	0.44
42:S60:1167:C:H4'	68:SS0:91:MET:C	2.38	0.44
47:SC0:130:PRO:CB	71:SV0:4:PHE:CE1	2.98	0.44
35:LU0:39:ILE:HG23	35:LU0:48:LEU:HD21	2.00	0.44
47:SC0:148:VAL:HG21	72:SW0:97:PHE:CZ	2.53	0.44
64:SO0:27:HIS:HE1	64:SO0:36:THR:HG23	1.82	0.44
1:L50:1885:G:H1	1:L50:1933:C:H42	1.66	0.44
42:S60:431:G:H2'	42:S60:445:U:N3	2.32	0.44
42:S60:662:U:H1'	63:SN0:52:ASN:HD21	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:2416:G:H5"	1:L50:2416:G:H8	1.82	0.44
6:LC0:328:ILE:HG13	12:LF0:53:ILE:HG22	1.99	0.44
43:SA0:214:LEU:HD13	67:SR0:86:PRO:HG3	2.00	0.44
50:SDD:16:PHE:HE1	65:SP0:66:GLY:HA3	1.82	0.44
58:SI0:69:THR:HG21	61:SL0:22:TYR:CE2	2.52	0.44
1:L50:158:A:N6	1:L50:168:G:H1'	2.32	0.44
5:LB0:133:LEU:H	5:LB0:133:LEU:HG	1.69	0.44
42:S60:1144:G:O2'	42:S60:1145:G:H5'	2.17	0.44
42:S60:1199:C:OP2	50:SDD:41:ARG:NH2	2.47	0.44
1:L50:2551:C:H2'	1:L50:2552:G:O4'	2.18	0.43
17:LHH:113:LYS:HE2	22:LL0:46:ASN:HD22	1.83	0.43
41:MD1:17:ILE:HD12	41:MD1:95:TYR:CD2	2.53	0.43
43:SA0:63:ARG:CD	71:SV0:30:LEU:CG	2.95	0.43
67:SR0:36:ILE:HD11	67:SR0:44:LYS:HZ2	1.83	0.43
26:LN0:14:LYS:HE2	26:LN0:120:TRP:CZ3	2.53	0.43
41:MD1:106:TYR:HE2	41:MD1:108:GLU:HA	1.83	0.43
42:S60:1107:U:H2'	42:S60:1108:C:C6	2.53	0.43
42:S60:1230:U:O3'	44:SAA:88:SER:HA	2.18	0.43
3:LA0:238:LYS:NZ	42:S60:714:U:H5"	2.32	0.43
27:LO0:84:LYS:HE2	27:LO0:89:HIS:CD2	2.54	0.43
42:S60:1085:G:OP1	65:SP0:99:ARG:NE	2.46	0.43
42:S60:1149:U:C5	68:SS0:140:ARG:CZ	3.00	0.43
47:SC0:148:VAL:HG22	72:SW0:94:SER:HB2	2.00	0.43
47:SC0:167:GLY:HA3	59:SJ0:103:LEU:O	2.17	0.43
49:SD0:30:ALA:HB2	70:SU0:60:PHE:CE2	2.53	0.43
68:SS0:24:PHE:CE2	68:SS0:79:ILE:HG21	2.53	0.43
70:SU0:116:THR:O	70:SU0:117:LEU:HG	2.18	0.43
1:L50:2525:G:H5'	29:LP0:71:PRO:HD3	2.00	0.43
1:L50:2462:A:H2'	1:L50:2463:A:C8	2.54	0.43
37:LW0:98:ASN:HD22	55:SG0:147:PHE:N	2.10	0.43
42:S60:50:U:H2'	42:S60:51:G:C8	2.54	0.43
42:S60:94:U:H3'	42:S60:263:A:H61	1.83	0.43
42:S60:933:G:H8	42:S60:933:G:O5'	2.02	0.43
72:SW0:26:ARG:O	72:SW0:26:ARG:HG2	2.18	0.43
74:SY0:116:ARG:NH1	74:SY0:120:LYS:HZ2	2.16	0.43
11:LEE:133:LEU:HG	11:LEE:133:LEU:O	2.19	0.43
14:LG0:174:PHE:CE2	14:LG0:178:ILE:HD11	2.53	0.43
44:SAA:51:ASP:OD2	48:SCC:57:GLU:C	2.57	0.43
42:S60:914:U:C5	42:S60:916:G:C5	3.06	0.43
42:S60:916:G:O3'	42:S60:917:U:O2	2.37	0.43
43:SA0:50:ASP:OD1	67:SR0:109:TYR:OH	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SE0:54:VAL:CG2	74:SY0:23:LEU:HD11	2.47	0.43
58:SI0:123:ASP:HB2	61:SL0:22:TYR:HE1	1.84	0.43
1:L50:21:U:H5'	1:L50:1087:G:OP1	2.19	0.43
1:L50:88:A:H5'	21:LJJ:75:ALA:HB2	2.01	0.43
1:L50:1089:U:H2'	1:L50:1090:A:H8	1.84	0.43
1:L50:1875:G:H2'	1:L50:1876:A:C8	2.53	0.43
42:S60:926:G:H2'	42:S60:927:G:C8	2.54	0.43
1:L50:555:G:H1'	6:LC0:71:ARG:NH1	2.34	0.43
6:LC0:2:SER:O	6:LC0:3:ARG:HG2	2.19	0.43
42:S60:173:A:N7	51:SE0:131:VAL:CG1	2.82	0.43
42:S60:218:A:H4'	42:S60:219:U:H5"	2.00	0.43
42:S60:1033:A:H2'	42:S60:1034:A:H5'	2.00	0.43
43:SA0:43:GLU:HG2	67:SR0:120:LYS:HE2	2.01	0.43
49:SD0:94:GLN:NE2	60:SK0:19:SER:HB3	2.32	0.43
58:SI0:69:THR:HG22	61:SL0:20:ASN:OD1	2.18	0.43
43:SA0:50:ASP:OD1	67:SR0:109:TYR:CE2	2.72	0.43
1:L50:597:A:H4'	63:SN0:123:TYR:CD1	2.53	0.42
4:LAA:144:VAL:HG21	22:LL0:163:TYR:O	2.19	0.42
47:SC0:166:LYS:O	59:SJ0:103:LEU:HB3	2.18	0.42
58:SI0:68:LYS:HE2	58:SI0:152:TYR:CD2	2.54	0.42
62:SM0:15:LEU:CB	62:SM0:122:PHE:HE2	2.31	0.42
1:L50:1933:C:H2'	1:L50:1934:C:C6	2.55	0.42
12:LF0:69:LYS:HD3	34:LT0:141:GLU:CG	2.49	0.42
37:LW0:67:HIS:HB2	42:S60:1282:A:N3	2.34	0.42
42:S60:705:A:H2'	42:S60:707:A:N7	2.34	0.42
1:L50:1325:G:H1	1:L50:1370:U:H3	1.67	0.42
1:L50:1441:U:H4'	38:LX0:64:ILE:CD1	2.49	0.42
5:LB0:265:ARG:NH1	27:LO0:62:SER:OG	2.53	0.42
42:S60:1107:U:H2'	42:S60:1108:C:H6	1.84	0.42
42:S60:1208:G:H2'	42:S60:1209:C:H5'	2.01	0.42
43:SA0:33:LEU:HD13	43:SA0:150:THR:HA	2.00	0.42
49:SD0:94:GLN:NE2	60:SK0:19:SER:CB	2.81	0.42
67:SR0:103:MET:SD	67:SR0:117:LEU:HG	2.59	0.42
1:L50:1691:A:H62	42:S60:1248:G:H4'	1.71	0.42
42:S60:517:U:C5'	51:SE0:219:SER:O	2.66	0.42
42:S60:790:G:H5"	42:S60:790:G:H8	1.84	0.42
49:SD0:34:LYS:CE	70:SU0:60:PHE:HB3	2.49	0.42
74:SY0:116:ARG:CZ	74:SY0:120:LYS:HZ2	2.33	0.42
42:S60:189:A:H2'	42:S60:190:A:H4'	2.01	0.42
42:S60:502:A:O3'	72:SW0:4:LYS:NZ	2.52	0.42
42:S60:696:G:H1	42:S60:712:A:H2	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:1160:A:P	65:SP0:62:SER:HG	2.41	0.42
42:S60:1262:A:C8	42:S60:1262:A:H5”	2.54	0.42
42:S60:1023:A:P	67:SR0:3:GLN:OE1	2.78	0.42
1:L50:145:A:H5”	21:LJJ:46:LYS:HD2	2.01	0.42
1:L50:1298:A:H5’	1:L50:1299:A:OP2	2.20	0.42
1:L50:2170:A:C8	28:LOO:54:PRO:HB3	2.55	0.42
17:LHH:6:LYS:HG3	17:LHH:7:ASP:OD1	2.19	0.42
42:S60:954:G:H5’	42:S60:980:G:OP1	2.20	0.42
47:SC0:130:PRO:CG	71:SV0:4:PHE:CE1	3.03	0.42
42:S60:1024:G:C2	42:S60:1025:G:C8	3.08	0.42
42:S60:1230:U:O3’	44:SAA:88:SER:CB	2.68	0.42
43:SA0:215:TYR:CE1	67:SR0:84:PHE:CZ	3.08	0.42
56:SGG:147:ASN:N	56:SGG:147:ASN:HD22	2.17	0.42
1:L50:32:G:H21	1:L50:377:A:H62	1.66	0.42
1:L50:1698:A:H1’	42:S60:1247:C:H1’	2.01	0.42
1:L50:1936:U:HO2’	1:L50:1937:G:H8	1.66	0.42
1:L50:2160:G:H5”	28:LOO:65:LYS:HD2	2.02	0.42
1:L50:2492:U:H2’	1:L50:2493:G:C8	2.55	0.42
1:L50:2573:U:H2’	1:L50:2574:A:C8	2.55	0.42
42:S60:864:A:C6	65:SP0:118:ARG:HB2	2.55	0.42
42:S60:1231:U:H4’	44:SAA:86:VAL:CG1	2.50	0.42
50:SDD:7:LYS:CA	65:SP0:67:PHE:O	2.68	0.42
57:SH0:53:LEU:HB3	57:SH0:54:PRO:HD3	2.02	0.42
63:SN0:128:TYR:HE1	63:SN0:132:LYS:HZ2	1.66	0.42
1:L50:1691:A:C2	42:S60:1248:G:H1’	2.55	0.42
17:LHH:66:LEU:HD12	38:LX0:22:ILE:HD11	2.01	0.42
31:LQ0:164:TYR:CE2	31:LQ0:177:ARG:HD2	2.55	0.42
47:SC0:228:GLU:O	71:SV0:42:ILE:HG21	2.20	0.42
1:L50:2610:U:H2’	1:L50:2611:C:C6	2.55	0.41
42:S60:132:C:H3’	42:S60:133:A:C8	2.53	0.41
42:S60:995:A:C3’	42:S60:996:G:H8	2.23	0.41
43:SA0:10:ASP:CB	67:SR0:112:ASN:OD1	2.67	0.41
28:LOO:64:LYS:HB3	28:LOO:64:LYS:HE2	1.92	0.41
42:S60:375:G:H8	42:S60:375:G:H5”	1.86	0.41
42:S60:1054:G:H2’	42:S60:1055:A:O4’	2.21	0.41
47:SC0:149:LYS:HB3	72:SW0:93:PRO:HA	2.01	0.41
65:SP0:132:ARG:CZ	68:SS0:127:LEU:HD22	2.50	0.41
1:L50:1296:C:H6	1:L50:1296:C:H5”	1.85	0.41
18:LI0:30:LYS:HE2	18:LI0:66:GLU:HG2	2.02	0.41
42:S60:830:G:O3’	42:S60:831:G:H8	2.02	0.41
42:S60:995:A:H2’	42:S60:996:G:H5’	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S60:996:G:H2'	42:S60:997:A:O4'	2.20	0.41
42:S60:1108:C:H5'	69:ST0:44:THR:OG1	2.20	0.41
49:SD0:184:ILE:HD12	49:SD0:215:MET:CE	2.50	0.41
42:S60:552:G:O2'	72:SW0:105:SER:HB3	2.20	0.41
42:S60:1262:A:H61	42:S60:1301:U:H3	1.68	0.41
53:SF0:49:THR:O	53:SF0:49:THR:HG22	2.20	0.41
61:SL0:144:ILE:HD13	61:SL0:147:LYS:HE2	2.03	0.41
62:SM0:15:LEU:C	62:SM0:15:LEU:HD12	2.41	0.41
1:L50:2026:G:C2	28:LOO:5:PRO:HG2	2.55	0.41
42:S60:924:U:H1'	42:S60:925:A:C8	2.55	0.41
43:SA0:184:TYR:CD2	71:SV0:35:ARG:HD3	2.54	0.41
1:L50:222:A:H2'	1:L50:223:A:C8	2.55	0.41
8:LD0:214:LEU:HD23	8:LD0:214:LEU:HA	1.94	0.41
42:S60:574:A:H1'	46:SBB:67:GLY:CA	2.51	0.41
42:S60:1168:A:H3'	42:S60:1169:G:C8	2.55	0.41
62:SM0:15:LEU:HB3	62:SM0:122:PHE:CE2	2.52	0.41
1:L50:1642:G:H2'	1:L50:1643:G:C8	2.56	0.41
1:L50:2211:A:H5"	1:L50:2212:G:N2	2.35	0.41
42:S60:156:U:H2'	42:S60:157:A:C8	2.55	0.41
1:L50:885:G:H5"	1:L50:885:G:H8	1.86	0.41
6:LC0:323:GLU:HG2	6:LC0:324:ILE:N	2.36	0.41
10:LE0:17:TYR:CE1	11:LEE:79:ARG:HD3	2.56	0.41
21:LJJ:40:PRO:O	38:LX0:3:LYS:HE3	2.21	0.41
37:LW0:102:LYS:HB3	55:SG0:150:ASP:HB3	2.03	0.41
42:S60:999:C:O2'	42:S60:1000:C:H5'	2.20	0.41
46:SBB:81:ILE:CD1	63:SN0:25:TYR:HB2	2.51	0.41
49:SD0:184:ILE:HD12	49:SD0:215:MET:HE3	2.03	0.41
1:L50:506:G:H2'	1:L50:508:A:N7	2.36	0.41
1:L50:1133:C:H4'	1:L50:1134:A:H5'	2.02	0.41
42:S60:967:A:H5"	42:S60:968:C:C6	2.55	0.41
42:S60:999:C:C4	42:S60:1000:C:C4	3.09	0.41
47:SC0:166:LYS:CB	59:SJ0:100:GLU:OE2	2.69	0.41
51:SE0:35:PRO:HD2	51:SE0:83:PRO:HG2	2.03	0.41
56:SGG:65:PHE:HZ	67:SR0:29:TYR:CE2	2.27	0.41
1:L50:763:U:H2'	1:L50:764:U:O4'	2.21	0.40
1:L50:2473:G:H2'	1:L50:2474:A:O4'	2.21	0.40
17:LHH:66:LEU:CD1	38:LX0:22:ILE:HD11	2.51	0.40
42:S60:933:G:C8	42:S60:933:G:O5'	2.74	0.40
73:SX0:41:ALA:HA	73:SX0:42:PRO:HD3	1.98	0.40
42:S60:1090:C:O2	65:SP0:146:HIS:HE1	2.02	0.40
44:SAA:51:ASP:OD2	48:SCC:58:ARG:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC0:230:ASN:CB	71:SV0:24:GLN:NE2	2.84	0.40
55:SG0:156:GLU:O	55:SG0:160:LYS:HG3	2.20	0.40
1:L50:158:A:H61	1:L50:168:G:H1'	1.87	0.40
1:L50:1940:C:H2'	1:L50:1941:A:H8	1.86	0.40
36:LV0:75:ARG:HH22	42:S60:1261:G:H5'	1.86	0.40
42:S60:1022:C:N3	42:S60:1024:G:C8	2.89	0.40
43:SA0:118:GLU:OE2	47:SC0:31:THR:CA	2.61	0.40
1:L50:885:G:H5"	1:L50:885:G:C8	2.56	0.40
14:LG0:16:PRO:HG2	26:LN0:32:GLN:HE21	1.86	0.40
16:LH0:129:THR:HG22	16:LH0:150:VAL:HG22	2.04	0.40
42:S60:405:A:H2'	42:S60:406:U:H6	1.84	0.40
42:S60:1023:A:H5"	67:SR0:3:GLN:CG	2.52	0.40
43:SA0:51:ILE:CG1	67:SR0:105:MET:CE	2.99	0.40
43:SA0:215:TYR:CG	67:SR0:84:PHE:CE2	3.05	0.40
53:SF0:95:THR:CG2	53:SF0:169:ILE:HG12	2.52	0.40
1:L50:101:C:H2'	1:L50:102:A:C8	2.56	0.40
1:L50:401:A:N1	6:LC0:80:THR:CG2	2.84	0.40
3:LA0:20:HIS:CD2	3:LA0:21:LYS:HG3	2.57	0.40
6:LC0:308:MET:HE3	12:LF0:155:LYS:HB3	2.02	0.40
42:S60:641:A:H2'	42:S60:642:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L50	2494/2618 (95%)	736 (29%)	0
2	L70	118/119 (99%)	36 (30%)	0
42	S60	1352/1368 (98%)	518 (38%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3964/4105 (96%)	1290 (32%)	0

All (1290) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L50	2	U
1	L50	3	A
1	L50	13	A
1	L50	15	G
1	L50	21	U
1	L50	22	U
1	L50	23	U
1	L50	24	G
1	L50	25	G
1	L50	31	G
1	L50	39	G
1	L50	43	G
1	L50	48	A
1	L50	51	A
1	L50	52	G
1	L50	59	A
1	L50	62	U
1	L50	63	G
1	L50	68	G
1	L50	70	A
1	L50	71	G
1	L50	73	A
1	L50	74	G
1	L50	75	C
1	L50	76	A
1	L50	77	G
1	L50	82	G
1	L50	87	C
1	L50	88	A
1	L50	98	A
1	L50	99	U
1	L50	100	A
1	L50	101	C
1	L50	113	G
1	L50	114	G
1	L50	118	A
1	L50	123	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	132	A
1	L50	135	A
1	L50	137	A
1	L50	151	G
1	L50	152	A
1	L50	157	A
1	L50	158	A
1	L50	159	A
1	L50	160	C
1	L50	165	G
1	L50	167	G
1	L50	169	A
1	L50	178	G
1	L50	181	G
1	L50	184	G
1	L50	186	G
1	L50	188	G
1	L50	191	A
1	L50	194	A
1	L50	201	A
1	L50	202	G
1	L50	204	C
1	L50	209	A
1	L50	210	G
1	L50	211	U
1	L50	212	G
1	L50	213	U
1	L50	214	A
1	L50	216	U
1	L50	221	A
1	L50	224	U
1	L50	225	G
1	L50	226	A
1	L50	233	G
1	L50	234	U
1	L50	237	A
1	L50	238	A
1	L50	239	A
1	L50	240	G
1	L50	241	G
1	L50	242	A
1	L50	246	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	247	G
1	L50	255	U
1	L50	258	G
1	L50	266	A
1	L50	267	G
1	L50	268	C
1	L50	273	C
1	L50	276	U
1	L50	277	A
1	L50	284	G
1	L50	285	A
1	L50	286	U
1	L50	287	A
1	L50	289	U
1	L50	298	G
1	L50	309	U
1	L50	311	C
1	L50	312	G
1	L50	314	U
1	L50	315	G
1	L50	316	A
1	L50	317	G
1	L50	330	G
1	L50	331	U
1	L50	332	A
1	L50	333	A
1	L50	340	G
1	L50	343	A
1	L50	345	G
1	L50	346	A
1	L50	347	G
1	L50	352	C
1	L50	353	A
1	L50	358	G
1	L50	366	G
1	L50	373	U
1	L50	382	A
1	L50	384	A
1	L50	385	C
1	L50	392	C
1	L50	396	G
1	L50	397	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	400	U
1	L50	416	A
1	L50	434	G
1	L50	438	A
1	L50	449	U
1	L50	450	C
1	L50	453	G
1	L50	454	C
1	L50	467	A
1	L50	478	A
1	L50	488	C
1	L50	495	A
1	L50	499	G
1	L50	503	A
1	L50	504	G
1	L50	507	G
1	L50	508	A
1	L50	509	A
1	L50	510	G
1	L50	517	A
1	L50	523	A
1	L50	524	G
1	L50	527	A
1	L50	530	A
1	L50	533	G
1	L50	534	A
1	L50	535	A
1	L50	536	A
1	L50	542	G
1	L50	556	A
1	L50	562	U
1	L50	563	U
1	L50	564	G
1	L50	567	A
1	L50	568	A
1	L50	569	C
1	L50	570	U
1	L50	580	U
1	L50	581	G
1	L50	587	A
1	L50	601	C
1	L50	612	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	618	G
1	L50	620	C
1	L50	625	U
1	L50	630	U
1	L50	631	G
1	L50	642	G
1	L50	643	C
1	L50	646	A
1	L50	647	A
1	L50	658	G
1	L50	659	G
1	L50	660	G
1	L50	661	G
1	L50	665	A
1	L50	667	G
1	L50	668	A
1	L50	675	G
1	L50	676	A
1	L50	684	A
1	L50	685	G
1	L50	688	G
1	L50	689	C
1	L50	695	C
1	L50	710	A
1	L50	711	U
1	L50	714	G
1	L50	715	G
1	L50	720	C
1	L50	726	C
1	L50	729	A
1	L50	732	G
1	L50	736	A
1	L50	739	A
1	L50	742	G
1	L50	749	A
1	L50	750	U
1	L50	763	U
1	L50	764	U
1	L50	765	A
1	L50	766	A
1	L50	767	G
1	L50	768	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	772	C
1	L50	776	C
1	L50	778	A
1	L50	779	A
1	L50	781	U
1	L50	782	G
1	L50	784	G
1	L50	795	U
1	L50	796	C
1	L50	801	A
1	L50	802	U
1	L50	803	G
1	L50	806	A
1	L50	816	G
1	L50	822	U
1	L50	828	A
1	L50	830	G
1	L50	834	G
1	L50	838	G
1	L50	840	C
1	L50	843	A
1	L50	848	A
1	L50	849	A
1	L50	852	A
1	L50	854	C
1	L50	858	G
1	L50	859	C
1	L50	865	G
1	L50	866	C
1	L50	867	U
1	L50	871	G
1	L50	877	A
1	L50	878	A
1	L50	879	U
1	L50	885	G
1	L50	889	G
1	L50	893	C
1	L50	900	A
1	L50	905	G
1	L50	910	A
1	L50	980	A
1	L50	990	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	998	U
1	L50	1001	A
1	L50	1002	U
1	L50	1010	A
1	L50	1017	A
1	L50	1018	U
1	L50	1021	G
1	L50	1022	A
1	L50	1023	U
1	L50	1024	G
1	L50	1030	U
1	L50	1032	A
1	L50	1033	G
1	L50	1034	C
1	L50	1037	G
1	L50	1050	U
1	L50	1053	C
1	L50	1055	A
1	L50	1056	C
1	L50	1061	G
1	L50	1062	A
1	L50	1070	G
1	L50	1075	A
1	L50	1082	G
1	L50	1085	G
1	L50	1087	G
1	L50	1089	U
1	L50	1090	A
1	L50	1096	A
1	L50	1099	G
1	L50	1100	C
1	L50	1102	G
1	L50	1105	C
1	L50	1111	G
1	L50	1117	A
1	L50	1118	G
1	L50	1120	G
1	L50	1121	A
1	L50	1123	A
1	L50	1124	A
1	L50	1130	C
1	L50	1131	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1133	C
1	L50	1134	A
1	L50	1135	G
1	L50	1136	C
1	L50	1142	A
1	L50	1144	A
1	L50	1148	A
1	L50	1149	G
1	L50	1150	G
1	L50	1151	A
1	L50	1155	G
1	L50	1163	U
1	L50	1169	C
1	L50	1170	A
1	L50	1171	U
1	L50	1172	A
1	L50	1173	A
1	L50	1175	A
1	L50	1177	G
1	L50	1181	G
1	L50	1182	A
1	L50	1183	G
1	L50	1189	U
1	L50	1191	U
1	L50	1192	A
1	L50	1193	A
1	L50	1194	G
1	L50	1196	G
1	L50	1213	A
1	L50	1217	A
1	L50	1218	A
1	L50	1221	A
1	L50	1224	A
1	L50	1231	U
1	L50	1232	G
1	L50	1233	A
1	L50	1235	A
1	L50	1236	U
1	L50	1237	U
1	L50	1243	G
1	L50	1247	G
1	L50	1250	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1252	G
1	L50	1254	C
1	L50	1256	U
1	L50	1257	A
1	L50	1264	C
1	L50	1267	G
1	L50	1268	U
1	L50	1269	A
1	L50	1270	U
1	L50	1274	C
1	L50	1277	G
1	L50	1278	U
1	L50	1282	C
1	L50	1283	A
1	L50	1284	C
1	L50	1296	C
1	L50	1299	A
1	L50	1304	A
1	L50	1305	A
1	L50	1308	A
1	L50	1309	C
1	L50	1317	G
1	L50	1318	U
1	L50	1327	A
1	L50	1332	G
1	L50	1333	A
1	L50	1340	A
1	L50	1341	G
1	L50	1342	A
1	L50	1346	A
1	L50	1350	U
1	L50	1355	C
1	L50	1356	G
1	L50	1359	G
1	L50	1361	G
1	L50	1362	G
1	L50	1374	U
1	L50	1375	G
1	L50	1384	U
1	L50	1385	G
1	L50	1386	A
1	L50	1387	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1395	U
1	L50	1396	G
1	L50	1402	G
1	L50	1411	C
1	L50	1412	C
1	L50	1414	U
1	L50	1416	A
1	L50	1427	A
1	L50	1429	A
1	L50	1430	U
1	L50	1431	G
1	L50	1432	G
1	L50	1440	G
1	L50	1447	C
1	L50	1449	A
1	L50	1450	A
1	L50	1453	G
1	L50	1455	A
1	L50	1457	C
1	L50	1458	A
1	L50	1466	A
1	L50	1467	A
1	L50	1468	G
1	L50	1474	G
1	L50	1475	A
1	L50	1479	U
1	L50	1485	G
1	L50	1486	G
1	L50	1488	U
1	L50	1489	G
1	L50	1490	U
1	L50	1491	U
1	L50	1492	U
1	L50	1499	U
1	L50	1513	G
1	L50	1524	G
1	L50	1527	U
1	L50	1533	C
1	L50	1534	G
1	L50	1535	G
1	L50	1536	G
1	L50	1538	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1547	G
1	L50	1554	U
1	L50	1555	G
1	L50	1556	U
1	L50	1557	G
1	L50	1563	A
1	L50	1564	U
1	L50	1565	U
1	L50	1566	G
1	L50	1568	G
1	L50	1569	A
1	L50	1571	A
1	L50	1573	G
1	L50	1574	G
1	L50	1575	G
1	L50	1583	A
1	L50	1591	G
1	L50	1592	U
1	L50	1602	G
1	L50	1610	A
1	L50	1611	A
1	L50	1612	G
1	L50	1613	A
1	L50	1614	G
1	L50	1617	A
1	L50	1619	G
1	L50	1624	G
1	L50	1626	G
1	L50	1638	G
1	L50	1643	G
1	L50	1644	U
1	L50	1645	C
1	L50	1646	G
1	L50	1649	A
1	L50	1651	A
1	L50	1653	G
1	L50	1665	A
1	L50	1668	A
1	L50	1674	G
1	L50	1675	G
1	L50	1680	A
1	L50	1682	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1685	G
1	L50	1686	G
1	L50	1689	G
1	L50	1692	A
1	L50	1693	C
1	L50	1697	G
1	L50	1698	A
1	L50	1699	C
1	L50	1705	U
1	L50	1708	G
1	L50	1709	G
1	L50	1710	U
1	L50	1711	A
1	L50	1717	A
1	L50	1718	C
1	L50	1720	C
1	L50	1724	G
1	L50	1733	A
1	L50	1735	G
1	L50	1739	A
1	L50	1742	C
1	L50	1743	G
1	L50	1746	U
1	L50	1749	A
1	L50	1751	G
1	L50	1755	U
1	L50	1760	A
1	L50	1770	U
1	L50	1772	U
1	L50	1797	A
1	L50	1799	U
1	L50	1800	U
1	L50	1801	C
1	L50	1808	A
1	L50	1809	A
1	L50	1810	C
1	L50	1811	G
1	L50	1820	C
1	L50	1821	G
1	L50	1822	G
1	L50	1828	G
1	L50	1832	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1833	A
1	L50	1835	G
1	L50	1836	A
1	L50	1837	A
1	L50	1838	G
1	L50	1839	A
1	L50	1846	U
1	L50	1854	A
1	L50	1858	U
1	L50	1860	G
1	L50	1868	A
1	L50	1869	A
1	L50	1870	G
1	L50	1872	U
1	L50	1873	G
1	L50	1874	U
1	L50	1881	U
1	L50	1883	A
1	L50	1885	G
1	L50	1887	G
1	L50	1888	A
1	L50	1931	C
1	L50	1934	C
1	L50	1935	A
1	L50	1937	G
1	L50	1938	A
1	L50	1939	U
1	L50	1940	C
1	L50	1941	A
1	L50	1942	U
1	L50	1943	C
1	L50	1946	G
1	L50	1949	A
1	L50	1950	C
1	L50	1955	G
1	L50	1956	U
1	L50	1957	U
1	L50	1958	U
1	L50	1959	A
1	L50	1960	A
1	L50	1961	G
1	L50	1963	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1966	A
1	L50	1967	A
1	L50	1968	G
1	L50	1973	G
1	L50	1977	G
1	L50	1978	G
1	L50	1985	G
1	L50	1991	G
1	L50	1995	G
1	L50	1997	A
1	L50	2007	A
1	L50	2008	A
1	L50	2011	A
1	L50	2013	A
1	L50	2019	G
1	L50	2020	U
1	L50	2022	G
1	L50	2023	A
1	L50	2027	A
1	L50	2030	G
1	L50	2031	U
1	L50	2032	A
1	L50	2036	A
1	L50	2037	C
1	L50	2039	G
1	L50	2042	A
1	L50	2043	G
1	L50	2045	C
1	L50	2046	G
1	L50	2047	A
1	L50	2048	G
1	L50	2049	A
1	L50	2052	A
1	L50	2057	U
1	L50	2059	U
1	L50	2060	A
1	L50	2061	G
1	L50	2062	A
1	L50	2063	G
1	L50	2065	A
1	L50	2067	A
1	L50	2073	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2075	A
1	L50	2076	A
1	L50	2077	G
1	L50	2078	A
1	L50	2085	G
1	L50	2087	G
1	L50	2093	G
1	L50	2096	C
1	L50	2097	U
1	L50	2098	A
1	L50	2099	C
1	L50	2108	U
1	L50	2109	G
1	L50	2110	A
1	L50	2111	G
1	L50	2114	G
1	L50	2122	G
1	L50	2124	C
1	L50	2130	G
1	L50	2131	A
1	L50	2136	A
1	L50	2140	A
1	L50	2141	U
1	L50	2142	A
1	L50	2145	A
1	L50	2146	G
1	L50	2149	A
1	L50	2150	C
1	L50	2152	U
1	L50	2160	G
1	L50	2162	G
1	L50	2164	G
1	L50	2167	A
1	L50	2168	G
1	L50	2169	A
1	L50	2170	A
1	L50	2171	A
1	L50	2177	C
1	L50	2178	C
1	L50	2185	A
1	L50	2189	C
1	L50	2211	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2212	G
1	L50	2213	A
1	L50	2217	C
1	L50	2221	G
1	L50	2224	G
1	L50	2228	U
1	L50	2229	U
1	L50	2234	U
1	L50	2235	C
1	L50	2239	G
1	L50	2241	U
1	L50	2243	U
1	L50	2253	C
1	L50	2254	U
1	L50	2255	A
1	L50	2257	C
1	L50	2260	G
1	L50	2262	C
1	L50	2266	G
1	L50	2272	G
1	L50	2275	G
1	L50	2279	A
1	L50	2286	G
1	L50	2291	U
1	L50	2293	C
1	L50	2296	C
1	L50	2303	C
1	L50	2304	A
1	L50	2306	G
1	L50	2309	A
1	L50	2310	C
1	L50	2313	G
1	L50	2319	G
1	L50	2322	U
1	L50	2323	U
1	L50	2325	G
1	L50	2337	A
1	L50	2339	A
1	L50	2340	G
1	L50	2345	G
1	L50	2347	U
1	L50	2351	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2355	A
1	L50	2358	G
1	L50	2364	A
1	L50	2376	A
1	L50	2377	G
1	L50	2379	G
1	L50	2394	A
1	L50	2399	A
1	L50	2401	C
1	L50	2410	A
1	L50	2412	C
1	L50	2413	U
1	L50	2416	G
1	L50	2419	G
1	L50	2420	C
1	L50	2423	C
1	L50	2424	G
1	L50	2432	G
1	L50	2434	A
1	L50	2436	G
1	L50	2437	U
1	L50	2441	A
1	L50	2447	A
1	L50	2451	U
1	L50	2452	A
1	L50	2453	C
1	L50	2459	C
1	L50	2460	U
1	L50	2473	G
1	L50	2475	A
1	L50	2476	G
1	L50	2477	C
1	L50	2482	A
1	L50	2487	A
1	L50	2490	A
1	L50	2491	A
1	L50	2501	A
1	L50	2503	U
1	L50	2508	A
1	L50	2509	A
1	L50	2518	G
1	L50	2519	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2520	A
1	L50	2529	C
1	L50	2532	A
1	L50	2533	G
1	L50	2534	U
1	L50	2535	U
1	L50	2538	C
1	L50	2539	A
1	L50	2548	G
1	L50	2555	A
1	L50	2558	A
1	L50	2559	G
1	L50	2562	U
1	L50	2563	U
1	L50	2565	U
1	L50	2568	U
1	L50	2578	G
1	L50	2588	G
1	L50	2593	A
1	L50	2595	U
1	L50	2596	G
1	L50	2597	G
1	L50	2598	U
1	L50	2600	G
1	L50	2605	C
1	L50	2606	A
1	L50	2612	G
2	L70	2	G
2	L70	10	C
2	L70	14	U
2	L70	15	C
2	L70	18	C
2	L70	22	A
2	L70	25	A
2	L70	27	A
2	L70	32	A
2	L70	33	U
2	L70	35	C
2	L70	41	G
2	L70	42	A
2	L70	49	A
2	L70	50	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L70	51	G
2	L70	53	U
2	L70	63	A
2	L70	64	G
2	L70	65	A
2	L70	67	C
2	L70	69	A
2	L70	88	C
2	L70	89	G
2	L70	91	C
2	L70	93	A
2	L70	100	A
2	L70	101	A
2	L70	104	C
2	L70	105	G
2	L70	107	G
2	L70	108	G
2	L70	109	U
2	L70	110	G
2	L70	115	A
2	L70	119	U
42	S60	7	U
42	S60	8	U
42	S60	14	U
42	S60	17	C
42	S60	26	A
42	S60	32	G
42	S60	37	A
42	S60	39	A
42	S60	40	G
42	S60	41	A
42	S60	43	U
42	S60	44	U
42	S60	45	A
42	S60	48	C
42	S60	52	C
42	S60	54	U
42	S60	55	G
42	S60	56	U
42	S60	66	G
42	S60	70	U
42	S60	71	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	72	A
42	S60	73	G
42	S60	75	G
42	S60	76	A
42	S60	77	A
42	S60	83	G
42	S60	86	A
42	S60	88	G
42	S60	92	A
42	S60	94	U
42	S60	97	C
42	S60	98	G
42	S60	99	G
42	S60	102	G
42	S60	104	G
42	S60	106	A
42	S60	107	U
42	S60	110	A
42	S60	112	U
42	S60	116	U
42	S60	118	G
42	S60	119	A
42	S60	120	A
42	S60	121	C
42	S60	124	G
42	S60	127	A
42	S60	128	A
42	S60	132	C
42	S60	133	A
42	S60	134	G
42	S60	138	A
42	S60	140	A
42	S60	141	G
42	S60	142	A
42	S60	147	A
42	S60	148	A
42	S60	150	A
42	S60	153	G
42	S60	155	G
42	S60	157	A
42	S60	161	G
42	S60	167	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	172	U
42	S60	173	A
42	S60	174	G
42	S60	180	G
42	S60	181	A
42	S60	184	A
42	S60	186	A
42	S60	187	A
42	S60	189	A
42	S60	190	A
42	S60	191	C
42	S60	192	A
42	S60	193	G
42	S60	197	A
42	S60	198	G
42	S60	199	G
42	S60	204	U
42	S60	206	A
42	S60	219	U
42	S60	220	C
42	S60	222	G
42	S60	226	G
42	S60	228	A
42	S60	238	A
42	S60	241	G
42	S60	242	C
42	S60	247	U
42	S60	254	U
42	S60	255	A
42	S60	256	G
42	S60	259	G
42	S60	262	U
42	S60	263	A
42	S60	264	C
42	S60	268	G
42	S60	271	U
42	S60	283	U
42	S60	284	C
42	S60	290	A
42	S60	292	G
42	S60	299	G
42	S60	300	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	303	G
42	S60	304	A
42	S60	305	C
42	S60	307	G
42	S60	311	C
42	S60	314	G
42	S60	315	G
42	S60	318	C
42	S60	319	A
42	S60	320	A
42	S60	326	G
42	S60	327	C
42	S60	328	A
42	S60	329	G
42	S60	335	G
42	S60	338	A
42	S60	340	A
42	S60	341	A
42	S60	342	U
42	S60	344	A
42	S60	345	C
42	S60	347	G
42	S60	348	A
42	S60	355	C
42	S60	356	A
42	S60	357	A
42	S60	358	G
42	S60	362	G
42	S60	363	C
42	S60	364	G
42	S60	367	A
42	S60	368	G
42	S60	371	A
42	S60	372	A
42	S60	373	G
42	S60	374	A
42	S60	375	G
42	S60	377	C
42	S60	378	G
42	S60	380	G
42	S60	382	A
42	S60	383	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	384	A
42	S60	385	C
42	S60	388	G
42	S60	395	U
42	S60	396	A
42	S60	398	A
42	S60	399	A
42	S60	402	C
42	S60	407	G
42	S60	408	A
42	S60	409	G
42	S60	412	A
42	S60	414	U
42	S60	416	G
42	S60	422	A
42	S60	424	G
42	S60	425	G
42	S60	426	C
42	S60	431	G
42	S60	432	C
42	S60	437	A
42	S60	441	G
42	S60	444	G
42	S60	445	U
42	S60	446	A
42	S60	449	A
42	S60	450	C
42	S60	452	A
42	S60	453	G
42	S60	454	C
42	S60	461	A
42	S60	471	A
42	S60	473	G
42	S60	474	A
42	S60	476	U
42	S60	477	G
42	S60	478	C
42	S60	481	C
42	S60	482	G
42	S60	486	A
42	S60	487	A
42	S60	490	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	491	G
42	S60	501	G
42	S60	506	A
42	S60	509	G
42	S60	510	U
42	S60	511	A
42	S60	512	C
42	S60	521	A
42	S60	527	G
42	S60	530	U
42	S60	535	A
42	S60	536	G
42	S60	540	C
42	S60	541	G
42	S60	543	A
42	S60	544	U
42	S60	547	A
42	S60	550	G
42	S60	553	A
42	S60	554	A
42	S60	565	U
42	S60	566	A
42	S60	567	A
42	S60	568	G
42	S60	575	A
42	S60	578	A
42	S60	579	G
42	S60	590	U
42	S60	593	A
42	S60	598	C
42	S60	599	G
42	S60	600	A
42	S60	601	G
42	S60	602	A
42	S60	608	A
42	S60	609	A
42	S60	610	U
42	S60	616	G
42	S60	621	G
42	S60	622	C
42	S60	623	U
42	S60	624	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	625	A
42	S60	630	U
42	S60	633	C
42	S60	635	G
42	S60	637	G
42	S60	644	G
42	S60	647	C
42	S60	661	A
42	S60	662	U
42	S60	665	G
42	S60	668	G
42	S60	671	C
42	S60	673	A
42	S60	686	G
42	S60	687	A
42	S60	688	G
42	S60	690	A
42	S60	694	A
42	S60	700	A
42	S60	702	U
42	S60	705	A
42	S60	706	G
42	S60	707	A
42	S60	722	G
42	S60	724	A
42	S60	725	G
42	S60	727	A
42	S60	728	A
42	S60	730	C
42	S60	731	G
42	S60	733	U
42	S60	734	G
42	S60	738	A
42	S60	740	G
42	S60	749	G
42	S60	752	A
42	S60	753	U
42	S60	754	G
42	S60	755	A
42	S60	757	C
42	S60	771	A
42	S60	775	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	776	A
42	S60	780	G
42	S60	789	G
42	S60	790	G
42	S60	791	A
42	S60	795	U
42	S60	806	G
42	S60	810	U
42	S60	817	A
42	S60	818	A
42	S60	820	G
42	S60	821	G
42	S60	823	A
42	S60	825	U
42	S60	831	G
42	S60	836	A
42	S60	839	C
42	S60	840	C
42	S60	841	A
42	S60	846	G
42	S60	848	G
42	S60	866	U
42	S60	868	U
42	S60	871	C
42	S60	872	U
42	S60	874	A
42	S60	875	A
42	S60	877	G
42	S60	878	C
42	S60	880	G
42	S60	881	G
42	S60	883	C
42	S60	884	A
42	S60	890	C
42	S60	898	G
42	S60	899	A
42	S60	905	G
42	S60	908	U
42	S60	909	G
42	S60	911	G
42	S60	915	A
42	S60	916	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	917	U
42	S60	918	A
42	S60	924	U
42	S60	925	A
42	S60	926	G
42	S60	927	G
42	S60	928	U
42	S60	929	C
42	S60	930	A
42	S60	932	A
42	S60	933	G
42	S60	934	A
42	S60	936	U
42	S60	940	G
42	S60	941	C
42	S60	942	A
42	S60	952	A
42	S60	953	C
42	S60	955	A
42	S60	957	G
42	S60	958	A
42	S60	959	G
42	S60	962	G
42	S60	966	G
42	S60	967	A
42	S60	968	C
42	S60	970	U
42	S60	971	U
42	S60	972	U
42	S60	974	G
42	S60	976	U
42	S60	978	A
42	S60	980	G
42	S60	987	A
42	S60	991	A
42	S60	995	A
42	S60	998	U
42	S60	999	C
42	S60	1003	A
42	S60	1006	A
42	S60	1007	U
42	S60	1008	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	1011	A
42	S60	1012	A
42	S60	1013	A
42	S60	1014	G
42	S60	1017	A
42	S60	1018	U
42	S60	1019	C
42	S60	1021	A
42	S60	1023	A
42	S60	1024	G
42	S60	1028	U
42	S60	1029	U
42	S60	1033	A
42	S60	1039	G
42	S60	1041	A
42	S60	1042	A
42	S60	1044	G
42	S60	1045	A
42	S60	1046	A
42	S60	1047	G
42	S60	1052	A
42	S60	1053	A
42	S60	1054	G
42	S60	1056	A
42	S60	1057	C
42	S60	1058	A
42	S60	1059	G
42	S60	1060	G
42	S60	1062	C
42	S60	1063	A
42	S60	1064	G
42	S60	1066	G
42	S60	1075	A
42	S60	1076	G
42	S60	1077	A
42	S60	1078	U
42	S60	1088	U
42	S60	1089	G
42	S60	1090	C
42	S60	1092	C
42	S60	1094	C
42	S60	1099	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	1100	A
42	S60	1102	A
42	S60	1103	G
42	S60	1104	U
42	S60	1105	G
42	S60	1106	G
42	S60	1111	A
42	S60	1112	G
42	S60	1116	A
42	S60	1117	A
42	S60	1118	A
42	S60	1119	C
42	S60	1120	A
42	S60	1121	A
42	S60	1122	A
42	S60	1123	U
42	S60	1124	A
42	S60	1125	G
42	S60	1126	A
42	S60	1127	A
42	S60	1128	G
42	S60	1129	U
42	S60	1130	A
42	S60	1135	U
42	S60	1136	G
42	S60	1137	A
42	S60	1139	C
42	S60	1141	A
42	S60	1142	G
42	S60	1146	G
42	S60	1152	G
42	S60	1154	A
42	S60	1158	U
42	S60	1159	A
42	S60	1160	A
42	S60	1161	U
42	S60	1162	G
42	S60	1170	G
42	S60	1171	A
42	S60	1175	A
42	S60	1176	G
42	S60	1177	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	1179	A
42	S60	1182	G
42	S60	1185	A
42	S60	1191	C
42	S60	1192	G
42	S60	1194	U
42	S60	1195	A
42	S60	1196	U
42	S60	1202	U
42	S60	1203	A
42	S60	1204	A
42	S60	1205	G
42	S60	1210	G
42	S60	1211	A
42	S60	1214	A
42	S60	1216	U
42	S60	1217	G
42	S60	1219	G
42	S60	1223	C
42	S60	1225	G
42	S60	1227	U
42	S60	1230	U
42	S60	1237	C
42	S60	1238	A
42	S60	1239	C
42	S60	1240	C
42	S60	1241	G
42	S60	1243	C
42	S60	1246	U
42	S60	1249	U
42	S60	1250	U
42	S60	1251	A
42	S60	1260	G
42	S60	1262	A
42	S60	1263	A
42	S60	1264	C
42	S60	1266	A
42	S60	1267	G
42	S60	1270	G
42	S60	1274	A
42	S60	1275	C
42	S60	1276	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	S60	1280	G
42	S60	1282	A
42	S60	1283	A
42	S60	1284	G
42	S60	1287	A
42	S60	1294	G
42	S60	1295	C
42	S60	1296	A
42	S60	1297	G
42	S60	1301	U
42	S60	1302	C
42	S60	1307	U
42	S60	1310	G
42	S60	1314	C
42	S60	1315	A
42	S60	1316	A
42	S60	1317	G
42	S60	1320	G
42	S60	1322	A
42	S60	1326	A
42	S60	1327	G
42	S60	1328	G
42	S60	1329	C
42	S60	1331	G
42	S60	1340	G
42	S60	1341	A
42	S60	1342	A
42	S60	1343	C
42	S60	1348	A
42	S60	1352	G
42	S60	1353	G
42	S60	1354	A
42	S60	1355	U
42	S60	1356	C
42	S60	1357	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

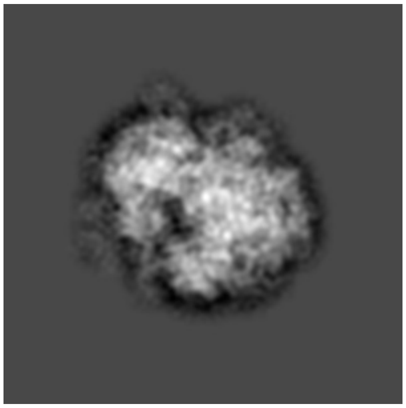
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17448. These allow visual inspection of the internal detail of the map and identification of artifacts.

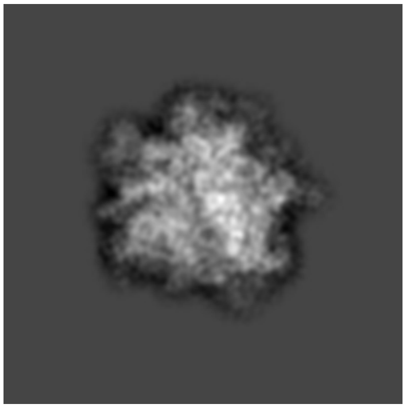
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

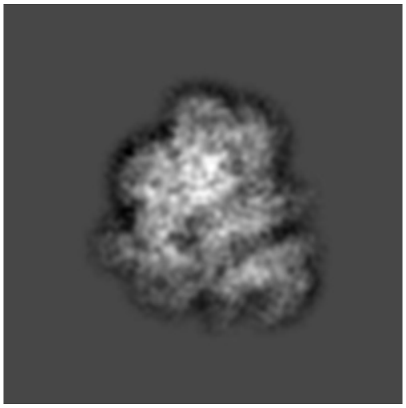
6.1.1 Primary map



X

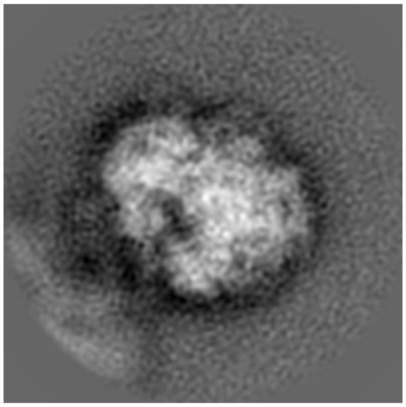


Y

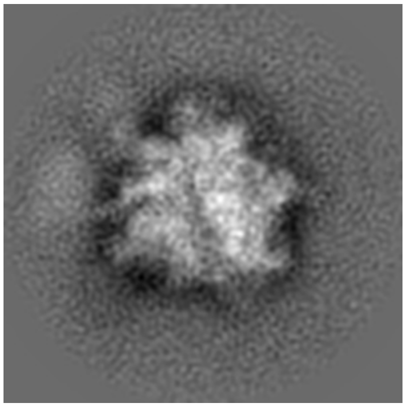


Z

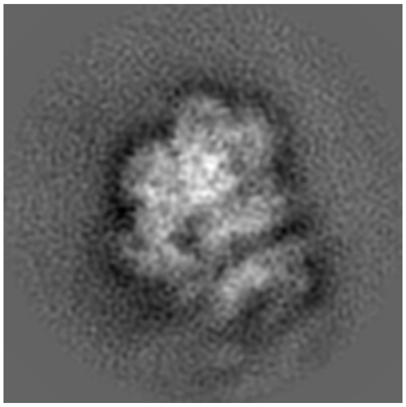
6.1.2 Raw map



X



Y

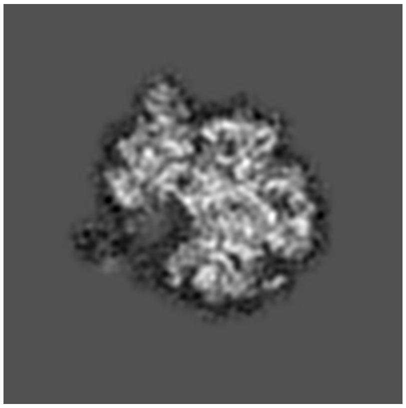


Z

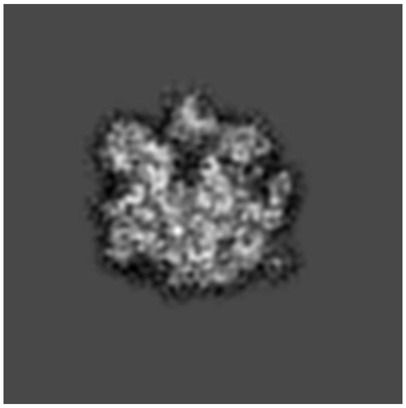
The images above show the map projected in three orthogonal directions.

6.2 Central slices

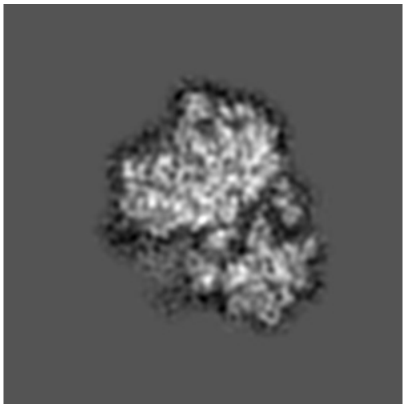
6.2.1 Primary map



X Index: 50

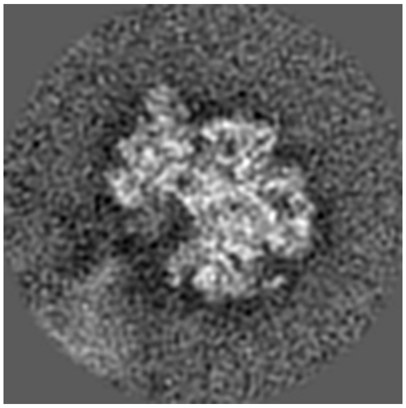


Y Index: 50

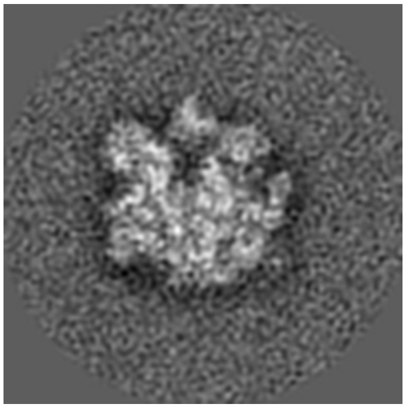


Z Index: 50

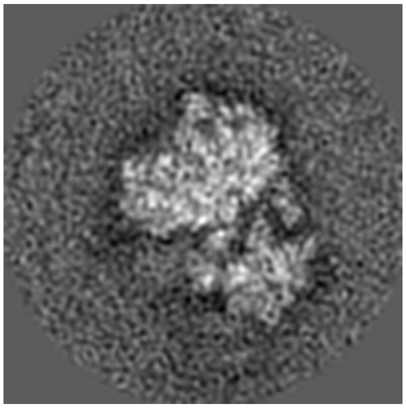
6.2.2 Raw map



X Index: 50



Y Index: 50

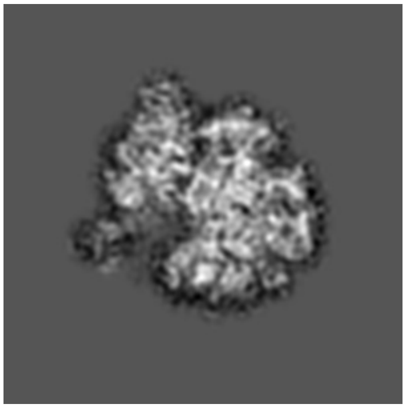


Z Index: 50

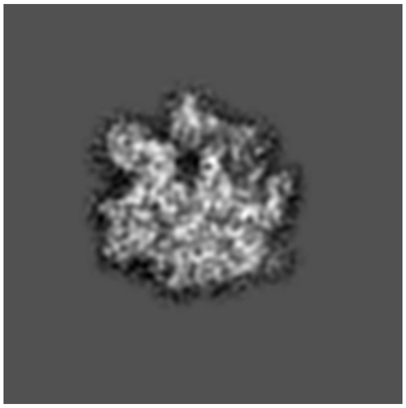
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

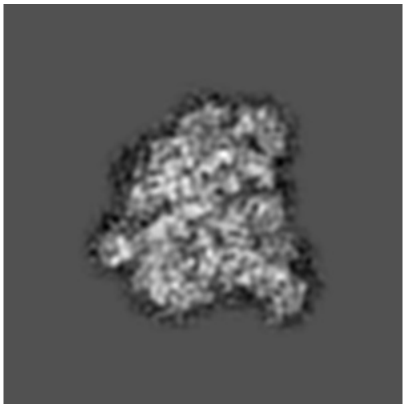
6.3.1 Primary map



X Index: 51

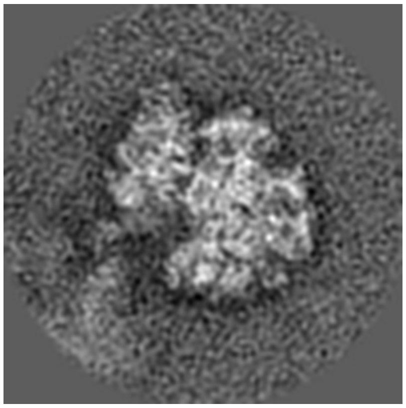


Y Index: 51

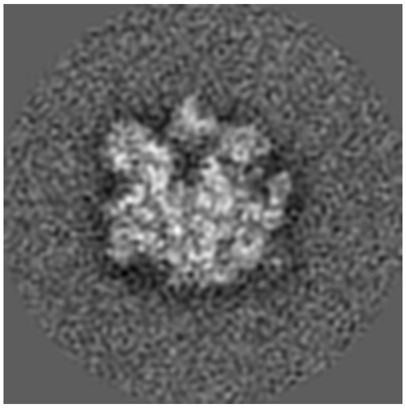


Z Index: 57

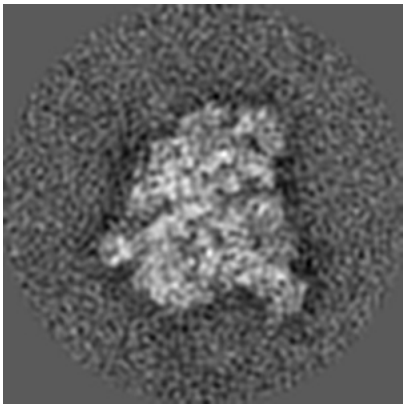
6.3.2 Raw map



X Index: 51



Y Index: 50

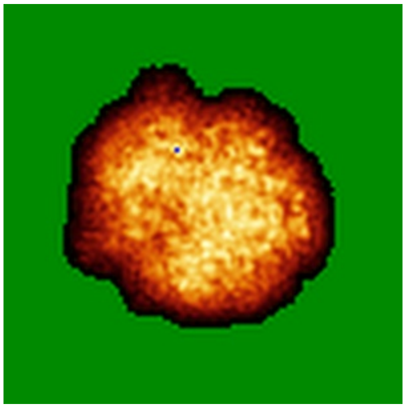


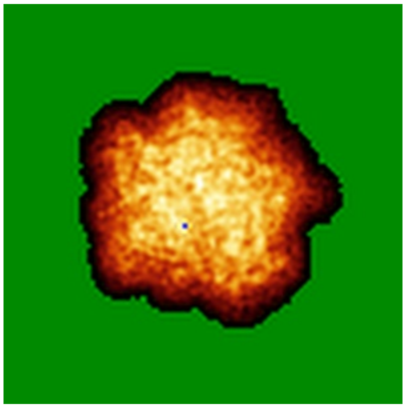
Z Index: 57

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

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

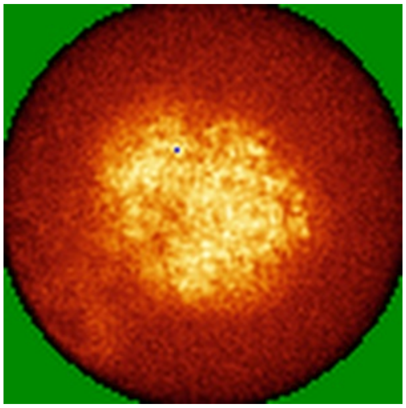
6.4.1 Primary map

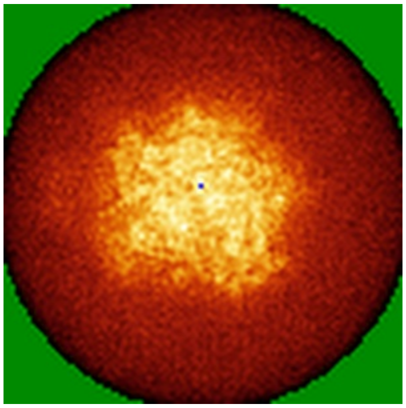

X

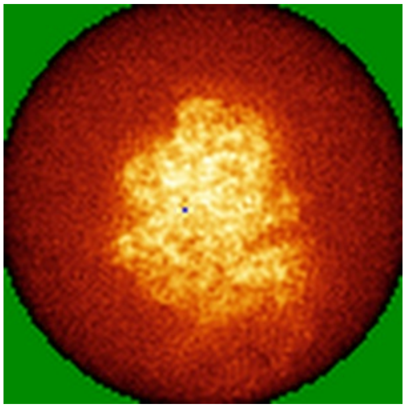

Y


Z

6.4.2 Raw map


X

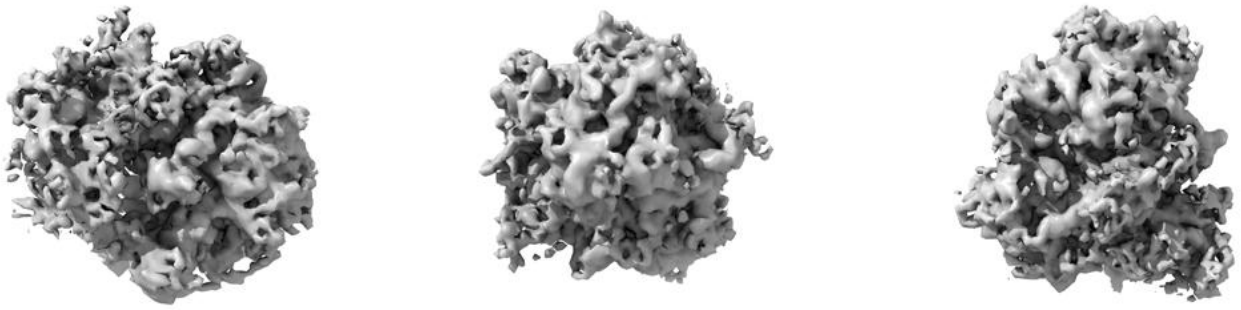

Y


Z

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

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

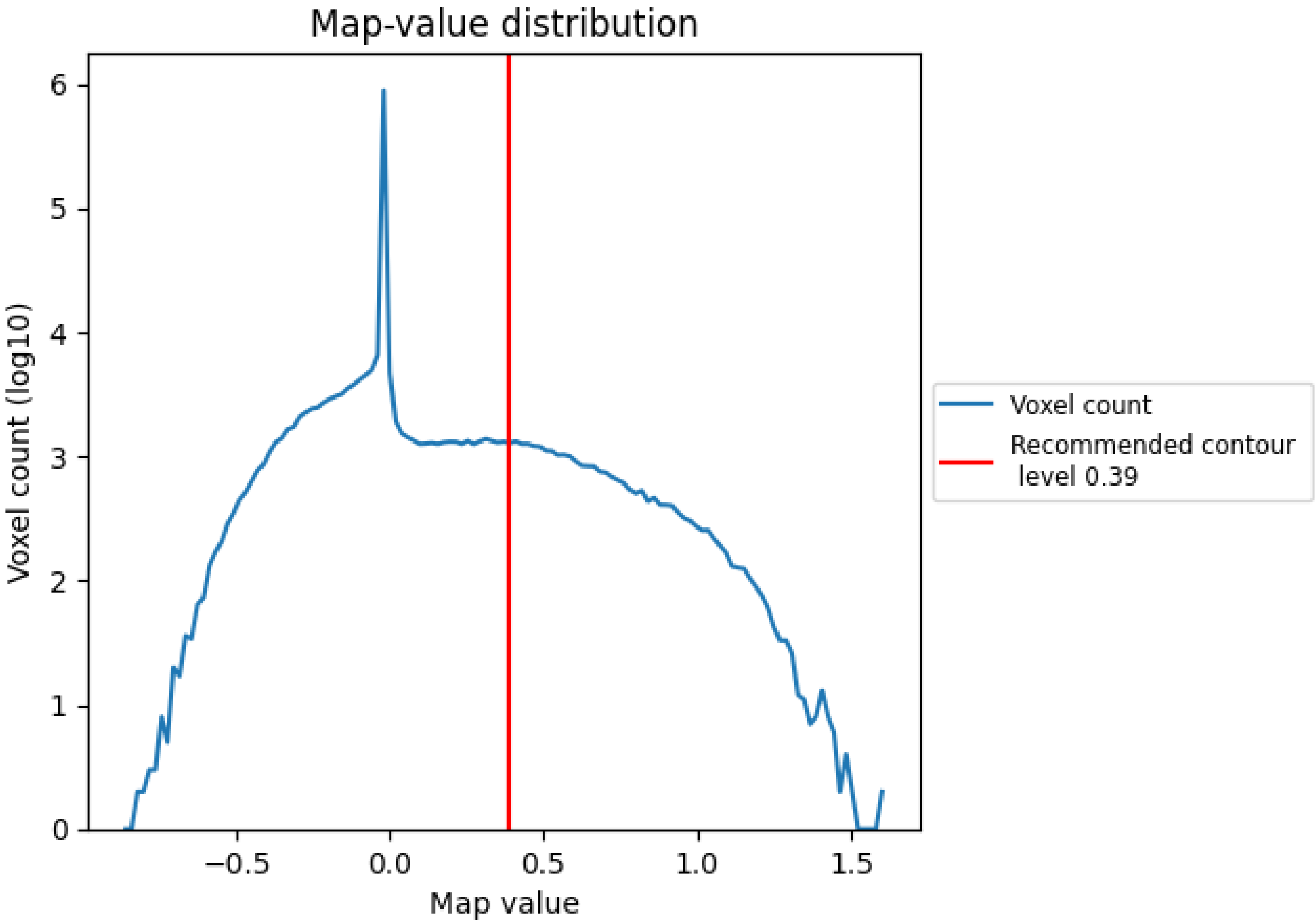
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

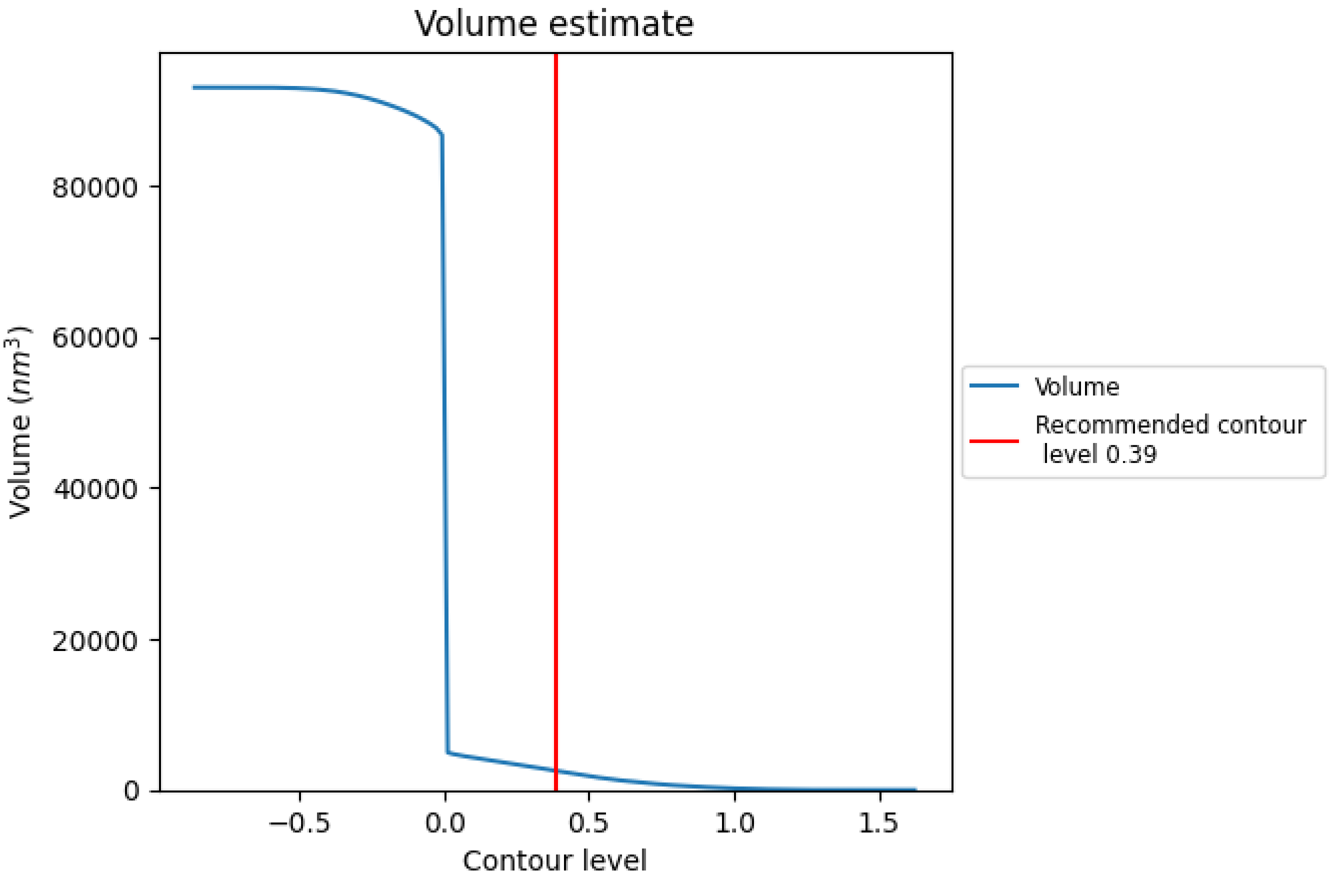
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

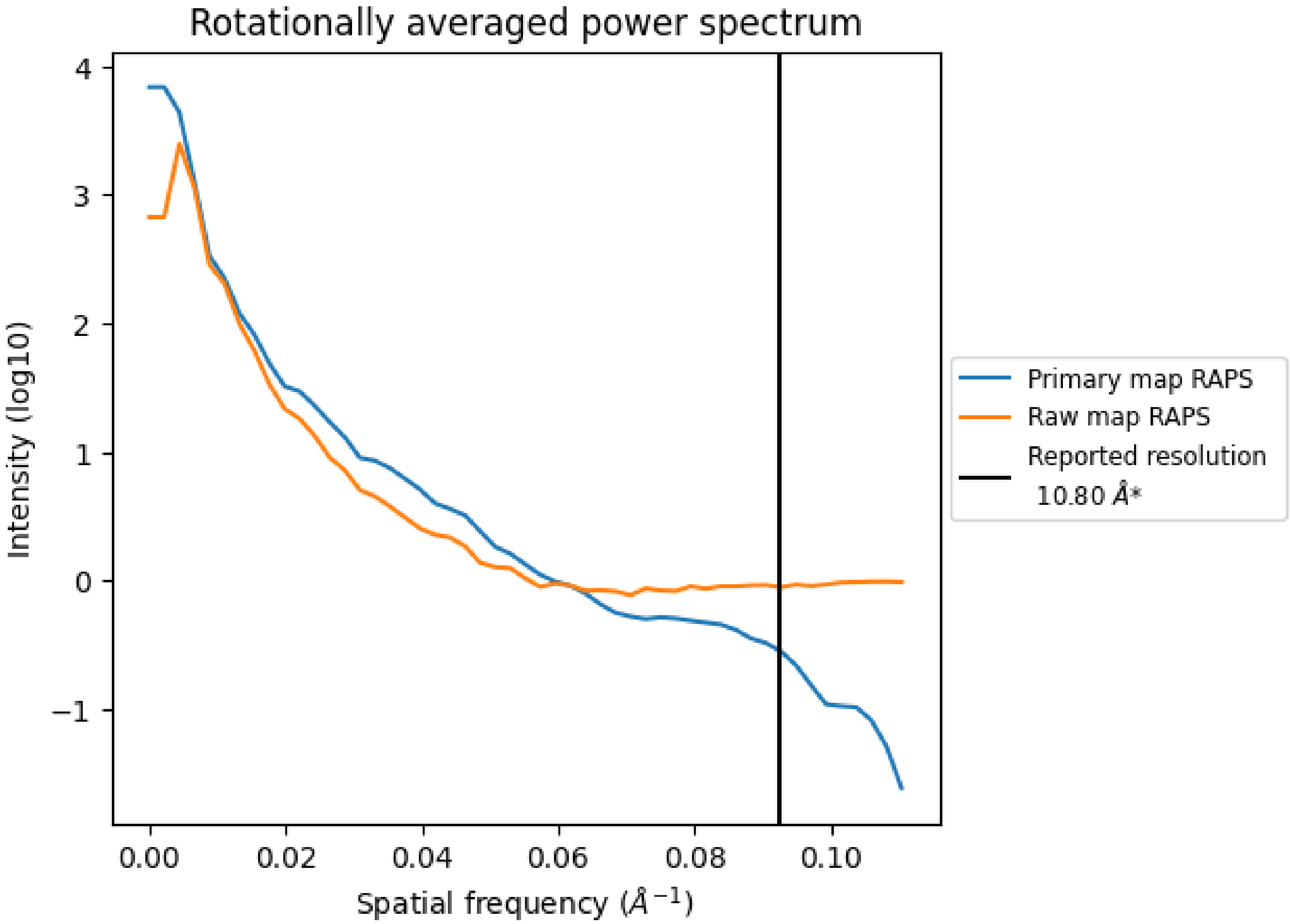
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2482 nm^3; this corresponds to an approximate mass of 2242 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 ⓘ

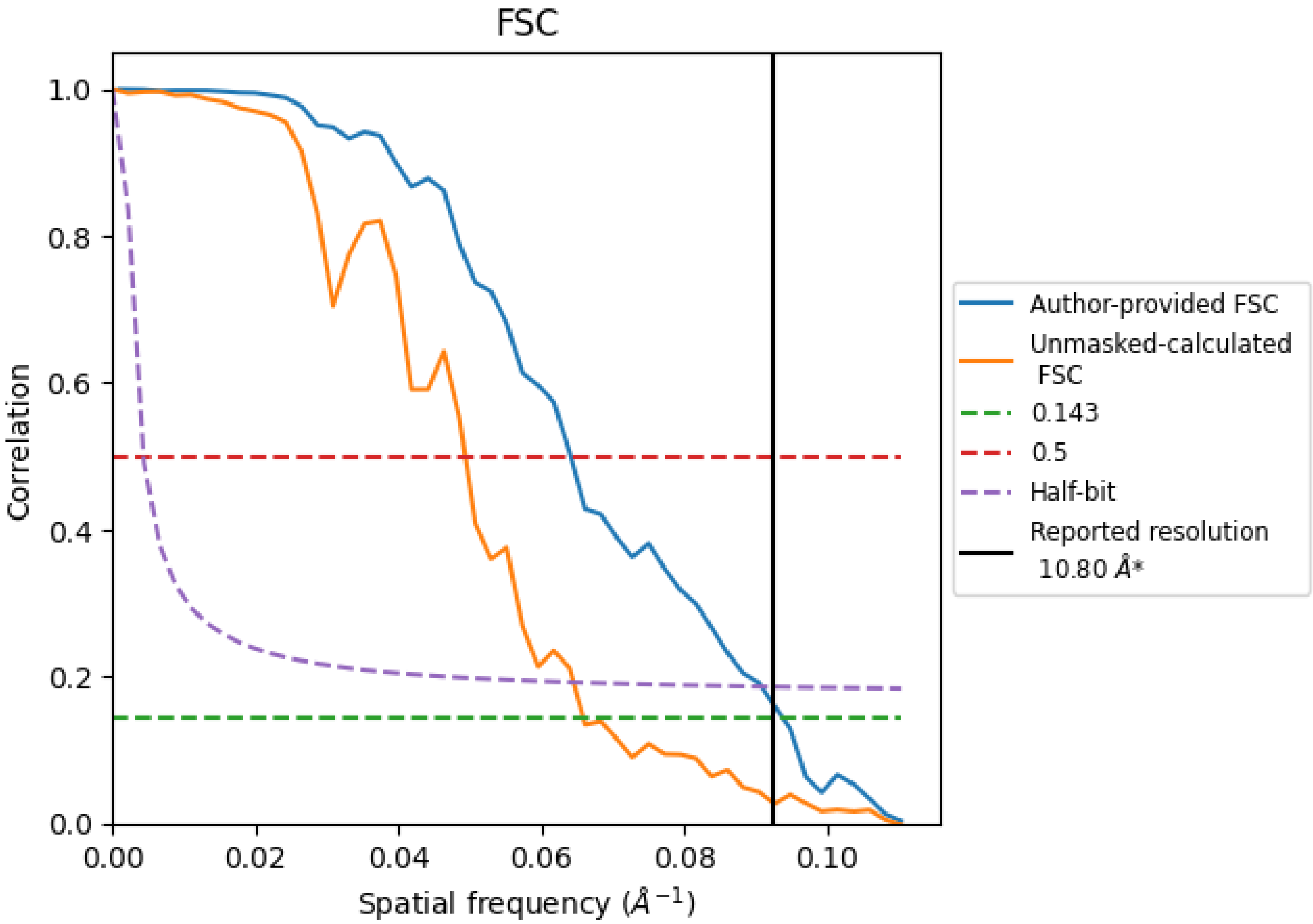


*Reported resolution corresponds to spatial frequency of 0.093 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.093 Å^{-1}

8.2 Resolution estimates ⓘ

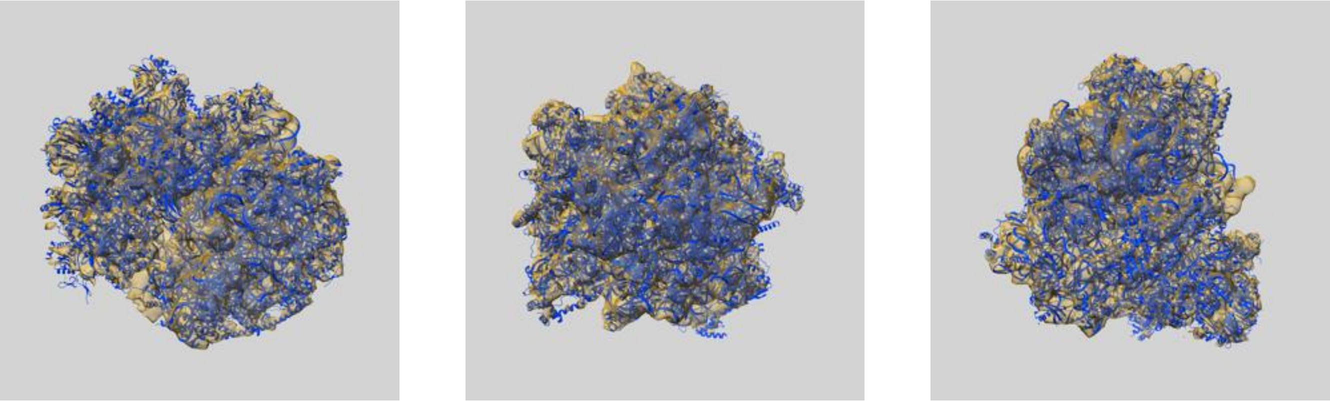
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	10.80	-	-
Author-provided FSC curve	10.65	15.58	11.00
Unmasked-calculated*	15.15	20.24	15.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.15 differs from the reported value 10.8 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17448 and PDB model 8P5D. Per-residue inclusion information can be found in section 3 on page 18.

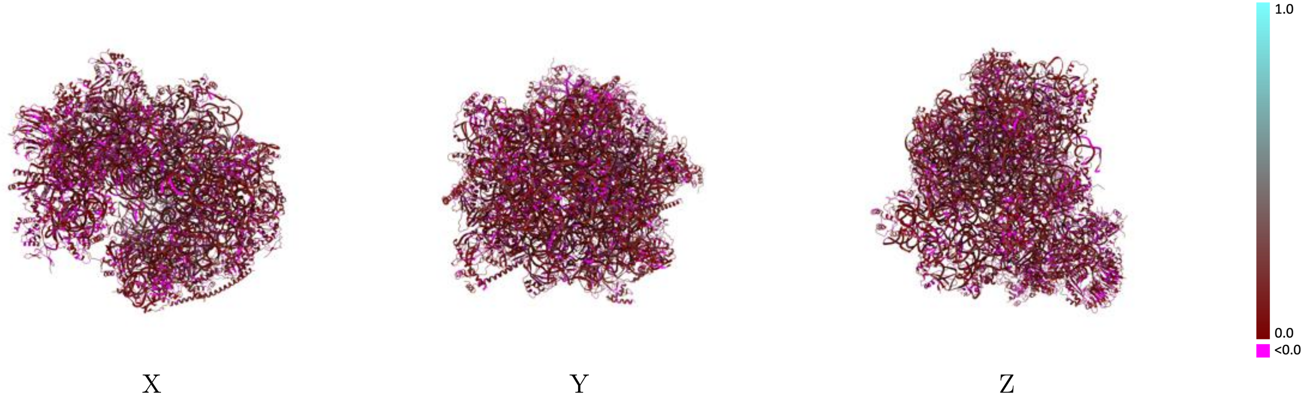
9.1 Map-model overlay ⓘ



X Y Z

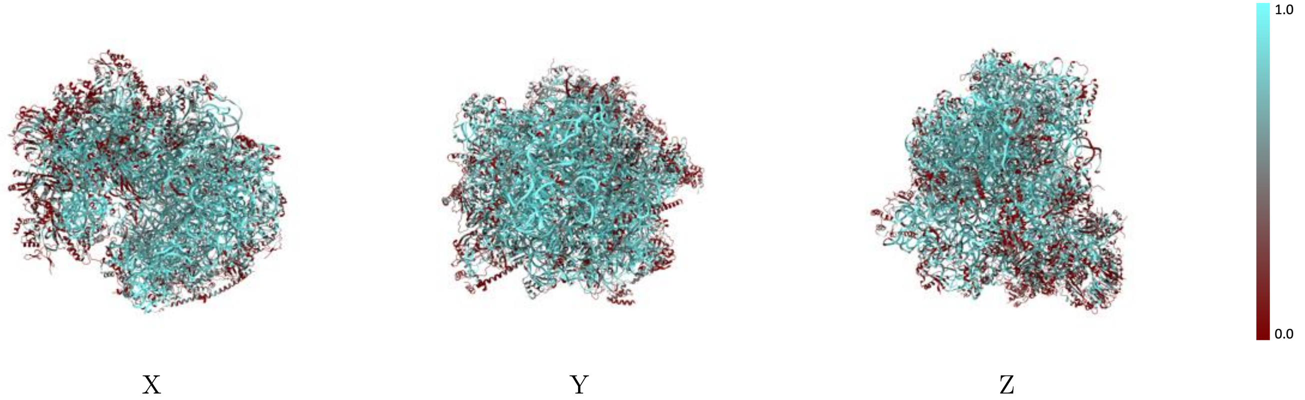
The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



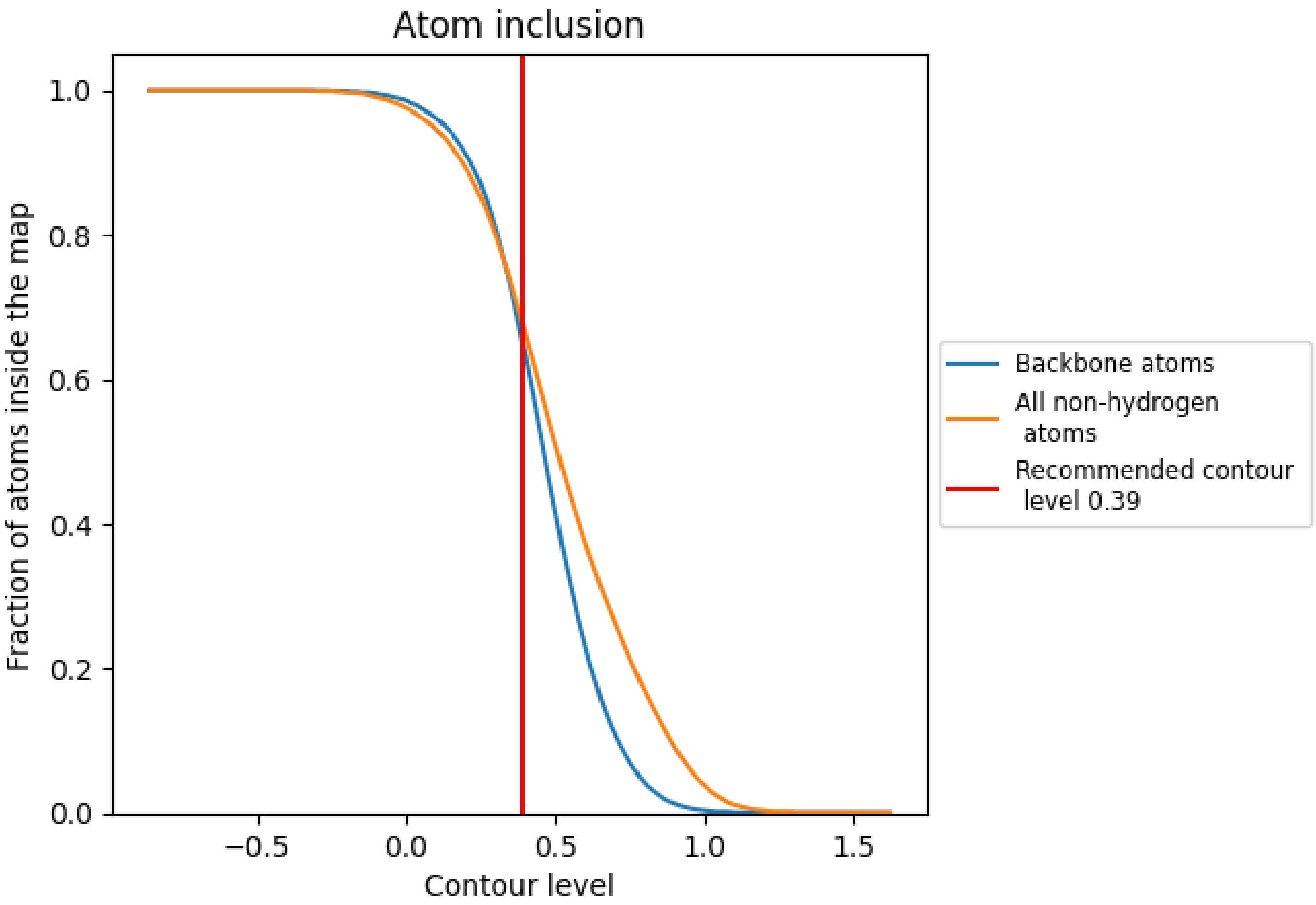
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.39).

9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.0880
L50	0.9150	0.1100
L70	0.9040	0.1200
LA0	0.5280	0.0500
LAA	0.7060	0.0460
LB0	0.5470	0.0550
LC0	0.5060	0.0530
LCC	0.4150	0.0890
LD0	0.5650	0.0600
LDD	0.5200	0.0830
LE0	0.3100	0.0940
LEE	0.5220	0.0490
LF0	0.4930	0.0820
LFF	0.5130	0.0670
LG0	0.4810	0.0950
LGG	0.5720	0.0420
LH0	0.4950	0.0810
LHH	0.5640	0.0950
LI0	0.5460	0.0630
LII	0.5210	0.0730
LJ0	0.5060	0.0720
LJJ	0.7270	0.0670
LL0	0.5870	0.0660
LLL	0.5270	0.0420
LM0	0.3300	0.0970
LMM	0.6050	0.0700
LN0	0.7350	0.0210
LO0	0.4870	0.0860
LOO	0.5920	0.0590
LP0	0.5630	0.0720
LPP	0.5880	0.0790
LQ0	0.5240	0.0650
LR0	0.4620	0.0860
LS0	0.4650	0.0850
LT0	0.5090	0.0430

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LU0	0.5760	0.0960
LV0	0.3960	0.0630
LW0	0.2860	0.0700
LX0	0.4370	0.0780
LY0	0.5510	0.0880
LZ0	0.3690	0.0760
MD1	0.2650	0.0630
S60	0.8810	0.1040
SA0	0.2730	0.0810
SAA	0.4940	0.0590
SB0	0.3950	0.0660
SBB	0.4690	0.0830
SC0	0.4390	0.0860
SCC	0.1420	0.0520
SD0	0.2890	0.0880
SDD	0.5110	0.0520
SE0	0.4240	0.0690
SEE	0.3990	0.0730
SF0	0.4840	0.0640
SFF	0.0260	0.0160
SG0	0.3730	0.0740
SGG	0.3450	0.0650
SH0	0.2640	0.0870
SI0	0.4300	0.0500
SJ0	0.4350	0.0830
SK0	0.2860	0.0660
SL0	0.3800	0.0780
SM0	0.1760	0.0430
SN0	0.4590	0.0740
SO0	0.5000	0.0440
SP0	0.3270	0.0440
SQ0	0.4240	0.0520
SR0	0.2240	0.0710
SS0	0.4530	0.0570
ST0	0.4690	0.0750
SU0	0.3330	0.0770
SV0	0.3190	0.0940
SW0	0.4180	0.0710
SX0	0.2580	0.0350
SY0	0.4020	0.0650
SZ0	0.4930	0.0580