



wwPDB EM Map/Model Validation Report ⓘ

Apr 28, 2016 – 12:16 PM EDT

PDB ID : 5GAK
EMDB ID: : EMD-3227
Title : Yeast 60S ribosomal subunit with A-site tRNA, P-site tRNA and eIF-5A
Authors : Schmidt, C.; Becker, T.
Deposited on : 2015-12-09
Resolution : 3.88 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

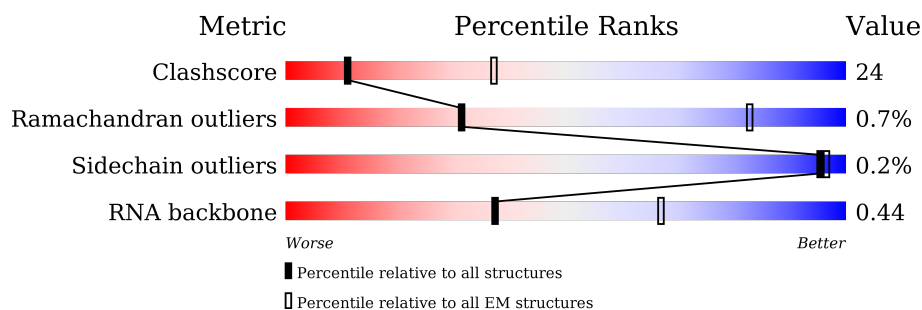
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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.




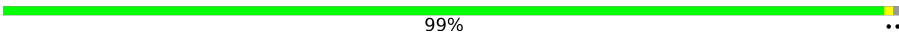

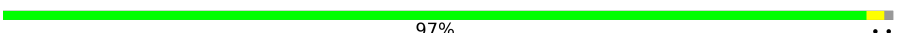

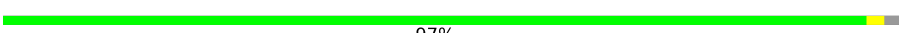










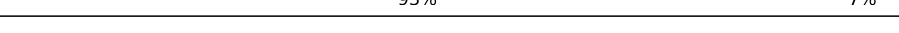

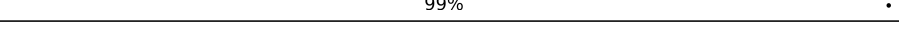

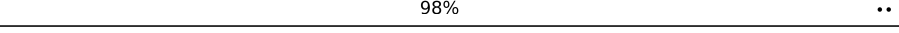

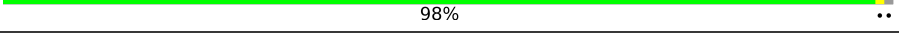

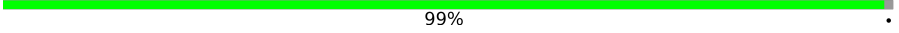
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	3396	18% 44% 30% • 7%
2	X	137	59% 40% •
3	3	121	21% 55% 23%
4	Y	155	46% 17% 37%
5	4	158	20% 49% 30% •
6	Z	142	52% 32% • 15%
7	A	76	12% 39% 46% •
8	a	127	98% ••

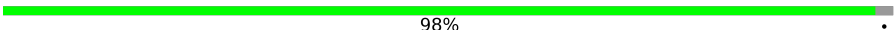
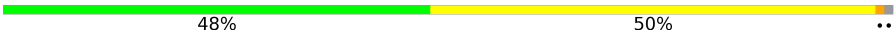


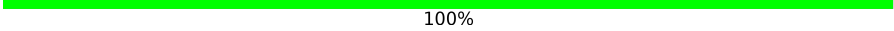



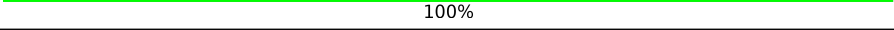

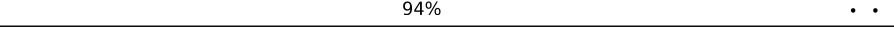


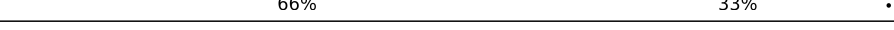

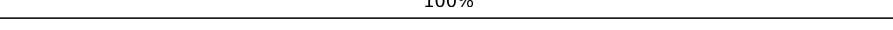
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Mol	Chain	Length	Quality of chain
9	B	77	
10	b	136	
11	C	106	
12	c	149	
13	D	92	
14	d	59	
15	E	254	
16	e	105	
17	F	387	
18	f	109	
19	G	362	
20	g	130	
21	H	297	
22	h	107	
23	I	176	
24	i	121	
25	J	244	
26	j	120	
27	K	256	
28	k	100	
29	L	191	
30	l	88	
31	M	174	
32	m	78	
33	N	199	

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Mol	Chain	Length	Quality of chain
34	n	51	 98% .
35	O	138	 48% 50% ..
36	o	128	 41% 59%
37	P	204	 59% 41%
38	p	25	 100%
39	Q	199	 64% 35% .
40	q	157	 89% 8% ..
41	R	184	 62% 38% .
42	r	210	 100%
43	S	186	 66% 33% ..
44	s	221	 94% . .
45	T	189	 65% 34% .
46	U	172	 64% 36%
47	V	160	 66% 33% ..
48	W	121	 52% 31% 17%
49	z	23	 100%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 128975 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3165	Total	C	N	O	P	0	0
			67695	30238	12201	22091	3165		

- Molecule 2 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 4 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 6 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 7 is a RNA chain called The A-site tRNA was modeled based on an E. coli tRNA-Lys.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	76	Total	C	N	O	P	0	0
			1611	721	281	534	75		

- Molecule 8 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 9 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	77	Total	C	N	O	P	0	0
			1644	731	290	546	77		

- Molecule 10 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 11 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 12 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 13 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 14 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	d	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 15 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	e	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 17 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 18 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 19 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 21 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 22 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 23 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 24 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 25 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 27 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 28 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 29 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 30 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 31 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 32 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	m	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 33 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 34 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 35 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 36 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 37 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 38 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 39 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	154	Total	C	N	O	S	0	0
			1143	709	195	230	9		

- Molecule 41 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	183	Total	C	N	O		0	0
			1420	882	281	257			

- Molecule 42 is a protein called ribosomal protein RPL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 43 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 44 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 45 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	T	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 46 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	U	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 47 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

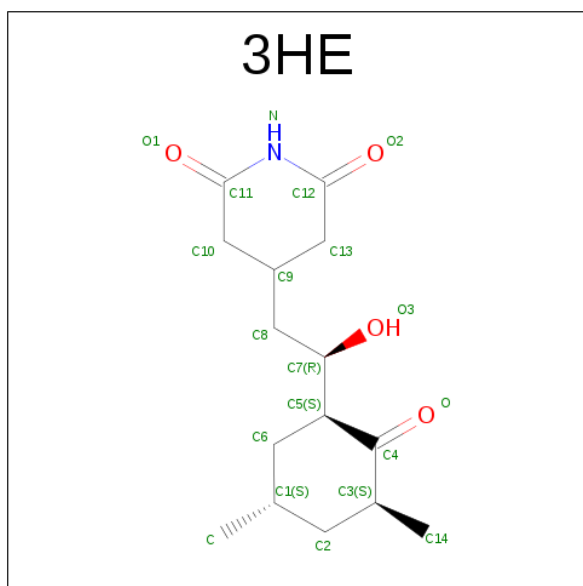
- Molecule 48 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	W	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 49 is a protein called nascent polypeptide chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	23	Total	C	N	O	0	0
			115	69	23	23		

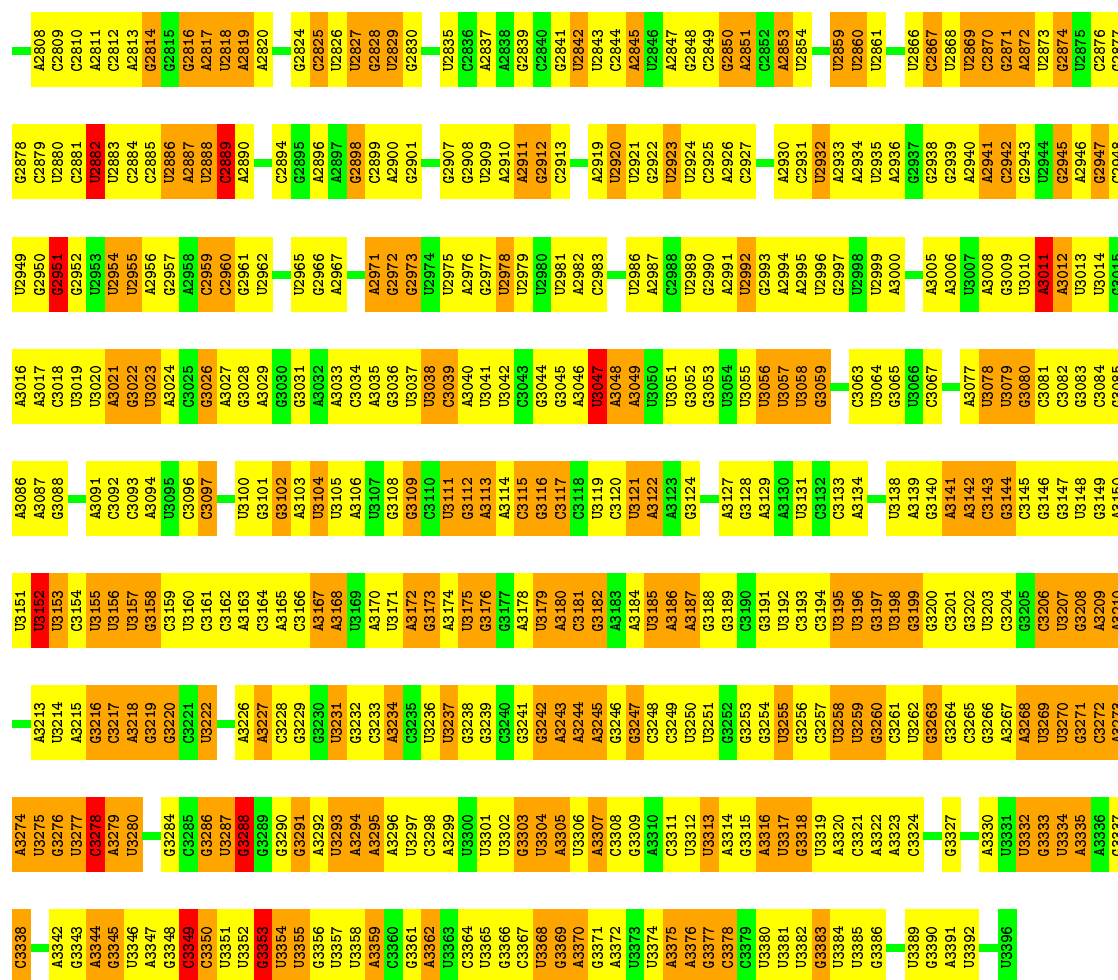
- Molecule 50 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C₁₅H₂₃NO₄).



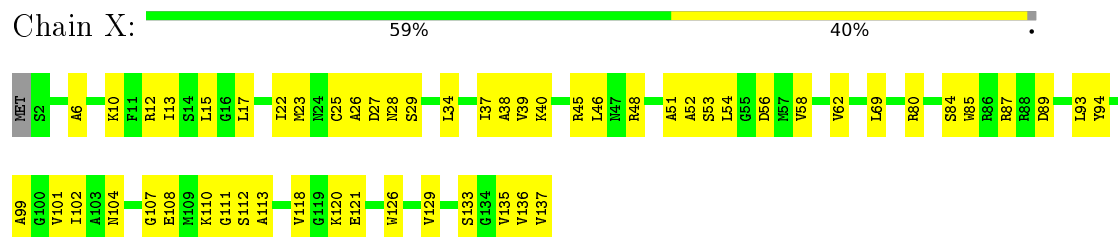
Mol	Chain	Residues	Atoms				AltConf
50	1	1	Total	C	N	O	0
			20	15	1	4	

U1717	U1651	G1528	G1468	G1401	G1339	C1275	G1213	A1143	A1079	C1017	C957	G891	A828	U767
G1718	G1652	A1529	G1469	C1402	G1340	U1276	U1214	U1444	A1080	G1018	C958	U892	U829	C768
G1719	G1653	U1630	U1470	U1403	U1341	C1277	A1217	G1145	U1081	G1019	C959	G893	A830	C769
U1720	A1654	C1531	U1471	G1404	C1342	A1278		U1082	U1082	G1020	U960	G894	G831	G770
U1721	G1655	C1532	U1472		A1343	C1279		G1147	G1083	U1021	C961	A895	G832	U771
U1722	A1656	U1533	G1473	A1407	G1344	C1280	U1220	G1148	A1084	U1022	A962	A896		U772
A1723	C1657	A1534	A1474	G1408	G1345	G1281	A1221	G1149	A1085	C1023	C963	U897	G835	G773
U1724	G1658	U1535	A1475	G1409	U1346	G1282	G1222	A1150	C1086	G1024	G964		A836	G774
C1725	U1659	G1536	G1476		U1347	C1283	A1223	U1151	U1087	A1025	A965	G900	A837	A775
G1726	G1660	A1537	A1477	G1412	U1348	C1284	C1224	U1152	U1088	A1026	U966	G901	G838	U776
G1727	G1661	G1538	C1478	G1413	U1349	G1285	A1225	A1153	G1089	A1027	A967	G902	G839	U777
G1728	G1662	U1539	U1479	G1414	A1350	A1286	C1226	A1154	G1090	U1028	G968	U903	C840	
A1729	C1663	U1540	U1480	U1415	U1351	A1287	C1227	C1155	A1091	G1029	C969	A904	C841	
G1730	G1664	G1541	A1481	C1416	A1352	U1288	G1228		C1092	A1030	A970	U905	G842	A780
A1731	C1665	G1542	G1482	G1417	U1353	G1289	G1229	A1158	A1093	C1031	G971	A906		G781
U1732	G1666	G1543	G1483	A1418	U1354	A1290	G1230	A1159	U1094	C1032	A972	G907	G845	U782
G1733	A1667	A1544	U1484	A1419	U1355	A1291	C1231	C1160	U1095	U1033	A973	G908	A846	A784
G1734	G1668	G1545	G1485	C1420	U1356	C1292	A1232	U1173	U1096	U1034	G974	G909	A847	G785
		A1546	G1486	G1421	G1357	U1293	G1233	A1169	G1097	G1035	C975	G910	A848	A786
			G1487	G1422	C1358	A1294	G1234	A1170	A1098	A1036	U976	C911	C849	G787
			C1423	C1423	C1359		U1235	G1171	A1099	C1037	C977	G912	U850	G788
			C1424		U1360	A1301	G1236	G1172	U1100	C1038	G978	A913	C851	A789
				U1427	A1362	A1302	C1238	G1174	A1102	U1040	A980	A915	G853	A791
			G1428	G1429	A1363	A1303	C1239	C1175	A1103	U1041	U981	G916	G854	G792
			U1430	U1431	C1364	A1304	A1240	G1176	G1104	U1042	C982	A917	U855	C793
			G1431	G1432	U1365	U1305	U1241	G1177	A1105	U1043	A983	C918	G857	U794
			U1432	U1433	A1366	G1306	G1242	G1178	G1106	U1044	U985	A920	A858	U796
			C1432	U1433	G1367	G1307	G1243	A1179	C1107	U1045	U986	A921	G859	U797
			U1433	U1434	U1368	A1308	A1244	A1180	U1108	A1046	U987	U922	G860	G798
			G1434	G1435	U1369	U1309	U1245	U1181	U1109	U1047	U988	C923	C861	G799
			U1435	U1436	G1371	G1310	G1246	A1182	U1110	A1048	U989	G924	U862	G800
			U1436	U1437	C1372	G1311	U1247	A1183	U1111	C1049	A990	G925	C862	A801
			C1437	U1438	A1373	C1312	G1248	A1184	A1112	U1050	U991	A926	C863	C802
			U1439		G1374	G1313	G1249	G1185	G1113	U1051	G991			
					U1375	C1314	G1250	G1186	U1114	U1052	A992	C927	A866	C803
					C1376	U1315	A1251	C1187	G1115	A1053	G993	C928	G867	C804
					G1377	C1316	A1252	U1188	G1116	A1054	G994	A929	C868	G805
					U1378	A1317	U1253	C1189	G1117	A1055	U995	U930	G869	A806
				U1443	U1379	A1318	C1254	A1190	C1118	U1056	A996	C931	G870	A807
				U1444	G1380	G1319	C1255	U1191	C1119		A997	U932	U871	A808
				G1446	U1381	G1320	G1256	C1192	A1120	G1066	A998	A933	U872	C809
				G1447	A1381	G1321	C1257	A1193	G999	G1059	G999	G934	C873	A810
				U1448	G1382	U1322	U1258	A1194	U1121			U935	U874	U811
				U1449		G1323	A1259	A1195		G1062	G1000	A936	G875	G812
				G1450	U1385	U1324	A1260	C1196	G1127	G1063	A1001	A937	A876	G813
					A1386	G1325	G1261	A1197	U1128	A1064	A1002	C937	U876	G814
					G1387	A1326	G1262	C1198	A1129	A1065	A1003	C938	C877	U814
					U1388	A1326	C1263	G1199	A1130	G1066	U1004	U939	G878	G815
					G1389	C1327	A1264	A1200	G1131	U1067	G1005	G940	U879	A816
					A1390	C1328	G1265	A1201	C1132	C1068	A1006	G941	G880	A817
					U1391	U1329	U1265	C1201	A1133	C1069	U1007	U942	C881	C818
					U1392	A1330	G1266	A1202	G1134	U1070	U1008	U943	A882	U819
					A1393	U1331	U1267	A1203	U1135	U1071	A1009	C944	A883	A820
					A1394	A1332	G1268	A1204	A1136	G1072	A1010		A884	U821
					G1395	C1333	U1269		C1137	U1073	A1011	G950	U885	G822
					U1396	U1334	A1270	U1208	U1138	U1074	A1012	A951	C886	C823
					C1397	G1335	A1271	G1209	G1139	A1075	G1013	A952	G887	C824
					U1398	U1336	C1272	U1210	G1140	C1076	G953	A954	A888	U825
					A1399	A1337	A1273	U1211	C1141	U1077	U1015	U954	U889	G826
					G1400	C1338	A1274	A1212	G1142	U1078			C990	A827

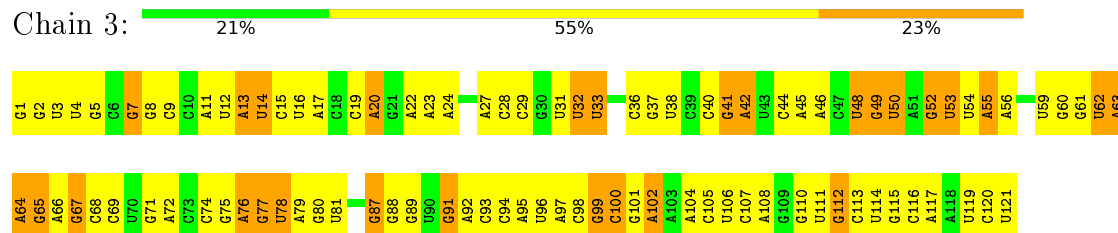
A2749	C2675	G2602	U2536	U2410	U2347	U2280	U2217	C2151	G	U	A	A1842	C1779
A2740	A2676	G2603	U2537	U2411	A2948	A2281	G2218	A2152	G	A	A	A1843	G1780
C2741	G2677	U2604	U2538	A2412	U2949	U2282	A2219	U2153	U	U	U	A1844	C1781
C2742	C2678	G2605	C2539	G2413	C2350	G2283	A2220	U2154	C	U	C	G1845	U1782
A2743	A2679	G2606	U2540	G2414	C2351	C2284	G2221	G2155	U	A	A	C1846	U1783
U2744	A2680	C2607	U2541	C2415	G2353	C2285	A2222	C2156	C	G	G	A1847	G1784
C2745	U2681	G2608	U2542	U2416	C2354	U2286	A2223	G2157	C	A	A	G1848	U1785
A2746	C2682	A2609	U2543	U2417	G2355	C2287	A2224	A2158	C	C	C	G1849	G1786
A2747	U2683	G2610	U2544	G2418	A2356	G2288	U2225	U2159	U	U	G	A1850	A1787
A2748	C2684	U2611	C2545	G2419	A2357	U2289	G2226	G2160	C	C	C	G1851	C1788
G2749	A2685	U2612	C2546	A	A2358	U2290	C2227	G2161	U	U	A	G1852	G1789
	A2686	G2613	A2547	A	C2359	A2291	A2228	U2162	C	C	C	U1853	G1790
U2752	C2687	U2614	C2548	A	U2292	U2292	A2229	U2163	U	U	U	C1854	
G2753	U2688	G2615	G2549	U	C2362	U2293	G2230		U	G	G	A1858	C1793
G2754	A2689	C2616	U2550	U	A2363	U2294	C2231	A2166	G	U	A	A1859	G1794
C2755	U2617	U2551	U2551	C	G2364	U2295	A2232	A2167	G	G	U	U1795	U1795
C2756	G2690	G2618	C2552	A	G2429	A2296	A2233	G2168	U	C	C	G1860	G1796
U2757	A2691	G2619	U2553	A	C2365	U2297	A2234	G2169	G	G	G	A1861	A1797
	A2692	G2620	U2554		C2367	U2298	G2236	U2170	U	U	U	U1862	A1798
C2760	A2695		G2555	U2433	A2368	A2299	G2237	A2171	C	A	A	G1863	A1799
G2761	C2625	G2625	U2556	U2434	G2369		G2238	A2172	G	G	U	A1864	A1800
A2762	A2626	U2627	A2557	G2435	G2370	G2302	G2239	U2173	A	U	A	A1865	
U2763	C2627	U2558	U2558	U2436	G2371		G2240	G2174	C	U	U	C1866	G1928
C2764	A2628	U2559	U2559	G2437	A2372	G2305	U2241	U2175	G	U	G	A1867	U1925
U2765	U2629	C2560		G2438	C2373	C2306	A2242	U2176	G	U	U	G1868	C1805
U2766	C2630		U2565	A2439	C2374	G2307	A2243	G2177	C	G	C	C1869	A1806
C2767	A2635	U2631	C2568	U2440	G2375	C2308	A2244	A2178	C	G	C	C1870	G1807
U2768	G2632		U2569	A2441	G2376	A2309	C2245	C2179	U	U	A	G1871	G1808
G2769	U2633	A2635	C2569	G2442	G2377	U2310	G2246	G2180	U	U	C	C1872	A1809
C2770	A2636	U2634	U2570	G2443	C2378	G2311	C2247	G2181	G	U	U	A1873	A1810
U2771	C2637	U2635	U2571	C2444	U2379	A2312	C2248	A2182	G	U	A	A1874	G1811
C2772	G2638		C2572	U2445	U2380	A2313	C2249	A2183	U	C	C	G1875	G1812
U2773	A2643	U2506	U2573	U2446	C2381	U2314	G2250	U2184	A	U	A	G1876	A1813
C2774	G2644	C2507	G2574	A2447	G2382	G2315	G2251	G2185	U	U	C	U1877	A1814
U2775	U2645	U2508	G2575	G2448	C2383	G2316	A2252	U2186	G	U	G	G1878	U1815
C2776	G2646	U2509	G2576	A2449	A2384	G2319	G2253	G2187	U	U	C	A1879	A1816
G2777	U2647	U2510	C2577	G2450	G2385	U2319	U2254	A2188	C	U	C	G1880	G1817
U2778	A2647	A2511	C2578	G2451	A2386	A2320	A2255		U	U	U	A1881	U1818
A2779	G2648	C2512	U2579	U	A2387		A2256		C	C	C	G1882	U1819
U2780	U2651	U2513	G2579	G2452	U2388	G2323	A2257	U2193	U	U	G	U1820	U1820
U2781	U2652	U2514	A2580	U	C2389	A2324	U2258	G2194	C	U	C	U1821	A1821
	G2720	U2651	U2581	A	A2390	G2325	A2259	C2196	U	U	G	A1886	C1822
		U2516		G	C2392	A2326	U2260	C2197	A	U	U	A1887	A1823
		U2517		A	C2393		A2261	A2198	C	U	G	G1888	U1824
			G2584	A	G2393		A2262	G2199	G	G	G	G1889	G1825
			G2585	A	C2396		C2263	U2200	A	C	A	G1890	C1826
			G2586	U	G2396		U2264	G2201	C	U	C	A1891	C1827
			U2587	U	A2397		G2265	C2202	C	C	C	G1892	A1828
			U2588	A	A2398		U2266	U2203	G	U	A	A1893	G1829
			G2589	A	A2399		C2267	C2204	U	U	C	U1894	G1830
			A2590	G	A2399			U2205	C	C	C	A1895	U1831
			A2591	U	G2400			U2141	C	U	U	A1896	C1832
			G2592	U	A2401		A2270	A2142	G	U	G	A1897	G1833
			G2593	G	A2402		A2271	A2143	C	A	A	G1898	U1834
			C2594	G	G2403		G2272	A2144	U	G	G	A1899	A1835
				A	A2404		G2273	U2209	U	U	C	A1900	C1836
				G	C2405		U2274	G2210	G	C	C	A1901	
			U2597	C	C2406		A2275	A2146	C	G	C	A1902	A1839
			G2598	U	C2407		G2276	A2148	U	U	U	G1903	U1840
			U2599	U	G2408			A2214	A	A	C	U1903	
			C2600	U	A2345								
			A2601	C	C2346		A2279	G2150					



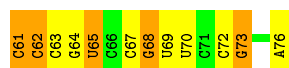
• Molecule 2: 60S ribosomal protein L23-A



• Molecule 3: 5S rRNA



• Molecule 4: 60S ribosomal protein L24-A



- Molecule 10: 60S ribosomal protein L27-A

Chain b: 99%



- Molecule 11: 60S ribosomal protein L42-A

Chain C: 70% 29%



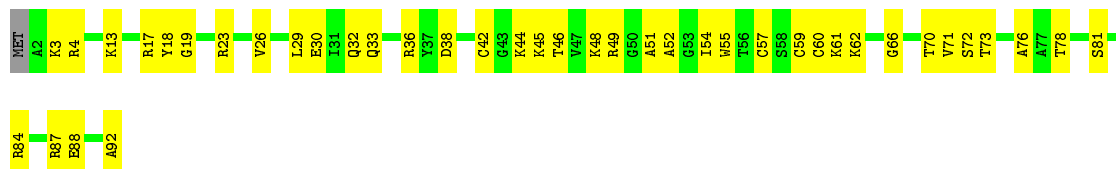
- Molecule 12: 60S ribosomal protein L28

Chain c: 97%



- Molecule 13: 60S ribosomal protein L43-A

Chain D: 54% 45%



- Molecule 14: 60S ribosomal protein L29

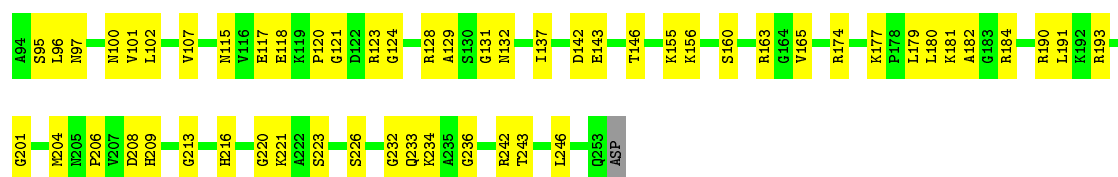
Chain d: 97%



- Molecule 15: 60S ribosomal protein L2-A

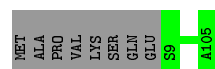
Chain E: 62% 37%





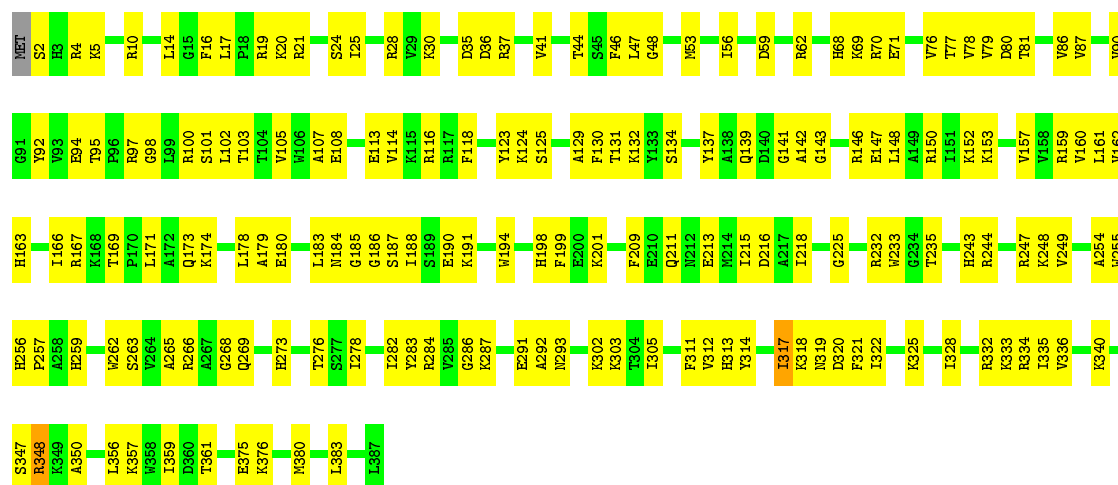
- Molecule 16: 60S ribosomal protein L30

Chain e: 92% 8%



- Molecule 17: 60S ribosomal protein L3

Chain F: 56% 43%



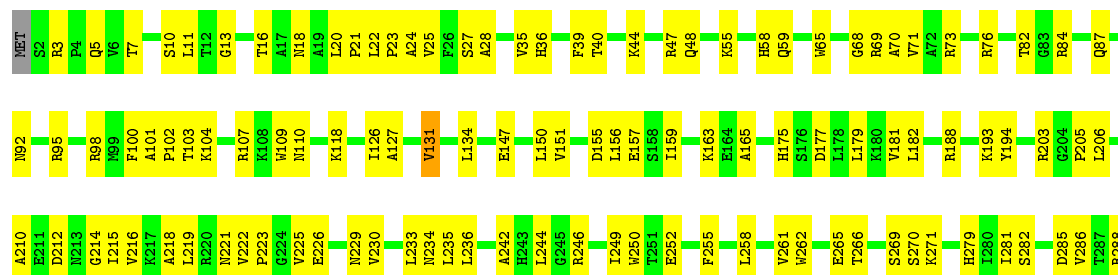
- Molecule 18: 60S ribosomal protein L31-A

Chain f: 100%

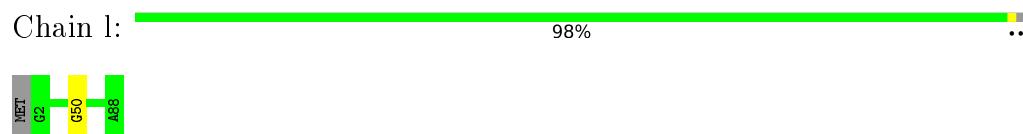
There are no outlier residues recorded for this chain.

- Molecule 19: 60S ribosomal protein L4-A

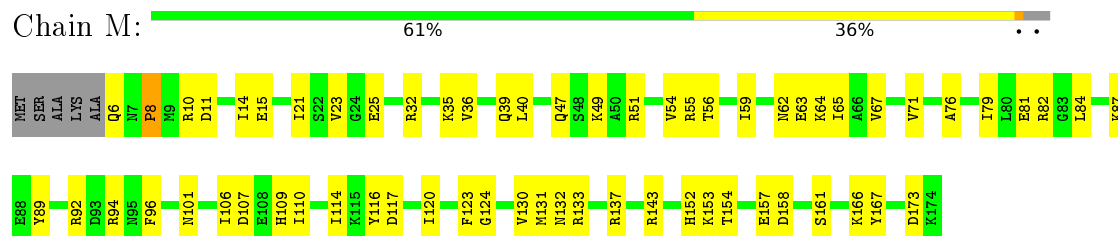
Chain G: 63% 36%



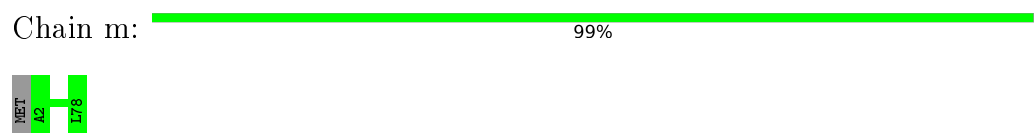
- Molecule 30: 60S ribosomal protein L37-A



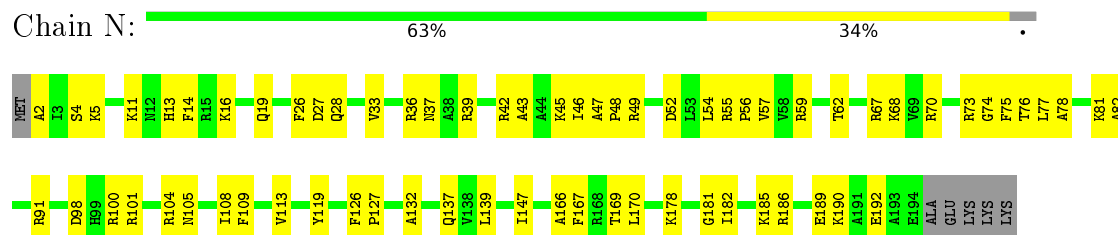
- Molecule 31: 60S ribosomal protein L11-A



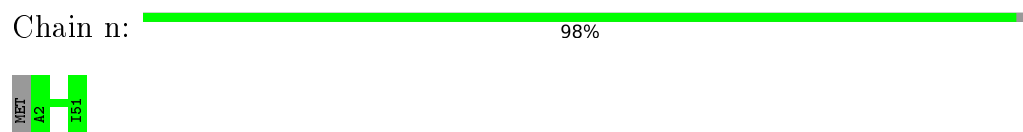
- Molecule 32: 60S ribosomal protein L38



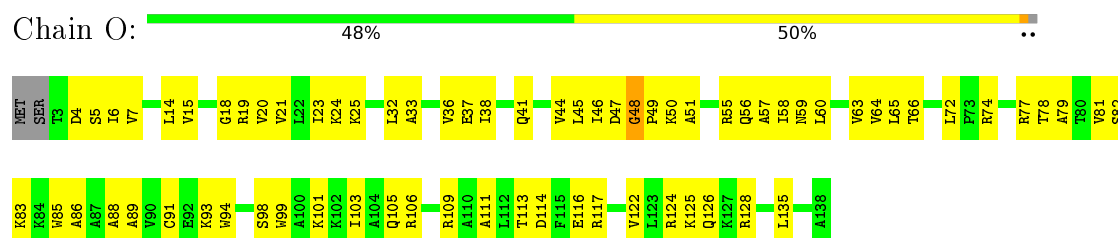
- Molecule 33: 60S ribosomal protein L13-A



- Molecule 34: 60S ribosomal protein L39

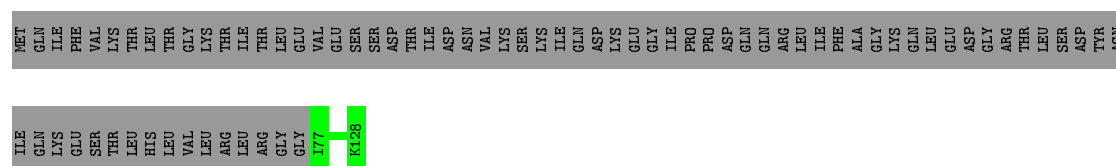


- Molecule 35: 60S ribosomal protein L14-B



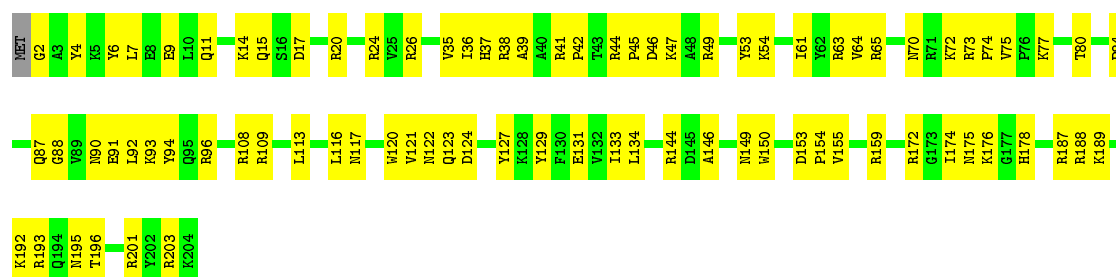
- Molecule 36: Ubiquitin-60S ribosomal protein L40

Chain o:  41% 59%



- Molecule 37: 60S ribosomal protein L15-A

Chain P:  59% 41%



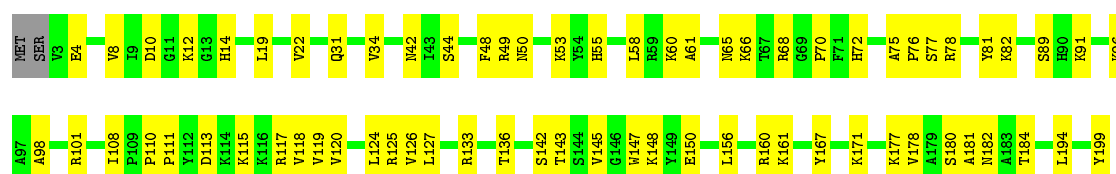
- Molecule 38: 60S ribosomal protein L41-A

Chain p:  100%


There are no outlier residues recorded for this chain.

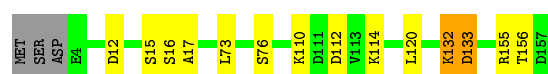
- Molecule 39: 60S ribosomal protein L16-A

Chain Q:  64% 35%



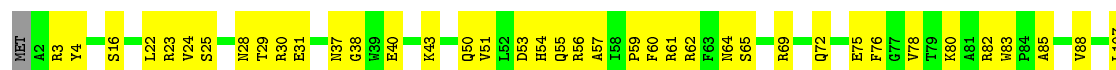
- Molecule 40: Eukaryotic translation initiation factor 5A-1

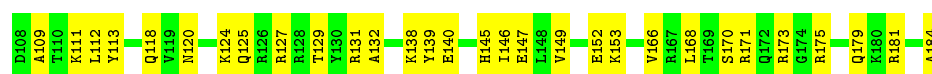
Chain q:  89% 8%



- Molecule 41: 60S ribosomal protein L17-A

Chain R:  62% 38%





- Molecule 42: ribosomal protein RPL1

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 60S ribosomal protein L18-A

Chain S:  66%  33% ..



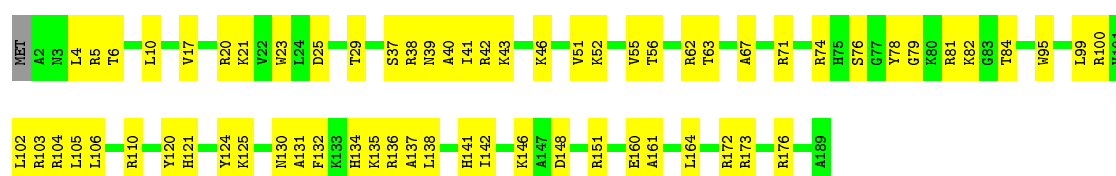
- Molecule 44: 60S ribosomal protein L10

Chain s:  94% ..



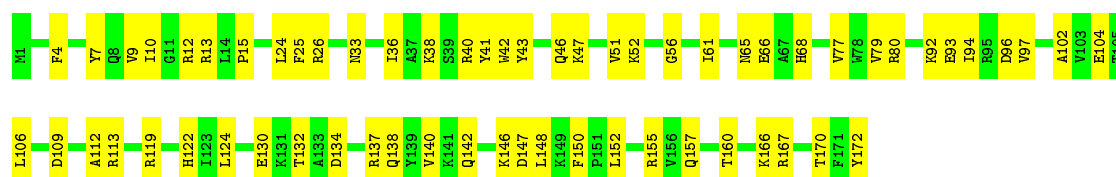
- Molecule 45: 60S ribosomal protein L19-A

Chain T:  65%  34% .



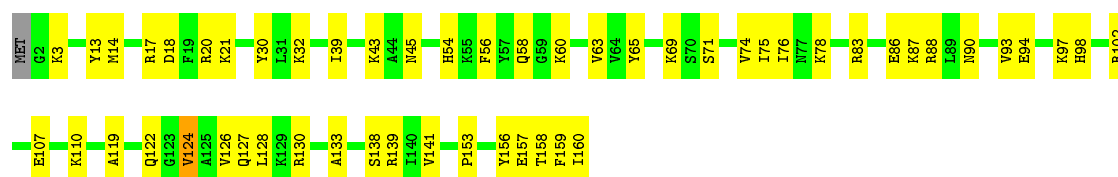
- Molecule 46: 60S ribosomal protein L20-A

Chain U:  64%  36%



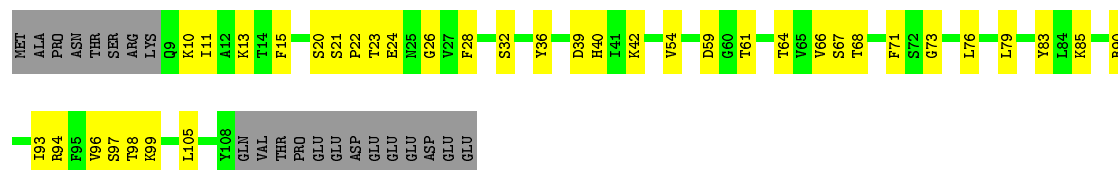
- Molecule 47: 60S ribosomal protein L21-A

Chain V:  66%  33% ..



- Molecule 48: 60S ribosomal protein L22-A

Chain W: 52% 31% 17%



- Molecule 49: nascent polypeptide chain

Chain z: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	62532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5CT, 3HE

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.73	0/75774	1.03	156/118137 (0.1%)
10	b	0.35	0/1118	0.51	0/1497
11	C	0.37	0/860	0.53	0/1136
12	c	0.40	0/1204	0.54	0/1612
13	D	0.42	0/701	0.60	0/934
14	d	0.36	0/473	0.48	0/629
15	E	0.41	0/1948	0.56	0/2617
16	e	0.34	0/751	0.50	0/1008
17	F	0.40	0/3146	0.55	0/4228
18	f	0.40	0/890	0.54	0/1196
19	G	0.39	0/2800	0.53	0/3790
2	X	0.39	0/1018	0.52	0/1369
20	g	0.39	0/1041	0.54	0/1394
21	H	0.34	0/2425	0.50	0/3271
22	h	0.45	0/868	0.53	0/1168
23	I	0.34	0/1260	0.47	0/1694
24	i	0.39	0/890	0.52	0/1189
25	J	0.41	0/1821	0.50	0/2451
26	j	0.33	0/978	0.47	0/1301
27	K	0.35	0/1836	0.52	0/2481
28	k	0.31	0/778	0.50	0/1034
29	L	0.37	0/1539	0.53	0/2073
3	3	0.61	0/2883	0.94	0/4491
30	l	0.44	0/696	0.54	0/923
31	M	0.33	0/1374	0.51	0/1842
32	m	0.31	0/618	0.53	0/826
33	N	0.36	0/1568	0.52	0/2106
34	n	0.36	0/443	0.51	0/588
35	O	0.34	0/1068	0.52	0/1438
36	o	0.37	0/423	0.52	0/562
37	P	0.45	0/1757	0.58	0/2354
38	p	0.29	0/234	0.52	0/300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	Q	0.41	0/1585	0.54	0/2128
4	Y	0.32	0/712	0.50	0/958
40	q	0.32	0/1142	0.61	0/1537
41	R	0.40	0/1443	0.55	0/1944
43	S	0.37	0/1465	0.54	0/1965
44	s	0.40	0/1807	0.54	0/2425
45	T	0.34	0/1538	0.48	0/2050
46	U	0.43	0/1481	0.55	0/1990
47	V	0.39	0/1300	0.54	0/1743
48	W	0.36	0/812	0.52	0/1099
5	4	0.73	0/3746	0.99	8/5832 (0.1%)
6	Z	0.39	0/979	0.54	0/1321
7	A	0.52	0/1799	1.03	4/2801 (0.1%)
8	a	0.34	0/1004	0.55	1/1341 (0.1%)
9	B	0.57	1/1835 (0.1%)	1.01	1/2858 (0.0%)
All	All	0.61	1/137831 (0.0%)	0.89	170/203631 (0.1%)

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
17	F	0	1
25	J	0	1
27	K	0	1
30	l	0	1
35	O	0	1
39	Q	0	1
40	q	0	1
43	S	0	1
44	s	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1	G	OP3-P	-10.85	1.48	1.61

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	922	U	C2-N1-C1'	8.41	127.79	117.70
1	1	3278	C	C2-N1-C1'	7.92	127.51	118.80
1	1	1836	C	N3-C2-O2	-7.81	116.43	121.90
1	1	2867	C	N1-C2-O2	7.79	123.57	118.90
1	1	1836	C	N1-C2-O2	7.77	123.56	118.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	F	348	ARG	Peptide
25	J	108	LEU	Peptide
27	K	76	ALA	Peptide
35	O	48	GLY	Peptide
30	l	50	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	1	67695	0	34019	2941	0
2	X	1003	0	1048	42	0
3	3	2579	0	1304	112	0
4	Y	699	0	640	23	0
5	4	3353	0	1695	138	0
6	Z	964	0	1025	40	0
7	A	1611	0	816	88	0
8	a	993	0	1081	0	0
9	B	1644	0	831	69	0
10	b	1092	0	1155	0	0
11	C	847	0	918	46	0
12	c	1173	0	1215	0	0
13	D	694	0	738	44	0
14	d	462	0	491	0	0
15	E	1914	0	1981	95	0
16	e	743	0	797	0	0
17	F	3075	0	3142	155	0
18	f	876	0	912	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	2748	0	2859	122	0
20	g	1020	0	1090	0	0
21	H	2375	0	2325	147	0
22	h	850	0	880	0	0
23	I	1239	0	1326	63	0
24	i	880	0	945	0	0
25	J	1784	0	1862	70	0
26	j	969	0	1078	0	0
27	K	1804	0	1877	99	0
28	k	771	0	849	0	0
29	L	1518	0	1587	66	0
30	l	681	0	687	0	0
31	M	1353	0	1383	52	0
32	m	612	0	682	0	0
33	N	1543	0	1608	71	0
34	n	436	0	475	0	0
35	O	1053	0	1149	79	0
36	o	417	0	459	0	0
37	P	1720	0	1779	104	0
38	p	233	0	284	0	0
39	Q	1555	0	1659	54	0
40	q	1143	0	1107	0	0
41	R	1420	0	1437	67	0
42	r	1050	0	222	0	0
43	S	1441	0	1543	74	0
44	s	1770	0	1808	0	0
45	T	1521	0	1617	70	0
46	U	1445	0	1487	63	0
47	V	1276	0	1323	50	0
48	W	796	0	812	25	0
49	z	115	0	37	0	0
50	1	20	0	23	2	0
All	All	128975	0	92067	4460	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 24.

The worst 5 of 4460 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)
1:1:520:U:OP2	25:J:70:LYS:NZ	1.71	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:208:C:OP2	19:G:163:LYS:NZ	1.75	1.20
45:T:103:ARG:NH1	45:T:124:TYR:OH	1.82	1.13
1:1:1382:G:OP2	19:G:188:ARG:NH1	1.84	1.11
1:1:73:C:N3	33:N:59:ARG:NH1	1.99	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
4	Y	96/155 (62%)	86 (90%)	10 (10%)	0	100	100
6	Z	119/142 (84%)	111 (93%)	7 (6%)	1 (1%)	24	68
8	a	124/127 (98%)	109 (88%)	15 (12%)	0	100	100
10	b	133/136 (98%)	120 (90%)	12 (9%)	1 (1%)	24	68
11	C	103/106 (97%)	88 (85%)	15 (15%)	0	100	100
12	c	146/149 (98%)	128 (88%)	15 (10%)	3 (2%)	9	51
13	D	89/92 (97%)	79 (89%)	10 (11%)	0	100	100
14	d	56/59 (95%)	48 (86%)	7 (12%)	1 (2%)	11	54
15	E	250/254 (98%)	230 (92%)	20 (8%)	0	100	100
16	e	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
17	F	384/387 (99%)	358 (93%)	25 (6%)	1 (0%)	46	82
18	f	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
19	G	359/362 (99%)	319 (89%)	38 (11%)	2 (1%)	30	73
20	g	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
21	H	294/297 (99%)	260 (88%)	31 (10%)	3 (1%)	19	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	h	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
23	I	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	26	70
24	i	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
25	J	220/244 (90%)	202 (92%)	18 (8%)	0	100	100
26	j	117/120 (98%)	103 (88%)	14 (12%)	0	100	100
27	K	231/256 (90%)	205 (89%)	23 (10%)	3 (1%)	15	60
28	k	97/100 (97%)	80 (82%)	16 (16%)	1 (1%)	19	64
29	L	189/191 (99%)	169 (89%)	20 (11%)	0	100	100
30	l	85/88 (97%)	74 (87%)	11 (13%)	0	100	100
31	M	167/174 (96%)	145 (87%)	20 (12%)	2 (1%)	16	61
32	m	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
33	N	191/199 (96%)	171 (90%)	20 (10%)	0	100	100
34	n	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
35	O	134/138 (97%)	119 (89%)	15 (11%)	0	100	100
36	o	50/128 (39%)	46 (92%)	4 (8%)	0	100	100
37	P	201/204 (98%)	176 (88%)	25 (12%)	0	100	100
38	p	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
39	Q	195/199 (98%)	179 (92%)	16 (8%)	0	100	100
40	q	151/157 (96%)	127 (84%)	14 (9%)	10 (7%)	1	25
41	R	181/184 (98%)	166 (92%)	15 (8%)	0	100	100
43	S	183/186 (98%)	169 (92%)	14 (8%)	0	100	100
44	s	218/221 (99%)	180 (83%)	29 (13%)	9 (4%)	3	36
45	T	186/189 (98%)	169 (91%)	16 (9%)	1 (0%)	34	76
46	U	170/172 (99%)	151 (89%)	18 (11%)	1 (1%)	30	73
47	V	157/160 (98%)	150 (96%)	6 (4%)	1 (1%)	30	73
48	W	98/121 (81%)	86 (88%)	11 (11%)	1 (1%)	19	64
All	All	6347/6736 (94%)	5722 (90%)	583 (9%)	42 (1%)	31	70

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	c	48	TYR
23	I	98	VAL

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Mol	Chain	Res	Type
40	q	110	LYS
40	q	112	ASP
40	q	133	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	104/105 (99%)	104 (100%)	0	100	100
4	Y	57/129 (44%)	57 (100%)	0	100	100
6	Z	104/118 (88%)	104 (100%)	0	100	100
8	a	109/110 (99%)	109 (100%)	0	100	100
10	b	115/116 (99%)	115 (100%)	0	100	100
11	C	90/91 (99%)	90 (100%)	0	100	100
12	c	118/119 (99%)	118 (100%)	0	100	100
13	D	71/72 (99%)	71 (100%)	0	100	100
14	d	46/47 (98%)	46 (100%)	0	100	100
15	E	193/196 (98%)	193 (100%)	0	100	100
16	e	81/88 (92%)	81 (100%)	0	100	100
17	F	320/323 (99%)	319 (100%)	1 (0%)	94	97
18	f	92/96 (96%)	92 (100%)	0	100	100
19	G	288/289 (100%)	288 (100%)	0	100	100
20	g	109/111 (98%)	109 (100%)	0	100	100
21	H	244/245 (100%)	243 (100%)	1 (0%)	93	97
22	h	90/91 (99%)	90 (100%)	0	100	100
23	I	134/153 (88%)	134 (100%)	0	100	100
24	i	95/103 (92%)	95 (100%)	0	100	100
25	J	186/205 (91%)	186 (100%)	0	100	100
26	j	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	K	187/208 (90%)	187 (100%)	0	100	100
28	k	81/82 (99%)	81 (100%)	0	100	100
29	L	171/171 (100%)	171 (100%)	0	100	100
30	l	70/71 (99%)	70 (100%)	0	100	100
31	M	147/150 (98%)	147 (100%)	0	100	100
32	m	68/69 (99%)	68 (100%)	0	100	100
33	N	154/159 (97%)	154 (100%)	0	100	100
34	n	45/46 (98%)	45 (100%)	0	100	100
35	O	107/109 (98%)	107 (100%)	0	100	100
36	o	47/116 (40%)	47 (100%)	0	100	100
37	P	175/176 (99%)	175 (100%)	0	100	100
38	p	23/23 (100%)	23 (100%)	0	100	100
39	Q	160/162 (99%)	160 (100%)	0	100	100
40	q	118/132 (89%)	113 (96%)	5 (4%)	36	72
41	R	140/146 (96%)	140 (100%)	0	100	100
43	S	150/151 (99%)	150 (100%)	0	100	100
44	s	184/187 (98%)	178 (97%)	6 (3%)	45	77
45	T	153/154 (99%)	153 (100%)	0	100	100
46	U	156/156 (100%)	156 (100%)	0	100	100
47	V	136/137 (99%)	136 (100%)	0	100	100
48	W	87/107 (81%)	87 (100%)	0	100	100
All	All	5309/5624 (94%)	5296 (100%)	13 (0%)	95	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	q	133	ASP
40	q	155	ARG
44	s	108	ASP
40	q	132	LYS
44	s	104	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
19	G	221	ASN
27	K	38	GLN
44	s	112	GLN
19	G	279	HIS
21	H	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3162/3396 (93%)	1117 (35%)	336 (10%)
3	3	120/121 (99%)	30 (25%)	7 (5%)
5	4	157/158 (99%)	58 (36%)	20 (12%)
7	A	75/76 (98%)	40 (53%)	7 (9%)
9	B	76/77 (98%)	35 (46%)	6 (7%)
All	All	3590/3828 (93%)	1280 (35%)	376 (10%)

5 of 1280 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	11	A
1	1	13	A
1	1	14	U
1	1	15	C

5 of 376 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1656	A
1	1	2174	G
5	4	38	U
1	1	1724	U
1	1	1842	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
40	5CT	q	51	40	12,14,15	0.37	0	12,15,17	1.38	3 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	5CT	q	51	40	-	0/12/14/16	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
40	q	51	5CT	C4-C3-C2	-2.60	109.16	113.70
40	q	51	5CT	C1-NZ-CE	-2.38	108.23	113.83
40	q	51	5CT	O-C-CA	-2.01	120.33	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	3HE	1	3401	-	21,21,21	0.83	1 (4%)	18,30,30	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3HE	1	3401	-	-	0/8/36/36	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	3401	3HE	C5-C7	3.15	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	1	3401	3HE	2	0

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.