



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:34 AM UTC

PDB ID : 7ASE / pdb_00007ase
EMDB ID : EMD-11893
Title : 43S preinitiation complex from Trypanosoma cruzi with the kDDX60 helicase
Authors : Bochler, A.; Brito Querido, J.; Prilepskaja, T.; Soufari, H.; Del Cistia, M.L.; Kuhn, L.; Rimoldi Ribeiro, A.; Valasek, L.S.; Hashem, Y.
Deposited on : 2020-10-27
Resolution : 3.33 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

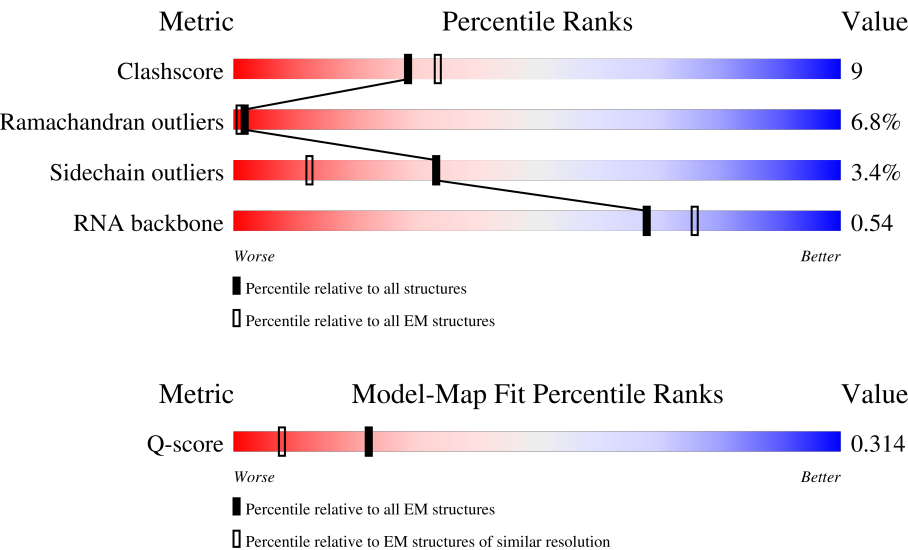
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.33 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14484 (2.83 - 3.83)

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 $\leq 5\%$. 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	f	2174	54% 46% 16% 5% • 30%
2	1	75	13% 83% 11% • •
3	0	2319	18% 72% 18% • 7%

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Mol	Chain	Length	Quality of chain
4	y	137	
5	s	418	
6	j	150	
7	n	343	
8	p	318	
9	r	149	
10	u	153	
11	m	143	
12	Z	221	
13	o	190	
14	q	211	
15	R	151	
16	S	86	
17	t	112	
18	U	91	
19	v	144	
20	X	173	
21	B	190	
22	F	245	
23	d	263	
24	g	247	
25	a	110	
26	J	257	
27	h	141	
28	5	477	

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Mol	Chain	Length	Quality of chain
29	P	250	
30	i	141	
31	L	117	
32	M	214	
33	N	161	
34	O	167	
35	b	145	
36	c	66	
37	V	109	
38	w	166	
39	E	407	
40	Y	379	
41	Q	57	
42	D	34	
43	G	345	
44	K	203	
45	T	152	
46	C	716	
47	8	762	
48	W	254	
49	I	489	
50	H	334	
51	A	502	
52	l	273	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	GNP	5	502	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 136847 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 protein called kDDX60.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	1523	Total	C	N	O	S	0	0
			12257	7734	2165	2292	66		

- Molecule 2 is a RNA chain called initiator tRNA-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	75	Total	C	N	O	P	0	0
			1606	718	300	514	74		

- Molecule 3 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	2150	Total	C	N	O	P	0	0
			45795	20471	8144	15037	2143		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	143	C	A	conflict	GB 320364483
0	805	C	U	conflict	GB 320364483
0	2321	U	-	insertion	GB 320364483
0	2322	U	-	insertion	GB 320364483
0	2323	U	-	insertion	GB 320364483

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	123	Total	C	N	O	S	0	0
			989	628	194	165	2		

- Molecule 5 is a protein called Elongation initiation factor 2 alpha subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	s	295	Total	C	N	O	S	0	0
			2365	1489	436	427	13		

- Molecule 6 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	79	Total	C	N	O	S	0	0
			644	409	123	106	6		

- Molecule 7 is a protein called Translation initiation factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	225	Total	C	N	O	S	0	0
			1796	1111	335	339	11		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	310	Total	C	N	O	S	0	0
			2405	1505	424	463	13		

- Molecule 9 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	140	Total	C	N	O	S	0	0
			1113	706	212	192	3		

- Molecule 10 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	u	136	Total	C	N	O	S	0	0
			1108	689	224	190	5		

- Molecule 11 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	142	Total	C	N	O	S	0	0
			1116	706	220	188	2		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	175	Total	C	N	O	S	0	0
			1404	885	283	233	3		

- Molecule 13 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	190	Total	C	N	O	S	0	0
			1493	932	286	269	6		

- Molecule 14 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	200	Total	C	N	O	S	0	0
			1670	1063	324	277	6		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	141	Total	C	N	O	S	0	0
			1143	724	221	190	8		

- Molecule 16 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	82	Total	C	N	O	S	0	0
			630	384	121	116	9		

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	104	Total	C	N	O	S	0	0
			829	510	177	132	10		

- Molecule 18 is a protein called 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	68	Total	C	N	O	S	0	0
			526	315	107	100	4		

- Molecule 19 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	135	Total	C	N	O	S	0	0
			1011	620	195	187	9		

- Molecule 20 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	148	Total	C	N	O	S	0	0
			1212	760	239	207	6		

- Molecule 21 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	179	Total	C	N	O	S	0	0
			1483	935	297	243	8		

- Molecule 22 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	207	Total	C	N	O	S	0	0
			1658	1060	299	288	11		

- Molecule 23 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	223	Total	C	N	O	S	0	0
			1726	1098	304	314	10		

- Molecule 24 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	83	Total	C	N	O	S	0	0
			635	395	116	122	2		

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	70	Total	C	N	O	S	0	0
			553	356	97	97	3		

- Molecule 26 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	173	Total	C	N	O	S	0	0
			1358	862	259	234	3		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	121	Total	C	N	O	S	0	0
			958	594	174	185	5		

- Molecule 28 is a protein called Eukaryotic translation initiation factor 2 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	421	Total	C	N	O	S	0	0
			3245	2049	581	596	19		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	249	Total	C	N	O	S	0	0
			1983	1244	402	333	4		

- Molecule 30 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	121	Total	C	N	O	S	0	0
			992	623	190	174	5		

- Molecule 31 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	99	Total	C	N	O	S	0	0
			784	497	144	140	3		

- Molecule 32 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	200	Total	C	N	O	S	0	0
			1587	995	302	279	11		

- Molecule 33 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	93	Total	C	N	O	S	0	0
			780	508	136	132	4		

- Molecule 34 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	140	Total	C	N	O	S	0	0
			1116	702	221	185	8		

- Molecule 35 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	129	Total	C	N	O	S	0	0
			1019	647	188	176	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	83	THR	ALA	conflict	UNP Q4CXX2

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	60	Total	C	N	O	S	0	0
			480	303	98	78	1		

- Molecule 37 is a protein called Protein translation factor SUI1 homolog, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	97	Total	C	N	O	S	0	0
			789	490	152	145	2		

- Molecule 38 is a protein called Putative eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	147	Total	C	N	O	S	0	0
			1162	716	209	236	1		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	391	Total	C	N	O	S	0	0
			3119	1977	536	593	13		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	174	Total	C	N	O	S	0	0
			1387	872	243	260	12		

- Molecule 41 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	57	Total	C	N	O	S	0	0
			462	283	96	77	6		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	33	Total	C	N	O	S	0	0
			294	178	76	38	2		

- Molecule 43 is a protein called JAB_MPN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	308	Total	C	N	O	S	0	0
			2414	1492	442	466	14		

- Molecule 44 is a protein called CSN8_PSD8_EIF3K domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	K	201	Total	C	N	O	S	0	0
			1566	1001	256	304	5		

- Molecule 45 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	132	Total	C	N	O	S	0	0
			1057	670	204	179	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit 8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C	696	Total	C	N	O	S	0	0
			5630	3542	973	1092	23		

- Molecule 47 is a protein called eIF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	8	576	Total	C	N	O	S	0	0
			4596	2882	845	847	22		

- Molecule 48 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	217	Total	C	N	O	S	0	0
			1781	1124	337	313	7		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	I	344	Total	C	N	O	S	0	0
			2770	1771	479	503	17		

- Molecule 50 is a protein called eIF3H.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	H	297	Total	C	N	O	S	0	0
			2388	1498	421	451	18		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit 7-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	483	Total	C	N	O	S	0	0
			3891	2446	691	729	25		

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	258	Total	C	N	O	S	0	0
			2038	1290	383	354	11		

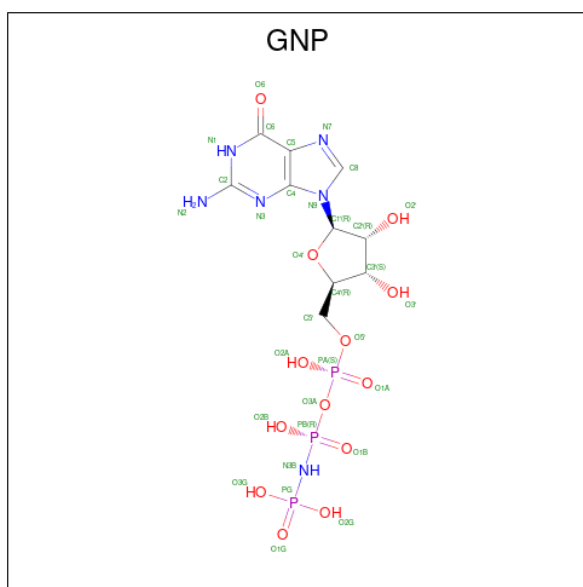
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	n	1	Total	Zn	0
			1	1	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	5	1	Total	Mg	0
			1	1	

- Molecule 55 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

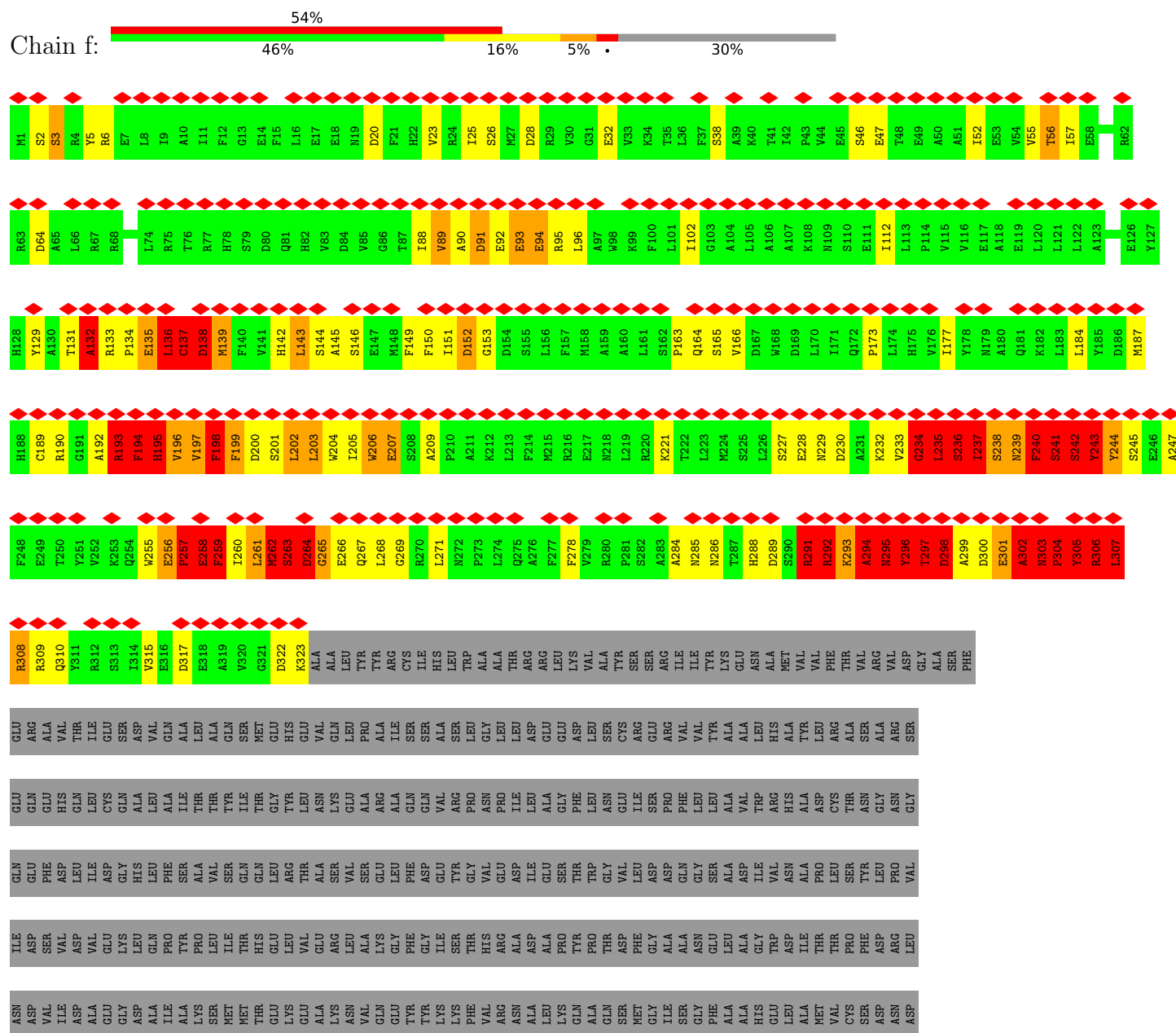


Mol	Chain	Residues	Atoms					AltConf
55	5	1	Total	C	N	O	P	0
			32	10	6	13	3	

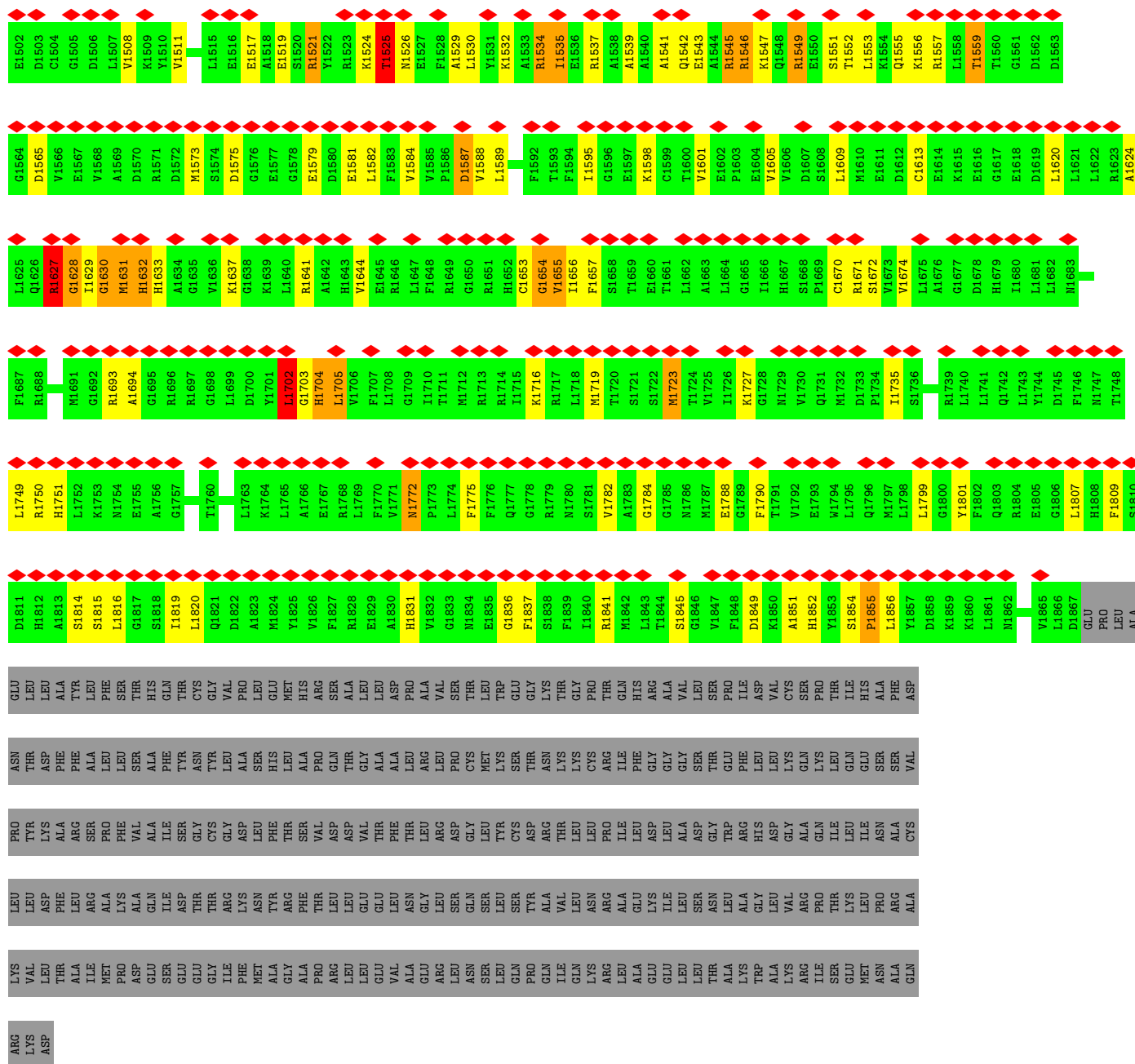
3 Residue-property plots

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.

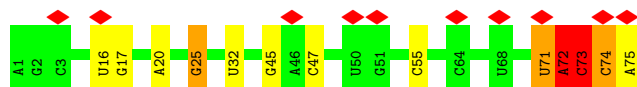
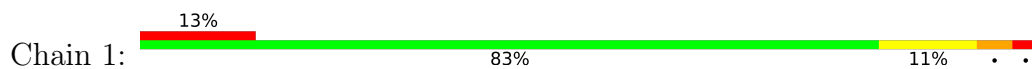
• Molecule 1: kDDX60



E1440	E1441	M1442	M1443	E1444	Q1445	S1447	E1448	E1449	Q1450	G1451	G1452	A1453	Q1454	E1455	E1456	E1457	Q1458	E1459	K1460	E1461	T1462	V1463	G1464	S1465	V1466	S1467	F1468	P1469	D1470	G1471	R1472	Q1473	F1474	L1475	R1476	E1477	H1478	I1479	L1483	R1484	E1485	L1486	I1487	A1488	R1489	D1490	M1491	G1492	P1493	T1494	V1495	F1497	S1498	F1499	E1500	S1501	
A1380	S1381	M1382	N1383	A1384	V1386	E1387	S1388	I1389	L1390	R1391	T1392	F1393	A1394	Q1395	K1396	L1397	N1398	E1399	D1400	E1401	A1402	L1403	L1404	E1405	R1406	A1407	A1408	A1409	D1410	G1411	M1412	E1413	K1414	K1415	L1416	R1417	M1418	L1419	L1420	R1421	Q1422	Q1423	H1424	L1425	Q1426	L1427	Q1429	Q1430	E1431	E1432	Q1433	E1434	N1435	E1436	P1437	Q1439	
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K1253	A1254	Q1255	Y1256	N1257	N1258	C1259	I1261	R1262	D1263	L1264	H1265	P1266	S1267	S1268	I1269	L1270	T1271	A1272	D1273	Q1274	L1275	Q1276	R1277	G1278	F1279	P1280	P1281	D1282	I1283	S1284	L1285	V1286	P1287	S1288	E1289	V1290	V1291	S1292	E1295	K1296	M1297	H1298	S1299	K1300	F1301	N1302	E1303	V1304	V1305	V1306	P1307	N1308	Y1309	S1310	S1311	L1312	Q1313
L1314	A1315	K1316	T1317	L1318	R1319	A1320	Q1321	L1322	M1323	L1324	I1325	E1326	P1327	S1328	K1329	L1330	F1331	E1332	A1333	E1334	T1335	Y1336	I1337	T1338	Q1339	E1340	R1341	Q1344	E1345	V1349	K1350	N1351	A1352	F1353	Y1358	L1359	G1360	H1361	E1362	G1363	C1364	E1365	L1366	P1367	E1368	N1369	L1370	V1371	E1372	E1373	D1374	L1375	D1376	D1377	F1378	S1379	
A1380	S1381	M1382	N1383	A1384	V1386	E1387	S1388	I1389	L1390	R1391	T1392	F1393	A1394	Q1395	K1396	L1397	N1398	E1399	D1400	E1401	A1402	L1403	L1404	E1405	R1406	A1407	A1408	A1409	D1410	G1411	M1412	E1413	K1414	K1415	L1416	R1417	M1418	L1419	L1420	R1421	Q1422	Q1423	H1424	L1425	Q1426	L1427	Q1429	Q1430	E1431	E1432	Q1433	E1434	N1435	E1436	P1437	Q1439	
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L792	V793	A794	R795	S796	Q797	L798	R799	E800	V801	E802	F803	A804	F805	A806	M807	E808	D809	L812	K813	A816	K820	K821	K822	D823	S824	K825	S826	E827	Y828	K829	M830	L831	Y832	G833	E834	H835	V836	I837	N838	Q839	F840	R843	E844	V846	K847	G848	N849	H850	W851	G852	Q853	L854	D855	P856			
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E1129	T1130	F1131	W1134	S1137	P1138	K1139	Y1140	T1141	D1142	W1143	V1144	E1145	L1146	I1147	D1148	V1149	I1151	L1152	D1153	E1154	I1155	H1156	S1157	M1158	E1159	S1160	N1161	G1162	N1163	G1164	D1165	V1166	W1167	E1168	R1169	L1170	L1171	A1172	L1173	L1174	P1175	C1176	P1177	F1178	V1179	A1180	L1181	S1182	A1183	T1184	L1185	G1186	E1187	T1188	Q1189	Q1190	
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A1380	S1381	M1382	N1383	A1384	V1386	E1387	S1388	I1389	L1390	R1391	T1392	F1393	A1394	Q1395	K1396	L1397	N1398	E1399	D1400	E1401	A1402	L1403	L1404	E1405	R1406	A1407	A1408	A1409	D1410	G1411	M1412	E1413	K1414	K1415	L1416	R1417	M1418	L1419	L1420	R1421	Q1422	Q1423	H1424	L1425	Q1426	L1427	Q1429	Q1430	E1431	E1432	Q1433	E1434	N1435	E1436	P1437	Q1439	
E1440	E1441	M1442	M1443	E1444	Q1445	S1447	E1448	E1449	Q1450	G1451	G1452	A1453	Q1454	E1455	E1456	E1457	Q1458	E1459	K1460	E1461	T1462	V1463	G1464	S1465	V1466	S1467	F1468	P1469	D1470	G1471	R1472	Q1473	F1474	L1475	R1476	E1477	H1478	I1479	L1483	R1484	E1485	L1486	I1487	A1488	R1489	D1490	M1491	G1492	P1493	T1494	V1495	F1497	S1498	F1499	E1500	S1501	

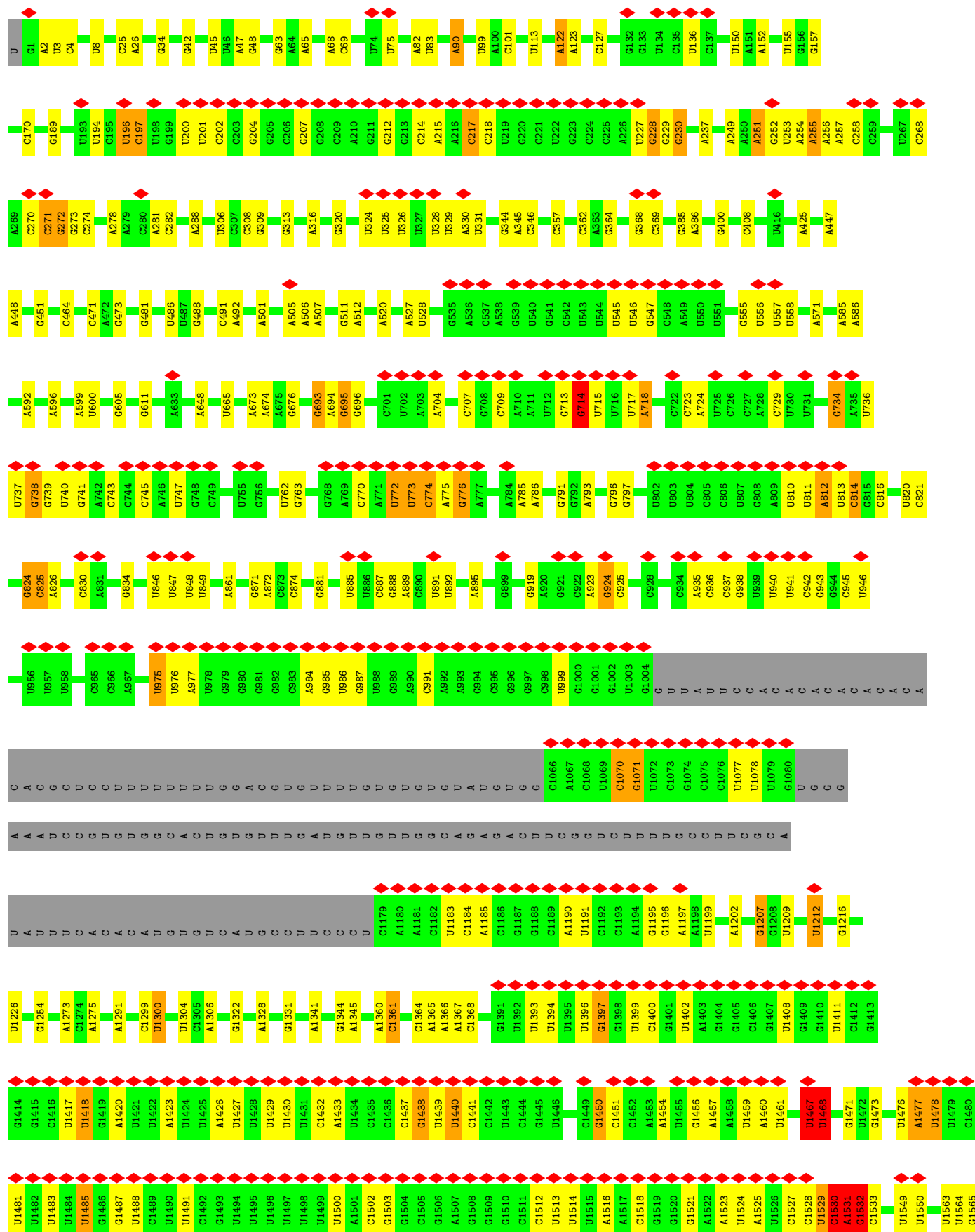


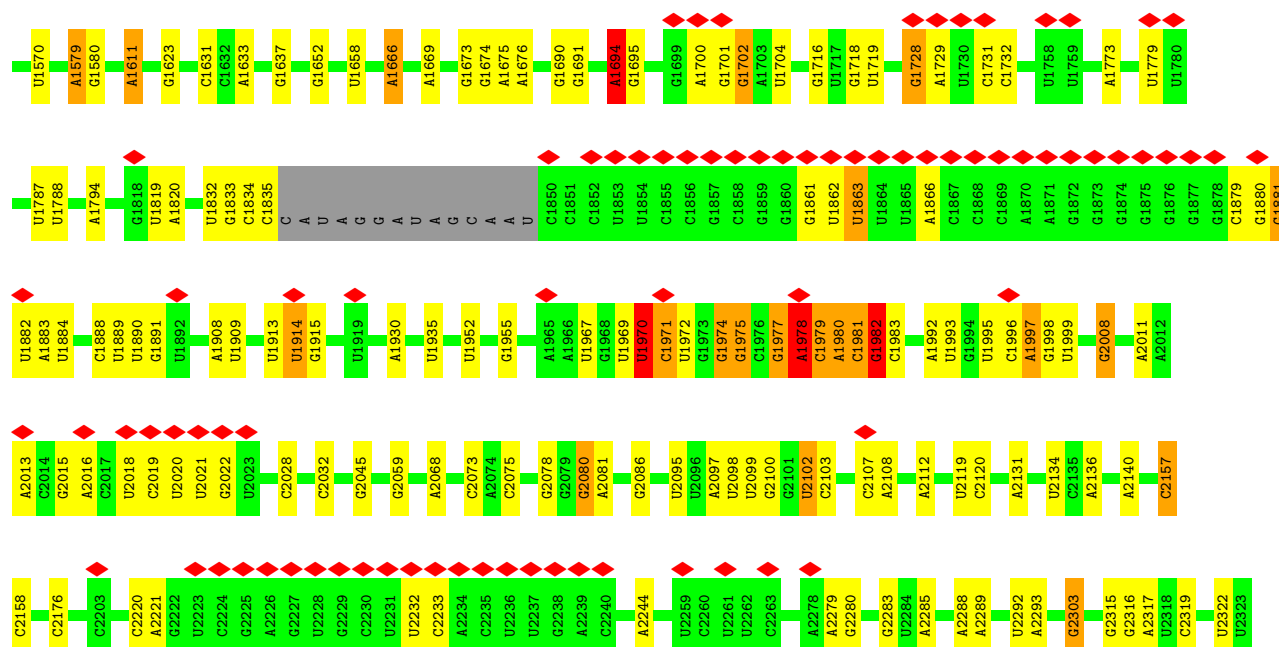
• Molecule 2: initiator tRNA-Met



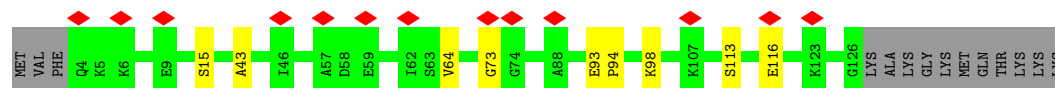
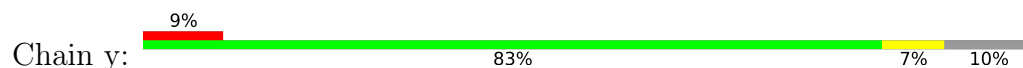
• Molecule 3: 18S



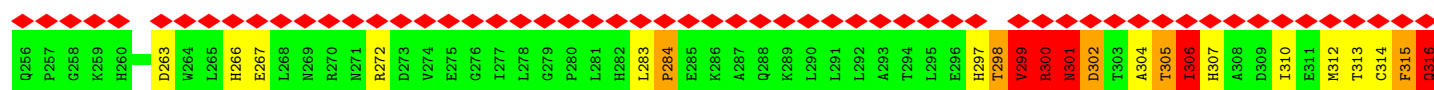
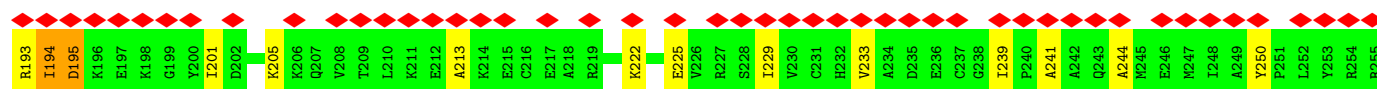
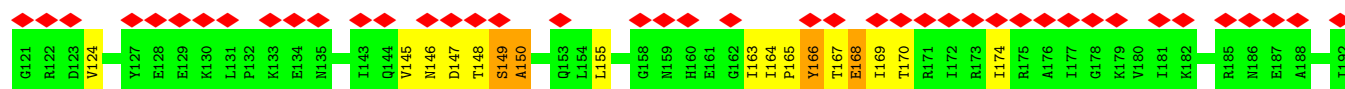
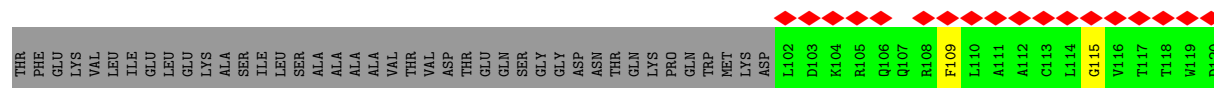
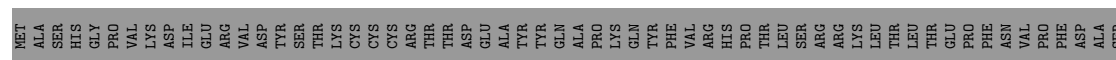


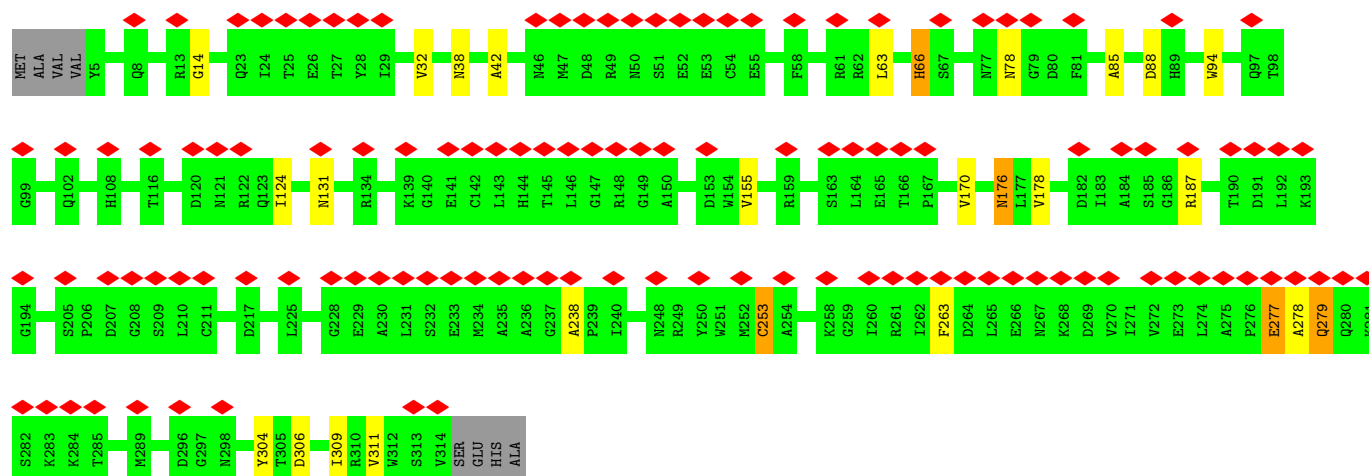


• Molecule 4: 40S ribosomal protein S24

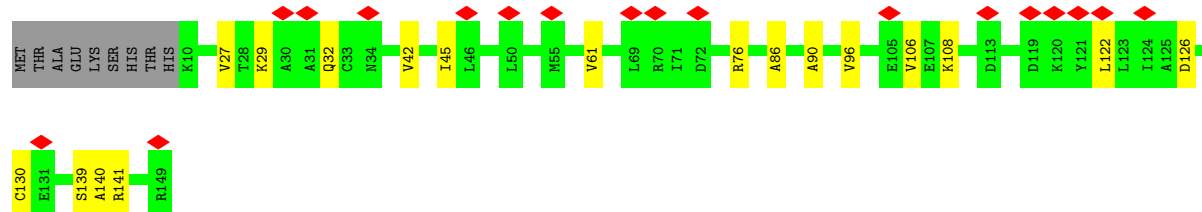
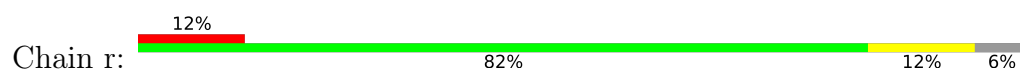


• Molecule 5: Elongation initiation factor 2 alpha subunit, putative

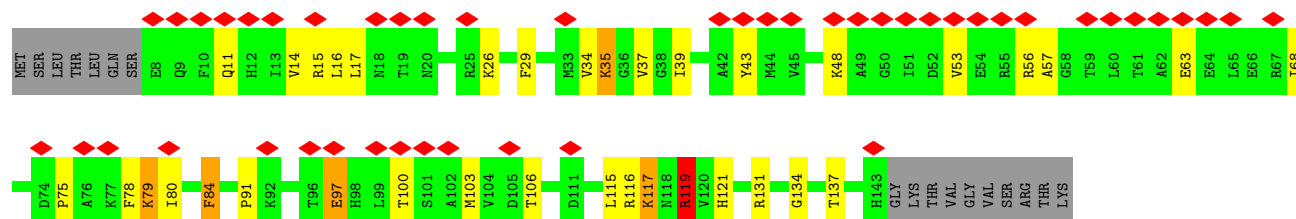




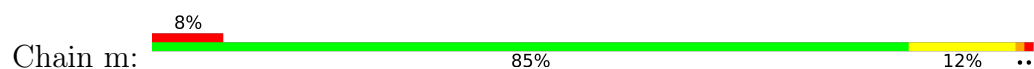
- Molecule 9: 40S ribosomal protein S16, putative



- Molecule 10: 40S ribosomal protein S18, putative

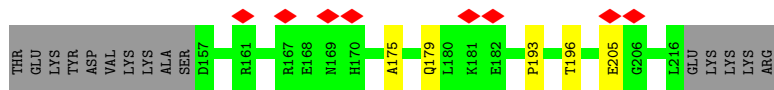


- Molecule 11: 40S ribosomal protein S23, putative

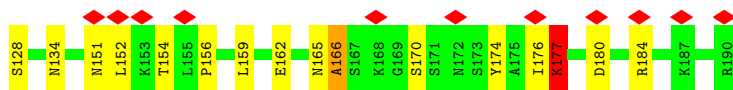


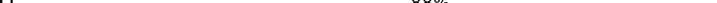
- Molecule 12: 40S ribosomal protein S8



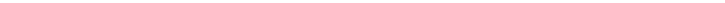


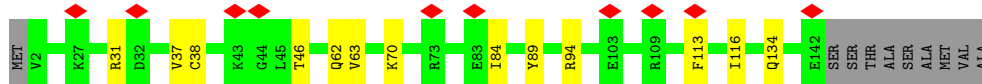
- Chain of thought: 22% 83% 16% ...

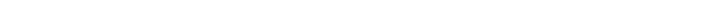


- Chain q: 



- Chain R:  7% 85% 9% 7%



- Chain S:  9% 71% 21% 5%



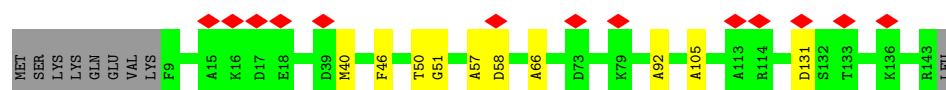
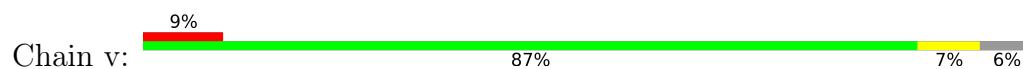
- Chain t:  10% 88% 5% 7%



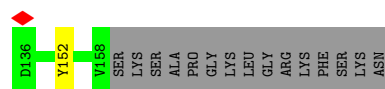
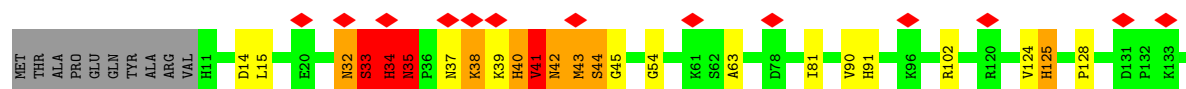
- Molecule 18: 40S ribosomal protein S33



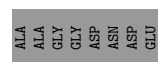
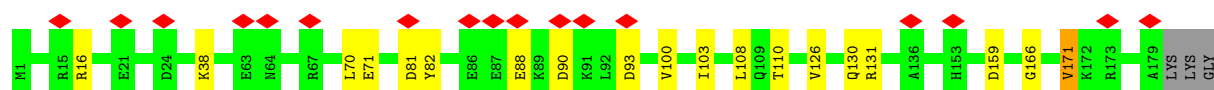
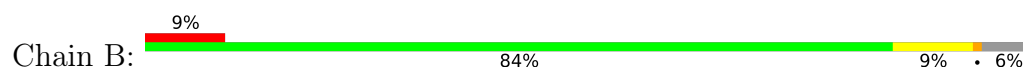
- Molecule 19: 40S ribosomal protein S14, putative



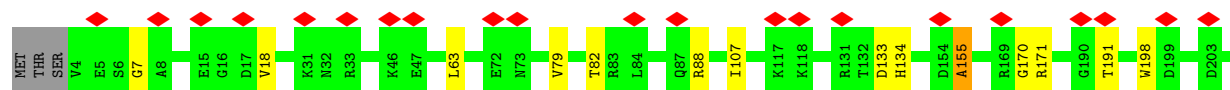
- Molecule 20: 40S ribosomal protein S11, putative

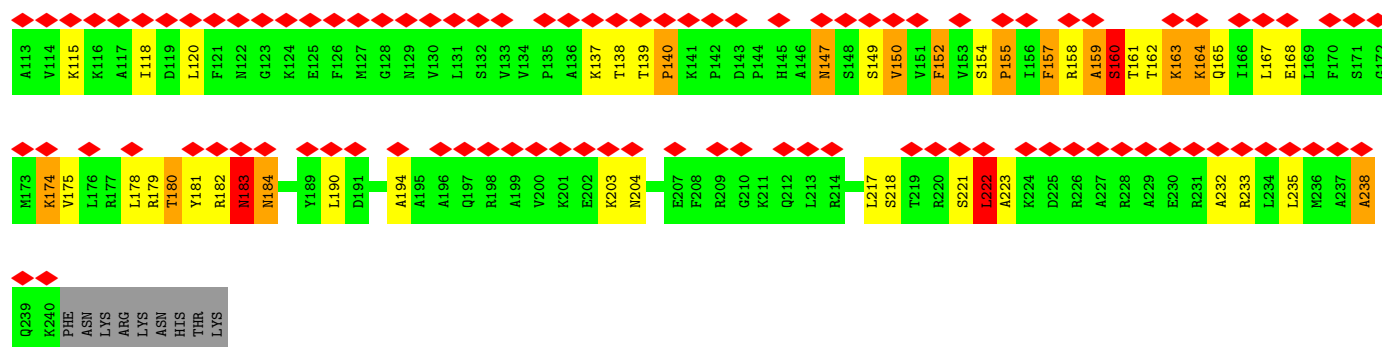


- Molecule 21: Putative 40S ribosomal protein S9

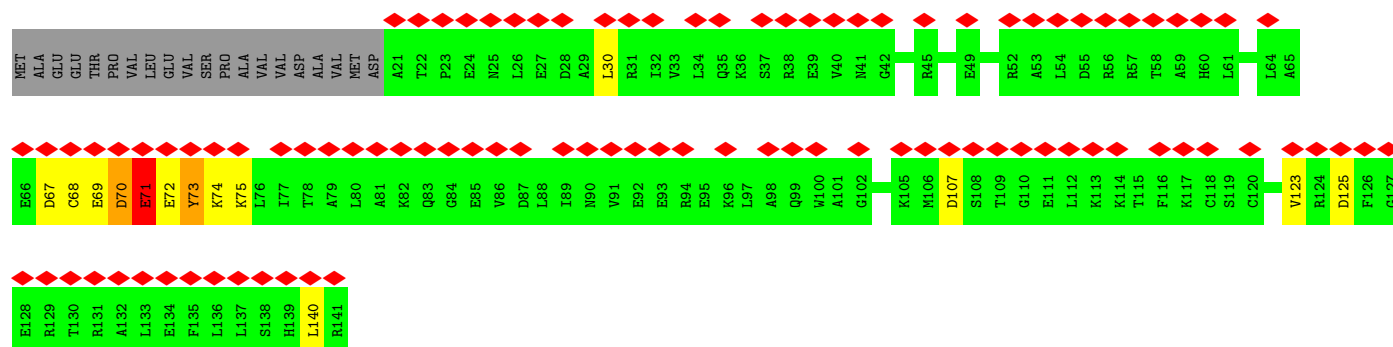
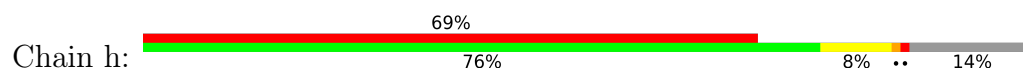


- Molecule 22: 40S ribosomal protein SA

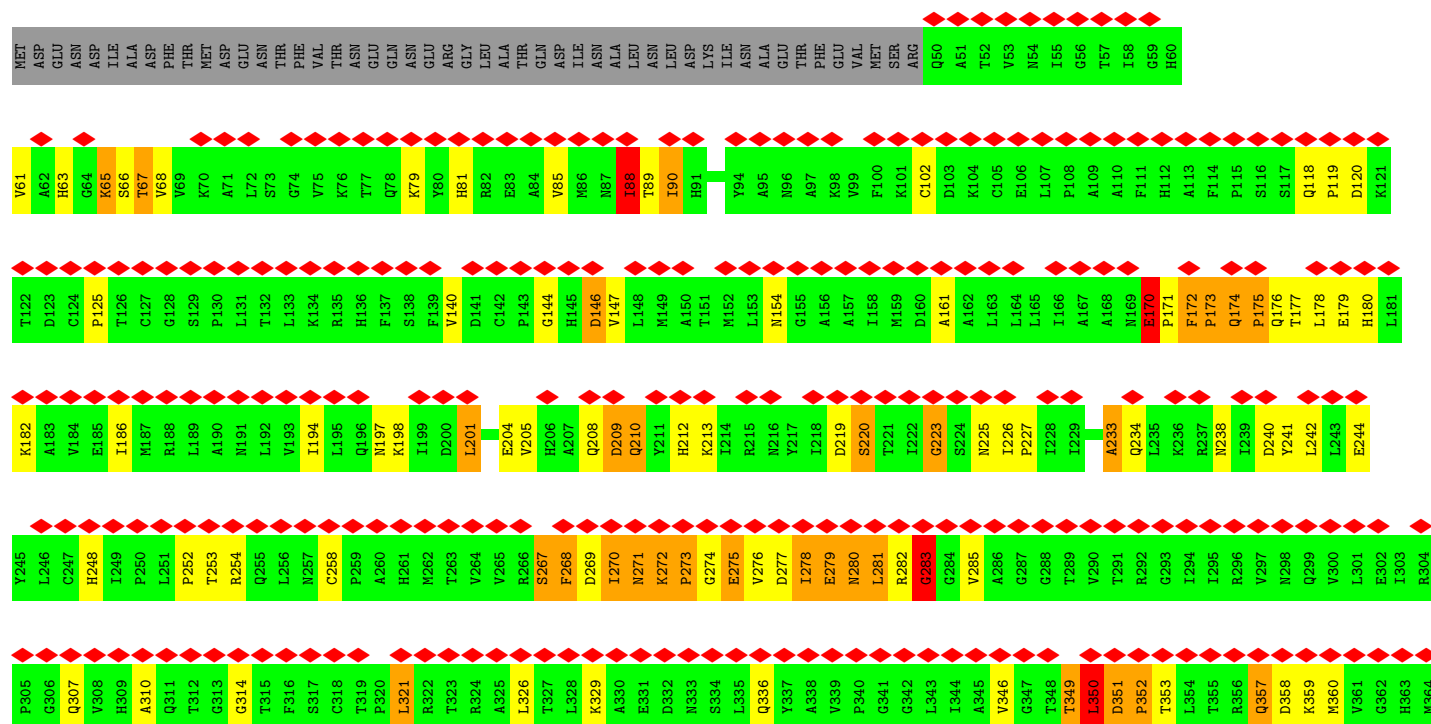
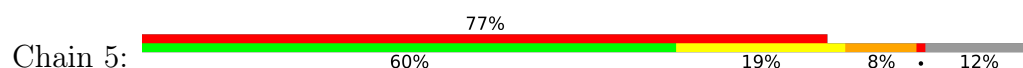


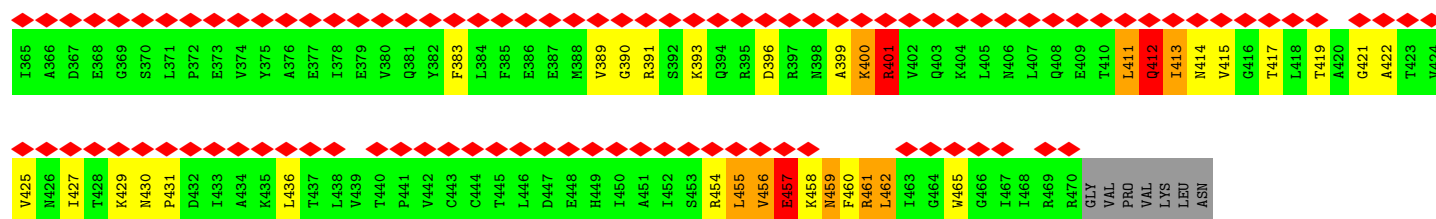


• Molecule 27: 40S ribosomal protein S12

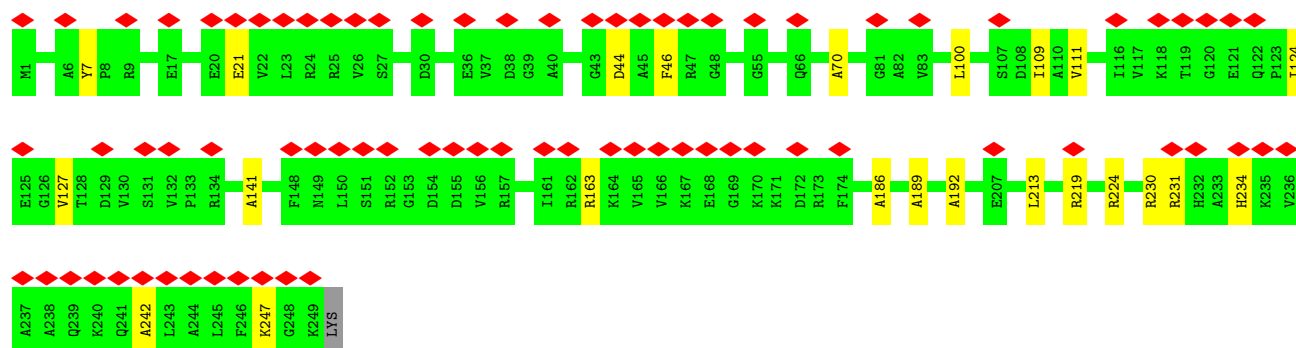
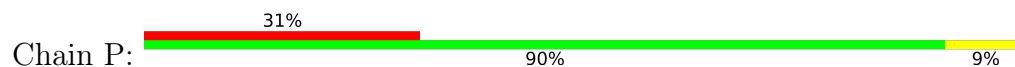


• Molecule 28: Eukaryotic translation initiation factor 2 subunit, putative

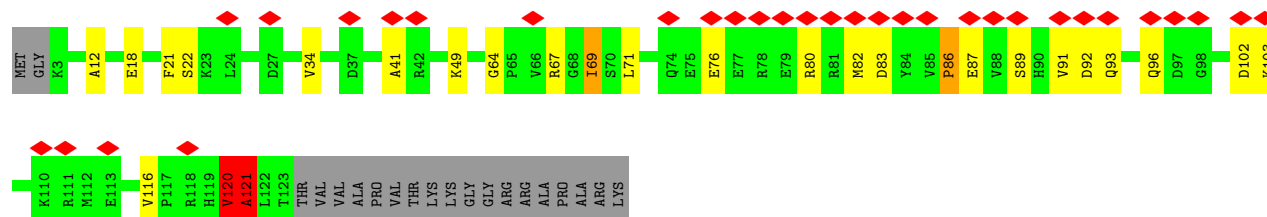




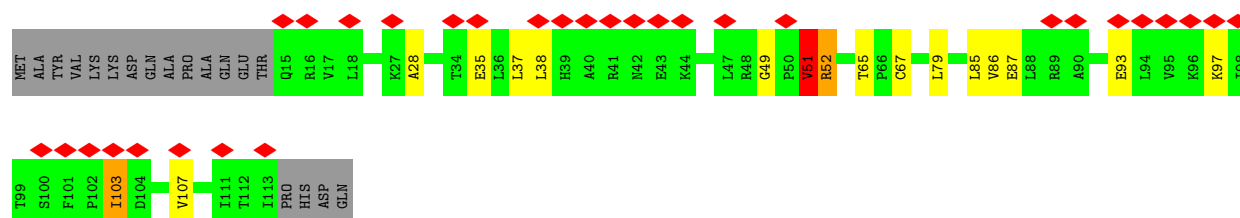
• Molecule 29: 40S ribosomal protein S6



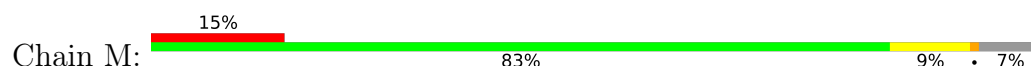
• Molecule 30: 40S ribosomal protein S17, putative

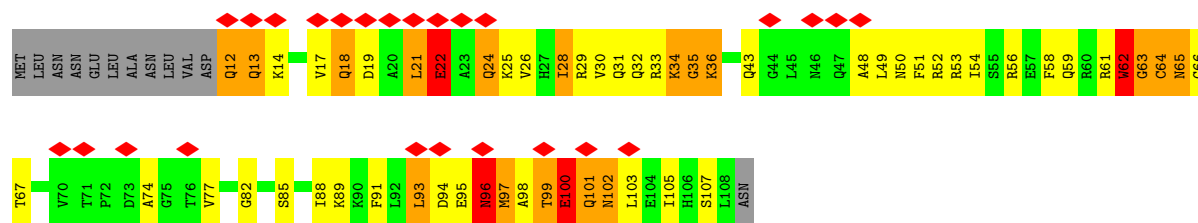


• Molecule 31: Ribosomal protein S20, putative

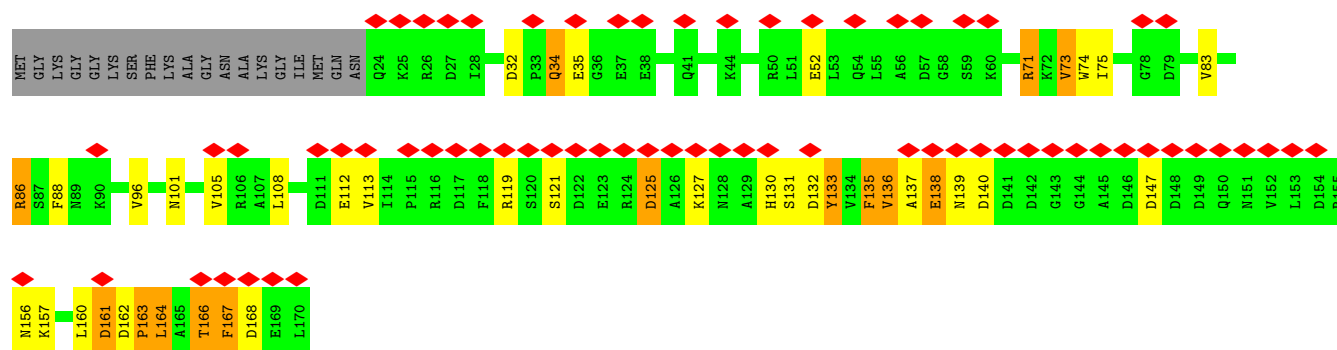
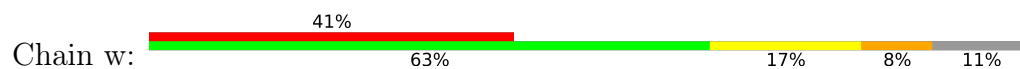


• Molecule 32: 40S ribosomal protein S3, putative

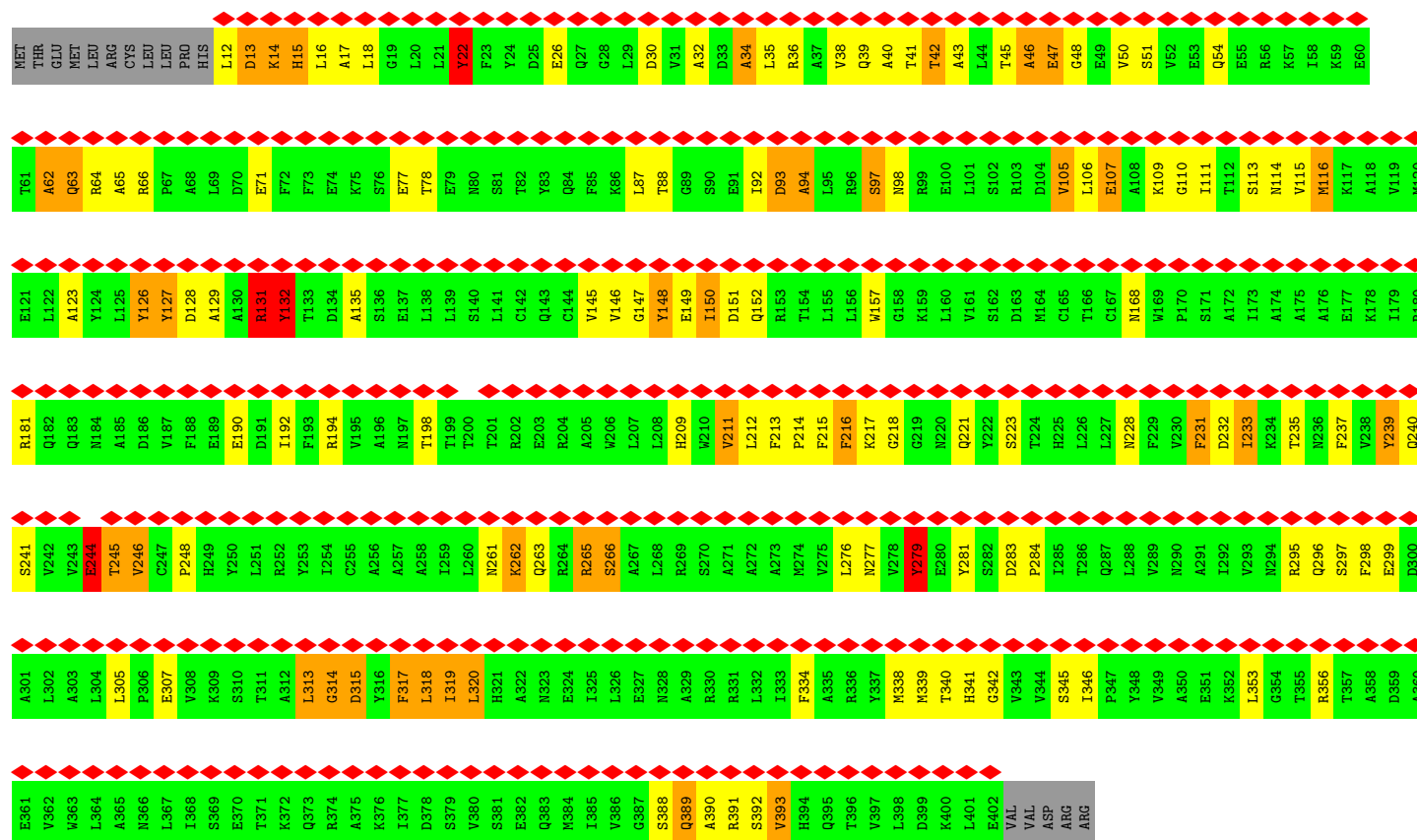


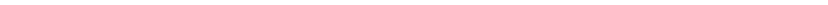


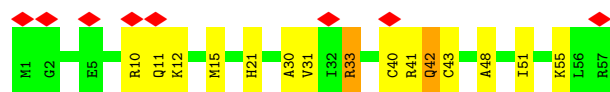
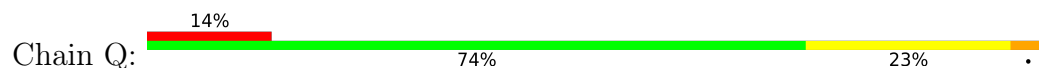
• Molecule 38: Putative eukaryotic translation initiation factor 1A



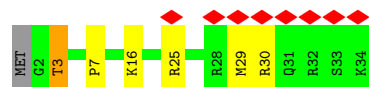
• Molecule 39: Eukaryotic translation initiation factor 3 subunit E

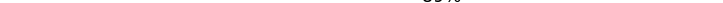


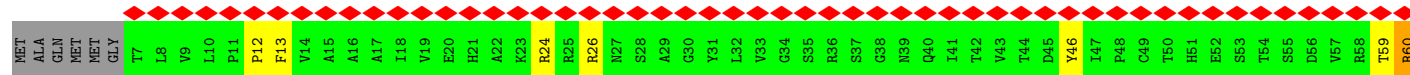
- Chain Y: 

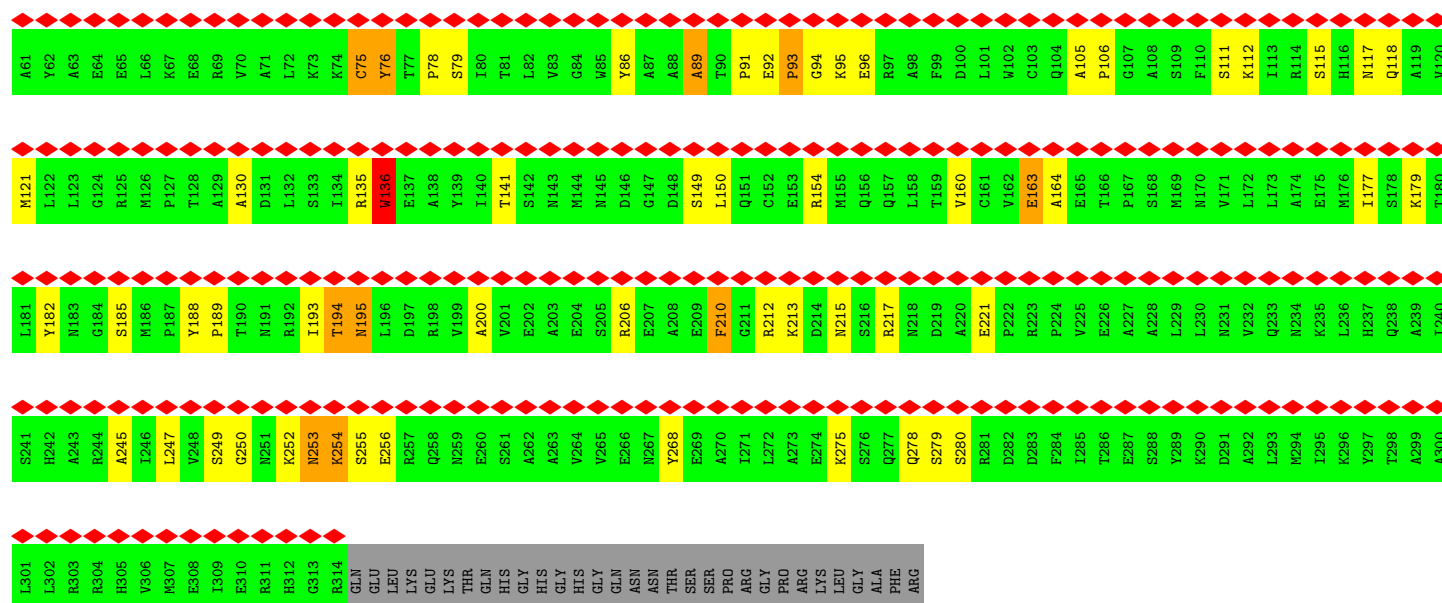


- Chain D:  24% 79% 15% . .

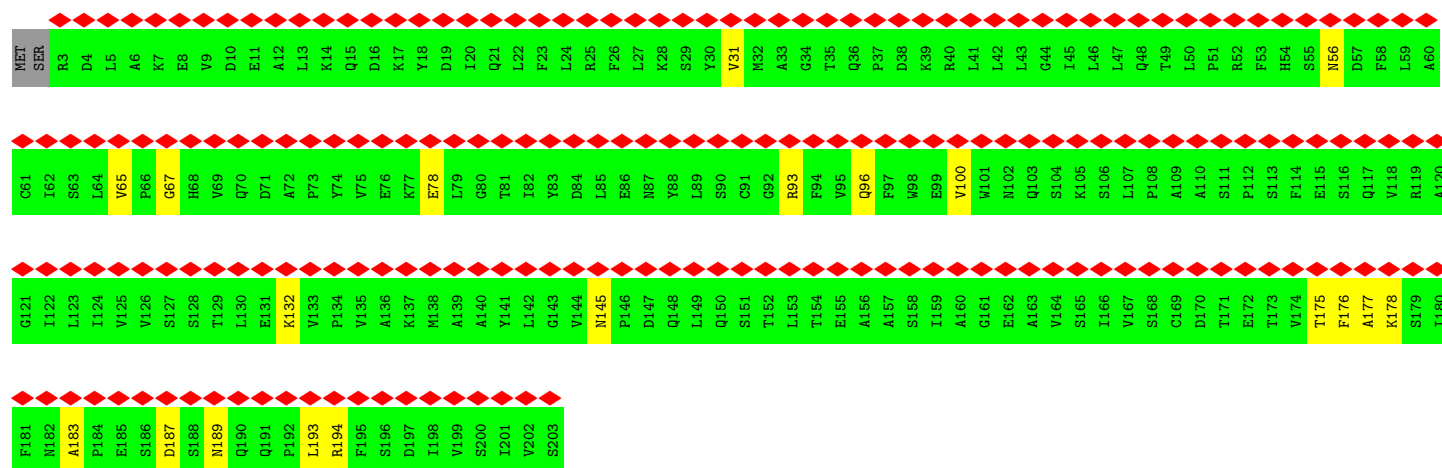
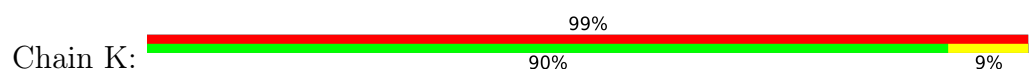


- Chain G:  89% 70% 16% 11%

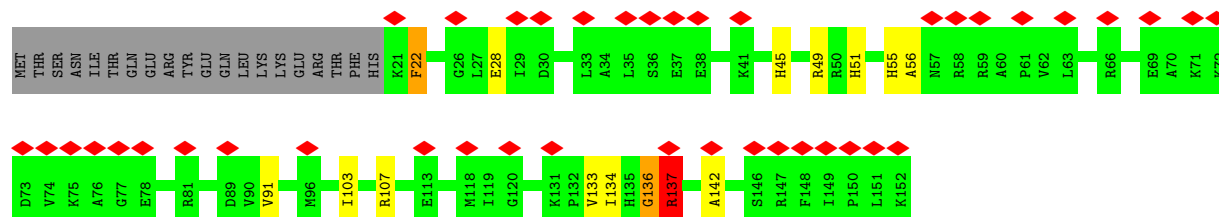
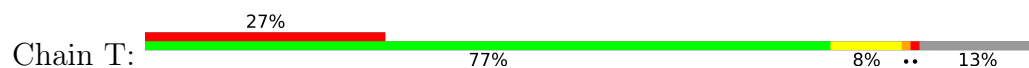




• Molecule 44: CSN8_PSD8_EIF3K domain-containing protein

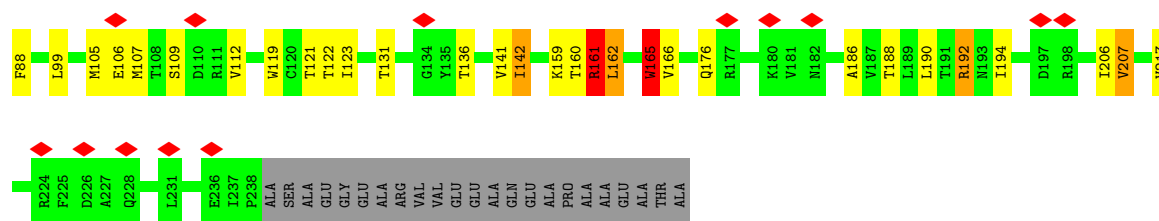


• Molecule 45: 40S ribosomal protein S15, putative

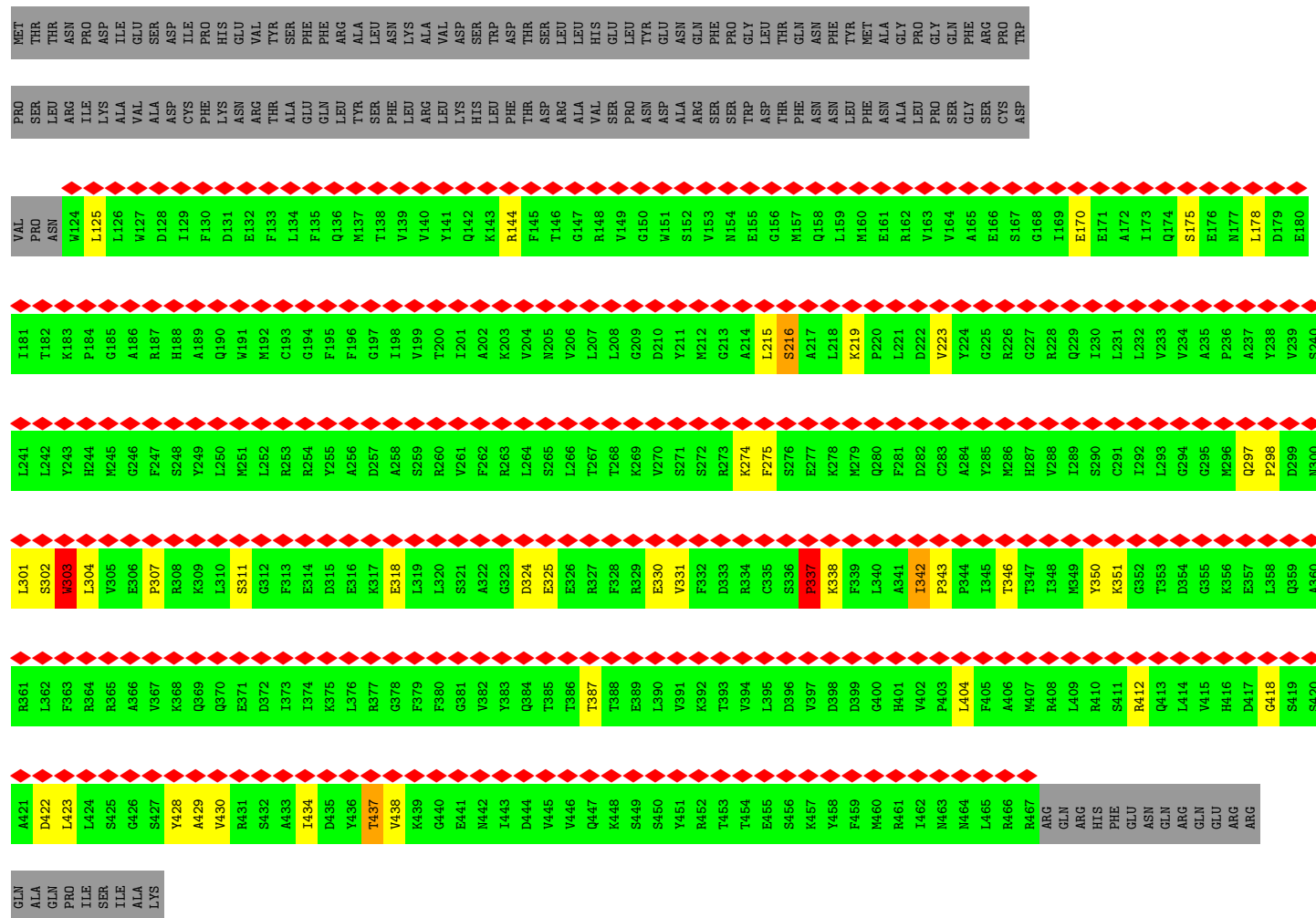


• Molecule 46: Eukaryotic translation initiation factor 3 subunit 8, putative

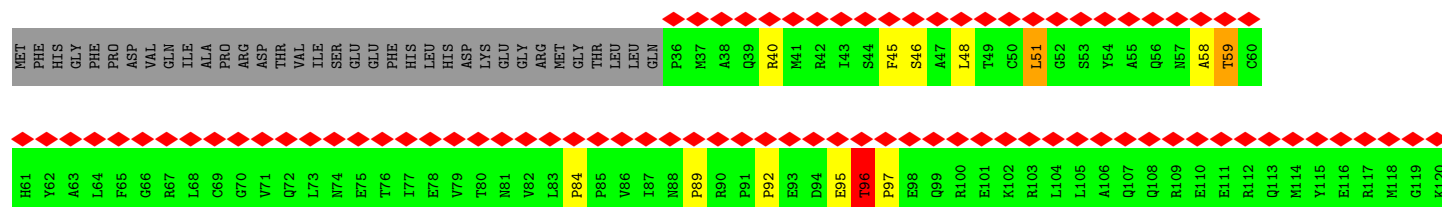




- Molecule 49: Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative

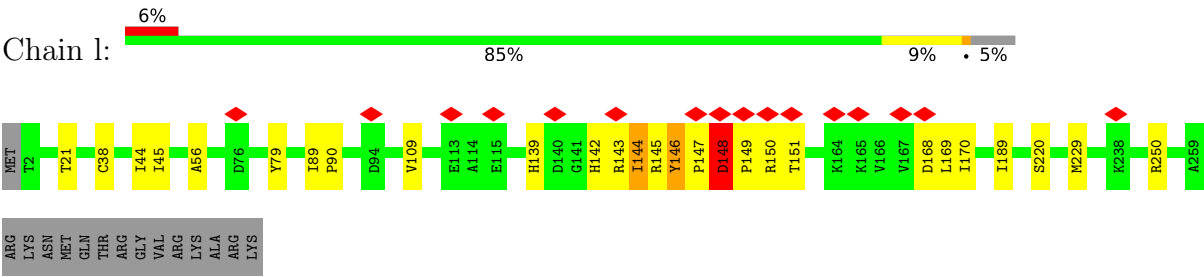


- Molecule 50: eIF3H





● Molecule 52: 40S ribosomal protein S4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0193	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	f	1.78	106/12510 (0.8%)	2.20	379/16884 (2.2%)
2	l	0.89	0/1798	1.06	5/2803 (0.2%)
3	o	0.89	2/51207 (0.0%)	1.03	53/79792 (0.1%)
4	y	1.30	1/1004 (0.1%)	1.52	10/1335 (0.7%)
5	s	1.21	1/2405 (0.0%)	1.63	34/3247 (1.0%)
6	j	1.23	0/658	1.38	4/871 (0.5%)
7	n	1.15	1/1818 (0.1%)	1.44	9/2433 (0.4%)
8	p	1.24	0/2461	1.45	21/3347 (0.6%)
9	r	1.28	0/1131	1.61	8/1520 (0.5%)
10	u	1.35	0/1126	1.72	19/1508 (1.3%)
11	m	1.25	0/1137	1.48	8/1520 (0.5%)
12	Z	1.35	0/1424	1.47	9/1904 (0.5%)
13	o	1.23	0/1515	1.60	20/2034 (1.0%)
14	q	1.33	0/1703	1.58	15/2290 (0.7%)
15	R	1.29	0/1164	1.72	19/1559 (1.2%)
16	S	1.24	0/641	1.38	4/858 (0.5%)
17	t	1.42	0/845	1.51	5/1129 (0.4%)
18	U	1.35	0/527	1.32	2/702 (0.3%)
19	v	1.33	0/1026	1.53	9/1376 (0.7%)
20	X	1.36	2/1238 (0.2%)	1.47	12/1662 (0.7%)
21	B	1.33	0/1513	1.67	19/2030 (0.9%)
22	F	1.26	0/1693	1.60	15/2290 (0.7%)
23	d	1.23	0/1760	1.55	16/2376 (0.7%)
24	g	1.24	0/644	1.46	2/875 (0.2%)
25	a	1.21	0/559	1.52	5/748 (0.7%)
26	J	1.32	0/1381	1.75	29/1857 (1.6%)
27	h	1.25	0/966	1.49	5/1295 (0.4%)
28	5	1.32	4/3302 (0.1%)	2.06	45/4483 (1.0%)
29	P	1.35	0/2008	1.57	23/2678 (0.9%)
30	i	1.28	0/1005	1.85	23/1341 (1.7%)
31	L	1.30	0/794	1.46	10/1076 (0.9%)
32	M	1.33	0/1606	1.56	17/2141 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	N	1.22	0/804	1.68	12/1082 (1.1%)
34	O	1.29	0/1140	1.64	14/1524 (0.9%)
35	b	1.26	0/1037	1.55	11/1391 (0.8%)
36	c	1.15	0/488	1.53	4/644 (0.6%)
37	V	0.96	0/799	1.26	6/1072 (0.6%)
38	w	1.16	0/1177	1.31	6/1588 (0.4%)
39	E	1.40	6/3174 (0.2%)	1.82	74/4304 (1.7%)
40	Y	1.16	0/1406	1.56	12/1890 (0.6%)
41	Q	1.37	0/468	1.60	4/618 (0.6%)
42	D	1.56	0/298	1.65	8/385 (2.1%)
43	G	1.28	0/2455	1.68	28/3323 (0.8%)
44	K	1.14	0/1597	1.67	23/2170 (1.1%)
45	T	1.27	0/1079	1.58	4/1447 (0.3%)
46	C	2.10	4/5724 (0.1%)	1.72	90/7724 (1.2%)
47	8	1.24	0/4685	1.79	91/6327 (1.4%)
48	W	1.35	5/1809 (0.3%)	1.67	30/2437 (1.2%)
49	I	1.22	0/2826	1.67	32/3809 (0.8%)
50	H	1.28	0/2431	1.69	40/3285 (1.2%)
51	A	1.24	3/3971 (0.1%)	1.58	30/5366 (0.6%)
52	l	1.31	0/2073	1.46	14/2787 (0.5%)
All	All	1.25	135/144010 (0.1%)	1.48	1387/205137 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	f	3	200
3	0	2	52
4	y	0	1
5	s	0	17
6	j	0	2
7	n	0	1
8	p	0	2
9	r	0	4
10	u	0	2
11	m	0	2
12	Z	0	2
13	o	0	1
17	t	0	1
19	v	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	X	0	10
21	B	0	4
22	F	0	3
23	d	0	3
24	g	0	1
26	J	0	21
28	5	0	12
29	P	0	4
31	L	0	7
32	M	0	2
33	N	0	1
34	O	0	6
35	b	0	1
36	c	0	3
38	w	0	6
39	E	1	73
40	Y	0	4
41	Q	0	3
42	D	0	1
43	G	0	36
44	K	0	2
45	T	0	1
46	C	1	137
47	8	0	69
48	W	0	2
49	I	2	6
50	H	0	26
51	A	0	16
52	l	0	10
All	All	9	759

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	C	411	ARG	CD-NE	128.69	3.26	1.46
1	f	301	GLU	CA-C	-37.30	1.02	1.52
1	f	1149	TYR	C-N	30.50	1.72	1.33
1	f	301	GLU	C-O	-30.05	0.86	1.24
1	f	304	PRO	CA-C	-28.52	1.19	1.52

The worst 5 of 1387 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	412	GLN	O-C-N	-66.91	66.11	121.65
1	f	234	GLY	O-C-N	-39.58	66.87	122.68
28	5	411	LEU	CA-C-N	-38.02	82.45	123.13
28	5	411	LEU	C-N-CA	-38.02	82.45	123.13
1	f	1147	ILE	O-C-N	32.67	160.84	122.62

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	f	296	TYR	CA
1	f	305	TYR	CA
1	f	772	TYR	CA
3	0	974	A	C1'
3	0	1833	G	C1'

5 of 759 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	f	26	SER	Peptide
1	f	38	SER	Peptide
1	f	46	SER	Peptide
1	f	55	VAL	Peptide
1	f	56	THR	Peptide

5.2 Too-close contacts [i](#)

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	f	12257	0	12096	627	0
2	1	1606	0	816	23	0
3	0	45795	0	23111	114	0
4	y	989	0	1065	0	0
5	s	2365	0	2421	216	0
6	j	644	0	677	18	0
7	n	1796	0	1824	136	0
8	p	2405	0	2323	7	0
9	r	1113	0	1175	1	0
10	u	1108	0	1144	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	1116	0	1169	28	0
12	Z	1404	0	1503	0	0
13	o	1493	0	1562	25	0
14	q	1670	0	1778	1	0
15	R	1143	0	1226	0	0
16	S	630	0	630	51	0
17	t	829	0	866	0	0
18	U	526	0	550	34	0
19	v	1011	0	1019	0	0
20	X	1212	0	1250	23	0
21	B	1483	0	1548	1	0
22	F	1658	0	1704	0	0
23	d	1726	0	1774	2	0
24	g	635	0	631	0	0
25	a	553	0	608	1	0
26	J	1358	0	1419	38	0
27	h	958	0	981	16	0
28	5	3245	0	3326	289	0
29	P	1983	0	2131	1	0
30	i	992	0	1054	1	0
31	L	784	0	848	3	0
32	M	1587	0	1662	2	0
33	N	780	0	771	0	0
34	O	1116	0	1166	2	0
35	b	1019	0	1050	0	0
36	c	480	0	532	18	0
37	V	789	0	800	128	0
38	w	1162	0	1128	82	0
39	E	3119	0	3106	40	0
40	Y	1387	0	1429	70	0
41	Q	462	0	475	0	0
42	D	294	0	336	0	0
43	G	2414	0	2396	2	0
44	K	1566	0	1566	0	0
45	T	1057	0	1099	6	0
46	C	5630	0	5586	327	0
47	8	4596	0	4584	177	0
48	W	1781	0	1852	97	0
49	I	2770	0	2786	1	0
50	H	2388	0	2377	5	0
51	A	3891	0	3874	264	0
52	l	2038	0	2142	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	n	1	0	0	0	0
54	5	1	0	0	0	0
55	5	32	0	13	21	0
All	All	136847	0	114959	2365	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 9.

The worst 5 of 2365 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)
39:E:279:TYR:CE1	39:E:279:TYR:CZ	1.75	1.69
39:E:279:TYR:CZ	39:E:279:TYR:CE2	1.75	1.69
39:E:279:TYR:CD1	39:E:279:TYR:CG	1.75	1.69
39:E:279:TYR:CG	39:E:279:TYR:CD2	1.74	1.68
7:n:326:TYR:CD2	37:V:77:VAL:HG21	1.27	1.67

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	
1	f	1519/2174 (70%)	1094 (72%)	295 (19%)	130 (9%)	0	4
4	y	121/137 (88%)	109 (90%)	10 (8%)	2 (2%)	7	30
5	s	293/418 (70%)	207 (71%)	51 (17%)	35 (12%)	0	2
6	j	77/150 (51%)	68 (88%)	6 (8%)	3 (4%)	2	16
7	n	223/343 (65%)	179 (80%)	33 (15%)	11 (5%)	1	12
8	p	308/318 (97%)	268 (87%)	31 (10%)	9 (3%)	3	21
9	r	138/149 (93%)	101 (73%)	29 (21%)	8 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	u	134/153 (88%)	87 (65%)	33 (25%)	14 (10%)	0	2
11	m	140/143 (98%)	120 (86%)	18 (13%)	2 (1%)	9	34
12	Z	171/221 (77%)	145 (85%)	20 (12%)	6 (4%)	3	18
13	o	188/190 (99%)	147 (78%)	33 (18%)	8 (4%)	2	14
14	q	198/211 (94%)	168 (85%)	28 (14%)	2 (1%)	12	41
15	R	139/151 (92%)	121 (87%)	15 (11%)	3 (2%)	5	26
16	S	80/86 (93%)	69 (86%)	9 (11%)	2 (2%)	4	24
17	t	102/112 (91%)	82 (80%)	19 (19%)	1 (1%)	12	41
18	U	66/91 (72%)	54 (82%)	10 (15%)	2 (3%)	3	21
19	v	133/144 (92%)	121 (91%)	10 (8%)	2 (2%)	8	33
20	X	146/173 (84%)	121 (83%)	20 (14%)	5 (3%)	3	19
21	B	177/190 (93%)	149 (84%)	23 (13%)	5 (3%)	4	22
22	F	205/245 (84%)	180 (88%)	23 (11%)	2 (1%)	12	41
23	d	221/263 (84%)	191 (86%)	28 (13%)	2 (1%)	14	43
24	g	81/247 (33%)	68 (84%)	12 (15%)	1 (1%)	10	37
25	a	68/110 (62%)	56 (82%)	12 (18%)	0	100	100
26	J	171/257 (66%)	132 (77%)	24 (14%)	15 (9%)	0	4
27	h	119/141 (84%)	96 (81%)	19 (16%)	4 (3%)	3	19
28	5	417/477 (87%)	325 (78%)	62 (15%)	30 (7%)	1	6
29	P	247/250 (99%)	219 (89%)	25 (10%)	3 (1%)	10	37
30	i	119/141 (84%)	91 (76%)	16 (13%)	12 (10%)	0	3
31	L	97/117 (83%)	75 (77%)	20 (21%)	2 (2%)	5	27
32	M	198/214 (92%)	160 (81%)	31 (16%)	7 (4%)	3	18
33	N	91/161 (56%)	78 (86%)	10 (11%)	3 (3%)	3	19
34	O	138/167 (83%)	103 (75%)	27 (20%)	8 (6%)	1	9
35	b	127/145 (88%)	108 (85%)	18 (14%)	1 (1%)	16	46
36	c	58/66 (88%)	47 (81%)	10 (17%)	1 (2%)	7	30
37	V	95/109 (87%)	70 (74%)	15 (16%)	10 (10%)	0	2
38	w	145/166 (87%)	105 (72%)	30 (21%)	10 (7%)	1	7
39	E	389/407 (96%)	288 (74%)	46 (12%)	55 (14%)	0	1
40	Y	172/379 (45%)	139 (81%)	27 (16%)	6 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Q	55/57 (96%)	40 (73%)	8 (14%)	7 (13%)	0	1
42	D	31/34 (91%)	25 (81%)	5 (16%)	1 (3%)	3	19
43	G	306/345 (89%)	254 (83%)	33 (11%)	19 (6%)	1	8
44	K	199/203 (98%)	185 (93%)	10 (5%)	4 (2%)	6	28
45	T	130/152 (86%)	100 (77%)	21 (16%)	9 (7%)	1	7
46	C	694/716 (97%)	490 (71%)	82 (12%)	122 (18%)	0	0
47	8	574/762 (75%)	462 (80%)	57 (10%)	55 (10%)	0	3
48	W	215/254 (85%)	181 (84%)	27 (13%)	7 (3%)	3	19
49	I	342/489 (70%)	302 (88%)	21 (6%)	19 (6%)	1	10
50	H	295/334 (88%)	231 (78%)	41 (14%)	23 (8%)	1	5
51	A	481/502 (96%)	341 (71%)	89 (18%)	51 (11%)	0	2
52	l	256/273 (94%)	216 (84%)	30 (12%)	10 (4%)	2	16
All	All	11089/13737 (81%)	8768 (79%)	1572 (14%)	749 (7%)	2	7

5 of 749 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	56	THR
1	f	91	ASP
1	f	190	ARG
1	f	203	LEU
1	f	235	LEU

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	
1	f	1318/1862 (71%)	1272 (96%)	46 (4%)	32	58
4	y	104/116 (90%)	104 (100%)	0	100	100
5	s	252/362 (70%)	240 (95%)	12 (5%)	23	52
6	j	69/123 (56%)	65 (94%)	4 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	n	196/289 (68%)	182 (93%)	14 (7%)	13	41
8	p	262/268 (98%)	259 (99%)	3 (1%)	65	75
9	r	113/121 (93%)	113 (100%)	0	100	100
10	u	117/132 (89%)	108 (92%)	9 (8%)	12	38
11	m	116/117 (99%)	112 (97%)	4 (3%)	32	59
12	Z	143/184 (78%)	143 (100%)	0	100	100
13	o	160/160 (100%)	157 (98%)	3 (2%)	50	68
14	q	188/195 (96%)	186 (99%)	2 (1%)	65	75
15	R	125/132 (95%)	125 (100%)	0	100	100
16	S	70/73 (96%)	69 (99%)	1 (1%)	59	72
17	t	87/93 (94%)	86 (99%)	1 (1%)	65	75
18	U	57/74 (77%)	50 (88%)	7 (12%)	4	20
19	v	103/112 (92%)	102 (99%)	1 (1%)	68	75
20	X	137/157 (87%)	134 (98%)	3 (2%)	45	65
21	B	159/165 (96%)	159 (100%)	0	100	100
22	F	182/212 (86%)	181 (100%)	1 (0%)	81	82
23	d	187/208 (90%)	187 (100%)	0	100	100
24	g	68/197 (34%)	65 (96%)	3 (4%)	25	53
25	a	64/96 (67%)	63 (98%)	1 (2%)	55	71
26	J	138/191 (72%)	127 (92%)	11 (8%)	11	37
27	h	103/120 (86%)	101 (98%)	2 (2%)	50	68
28	5	358/408 (88%)	338 (94%)	20 (6%)	19	47
29	P	204/205 (100%)	201 (98%)	3 (2%)	57	71
30	i	110/124 (89%)	104 (94%)	6 (6%)	19	48
31	L	89/104 (86%)	88 (99%)	1 (1%)	65	75
32	M	167/179 (93%)	164 (98%)	3 (2%)	51	69
33	N	84/125 (67%)	82 (98%)	2 (2%)	43	65
34	O	118/139 (85%)	117 (99%)	1 (1%)	73	78
35	b	110/123 (89%)	109 (99%)	1 (1%)	70	77
36	c	49/53 (92%)	47 (96%)	2 (4%)	27	55
37	V	86/97 (89%)	68 (79%)	18 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	w	125/137 (91%)	117 (94%)	8 (6%)	16	44
39	E	334/350 (95%)	327 (98%)	7 (2%)	47	66
40	Y	152/327 (46%)	146 (96%)	6 (4%)	28	56
41	Q	49/49 (100%)	46 (94%)	3 (6%)	17	46
42	D	30/31 (97%)	29 (97%)	1 (3%)	33	59
43	G	260/289 (90%)	257 (99%)	3 (1%)	63	74
44	K	176/178 (99%)	174 (99%)	2 (1%)	65	75
45	T	111/131 (85%)	109 (98%)	2 (2%)	51	69
46	C	616/628 (98%)	585 (95%)	31 (5%)	22	50
47	8	485/648 (75%)	467 (96%)	18 (4%)	30	57
48	W	194/217 (89%)	186 (96%)	8 (4%)	27	55
49	I	300/430 (70%)	295 (98%)	5 (2%)	53	70
50	H	266/299 (89%)	263 (99%)	3 (1%)	65	75
51	A	425/441 (96%)	384 (90%)	41 (10%)	8	30
52	l	217/230 (94%)	215 (99%)	2 (1%)	70	77
All	All	9633/11701 (82%)	9308 (97%)	325 (3%)	33	59

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	C	207	LYS
51	A	28	MET
46	C	274	LYS
47	8	263	HIS
51	A	207	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 283 such sidechains are listed below:

Mol	Chain	Res	Type
47	8	270	GLN
47	8	542	HIS
50	H	282	HIS
20	X	19	HIS
17	t	24	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	74/75 (98%)	11 (14%)	1 (1%)
3	0	2144/2319 (92%)	394 (18%)	28 (1%)
All	All	2218/2394 (92%)	405 (18%)	29 (1%)

5 of 405 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	16	U
2	1	17	G
2	1	20	A
2	1	25	G
2	1	32	U

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	0	1196	G
3	0	2073	C
3	0	1450	G
3	0	1979	C
3	0	1393	U

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
55	GNP	5	502	54	34,34,34	2.21	7 (20%)	47,54,54	1.07	4 (8%)

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
55	GNP	5	502	54	-	6/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	502	GNP	PA-O3A	-7.78	1.51	1.59
55	5	502	GNP	PB-O3A	-7.57	1.49	1.59
55	5	502	GNP	PB-O2B	-3.67	1.47	1.56
55	5	502	GNP	PG-O3G	-2.48	1.50	1.56
55	5	502	GNP	PG-N3B	-2.26	1.57	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	502	GNP	O3G-PG-O1G	-3.59	104.44	113.45
55	5	502	GNP	O2B-PB-O1B	2.75	115.76	109.87
55	5	502	GNP	C3'-C2'-C1'	2.44	106.07	101.46
55	5	502	GNP	O2G-PG-O3G	2.12	113.29	107.59

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

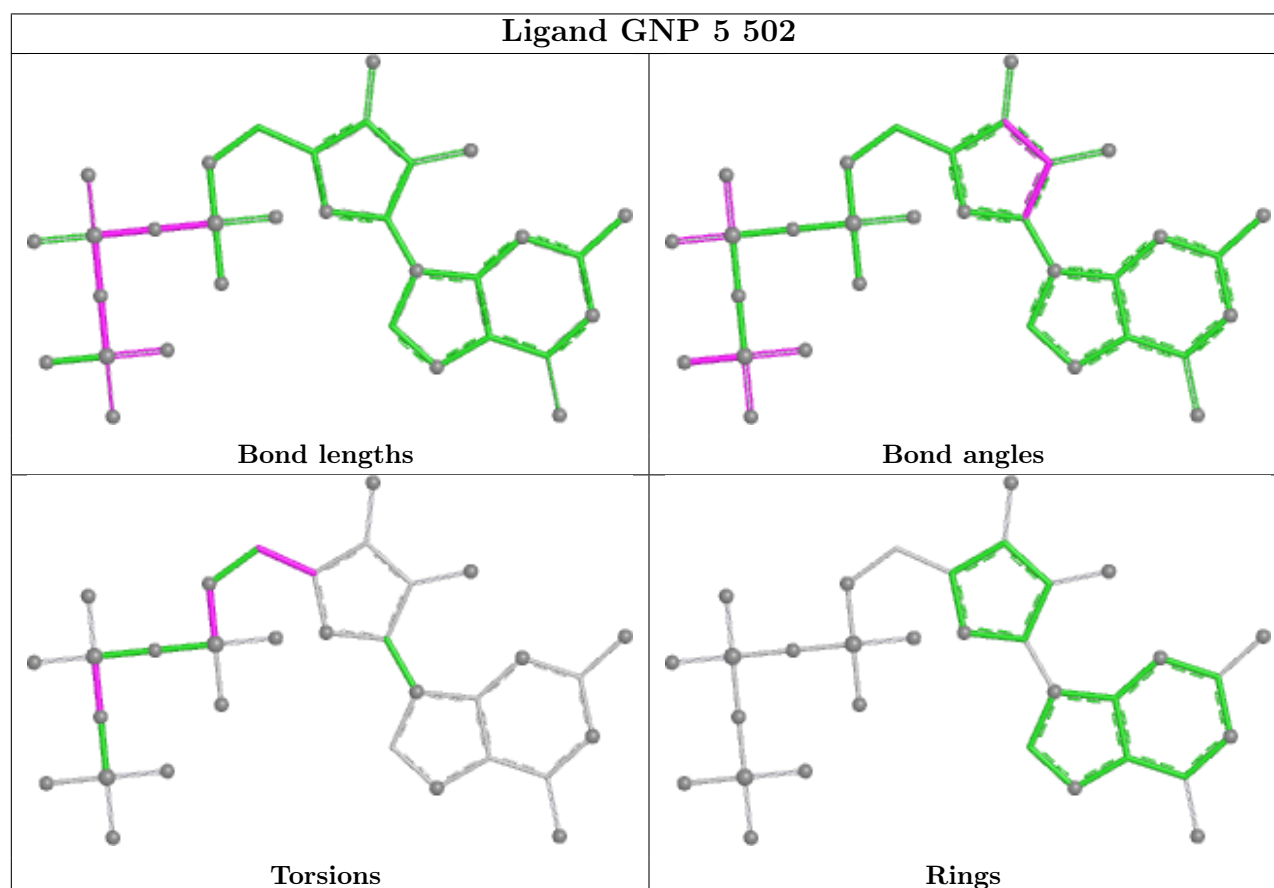
Mol	Chain	Res	Type	Atoms
55	5	502	GNP	PG-N3B-PB-O1B
55	5	502	GNP	PG-N3B-PB-O3A
55	5	502	GNP	C5'-O5'-PA-O3A
55	5	502	GNP	O4'-C4'-C5'-O5'
55	5	502	GNP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	5	502	GNP	21	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	20
28	5	2
46	C	1
48	W	1

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	282:ARG	C	283:GLY	N	2.09
1	f	1149:TYR	C	1150:VAL	N	1.72
1	f	1221:LEU	C	1222:PRO	N	1.71
1	f	1254:ALA	C	1255:GLN	N	1.68
1	C	53:ARG	C	54:ASN	N	1.67

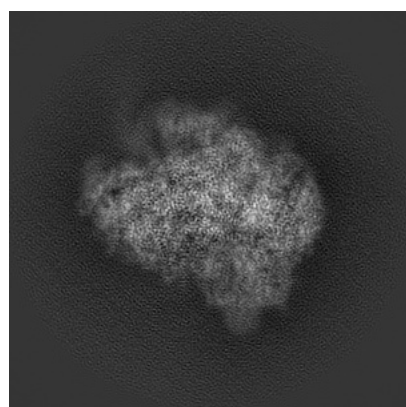
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11893. These allow visual inspection of the internal detail of the map and identification of artifacts.

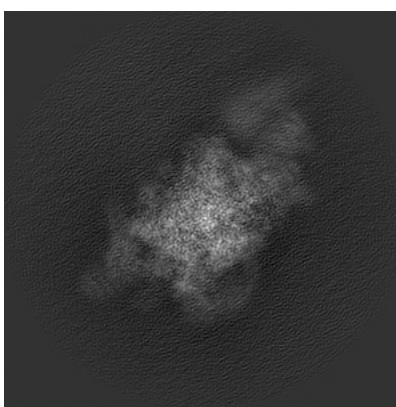
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

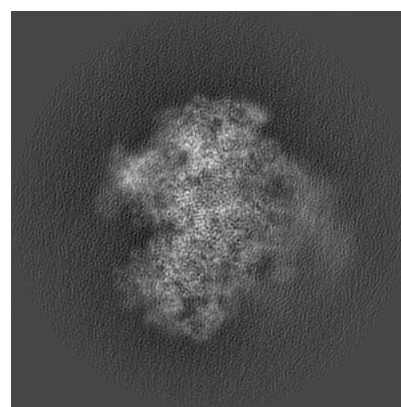
6.1.1 Primary map



X



Y

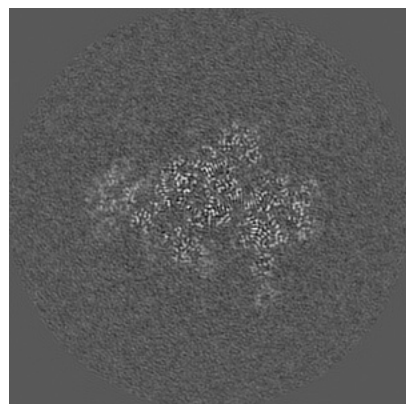


Z

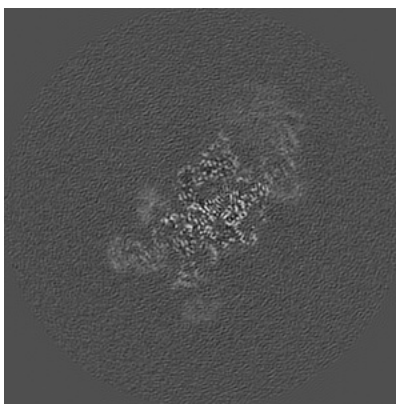
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

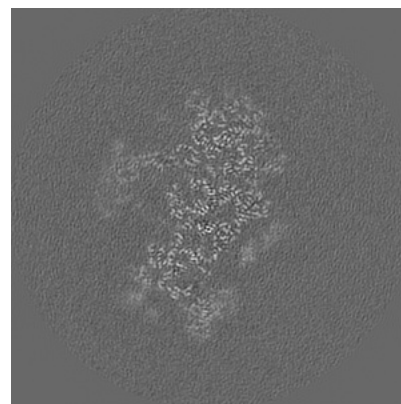
6.2.1 Primary map



X Index: 200



Y Index: 200

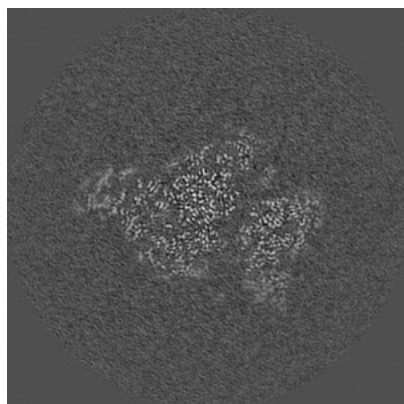


Z Index: 200

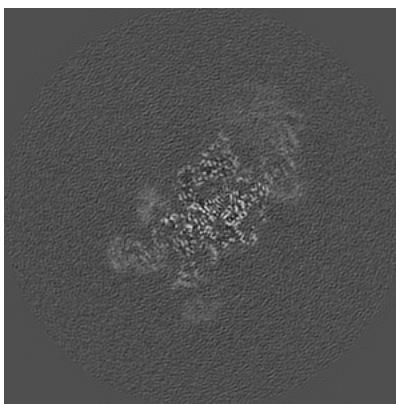
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

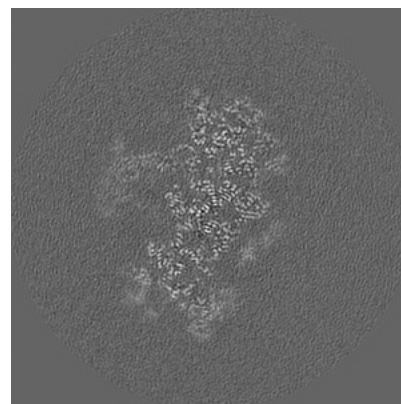
6.3.1 Primary map



X Index: 188



Y Index: 200

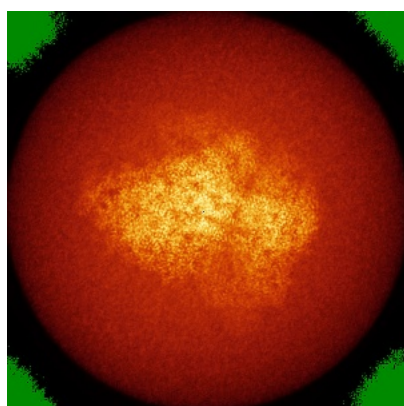


Z Index: 199

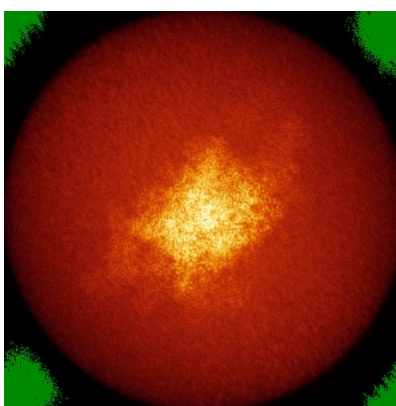
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

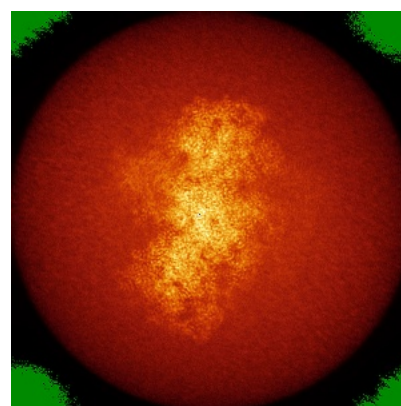
6.4.1 Primary map



X



Y

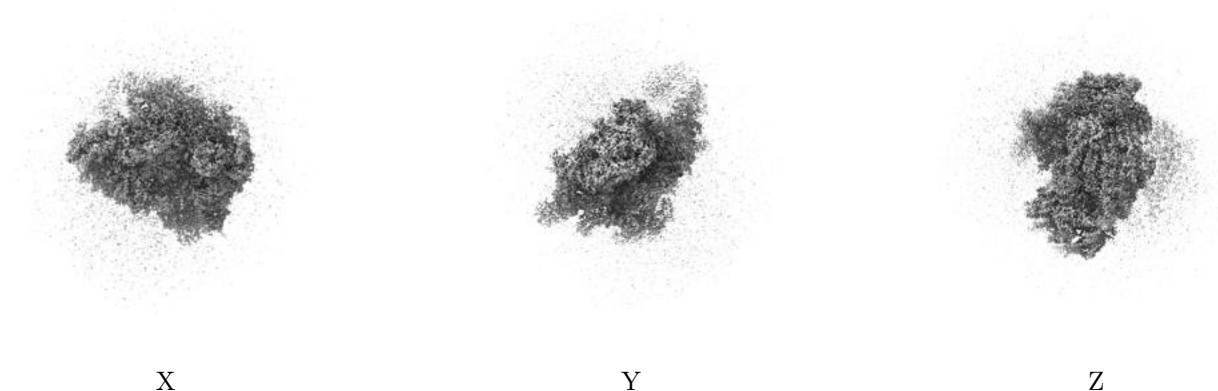


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

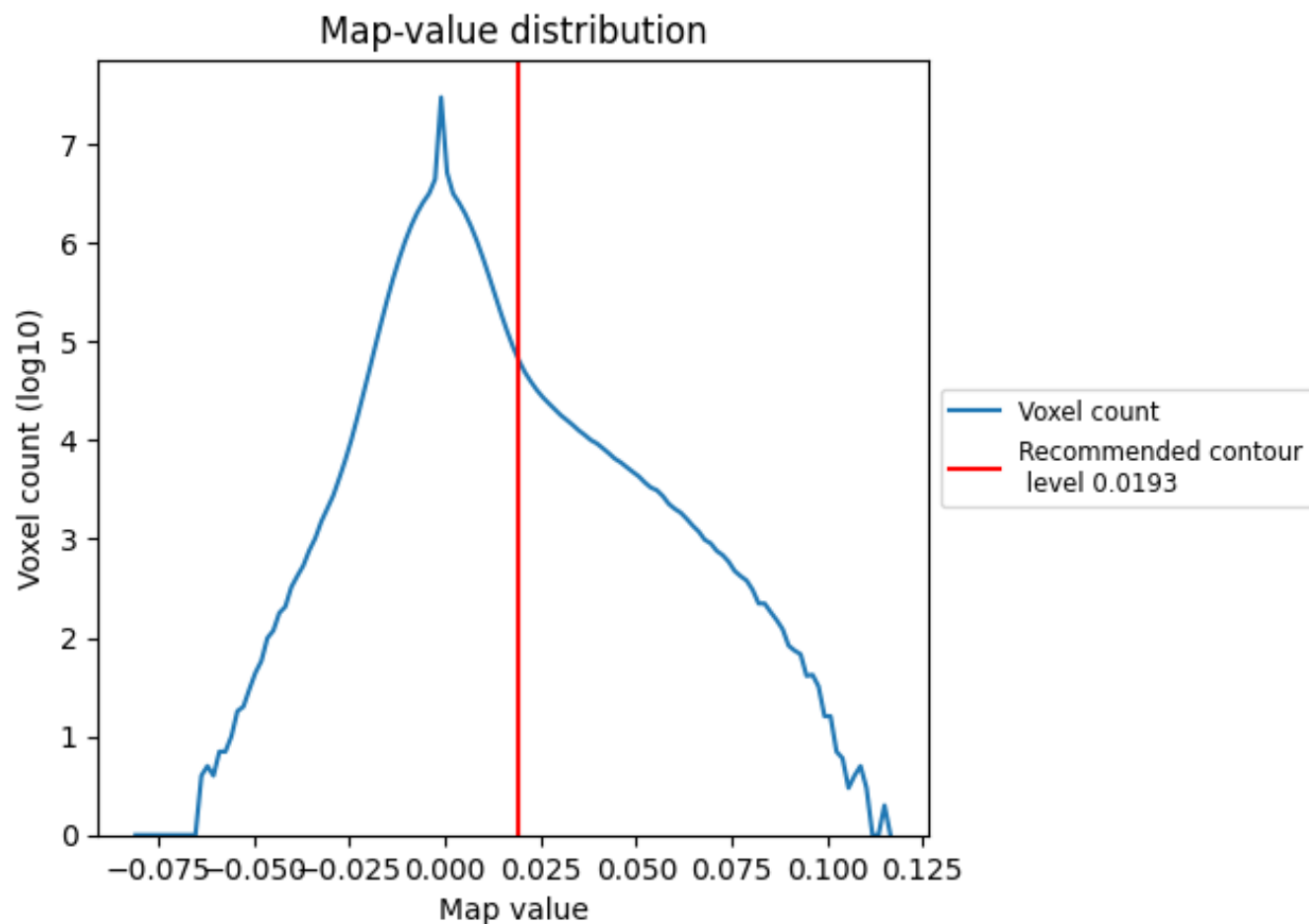
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

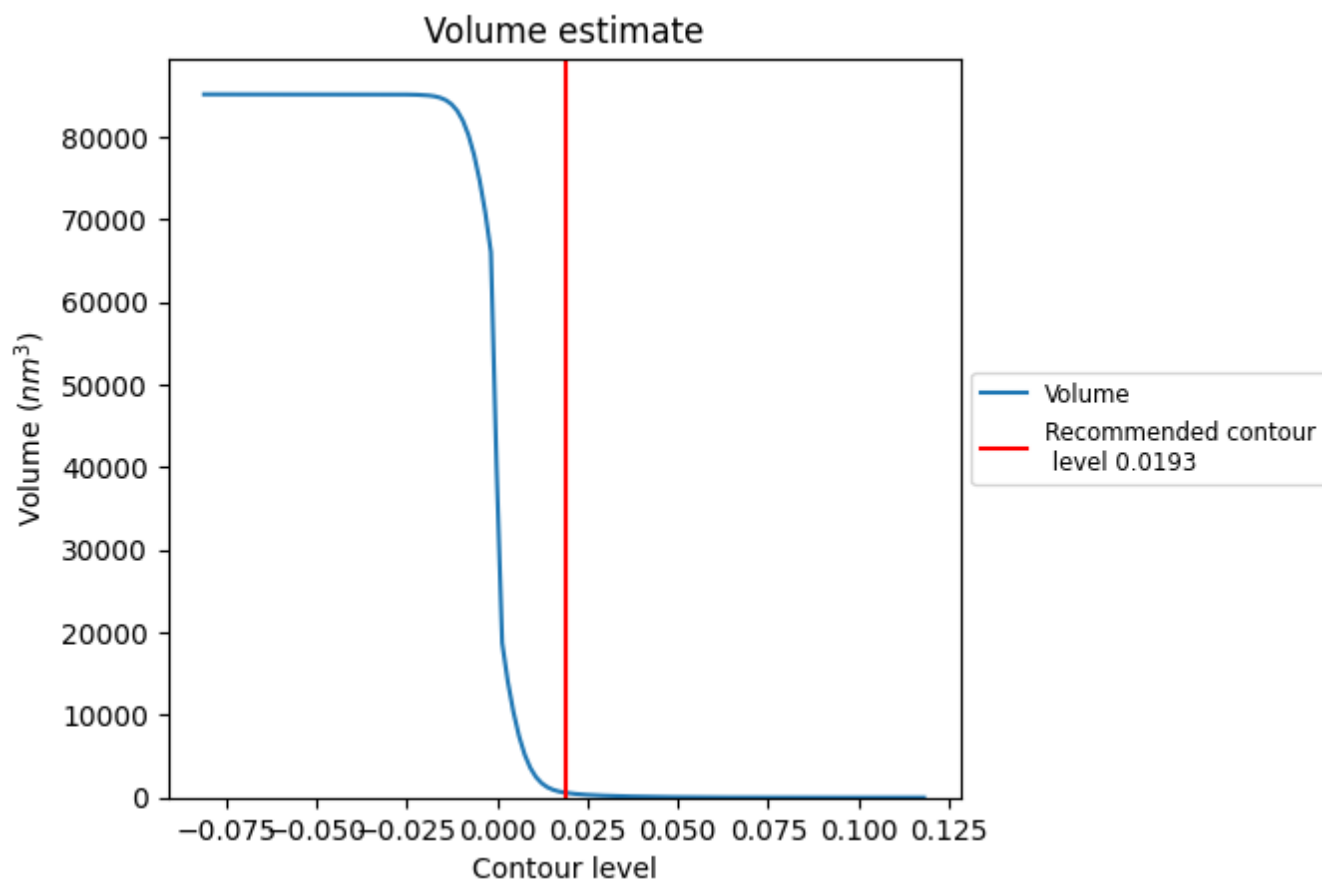
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

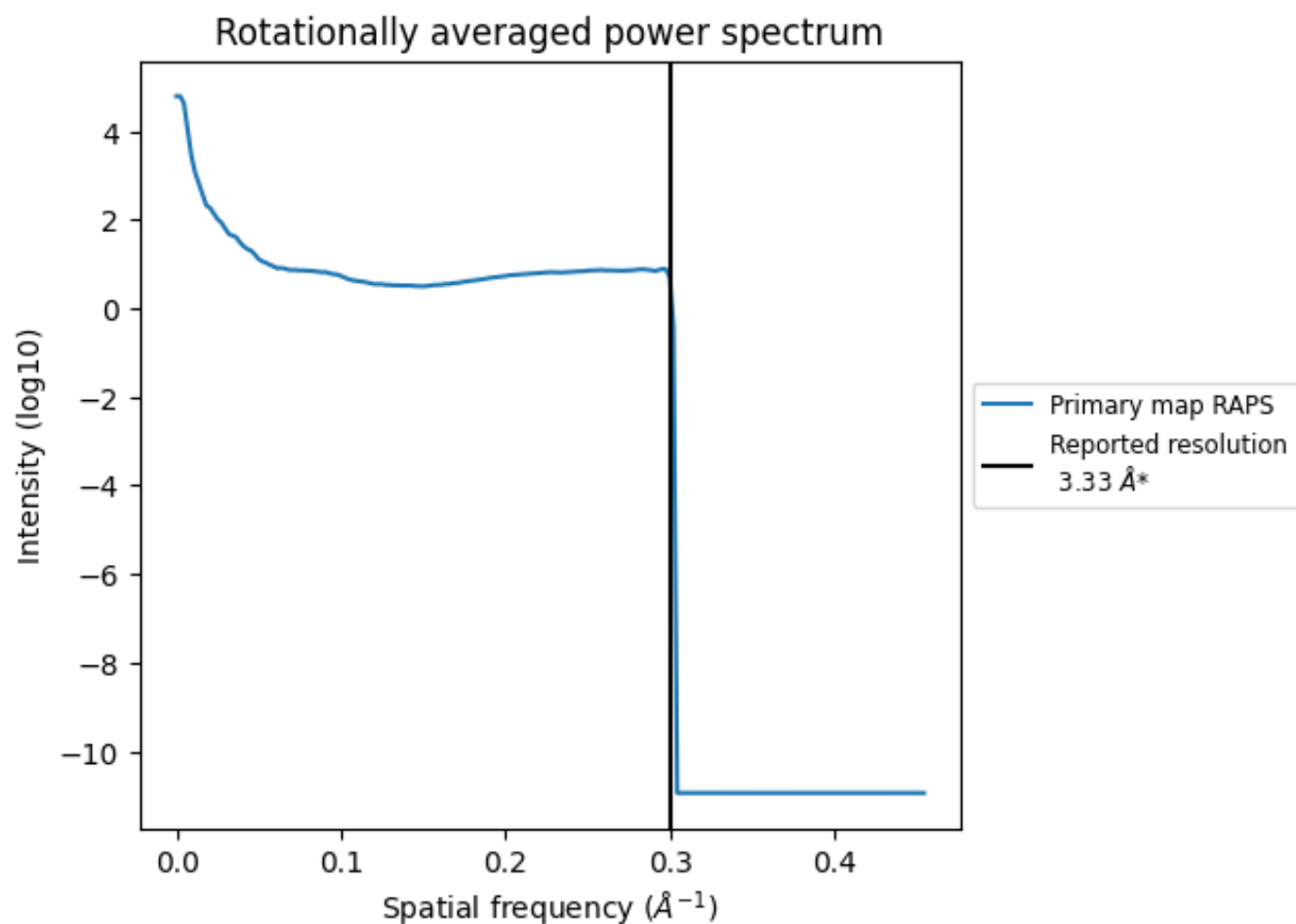
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 566 nm^3 ; this corresponds to an approximate mass of 511 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 0.300 $\text{\AA}^{-1}$

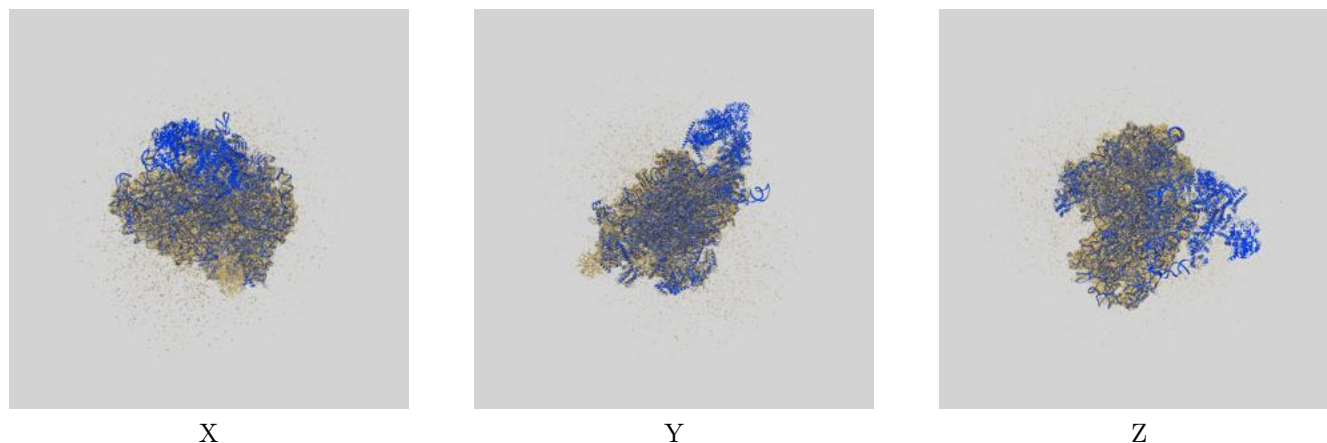
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

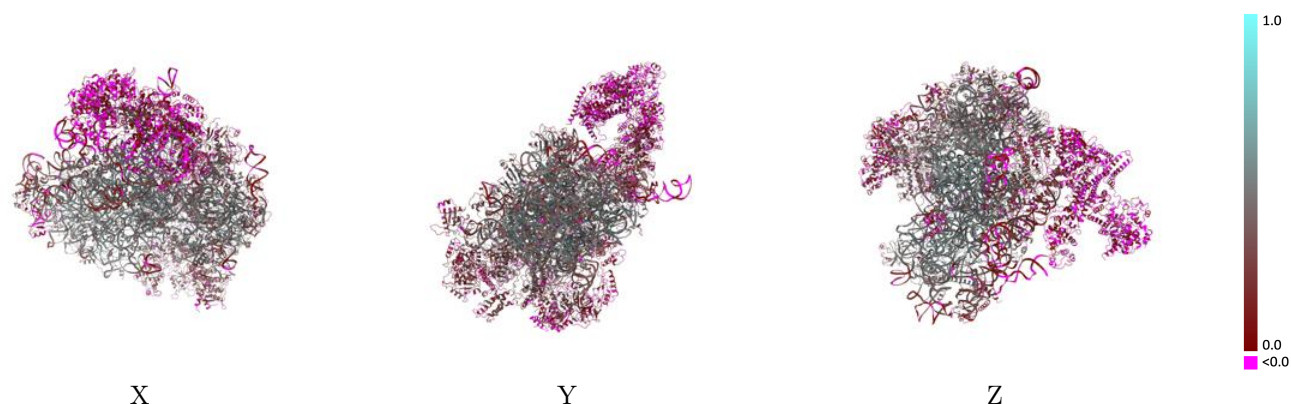
This section contains information regarding the fit between EMDB map EMD-11893 and PDB model 7ASE. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



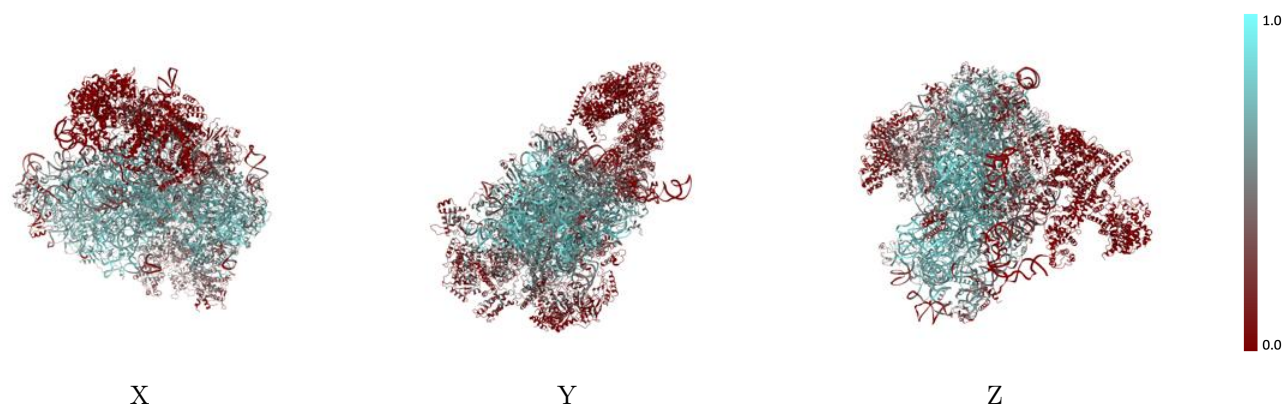
The images above show the 3D surface view of the map at the recommended contour level 0.0193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



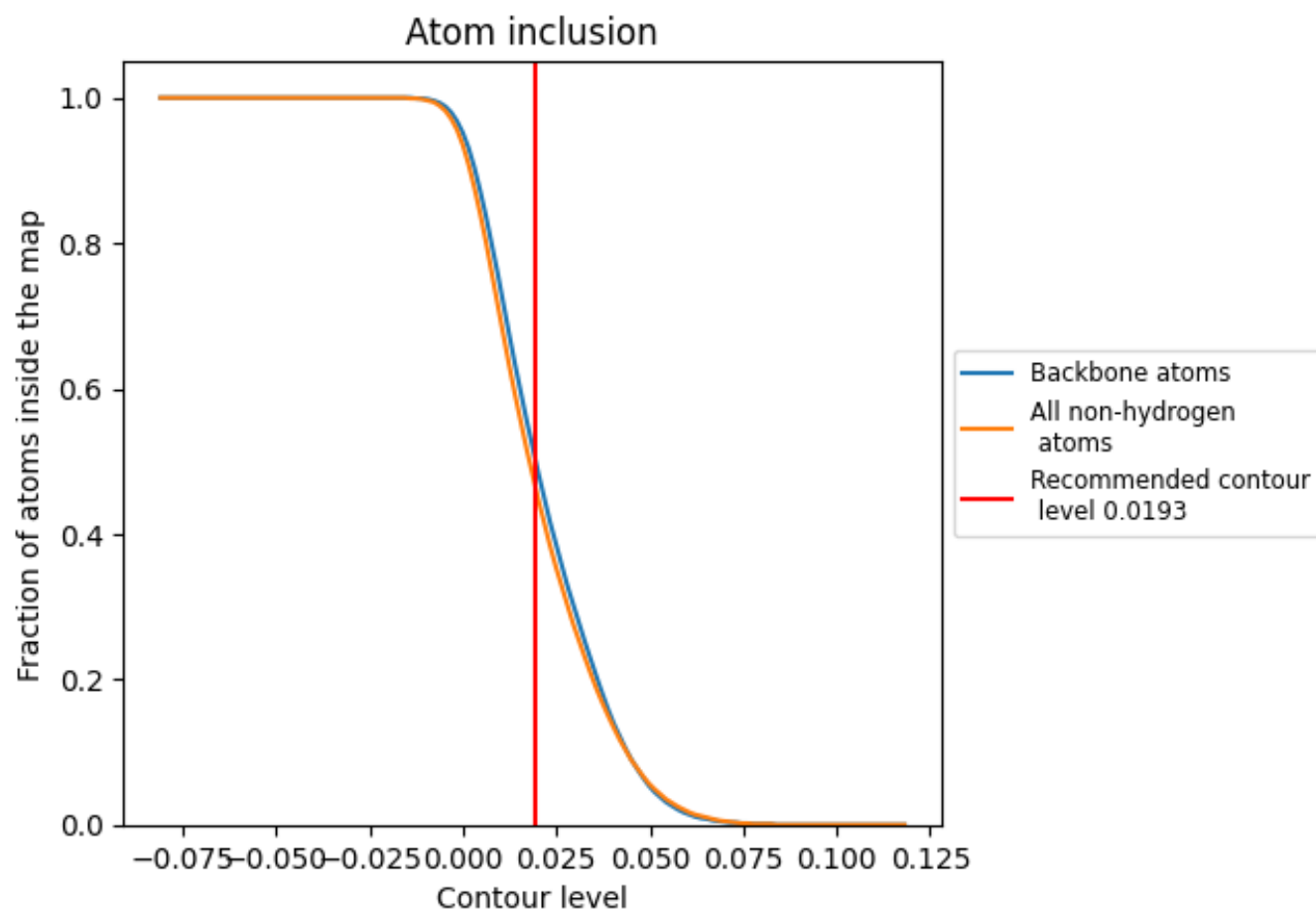
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0193).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 46% 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 (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4650	 0.3140
0	 0.6860	 0.4100
1	 0.6240	 0.3900
5	 0.1770	 0.1970
8	 0.1050	 0.1110
A	 0.1800	 0.2290
B	 0.6630	 0.4450
C	 0.1370	 0.1530
D	 0.6490	 0.4030
E	 0.0180	 0.0580
F	 0.6590	 0.4440
G	 0.0090	 0.0310
H	 0.0060	 0.0140
I	 0.0000	 0.0270
J	 0.2140	 0.1620
K	 0.0000	 0.0090
L	 0.5220	 0.3740
M	 0.5820	 0.4010
N	 0.5150	 0.3200
O	 0.5160	 0.2710
P	 0.5250	 0.3680
Q	 0.6170	 0.3660
R	 0.6710	 0.4560
S	 0.6560	 0.4530
T	 0.5680	 0.3920
U	 0.4510	 0.3740
V	 0.5590	 0.4390
W	 0.6410	 0.4440
X	 0.7030	 0.4570
Y	 0.0510	 0.1140
Z	 0.6630	 0.4390
a	 0.4440	 0.3150
b	 0.7230	 0.4770
c	 0.5110	 0.3610
d	 0.6770	 0.4640



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Chain	Atom inclusion	Q-score
f	 0.2540	 0.2210
g	 0.6680	 0.4600
h	 0.2370	 0.1980
i	 0.5450	 0.3570
j	 0.3190	 0.2750
l	 0.6780	 0.4450
m	 0.7000	 0.4630
n	 0.2780	 0.2490
o	 0.5770	 0.3930
p	 0.4880	 0.3530
q	 0.6080	 0.4110
r	 0.6470	 0.4160
s	 0.2070	 0.1950
t	 0.6920	 0.4720
u	 0.5260	 0.3220
v	 0.6550	 0.4420
w	 0.3930	 0.3050
y	 0.6420	 0.4190