



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 12:19 pm BST

PDB ID : 8R3V / pdb_00008r3v
EMDB ID : EMD-18875
Title : Escherichia coli paused disome complex (non-rotated disome interface)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-11-10
Resolution : 3.28 Å(reported)
Based on initial model : 7N1P

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:

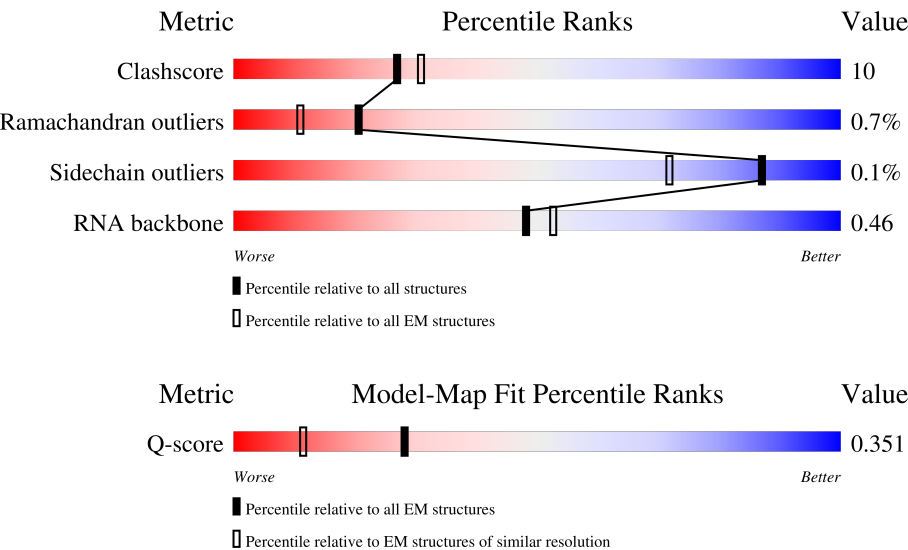
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 3.28 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.



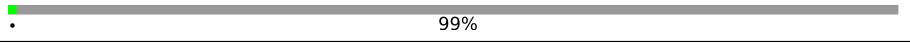
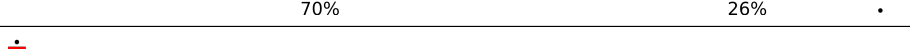
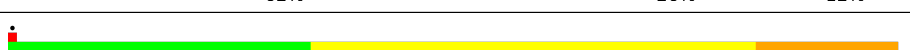
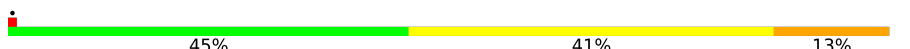
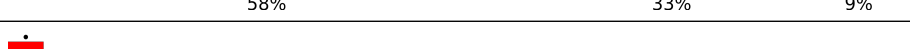
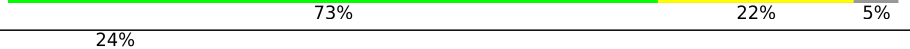
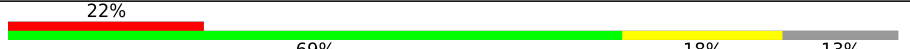
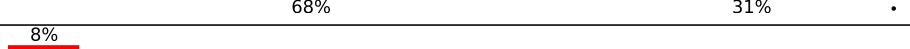
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	12	78	5% 77% 22% .
2	32	59	7% 71% 27% .
3	4	70	23% 61% 33% ..

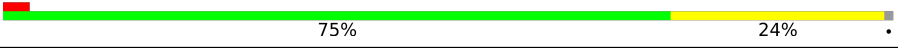
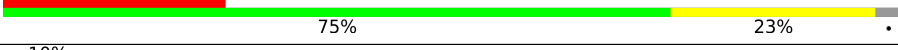
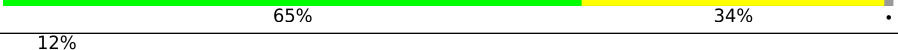
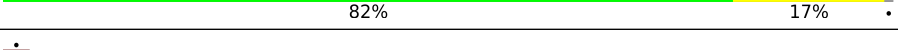
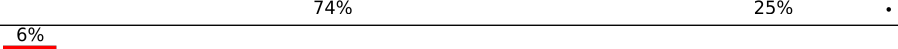
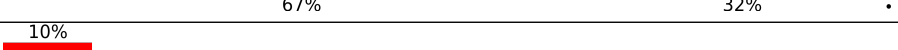
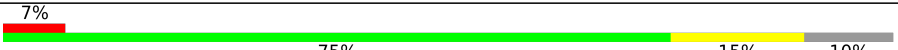
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Mol	Chain	Length	Quality of chain
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	
7	A1	1542	
7	A2	1542	
8	B	241	
8	B2	241	
9	C1	233	
9	C2	233	
10	D1	206	
10	D2	206	
11	E1	167	
11	E2	167	
12	F1	135	
12	F2	135	
13	G1	179	
13	G2	179	
14	H1	130	
14	H2	130	
15	I1	130	
15	I2	130	
16	J1	103	
16	J2	103	
17	K1	129	

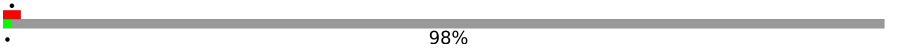
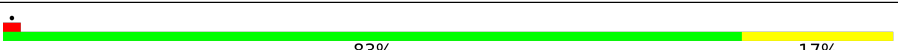
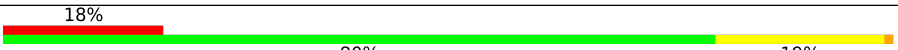
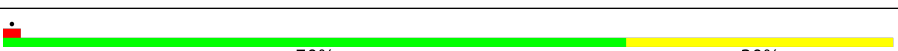
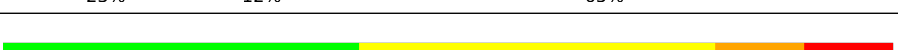
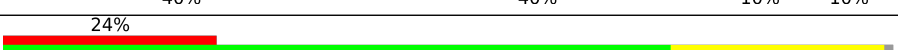
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Mol	Chain	Length	Quality of chain
17	K2	129	
18	L1	124	
18	L2	124	
19	M1	118	
19	M2	118	
20	N1	101	
20	N2	101	
21	O1	89	
21	O2	89	
22	P1	82	
23	Q1	84	
23	Q2	84	
24	R1	75	
24	R2	75	
25	S1	92	
25	S2	92	
26	T1	87	
27	U1	71	
27	U2	71	
28	V2	64	
29	W	76	
30	W1	76	
31	X2	77	
32	Y1	76	
33	Y2	76	

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Mol	Chain	Length	Quality of chain
34	Z1	557	
35	a2	234	
36	b2	273	
37	e2	179	
38	g2	55	
39	h2	136	
40	i2	149	
41	l2	46	
42	o2	144	
43	p	10	
44	r2	117	
45	z2	85	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 188607 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 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	30	Total	C	N	O	P	0	0
			644	288	119	207	30		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	94	Total	C	N	O	S	0	0
			756	474	147	134	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

- Molecule 29 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	2		

- Molecule 31 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	X2	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

- Molecule 32 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y1	36	Total	C	N	O	P	0	0
			778	348	142	252	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y2	76	Total	C	N	O	P	0	0
			1628	726	293	533	76		

- Molecule 34 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 38 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 41 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 43 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r2	116	Total	C	N	O	0	0
			891	552	178	161		

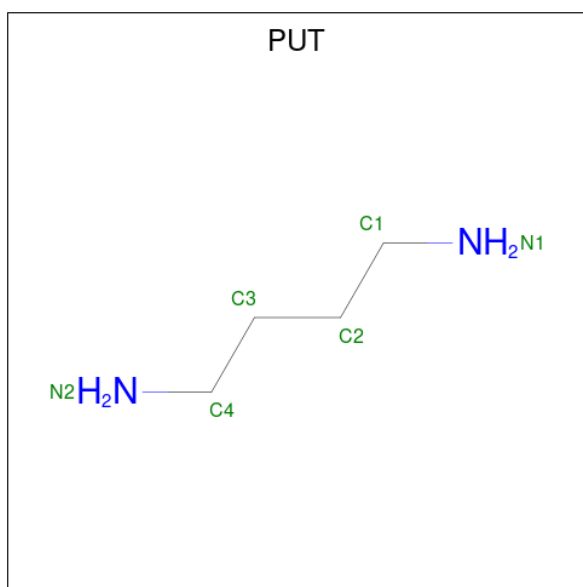
- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

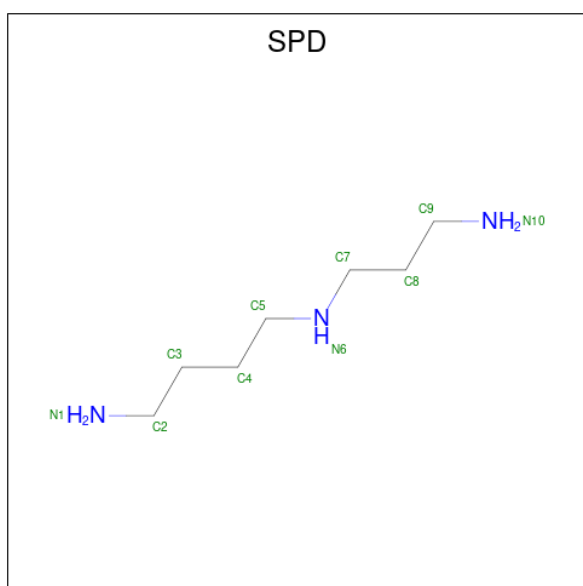
Mol	Chain	Residues	Atoms		AltConf
46	4	1	Total	Zn	0
			1	1	
46	B	1	Total	Zn	0
			1	1	

- Molecule 47 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			6	4	2	
47	72	1	Total	C	N	0
			6	4	2	

- Molecule 48 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

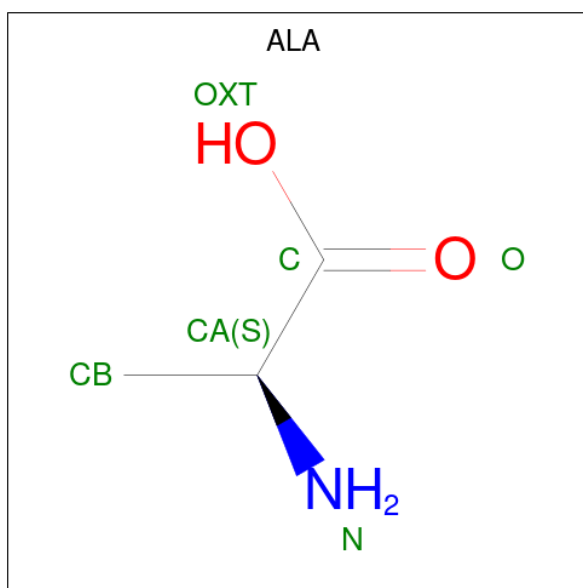


Mol	Chain	Residues	Atoms			AltConf
48	72	1	Total	C	N	0
			10	7	3	

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

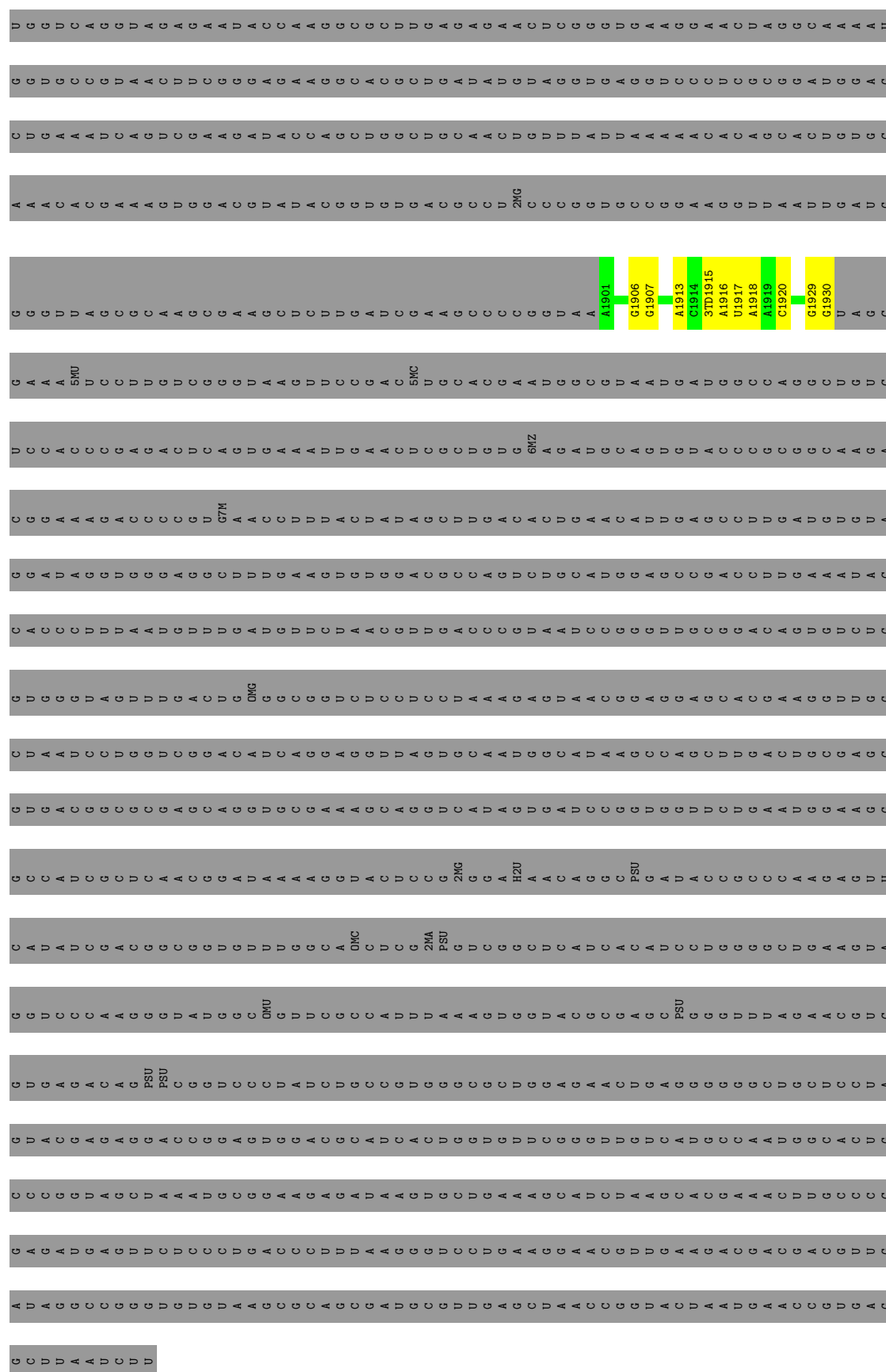
Mol	Chain	Residues	Atoms		AltConf
49	72	190	Total	Mg	0
			190	190	
49	82	1	Total	Mg	0
			1	1	
49	A1	60	Total	Mg	0
			60	60	
49	A2	42	Total	Mg	0
			42	42	
49	W	1	Total	Mg	0
			1	1	
49	Y2	1	Total	Mg	0
			1	1	
49	h2	1	Total	Mg	0
			1	1	
49	o2	1	Total	Mg	0
			1	1	

- Molecule 50 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



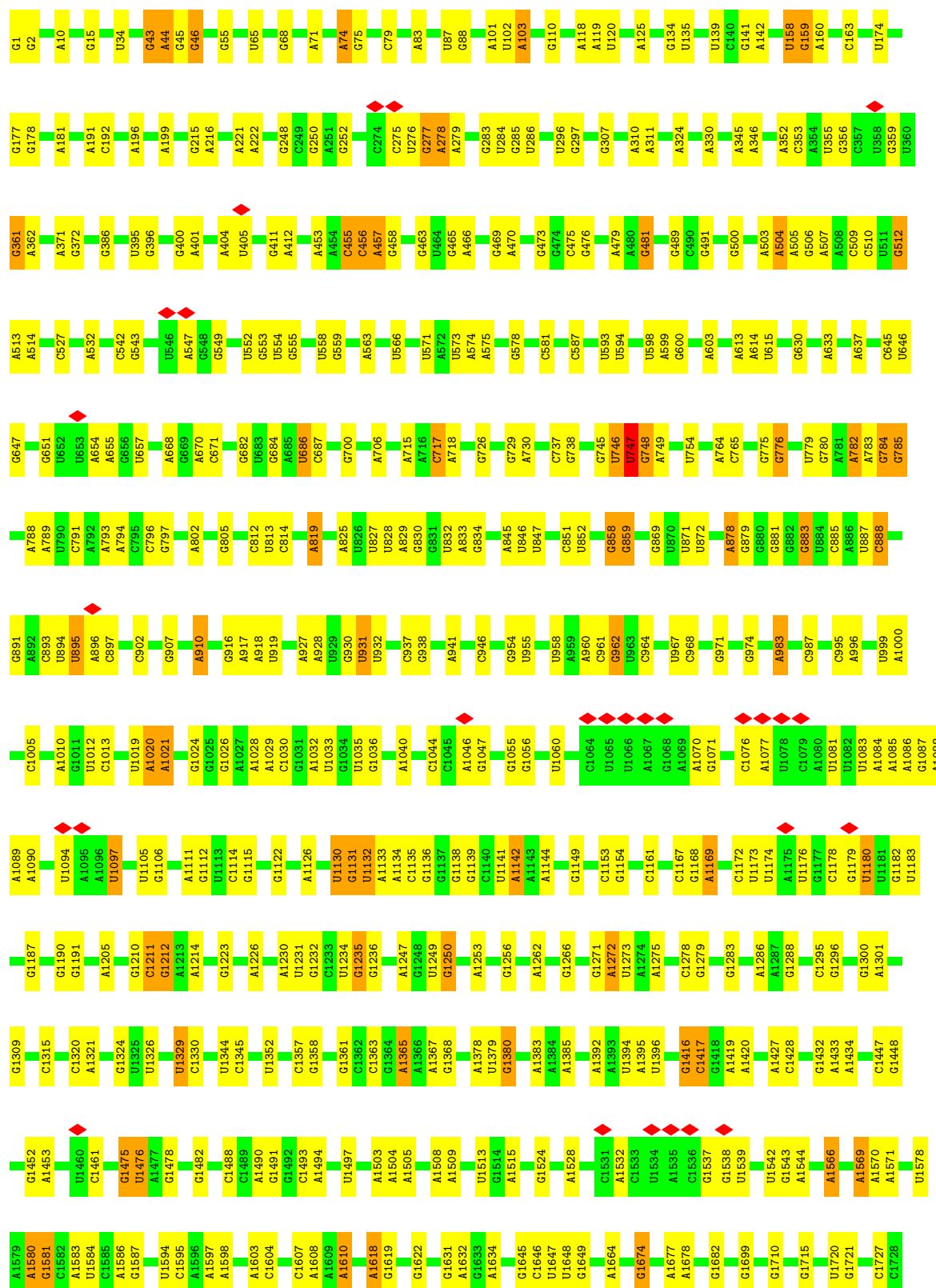
Mol	Chain	Residues	Atoms				AltConf
50	Y2	1	Total	C	N	O	0
			5	3	1	1	

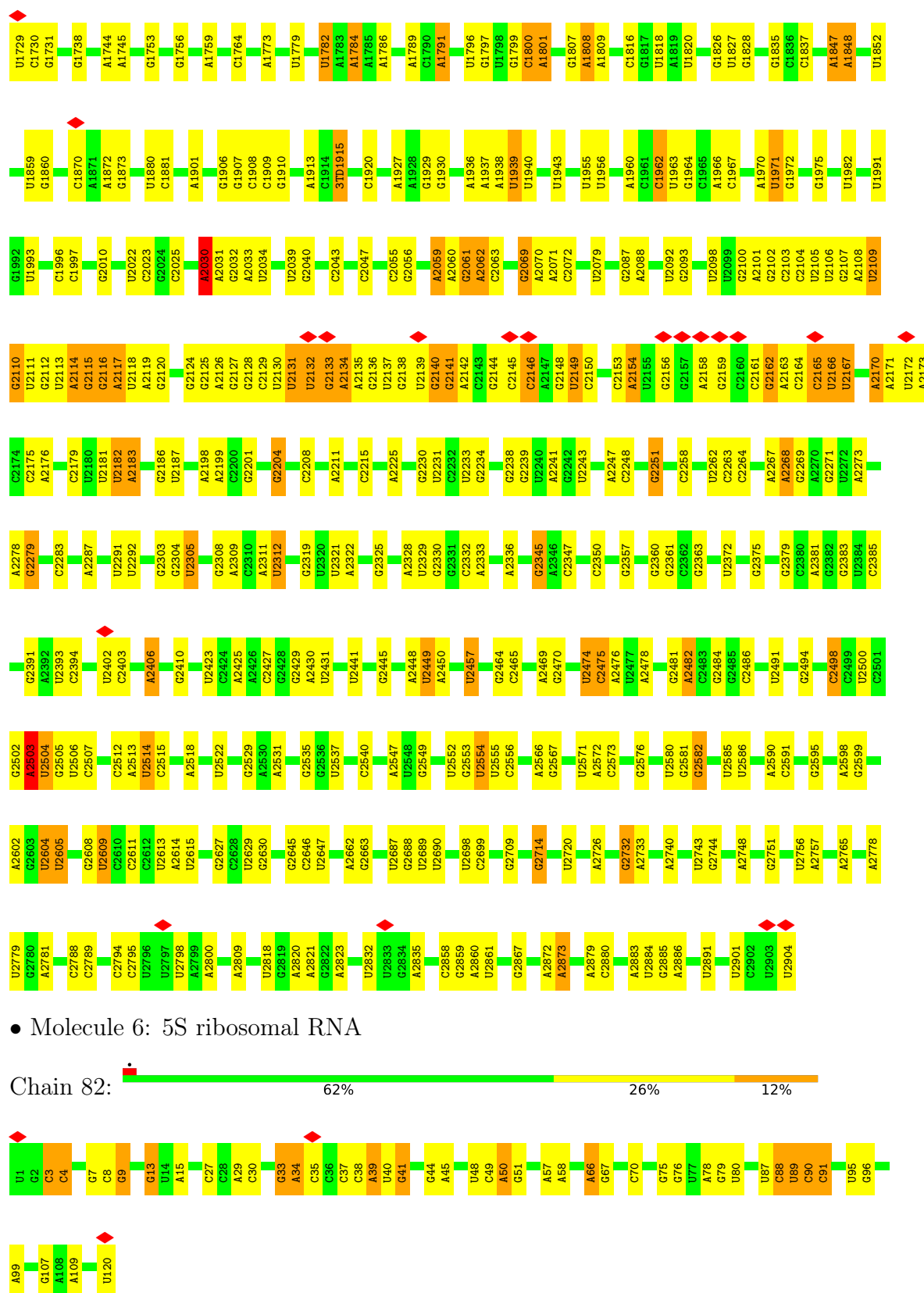


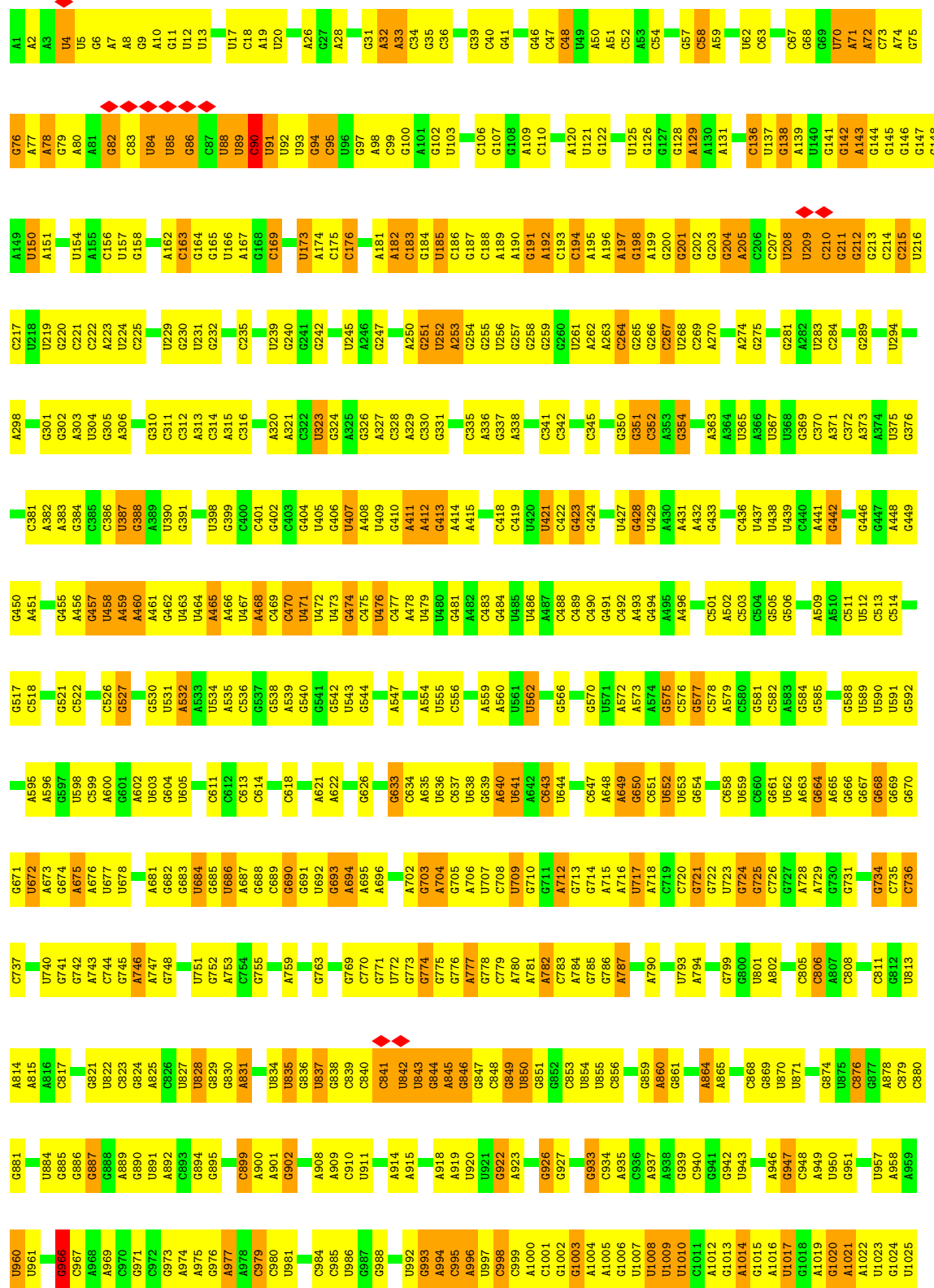


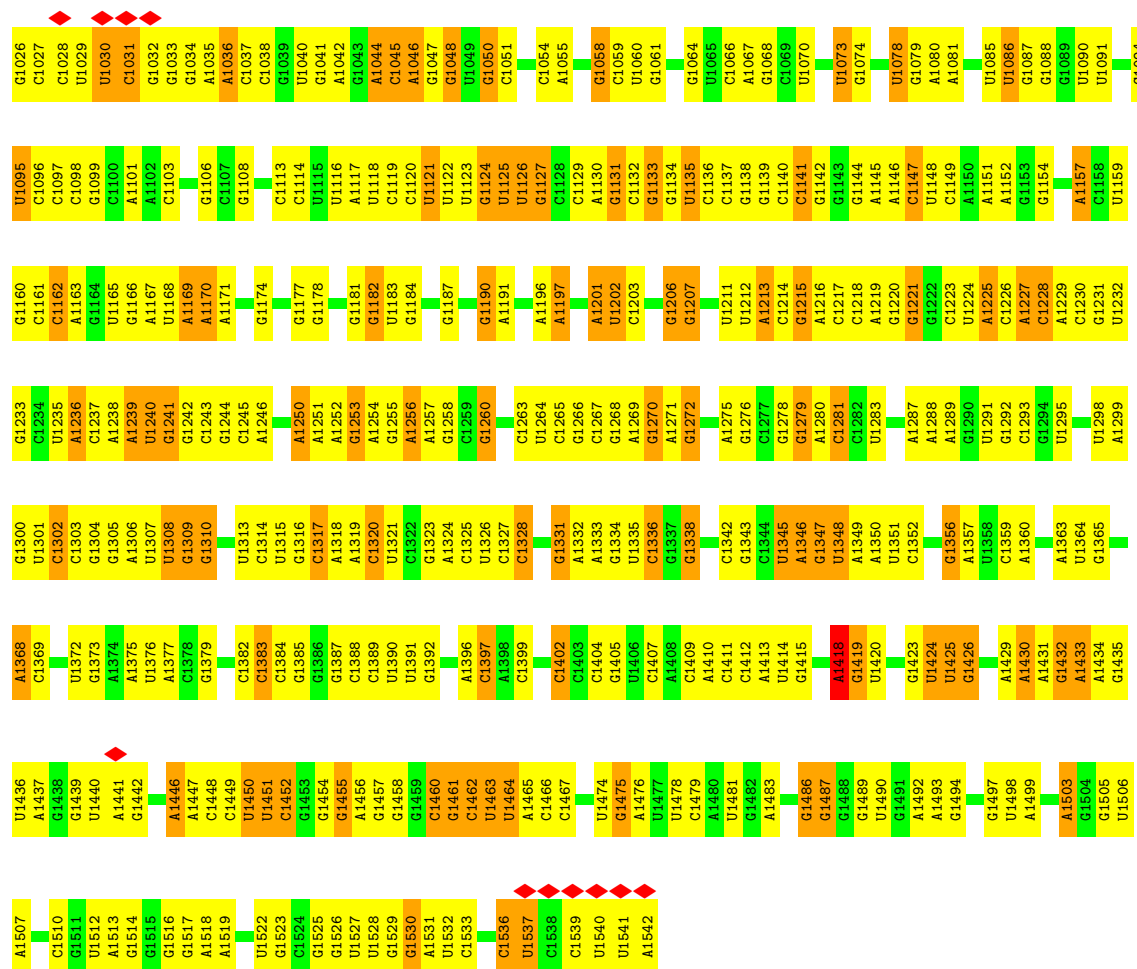
- Molecule 5: 23S ribosomal RNA

Chain 72:  70% 26%

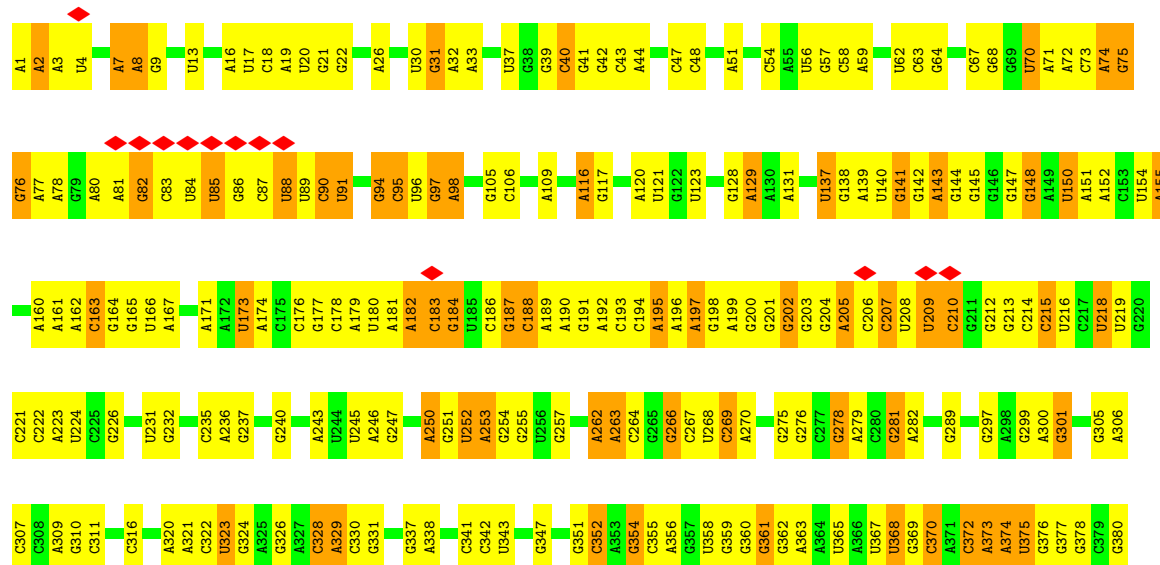






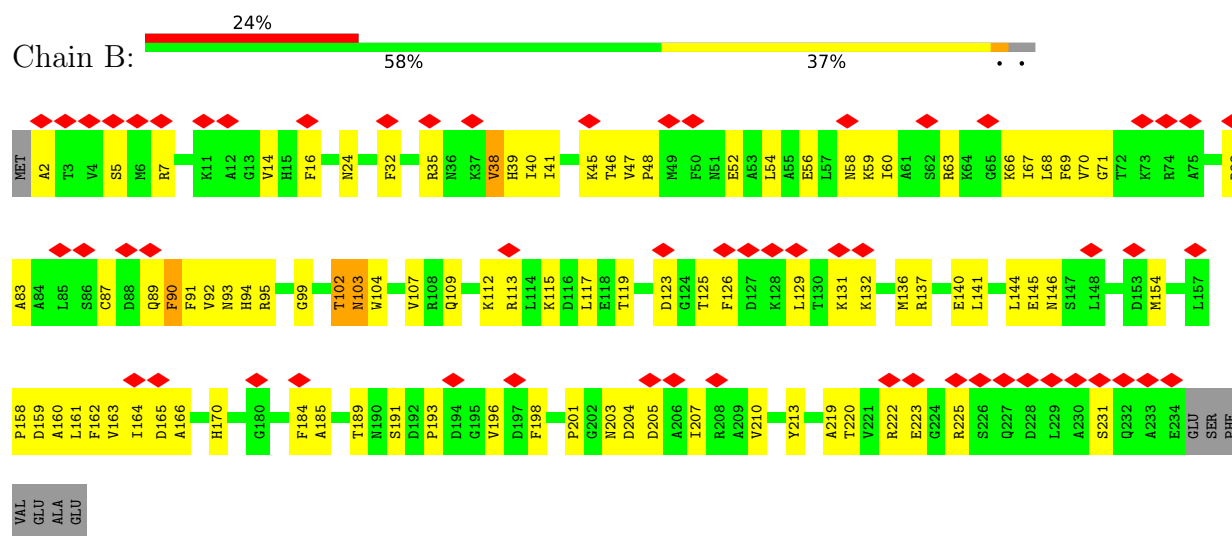


• Molecule 7: 16S ribosomal RNA

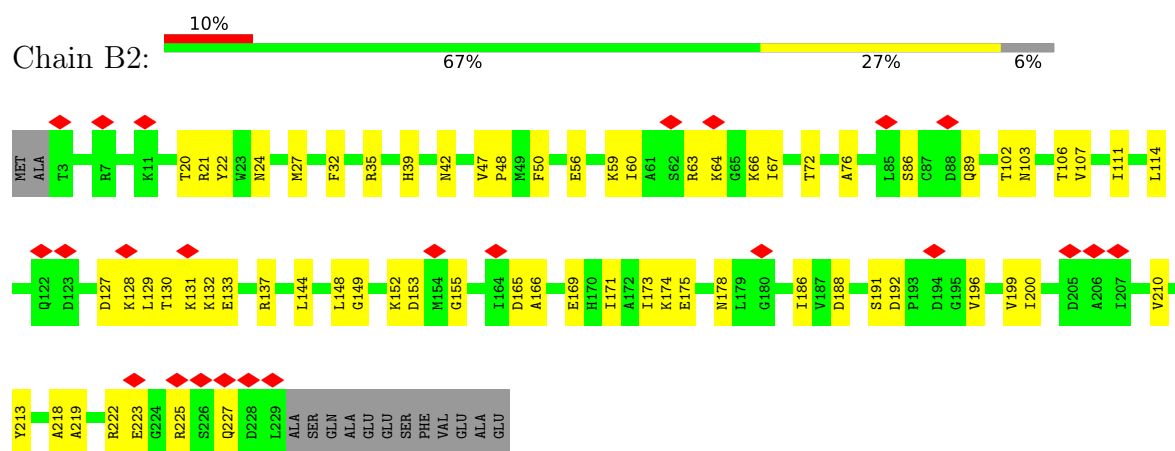


G1515	G1379	U1240	A1169	A1101	U1025	G953	A831	G722	A573	G506	G444	C381
G1516	U1380	G1241	A1170	C1103	C1027	G954	G832	U723	A574	C507	G445	A382
G1517	U1381		A1171	C1103	C1027	G954	G832	U723	A574	U508		A383
A1518	C1382	G1244	C1172	G1104	U1029	U960	U835	G725	C576	A509	A448	G384
A1519	C1314	C1245	C1173	A1105	U1029	U961	U835	U961	C577	A510	G449	G385
	C1316	A1246	G1174	G1106	U1030	C962	G838	C726	C578	C511	G450	C386
G1526	C1317	U1247	G1175	C1107	U1030	G963	C839	G731	A579	U512	A451	U387
	A1318	A1248	A1176	G1108	G1032	G963	C839	G731	A579	U512	A451	U387
G1529	A1319	C1249	G1177	C1113	G1033	G966	C841	C732	A579	C513	A452	G388
G1530	C1320	A1250	G1177	C1114	G1033	A968	U842	G734	U598	C514	G453	A389
U1531	C1321	A1251	U1182	C1114	A1035	A969	U843	C735	G601	U516	G454	U390
U1532	C1322	A1252	G1183	U1115	A1036	A969	G844	C735	A602	G517	G455	G391
C1533	G1233	G1283	G1184				G844			C518	G457	A393
A1534	A1324	A1294	G1185	U1118	U1040	C972	A845	C739	G606	C519	G458	A397
C1535	C1325	G1255	G1186	C1119	G1041	A974	G846	U740	U520	A459		A397
U1406	U1326	A1256	G1187	C1120	A1042	A975	C847	G741	A520	A459		A397
C1407	C1327	A1257	U1188	U1121	G1043	A976	C848	G748	C612	A460	A461	U398
	C1328	G1258	G1189	U1122	A1044	G976	G849	A749	C620	A461	G462	C400
C	A1329	C1259	U1190	U1123	C1045	A977	U855		A621	G524	U463	C401
U		G1260	A1191	G1124	A1046			G752	U632		U464	
U	A1332	A1261	C1192	U1125	G1063	A983	G859	C754	U632	G527	A465	G404
A	A1429	C1262	G1193	U1126	C1054	A983	G859	G755	G633	C528	A466	U405
		C1263	G1127	C1054	U1055	U986	A865		A642	G530	U467	G406
U1436	C1337	U1264	A1196	C1128	U1056	G987	A865	G765	C643	G530	A468	U407
A1437	G1338	C1265	A1197	C1129	U1057	G988	C868	A766		U531	C469	A408
	A1339	G1266	G1198	A1130	G1057	G989	C869			A532		U409
A1441	A1340	C1267	U1199	G1131	G1058	C990	U870	G769	U652	A533	C470	U410
		G1268	C1200	C1132	C1059	U991	U871		U653	A534	U472	G411
U1446	U1345	A1269	A1201	G1133	U1060	G992	U871	G776	G654	U534	U472	A412
A1447	A1346	A1270	U1202	G1134	G1061	G993	C876	A777	C475	G536	G474	G413
C1448	G1347	A1271	C1206	U1135	U1062	A994	C876	G778	U476	G538	U476	A414
U1449	U1348	C1272	C1207	C1136	C1063	C995	C880		C477	A539		G415
U1450	A1349	C1273	C1208	G1137	G1064	A996	G898	A787	G478	G540	A478	G416
U1451	U1350	A1274	C1209	C1138	U1065	U997	G898	U789	G666	G541	U480	C418
C1452	U1351		C1209	G1139	G1066	C998	A901	A790		U543	G481	C419
G1453	C1352	G1279		C1140	A1067	C1066	G902			G544	U420	G482
G1454	G1353	A1280	U1213	C1141	C1071	A1000	G902	U793	G671	C545	C483	U421
	U1354	C1281	A1212	G1142	G1072	A1004	A914	A794	U672	A546	G484	G422
U1477	G1355	A1282	C1214	G1143	G1072	A1005	A914	A794	A673	U547	U485	G423
U1478	G1356	U1286	G1215	G1144	G1072	A1006	G922	C797	A675	G548	U486	G424
C1479	A1357	A1287	C1218	A1145	U1073	G1006	G922	C797	A676	C549	U487	G425
	U1358	A1287	C1218	C1147	U1075	U1007	G926	C808	U677	C488	U427	U426
G1487	C1359	A1287	A1219	U1148	U1076	U1008	G926	C808	U677	G550	U427	U426
	A1360	U1291	G1220	C1149	U1078	U1009	C932	C811	G691	U551	G428	G428
A1492		C1292	U1292	A1150	U1078	U1010	C932	C811	G691	U552	C490	U429
A1493	A1363	C1293	G1222	A1151	C1079	C1011	C933	G812	U692	A553	G491	A430
	U1364	G1297	G1222	A1152	A1080	A1081	C934	G812	U692	A554	C492	A431
G1497	U1364	U1298	A1225	A1157	G1084	G1013	A935	A815	A694	U555	A493	G432
U1498	C1365	C1298	C1226	C1157	U1086	G1013	A935	A815	A694	C556	G494	G433
A1499	C1367	G1300	A1227	C1158	U1086	A1014	G941	A816	G703	G557	U434	A432
A1500	A1368	U1301	C1228	U1159	U1085	A1016	G942	C817	G703	G558	A495	A435
	C1369	C1302	A1229	G1160	U1085	A1016	G942	C817	G703	G558	A495	A435
A1503	G1370	C1302	A1229	G1160	U1085	A1016	G942	C817	G703	G558	A495	A435
	G1371	C1303	U1232	C1161	U1086	A1016	G942	C817	G703	G558	A495	A435
U1506	U1372	G1304	U1232	C1162	G1094	U1017	G945	G821	G710	A559	A496	C436
A1507	A1375	G1305	U1236	A1163	U1095	U1017	G945	G821	G710	A559	A496	C436
A1508	A1376	A1306	A1236	A1163	U1096	U1017	G945	G821	G710	A559	A496	C436
U1509	U1376	U1307	G1237	C1162	C1096	U1017	G945	G821	G710	A559	A496	C436
A1513	A1377	U1308	G1238	G1166	C1097	U1017	G945	G821	G710	A559	A496	C436
		A1378	A1239	A1167	U1098	U1017	G945	G821	G710	A559	A496	C436
G1514	G1378	G1309	A1239	U1168	G1100	G1024	U952	G830	G721	A572	C503	C443

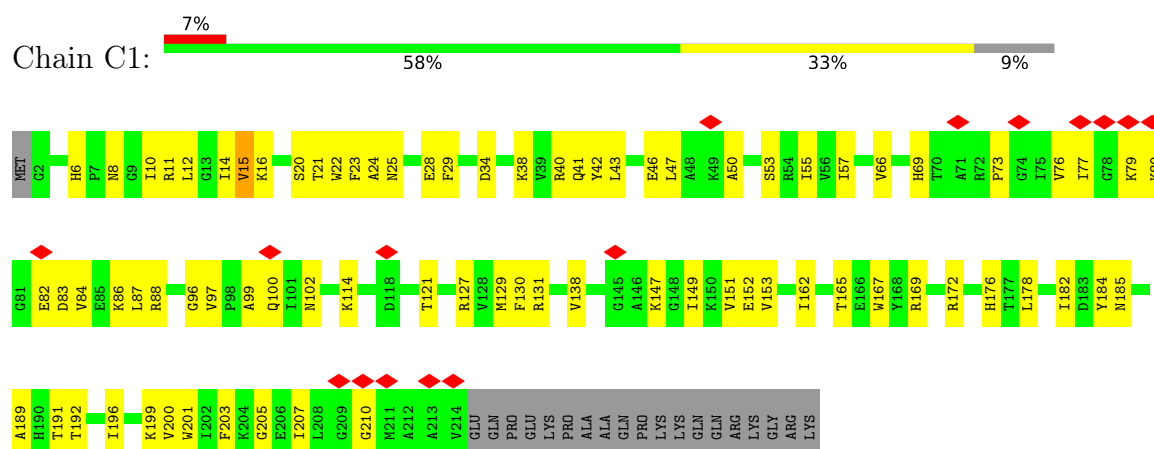
- Molecule 8: Small ribosomal subunit protein uS2



- Molecule 8: Small ribosomal subunit protein uS2

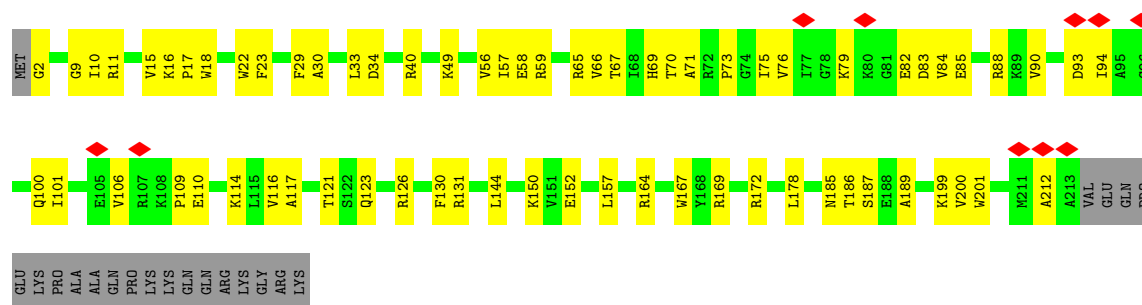


- Molecule 9: Small ribosomal subunit protein uS3

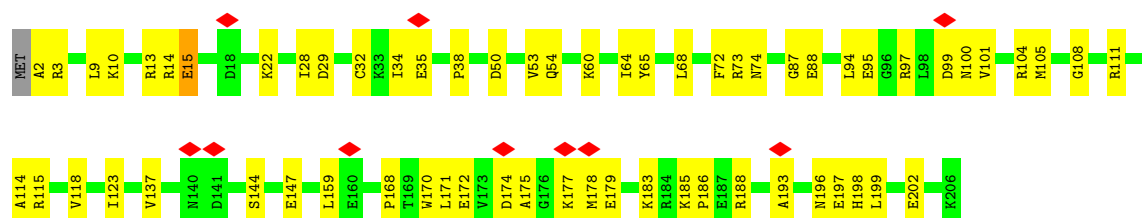
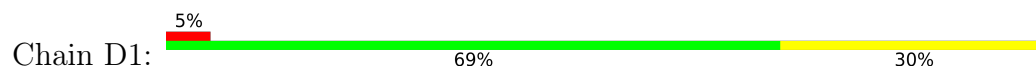


- Molecule 9: Small ribosomal subunit protein uS3

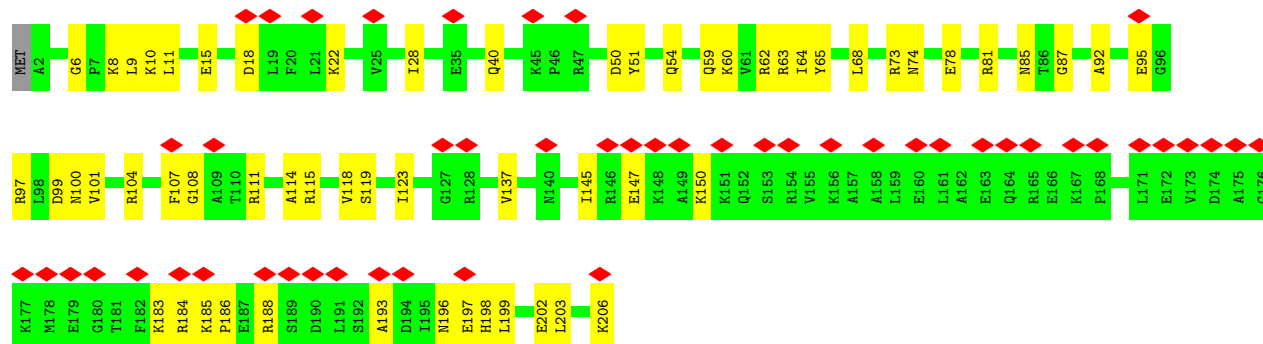




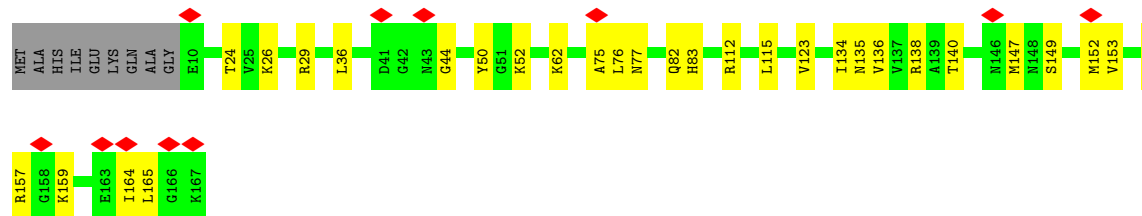
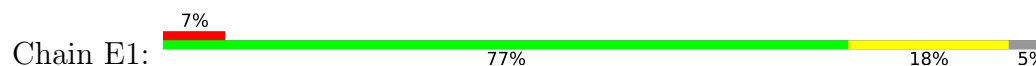
- Molecule 10: Small ribosomal subunit protein uS4



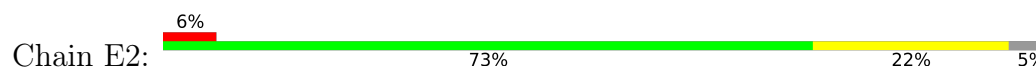
- Molecule 10: Small ribosomal subunit protein uS4

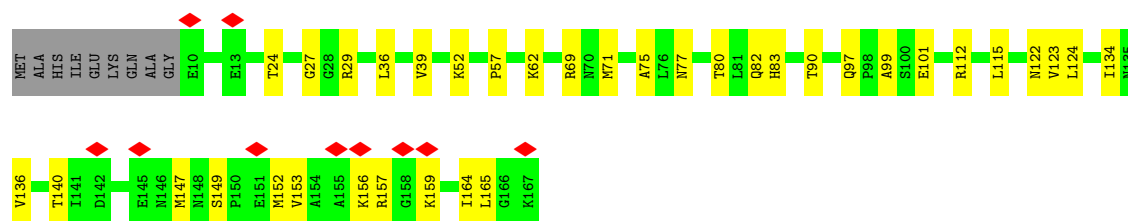


- Molecule 11: Small ribosomal subunit protein uS5

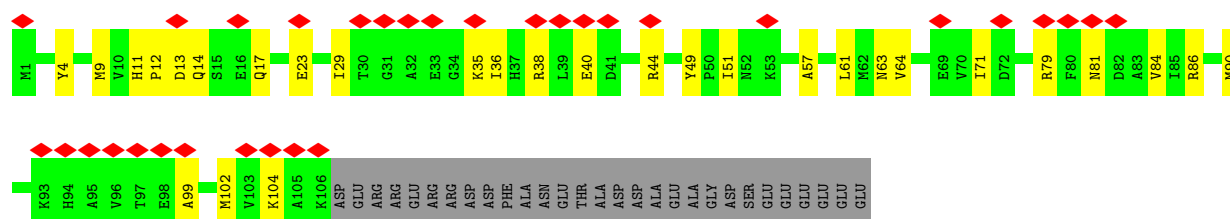


- Molecule 11: Small ribosomal subunit protein uS5

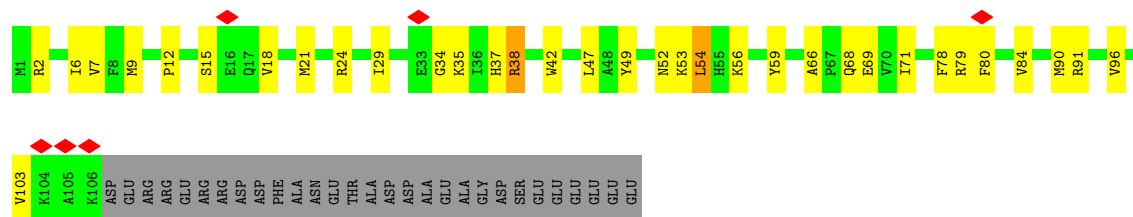




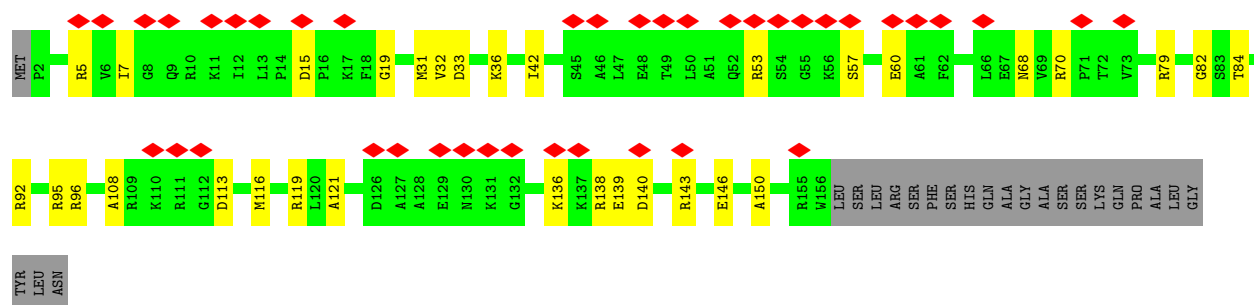
- Molecule 12: 30S ribosomal protein S6



- Molecule 12: 30S ribosomal protein S6

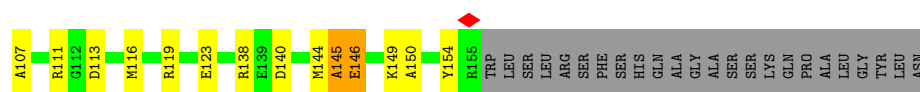


- Molecule 13: 30S ribosomal protein S7

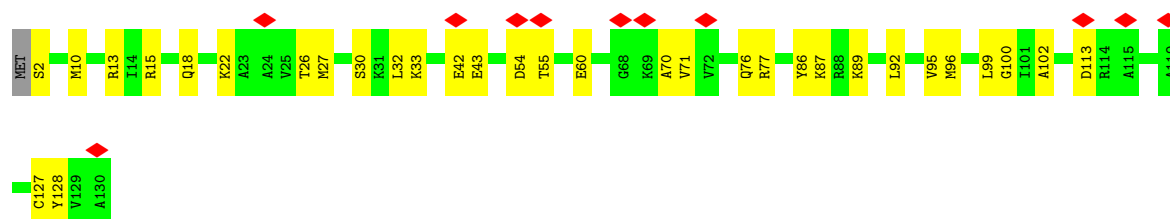
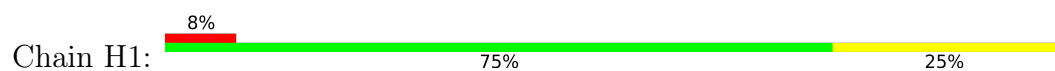


- Molecule 13: 30S ribosomal protein S7

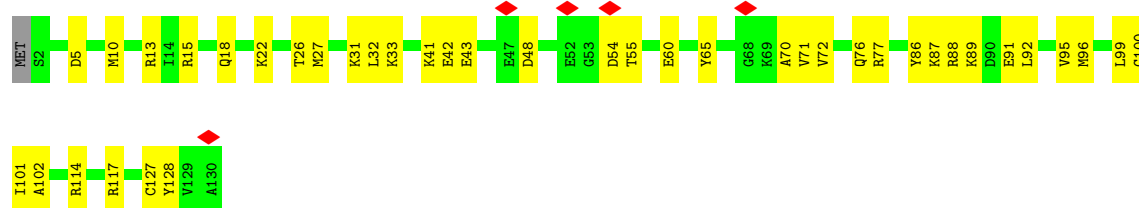




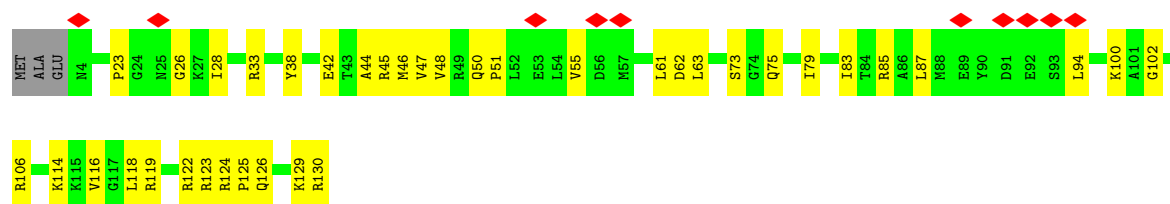
- Molecule 14: Small ribosomal subunit protein uS8



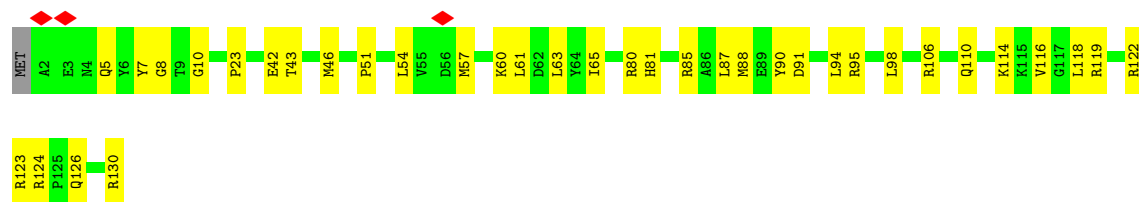
- Molecule 14: Small ribosomal subunit protein uS8



- Molecule 15: Small ribosomal subunit protein uS9

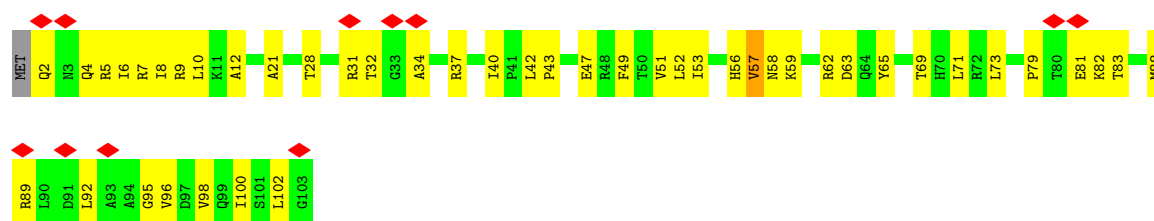


- Molecule 15: Small ribosomal subunit protein uS9



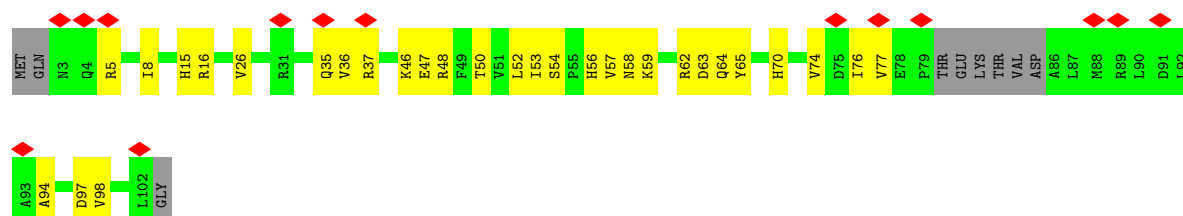
- Molecule 16: 30S ribosomal protein S10

Chain J1: 



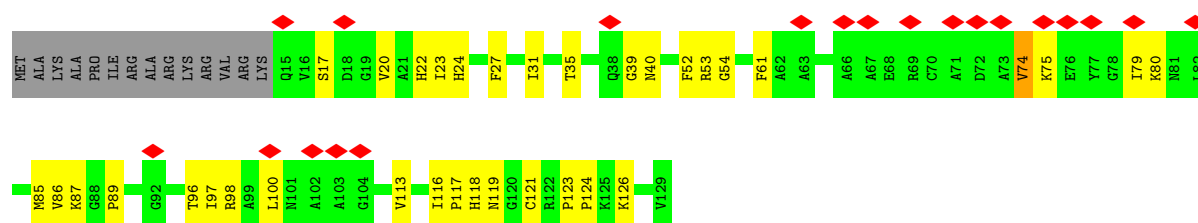
- Molecule 16: 30S ribosomal protein S10

Chain J2: 



- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 



- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 



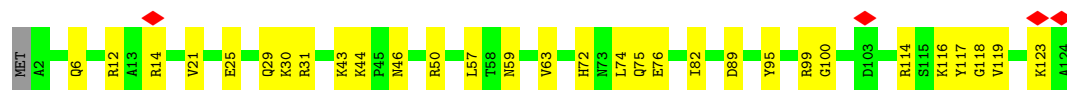
- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 

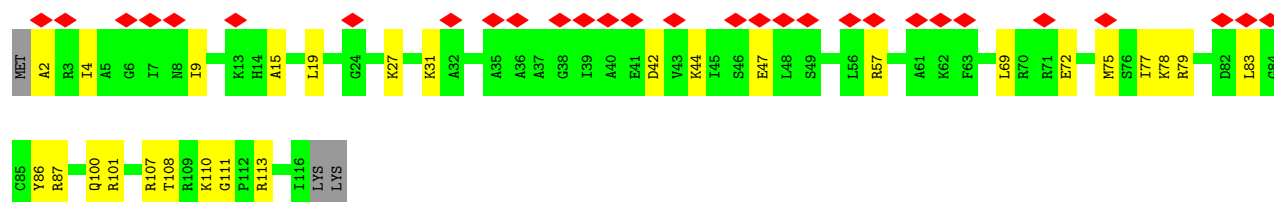
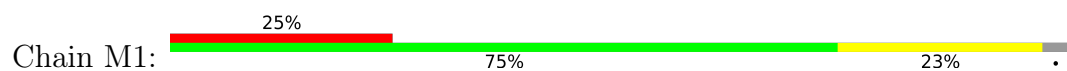


- Molecule 18: Small ribosomal subunit protein uS12

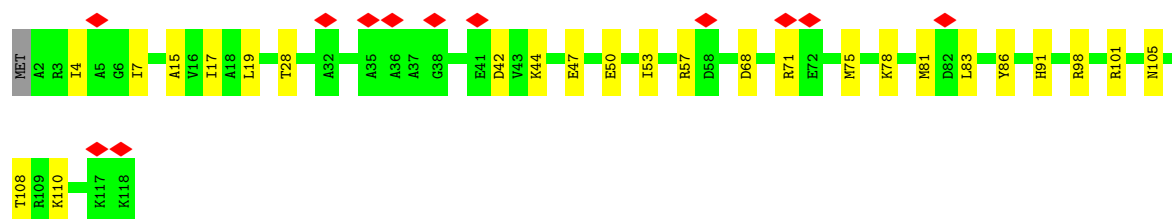
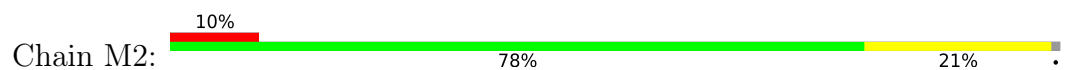
Chain L2: 



- Molecule 19: Small ribosomal subunit protein uS13



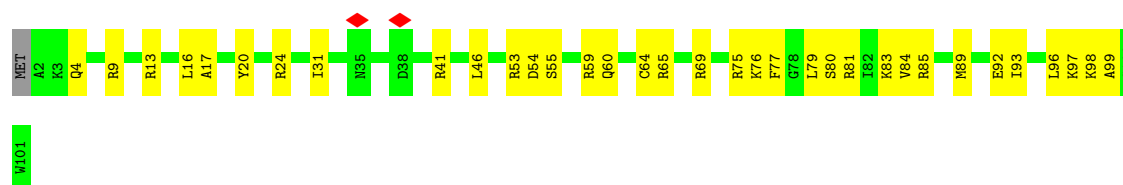
- Molecule 19: Small ribosomal subunit protein uS13



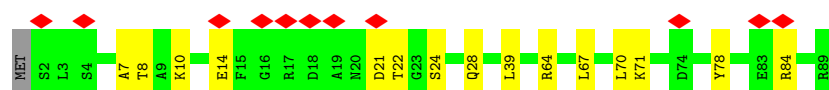
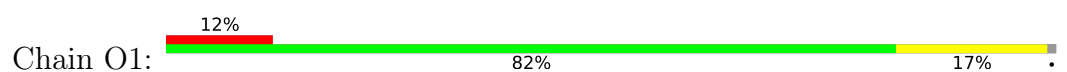
- Molecule 20: Small ribosomal subunit protein uS14



- Molecule 20: Small ribosomal subunit protein uS14

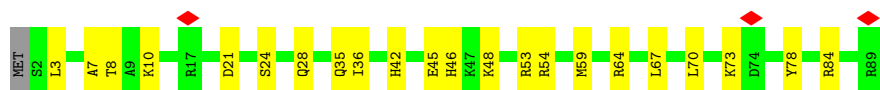


- Molecule 21: 30S ribosomal protein S15



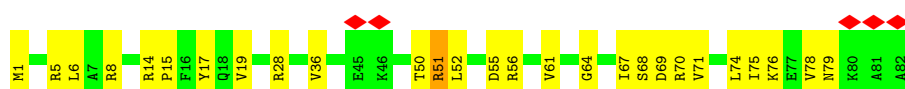
- Molecule 21: 30S ribosomal protein S15

Chain O2:  74% 25%



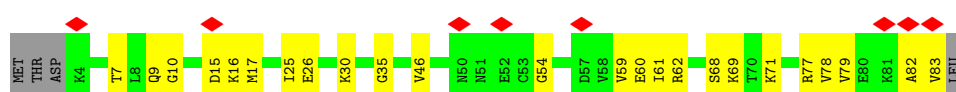
- Molecule 22: 30S ribosomal protein S16

Chain P1:  6% 67% 32%



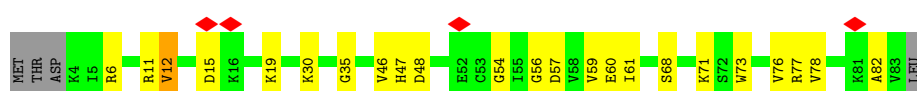
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q1:  10% 67% 29% 5%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q2:  5% 68% 26% 5%



- Molecule 24: Small ribosomal subunit protein bS18

Chain R1:  15% 69% 29%



- Molecule 24: Small ribosomal subunit protein bS18

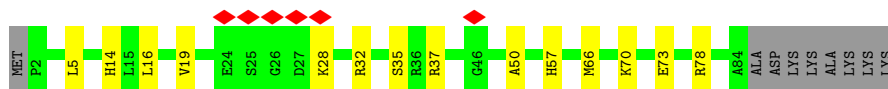
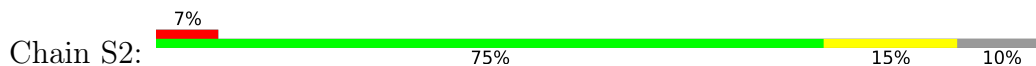
Chain R2:  9% 65% 33%



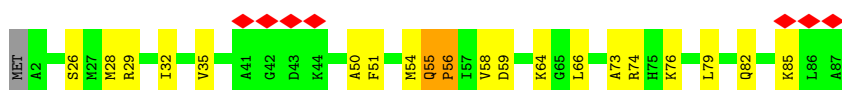
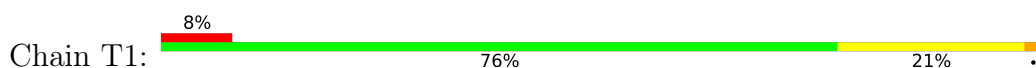
- Molecule 25: Small ribosomal subunit protein uS19

Chain S1:  24% 68% 22% 10%

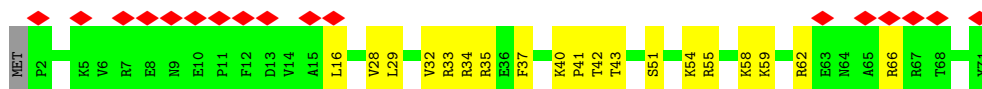
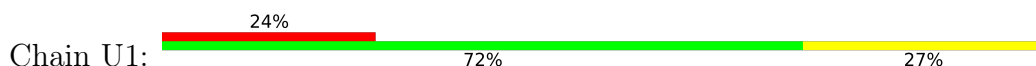
- Molecule 25: Small ribosomal subunit protein uS19



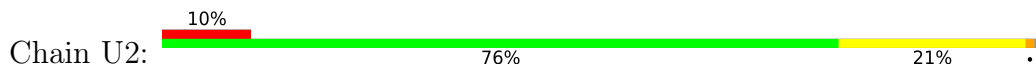
- Molecule 26: Small ribosomal subunit protein bS20



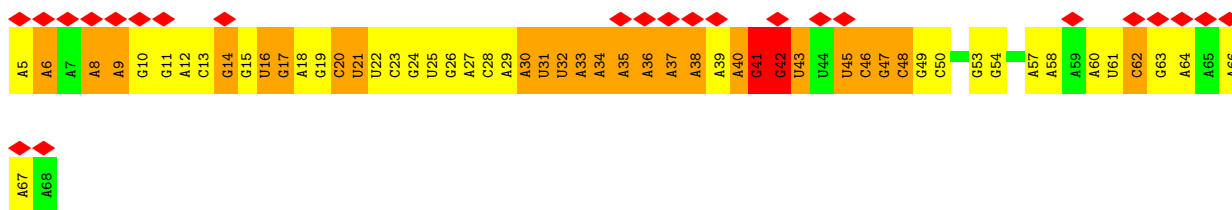
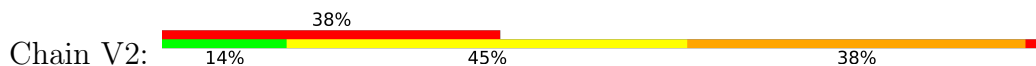
- Molecule 27: 30S ribosomal protein S21



- Molecule 27: 30S ribosomal protein S21

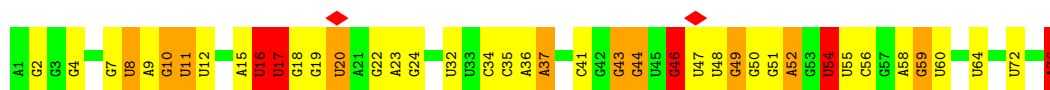


- Molecule 28: messenger RNA

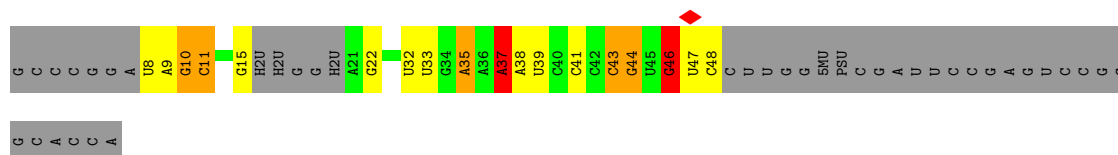
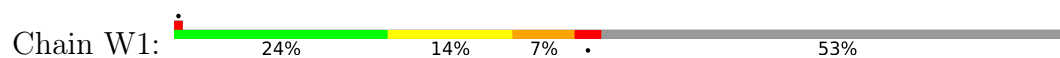


- Molecule 29: tRNA-Trp (P-site)

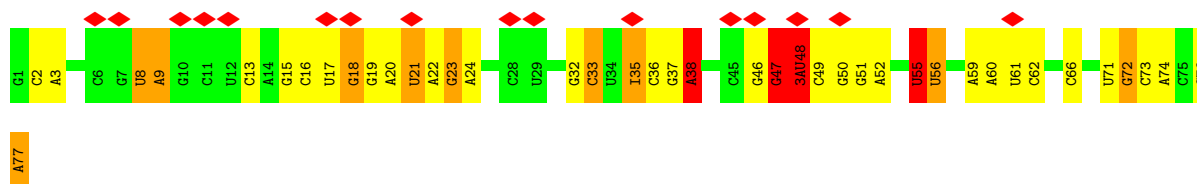




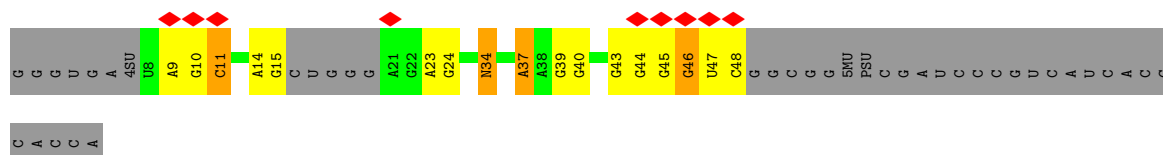
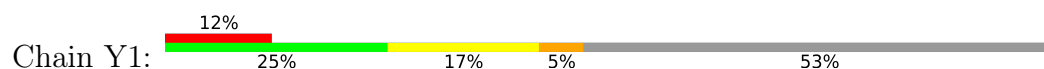
- Molecule 30: tRNA-Phe (P-site)



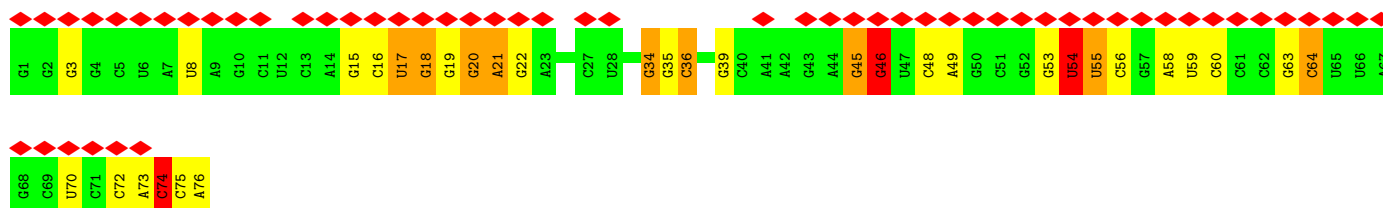
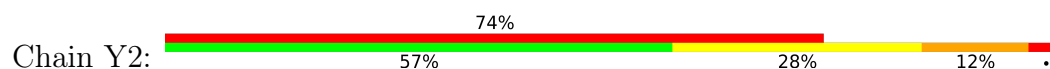
- Molecule 31: tRNA-Arg (E-site)



- Molecule 32: tRNA-Val (A-site)



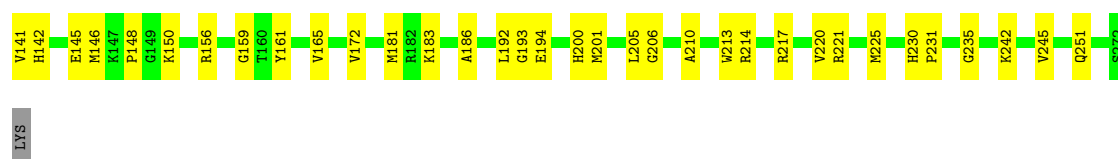
- Molecule 33: tRNA-Ala (A-site)



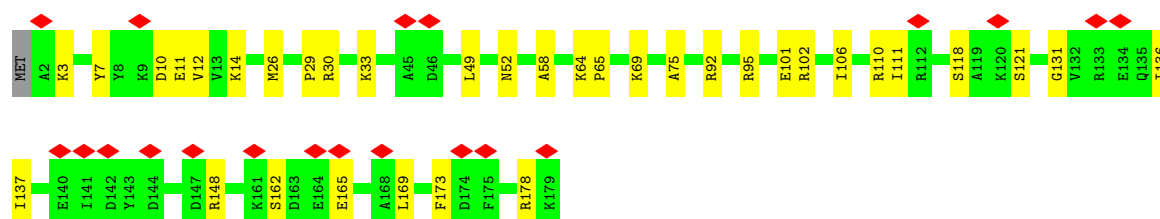
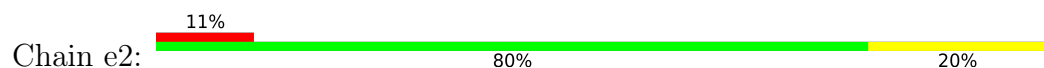
- Molecule 34: 30S ribosomal protein S1



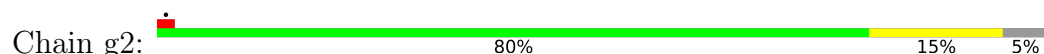




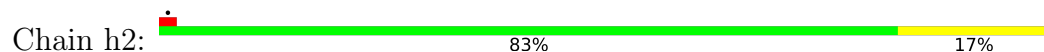
- Molecule 37: 50S ribosomal protein L5



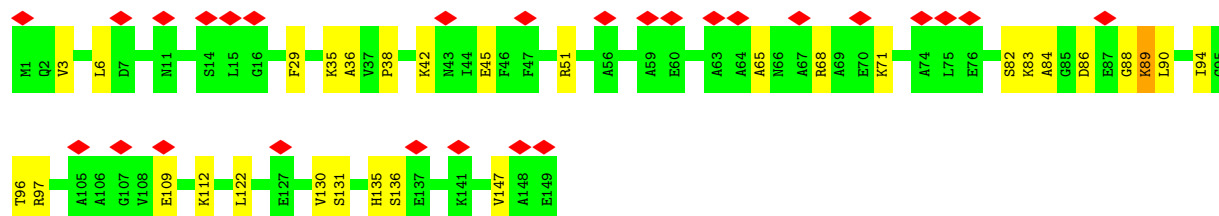
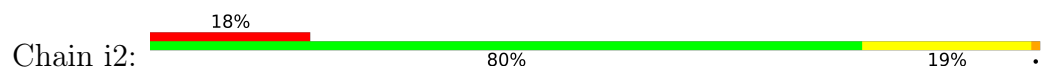
- Molecule 38: 50S ribosomal protein L33



- Molecule 39: 50S ribosomal protein L16



- Molecule 40: 50S ribosomal protein L9

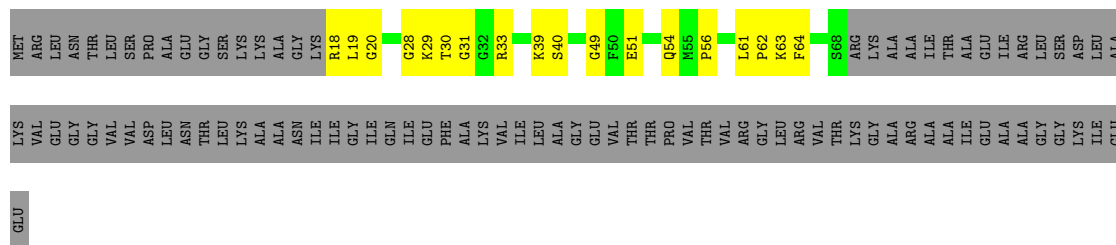


- Molecule 41: 50S ribosomal protein L34

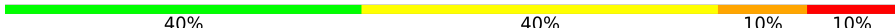


- Molecule 42: 50S ribosomal protein L15

Chain o2:  23% 12% 65%



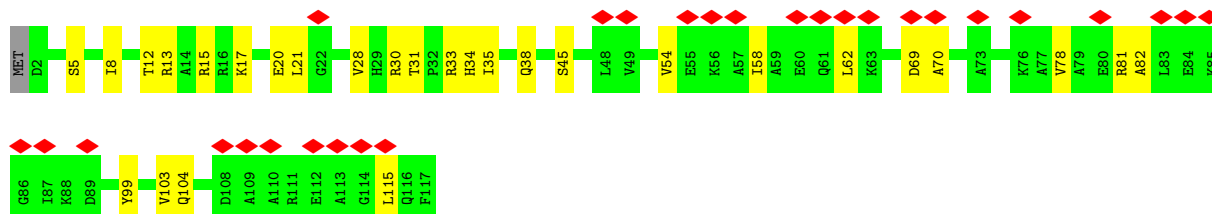
- Molecule 43: Nascent chain

Chain p:  40% 40% 10% 10%



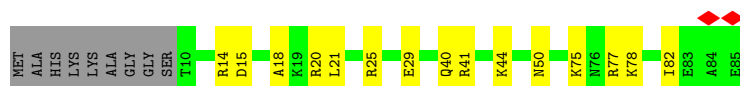
- Molecule 44: 50S ribosomal protein L18

Chain r2:  24% 75% 24%



- Molecule 45: 50S ribosomal protein L27

Chain z2:  72% 18% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.865	Depositor
Minimum map value	-5.986	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.7	Depositor
Map size (Å)	744.11993, 744.11993, 744.11993	wwPDB
Map dimensions	702, 702, 702	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, RSP, OMC, 5MC, MA6, 2MA, PUT, 7MG, H2U, 5MU, 1MG, G7M, SPD, OMU, 3AU, ZN, 3TD, 2MG, MIA, 6MZ, PSU, 4OC, OMG, CM0, MG, UR3

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	12	0.11	0/635	0.34	0/848
2	32	0.10	0/453	0.34	0/605
3	4	0.24	0/539	0.66	0/721
4	62	0.09	0/513	0.33	0/676
5	71	0.09	0/696	0.26	0/1081
5	72	0.10	0/69306	0.21	0/108116
6	82	0.16	1/2872 (0.0%)	0.27	0/4478
7	A1	0.17	0/36794	0.35	2/57392 (0.0%)
7	A2	0.16	0/36681	0.31	3/57217 (0.0%)
8	B	0.17	0/1846	0.50	0/2488
8	B2	0.16	0/1807	0.46	0/2435
9	C1	0.13	0/1692	0.41	0/2280
9	C2	0.13	0/1685	0.38	0/2270
10	D1	0.12	0/1665	0.40	0/2227
10	D2	0.10	0/1665	0.33	0/2227
11	E1	0.13	0/1179	0.34	0/1584
11	E2	0.13	0/1179	0.34	0/1584
12	F1	0.10	0/881	0.30	0/1189
12	F2	0.13	0/881	0.40	0/1189
13	G1	0.10	0/1246	0.33	0/1672
13	G2	0.13	0/1230	0.45	0/1649
14	H1	0.11	0/989	0.33	0/1326
14	H2	0.11	0/989	0.34	0/1326
15	I1	0.11	0/1034	0.36	0/1375
15	I2	0.12	0/1048	0.36	0/1394
16	J1	0.17	0/827	0.43	0/1117
16	J2	0.19	0/765	0.59	1/1033 (0.1%)
17	K1	0.11	0/873	0.34	0/1180
17	K2	0.12	0/900	0.33	0/1215
18	L1	0.12	0/969	0.37	0/1300
18	L2	0.12	0/969	0.37	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M1	0.10	0/900	0.32	0/1204
19	M2	0.12	0/919	0.36	0/1226
20	N1	0.14	0/817	0.39	0/1088
20	N2	0.13	0/817	0.40	0/1088
21	O1	0.10	0/722	0.33	0/964
21	O2	0.11	0/722	0.36	0/964
22	P1	0.12	0/659	0.33	0/884
23	Q1	0.13	0/657	0.40	0/881
23	Q2	0.13	0/657	0.41	0/881
24	R1	0.11	0/635	0.36	0/849
24	R2	0.16	0/637	0.48	0/851
25	S1	0.11	0/680	0.34	0/915
25	S2	0.13	0/680	0.35	0/915
26	T1	0.15	0/676	0.41	0/895
27	U1	0.13	0/598	0.45	0/792
27	U2	0.14	0/592	0.41	0/785
28	V2	0.29	0/1552	0.59	3/2419 (0.1%)
29	W	0.24	0/1604	0.39	2/2496 (0.1%)
30	W1	0.27	0/747	0.28	0/1161
31	X2	0.41	2/1628 (0.1%)	0.41	0/2526
32	Y1	0.13	0/786	0.37	0/1216
33	Y2	0.22	0/1725	0.34	1/2687 (0.0%)
34	Z1	0.11	0/76	0.23	0/101
35	a2	0.07	0/1033	0.23	0/1387
36	b2	0.12	0/2121	0.35	0/2852
37	e2	0.10	0/1444	0.30	0/1937
38	g2	0.09	0/434	0.34	0/576
39	h2	0.10	0/1104	0.29	0/1474
40	i2	0.17	0/1122	0.41	0/1515
41	l2	0.08	0/380	0.29	0/498
42	o2	0.11	0/383	0.40	0/501
43	p	0.81	0/77	1.11	0/104
44	r2	0.11	0/901	0.37	0/1209
45	z2	0.08	0/589	0.30	0/779
All	All	0.14	3/203882 (0.0%)	0.31	12/307114 (0.0%)

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
10	D1	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	D2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X2	35	I	C5-C6	7.32	1.54	1.39
31	X2	35	I	N3-C4	7.01	1.50	1.35
6	82	120	U	Cl1'-N1	6.15	1.57	1.48

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	848	C	P-O3'-C3'	-7.90	108.34	120.20
7	A2	1532	U	P-O3'-C3'	-7.82	108.47	120.20
28	V2	43	U	P-O3'-C3'	-7.30	109.25	120.20
28	V2	41	G	P-O3'-C3'	-7.29	109.26	120.20
7	A2	1533	C	P-O3'-C3'	-6.82	109.96	120.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain

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	12	625	0	652	16	0
2	32	449	0	491	14	0
3	4	529	0	527	21	0
4	62	504	0	572	8	0
5	71	644	0	328	4	0
5	72	62355	0	31379	364	0
6	82	2569	0	1301	26	0
7	A1	33092	0	16676	765	0
7	A2	32990	0	16623	530	0
8	B	1815	0	1836	75	0
8	B2	1776	0	1802	51	0
9	C1	1665	0	1741	63	0
9	C2	1658	0	1732	57	0
10	D1	1643	0	1707	45	0
10	D2	1643	0	1707	37	0
11	E1	1166	0	1212	27	0
11	E2	1166	0	1212	33	0
12	F1	862	0	864	20	0
12	F2	862	0	864	26	0
13	G1	1228	0	1277	23	0
13	G2	1214	0	1267	40	0
14	H1	979	0	1031	29	0
14	H2	979	0	1031	38	0
15	I1	1022	0	1070	33	0
15	I2	1036	0	1081	35	0
16	J1	817	0	853	36	0
16	J2	756	0	795	22	0
17	K1	857	0	861	27	0
17	K2	884	0	896	15	0
18	L1	955	0	1016	24	0
18	L2	955	0	1016	26	0
19	M1	891	0	952	25	0
19	M2	910	0	978	25	0
20	N1	805	0	844	42	0
20	N2	805	0	844	32	0
21	O1	714	0	734	11	0
21	O2	714	0	734	14	0
22	P1	649	0	666	21	0
23	Q1	648	0	691	16	0
23	Q2	648	0	691	15	0
24	R1	624	0	652	17	0
24	R2	626	0	648	20	0
25	S1	663	0	688	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S2	663	0	688	15	0
26	T1	670	0	719	18	0
27	U1	590	0	629	16	0
27	U2	584	0	618	8	0
28	V2	1382	0	694	42	0
29	W	1630	0	839	25	0
30	W1	781	0	405	12	0
31	X2	1654	0	848	21	0
32	Y1	778	0	399	10	0
33	Y2	1628	0	827	12	0
34	Z1	75	0	65	2	0
35	a2	1026	0	1092	6	0
36	b2	2082	0	2154	54	0
37	e2	1420	0	1457	23	0
38	g2	427	0	464	7	0
39	h2	1085	0	1169	16	0
40	i2	1111	0	1148	19	0
41	l2	377	0	418	11	0
42	o2	377	0	389	19	0
43	p	76	0	75	6	0
44	r2	891	0	923	18	0
45	z2	582	0	599	14	0
46	4	1	0	0	0	0
46	B	1	0	0	0	0
47	72	12	0	24	0	0
48	72	10	0	19	1	0
49	72	190	0	0	0	0
49	82	1	0	0	0	0
49	A1	60	0	0	0	0
49	A2	42	0	0	0	0
49	W	1	0	0	0	0
49	Y2	1	0	0	0	0
49	h2	1	0	0	0	0
49	o2	1	0	0	0	0
50	Y2	5	0	4	2	0
All	All	188607	0	121208	2764	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 10.

The worst 5 of 2764 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)
31:X2:55:5MU:C4	31:X2:55:5MU:C5	1.80	1.68
5:72:747:5MU:C4	5:72:747:5MU:C5	1.80	1.67
29:W:54:5MU:C4	29:W:54:5MU:C5	1.80	1.62
33:Y2:54:5MU:C4	33:Y2:54:5MU:C5	1.80	1.61
5:72:1939:5MU:C4	5:72:1939:5MU:C5	1.80	1.59

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	12	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	30
3	4	65/70 (93%)	50 (77%)	14 (22%)	1 (2%)	8	33
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	191 (83%)	35 (15%)	5 (2%)	5	25
8	B2	225/241 (93%)	188 (84%)	36 (16%)	1 (0%)	30	60
9	C1	211/233 (91%)	185 (88%)	24 (11%)	2 (1%)	14	43
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100	100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	24	55
10	D2	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E1	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
11	E2	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	79 (76%)	22 (21%)	3 (3%)	3	20
13	G1	153/179 (86%)	150 (98%)	3 (2%)	0	100	100
13	G2	152/179 (85%)	119 (78%)	27 (18%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	J1	100/103 (97%)	91 (91%)	8 (8%)	1 (1%)	12	40
16	J2	90/103 (87%)	81 (90%)	8 (9%)	1 (1%)	11	39
17	K1	113/129 (88%)	97 (86%)	14 (12%)	2 (2%)	6	30
17	K2	116/129 (90%)	100 (86%)	14 (12%)	2 (2%)	7	30
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16	44
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	1 (1%)	2 (3%)	4	22
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	34
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	34
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	4	24
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100	100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3	20
34	Z1	7/557 (1%)	7 (100%)	0	0	100	100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
38	g2	50/55 (91%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h2	135/136 (99%)	135 (100%)	0	0	100	100
40	i2	147/149 (99%)	117 (80%)	27 (18%)	3 (2%)	6	27
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	z2	74/85 (87%)	74 (100%)	0	0	100	100
All	All	6094/7240 (84%)	5593 (92%)	461 (8%)	40 (1%)	20	48

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
12	F2	38	ARG
13	G2	17	LYS
13	G2	18	PHE
13	G2	35	LYS

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	12	67/68 (98%)	67 (100%)	0	100	100
2	32	48/49 (98%)	48 (100%)	0	100	100
3	4	60/62 (97%)	60 (100%)	0	100	100
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	188 (100%)	1 (0%)	81	83
9	C1	173/190 (91%)	173 (100%)	0	100	100
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D2	172/173 (99%)	172 (100%)	0	100	100
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	82/90 (91%)	82 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	91 (100%)	0	100	100
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	83 (100%)	0	100	100
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	63 (98%)	1 (2%)	55	72
24	R2	64/65 (98%)	64 (100%)	0	100	100
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	U1	60/61 (98%)	60 (100%)	0	100	100
27	U2	59/61 (97%)	59 (100%)	0	100	100
34	Z1	8/461 (2%)	8 (100%)	0	100	100
35	a2	110/181 (61%)	110 (100%)	0	100	100
36	b2	216/218 (99%)	216 (100%)	0	100	100
37	e2	149/150 (99%)	149 (100%)	0	100	100
38	g2	47/49 (96%)	47 (100%)	0	100	100
39	h2	110/109 (101%)	110 (100%)	0	100	100
40	i2	114/114 (100%)	114 (100%)	0	100	100
41	l2	38/38 (100%)	38 (100%)	0	100	100
42	o2	35/103 (34%)	35 (100%)	0	100	100
43	p	5/5 (100%)	4 (80%)	1 (20%)	1	6
44	r2	86/87 (99%)	86 (100%)	0	100	100
45	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5101/5932 (86%)	5098 (100%)	3 (0%)	87	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B2	137	ARG
24	R1	14	THR
43	p	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
14	H1	18	GLN
17	K2	22	HIS
39	h2	13	HIS
15	I1	126	GLN
18	L2	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	75/76 (98%)	24 (32%)	4 (5%)
30	W1	34/76 (44%)	9 (26%)	2 (5%)
31	X2	74/77 (96%)	27 (36%)	5 (6%)
32	Y1	34/76 (44%)	5 (14%)	2 (5%)
33	Y2	75/76 (98%)	22 (29%)	2 (2%)
5	71	29/2904 (0%)	4 (13%)	0
5	72	2903/2904 (99%)	462 (15%)	30 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1541/1542 (99%)	455 (29%)	39 (2%)
7	A2	1536/1542 (99%)	403 (26%)	33 (2%)
All	All	6483/9457 (68%)	1474 (22%)	129 (1%)

5 of 1474 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A

5 of 129 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	W	18	G
30	W1	43	C
7	A1	438	U
7	A1	428	G
31	X2	22	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMC	72	2498	5,49	19,22,23	3.29	8 (42%)	26,31,34	0.78	0
29	G7M	W	46	29	23,26,27	2.84	8 (34%)	35,39,42	1.94	8 (22%)
30	G7M	W1	46	30	23,26,27	2.85	8 (34%)	35,39,42	1.93	8 (22%)
5	2MA	72	2503	5	22,25,26	4.08	8 (36%)	33,37,40	3.47	12 (36%)
33	PSU	Y2	55	33	18,21,22	4.66	8 (44%)	22,30,33	1.87	5 (22%)
31	G7M	X2	47	31	23,26,27	2.86	8 (34%)	35,39,42	1.94	8 (22%)
7	4OC	A1	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.91	1 (3%)
32	7MG	Y1	46	32	22,26,27	3.91	10 (45%)	29,39,42	2.09	9 (31%)
33	5MU	Y2	54	33	19,22,23	7.19	7 (36%)	28,32,35	3.33	9 (32%)
5	5MC	72	1962	5	18,22,23	4.03	7 (38%)	26,32,35	1.04	2 (7%)
5	6MZ	72	2030	5	22,25,26	2.85	4 (18%)	30,36,39	2.41	11 (36%)
5	H2U	72	2449	5,49	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
33	H2U	Y2	17	33	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
5	PSU	72	2580	5	18,21,22	4.66	8 (44%)	22,30,33	1.83	6 (27%)
7	MA6	A1	1519	7	23,26,27	1.35	3 (13%)	34,38,41	3.34	14 (41%)
31	5MU	X2	55	31	19,22,23	7.20	7 (36%)	28,32,35	3.31	9 (32%)
29	H2U	W	20	29	18,21,22	3.06	5 (27%)	21,30,33	2.01	5 (23%)
29	H2U	W	17	29	18,21,22	3.07	5 (27%)	21,30,33	2.00	5 (23%)
31	H2U	X2	17	31	18,21,22	3.06	5 (27%)	21,30,33	2.00	5 (23%)
5	3TD	71	1915	5	19,22,23	4.11	7 (36%)	21,32,35	1.64	2 (9%)
29	MIA	W	37	29	28,31,32	2.41	5 (17%)	40,44,47	2.74	17 (42%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
7	MA6	A2	1519	7	23,26,27	1.36	4 (17%)	34,38,41	3.33	14 (41%)
5	1MG	72	745	5	22,26,27	2.73	5 (22%)	33,39,42	2.31	8 (24%)
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.31	3 (9%)
5	5MU	72	1939	5	19,22,23	7.17	7 (36%)	28,32,35	3.46	10 (35%)
7	5MC	A1	1407	7	18,22,23	4.06	7 (38%)	26,32,35	1.00	2 (7%)
29	PSU	W	32	29	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
5	PSU	72	2605	5	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
5	PSU	72	2457	5	18,21,22	4.64	8 (44%)	22,30,33	1.91	5 (22%)
7	UR3	A2	1498	7	19,22,23	2.77	8 (42%)	26,32,35	1.31	3 (11%)
29	4SU	W	8	29	18,21,22	3.78	7 (38%)	26,30,33	2.25	5 (19%)
29	H2U	W	16	29	18,21,22	3.06	5 (27%)	21,30,33	1.90	5 (23%)
30	PSU	W1	32	30	18,21,22	4.67	8 (44%)	22,30,33	1.79	5 (22%)
7	5MC	A2	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	72	2604	5	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
5	PSU	72	2504	5,49	18,21,22	4.68	8 (44%)	22,30,33	1.84	5 (22%)
7	5MC	A1	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
5	2MG	72	1835	5	23,26,27	3.07	8 (34%)	32,38,41	2.53	11 (34%)
7	2MG	A1	1207	7	23,26,27	3.11	8 (34%)	32,38,41	2.52	11 (34%)
29	5MU	W	54	29	19,22,23	7.21	7 (36%)	28,32,35	3.32	9 (32%)
31	PSU	X2	56	31	18,21,22	4.70	8 (44%)	22,30,33	1.80	5 (22%)
32	CM0	Y1	34	32	23,26,27	3.74	6 (26%)	27,37,40	1.50	2 (7%)
30	MIA	W1	37	30	28,31,32	2.43	5 (17%)	40,44,47	2.83	13 (32%)
33	G7M	Y2	46	33	23,26,27	2.83	9 (39%)	35,39,42	1.74	7 (20%)
5	G7M	72	2069	5	23,26,27	2.84	9 (39%)	35,39,42	1.75	8 (22%)
7	2MG	A2	1207	7	23,26,27	3.12	8 (34%)	32,38,41	2.53	11 (34%)
30	PSU	W1	39	30	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
32	6MZ	Y1	37	32	22,25,26	2.81	4 (18%)	30,36,39	2.48	12 (40%)
7	2MG	A2	1516	7	23,26,27	3.10	8 (34%)	32,38,41	2.50	11 (34%)
5	PSU	72	746	5,49	18,21,22	4.70	8 (44%)	22,30,33	1.79	5 (22%)
7	MA6	A2	1518	7	23,26,27	1.36	3 (13%)	34,38,41	3.35	14 (41%)
5	2MG	72	2445	5	23,26,27	3.10	8 (34%)	32,38,41	2.50	10 (31%)
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.05	5 (23%)
31	RSP	X2	33	31	17,21,22	4.11	7 (41%)	22,30,33	0.80	0
7	5MC	A2	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.98	1 (3%)
29	PSU	W	55	29	18,21,22	4.68	8 (44%)	22,30,33	1.85	5 (22%)
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.26	4 (15%)
5	3TD	72	1915	5	19,22,23	4.05	7 (36%)	21,32,35	1.74	3 (14%)
7	4OC	A2	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.91	1 (3%)
7	2MG	A1	966	7	23,26,27	3.11	8 (34%)	32,38,41	2.57	11 (34%)
7	UR3	A1	1498	7	19,22,23	2.79	8 (42%)	26,32,35	1.31	3 (11%)
31	2MA	X2	38	31	22,25,26	4.14	8 (36%)	33,37,40	3.46	11 (33%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
5	6MZ	72	1618	5	22,25,26	2.78	4 (18%)	30,36,39	2.47	11 (36%)
7	MA6	A1	1518	7	23,26,27	1.35	3 (13%)	34,38,41	3.35	14 (41%)
5	OMG	72	2251	29,5	23,26,27	2.59	7 (30%)	33,38,41	2.43	10 (30%)
7	2MG	A2	966	7	23,26,27	3.12	8 (34%)	32,38,41	2.51	11 (34%)
7	G7M	A2	527	7	23,26,27	2.84	9 (39%)	35,39,42	1.74	8 (22%)
5	5MU	72	747	5	19,22,23	7.17	7 (36%)	28,32,35	3.47	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	G7M	A1	527	7	23,26,27	2.84	9 (39%)	35,39,42	1.78	8 (22%)
7	2MG	A1	1516	7	23,26,27	3.12	8 (34%)	32,38,41	2.53	11 (34%)
30	4SU	W1	8	30	18,21,22	3.81	7 (38%)	26,30,33	2.22	4 (15%)

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
5	OMC	72	2498	5,49	-	2/9/27/28	0/2/2/2
29	G7M	W	46	29	-	5/7/25/26	0/3/3/3
30	G7M	W1	46	30	-	5/7/25/26	0/3/3/3
5	2MA	72	2503	5	-	1/7/25/26	0/3/3/3
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2
31	G7M	X2	47	31	-	3/7/25/26	0/3/3/3
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
5	6MZ	72	2030	5	-	3/9/27/28	0/3/3/3
5	H2U	72	2449	5,49	-	0/7/38/39	0/2/2/2
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
7	MA6	A1	1519	7	-	4/11/29/30	0/3/3/3
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
29	MIA	W	37	29	-	3/15/33/34	0/3/3/3
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
7	MA6	A2	1519	7	-	2/11/29/30	0/3/3/3
5	1MG	72	745	5	-	0/7/25/26	0/3/3/3
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
5	5MU	72	1939	5	-	0/7/25/26	0/2/2/2
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
5	PSU	72	2504	5,49	-	0/7/25/26	0/2/2/2
7	5MC	A1	967	7	-	1/7/25/26	0/2/2/2
5	2MG	72	1835	5	-	0/9/27/28	0/3/3/3
7	2MG	A1	1207	7	-	0/9/27/28	0/3/3/3
29	5MU	W	54	29	-	2/7/25/26	0/2/2/2
31	PSU	X2	56	31	-	1/7/25/26	0/2/2/2
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
30	MIA	W1	37	30	-	6/15/33/34	0/3/3/3
33	G7M	Y2	46	33	-	2/7/25/26	0/3/3/3
5	G7M	72	2069	5	-	3/7/25/26	0/3/3/3
7	2MG	A2	1207	7	-	0/9/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/9/27/28	0/3/3/3
7	2MG	A2	1516	7	-	0/9/27/28	0/3/3/3
5	PSU	72	746	5,49	-	1/7/25/26	0/2/2/2
7	MA6	A2	1518	7	-	3/11/29/30	0/3/3/3
5	2MG	72	2445	5	-	0/9/27/28	0/3/3/3
31	H2U	X2	21	31	-	1/7/38/39	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
29	PSU	W	55	29	-	0/7/25/26	0/2/2/2
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	2MG	A1	966	7	-	0/9/27/28	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
31	2MA	X2	38	31	-	5/7/25/26	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/9/27/28	0/3/3/3
7	MA6	A1	1518	7	-	3/11/29/30	0/3/3/3
5	OMG	72	2251	29,5	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	2MG	A2	966	7	-	0/9/27/28	0/3/3/3
7	G7M	A2	527	7	-	3/7/25/26	0/3/3/3
5	5MU	72	747	5	-	1/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/7/25/26	0/3/3/3
7	2MG	A1	1516	7	-	0/9/27/28	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2

The worst 5 of 509 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	747	5MU	C4-C5	21.41	1.80	1.44
5	72	1939	5MU	C4-C5	21.37	1.80	1.44
31	X2	55	5MU	C4-C5	21.31	1.80	1.44
29	W	54	5MU	C4-C5	21.22	1.80	1.44
33	Y2	54	5MU	C4-C5	21.21	1.80	1.44

The worst 5 of 505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C8	-12.45	99.02	127.14
31	X2	38	2MA	C1'-N9-C8	-12.29	99.38	127.14
7	A1	1519	MA6	N1-C6-N6	-12.16	103.79	117.08
7	A1	1518	MA6	N1-C6-N6	-12.12	103.83	117.08
7	A2	1519	MA6	N1-C6-N6	-12.08	103.87	117.08

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	Y1	37	6MZ	N1-C6-N6-C9
33	Y2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	17	H2U	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C6
33	Y2	17	H2U	C2'-C1'-N1-C2

There are no ring outliers.

34 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	W	46	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	W1	46	G7M	1	0
5	72	2503	2MA	3	0
33	Y2	55	PSU	1	0
31	X2	47	G7M	1	0
7	A1	1402	4OC	1	0
33	Y2	54	5MU	2	0
5	72	1962	5MC	1	0
5	72	2030	6MZ	1	0
5	72	2449	H2U	1	0
31	X2	55	5MU	1	0
29	W	17	H2U	1	0
29	W	37	MIA	2	0
31	X2	48	3AU	2	0
5	72	1939	5MU	2	0
5	72	2605	PSU	1	0
7	A2	1498	UR3	1	0
29	W	16	H2U	3	0
5	72	2604	PSU	2	0
5	72	2504	PSU	1	0
7	A1	1207	2MG	2	0
29	W	54	5MU	1	0
31	X2	56	PSU	1	0
32	Y1	34	CM0	3	0
30	W1	37	MIA	2	0
33	Y2	46	G7M	1	0
32	Y1	37	6MZ	1	0
5	72	746	PSU	2	0
7	A2	1518	MA6	2	0
5	72	1915	3TD	1	0
7	A2	1402	4OC	2	0
7	A1	966	2MG	1	0
31	X2	38	2MA	2	0
5	72	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 299 are monoatomic - leaving 4 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$
50	ALA	Y2	102	33	3,4,5	1.17	0	2,4,6	3.10	1 (50%)
47	PUT	72	3002	-	5,5,5	0.25	0	4,4,4	0.55	0
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.51	0
48	SPD	72	3003	-	9,9,9	0.33	0	8,8,8	0.86	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	ALA	Y2	102	33	-	0/0/2/4	-
47	PUT	72	3002	-	-	0/3/3/3	-
47	PUT	72	3001	-	-	1/3/3/3	-
48	SPD	72	3003	-	-	0/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Y2	102	ALA	O-C-CA	-4.38	110.42	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	Y2	102	ALA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	72	3003	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

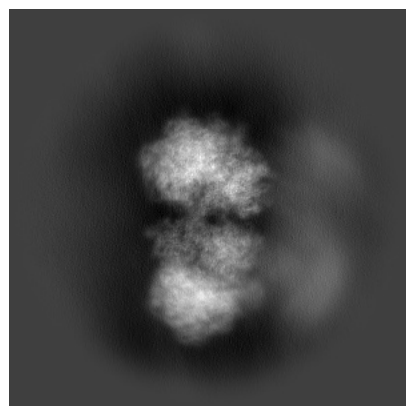
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18875. These allow visual inspection of the internal detail of the map and identification of artifacts.

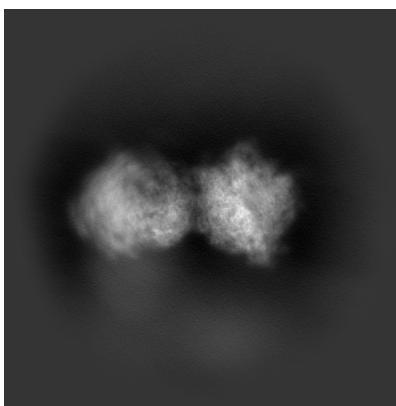
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

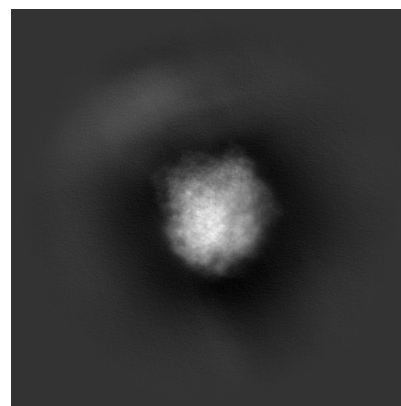
6.1.1 Primary map



X

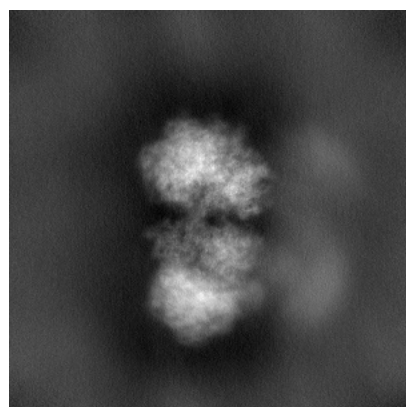


Y

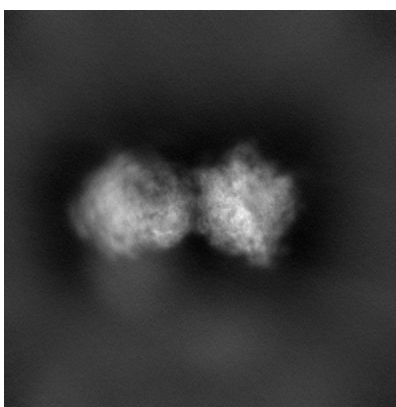


Z

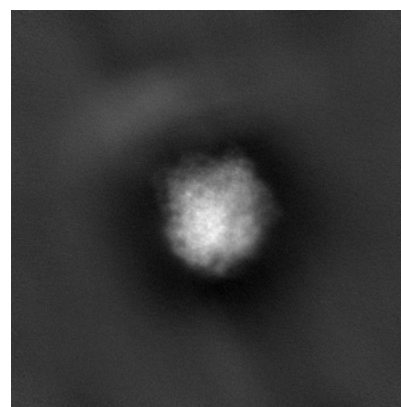
6.1.2 Raw map



X



Y

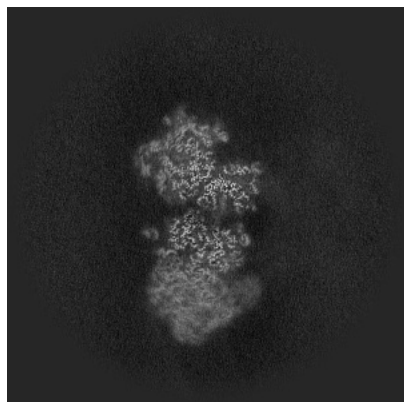


Z

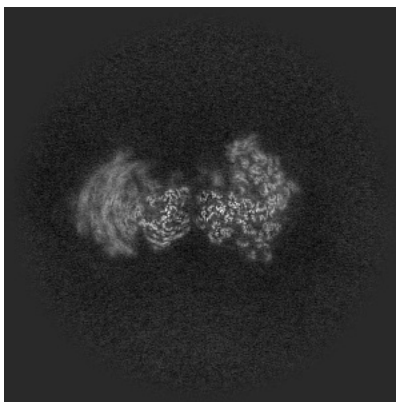
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

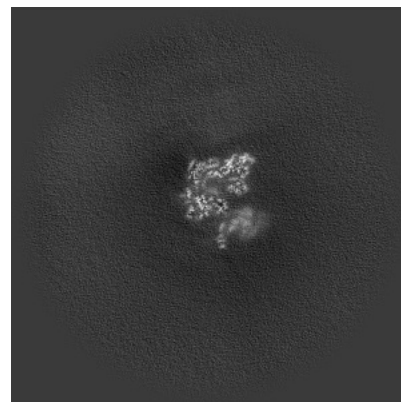
6.2.1 Primary map



X Index: 351

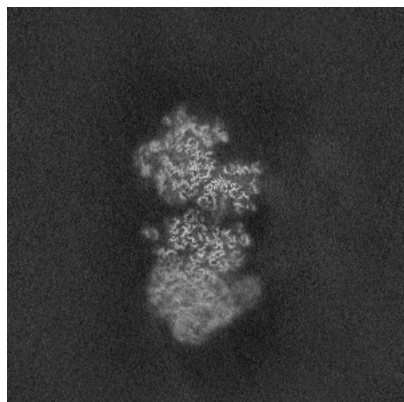


Y Index: 351

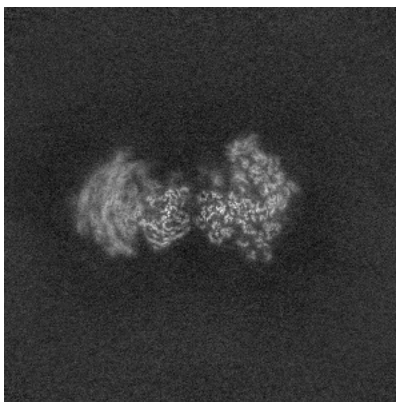


Z Index: 351

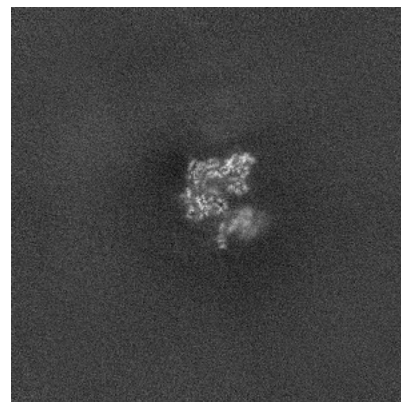
6.2.2 Raw map



X Index: 351



Y Index: 351

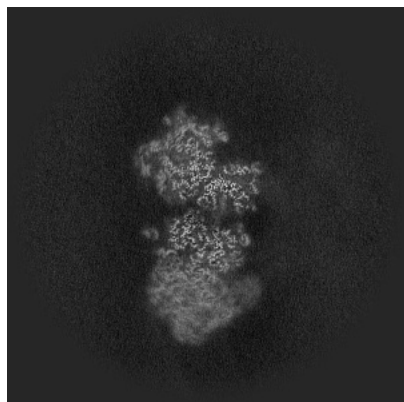


Z Index: 351

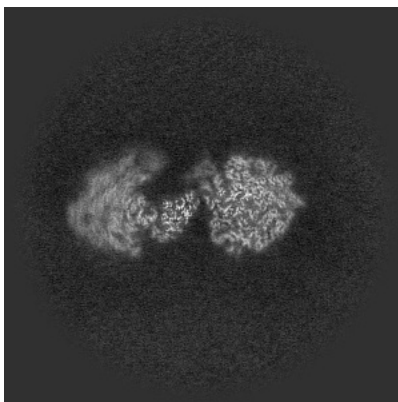
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

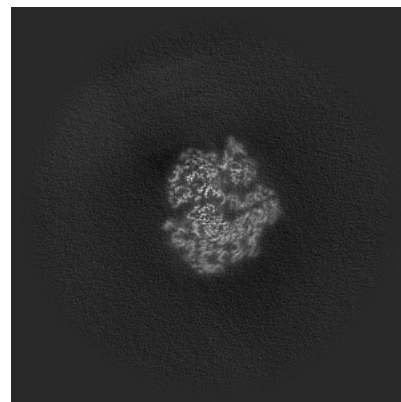
6.3.1 Primary map



X Index: 351

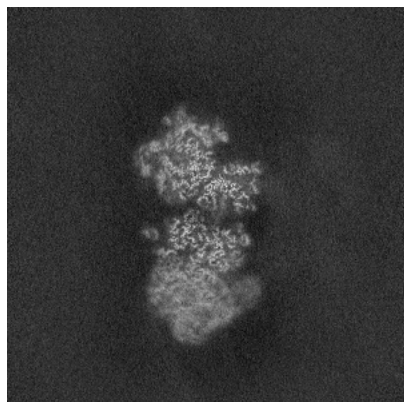


Y Index: 312

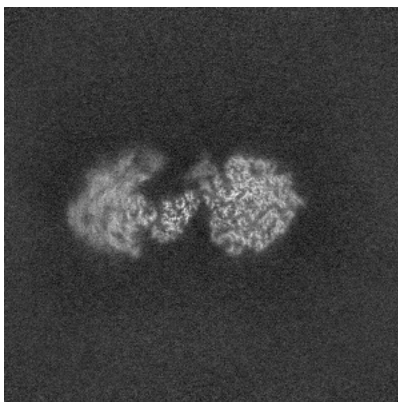


Z Index: 411

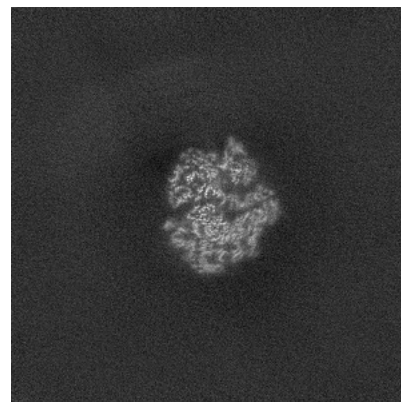
6.3.2 Raw map



X Index: 351



Y Index: 313

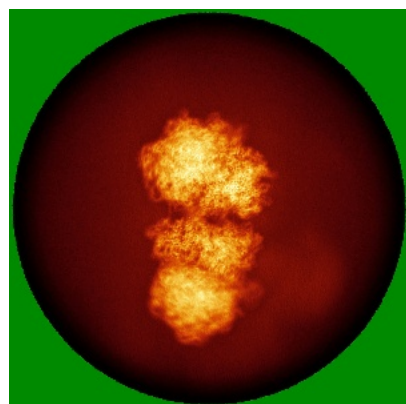


Z Index: 411

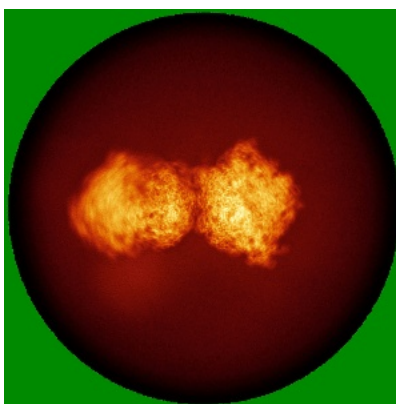
The images above show the largest variance slices of the map in three orthogonal directions.

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

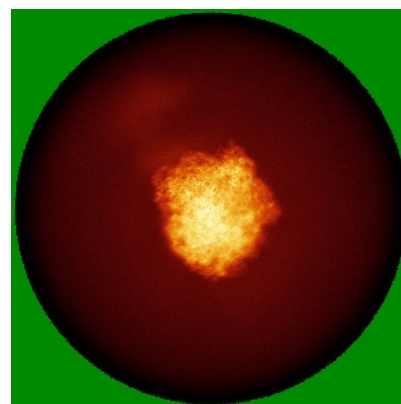
6.4.1 Primary map



X

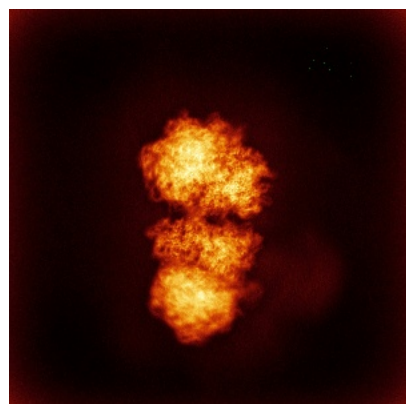


Y

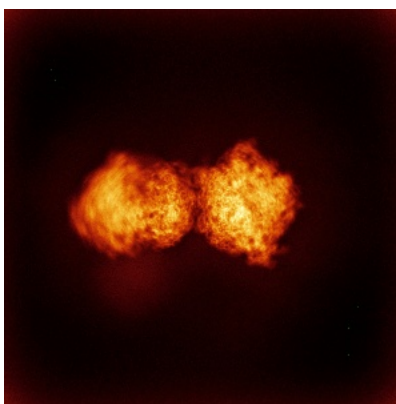


Z

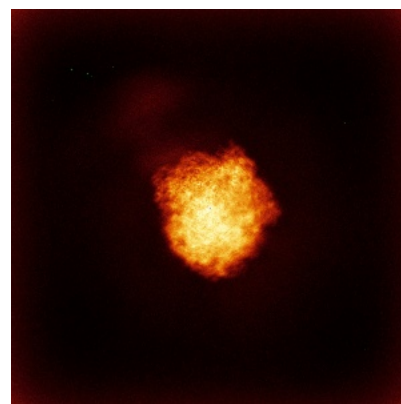
6.4.2 Raw map



X



Y

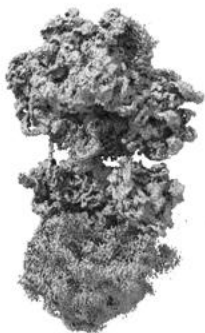


Z

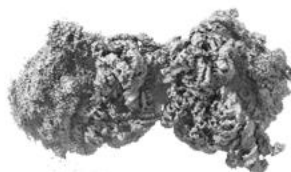
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

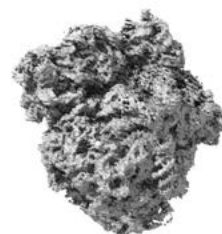
6.5.1 Primary map



X



Y



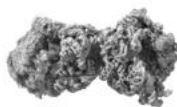
Z

The images above show the 3D surface view of the map at the recommended contour level 4.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

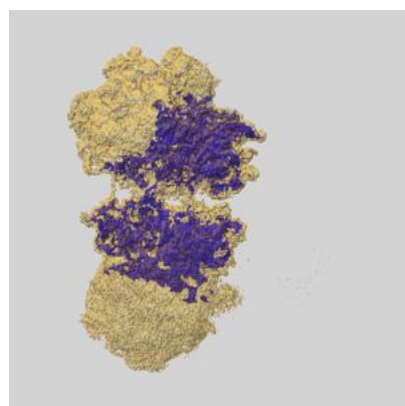
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

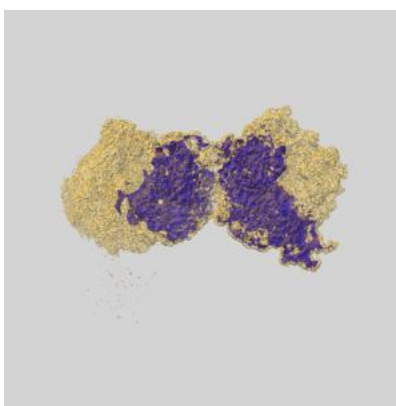
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

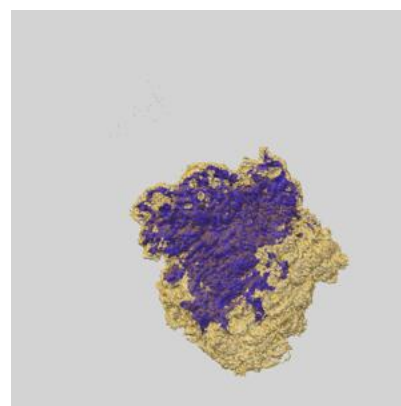
6.6.1 emd_18875_msk_1.map [i](#)



X



Y

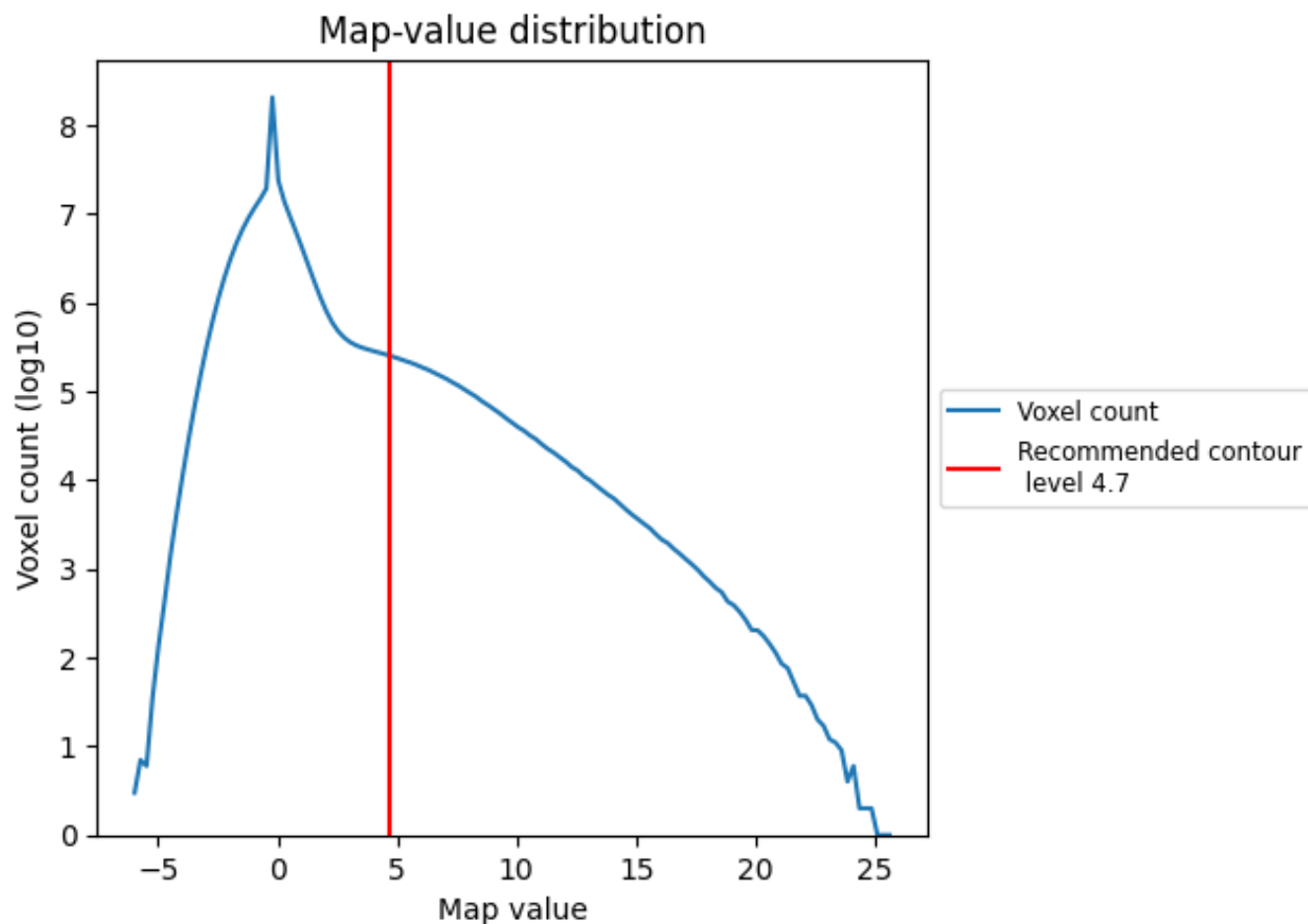


Z

7 Map analysis [i](#)

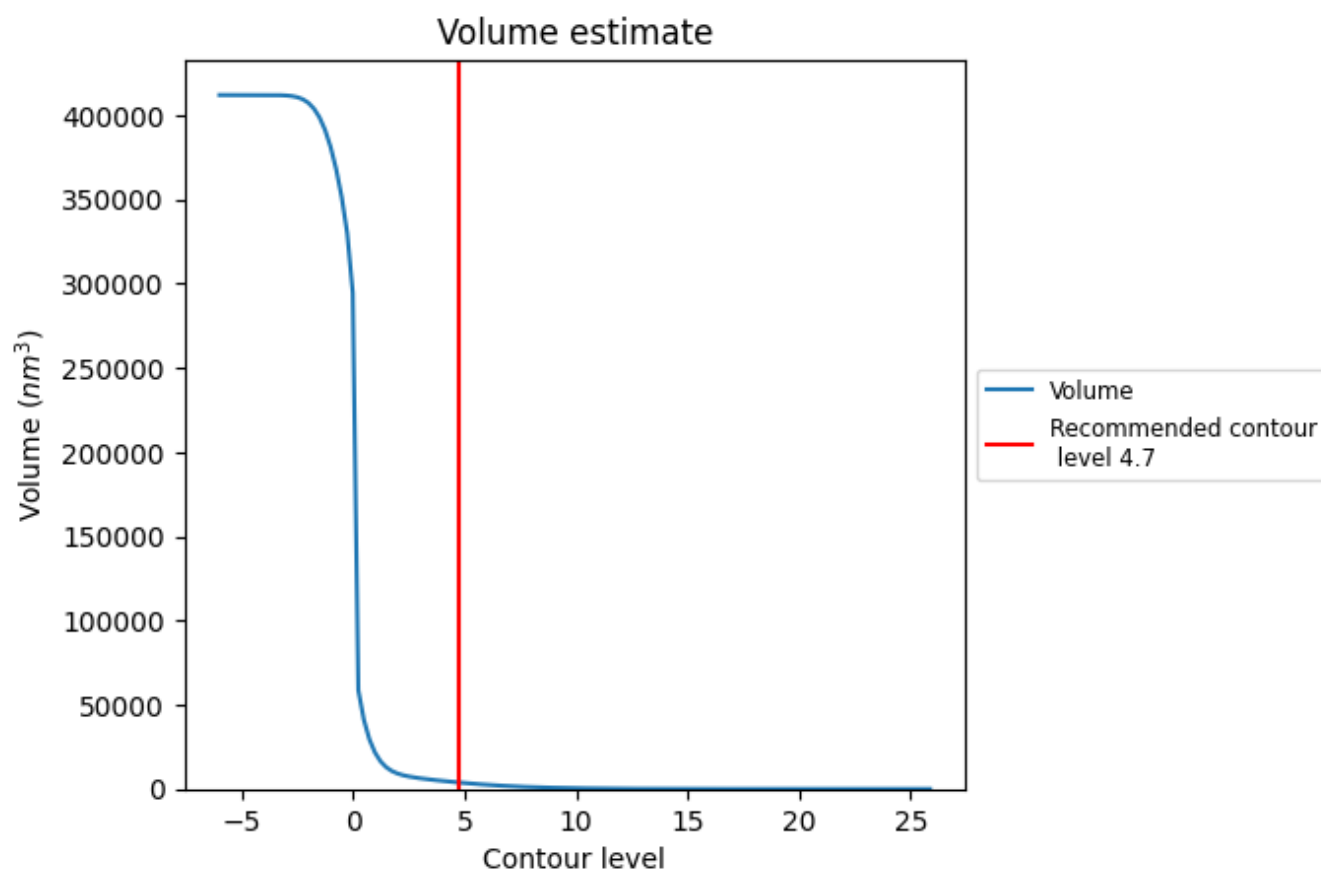
This section contains the results of statistical analysis of the map.

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.

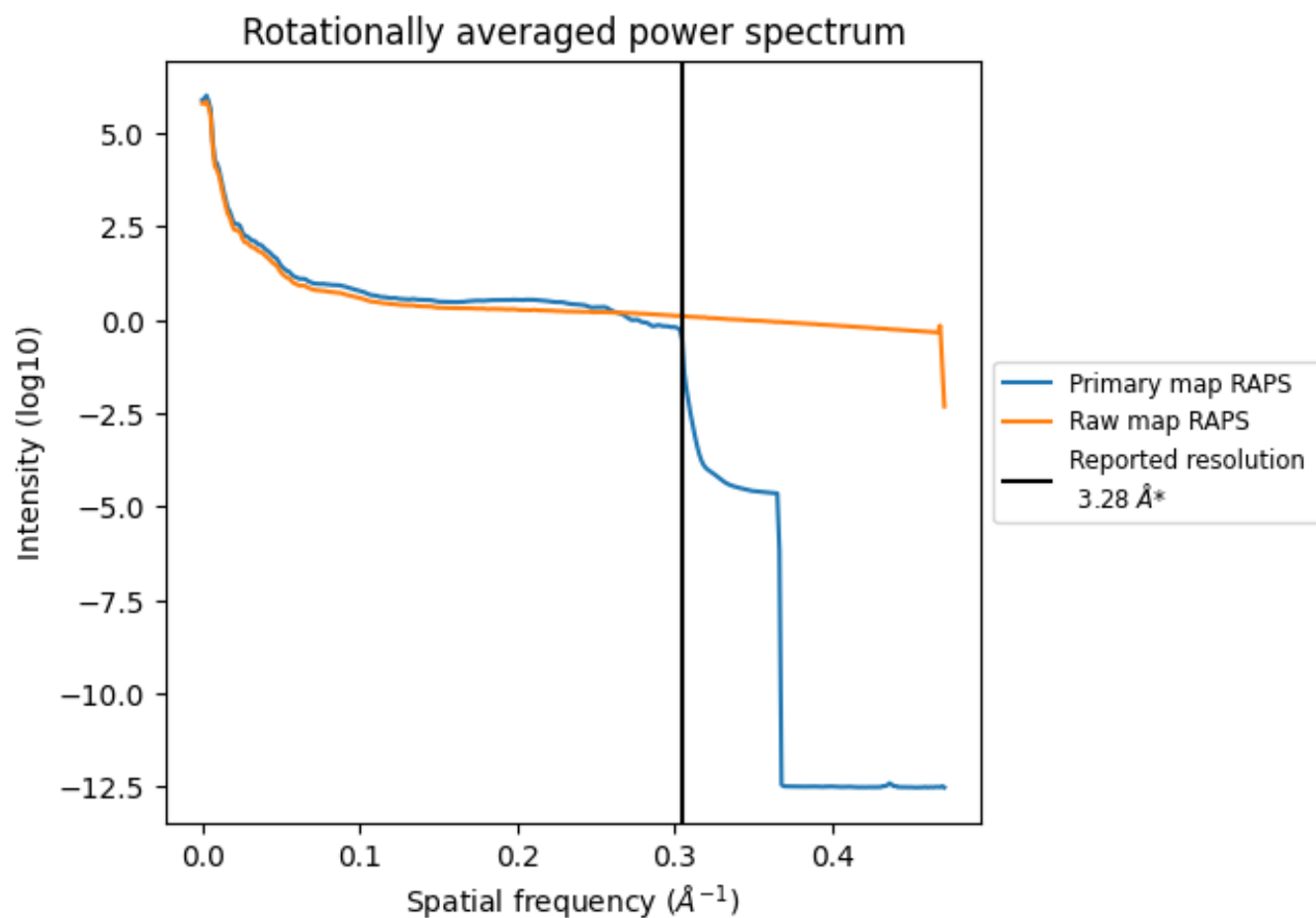
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3880 nm^3 ; this corresponds to an approximate mass of 3505 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 ⓘ

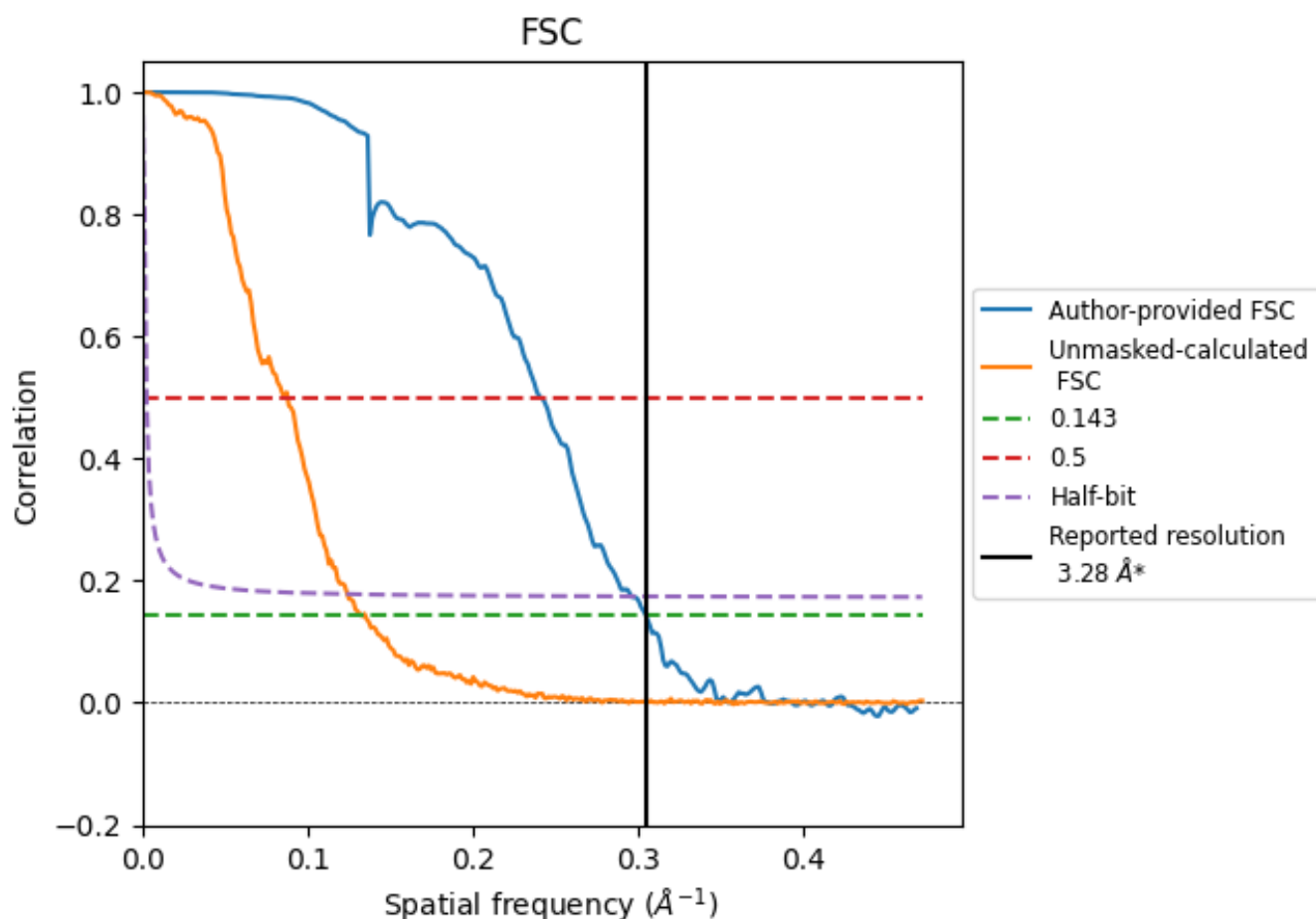


*Reported resolution corresponds to spatial frequency of 0.305 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

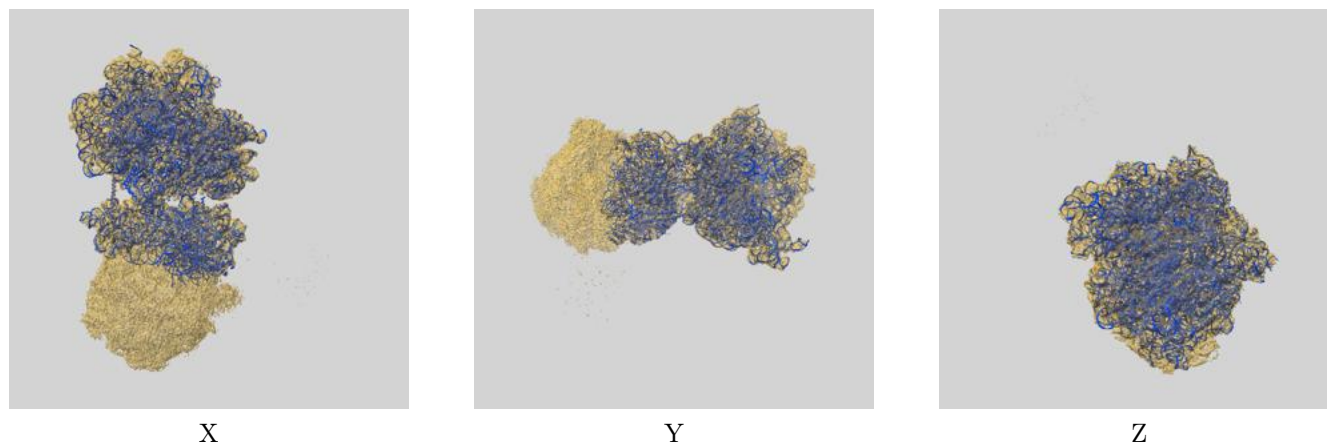
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	4.15	3.38
Unmasked-calculated*	7.55	11.38	8.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.55 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

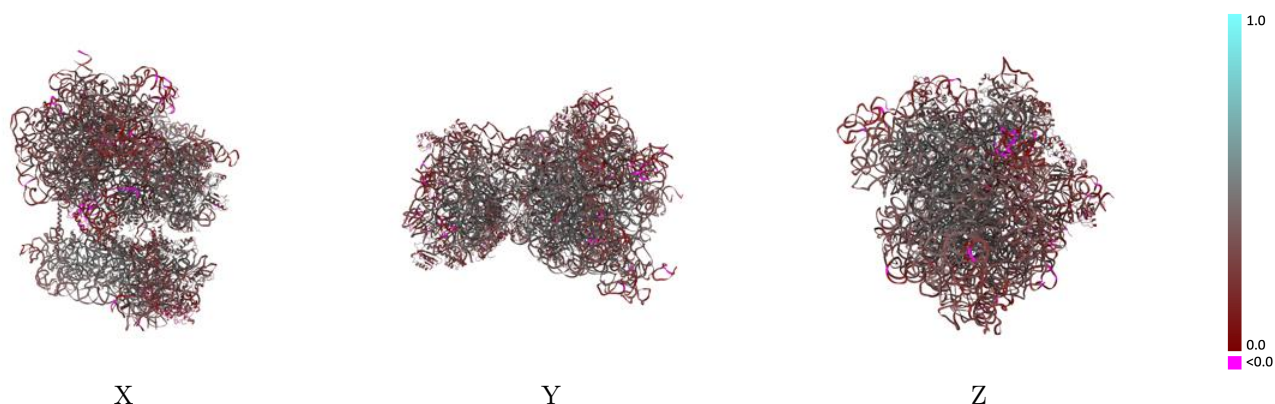
This section contains information regarding the fit between EMDB map EMD-18875 and PDB model 8R3V. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



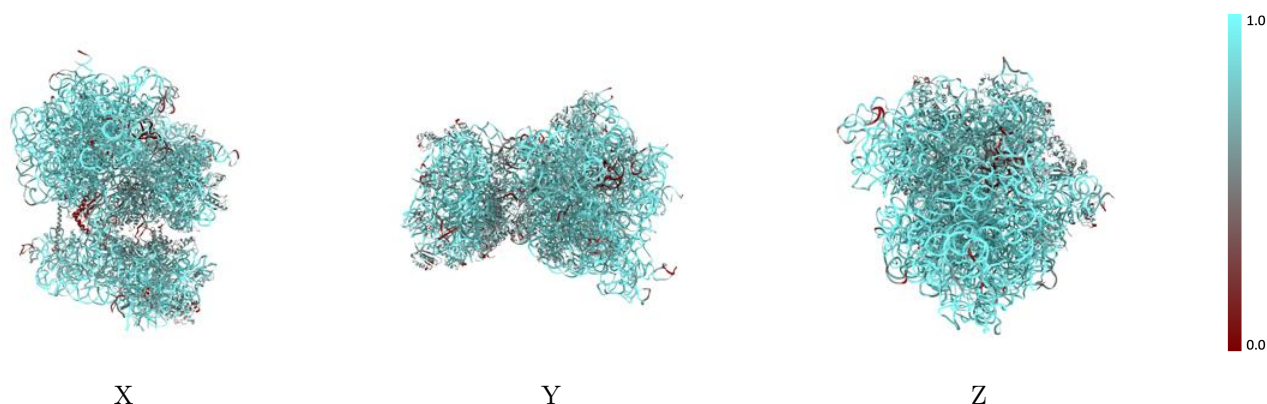
The images above show the 3D surface view of the map at the recommended contour level 4.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



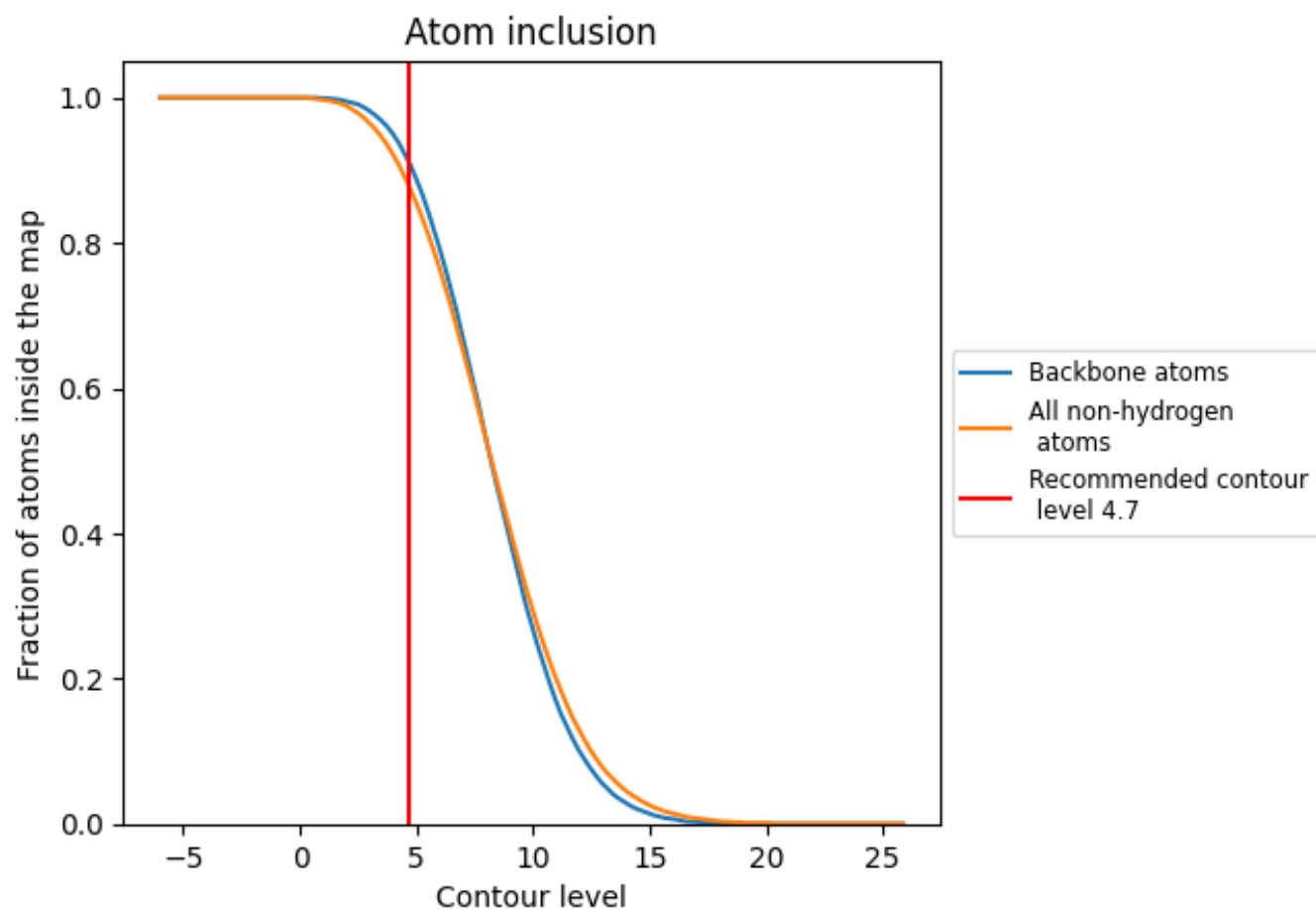
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 88% 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 (4.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.3510
12	 0.8220	 0.3680
32	 0.7960	 0.2690
4	 0.6150	 0.3020
62	 0.9080	 0.2980
71	 0.9810	 0.3000
72	 0.9500	 0.3430
82	 0.9120	 0.2260
A1	 0.9540	 0.3880
A2	 0.9490	 0.3980
B	 0.5500	 0.3150
B2	 0.6220	 0.3820
C1	 0.7140	 0.3890
C2	 0.7780	 0.3980
D1	 0.7670	 0.4060
D2	 0.6040	 0.2740
E1	 0.7400	 0.3760
E2	 0.7580	 0.4100
F1	 0.5400	 0.2680
F2	 0.7120	 0.4160
G1	 0.5980	 0.1750
G2	 0.7780	 0.3900
H1	 0.6850	 0.3020
H2	 0.7250	 0.3900
I1	 0.7220	 0.3410
I2	 0.8330	 0.4080
J1	 0.7150	 0.3830
J2	 0.7030	 0.3430
K1	 0.7130	 0.2460
K2	 0.7930	 0.4260
L1	 0.8340	 0.4030
L2	 0.8520	 0.3760
M1	 0.6410	 0.2210
M2	 0.7420	 0.2950
N1	 0.7570	 0.2950



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Chain	Atom inclusion	Q-score
N2	 0.7880	 0.3250
O1	 0.7450	 0.3030
O2	 0.7680	 0.3720
P1	 0.7810	 0.4070
Q1	 0.7230	 0.3120
Q2	 0.7390	 0.3950
R1	 0.6730	 0.3160
R2	 0.7330	 0.4210
S1	 0.6110	 0.1970
S2	 0.7650	 0.3250
T1	 0.7590	 0.3120
U1	 0.6340	 0.3010
U2	 0.7070	 0.3840
V2	 0.5570	 0.2240
W	 0.9470	 0.3130
W1	 0.8630	 0.2930
X2	 0.6230	 0.1440
Y1	 0.5670	 0.2240
Y2	 0.2600	 0.1860
Z1	 0.0270	 0.1910
a2	 0.1470	 0.0870
b2	 0.8640	 0.4220
e2	 0.7010	 0.2430
g2	 0.7970	 0.2770
h2	 0.8420	 0.3270
i2	 0.5980	 0.3770
l2	 0.9470	 0.3490
o2	 0.9720	 0.3630
p	 0.7470	 0.1210
r2	 0.6730	 0.1980
z2	 0.8820	 0.2520