



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:11 AM UTC

PDB ID : 6WDH / pdb_00006wdh
EMDB ID : EMD-21636
Title : Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Non-cognate Structure IV-B1)
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on : 2020-03-31
Resolution : 4.30 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
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

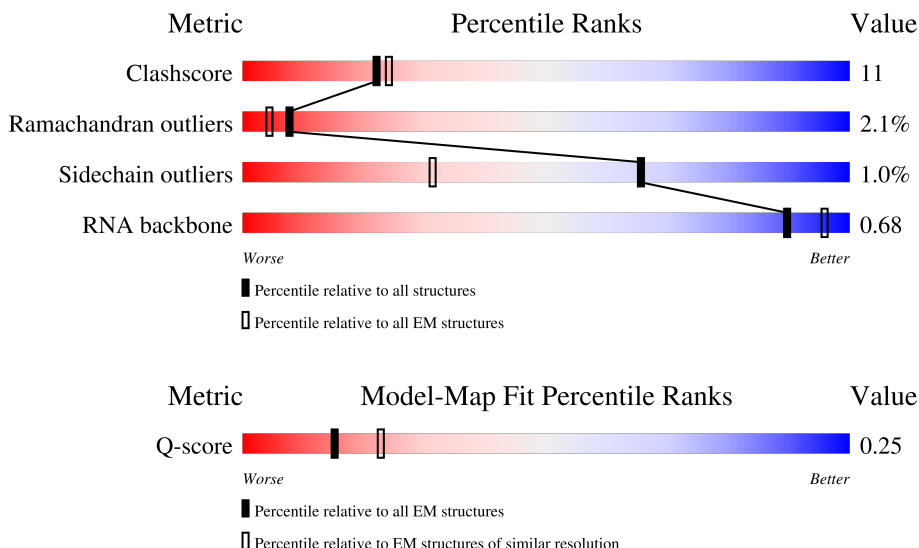
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.



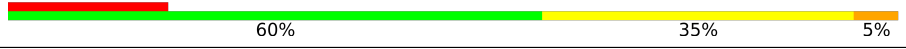
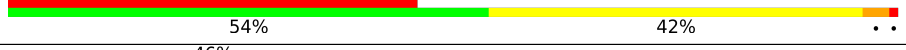
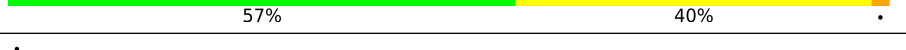
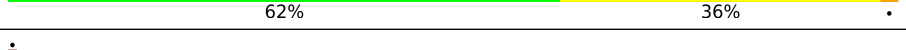
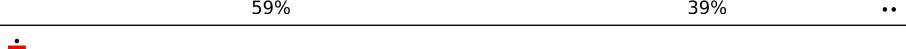
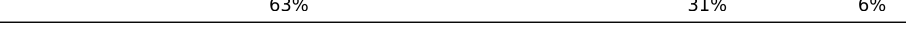
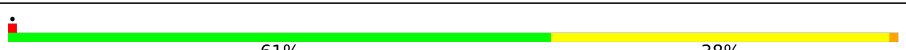
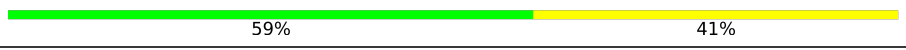
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	b	271	
2	c	209	
3	d	201	

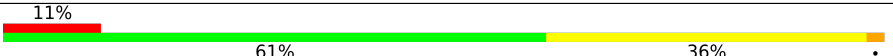
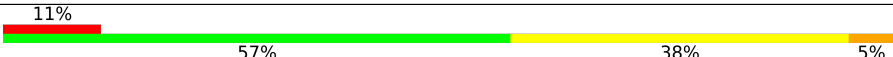
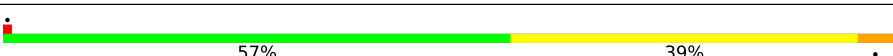
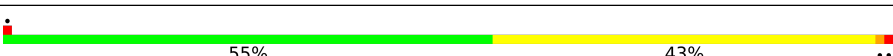
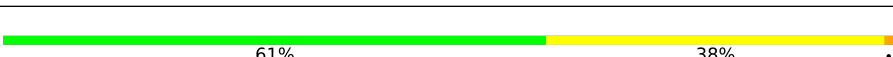
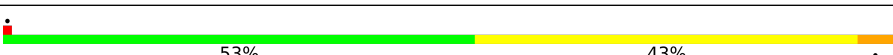
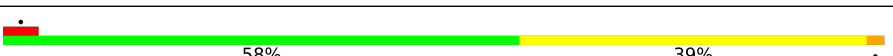
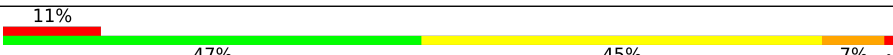
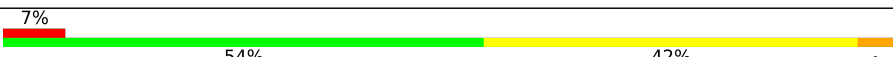
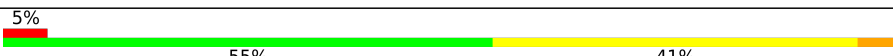
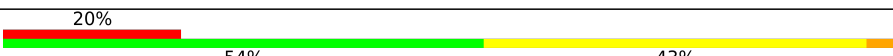
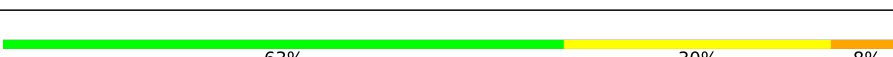
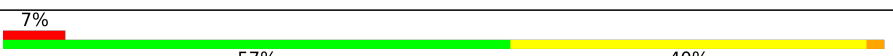
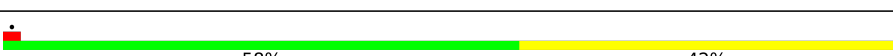
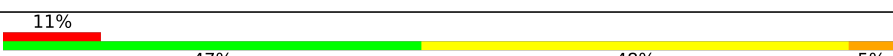
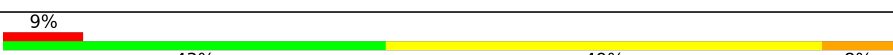
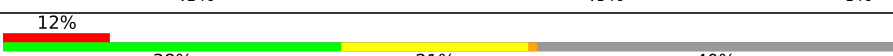
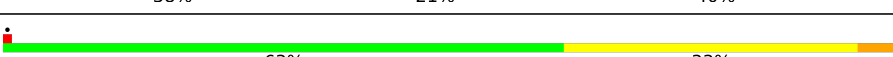
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Mol	Chain	Length	Quality of chain
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	
9	j	142	
10	k	122	
11	l	143	
12	m	136	
13	n	120	
14	o	116	
15	p	114	
16	q	117	
17	r	103	
18	s	110	
19	t	93	
20	u	102	
21	v	94	
22	w	75	
23	x	77	
24	y	63	
25	z	58	
26	B	56	
27	C	50	
28	D	46	

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Mol	Chain	Length	Quality of chain
29	E	64	
30	F	38	
31	G	225	
32	H	206	
33	I	205	
34	J	157	
35	K	100	
36	L	151	
37	M	129	
38	N	127	
39	O	98	
40	P	116	
41	Q	123	
42	R	114	
43	S	100	
44	T	88	
45	U	82	
46	V	80	
47	W	65	
48	X	79	
49	Y	85	
50	Z	65	
51	a	223	
52	3	1539	
53	1	2903	

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Mol	Chain	Length	Quality of chain
54	2	120	57% 38% 6%
55	5	77	5% 78% 19%
55	6	77	6% 64% 35%
56	4	18	11% 61% 33% 6%
57	7	76	76% 22% 7%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 150149 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	p	114	Total	C	N	O	S	0
			917	574	179	163	1	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	q	117	Total	C	N	O		0
			947	604	192	151		0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	103	Total	C	N	O	S	0
			816	516	153	145	2	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	s	110	Total	C	N	O	S	0
			857	532	166	156	3	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	t	93	Total	C	N	O	S	0
			739	466	139	132	2	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O		0
			780	492	146	142		0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 43 is a protein called 30S ribosomal protein S14.

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

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 55 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
55	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

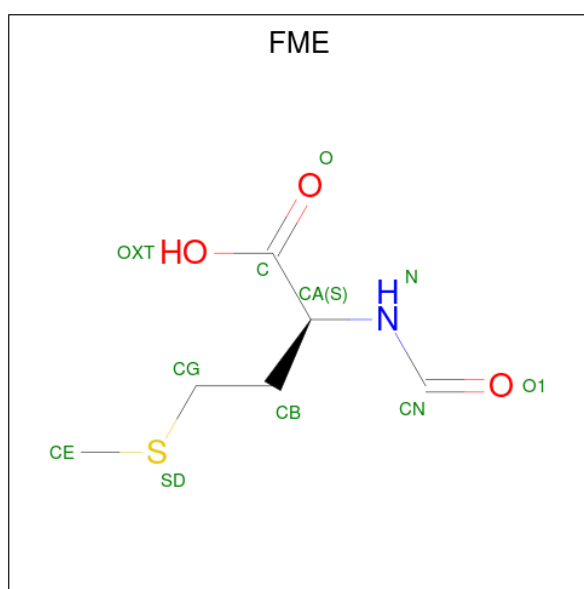
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	18	Total	C	N	O	P	0	0
			388	175	77	119	17		

- Molecule 57 is a RNA chain called tRNA^{Phe}.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	7	73	Total	C	N	O	P	0	0
			1557	695	279	511	72		

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).

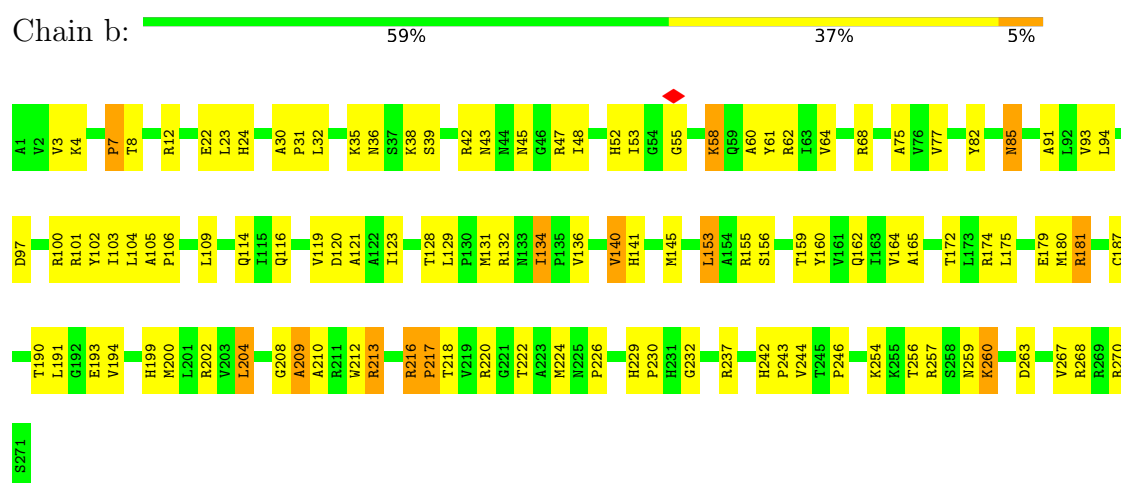


Mol	Chain	Residues	Atoms					AltConf
58	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

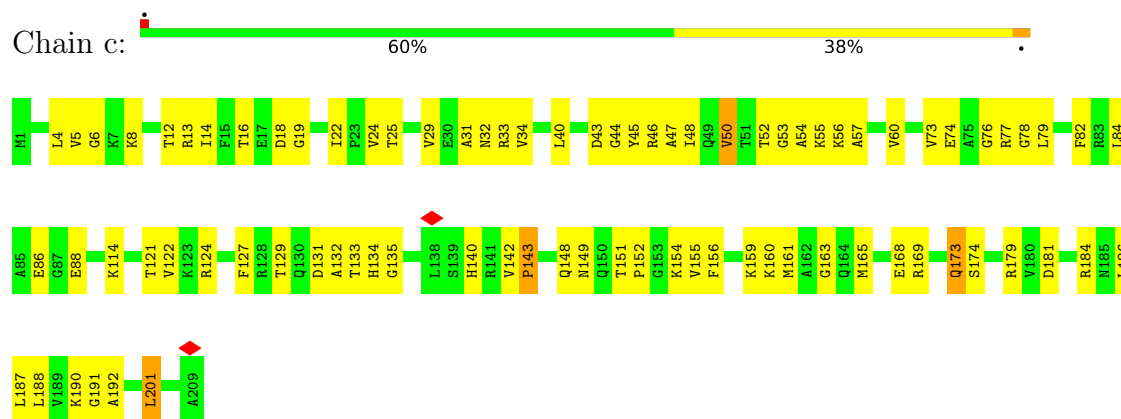
3 Residue-property plots

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.

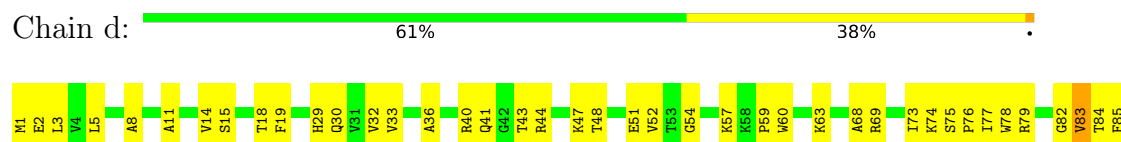
• Molecule 1: 50S ribosomal protein L2

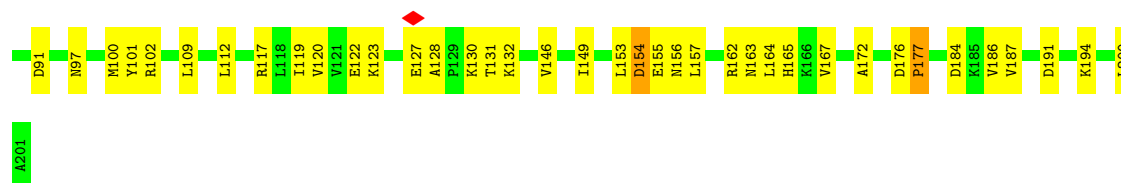


• Molecule 2: 50S ribosomal protein L3

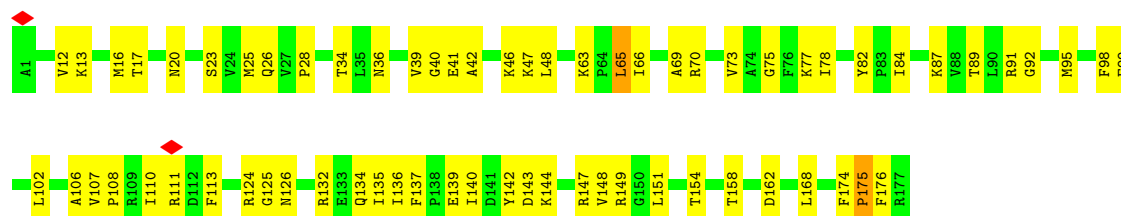


• Molecule 3: 50S ribosomal protein L4

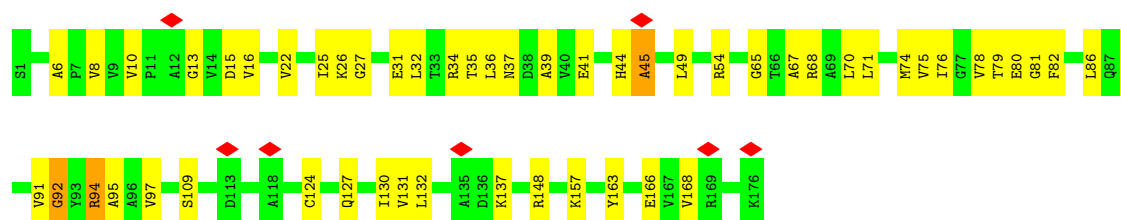




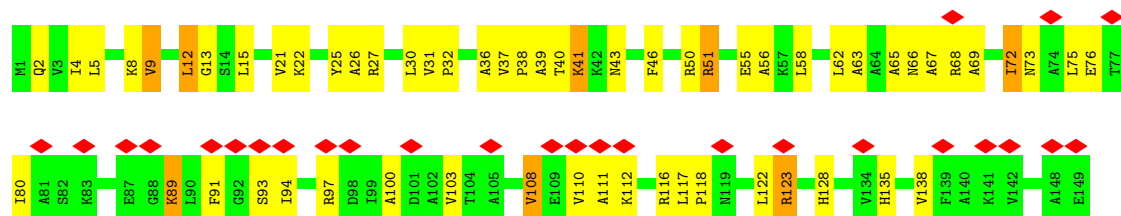
• Molecule 4: 50S ribosomal protein L5



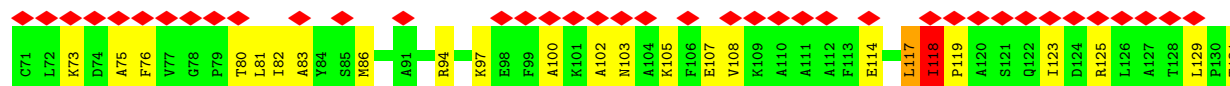
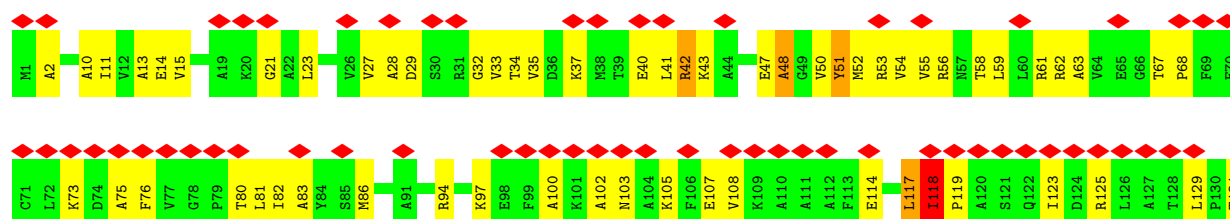
• Molecule 5: 50S ribosomal protein L6



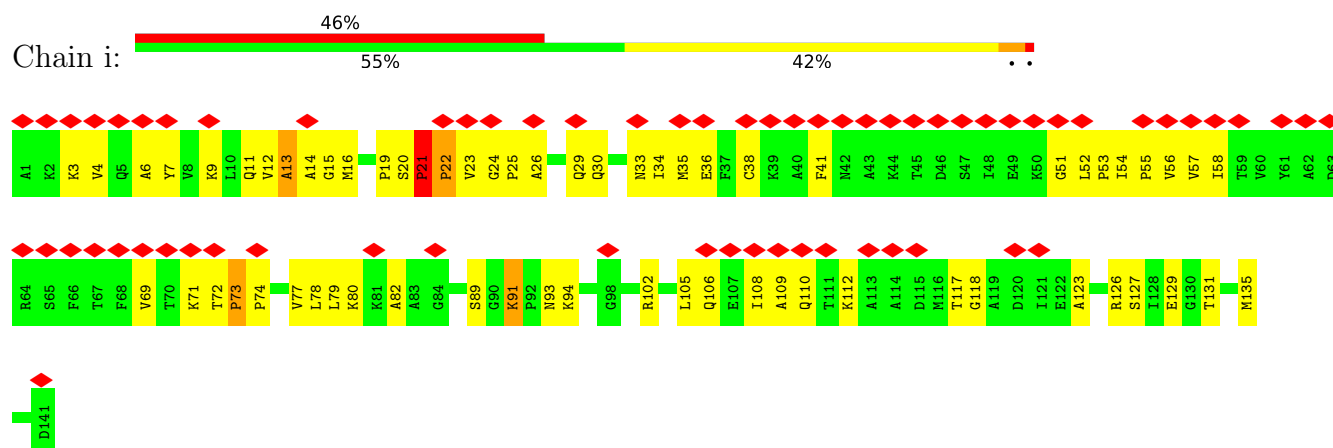
• Molecule 6: 50S ribosomal protein L9



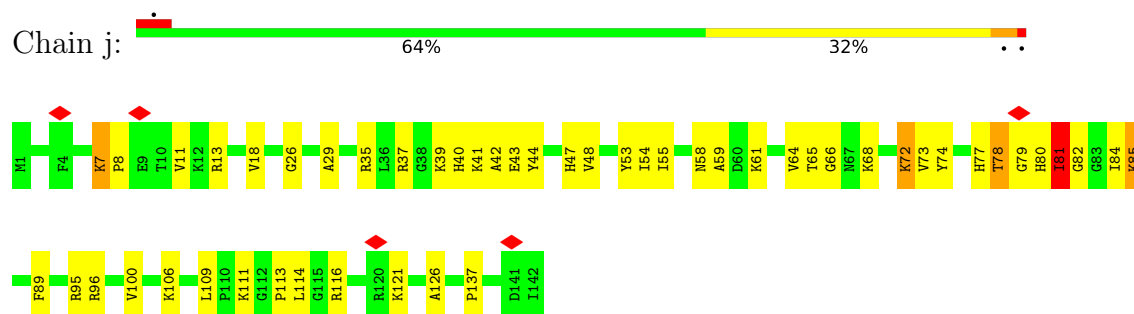
• Molecule 7: 50S ribosomal protein L10



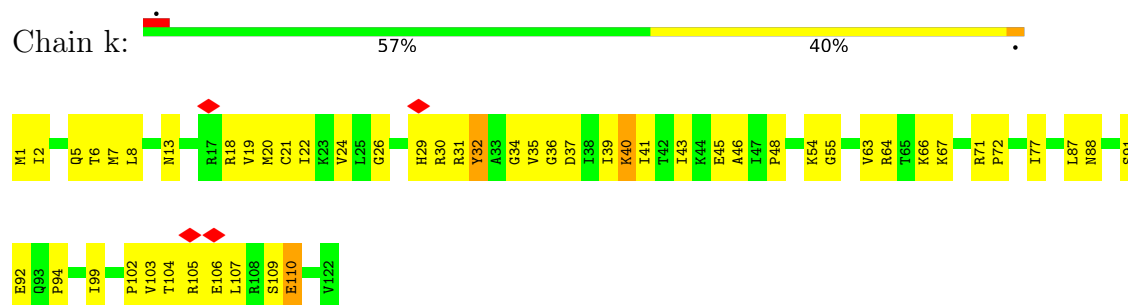
- Molecule 8: 50S ribosomal protein L11



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

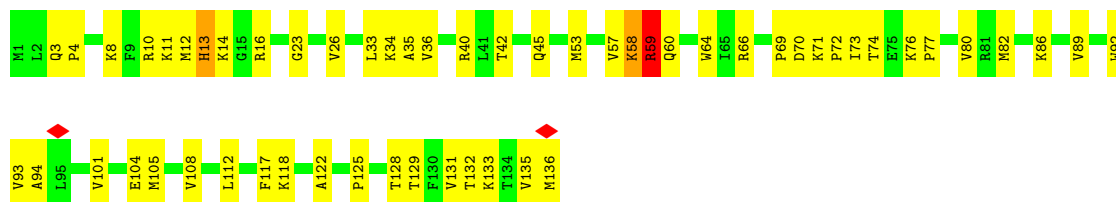


- Molecule 11: 50S ribosomal protein L15



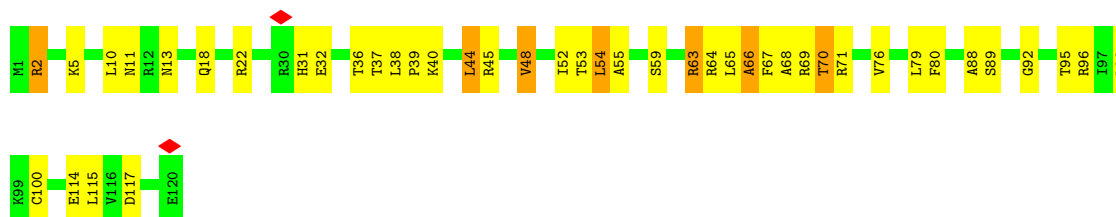
- Molecule 12: 50S ribosomal protein L16

Chain m:  59% 39% ..



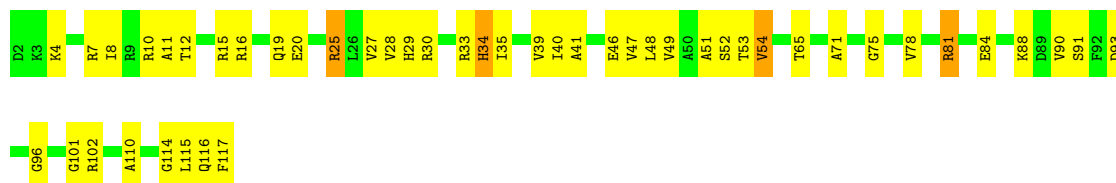
- Molecule 13: 50S ribosomal protein L17

Chain n:  63% 31% 6%



- Molecule 14: 50S ribosomal protein L18

Chain o:  59% 37% .



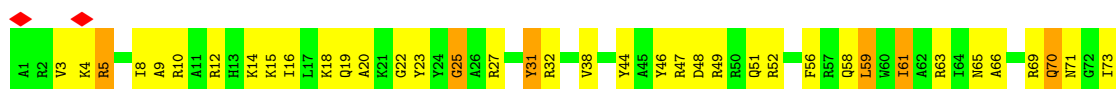
- Molecule 15: 50S ribosomal protein L19

Chain p:  62% 36% ..



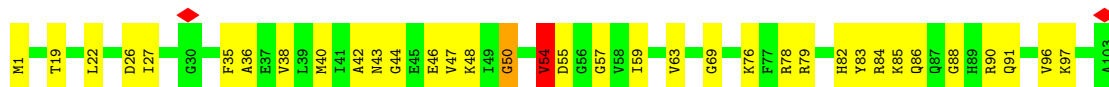
- Molecule 16: 50S ribosomal protein L20

Chain q:  59% 36% 5%





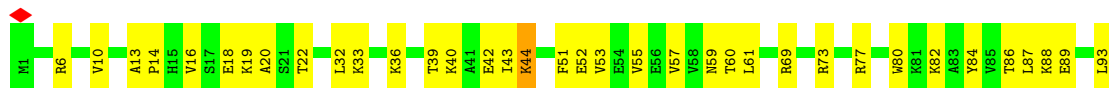
- Molecule 17: 50S ribosomal protein L21



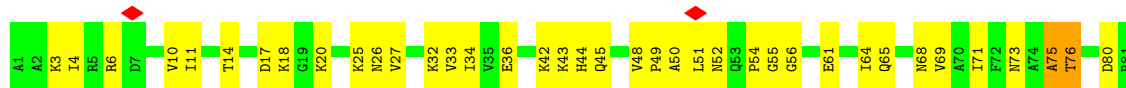
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

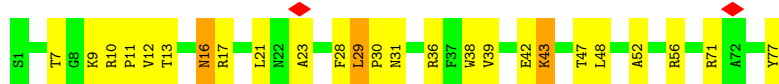


- Molecule 22: 50S ribosomal protein L27





- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



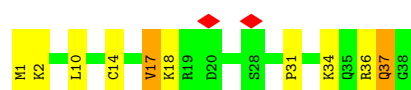
- Molecule 29: 50S ribosomal protein L35

Chain E: 



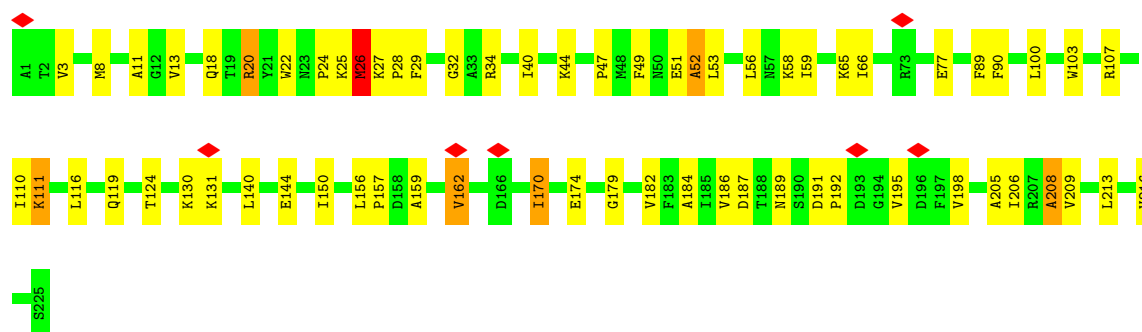
- Molecule 30: 50S ribosomal protein L36

Chain F: 



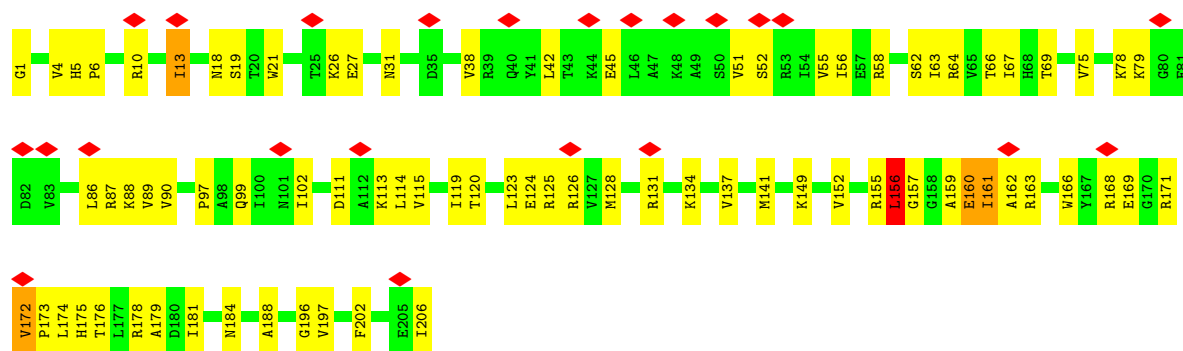
- Molecule 31: 30S ribosomal protein S2

Chain G: 



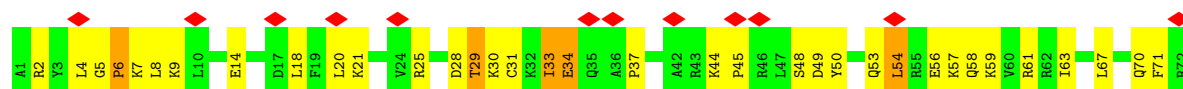
- Molecule 32: 30S ribosomal protein S3

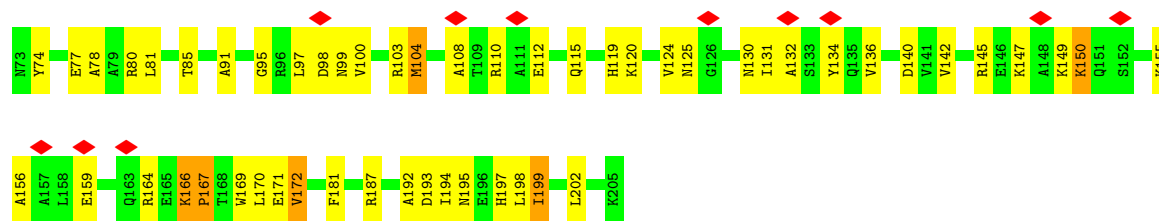
Chain H: 



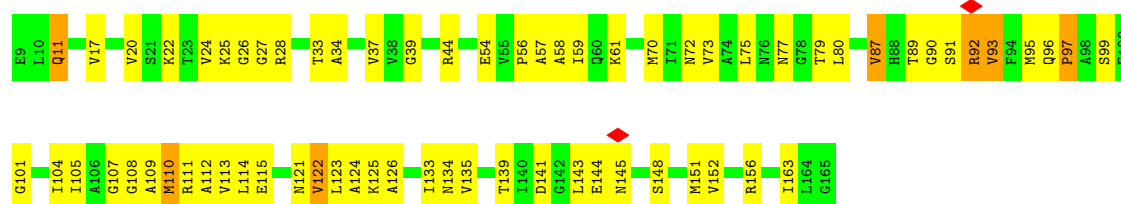
- Molecule 33: 30S ribosomal protein S4

Chain I: 

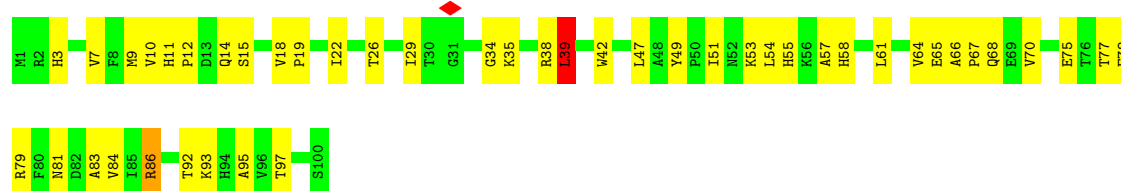




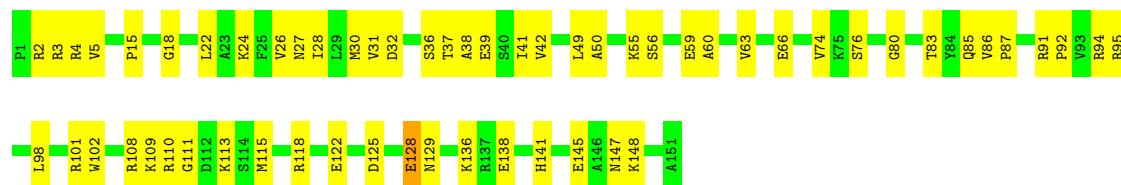
- Molecule 34: 30S ribosomal protein S5



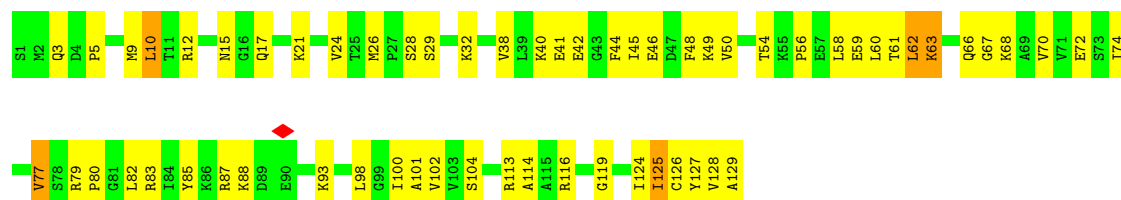
- Molecule 35: 30S ribosomal protein S6



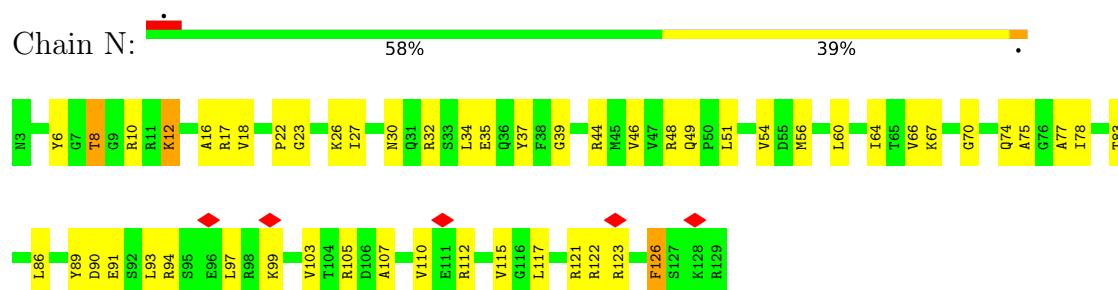
- Molecule 36: 30S ribosomal protein S7



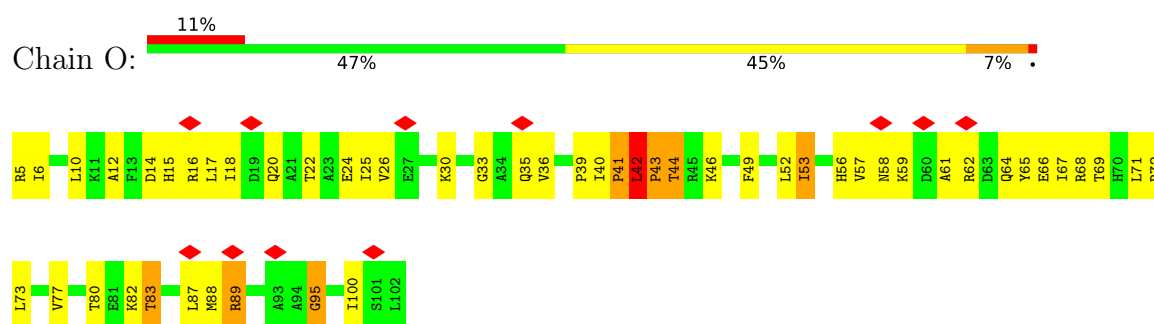
- Molecule 37: 30S ribosomal protein S8



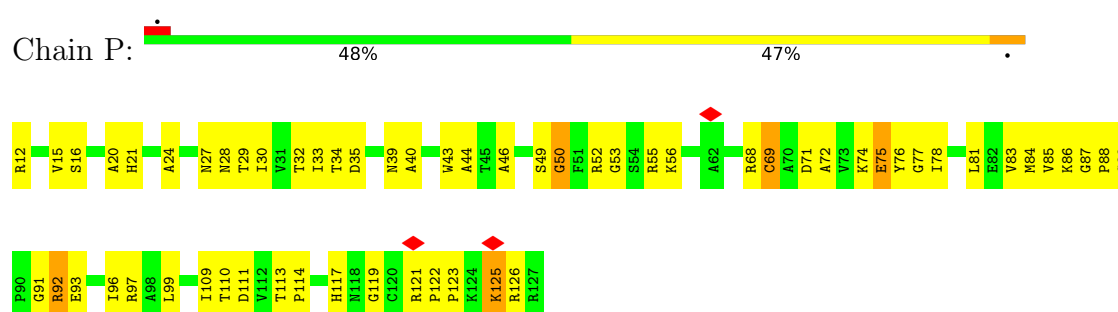
- Molecule 38: 30S ribosomal protein S9



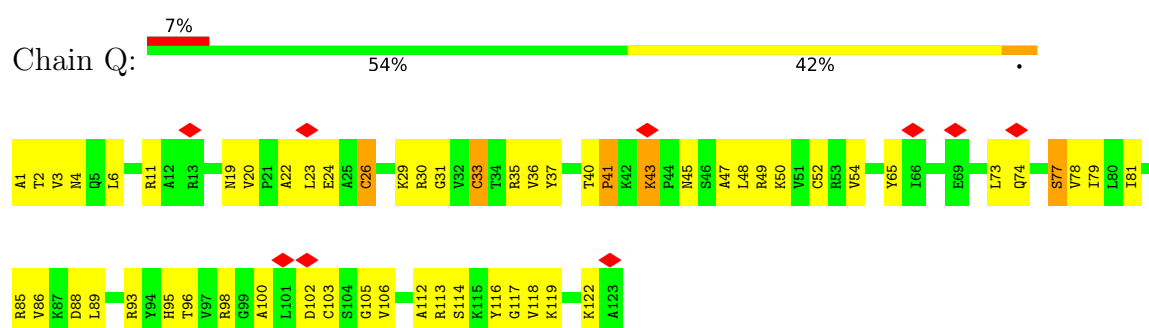
- Molecule 39: 30S ribosomal protein S10



- Molecule 40: 30S ribosomal protein S11

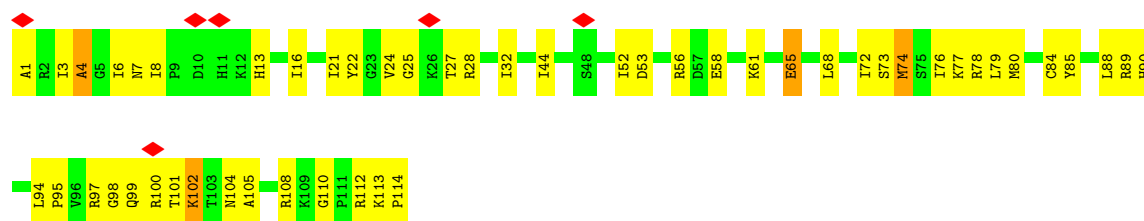


- Molecule 41: 30S ribosomal protein S12

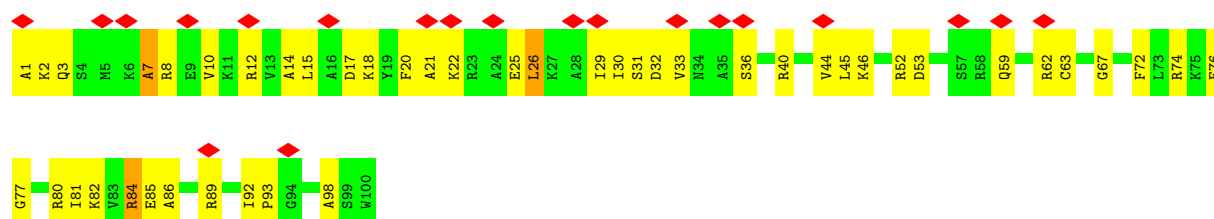


- Molecule 42: 30S ribosomal protein S13

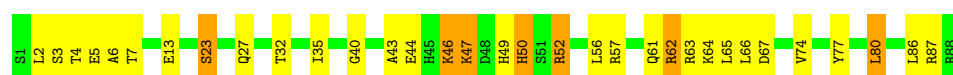




- Molecule 43: 30S ribosomal protein S14



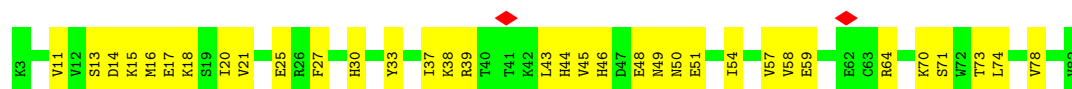
- Molecule 44: 30S ribosomal protein S15



- Molecule 45: 30S ribosomal protein S16



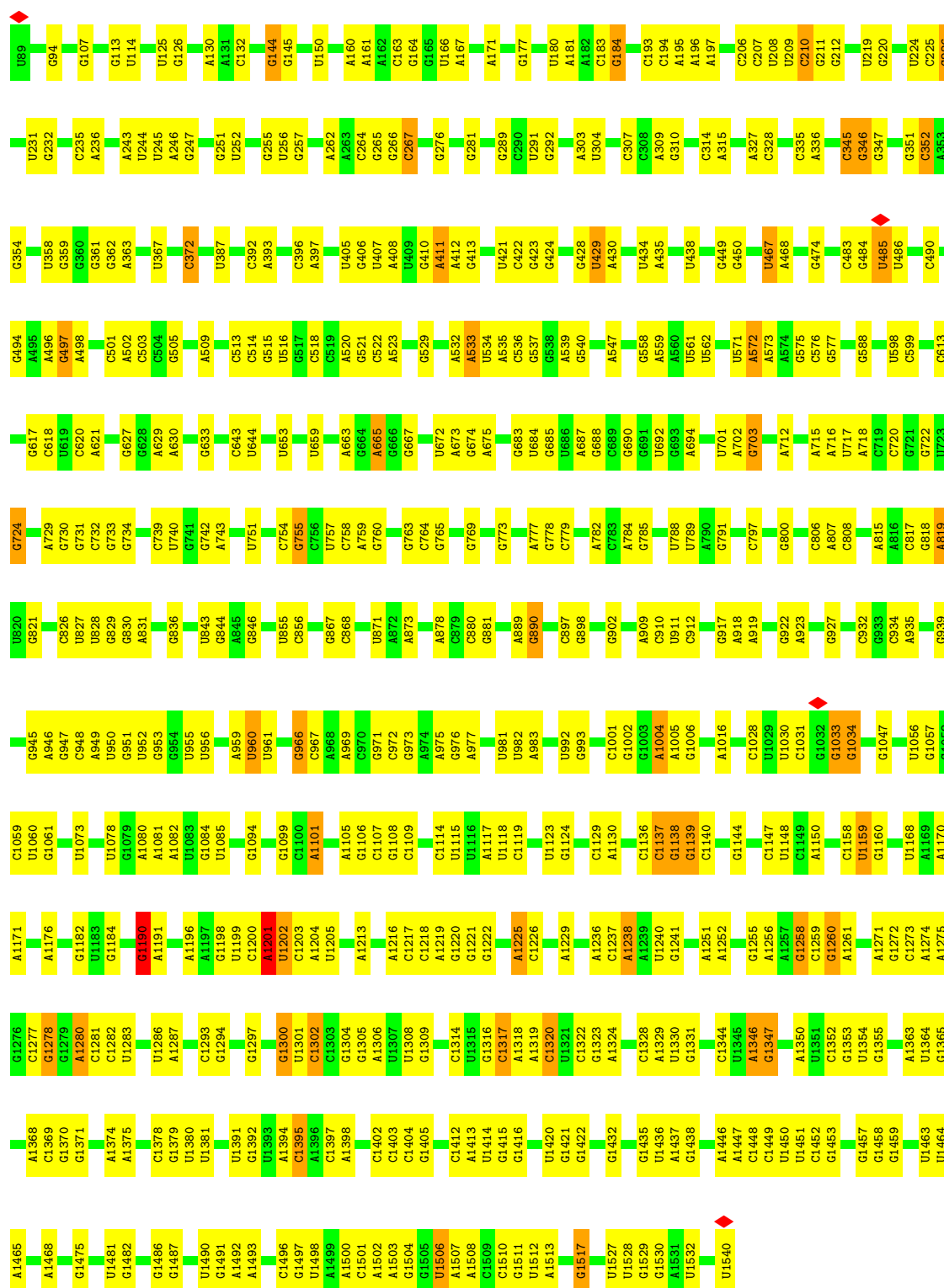
- Molecule 46: 30S ribosomal protein S17



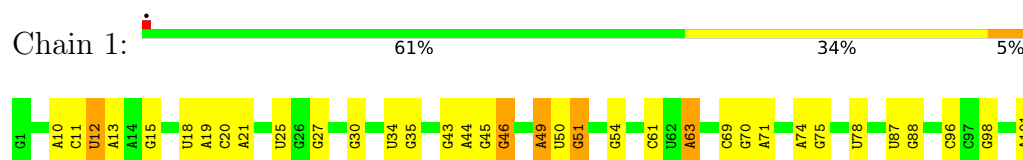
- Molecule 47: 30S ribosomal protein S18



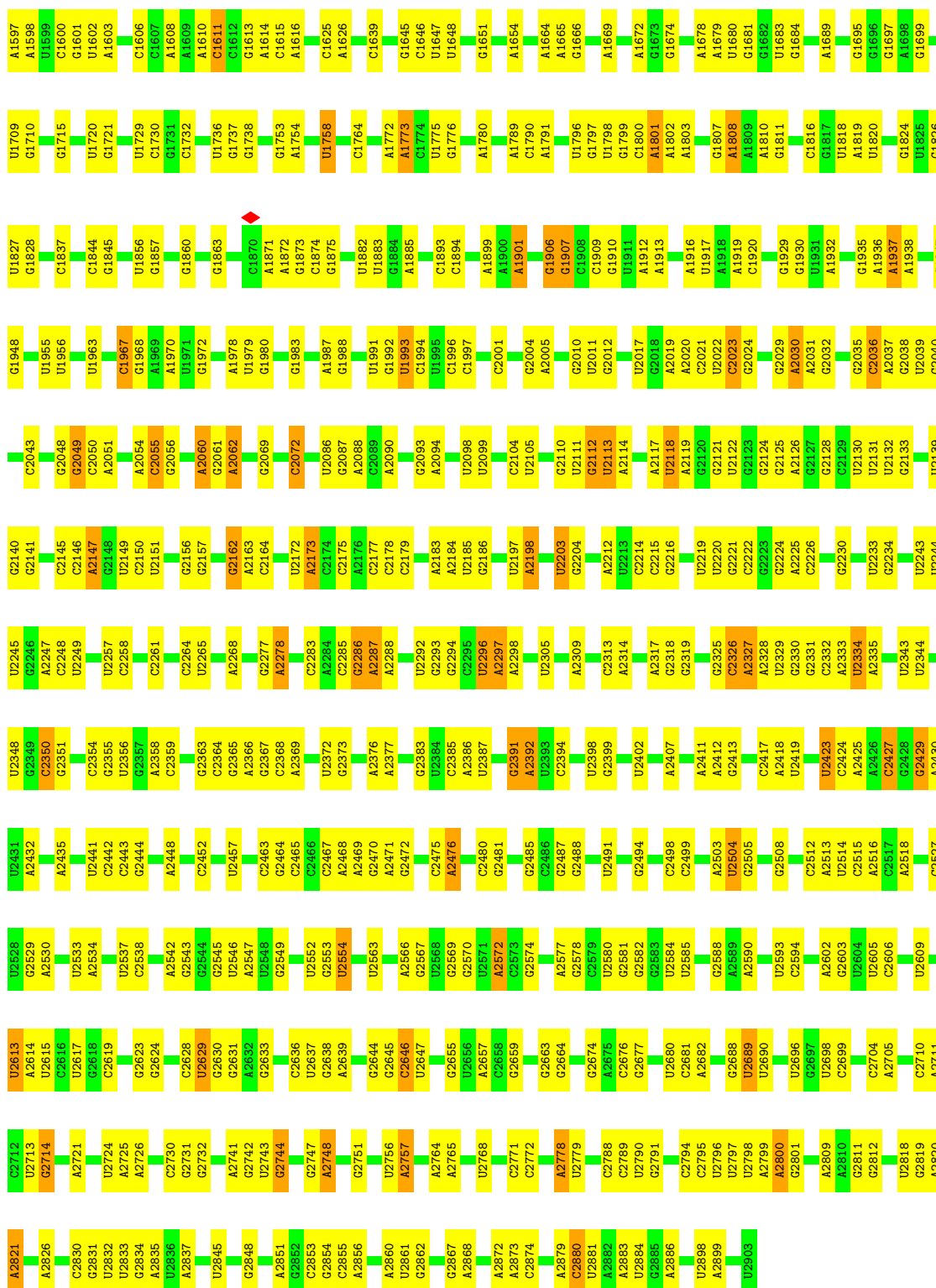
- Molecule 48: 30S ribosomal protein S19

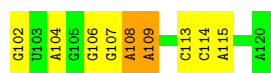


• Molecule 53: 23S ribosomal RNA

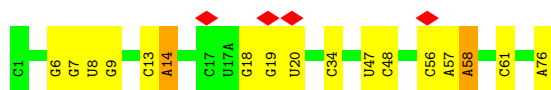
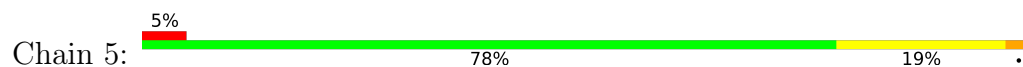


C1498	C1499	G1500	A1509	G1510	G1511	A1515	G1524	A1525	C1526	G1527	A1528	G1529	A1535	C1536	G1537	C1538	G1539	A1540	G1541	G1542	G1543	C1547	A1548	A1551	A1552	A1553	G1554	G1555	C1558	U1559	G1560	C1561	U1562	A1566	G1567	A1568	A1569	A1570	A1571	A1580	G1581	U1584	C1585	A1586	G1587	A1590	A1591					
G1368	G1369	C1370	G1371	G1372	A1373	C1376	G1377	A1378	U1379	G1380	A1383	C1398	U1415	C1416	G1417	C1418	A1419	A1420	G1424	G1425	G1429	G1430	A1431	G1432	A1433	A1434	G1435	U1440	G1441	U1442	U1443	G1444	G1445	C1454	C1461	U1474	G1475	U1476	G1482	U1487	C1488	C1489	A1490	G1491	G1492	C1493						
A1264	A1268	A1269	C1270	G1271	A1272	A1275	C1278	G1279	C1289	G1296	C1297	C1298	G1299	G1300	A1301	A1302	C1306	G1309	U1313	C1319	C1320	A1321	A1322	C1323	U1329	C1330	G1331	G1332	G1333	C1334	C1335	G1339	U1340	G1341	U1344	C1345	G1355	C1356	C1357	G1358	A1359	G1360	A1365	A1366	A1367							
G1157	G1162	G1163	C1170	G1171	A1175	U1176	G1177	C1178	U1077	C1079	A1080	U1081	U1082	U1083	G1186	G1187	U1188	A1189	G1190	U1201	G1202	G1210	C1211	G1212	G1216	U1217	U1219	G1220	C1221	U1222	G1225	U1231	G1232	C1233	U1234	G1235	G1248	C1251	G1252	A1253	A1254	U1255	G1256	C1257	U1258	G1259						
U1058	G1059	U1060	U1061	G1062	U1066	A1067	A1070	G1071	U1077	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1088	U1093	U1094	A1095	U1096	U1097	A1098	U1101	C1104	U1105	G1106	G1107	A1111	G1112	G1122	C1123	U1130	G1131	U1132	A1133	A1134	C1135	G1138	G1139	C1140	U1141	A1142	A1143	C1153							
G956	C957	C961	G962	U967	C968	G969	G974	A975	A983	A990	C991	C992	C995	A996	C997	A1001	G1002	A1009	U1012	C1013	A1014	U1019	A1020	A1021	G1022	U1023	G1026	A1027	U1033	G1034	U1035	G1036	A1040	C1043	C1044	G1045	A1046	G1047	C1052	C1053	A1054	G1055	G1056	A1057								
G859	U860	A861	G862	G869	U870	C873	G874	G875	C876	A877	A878	G881	G882	C885	A886	U887	C888	G891	A896	C897	A905	U906	A909	A910	C911	U912	U913	A917	C922	G928	U932	C937	G938	G939	G940	A941	G942	A943	C946	A947	C948	G949	G953	U954	U955							
A756	G763	A764	G771	C772	U773	G776	U779	G780	A781	A782	A783	G784	G785	A789	A792	A793	A794	C795	C796	G797	G801	G805	C806	U807	G808	C812	U813	C814	C817	G818	A819	A820	A821	G822	U826	U827	U828	A829	G830	G831	U832	A833	A845	U846	U847	C851						
U658	G659	C660	A661	G662	A668	G669	A670	C680	G681	G682	A685	U686	U688	A689	C690	C692	G695	A699	G700	U703	G704	G713	U714	A715	A718	C719	U720	A721	A727	G728	G729	A730	G731	C732	G733	U741	A742	A743	U744	G745	U746	C747	G748	A752	U755							
C239	C240	A241	A244	G248	C249	G250	A251	G252	C253	G254	A255	A256	A265	G266	C274	C275	U276	G277	A278	C281	U293	A294	G301	G307	A310	A311	G319	A320	U321	A322	C323	A324	G325	G326	G327	U328	A330	C331	C336	G337	G338	U339	A340	C341	A342							
C343	A344	A345	A346	A362	G363	G367	A368	A371	G372	A382	A483	C484	G488	C489	C490	C491	A492	G493	G494	U499	A503	A504	A505	G506	C509	C510	A613	U511	G512	C433	U434	C435	C436	U437	G438	A439	C440	U441	G442	A443	C444	G445	G446	U451	C452	C456	A457	G458	U464	G465	A466	G467
G122	G123	G124	A125	U138	U139	C140	G141	A142	C145	A146	U150	C151	U158	G159	A160	A161	U162	C163	G164	A165	U166	A167	G168	U171	A172	A173	U174	G175	A176	G177	A181	C184	G185	G186	G187	G188	A196	G195	G215	A216	A221	A222	C225	A226	A227	C228	C229					

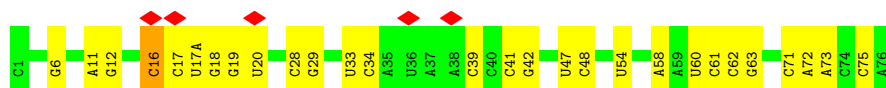




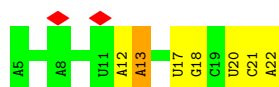
• Molecule 55: tRNAfMet



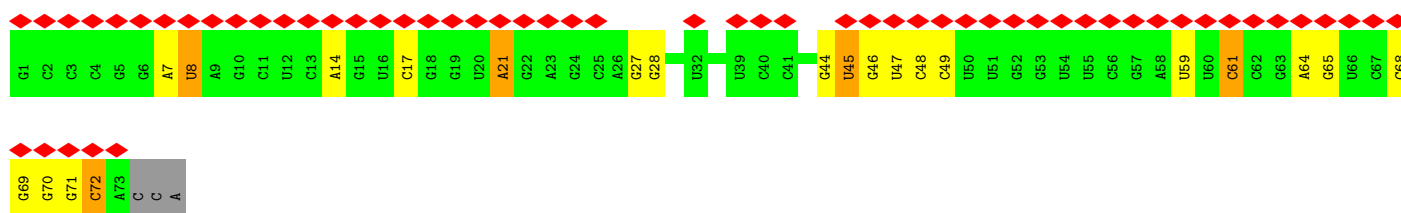
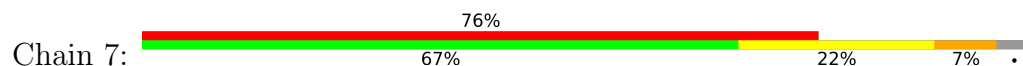
• Molecule 55: tRNAfMet



• Molecule 56: mRNA



• Molecule 57: tRNAPhe



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1699	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 ($e^-/\text{\AA}^2$)	35	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	18.877	Depositor
Minimum map value	-10.681	Depositor
Average map value	0.115	Depositor
Map value standard deviation	0.882	Depositor
Recommended contour level	1	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	b	0.30	0/2122	0.98	11/2852 (0.4%)
2	c	0.30	0/1586	0.85	2/2134 (0.1%)
3	d	0.30	0/1571	0.94	5/2113 (0.2%)
4	e	0.31	0/1435	0.91	4/1926 (0.2%)
5	f	0.30	0/1343	0.95	9/1816 (0.5%)
6	g	0.30	0/1122	1.01	8/1515 (0.5%)
7	h	0.33	0/1002	1.02	3/1350 (0.2%)
8	i	0.37	0/1046	1.01	10/1410 (0.7%)
9	j	0.30	0/1152	0.95	7/1551 (0.5%)
10	k	0.30	0/948	1.00	3/1268 (0.2%)
11	l	0.30	0/1054	1.00	5/1403 (0.4%)
12	m	0.32	0/1093	0.95	3/1460 (0.2%)
13	n	0.32	0/974	1.02	10/1301 (0.8%)
14	o	0.29	0/902	0.95	3/1209 (0.2%)
15	p	0.30	0/929	0.88	3/1242 (0.2%)
16	q	0.29	0/960	0.96	8/1278 (0.6%)
17	r	0.30	0/829	0.99	4/1107 (0.4%)
18	s	0.27	0/864	0.94	1/1156 (0.1%)
19	t	0.29	0/745	1.02	4/994 (0.4%)
20	u	0.31	0/788	1.01	5/1051 (0.5%)
21	v	0.29	0/766	0.89	3/1025 (0.3%)
22	w	0.31	0/582	0.90	1/769 (0.1%)
23	x	0.30	0/635	0.89	0/848
24	y	0.29	0/510	1.06	6/677 (0.9%)
25	z	0.30	0/453	1.06	4/605 (0.7%)
26	B	0.28	0/450	0.82	2/599 (0.3%)
27	C	0.34	0/417	0.82	0/554
28	D	0.32	0/380	0.92	1/498 (0.2%)
29	E	0.30	0/513	0.91	1/676 (0.1%)
30	F	0.31	0/303	0.92	0/397
31	G	0.29	0/1788	0.96	10/2408 (0.4%)
32	H	0.30	0/1652	0.97	8/2225 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/1665	1.02	11/2227 (0.5%)
34	J	0.34	0/1170	0.97	6/1573 (0.4%)
35	K	0.30	0/836	0.97	3/1128 (0.3%)
36	L	0.29	0/1196	0.90	1/1602 (0.1%)
37	M	0.30	0/989	0.90	3/1326 (0.2%)
38	N	0.30	0/1034	0.93	2/1375 (0.1%)
39	O	0.32	0/797	0.99	7/1077 (0.6%)
40	P	0.31	0/886	0.99	5/1195 (0.4%)
41	Q	0.30	0/969	1.02	6/1300 (0.5%)
42	R	0.32	0/893	0.99	5/1193 (0.4%)
43	S	0.29	0/817	0.96	4/1088 (0.4%)
44	T	0.29	0/722	0.99	5/964 (0.5%)
45	U	0.33	0/659	1.03	3/884 (0.3%)
46	V	0.29	0/658	0.89	2/881 (0.2%)
47	W	0.32	0/545	0.92	1/731 (0.1%)
48	X	0.31	0/653	0.90	2/877 (0.2%)
49	Y	0.29	0/671	1.06	7/888 (0.8%)
50	Z	0.34	0/551	1.03	4/728 (0.5%)
51	a	0.32	0/1034	0.85	1/1387 (0.1%)
52	3	0.40	0/36963	0.51	3/57662 (0.0%)
53	1	0.39	0/69796	0.50	1/108888 (0.0%)
54	2	0.40	0/2872	0.51	0/4479
55	5	0.39	0/1832	0.49	0/2855
55	6	0.39	0/1832	0.51	0/2855
56	4	0.40	0/436	0.48	0/679
57	7	0.40	0/1740	0.50	0/2712
All	All	0.37	0/163130	0.65	226/243971 (0.1%)

There are no bond length outliers.

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	r	50	GLY	N-CA-C	-9.72	102.40	114.16
31	G	20	ARG	N-CA-C	-8.80	102.67	113.50
34	J	92	ARG	N-CA-C	-8.70	102.80	113.50
6	g	72	ILE	N-CA-C	-8.33	102.75	111.58
7	h	117	LEU	N-CA-C	8.27	123.12	109.06

There are no chirality outliers.

There are no planarity outliers.

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	b	2083	0	2157	112	0
2	c	1565	0	1616	63	0
3	d	1552	0	1619	67	0
4	e	1411	0	1447	54	0
5	f	1323	0	1374	38	0
6	g	1111	0	1148	56	0
7	h	989	0	1025	60	0
8	i	1032	0	1088	53	0
9	j	1129	0	1162	38	0
10	k	939	0	1012	45	0
11	l	1045	0	1117	53	0
12	m	1074	0	1157	56	0
13	n	961	0	1000	29	0
14	o	892	0	923	31	0
15	p	917	0	965	35	0
16	q	947	0	1022	43	0
17	r	816	0	839	31	0
18	s	857	0	922	33	0
19	t	739	0	807	28	0
20	u	780	0	834	46	0
21	v	753	0	780	22	0
22	w	575	0	592	25	0
23	x	625	0	655	24	0
24	y	509	0	543	15	0
25	z	449	0	491	17	0
26	B	444	0	461	17	0
27	C	410	0	440	18	0
28	D	377	0	418	26	0
29	E	504	0	574	25	0
30	F	302	0	343	10	0
31	G	1757	0	1787	48	0
32	H	1625	0	1699	68	0
33	I	1643	0	1710	64	0
34	J	1157	0	1199	58	0
35	K	818	0	808	40	0
36	L	1182	0	1240	46	0
37	M	979	0	1034	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	1022	0	1070	48	0
39	O	787	0	828	41	0
40	P	870	0	878	49	0
41	Q	955	0	1019	49	0
42	R	884	0	944	43	0
43	S	805	0	847	42	0
44	T	714	0	737	25	0
45	U	649	0	666	33	0
46	V	649	0	691	27	0
47	W	536	0	552	20	0
48	X	638	0	665	33	0
49	Y	665	0	714	39	0
50	Z	545	0	579	29	0
51	a	1027	0	1092	45	0
52	3	33012	0	16618	454	0
53	1	62317	0	31346	876	0
54	2	2568	0	1303	54	0
55	5	1640	0	836	7	0
55	6	1640	0	837	18	0
56	4	388	0	197	9	0
57	7	1557	0	789	13	0
58	5	10	0	10	1	0
All	All	150149	0	101226	2886	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 11.

The worst 5 of 2886 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)
53:1:45:G:H5''	53:1:46:G:H5'	1.32	1.05
4:e:25:MET:HE1	54:2:55:U:H1'	1.40	1.03
11:l:47:ARG:HH11	53:1:195:A:H5''	1.30	0.97
37:M:21:LYS:HE3	52:3:827:U:H5''	1.48	0.96
10:k:48:PRO:HG3	52:3:1422:G:H5'	1.48	0.96

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	b	269/271 (99%)	226 (84%)	37 (14%)	6 (2%)	5	29
2	c	207/209 (99%)	173 (84%)	30 (14%)	4 (2%)	6	32
3	d	199/201 (99%)	172 (86%)	23 (12%)	4 (2%)	6	31
4	e	175/177 (99%)	153 (87%)	21 (12%)	1 (1%)	21	58
5	f	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
6	g	147/149 (99%)	123 (84%)	20 (14%)	4 (3%)	4	25
7	h	129/131 (98%)	97 (75%)	27 (21%)	5 (4%)	2	19
8	i	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3	23
9	j	140/142 (99%)	122 (87%)	15 (11%)	3 (2%)	5	30
10	k	120/122 (98%)	101 (84%)	16 (13%)	3 (2%)	4	26
11	l	141/143 (99%)	122 (86%)	16 (11%)	3 (2%)	5	30
12	m	134/136 (98%)	112 (84%)	18 (13%)	4 (3%)	3	22
13	n	118/120 (98%)	97 (82%)	20 (17%)	1 (1%)	16	52
14	o	114/116 (98%)	101 (89%)	11 (10%)	2 (2%)	6	33
15	p	112/114 (98%)	99 (88%)	11 (10%)	2 (2%)	6	33
16	q	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	35
17	r	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	6	31
18	s	108/110 (98%)	90 (83%)	16 (15%)	2 (2%)	6	32
19	t	91/93 (98%)	81 (89%)	9 (10%)	1 (1%)	11	45
20	u	100/102 (98%)	86 (86%)	13 (13%)	1 (1%)	12	47
21	v	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	11	45
22	w	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
23	x	75/77 (97%)	69 (92%)	4 (5%)	2 (3%)	4	25
24	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	37
25	z	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
27	C	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
28	D	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	5	28
29	E	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	3	21
30	F	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	4	24
31	G	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
32	H	204/206 (99%)	187 (92%)	16 (8%)	1 (0%)	24	62
33	I	203/205 (99%)	179 (88%)	19 (9%)	5 (2%)	4	26
34	J	155/157 (99%)	121 (78%)	27 (17%)	7 (4%)	2	17
35	K	98/100 (98%)	79 (81%)	16 (16%)	3 (3%)	3	22
36	L	149/151 (99%)	128 (86%)	16 (11%)	5 (3%)	3	21
37	M	127/129 (98%)	109 (86%)	16 (13%)	2 (2%)	7	37
38	N	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	3	21
39	O	96/98 (98%)	74 (77%)	16 (17%)	6 (6%)	1	13
40	P	114/116 (98%)	94 (82%)	19 (17%)	1 (1%)	14	49
41	Q	121/123 (98%)	99 (82%)	18 (15%)	4 (3%)	3	21
42	R	112/114 (98%)	92 (82%)	15 (13%)	5 (4%)	2	17
43	S	98/100 (98%)	81 (83%)	16 (16%)	1 (1%)	12	47
44	T	86/88 (98%)	72 (84%)	10 (12%)	4 (5%)	2	16
45	U	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	26
46	V	78/80 (98%)	61 (78%)	14 (18%)	3 (4%)	2	19
47	W	63/65 (97%)	58 (92%)	4 (6%)	1 (2%)	7	37
48	X	77/79 (98%)	60 (78%)	16 (21%)	1 (1%)	9	41
49	Y	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4	27
50	Z	63/65 (97%)	43 (68%)	13 (21%)	7 (11%)	0	6
51	a	130/223 (58%)	117 (90%)	13 (10%)	0	100	100
All	All	5919/6112 (97%)	5051 (85%)	741 (12%)	127 (2%)	8	30

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	58	LYS
3	d	83	VAL

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Mol	Chain	Res	Type
6	g	9	VAL
7	h	108	VAL
7	h	118	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	212 (98%)	4 (2%)	50	66
2	c	164/164 (100%)	163 (99%)	1 (1%)	78	80
3	d	165/165 (100%)	163 (99%)	2 (1%)	63	73
4	e	148/148 (100%)	146 (99%)	2 (1%)	59	71
5	f	137/137 (100%)	137 (100%)	0	100	100
6	g	114/114 (100%)	114 (100%)	0	100	100
7	h	100/100 (100%)	99 (99%)	1 (1%)	68	76
8	i	109/109 (100%)	109 (100%)	0	100	100
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	102 (99%)	1 (1%)	68	76
11	l	102/102 (100%)	102 (100%)	0	100	100
12	m	109/109 (100%)	109 (100%)	0	100	100
13	n	100/100 (100%)	97 (97%)	3 (3%)	36	57
14	o	86/86 (100%)	85 (99%)	1 (1%)	63	73
15	p	99/99 (100%)	98 (99%)	1 (1%)	68	76
16	q	89/89 (100%)	88 (99%)	1 (1%)	65	74
17	r	84/84 (100%)	83 (99%)	1 (1%)	63	73
18	s	93/93 (100%)	91 (98%)	2 (2%)	45	64
19	t	80/80 (100%)	80 (100%)	0	100	100
20	u	83/83 (100%)	83 (100%)	0	100	100
21	v	78/78 (100%)	77 (99%)	1 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	w	57/57 (100%)	56 (98%)	1 (2%)	51	67
23	x	67/67 (100%)	65 (97%)	2 (3%)	36	57
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	48 (100%)	0	100	100
26	B	47/47 (100%)	47 (100%)	0	100	100
27	C	45/45 (100%)	44 (98%)	1 (2%)	45	64
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51 (100%)	49 (96%)	2 (4%)	28	50
30	F	34/34 (100%)	32 (94%)	2 (6%)	18	41
31	G	186/186 (100%)	185 (100%)	1 (0%)	81	81
32	H	170/170 (100%)	167 (98%)	3 (2%)	51	67
33	I	172/172 (100%)	171 (99%)	1 (1%)	78	80
34	J	119/119 (100%)	119 (100%)	0	100	100
35	K	87/87 (100%)	86 (99%)	1 (1%)	65	74
36	L	124/124 (100%)	122 (98%)	2 (2%)	55	69
37	M	104/104 (100%)	100 (96%)	4 (4%)	29	51
38	N	105/105 (100%)	105 (100%)	0	100	100
39	O	86/86 (100%)	85 (99%)	1 (1%)	63	73
40	P	89/89 (100%)	89 (100%)	0	100	100
41	Q	103/103 (100%)	103 (100%)	0	100	100
42	R	92/92 (100%)	91 (99%)	1 (1%)	65	74
43	S	83/83 (100%)	82 (99%)	1 (1%)	63	73
44	T	76/76 (100%)	74 (97%)	2 (3%)	40	60
45	U	65/65 (100%)	64 (98%)	1 (2%)	57	70
46	V	74/74 (100%)	74 (100%)	0	100	100
47	W	56/56 (100%)	56 (100%)	0	100	100
48	X	70/70 (100%)	69 (99%)	1 (1%)	59	71
49	Y	65/65 (100%)	65 (100%)	0	100	100
50	Z	55/55 (100%)	55 (100%)	0	100	100
51	a	110/174 (63%)	108 (98%)	2 (2%)	51	67
All	All	4908/4972 (99%)	4858 (99%)	50 (1%)	65	76

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	F	17	VAL
36	L	115	MET
51	a	222	VAL
31	G	26	MET
32	H	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
18	s	40	ASN
44	T	41	HIS
24	y	41	HIS
44	T	36	ASN
39	O	99	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	139 (9%)	3 (0%)
53	1	2902/2903 (99%)	323 (11%)	8 (0%)
54	2	119/120 (99%)	11 (9%)	1 (0%)
55	5	76/77 (98%)	12 (15%)	0
55	6	76/77 (98%)	8 (10%)	0
56	4	17/18 (94%)	2 (11%)	0
57	7	72/76 (94%)	11 (15%)	0
All	All	4800/4810 (99%)	506 (10%)	12 (0%)

5 of 506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	7	A
52	3	9	G
52	3	22	G
52	3	31	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	2286	G
53	1	2296	U
54	2	88	C
53	1	2326	C
53	1	490	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	FME	5	101	55	8,9,10	0.81	0	8,9,11	0.70	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
58	FME	5	101	55	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	5	101	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	5	101	FME	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.

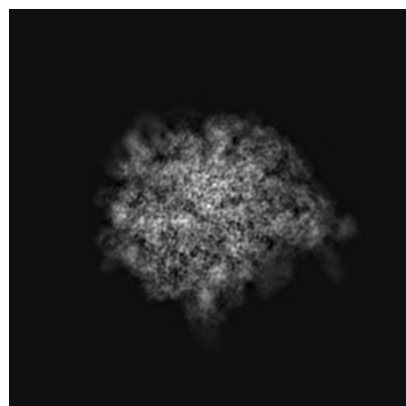
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21636. These allow visual inspection of the internal detail of the map and identification of artifacts.

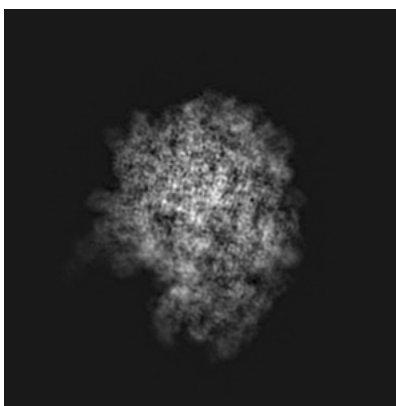
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

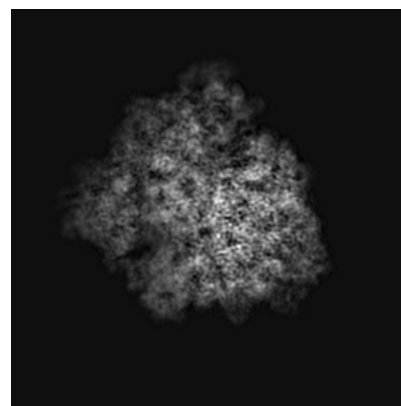
6.1.1 Primary map



X

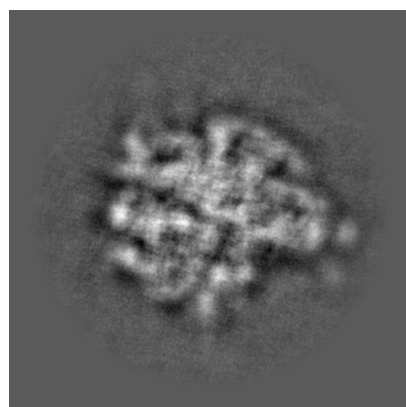


Y

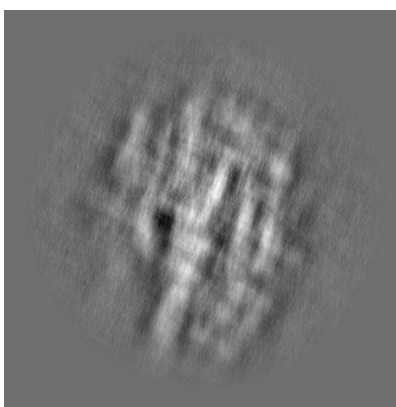


Z

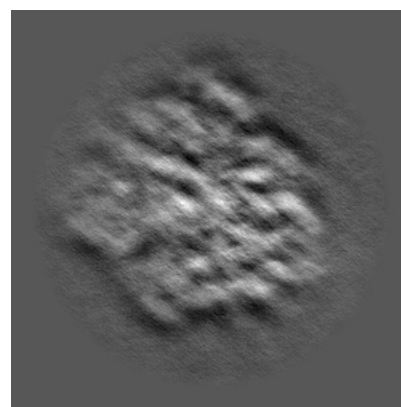
6.1.2 Raw map



X



Y

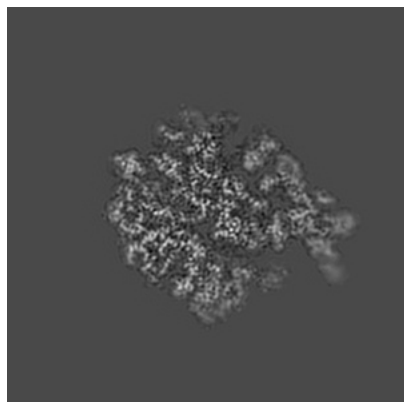


Z

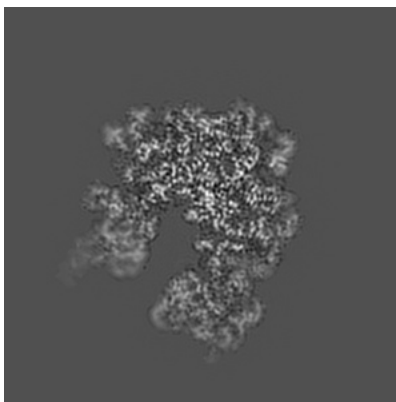
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

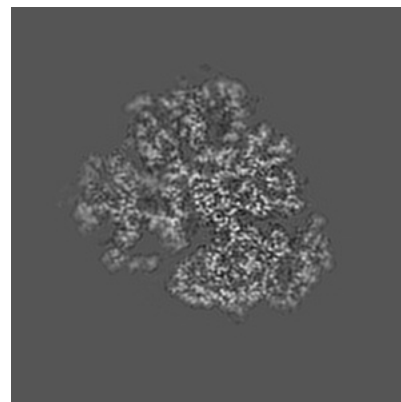
6.2.1 Primary map



X Index: 144

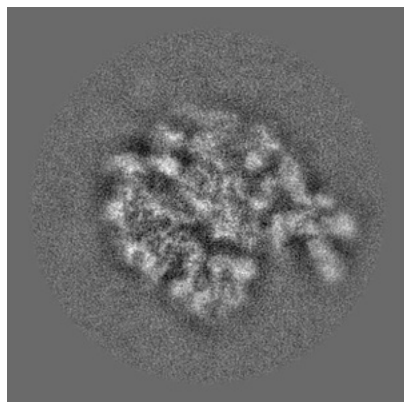


Y Index: 144

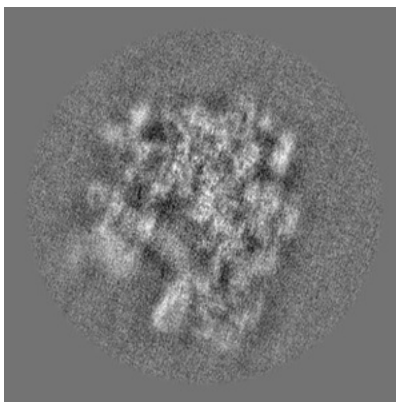


Z Index: 144

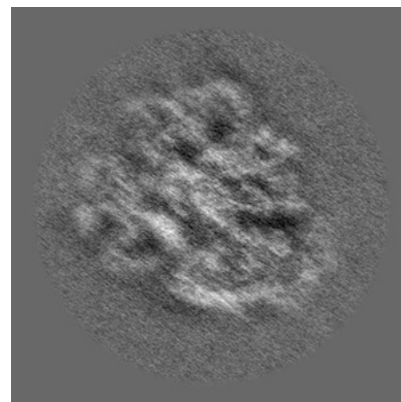
6.2.2 Raw map



X Index: 144



Y Index: 144

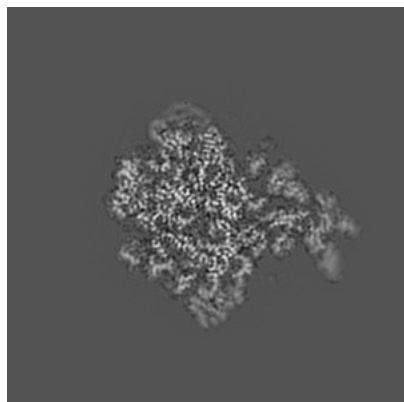


Z Index: 144

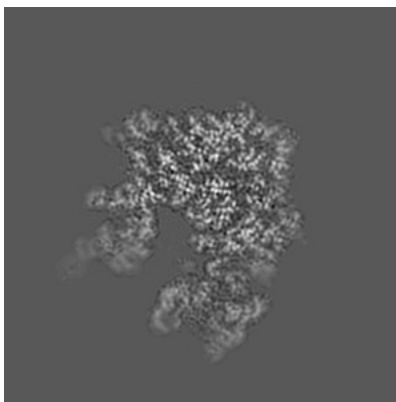
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

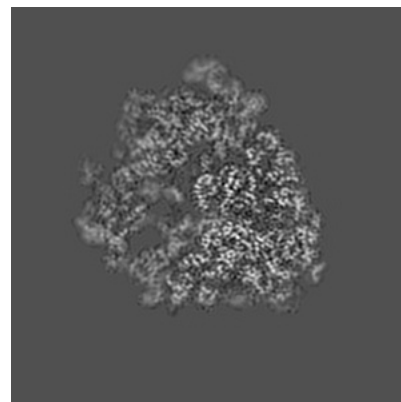
6.3.1 Primary map



X Index: 149

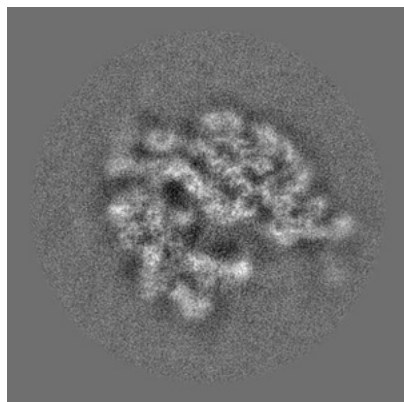


Y Index: 148

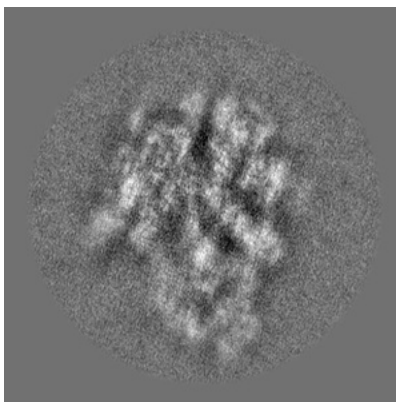


Z Index: 135

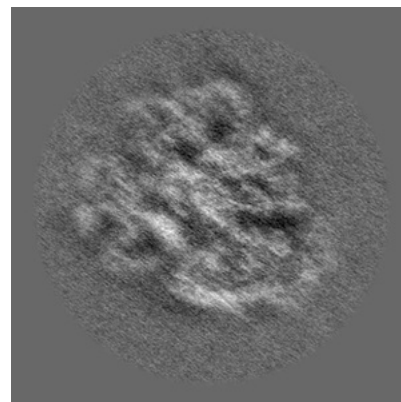
6.3.2 Raw map



X Index: 134



Y Index: 129

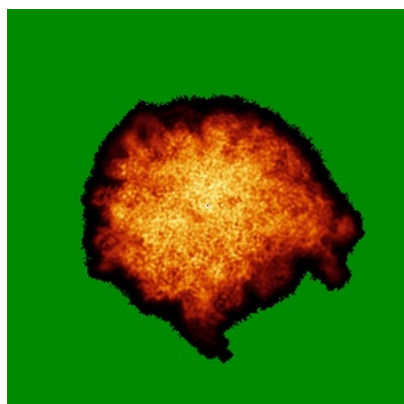


Z Index: 144

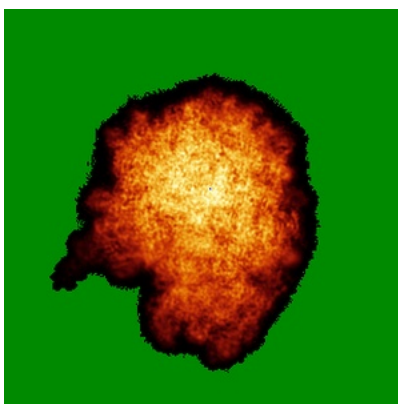
The images above show the largest variance slices of the map in three orthogonal directions.

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

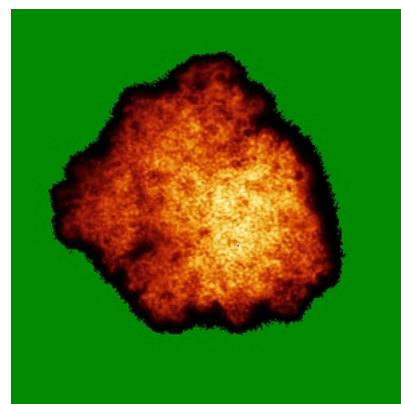
6.4.1 Primary map



X

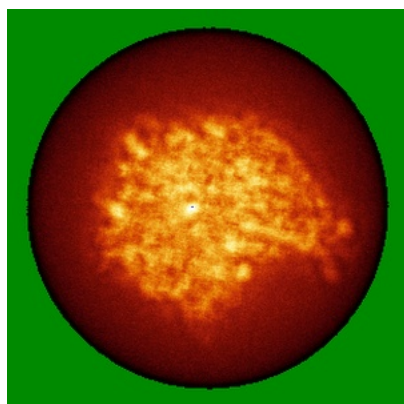


Y

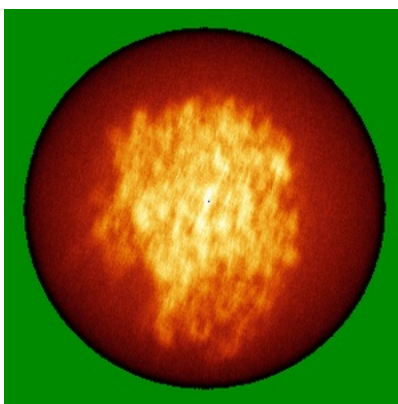


Z

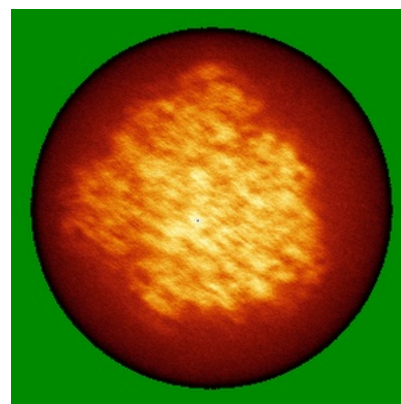
6.4.2 Raw map



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



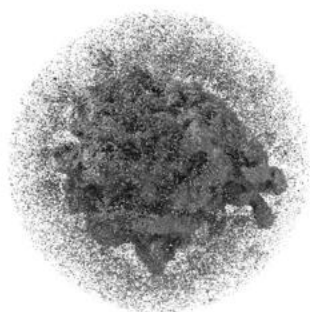
Y



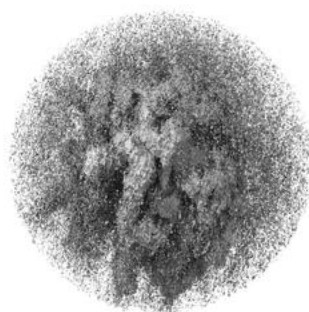
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

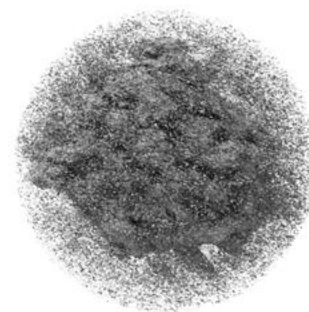
6.5.2 Raw map



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.

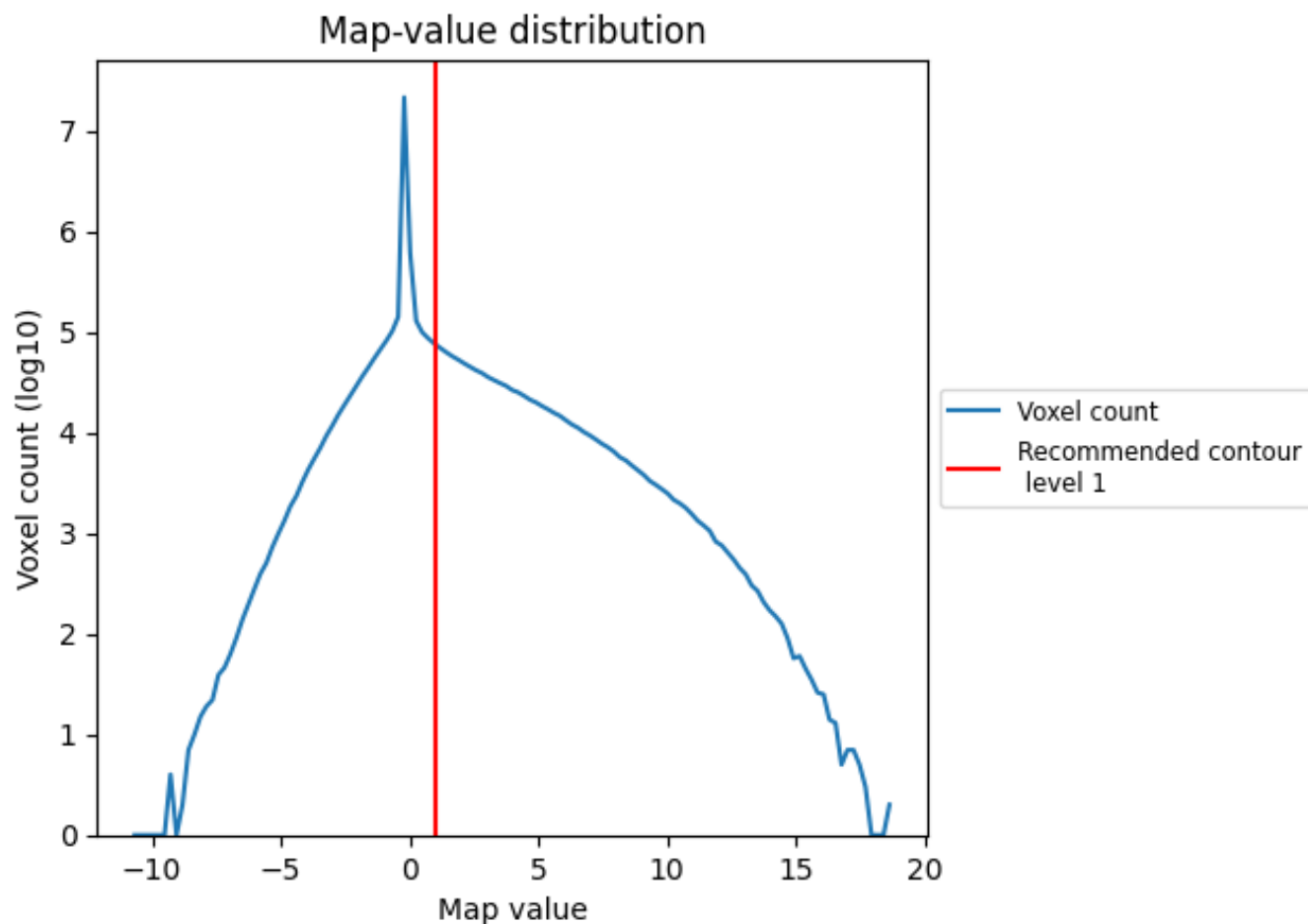
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

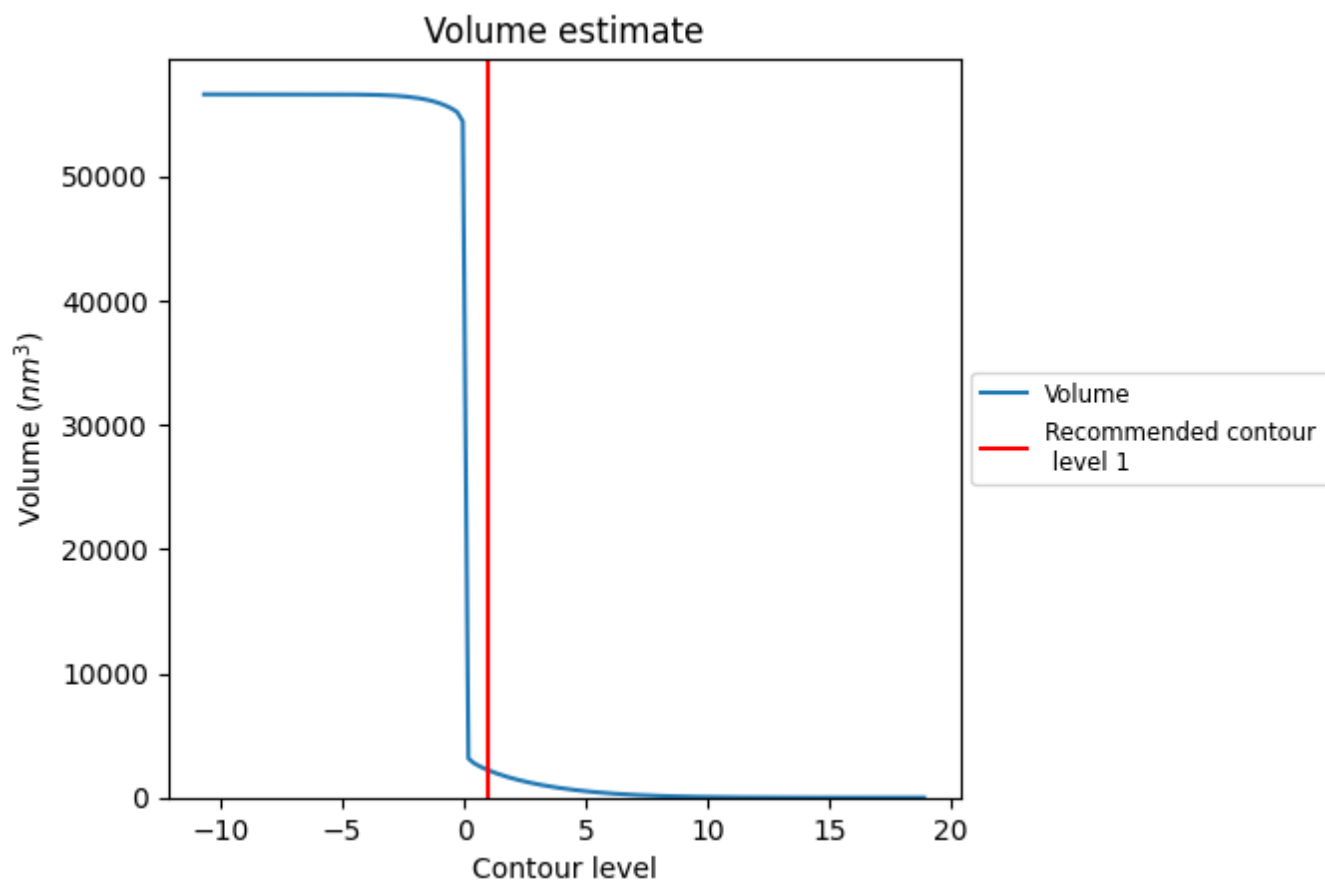
This section contains the results of statistical analysis of the map.

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.

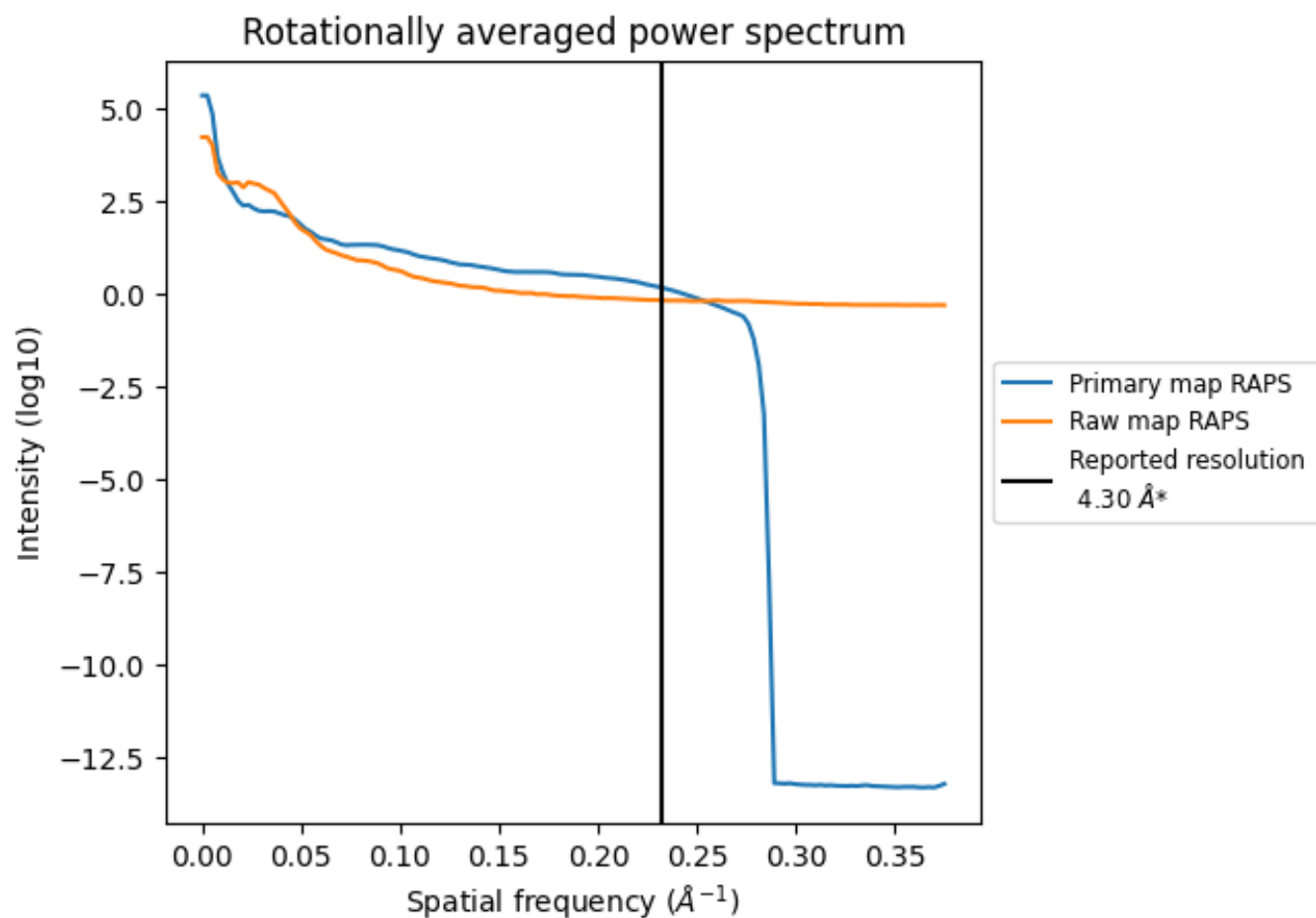
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2191 nm³; this corresponds to an approximate mass of 1979 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 ⓘ

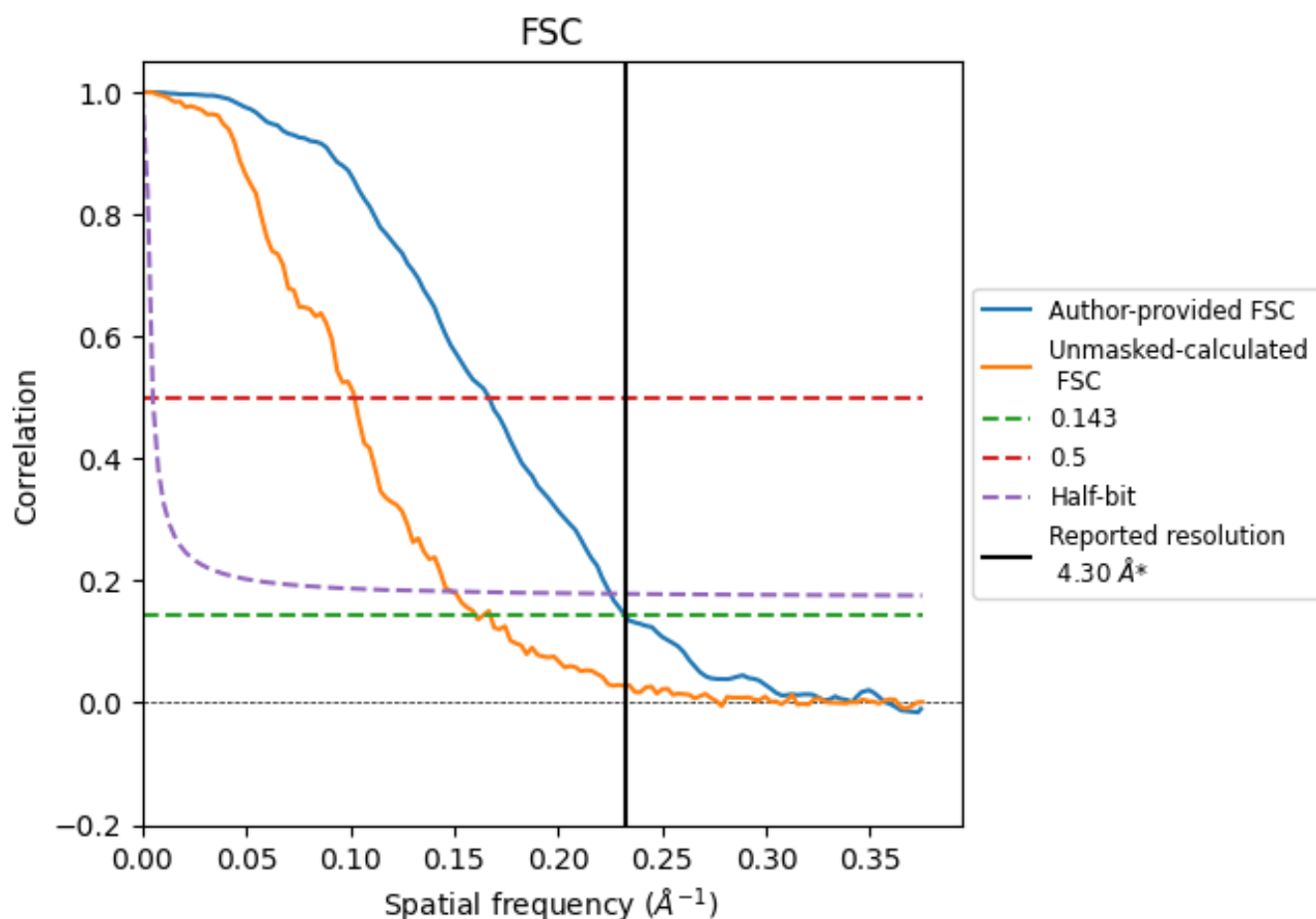


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

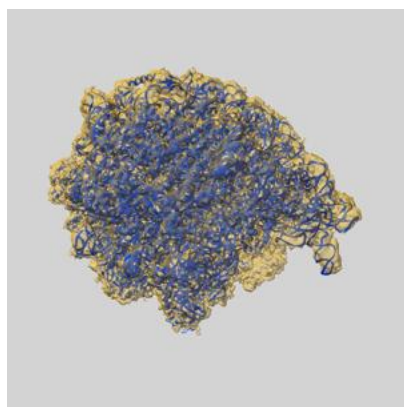
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.31	6.00	4.44
Unmasked-calculated*	6.24	9.80	6.71

*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 6.24 differs from the reported value 4.3 by more than 10 %

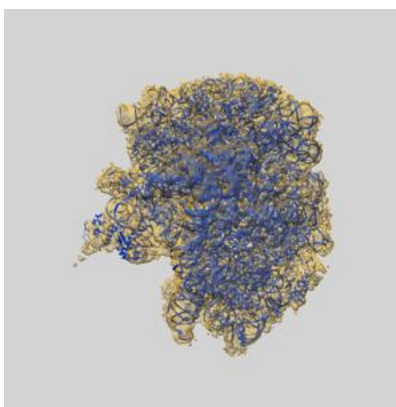
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21636 and PDB model 6WDH. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

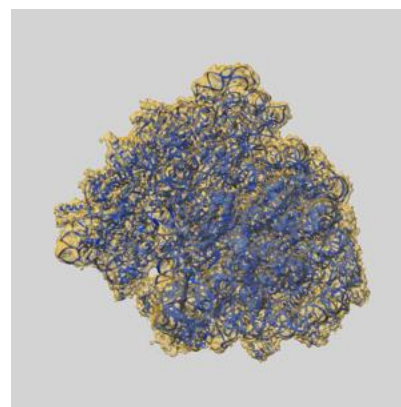
9.1 Map-model overlay [i](#)



X



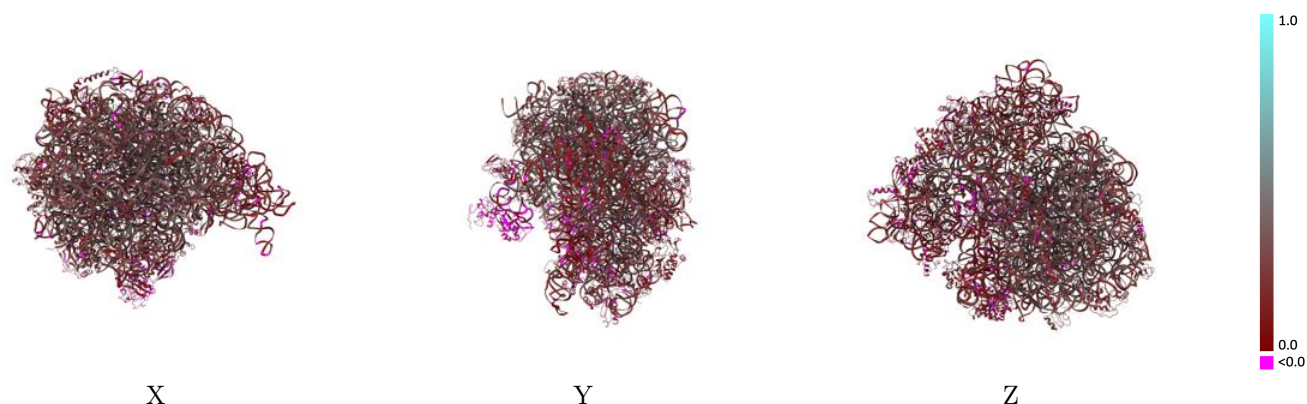
Y



Z

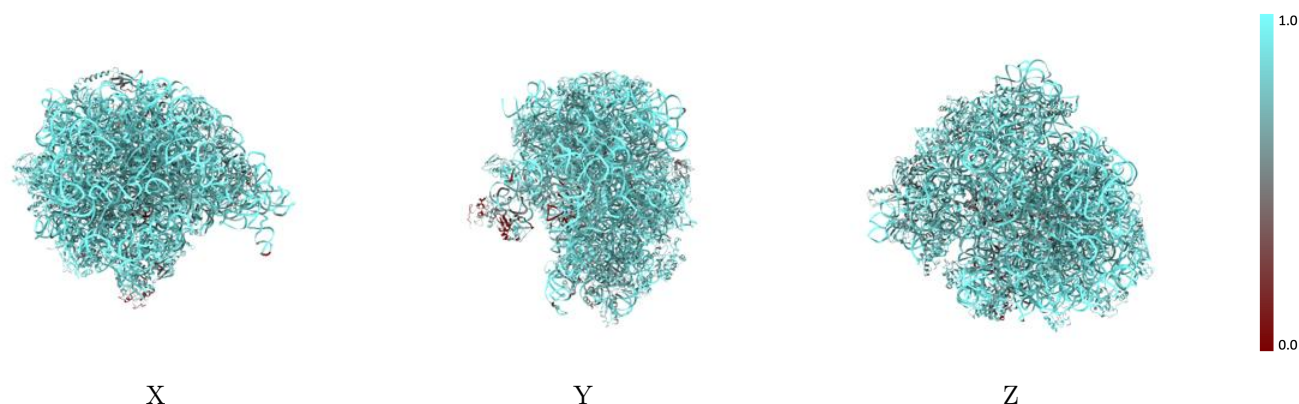
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



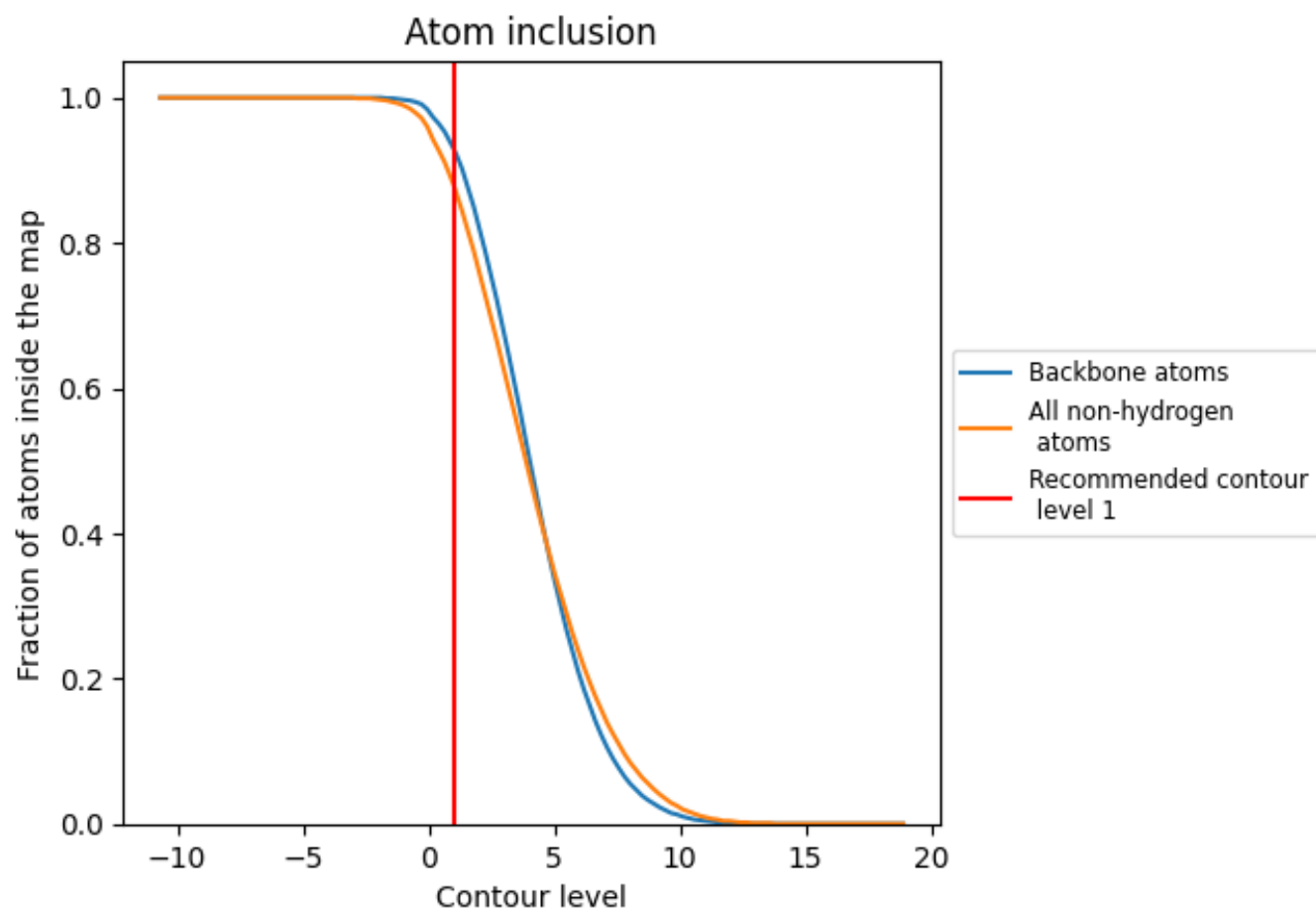
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.2500
1	 0.9430	 0.2970
2	 0.9620	 0.2790
3	 0.9230	 0.2450
4	 0.7370	 0.1340
5	 0.8580	 0.1950
6	 0.7560	 0.1010
7	 0.1770	 0.0080
B	 0.8460	 0.2570
C	 0.6770	 0.2030
D	 0.8000	 0.2850
E	 0.8450	 0.3030
F	 0.7430	 0.2230
G	 0.7950	 0.1920
H	 0.6960	 0.1960
I	 0.7300	 0.1220
J	 0.8340	 0.2760
K	 0.8470	 0.1870
L	 0.8120	 0.1590
M	 0.8150	 0.2300
N	 0.7750	 0.1600
O	 0.6780	 0.1550
P	 0.8320	 0.1910
Q	 0.7410	 0.1990
R	 0.8090	 0.1480
S	 0.6670	 0.1790
T	 0.8460	 0.2090
U	 0.7560	 0.1670
V	 0.8170	 0.1900
W	 0.8160	 0.2180
X	 0.8600	 0.1910
Y	 0.7060	 0.1320
Z	 0.7570	 0.1430
a	 0.6820	 0.0790
b	 0.8460	 0.2820



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Chain	Atom inclusion	Q-score
c	 0.8450	 0.2790
d	 0.8390	 0.2430
e	 0.8570	 0.2100
f	 0.8270	 0.1690
g	 0.6900	 0.1550
h	 0.4560	 0.0080
i	 0.4510	 -0.0090
j	 0.8150	 0.2350
k	 0.7880	 0.2560
l	 0.8400	 0.2800
m	 0.8000	 0.2460
n	 0.8470	 0.2850
o	 0.8520	 0.2370
p	 0.8040	 0.2350
q	 0.8450	 0.2820
r	 0.8360	 0.2300
s	 0.8330	 0.2720
t	 0.8310	 0.2550
u	 0.8310	 0.2450
v	 0.8440	 0.2440
w	 0.8180	 0.2750
x	 0.8600	 0.2790
y	 0.7950	 0.1930
z	 0.8600	 0.2590