



wwPDB EM Validation Summary Report ⓘ

Aug 12, 2024 – 06:15 pm BST

PDB ID : 8S1U
EMDB ID : EMD-19641
Title : YlmH bound to stalled 50S subunits with RqcH and PtRNA
Authors : Paternoga, H.; Wilson, D.N.
Deposited on : 2024-02-16
Resolution : 3.40 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

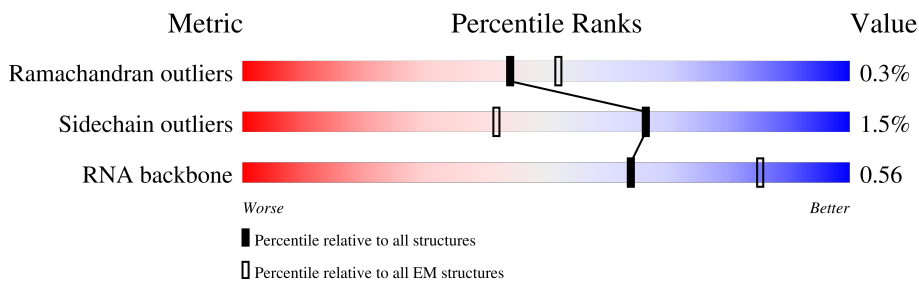
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	a	76	
1	c	76	
2	0	59	
3	1	49	
4	2	44	
5	3	66	
6	4	37	
7	6	66	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	B	112	43% 76% 22%
9	C	277	22% 95%
10	D	209	33% 97%
11	E	207	43% 99%
12	F	179	95% 99%
13	G	179	79% 97%
14	J	145	27% 98%
15	K	122	42% 98%
16	L	146	39% 99%
17	M	144	19% 92% 6%
18	N	120	29% 97%
19	O	120	68% 100%
20	P	115	44% 95%
21	Q	119	19% 97%
22	R	102	36% 100%
23	S	113	33% 94%
24	T	95	47% 96%
25	U	103	61% 97%
26	V	275	81% 89% 9%
27	W	94	16% 84% 15%
28	X	62	53% 95%
29	Y	66	70% 98%
30	Z	59	31% 95%
31	H	570	91% 91% 9%
32	A	2928	14% 80% 15% 5%

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 93269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	c	66	1413	628	254	465	66	0	0
1	a	69	1477	657	268	483	69	0	0

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0	53	418	258	84	69	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1	49	411	250	82	75	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	44	368	222	89	55	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	3	64	512	321	107	82	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	175	1342	835	248	257	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	143	1131	714	207	205	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	122	921	571	173	173	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	146	1082	671	207	202	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	135	1076	690	205	176	5	0	0

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	119	954	583	186	181	4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	120	913	564	176	172	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	113	922	588	177	156	1	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	118	950	597	191	158	4	0	0

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	102	795	506	140	148	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	110	850	530	165	151	4	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	91	733	458	135	137	3	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	102	770	482	143	141	4	0	0

- Molecule 26 is a protein called Putative RNA-binding protein YlmH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	249	1988	1256	350	376	6	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	258	GLY	-	expression tag	UNP P71020
V	259	SER	-	expression tag	UNP P71020
V	260	GLY	-	expression tag	UNP P71020
V	261	SER	-	expression tag	UNP P71020
V	262	GLY	-	expression tag	UNP P71020
V	263	SER	-	expression tag	UNP P71020
V	264	GLY	-	expression tag	UNP P71020
V	265	SER	-	expression tag	UNP P71020
V	266	GLY	-	expression tag	UNP P71020
V	267	SER	-	expression tag	UNP P71020
V	268	ASP	-	expression tag	UNP P71020
V	269	TYR	-	expression tag	UNP P71020
V	270	LYS	-	expression tag	UNP P71020
V	271	ASP	-	expression tag	UNP P71020
V	272	ASP	-	expression tag	UNP P71020
V	273	ASP	-	expression tag	UNP P71020
V	274	ASP	-	expression tag	UNP P71020
V	275	LYS	-	expression tag	UNP P71020

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	W	80	611	378	119	114	0	0

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	61	468	289	98	79	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	65	530	328	102	98	2	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	58	456	281	89	85	1	0	0

- Molecule 31 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	H	518	2567	1530	518	519	0	0

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	A	2789	59910	26733	11076	19313	2788	0	0

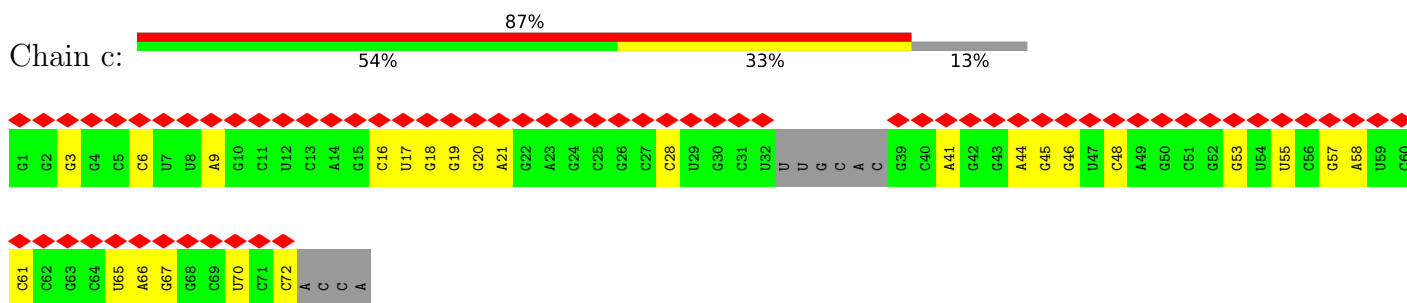
- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
33	A	15	Total	K	0
			15	15	

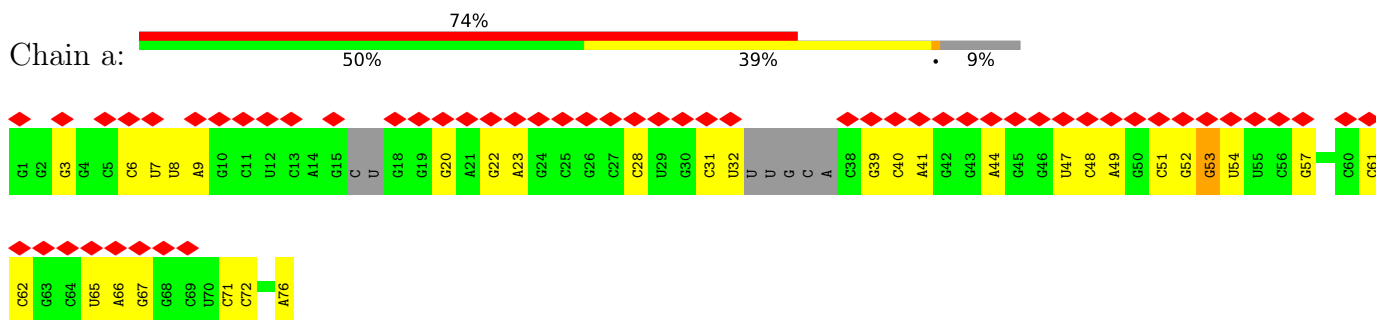
3 Residue-property plots [i](#)

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.

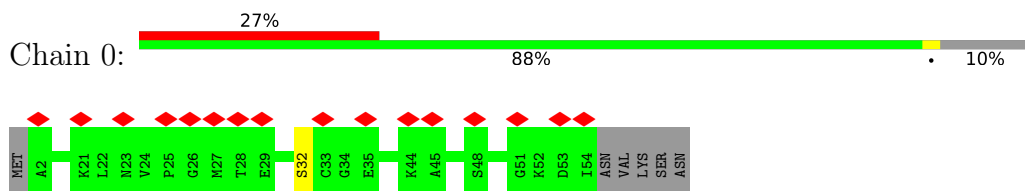
- Molecule 1: P-tRNA



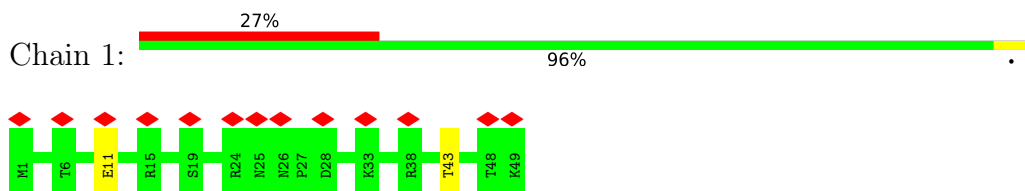
- Molecule 1: P-tRNA



- Molecule 2: 50S ribosomal protein L32



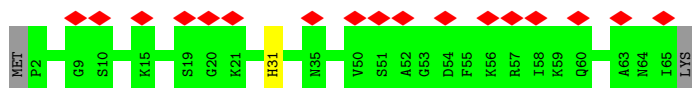
- Molecule 3: 50S ribosomal protein L33 1



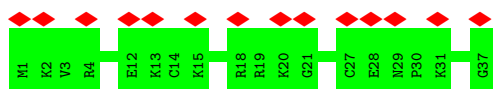
- Molecule 4: 50S ribosomal protein L34



- Molecule 5: 50S ribosomal protein L35



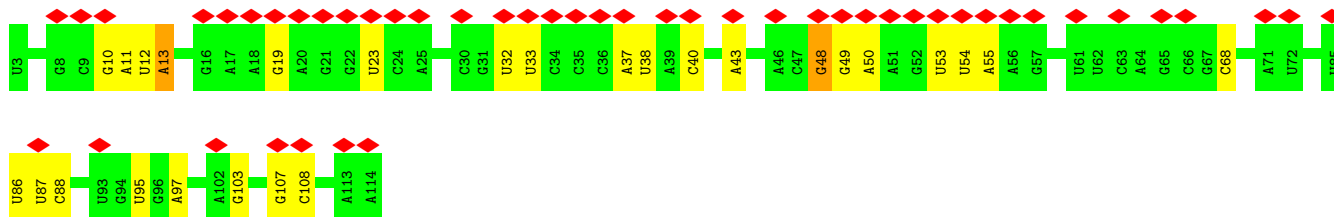
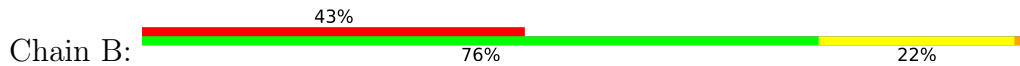
- Molecule 6: 50S ribosomal protein L36



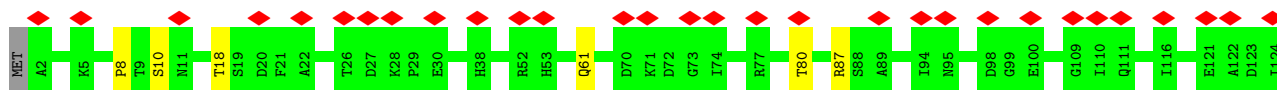
- Molecule 7: 50S ribosomal protein L31

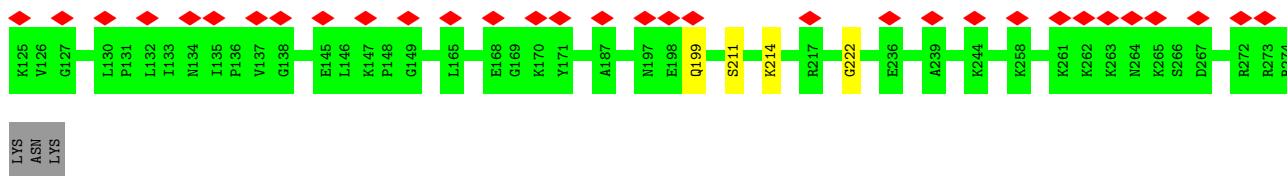


- Molecule 8: 5S rRNA

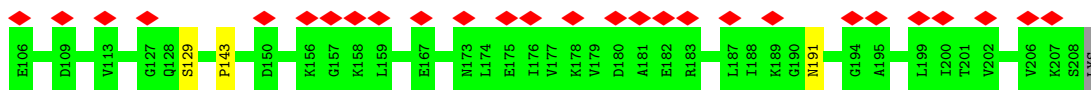
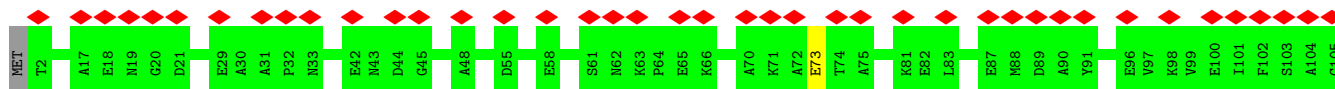


- Molecule 9: 50S ribosomal protein L2

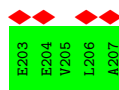
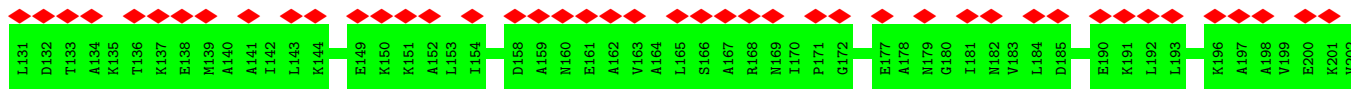
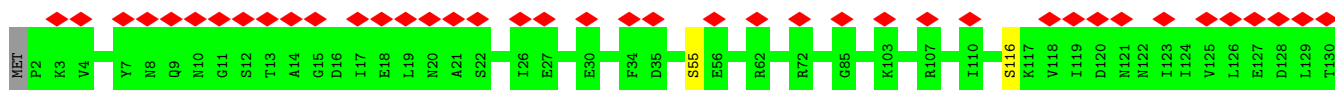
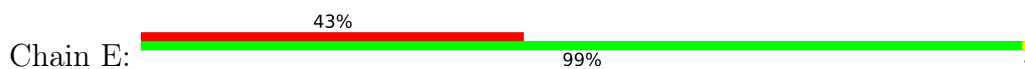




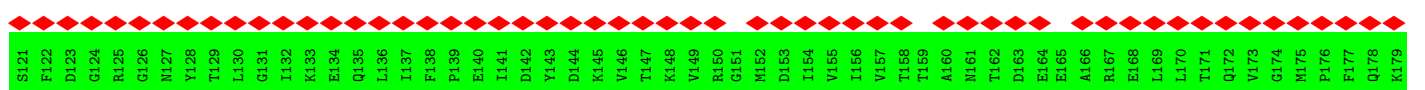
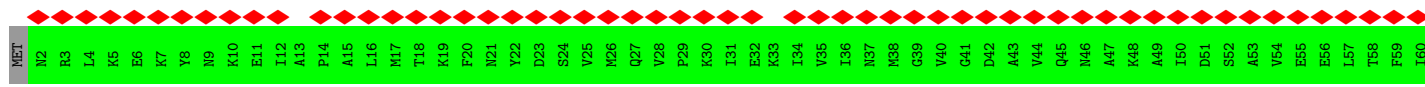
• Molecule 10: 50S ribosomal protein L3



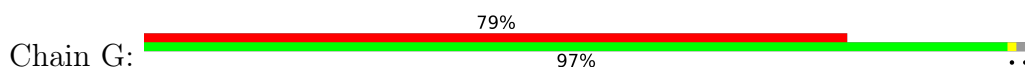
• Molecule 11: 50S ribosomal protein L4

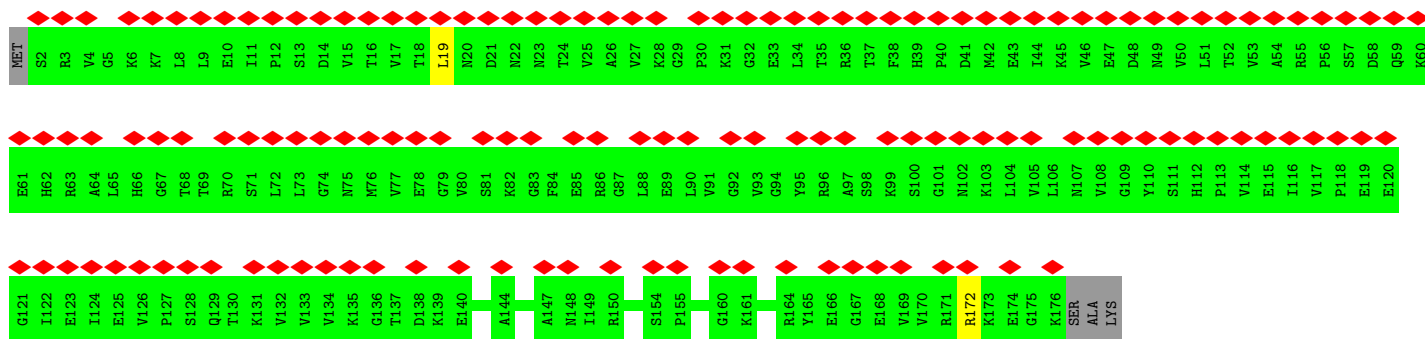


• Molecule 12: 50S ribosomal protein L5

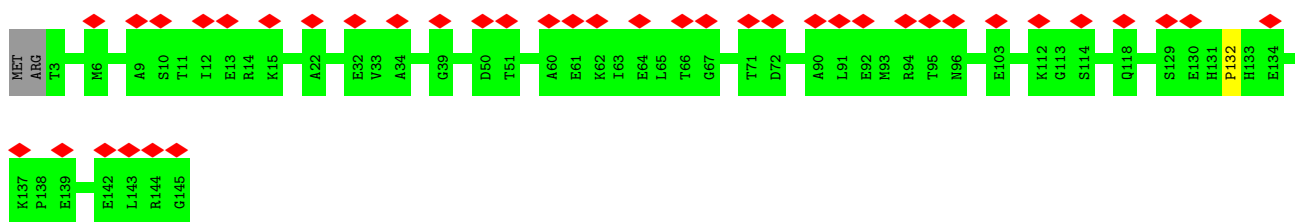


• Molecule 13: Large ribosomal subunit protein uL6

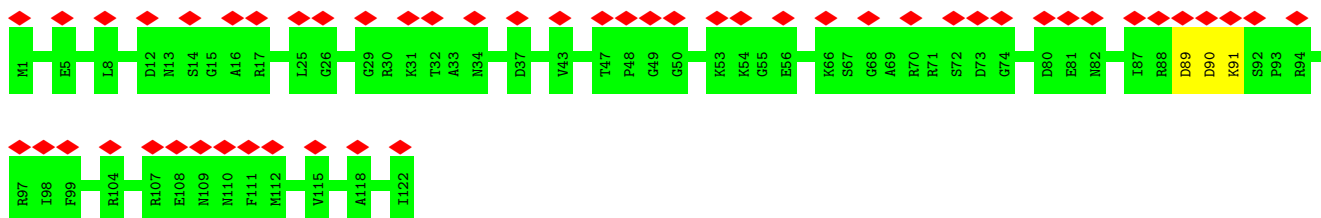
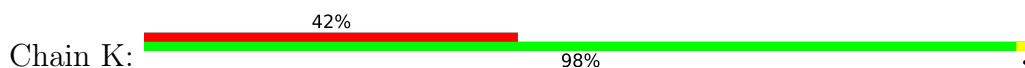




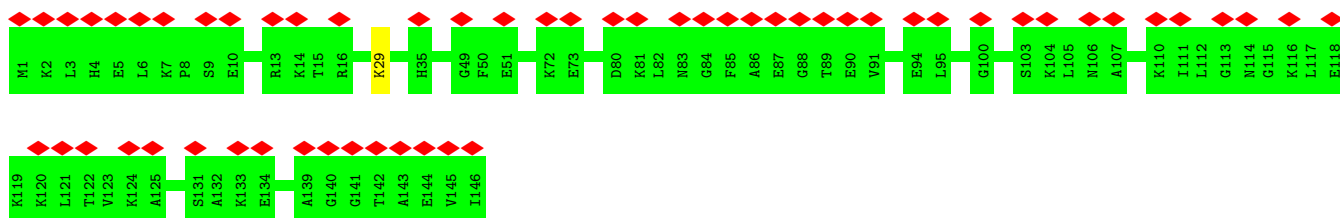
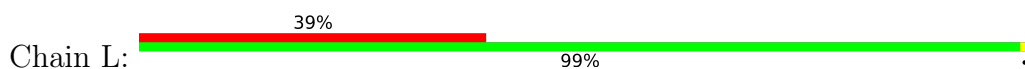
• Molecule 14: 50S ribosomal protein L13



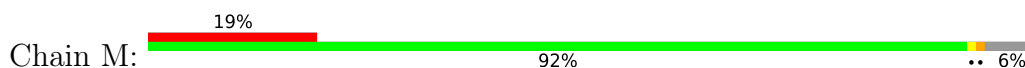
• Molecule 15: 50S ribosomal protein L14

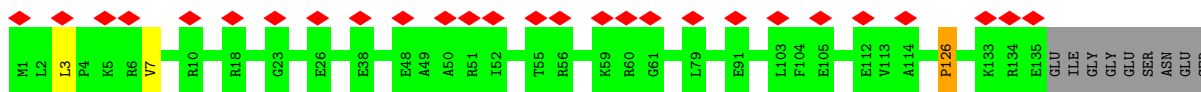


• Molecule 16: 50S ribosomal protein L15



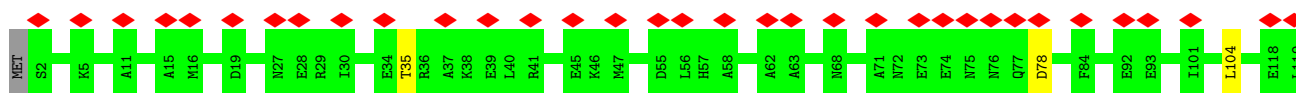
• Molecule 17: 50S ribosomal protein L16





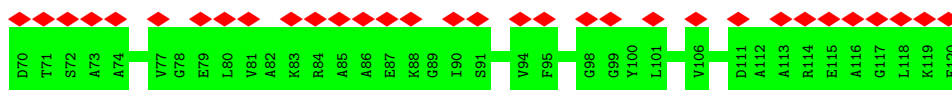
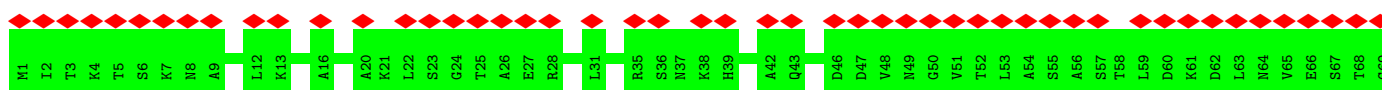
- Molecule 18: 50S ribosomal protein L17

Chain N: 29% 97%



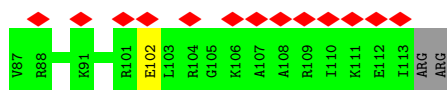
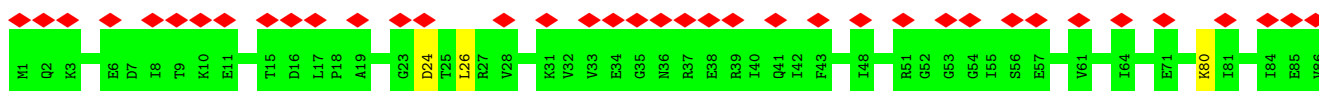
- Molecule 19: 50S ribosomal protein L18

Chain O: 68% 100%



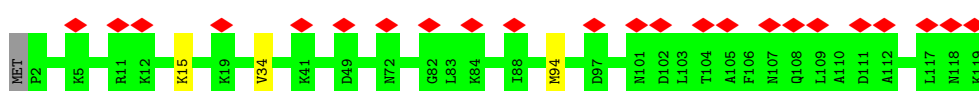
- Molecule 20: 50S ribosomal protein L19

Chain P: 44% 95%



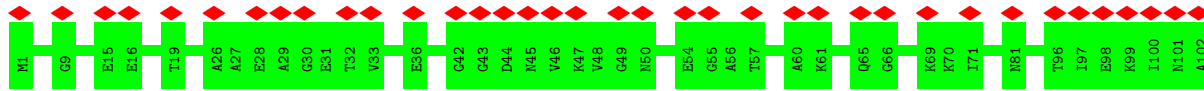
- Molecule 21: Large ribosomal subunit protein bL20

Chain Q: 19% 97%

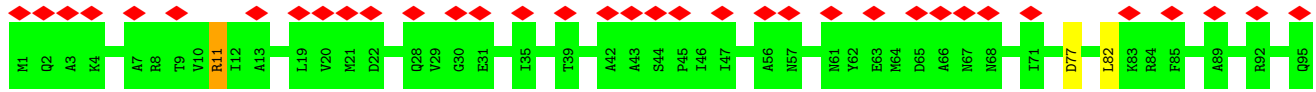
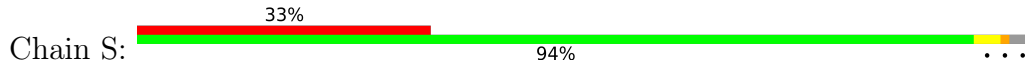


- Molecule 22: 50S ribosomal protein L21

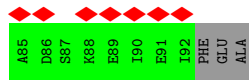
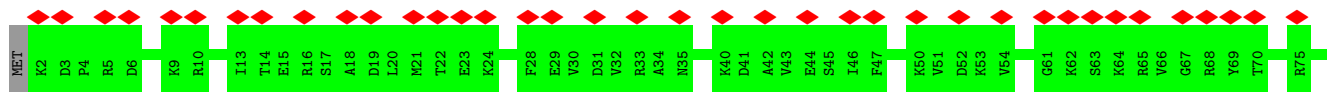
Chain R: 36% 100%



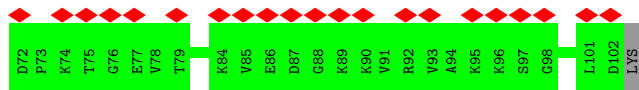
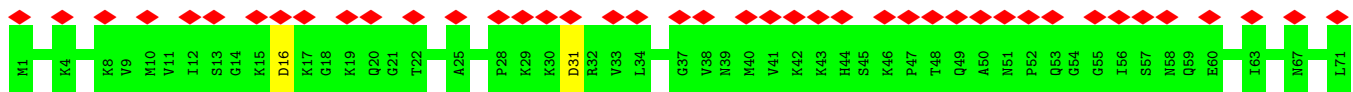
• Molecule 23: 50S ribosomal protein L22



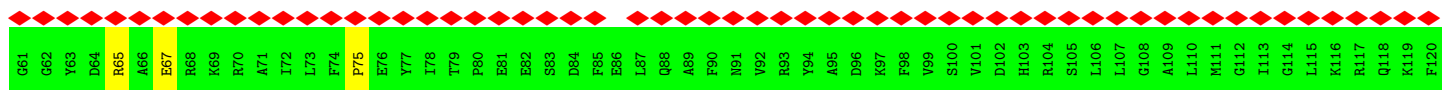
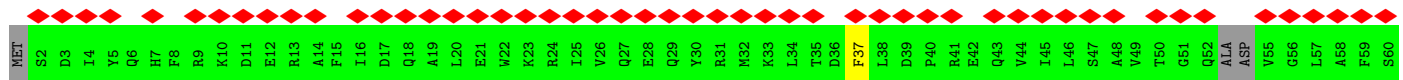
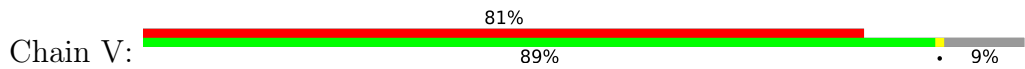
• Molecule 24: Large ribosomal subunit protein uL23

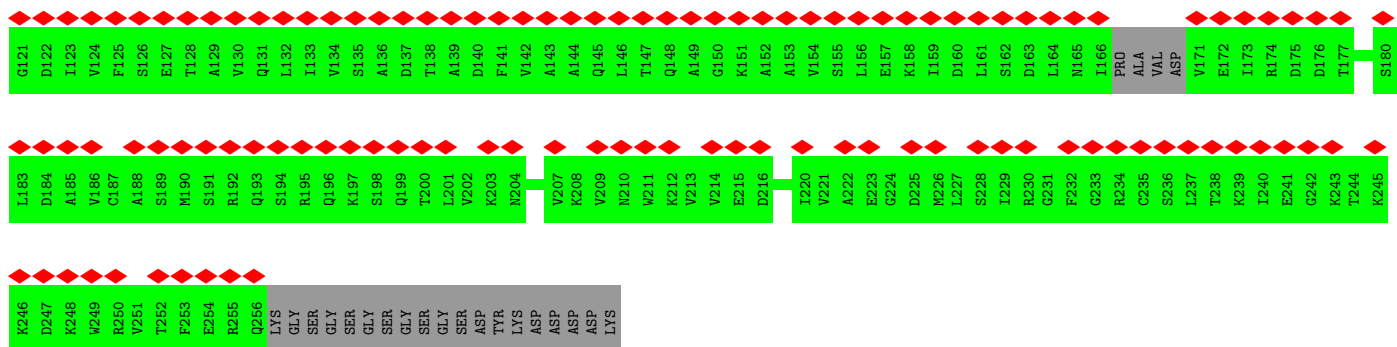


• Molecule 25: 50S ribosomal protein L24

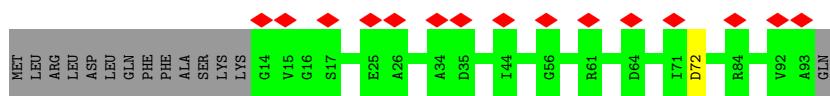
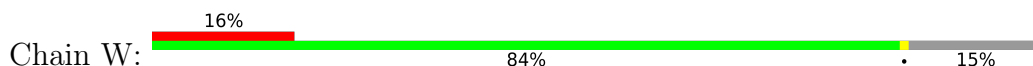


• Molecule 26: Putative RNA-binding protein YlmH

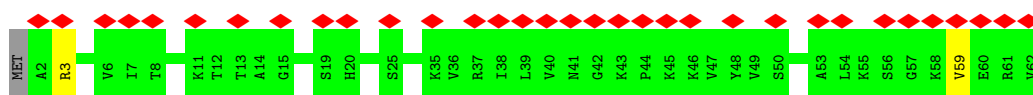




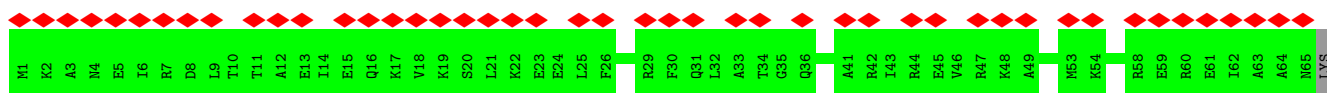
• Molecule 27: Large ribosomal subunit protein bL27



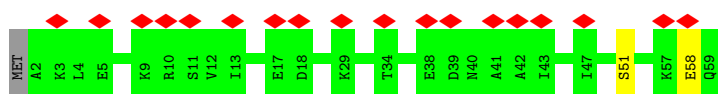
• Molecule 28: 50S ribosomal protein L28



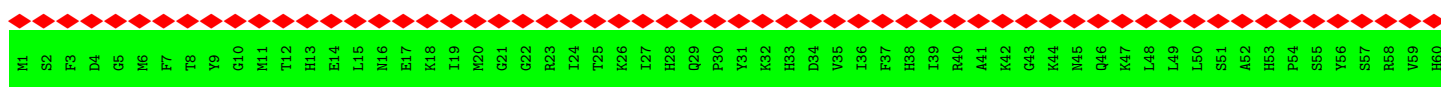
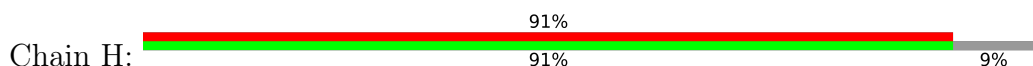
• Molecule 29: 50S ribosomal protein L29



• Molecule 30: Large ribosomal subunit protein uL30

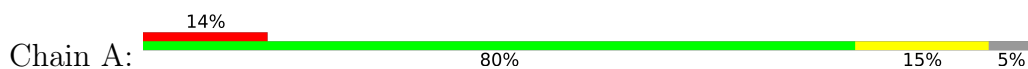


• Molecule 31: Rqc2 homolog RqcH

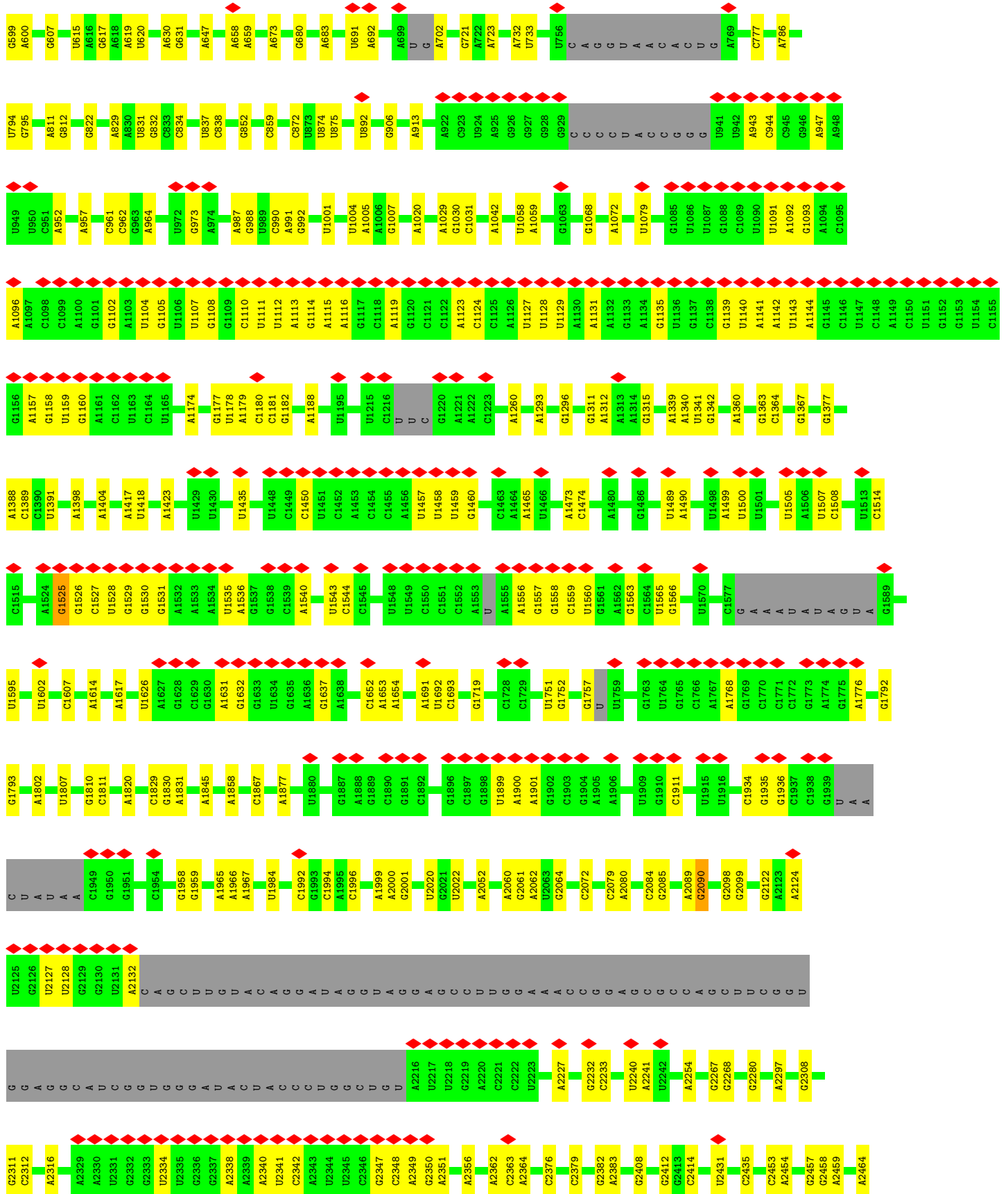


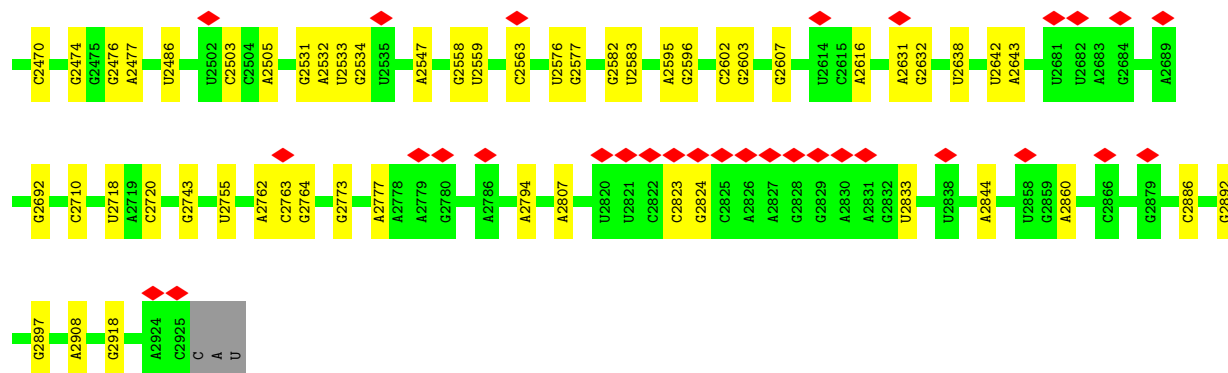
I61	T62	A63	Q64	A65	Y66	E67	N68	P69	S70	E71	P72	P73	M74	F76	C76	M77	L78	L79	R80	K81	H82	I83	E84	G86	F87	I88	E89	K90	I91	E92	Q93	A94	G95	L96	D97	R98	I99	M100	I101	F102	H103	I104	K105	S106	R107	N108	E109	I110	G111	D112	T113	T114	V115	R116	L118	Y119	V120																																																														
E121	I122	M123	G124	R125	H126	S127	N128	I129	I130	L131	T132	D133	A134	A135	E136	N137	V138	I139	I140	D141	G142	L143	K144	H145	L146	S147	P148	S149	M150	N151	S152	Y153	R154	T155	V156	L157	P158	G159	O160	D161	V162	K163	L164	P165	P166	A167	O168	D169	K170	I171	S172	P173	L174	E175	A176	S177	D178	F239																																																													
I181	L182	H184	R185	S186	F187	Q188	E189	G190	R191	L192	D193	K194	Q195	I196	L197	D198	H199	F200	S201	G202	V203	S204	P205	L206	F207	A208	K209	E210	A211	V212	H213	R214	A215	G216	L217	A218	N219	K220	V221	T222	L223	P224	K225	A226	L227	L228	A229	E230	F231	A232	E233	V234	K235	E236	H237	R238	F239																																																														
P241	N242	I243	T244	T245	V246	G248	K249	E250	Y251	F252	L253	L254	L255	E256	L257	T258	H259	L260	K261	G262	E263	A264	R265	R266	F267	D268	S269	L270	S271	E272	L273	L274	D275	R276	F277	Y278	F279	G280	K281	A282	E283	R284	D285	R286	V287	K288	Q289	Q290	A291	Q292	L293	L294	E295	R296	F297	V298	N300																																																														
E301	R302	K303	K304	N305	A306	N307	K308	I309	K310	K311	L312	E313	K314	T315	L316	E317	Y318	S319	E320	A321	K322	K323	E324	F325	Q326	L327	Y328	G329	E330	L331	L332	T333	A334	N335	L336	Y337	M338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	E391	E392	Q393	L394	R395	L396	A397	Q398	E399	E400	I401	E402	Y403	F404	D405	Q406	L407	L408	Q409	Q410	L411	S412	S413	A414	S415	P416	R417	D418	L419	S420
I4E	PRO	LEU	ASN	PRO	ASN	LYS	THR	P369	S370	E371	N372	A373	Q374	A375	Y376	F377	T378	K379	Y380	Q381	K382	A383	K384	N385	S386	V387	A388	V389	E391	E392	Q393	L394	R395	L396	A397	Q398	E399	E400	I401	E402	Y403	F404	D405	Q406	L407	L408	Q409	Q410	L411	S412	S413	A414	S415	P416	R417	D418	L419	S420																																																													
E421	L422	R423	E424	E425	L426	V427	E428	G429	L430	Y431	LEU	ARG	PRO	LYS	G436	G437	G438	L439	L440	L441	H442	PRO	VAL	E451	T452	Y453	E454	S455	T456	S457	G458	L459	T460	L461	L462	V463	G464	K465	M466	N467	R468	Q469	M470	E471	Y472	L473	T474	T475	R476	V477	A478	A479	R480																																																																		
D481	D482	I483	V484	L485	H486	T487	K488	D489	L490	P491	G492	S493	H494	V495	V496	I497	R498	S499	S500	E501	P502	D503	E504	Q505	T506	L507	M508	E509	A510	A511	T512	L513	A514	A515	Y516	F517	S518	K519	A520	K521	D522	S523	S524	S525	V526	V527	V528	D529	Y530	T531	K532	L533	E534	H535	V536	K537	P538	N540																																																													
G541	A542	K543	P544	G545	F546	V547	T548	Y549	D550	S551	Q552	H553	T554	V555	F556	V557	T558	P559	D560	A561	D562	T563	V564	L565	K566	L567	K568	K569	S570																																																																																										

• Molecule 32: 23S rRNA



C	C	U3	U4	A12	A13	A14	G15	U34	G45	C46	G60	A61	C62	G63	A71	U72	A73	U74	G75	U89	A90	A91	Q92	C93	U99	U100	G101	A117	A118	U119	C132	A133	C134	U135	U155	A156	U157	C158	U159	G160	U163	U164	C165	A166	A173	U174	G175			
A176	G177	A183	G184	A199	A202	U203	A207	A216	A219	A224	A225	A231	U232	G233	A236	G248	G251	A258	C267	C276	C277	A278	A279	G280	A281	G282	G283	C284	U285	U286	G287	C288	C289	U290	C291	U292	U293	G294	G295	G296	G300	U301	A302							
C306	A307	C308	U309	C310	U311	G312	U313	A314	C	G316	G317	A318	U321	A324	A325	A326	G327	G328	A329	A330	C331	G332	A333	G346	G347	U348	A355	C359	C360	G361	G368	A373	A374	G385	A389	U393	U394	C395	A578	G396	U397	U398	C399	U400	C401	U402	C403	C404	U405	G406
A407	G408	U409	G410	G411	A412	U413	C414	A418	G419	C430	G433	U450	C451	C452	A458	G459	C467	G471	C487	U498	C503	A504	C505	G528	G540	A543	G550	A551	U554	C555	G558	G568	G576	U577	A578	G579	A584	G595												





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3770	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0235	Depositor
Map size (\AA)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8, 0.8, 0.8	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5MU, G7M, PSU, 2MG, OMG, 2MA, H2U

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	a	0.62	0/1648	1.10	3/2564 (0.1%)
1	c	0.62	0/1577	1.03	1/2456 (0.0%)
2	0	0.43	0/425	0.75	0/563
3	1	0.42	0/416	0.83	0/551
4	2	0.51	0/371	0.84	0/483
5	3	0.44	0/519	0.76	0/680
6	4	0.42	0/300	0.77	0/393
7	6	0.40	0/363	0.56	0/485
8	B	0.57	0/2675	1.04	4/4170 (0.1%)
9	C	0.42	0/2131	0.77	0/2859
10	D	0.42	0/1597	0.76	0/2140
11	E	0.36	0/1586	0.70	0/2139
12	F	0.38	0/1424	0.64	0/1910
13	G	0.39	0/1360	0.66	0/1832
14	J	0.45	0/1154	0.72	0/1552
15	K	0.41	0/928	0.76	0/1245
16	L	0.41	0/1094	0.70	0/1457
17	M	0.41	0/1099	0.78	1/1468 (0.1%)
18	N	0.38	0/961	0.73	0/1284
19	O	0.38	0/922	0.71	0/1236
20	P	0.38	0/935	0.73	0/1251
21	Q	0.41	0/962	0.77	1/1277 (0.1%)
22	R	0.39	0/806	0.71	0/1080
23	S	0.39	0/859	0.75	1/1156 (0.1%)
24	T	0.42	0/739	0.78	0/985
25	U	0.38	0/780	0.68	0/1043
26	V	0.39	0/2016	0.67	0/2709
27	W	0.45	0/619	0.77	0/824
28	X	0.39	0/472	0.71	0/627
29	Y	0.35	0/531	0.71	0/707
30	Z	0.38	0/458	0.77	0/613
31	H	0.34	0/2564	0.50	0/3569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	A	0.61	0/66810	1.00	34/104210 (0.0%)
All	All	0.56	0/101101	0.94	45/151518 (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
9	C	0	1
20	P	0	1
23	S	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
32	A	1177	G	O3'-P-O5'	-6.51	91.62	104.00
32	A	207	A	O3'-P-O5'	-6.28	92.08	104.00
1	a	51	C	C2'-C3'-O3'	6.24	123.69	113.70
32	A	795	G	C1'-O4'-C4'	-6.07	105.04	109.90
32	A	2080	A	O3'-P-O5'	-6.01	92.58	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	80	THR	Peptide
20	P	26	LEU	Peptide
23	S	11	ARG	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	51/59 (86%)	44 (86%)	6 (12%)	1 (2%)	7	30
3	1	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	7	30
4	2	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
5	3	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
6	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
7	6	44/66 (67%)	44 (100%)	0	0	100	100
9	C	271/277 (98%)	254 (94%)	16 (6%)	1 (0%)	34	67
10	D	205/209 (98%)	187 (91%)	17 (8%)	1 (0%)	29	61
11	E	204/207 (99%)	193 (95%)	11 (5%)	0	100	100
12	F	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
13	G	173/179 (97%)	168 (97%)	5 (3%)	0	100	100
14	J	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
15	K	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	51
16	L	144/146 (99%)	133 (92%)	10 (7%)	1 (1%)	22	55
17	M	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
18	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
19	O	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
20	P	111/115 (96%)	104 (94%)	7 (6%)	0	100	100
21	Q	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
22	R	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
23	S	108/113 (96%)	105 (97%)	3 (3%)	0	100	100
24	T	89/95 (94%)	85 (96%)	4 (4%)	0	100	100
25	U	100/103 (97%)	91 (91%)	9 (9%)	0	100	100
26	V	243/275 (88%)	225 (93%)	14 (6%)	4 (2%)	9	34
27	W	78/94 (83%)	73 (94%)	5 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	X	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	21
29	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
30	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	H	512/570 (90%)	502 (98%)	10 (2%)	0	100	100
All	All	3718/3942 (94%)	3513 (94%)	193 (5%)	12 (0%)	44	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	222	GLY
10	D	73	GLU
26	V	37	PHE
26	V	65	ARG
2	0	32	SER

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	
2	0	47/53 (89%)	47 (100%)	0	100	100
3	1	47/47 (100%)	46 (98%)	1 (2%)	53	76
4	2	39/39 (100%)	39 (100%)	0	100	100
5	3	54/56 (96%)	53 (98%)	1 (2%)	57	78
6	4	35/35 (100%)	35 (100%)	0	100	100
7	6	39/55 (71%)	38 (97%)	1 (3%)	46	72
9	C	221/225 (98%)	213 (96%)	8 (4%)	35	63
10	D	168/170 (99%)	165 (98%)	3 (2%)	59	79
11	E	169/170 (99%)	167 (99%)	2 (1%)	71	85
12	F	153/154 (99%)	152 (99%)	1 (1%)	84	92
13	G	148/151 (98%)	146 (99%)	2 (1%)	67	83
14	J	121/123 (98%)	120 (99%)	1 (1%)	81	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	K	101/101 (100%)	99 (98%)	2 (2%)	55	77
16	L	110/110 (100%)	110 (100%)	0	100	100
17	M	109/116 (94%)	106 (97%)	3 (3%)	43	70
18	N	99/100 (99%)	96 (97%)	3 (3%)	41	68
19	O	93/93 (100%)	93 (100%)	0	100	100
20	P	98/100 (98%)	95 (97%)	3 (3%)	40	68
21	Q	97/98 (99%)	95 (98%)	2 (2%)	53	76
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	91/93 (98%)	88 (97%)	3 (3%)	38	66
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	86/87 (99%)	84 (98%)	2 (2%)	50	74
26	V	215/234 (92%)	215 (100%)	0	100	100
27	W	61/74 (82%)	60 (98%)	1 (2%)	62	81
28	X	49/50 (98%)	49 (100%)	0	100	100
29	Y	56/57 (98%)	56 (100%)	0	100	100
30	Z	52/53 (98%)	50 (96%)	2 (4%)	33	61
All	All	2724/2813 (97%)	2683 (98%)	41 (2%)	66	82

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	P	24	ASP
23	S	102	HIS
20	P	80	LYS
21	Q	34	VAL
25	U	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
26	V	7	HIS
28	X	17	ASN
28	X	23	ASN
26	V	204	ASN
15	K	3	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	66/76 (86%)	29 (43%)	0
1	c	64/76 (84%)	24 (37%)	0
32	A	2778/2928 (94%)	372 (13%)	53 (1%)
8	B	111/112 (99%)	24 (21%)	5 (4%)
All	All	3019/3192 (94%)	449 (14%)	58 (1%)

5 of 449 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	c	3	G
1	c	6	C
1	c	9	A
1	c	16	C
1	c	17	U

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	A	1339	A
32	A	2631	A
32	A	1536	A
32	A	2576	U
32	A	2348	C

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

12 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	$\# Z > 2$
32	H2U	A	2478	32	18,21,22	0.66	0	21,30,33	0.74	0
32	G7M	A	2603	32	20,26,27	0.99	1 (5%)	17,39,42	0.44	0
32	5MU	A	1968	32	19,22,23	0.49	0	28,32,35	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PSU	A	1001	32	18,21,22	0.83	1 (5%)	22,30,33	0.72	0
32	PSU	A	2486	32	18,21,22	0.97	1 (5%)	22,30,33	0.67	0
32	2MA	A	2532	33,32	17,25,26	1.06	2 (11%)	17,37,40	0.98	1 (5%)
32	5MU	A	794	32	19,22,23	0.28	0	28,32,35	0.33	0
32	PSU	A	2533	33,32	18,21,22	1.00	1 (5%)	22,30,33	0.75	0
32	OMG	A	2280	33,1,32	18,26,27	1.14	3 (16%)	19,38,41	0.80	0
32	5MU	A	620	33,32	19,22,23	0.36	0	28,32,35	0.66	2 (7%)
32	2MG	A	2474	32	18,26,27	1.17	3 (16%)	16,38,41	0.77	0
32	OMG	A	2582	32	18,26,27	1.04	3 (16%)	19,38,41	0.69	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
32	H2U	A	2478	32	-	0/7/38/39	0/2/2/2
32	G7M	A	2603	32	-	0/3/25/26	0/3/3/3
32	5MU	A	1968	32	-	0/7/25/26	0/2/2/2
32	PSU	A	1001	32	-	0/7/25/26	0/2/2/2
32	PSU	A	2486	32	-	0/7/25/26	0/2/2/2
32	2MA	A	2532	33,32	-	2/3/25/26	0/3/3/3
32	5MU	A	794	32	-	0/7/25/26	0/2/2/2
32	PSU	A	2533	33,32	-	0/7/25/26	0/2/2/2
32	OMG	A	2280	33,1,32	-	0/5/27/28	0/3/3/3
32	5MU	A	620	33,32	-	0/7/25/26	0/2/2/2
32	2MG	A	2474	32	-	0/5/27/28	0/3/3/3
32	OMG	A	2582	32	-	0/5/27/28	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	2533	PSU	C6-C5	3.82	1.39	1.35
32	A	2486	PSU	C6-C5	3.74	1.39	1.35
32	A	2603	G7M	C8-N9	3.13	1.38	1.33
32	A	1001	PSU	C6-C5	3.11	1.38	1.35
32	A	2280	OMG	C5-C6	-3.04	1.41	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	2532	2MA	CM2-C2-N1	2.84	122.54	116.23
32	A	620	5MU	O3'-C3'-C4'	-2.33	104.30	111.05
32	A	620	5MU	O3'-C3'-C2'	2.05	118.44	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	2532	2MA	C4'-C5'-O5'-P
32	A	2532	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

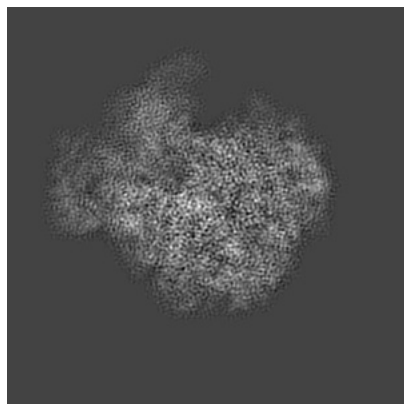
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19641. These allow visual inspection of the internal detail of the map and identification of artifacts.

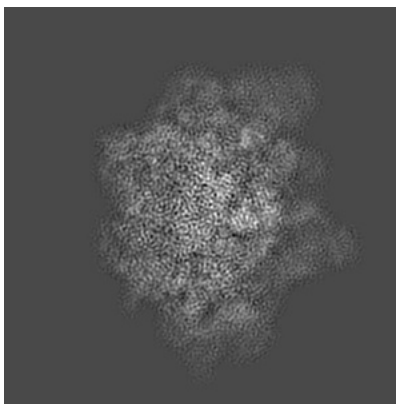
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

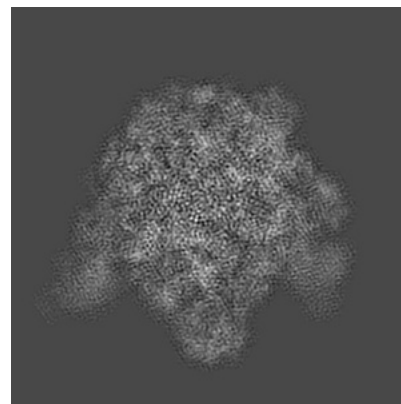
6.1.1 Primary map



X

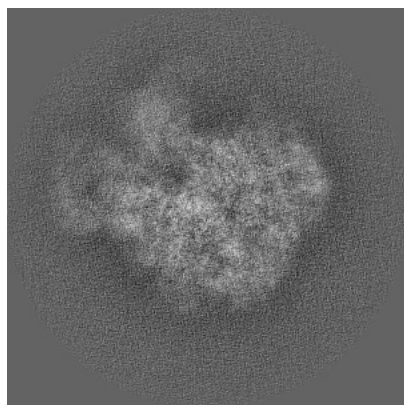


Y

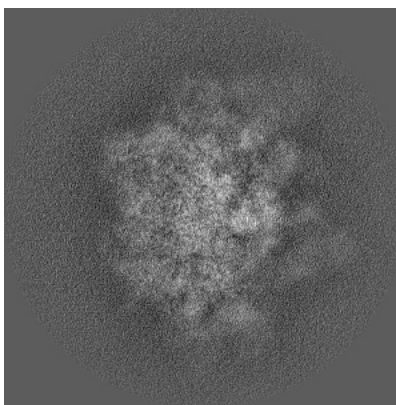


Z

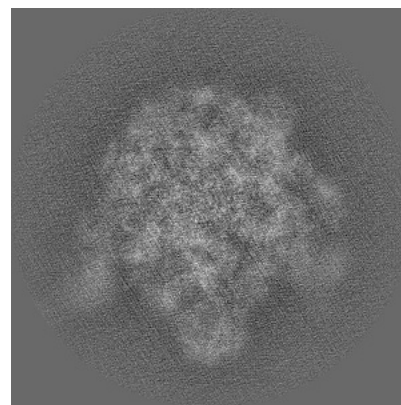
6.1.2 Raw map



X



Y

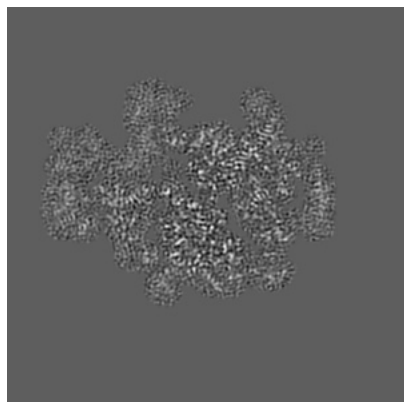


Z

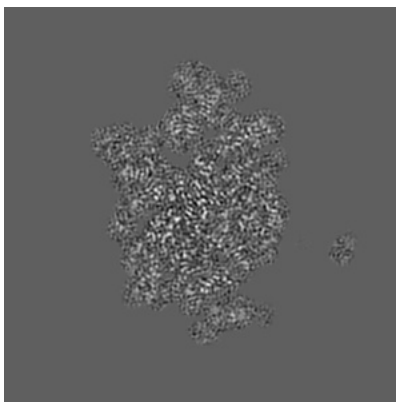
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

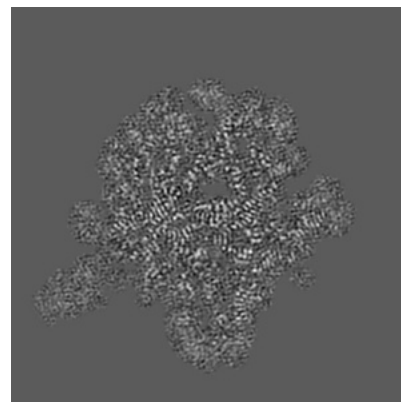
6.2.1 Primary map



X Index: 192

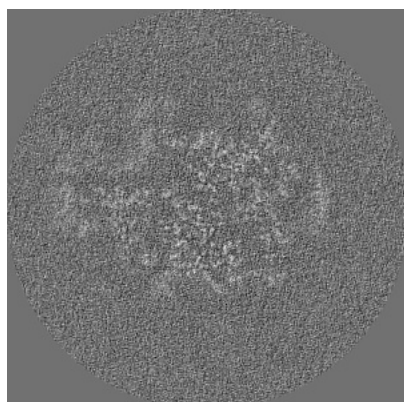


Y Index: 192

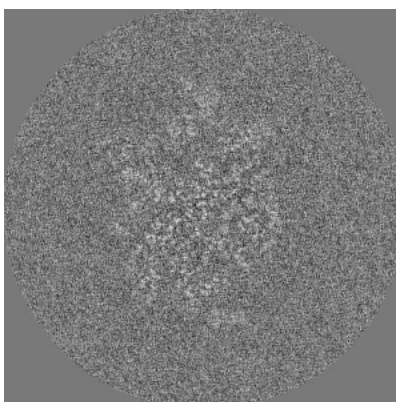


Z Index: 192

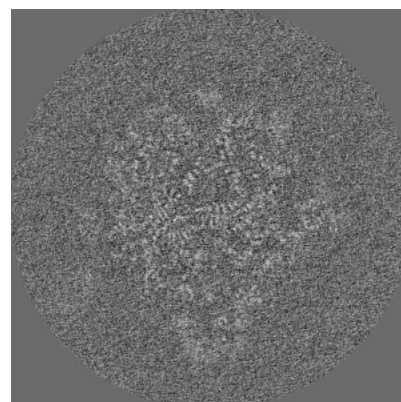
6.2.2 Raw map



X Index: 192



Y Index: 192

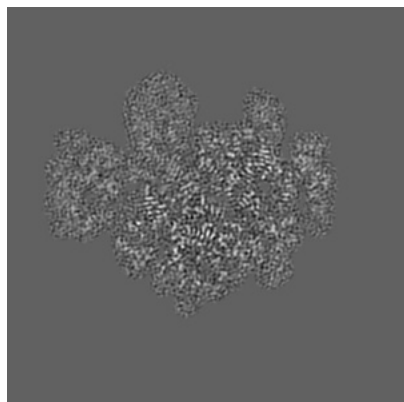


Z Index: 192

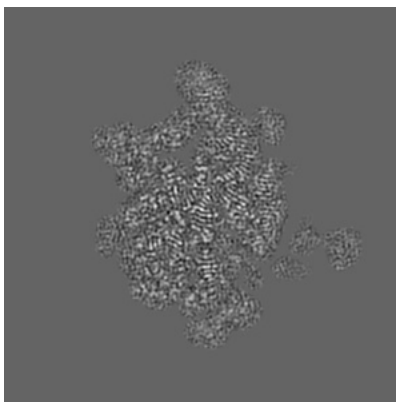
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

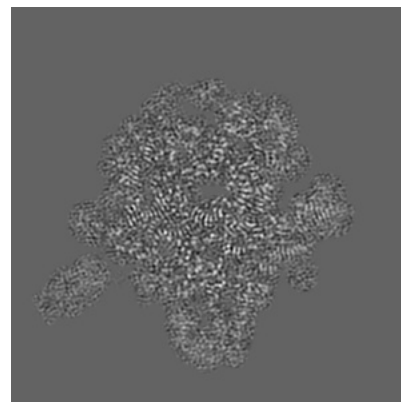
6.3.1 Primary map



X Index: 180

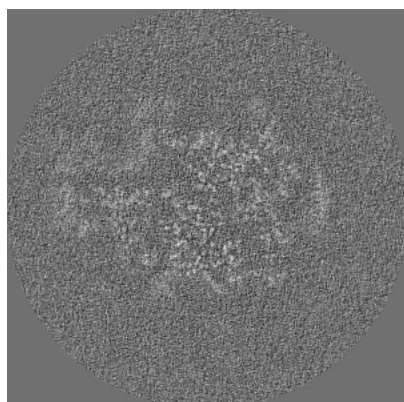


Y Index: 184

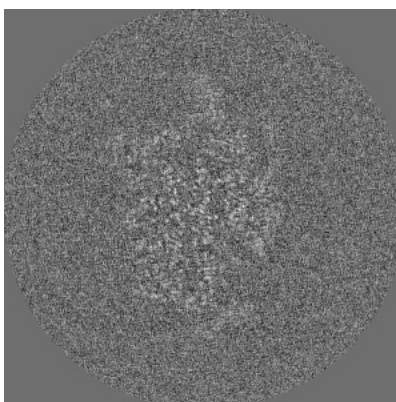


Z Index: 195

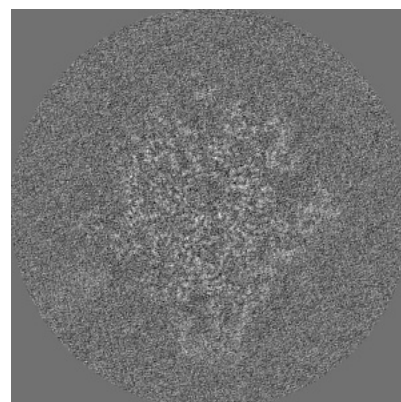
6.3.2 Raw map



X Index: 192



Y Index: 184

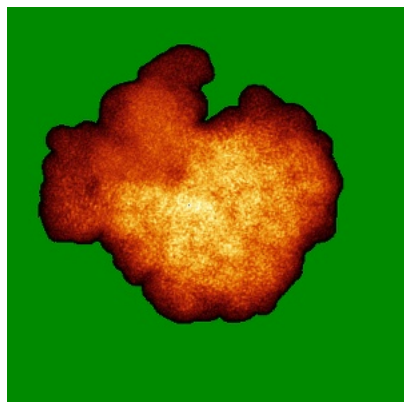


Z Index: 196

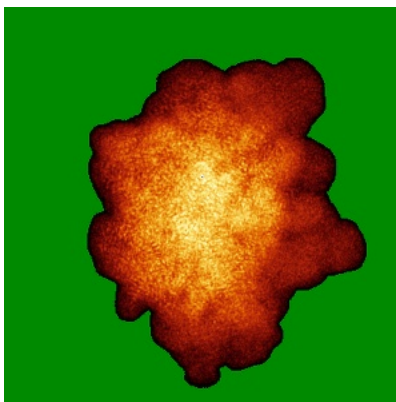
The images above show the largest variance slices of the map in three orthogonal directions.

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

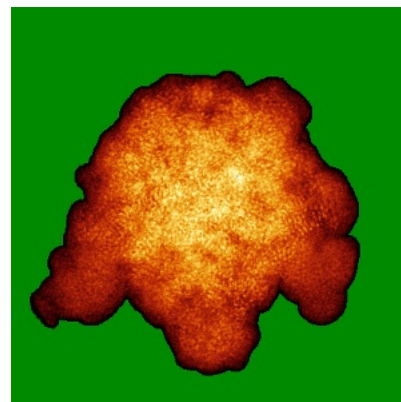
6.4.1 Primary map



X

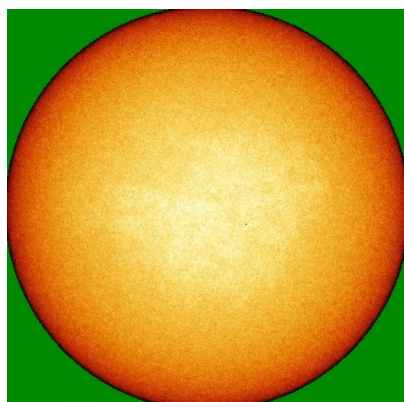


Y

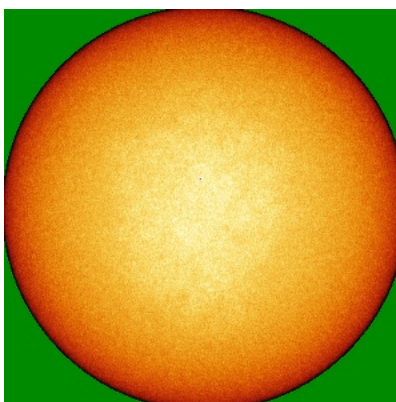


Z

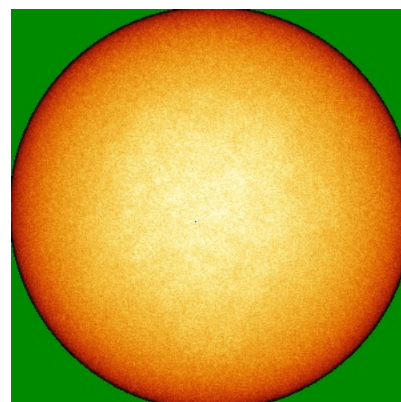
6.4.2 Raw map



X



Y

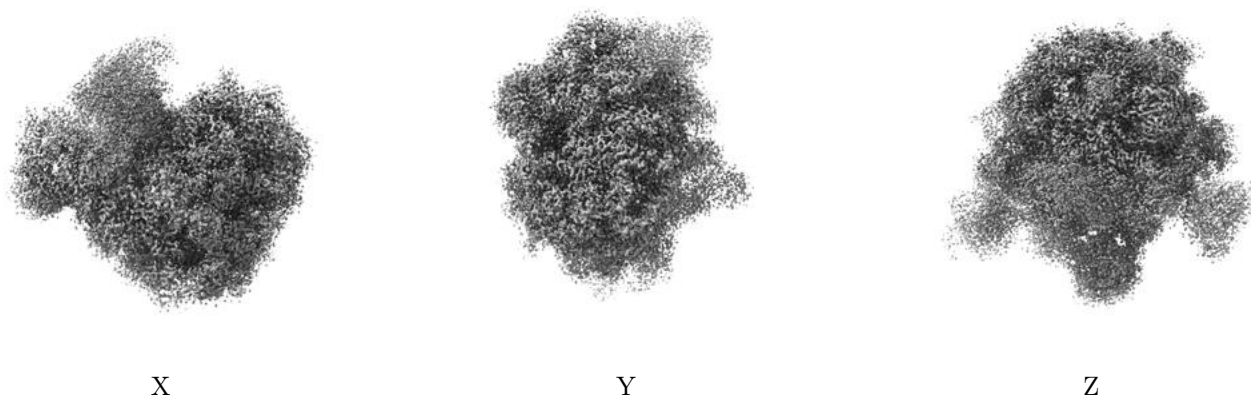


Z

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.

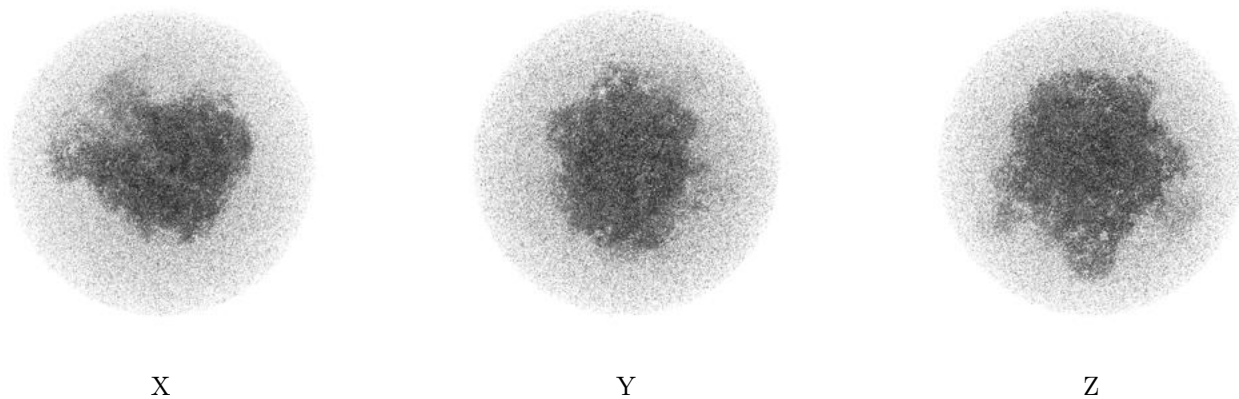
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0235. 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



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.

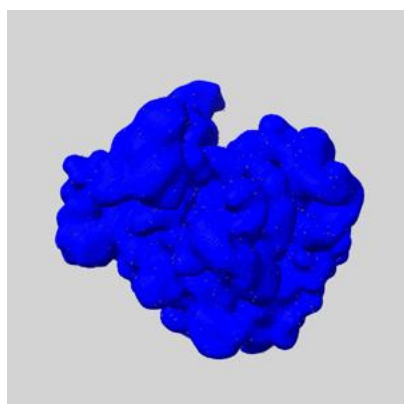
6.6 Mask visualisation [i](#)

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

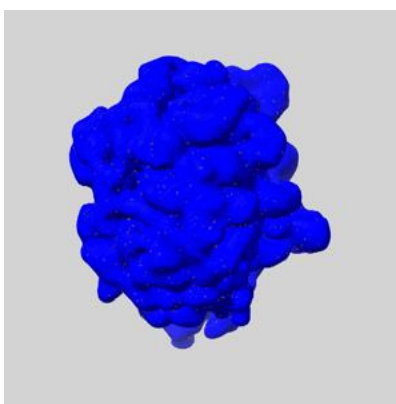
A mask typically either:

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

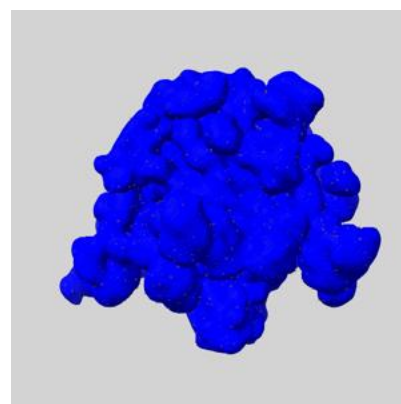
6.6.1 emd_19641_msk_1.map [i](#)



X



Y

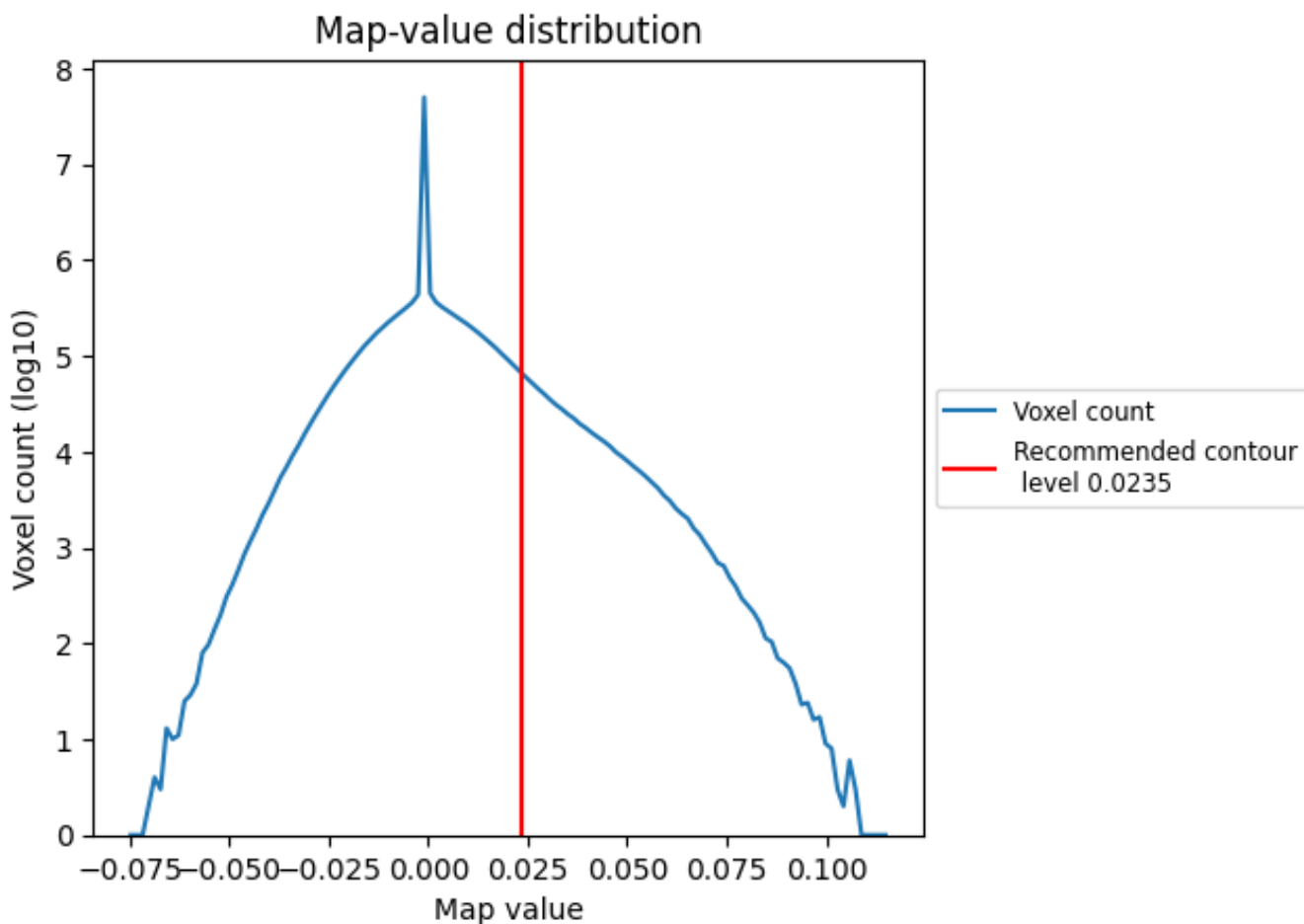


Z

7 Map analysis [i](#)

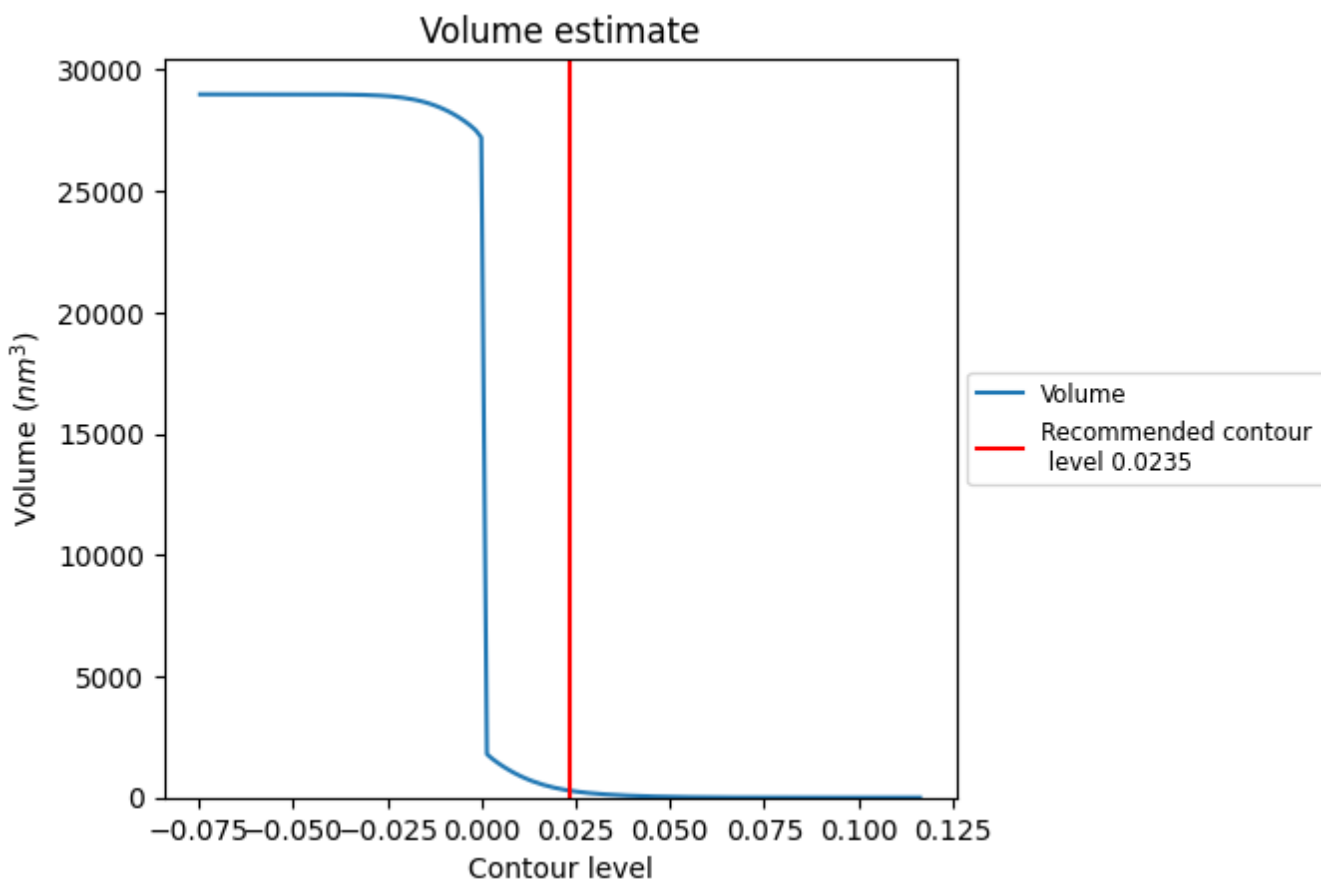
This section contains the results of statistical analysis of the map.

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.

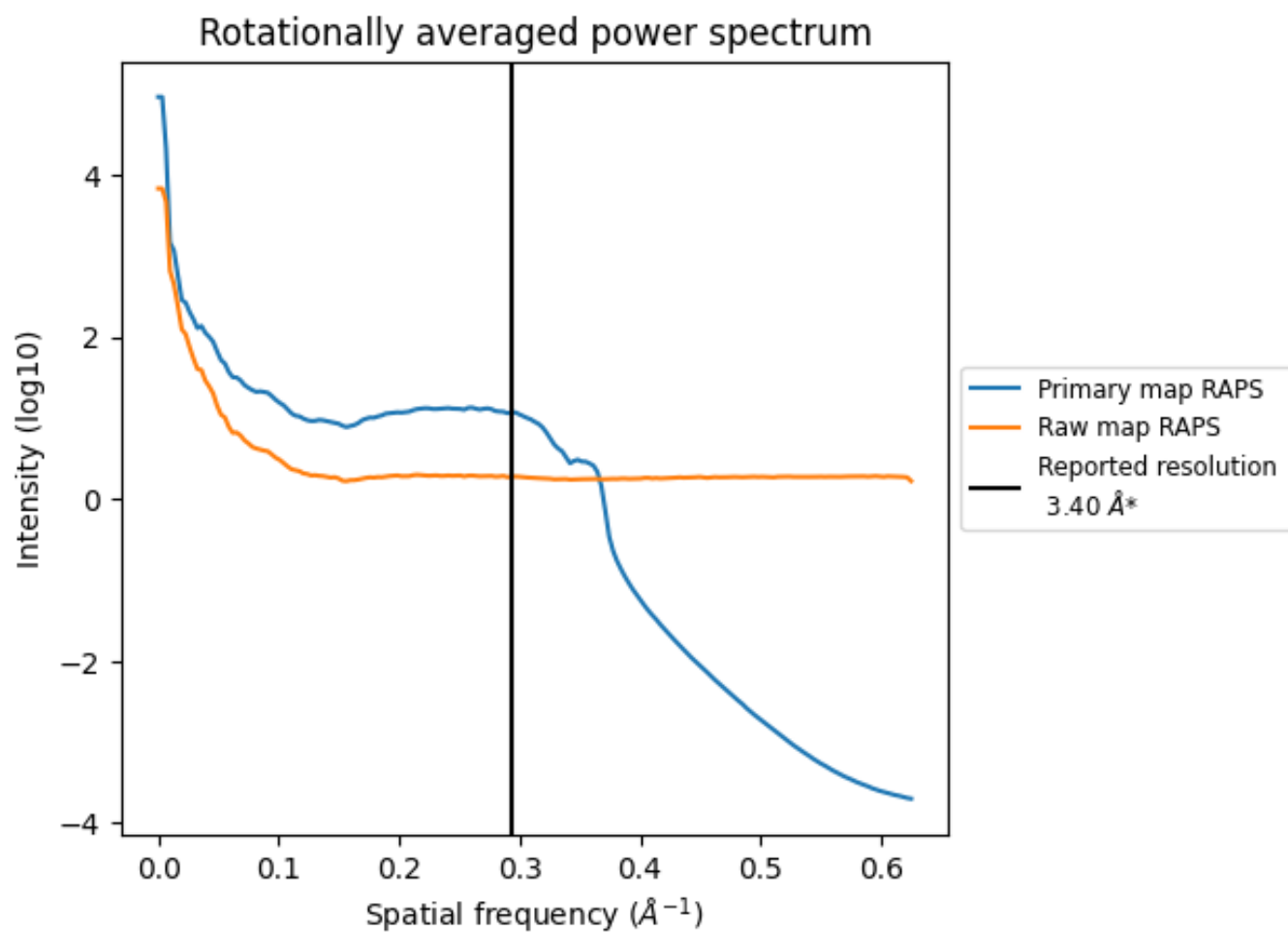
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 257 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 [i](#)

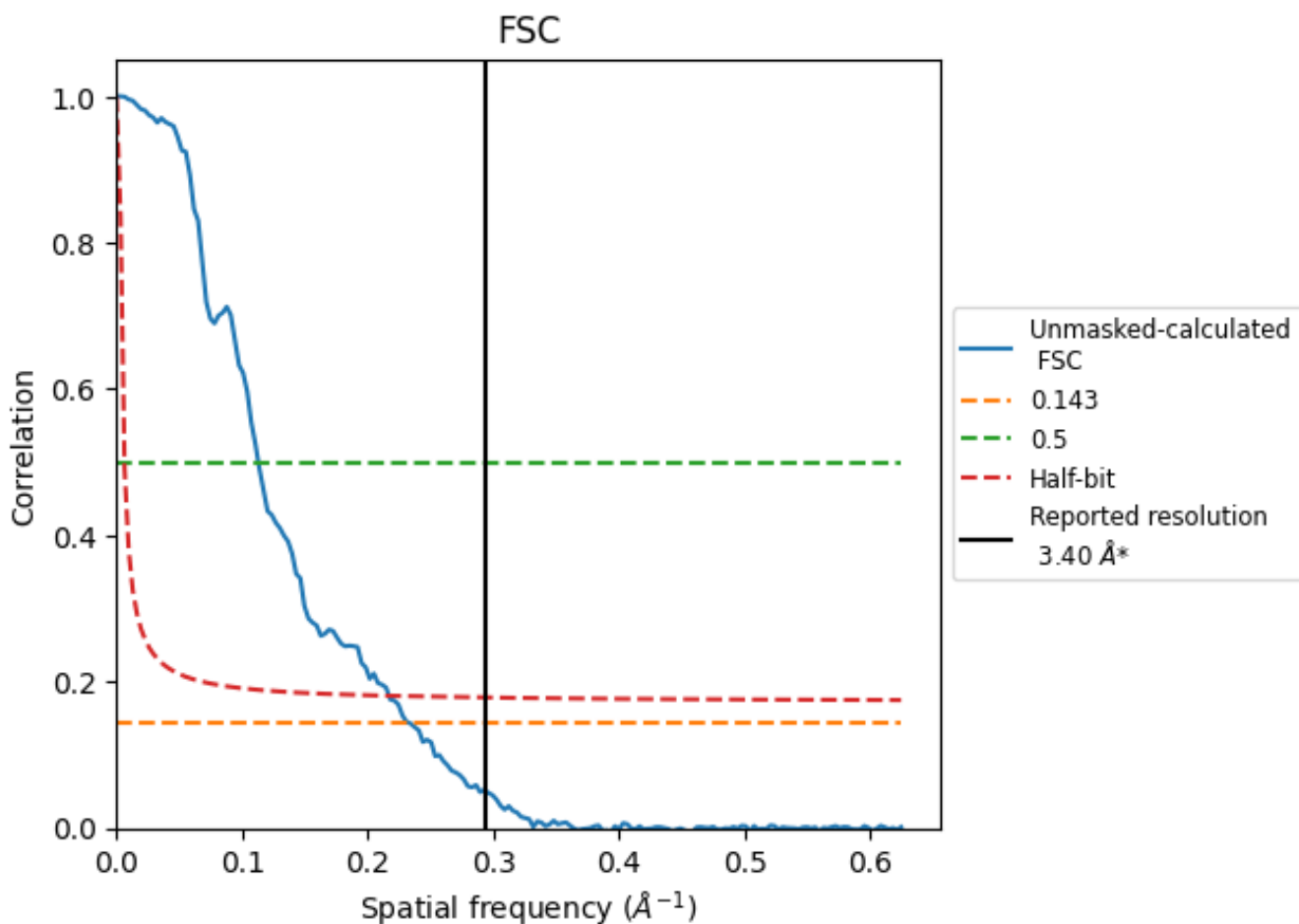


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

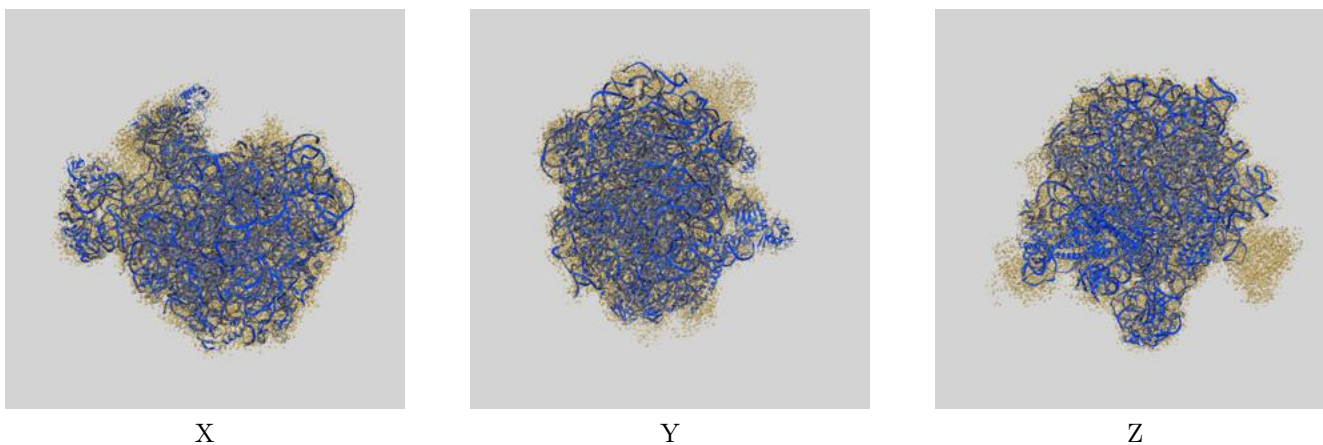
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	8.85	4.61

*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 4.28 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

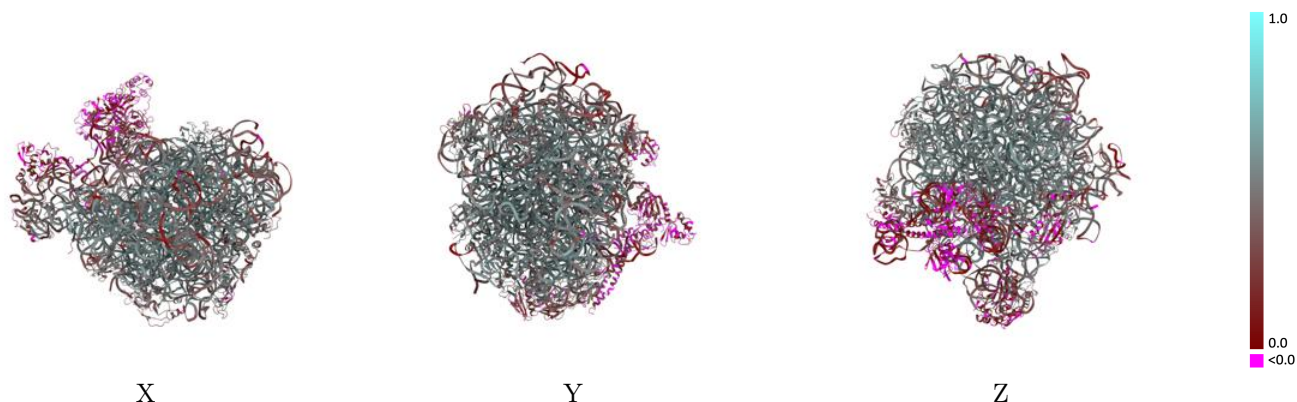
This section contains information regarding the fit between EMDB map EMD-19641 and PDB model 8S1U. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



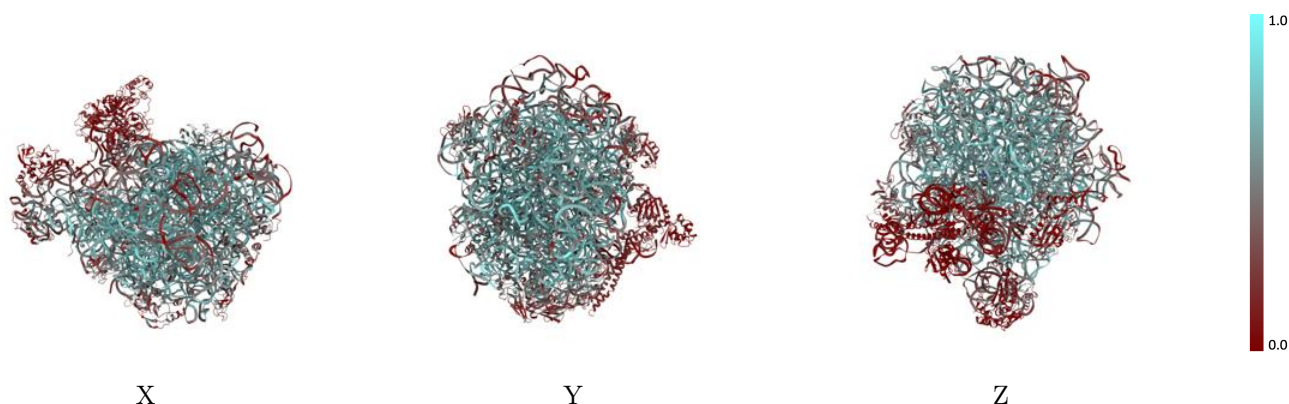
The images above show the 3D surface view of the map at the recommended contour level 0.0235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



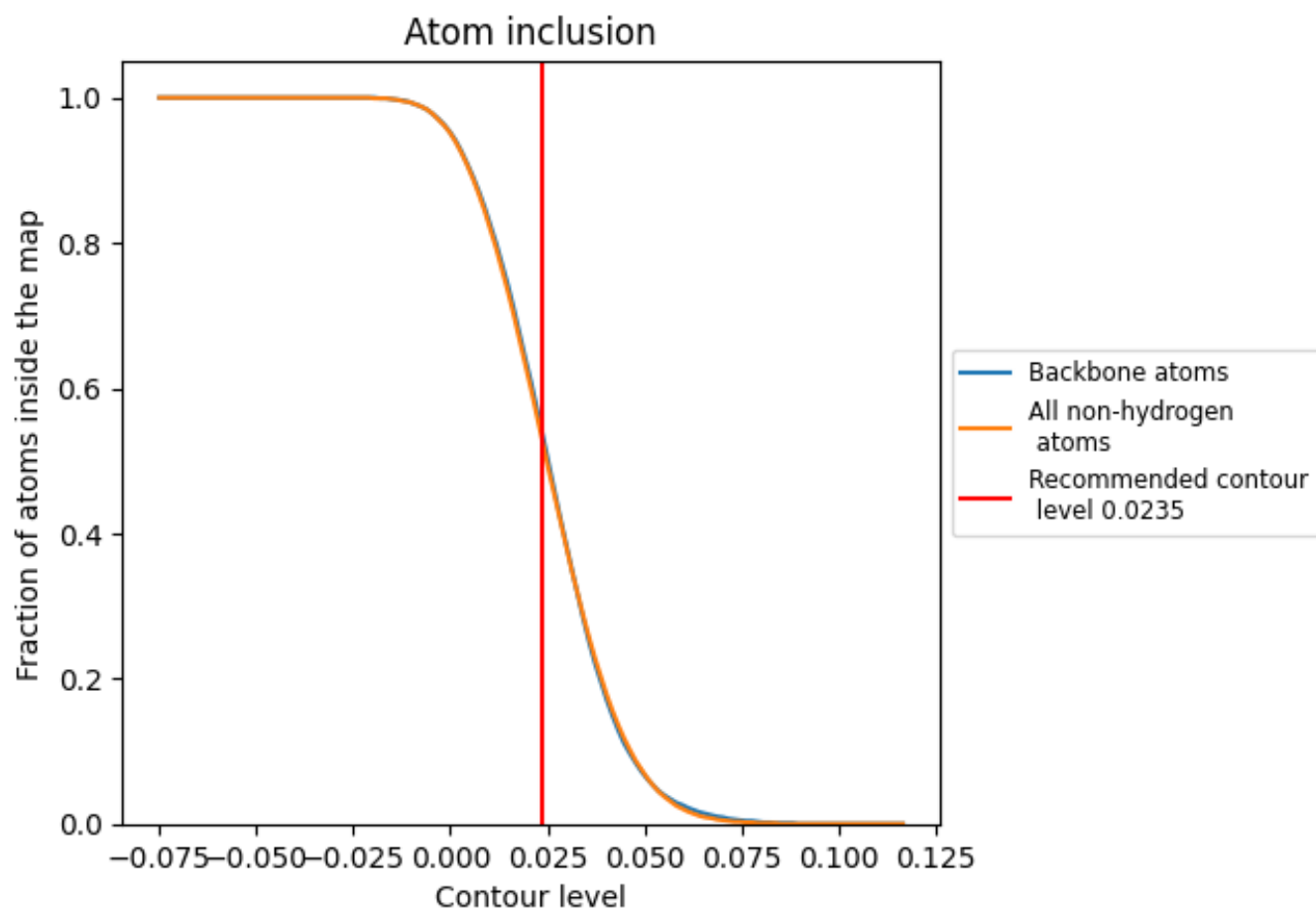
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0235).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5340	 0.4480
0	 0.5360	 0.4960
1	 0.5090	 0.4580
2	 0.6530	 0.5460
3	 0.5610	 0.5390
4	 0.4910	 0.5090
6	 0.0170	 0.0400
A	 0.6240	 0.4940
B	 0.4530	 0.4040
C	 0.5440	 0.5060
D	 0.5200	 0.4970
E	 0.4690	 0.4550
F	 0.1080	 0.1600
G	 0.2240	 0.2630
H	 0.0370	 0.0380
J	 0.5510	 0.4940
K	 0.4540	 0.4820
L	 0.4790	 0.4650
M	 0.5360	 0.4880
N	 0.5230	 0.4850
O	 0.3280	 0.3710
P	 0.4280	 0.4350
Q	 0.5880	 0.5220
R	 0.4650	 0.4590
S	 0.5010	 0.5090
T	 0.4130	 0.4250
U	 0.3360	 0.3740
V	 0.1560	 0.1900
W	 0.5640	 0.4970
X	 0.3920	 0.4570
Y	 0.3190	 0.3850
Z	 0.5090	 0.4560
a	 0.2490	 0.2530
c	 0.0570	 0.1180

