



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 11:10 am GMT

PDB ID : 7PAM
EMDB ID : EMD-13277
Title : 70S ribosome with A*- and P/E-site tRNAs in Mycoplasma pneumoniae cells
Authors : Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on : 2021-07-30
Resolution : 6.80 Å(reported)
Based on initial models : 7OOC, 4V7C, 7OOD

This is a Full wwPDB EM Validation 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:

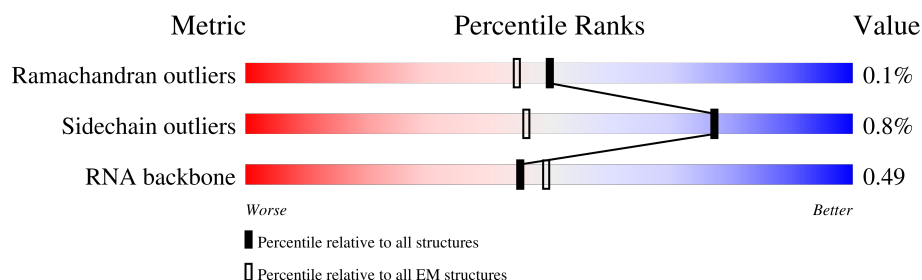
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 6.80 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	48	
2	1	59	
3	2	37	
4	A	294	
5	B	273	
6	C	205	
7	D	219	
8	E	215	

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Mol	Chain	Length	Quality of chain
9	F	155	
10	G	142	
11	H	132	
12	I	108	
13	J	121	
14	K	139	
15	L	124	
16	M	61	
17	N	86	
18	O	94	
19	P	85	
20	Q	104	
21	R	87	
22	S	87	
23	T	60	
24	a	287	
25	b	287	
26	c	212	
27	d	180	
28	e	184	
29	f	149	
30	g	161	
31	h	137	
32	i	146	
33	j	122	

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Mol	Chain	Length	Quality of chain
34	k	151	
35	l	139	
36	m	124	
37	n	116	
38	o	119	
39	p	127	
40	q	100	
41	r	159	
42	s	237	
43	t	111	
44	u	104	
45	v	65	
46	w	111	
47	x	97	
48	y	57	
49	z	53	
50	3	2907	
51	4	108	
52	5	1520	
53	6	76	
53	8	76	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 146120 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	47	Total	C	N	O	S	0	0
			380	236	81	61	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	240	Total	C	N	O	S	0	0
			1921	1226	334	352	9		

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	215	Total	C	N	O	S	0	0
			1698	1073	313	307	5		

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	203	Total	C	N	O	S	0	0
			1660	1051	314	290	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	118	Total	C	N	O		0	0
			951	594	191	166			

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	83	Total	C	N	O		0	0
			673	428	125	120			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	83	Total	C	N	O		0	0
			675	425	135	115			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	65	Total	C	N	O	S	0	0
			535	342	103	86	4		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	84	Total	C	N	O	S	0	0
			682	435	127	118	2		

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	77	Total	C	N	O	S	0	0
			629	383	135	111			

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	53	Total	C	N	O	S	0	0
			471	295	103	72	1		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	176	Total	C	N	O		
			1396	899	247	250	0	0

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	145	Total	C	N	O	S	
			1160	746	204	207	3	0

- Molecule 30 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	126	Total	C	N	O	S	
			960	612	167	178	3	0

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	h	128	Total	C	N	O	S	
			959	616	160	177	6	0

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	i	144	Total	C	N	O	S	
			1164	737	213	209	5	0

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	122	Total	C	N	O	S	
			944	595	178	167	4	0

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	k	148	Total	C	N	O		
			1153	731	226	196	0	0

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	112	Total	C	N	O	S	0	0
			889	557	175	155	2		

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	115	Total	C	N	O	S	0	0
			938	592	180	165	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	114	Total	C	N	O	S	0	0
			947	603	188	154	2		

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	92	Total	C	N	O	S	0	0
			720	475	122	122	1		

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	111	Total	C	N	O	S	0	0
			872	550	166	153	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	86	Total	C	N	O	S	0	0
			657	409	130	117	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	63	Total	C	N	O	S	0	0
			513	317	108	87	1		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	w	100	Total	C	N	O	0	0
			818	517	153	148		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 49 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 50 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

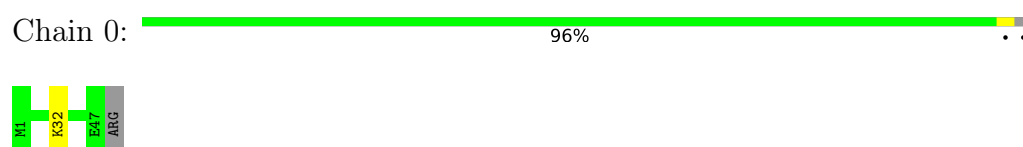
- Molecule 53 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		
53	8	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		

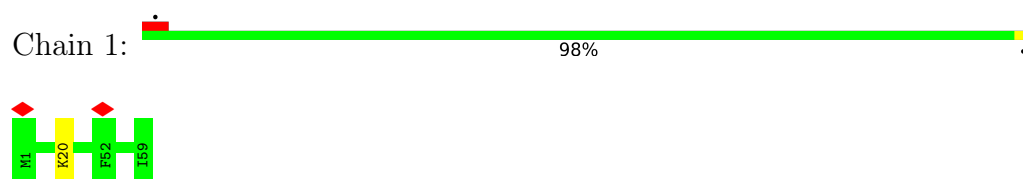
3 Residue-property plots [i](#)

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.

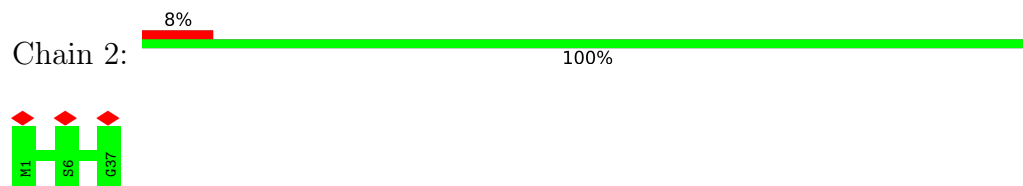
- Molecule 1: 50S ribosomal protein L34



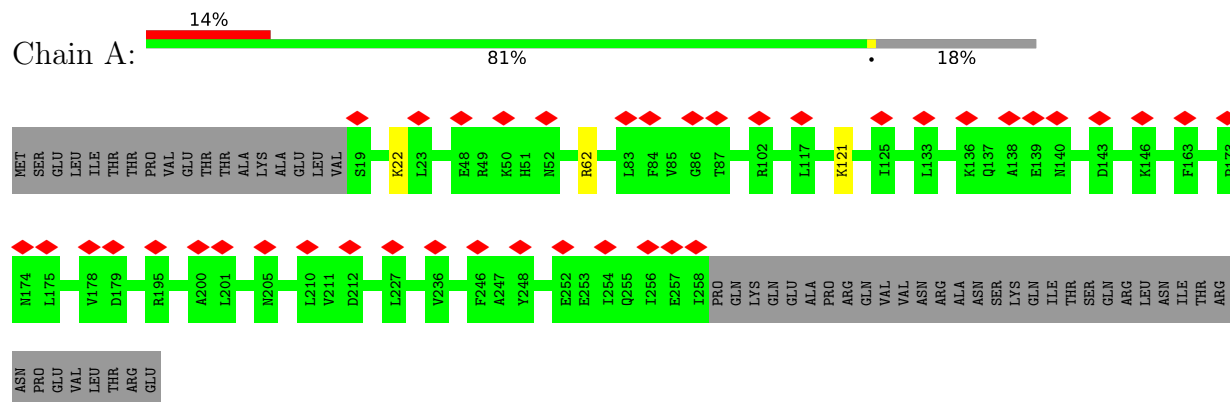
- Molecule 2: 50S ribosomal protein L35



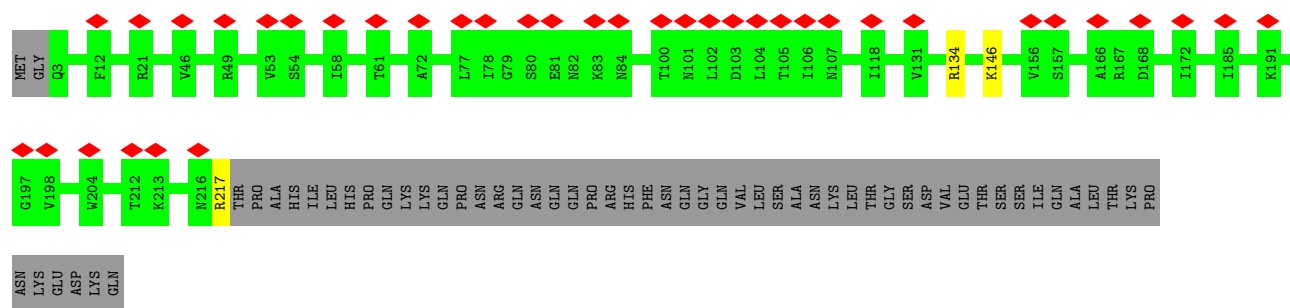
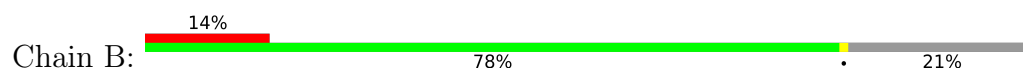
- Molecule 3: 50S ribosomal protein L36



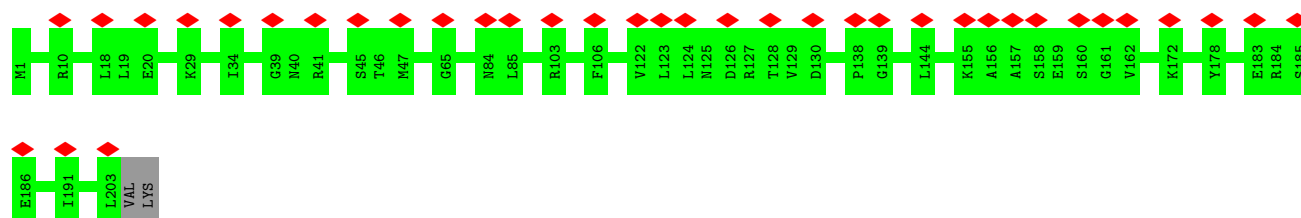
- Molecule 4: 30S ribosomal protein S2



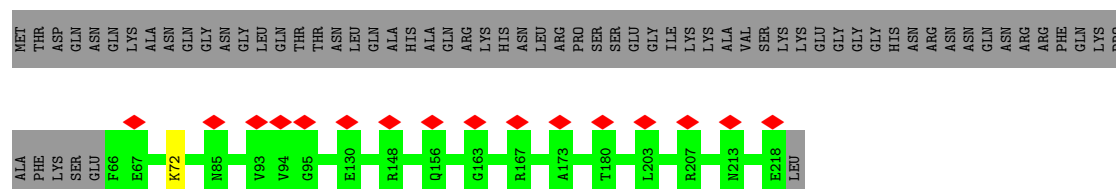
- Molecule 5: 30S ribosomal protein S3



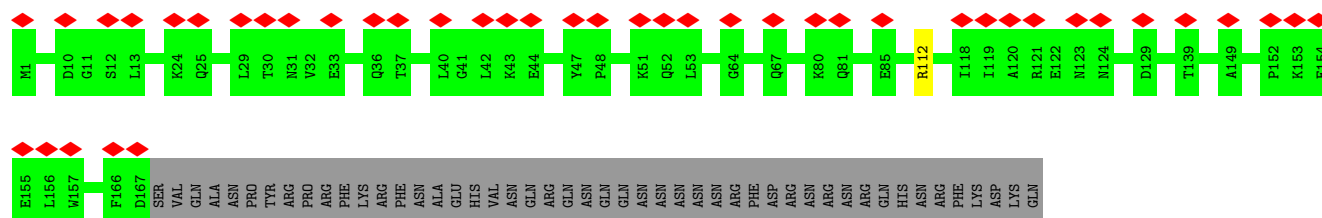
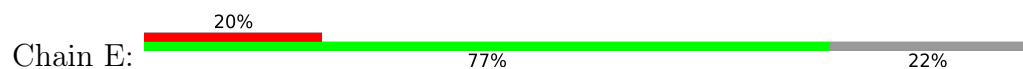
- Molecule 6: 30S ribosomal protein S4



- Molecule 7: 30S ribosomal protein S5

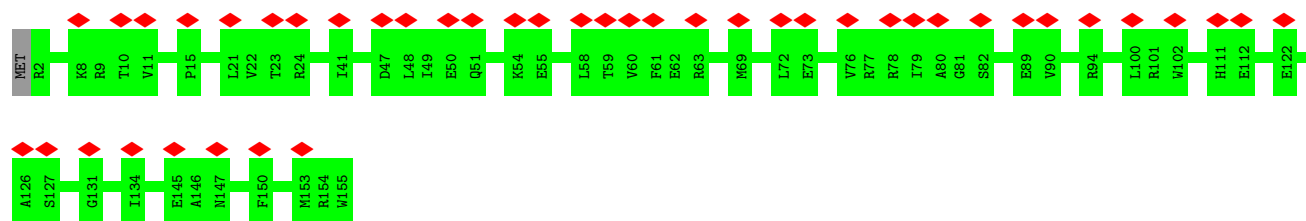


- Molecule 8: 30S ribosomal protein S6

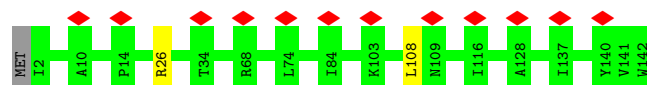


- Molecule 9: 30S ribosomal protein S7

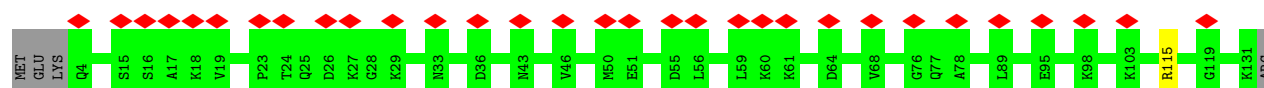




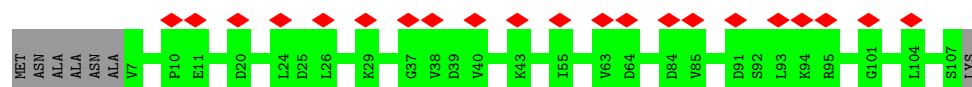
- Molecule 10: 30S ribosomal protein S8



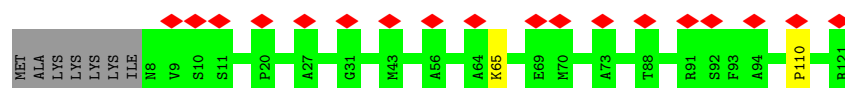
- Molecule 11: 30S ribosomal protein S9



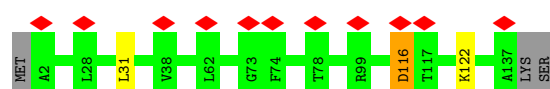
- Molecule 12: 30S ribosomal protein S10



- Molecule 13: 30S ribosomal protein S11

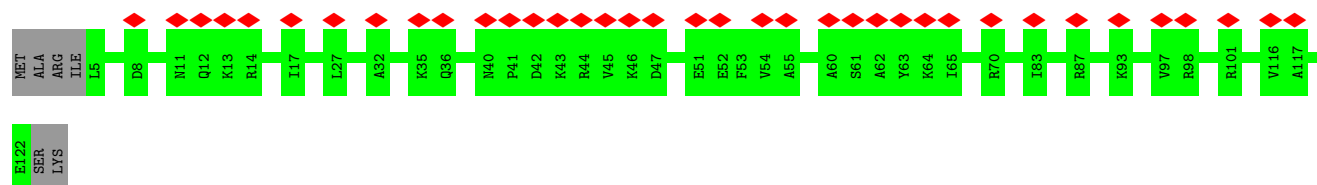


- Molecule 14: 30S ribosomal protein S12

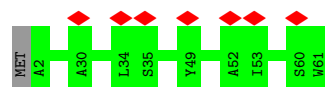


- Molecule 15: 30S ribosomal protein S13

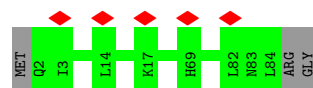




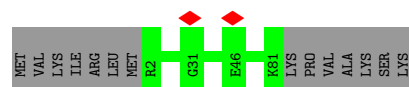
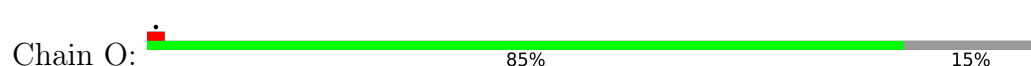
- Molecule 16: 30S ribosomal protein S14 type Z



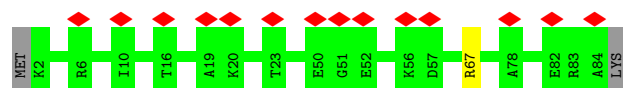
- Molecule 17: 30S ribosomal protein S15



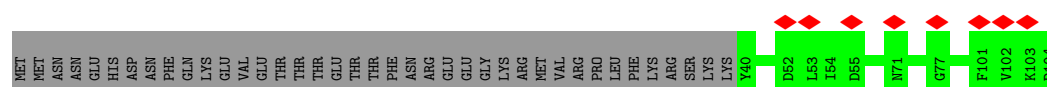
- Molecule 18: 30S ribosomal protein S16



- Molecule 19: 30S ribosomal protein S17

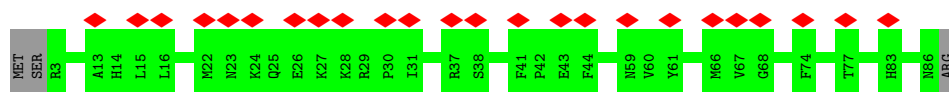


- Molecule 20: 30S ribosomal protein S18

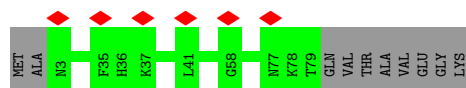
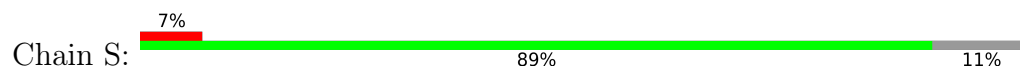


- Molecule 21: 30S ribosomal protein S19

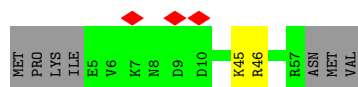
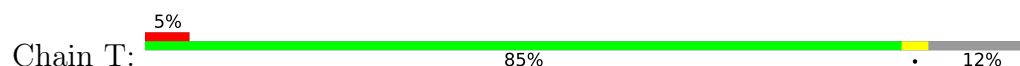




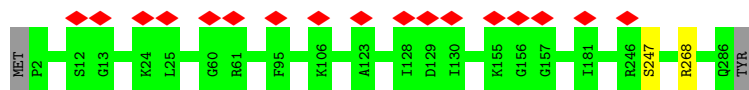
- Molecule 22: 30S ribosomal protein S20



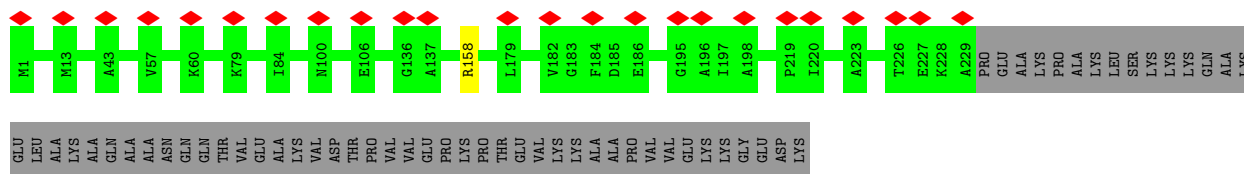
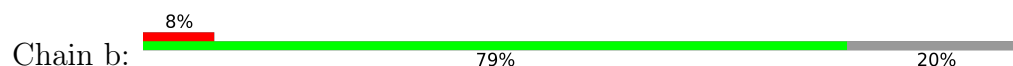
- Molecule 23: 30S ribosomal protein S21



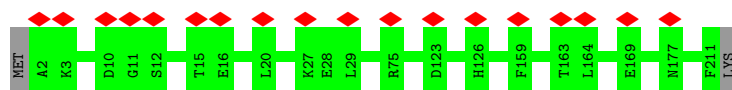
- Molecule 24: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L3

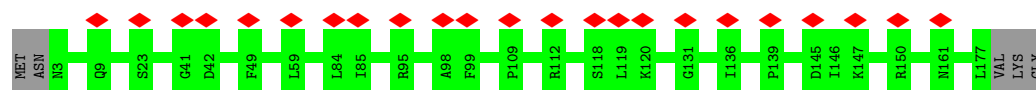


- Molecule 26: 50S ribosomal protein L4

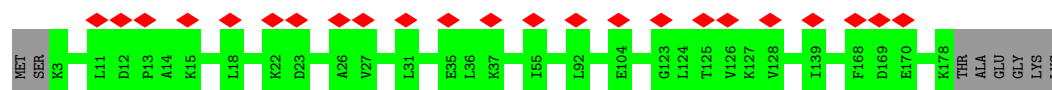


- Molecule 27: 50S ribosomal protein L5

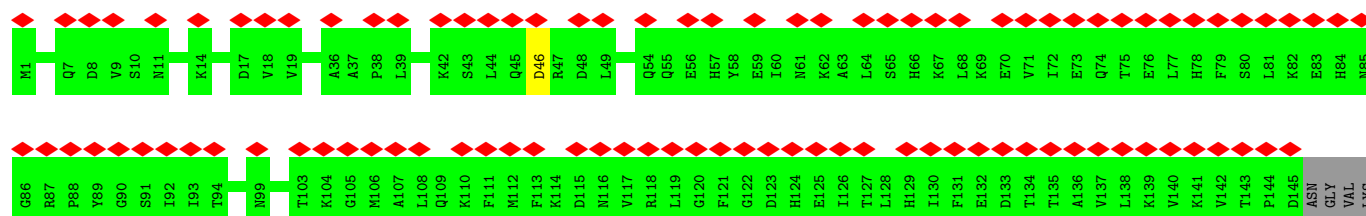




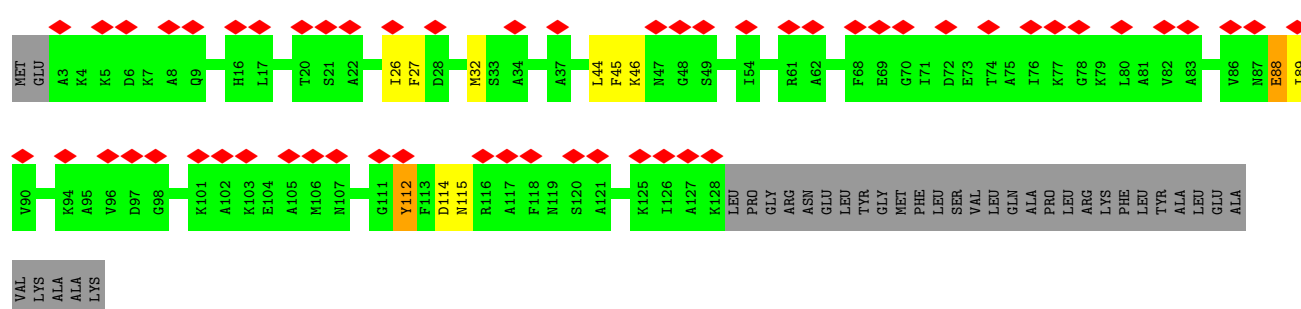
- Molecule 28: 50S ribosomal protein L6



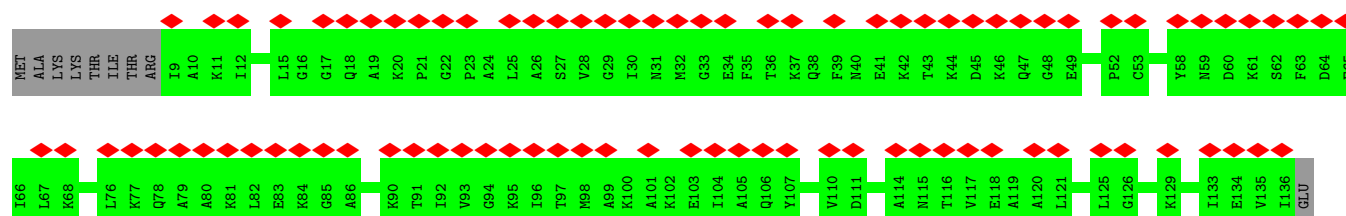
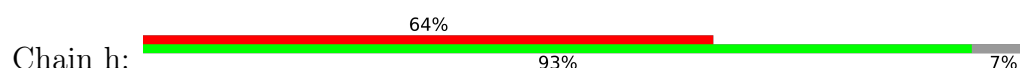
- Molecule 29: 50S ribosomal protein L9



- Molecule 30: 50S ribosomal protein L10



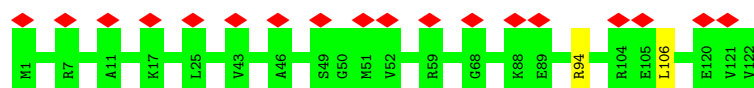
- Molecule 31: 50S ribosomal protein L11



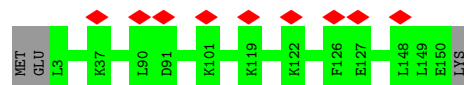
- Molecule 32: 50S ribosomal protein L13



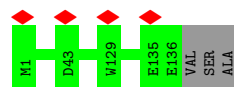
- Molecule 33: 50S ribosomal protein L14



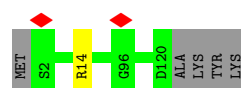
- Molecule 34: 50S ribosomal protein L15



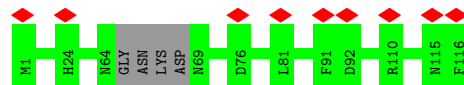
- Molecule 35: 50S ribosomal protein L16



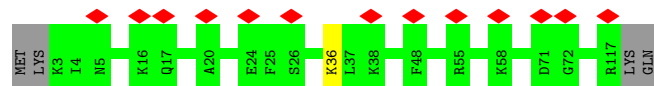
- Molecule 36: 50S ribosomal protein L17



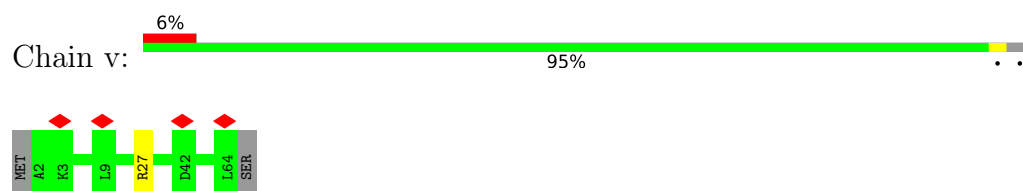
- Molecule 37: 50S ribosomal protein L18



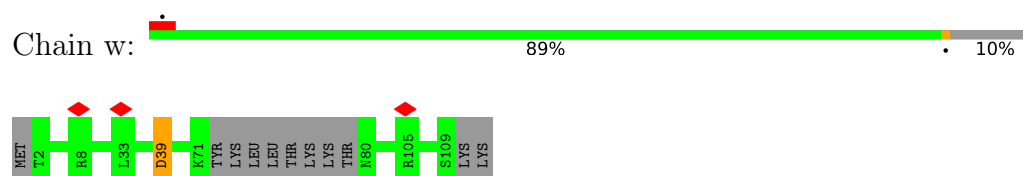
- Molecule 38: 50S ribosomal protein L19



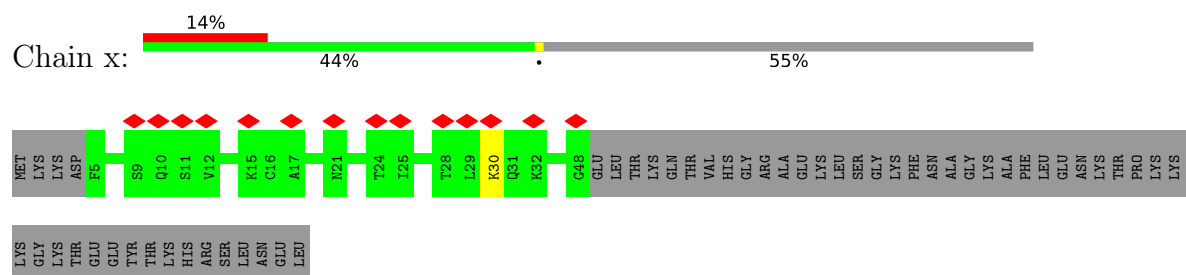
- Molecule 45: 50S ribosomal protein L28



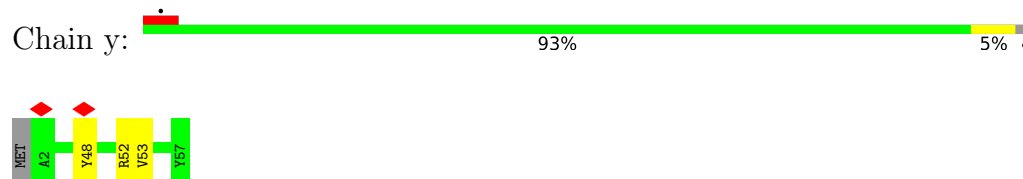
- Molecule 46: 50S ribosomal protein L29



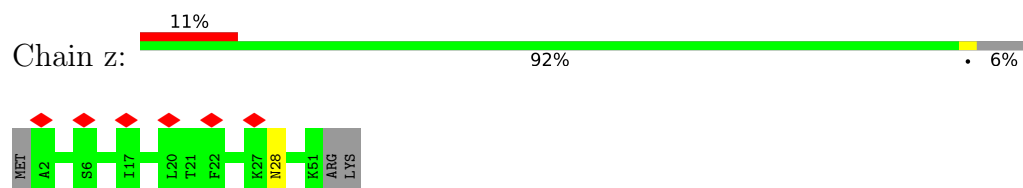
- Molecule 47: 50S ribosomal protein L31



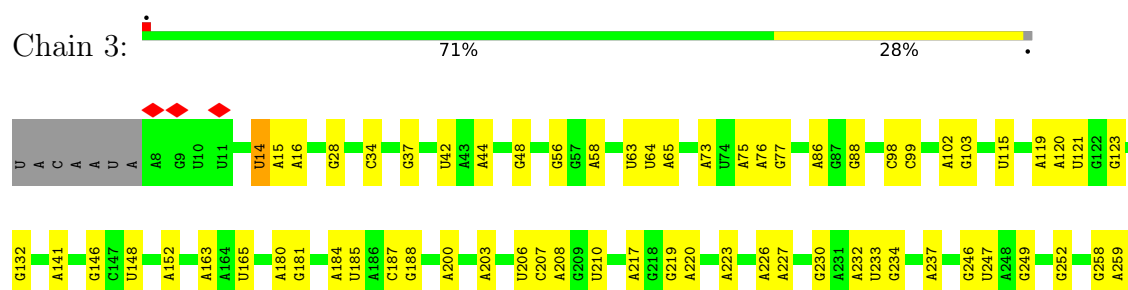
- Molecule 48: 50S ribosomal protein L32



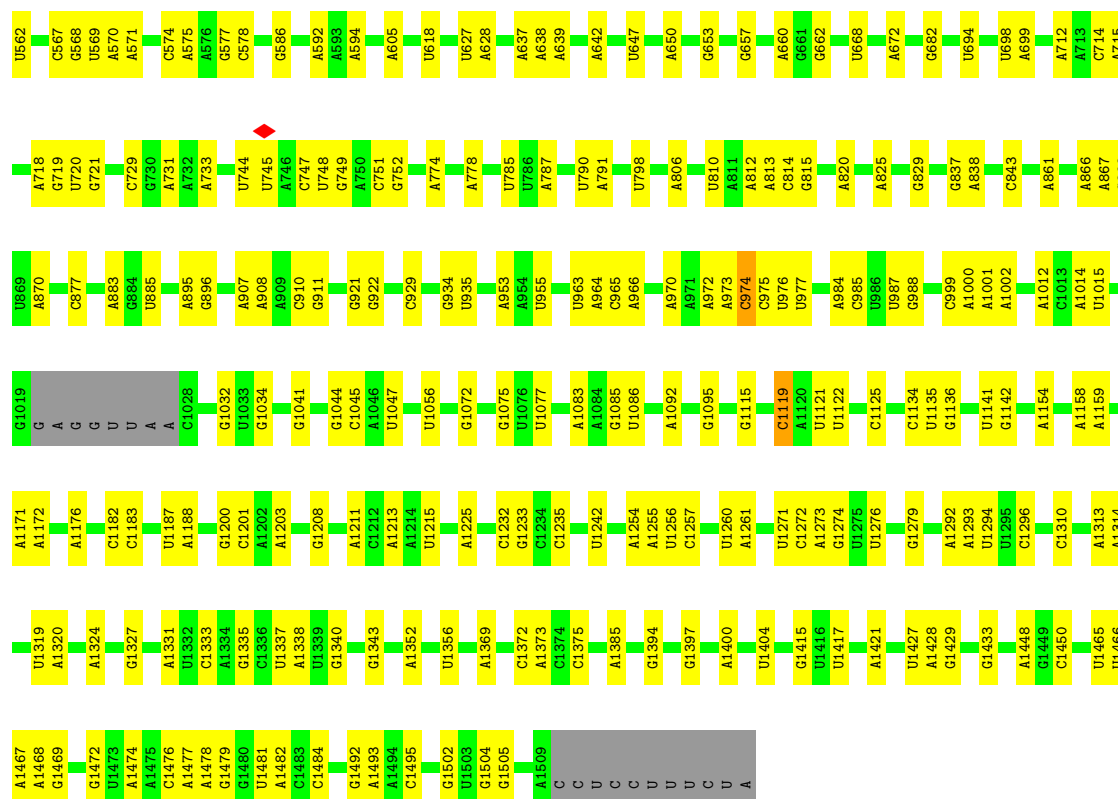
- Molecule 49: 50S ribosomal protein L33 1



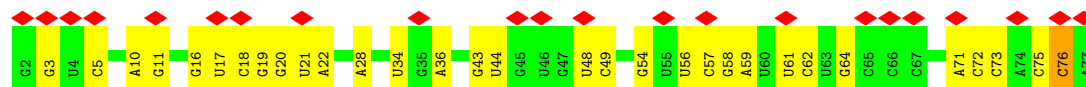
- Molecule 50: 23S ribosomal RNA



A2040	A1907	U1748	U1339	A1186	A1062	C949	A823	C659	A519	A402	A260
A2049	A1908	C1761	U1340	A1191	U1068	U950	A824	A688	U528	A403	A266
G2050	C1909	A1762	U1341	A1199	G1069	U952	U825	A673	U539	C404	A269
A2056	G1913	U1764	C1342	A1204	A1080	G953	A828	A673	U540	G408	G270
G2059	G1914	G1765	C1349	A1208	A1081	A954	A830	A679	A540	A409	A276
A1920	A1920	G1768	G1353	U1209	A1082	U967	C833	A680	U543	G410	
C2062	A1921	A1769	U1357	U1210	A1083	U968	C833	A681	U544	U411	
G2063	U1922	C1771	U1361	U1211	A1089	U970	G836	A682	C545	U284	
A2066	A1926	U1617	U1360	C1212	A1089	U970	A837	U688	U546	A421	
A2067	A1780	U1618	U1361	U1216	U1100	A977	G840	U689	A553	A422	
G2068	A1619	A1619	U1371	G1217	U1101	A981	C841	U690	G424	C423	
A1934	A1637	A1637	G1371	U1234	A1102	G982	C847	G691	U425	U426	
A1936	G1637	A1637	C1378	U1235	A1105	A993	A854	U701	C562	G432	
G1937	G1637	A1637	C1379	G1236	A1106	U994	A854	A703	A563	U295	
U1938	G1640	A1644	U1380	G1242	C1107	A995	A855	A705	A564	U296	
A1944	A1641	A1644	A1383	G1250	U1113	A996	U862	C706	C565	U297	
A1945	G1642	A1644	A1394	G1251	C1114	G997	U863	C707	G566	U298	
A1951	A1643	A1644	A1395	G1252	G1115	C998	U863	G708	U567	A437	
G1952	A1644	A1644	A1396	G1253	A1119	A1008	C868	A710	G568	U439	
U1953	C1651	A1651	C1404	G1256	A1123	A1009	C880	A710	A573	G442	
A1961	C1652	A1652	G1405	G1257	A1124	G1010	A881	G719	U579	C443	
U1962	C1653	A1653	A1406	G1262	U1125	A1011	C882	A720	U583	C444	
U1963	A1656	A1656	U1407	G1262	G1126	G1012	A883	G721	G584	G447	
C1964	G1667	A1667	G1408	G1266	C1132	G1013	A884	C722	A889	A448	
C1965	G1668	A1668	A1412	G1266	U1147	A1016	A885	C723	U889	U457	
U2110	G1681	A1681	U1422	U1268	U1148	A1017	A893	A724	G595	G460	
U2111	C1682	A1682	A1423	U1279	U1151	G1018	G894	C752	G596	G460	
C1966	U1693	A1693	U1424	G1280	U1154	G1020	U902	G761	G597	A464	
C1967	A1694	A1694	A1431	G1280	U1154	C1021	A903	A765	G598	A465	
U2112	C1697	A1697	U1434	A1283	G1157	A1024	U905	C766	U601	U484	
U2113	A1703	A1703	A1437	A1284	U1162	G1025	G906	A782	A605	C487	
G2113	C1706	A1706	G1438	U1285	A1163	U1027	C921	A786	G606	C492	
C2114	U1707	A1707	C1444	G1286	A1164	A1032	C922	A786	A607	A493	
A2115	G1708	A1708	U1445	U1296	A1165	C1042	A	G792	A608	G494	
U2116	A1715	A1715	U1446	U1297	G1166	A1045	C	A799	U609	U495	
G2117	U1716	A1716	U1448	U1298	U1167	A1046	U	G812	G612	G499	
U2118	U1727	A1727	A1455	A1298	A1168	A1047	A	C800	G620	U500	
A2119	A1728	A1728	C1456	G1301	A1169	A1048	G928	G810	G620	G501	
A2123	G1729	A1729	A1457	C1302	C1170	U1049	G811	G812	A623	C370	
A2124	G1733	A1733	G1463	A1322	G1171	A1052	A933	U637	G638	G510	
U2125	A1734	A1734	U1466	A1328	G1174	A1055	G936	A817	U641	U511	
U2126	G1737	A1737	U1467	U1329	C1175	A1056	U944	A818	U641	A514	
A2126	G1747	A1747	C1470	U1330	U1176	A1057	A947	U820	G656	A515	
G2127	G1906	A1906		G1338	G1179	A1061	A948	C822		A516	
G2131										G517	
G2132										A518	
A2133											
G2134											
U2138											
C2139											
G2140											
A2154											
A2165											
U2166											



• Molecule 53: tRNA-Phe



• Molecule 53: tRNA-Phe



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	6587	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 ($e^-/\text{\AA}^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.866	Depositor
Minimum map value	-0.639	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	0.47	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0	0.23	0/383	0.44	0/504
2	1	0.24	0/484	0.52	0/637
3	2	0.24	0/306	0.50	0/401
4	A	0.26	0/1954	0.50	0/2642
5	B	0.25	0/1721	0.50	0/2323
6	C	0.25	0/1691	0.48	0/2267
7	D	0.24	0/1188	0.47	0/1593
8	E	0.26	0/1384	0.50	0/1867
9	F	0.27	0/1266	0.49	0/1700
10	G	0.28	0/1126	0.59	0/1517
11	H	0.26	0/1044	0.52	0/1395
12	I	0.24	0/820	0.48	0/1103
13	J	0.57	2/844 (0.2%)	0.77	3/1136 (0.3%)
14	K	0.30	0/1094	0.60	1/1468 (0.1%)
15	L	0.25	0/962	0.47	0/1289
16	M	0.25	0/483	0.45	0/643
17	N	0.24	0/679	0.51	0/907
18	O	0.23	0/659	0.44	0/885
19	P	0.24	0/684	0.48	0/913
20	Q	0.24	0/545	0.48	0/730
21	R	0.25	0/698	0.47	0/936
22	S	0.24	0/631	0.41	0/838
23	T	0.24	0/475	0.48	0/621
24	a	0.24	0/2267	0.49	0/3044
25	b	0.25	0/1795	0.50	0/2412
26	c	0.24	0/1671	0.49	0/2246
27	d	0.27	0/1409	0.52	0/1894
28	e	0.25	0/1420	0.47	0/1912
29	f	0.25	0/1183	0.55	1/1587 (0.1%)
30	g	3.69	8/969 (0.8%)	0.90	6/1295 (0.5%)
31	h	0.25	0/968	0.48	0/1298
32	i	0.29	0/1186	0.58	1/1592 (0.1%)
33	j	0.27	0/953	0.54	1/1275 (0.1%)
34	k	0.27	0/1170	0.54	0/1559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	l	0.26	0/1104	0.52	0/1481
36	m	0.26	0/973	0.51	0/1309
37	n	0.30	0/897	0.57	0/1198
38	o	0.26	0/948	0.50	0/1262
39	p	0.25	0/961	0.46	0/1278
40	q	0.26	0/828	0.56	0/1111
41	r	0.26	0/1077	0.49	0/1441
42	s	0.27	0/732	0.51	0/988
43	t	0.25	0/879	0.51	0/1165
44	u	0.24	0/665	0.50	0/884
45	v	0.24	0/519	0.51	0/695
46	w	0.27	0/826	0.53	1/1104 (0.1%)
47	x	0.28	0/353	0.46	0/474
48	y	0.31	0/457	0.66	0/601
49	z	0.27	0/412	0.55	0/547
50	3	0.64	6/69073 (0.0%)	0.81	51/107710 (0.0%)
51	4	0.20	0/2505	0.80	2/3902 (0.1%)
52	5	0.20	0/35768	0.78	16/55764 (0.0%)
53	6	1.04	5/1808 (0.3%)	2.53	14/2817 (0.5%)
53	8	1.04	5/1808 (0.3%)	2.52	14/2817 (0.5%)
All	All	0.56	26/158705 (0.0%)	0.82	111/236977 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	G	0	1
24	a	0	1
30	g	0	1
44	u	0	1
All	All	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	3	2440	A	N3-C4	85.94	1.86	1.34
50	3	2440	A	C6-N1	72.66	1.86	1.35
30	g	112	TYR	CD1-CE1	67.07	2.40	1.39
50	3	2440	A	C5-C6	60.62	1.95	1.41
50	3	2440	A	C5-C4	59.55	1.80	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	3	2440	A	C2-N3	57.55	1.85	1.33
30	g	112	TYR	CD2-CE2	55.44	2.22	1.39
50	3	2440	A	N1-C2	51.12	1.80	1.34
30	g	112	TYR	CE1-CZ	42.69	1.94	1.38
30	g	112	TYR	CE2-CZ	38.98	1.89	1.38
30	g	112	TYR	CG-CD2	30.39	1.78	1.39
30	g	112	TYR	CG-CD1	30.09	1.78	1.39
53	6	76	C	N1-C6	27.30	1.53	1.37
53	8	76	C	N1-C6	27.29	1.53	1.37
53	8	76	C	C1'-N1	23.91	1.84	1.48
53	6	76	C	C1'-N1	23.76	1.84	1.48
53	8	76	C	N1-C2	21.04	1.61	1.40
53	6	76	C	N1-C2	21.00	1.61	1.40
30	g	115	ASN	N-CA	13.76	1.73	1.46
13	J	110	PRO	CG-CD	-12.09	1.10	1.50
30	g	114	ASP	C-N	10.27	1.57	1.34
53	6	76	C	C4-C5	-7.10	1.37	1.43
53	8	76	C	C4-C5	-7.09	1.37	1.43
13	J	110	PRO	N-CD	6.75	1.57	1.47
53	8	76	C	N3-C4	-6.32	1.29	1.33
53	6	76	C	N3-C4	-6.21	1.29	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	6	76	C	C6-N1-C2	-95.55	82.08	120.30
53	8	76	C	C6-N1-C2	-95.53	82.09	120.30
53	6	76	C	C5-C6-N1	57.84	149.92	121.00
53	8	76	C	C5-C6-N1	57.80	149.90	121.00
53	6	76	C	N3-C2-O2	-34.65	97.64	121.90
53	8	76	C	N3-C2-O2	-34.61	97.67	121.90
50	3	2440	A	N1-C2-N3	-27.97	115.31	129.30
53	6	76	C	N3-C4-C5	-23.88	112.35	121.90
50	3	2440	A	C2-N3-C4	23.85	122.53	110.60
53	8	76	C	N3-C4-C5	-23.76	112.39	121.90
53	6	76	C	N1-C2-N3	21.62	134.34	119.20
53	8	76	C	N1-C2-N3	21.61	134.33	119.20
53	6	76	C	C2-N1-C1'	19.44	140.19	118.80
53	8	76	C	C2-N1-C1'	19.43	140.17	118.80
30	g	114	ASP	C-N-CA	17.71	165.97	121.70
50	3	2440	A	N7-C8-N9	17.69	122.64	113.80
53	6	76	C	N1-C2-O2	15.20	128.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	8	76	C	N1-C2-O2	15.16	127.99	118.90
13	J	110	PRO	N-CD-CG	-14.43	81.55	103.20
53	8	76	C	C6-N1-C1'	13.91	137.49	120.80
53	6	76	C	C6-N1-C1'	13.90	137.49	120.80
53	6	76	C	C2-N3-C4	13.90	126.85	119.90
53	8	76	C	C2-N3-C4	13.80	126.80	119.90
50	3	2440	A	C4-C5-N7	-13.10	104.15	110.70
50	3	2440	A	N9-C4-C5	-12.85	100.66	105.80
50	3	2440	A	N3-C4-N9	12.51	137.41	127.40
50	3	2440	A	C6-N1-C2	11.89	125.73	118.60
53	6	76	C	O4'-C1'-N1	11.87	117.70	108.20
53	8	76	C	O4'-C1'-N1	11.80	117.64	108.20
13	J	110	PRO	CA-N-CD	-10.75	96.45	111.50
53	6	76	C	N1-C1'-C2'	10.20	127.26	114.00
53	8	76	C	N1-C1'-C2'	10.18	127.23	114.00
30	g	115	ASN	N-CA-CB	9.03	126.86	110.60
52	5	843	C	N3-C2-O2	-8.60	115.88	121.90
30	g	115	ASN	CB-CA-C	-8.23	93.94	110.40
50	3	99	C	N3-C2-O2	-8.16	116.19	121.90
50	3	2199	C	N3-C2-O2	-8.00	116.30	121.90
13	J	110	PRO	CA-CB-CG	-7.92	88.95	104.00
50	3	2440	A	N3-C4-C5	-7.78	121.35	126.80
50	3	2440	A	C6-C5-N7	7.77	137.74	132.30
52	5	1183	C	N3-C2-O2	-7.73	116.49	121.90
50	3	833	C	N3-C2-O2	-7.68	116.53	121.90
50	3	1965	C	N3-C2-O2	-7.58	116.59	121.90
50	3	98	C	N1-C2-O2	7.47	123.38	118.90
50	3	14	U	C2-N1-C1'	7.40	126.58	117.70
50	3	1507	G	O4'-C1'-N9	7.35	114.08	108.20
52	5	974	C	C2-N1-C1'	7.33	126.86	118.80
52	5	714	C	N3-C2-O2	-7.26	116.82	121.90
50	3	567	U	C2-N1-C1'	7.25	126.41	117.70
53	6	76	C	C5-C4-N4	7.25	125.27	120.20
53	8	76	C	C5-C4-N4	7.20	125.24	120.20
50	3	659	C	N3-C2-O2	-7.08	116.95	121.90
50	3	394	C	N3-C2-O2	-7.07	116.95	121.90
50	3	34	C	N3-C2-O2	-6.97	117.02	121.90
52	5	974	C	N1-C2-O2	6.97	123.08	118.90
50	3	1341	U	C2-N1-C1'	6.96	126.06	117.70
50	3	1341	U	N1-C2-O2	6.91	127.64	122.80
50	3	822	C	N3-C2-O2	-6.90	117.07	121.90
52	5	1484	C	N3-C2-O2	-6.90	117.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	3	567	U	N1-C2-O2	6.74	127.52	122.80
30	g	112	TYR	CD1-CE1-CZ	-6.62	113.84	119.80
50	3	444	C	N3-C2-O2	-6.60	117.28	121.90
50	3	98	C	N3-C2-O2	-6.54	117.32	121.90
50	3	2199	C	N1-C2-O2	6.51	122.81	118.90
52	5	843	C	N1-C2-O2	6.36	122.72	118.90
52	5	714	C	N1-C2-O2	6.36	122.71	118.90
50	3	1341	U	N3-C2-O2	-6.28	117.81	122.20
53	6	76	C	N3-C4-N4	6.26	122.38	118.00
53	8	76	C	N3-C4-N4	6.24	122.37	118.00
53	6	76	C	C4-C5-C6	-6.14	114.33	117.40
53	8	76	C	C4-C5-C6	-6.11	114.34	117.40
29	f	46	ASP	CB-CG-OD1	6.10	123.79	118.30
50	3	88	G	N1-C6-O6	-6.10	116.24	119.90
46	w	39	ASP	CB-CG-OD2	6.10	123.79	118.30
50	3	567	U	N3-C2-O2	-6.01	117.99	122.20
50	3	2612	G	N1-C6-O6	-5.99	116.31	119.90
50	3	2083	U	C2-N1-C1'	5.88	124.76	117.70
30	g	112	TYR	CB-CG-CD2	-5.73	117.56	121.00
52	5	1119	C	C2-N1-C1'	5.73	125.10	118.80
50	3	1965	C	C6-N1-C2	-5.71	118.02	120.30
51	4	58	C	N3-C2-O2	-5.69	117.92	121.90
50	3	14	U	N1-C2-O2	5.63	126.74	122.80
50	3	14	U	N3-C2-O2	-5.59	118.29	122.20
50	3	1010	G	O4'-C1'-N9	5.58	112.66	108.20
50	3	88	G	C5-C6-O6	5.55	131.93	128.60
52	5	1502	G	C5-C6-O6	5.54	131.92	128.60
50	3	812	G	N3-C4-N9	5.52	129.31	126.00
52	5	1502	G	N1-C6-O6	-5.46	116.62	119.90
33	j	106	LEU	CA-CB-CG	5.42	127.78	115.30
50	3	1262	G	N3-C4-N9	5.42	129.25	126.00
50	3	510	G	C5-C6-O6	5.39	131.84	128.60
52	5	1183	C	C6-N1-C2	-5.38	118.15	120.30
52	5	751	C	C2-N1-C1'	5.38	124.72	118.80
50	3	2612	G	C5-C6-O6	5.38	131.83	128.60
30	g	114	ASP	CA-C-O	-5.36	108.84	120.10
52	5	974	C	C6-N1-C1'	-5.36	114.37	120.80
14	K	31	LEU	CA-CB-CG	5.33	127.57	115.30
50	3	443	C	N1-C2-O2	5.31	122.09	118.90
50	3	1583	G	OP1-P-O3'	5.29	116.84	105.20
50	3	464	A	O4'-C1'-N9	5.28	112.42	108.20
51	4	78	C	O4'-C1'-N1	5.26	112.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	95	MET	CA-CB-CG	5.22	122.18	113.30
50	3	99	C	N1-C2-O2	5.19	122.02	118.90
52	5	1119	C	N1-C2-O2	5.17	122.00	118.90
50	3	88	G	N1-C2-N2	-5.15	111.57	116.20
50	3	426	U	C2-N1-C1'	5.14	123.87	117.70
52	5	1182	C	N1-C2-O2	5.11	121.96	118.90
50	3	833	C	C6-N1-C2	-5.10	118.26	120.30
50	3	1964	C	N1-C2-O2	5.07	121.94	118.90
50	3	444	C	C6-N1-C2	-5.07	118.27	120.30
50	3	1262	G	N3-C4-C5	-5.04	126.08	128.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	G	108	LEU	Peptide
24	a	247	SER	Peptide
30	g	112	TYR	Peptide
44	u	24	THR	Peptide

5.2 Too-close contacts [i](#)

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	
1	0	45/48 (94%)	40 (89%)	5 (11%)	0	100	100
2	1	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
3	2	35/37 (95%)	32 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	238/294 (81%)	215 (90%)	23 (10%)	0	100	100
5	B	213/273 (78%)	200 (94%)	13 (6%)	0	100	100
6	C	201/205 (98%)	192 (96%)	9 (4%)	0	100	100
7	D	151/219 (69%)	146 (97%)	5 (3%)	0	100	100
8	E	165/215 (77%)	153 (93%)	12 (7%)	0	100	100
9	F	152/155 (98%)	142 (93%)	10 (7%)	0	100	100
10	G	139/142 (98%)	121 (87%)	18 (13%)	0	100	100
11	H	126/132 (96%)	113 (90%)	13 (10%)	0	100	100
12	I	99/108 (92%)	89 (90%)	10 (10%)	0	100	100
13	J	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
14	K	134/139 (96%)	119 (89%)	14 (10%)	1 (1%)	19	57
15	L	116/124 (94%)	105 (90%)	11 (10%)	0	100	100
16	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
17	N	81/86 (94%)	79 (98%)	2 (2%)	0	100	100
18	O	78/94 (83%)	72 (92%)	6 (8%)	0	100	100
19	P	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
20	Q	63/104 (61%)	58 (92%)	5 (8%)	0	100	100
21	R	82/87 (94%)	75 (92%)	7 (8%)	0	100	100
22	S	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
23	T	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
24	a	283/287 (99%)	256 (90%)	27 (10%)	0	100	100
25	b	227/287 (79%)	213 (94%)	14 (6%)	0	100	100
26	c	208/212 (98%)	197 (95%)	11 (5%)	0	100	100
27	d	173/180 (96%)	161 (93%)	12 (7%)	0	100	100
28	e	174/184 (95%)	165 (95%)	9 (5%)	0	100	100
29	f	143/149 (96%)	136 (95%)	7 (5%)	0	100	100
30	g	124/161 (77%)	114 (92%)	9 (7%)	1 (1%)	16	55
31	h	126/137 (92%)	114 (90%)	12 (10%)	0	100	100
32	i	142/146 (97%)	131 (92%)	11 (8%)	0	100	100
33	j	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
34	k	146/151 (97%)	137 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	134/139 (96%)	124 (92%)	10 (8%)	0	100	100
36	m	117/124 (94%)	109 (93%)	8 (7%)	0	100	100
37	n	108/116 (93%)	97 (90%)	11 (10%)	0	100	100
38	o	113/119 (95%)	106 (94%)	7 (6%)	0	100	100
39	p	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
40	q	97/100 (97%)	82 (84%)	15 (16%)	0	100	100
41	r	137/159 (86%)	127 (93%)	10 (7%)	0	100	100
42	s	90/237 (38%)	87 (97%)	3 (3%)	0	100	100
43	t	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
44	u	84/104 (81%)	78 (93%)	6 (7%)	0	100	100
45	v	61/65 (94%)	55 (90%)	6 (10%)	0	100	100
46	w	96/111 (86%)	92 (96%)	3 (3%)	1 (1%)	13	49
47	x	42/97 (43%)	40 (95%)	2 (5%)	0	100	100
48	y	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	33
49	z	48/53 (91%)	48 (100%)	0	0	100	100
All	All	5820/6670 (87%)	5397 (93%)	419 (7%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	K	116	ASP
30	g	88	GLU
46	w	39	ASP
48	y	53	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	39 (98%)	1 (2%)	42	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	51/51 (100%)	50 (98%)	1 (2%)	50	68
3	2	35/35 (100%)	35 (100%)	0	100	100
4	A	212/262 (81%)	209 (99%)	3 (1%)	62	75
5	B	180/232 (78%)	177 (98%)	3 (2%)	56	72
6	C	181/183 (99%)	181 (100%)	0	100	100
7	D	123/178 (69%)	122 (99%)	1 (1%)	79	85
8	E	150/196 (76%)	149 (99%)	1 (1%)	81	87
9	F	131/132 (99%)	131 (100%)	0	100	100
10	G	123/124 (99%)	122 (99%)	1 (1%)	79	85
11	H	111/115 (96%)	110 (99%)	1 (1%)	75	83
12	I	95/99 (96%)	95 (100%)	0	100	100
13	J	91/97 (94%)	90 (99%)	1 (1%)	70	80
14	K	117/120 (98%)	115 (98%)	2 (2%)	56	72
15	L	100/105 (95%)	100 (100%)	0	100	100
16	M	47/48 (98%)	47 (100%)	0	100	100
17	N	76/78 (97%)	76 (100%)	0	100	100
18	O	69/82 (84%)	69 (100%)	0	100	100
19	P	73/75 (97%)	72 (99%)	1 (1%)	62	75
20	Q	56/94 (60%)	56 (100%)	0	100	100
21	R	74/77 (96%)	74 (100%)	0	100	100
22	S	70/77 (91%)	70 (100%)	0	100	100
23	T	49/56 (88%)	47 (96%)	2 (4%)	26	47
24	a	241/243 (99%)	240 (100%)	1 (0%)	89	91
25	b	186/233 (80%)	185 (100%)	1 (0%)	86	89
26	c	182/184 (99%)	182 (100%)	0	100	100
27	d	150/154 (97%)	150 (100%)	0	100	100
28	e	153/159 (96%)	153 (100%)	0	100	100
29	f	123/134 (92%)	123 (100%)	0	100	100
30	g	101/129 (78%)	93 (92%)	8 (8%)	10	29
31	h	102/110 (93%)	102 (100%)	0	100	100
32	i	126/128 (98%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	103/103 (100%)	102 (99%)	1 (1%)	73	82
34	k	123/126 (98%)	123 (100%)	0	100	100
35	l	113/115 (98%)	113 (100%)	0	100	100
36	m	105/109 (96%)	104 (99%)	1 (1%)	73	82
37	n	96/99 (97%)	96 (100%)	0	100	100
38	o	101/105 (96%)	100 (99%)	1 (1%)	73	82
39	p	100/108 (93%)	99 (99%)	1 (1%)	73	82
40	q	90/91 (99%)	90 (100%)	0	100	100
41	r	116/132 (88%)	116 (100%)	0	100	100
42	s	82/208 (39%)	82 (100%)	0	100	100
43	t	96/96 (100%)	96 (100%)	0	100	100
44	u	69/85 (81%)	67 (97%)	2 (3%)	37	56
45	v	58/60 (97%)	57 (98%)	1 (2%)	56	72
46	w	87/98 (89%)	87 (100%)	0	100	100
47	x	41/86 (48%)	40 (98%)	1 (2%)	44	62
48	y	48/49 (98%)	46 (96%)	2 (4%)	25	46
49	z	47/50 (94%)	46 (98%)	1 (2%)	48	66
All	All	5093/5751 (89%)	5054 (99%)	39 (1%)	77	85

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	32	LYS
2	1	20	LYS
4	A	22	LYS
4	A	62	ARG
4	A	121	LYS
5	B	134	ARG
5	B	146	LYS
5	B	217	ARG
7	D	72	LYS
8	E	112	ARG
10	G	26	ARG
11	H	115	ARG
13	J	65	LYS
14	K	116	ASP

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Mol	Chain	Res	Type
14	K	122	LYS
19	P	67	ARG
23	T	45	LYS
23	T	46	ARG
24	a	268	ARG
25	b	158	ARG
30	g	26	ILE
30	g	27	PHE
30	g	32	MET
30	g	44	LEU
30	g	45	PHE
30	g	46	LYS
30	g	88	GLU
30	g	89	ILE
33	j	94	ARG
36	m	14	ARG
38	o	36	LYS
39	p	84	LYS
44	u	26	ASN
44	u	55	ARG
45	v	27	ARG
47	x	30	LYS
48	y	48	TYR
48	y	52	ARG
49	z	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	70	ASN
4	A	137	GLN
5	B	193	GLN
6	C	121	HIS
8	E	17	GLN
9	F	39	GLN
9	F	67	ASN
9	F	85	GLN
11	H	77	GLN
19	P	5	GLN
22	S	50	GLN
24	a	58	GLN
24	a	219	ASN

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Mol	Chain	Res	Type
24	a	221	HIS
26	c	31	GLN
26	c	76	GLN
26	c	81	ASN
26	c	162	ASN
28	e	63	GLN
29	f	54	GLN
29	f	61	ASN
29	f	100	GLN
31	h	113	ASN
31	h	130	GLN
32	i	82	GLN
32	i	106	ASN
35	l	13	HIS
36	m	59	ASN
36	m	62	GLN
37	n	7	GLN
37	n	69	ASN
38	o	83	ASN
38	o	85	ASN
39	p	110	GLN
40	q	17	ASN
40	q	87	GLN
46	w	35	HIS
46	w	64	ASN
48	y	5	GLN
49	z	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	2876/2907 (98%)	774 (26%)	34 (1%)
51	4	103/108 (95%)	36 (34%)	3 (2%)
52	5	1490/1520 (98%)	353 (23%)	5 (0%)
53	6	75/76 (98%)	29 (38%)	4 (5%)
53	8	75/76 (98%)	29 (38%)	4 (5%)
All	All	4619/4687 (98%)	1221 (26%)	50 (1%)

All (1221) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	14	U
50	3	15	A
50	3	16	A
50	3	28	G
50	3	37	G
50	3	42	U
50	3	44	A
50	3	48	G
50	3	56	G
50	3	58	A
50	3	63	U
50	3	64	U
50	3	65	A
50	3	73	A
50	3	75	A
50	3	76	A
50	3	77	G
50	3	86	A
50	3	102	A
50	3	103	G
50	3	115	U
50	3	119	A
50	3	120	A
50	3	121	U
50	3	123	G
50	3	132	G
50	3	141	A
50	3	146	G
50	3	148	U
50	3	152	A
50	3	163	A
50	3	165	U
50	3	180	A
50	3	181	G
50	3	184	A
50	3	185	U
50	3	187	C
50	3	188	G
50	3	200	A
50	3	203	A
50	3	206	U
50	3	207	C
50	3	208	A

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Mol	Chain	Res	Type
50	3	210	U
50	3	217	A
50	3	219	G
50	3	220	A
50	3	223	A
50	3	226	A
50	3	227	A
50	3	230	G
50	3	232	A
50	3	233	U
50	3	234	G
50	3	237	A
50	3	246	G
50	3	247	U
50	3	249	G
50	3	252	G
50	3	258	G
50	3	259	A
50	3	260	A
50	3	266	A
50	3	269	A
50	3	270	G
50	3	276	A
50	3	284	U
50	3	286	A
50	3	287	G
50	3	293	G
50	3	295	U
50	3	296	U
50	3	297	G
50	3	298	U
50	3	299	A
50	3	309	A
50	3	310	U
50	3	312	U
50	3	314	G
50	3	318	U
50	3	319	G
50	3	325	G
50	3	326	A
50	3	336	C
50	3	345	A

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Mol	Chain	Res	Type
50	3	346	G
50	3	347	C
50	3	351	G
50	3	355	A
50	3	357	A
50	3	361	G
50	3	363	G
50	3	364	A
50	3	370	C
50	3	372	G
50	3	393	C
50	3	399	G
50	3	402	A
50	3	403	U
50	3	404	C
50	3	408	G
50	3	409	A
50	3	411	U
50	3	421	A
50	3	422	A
50	3	424	G
50	3	425	U
50	3	426	U
50	3	432	G
50	3	437	A
50	3	438	A
50	3	439	U
50	3	442	G
50	3	447	G
50	3	448	A
50	3	457	U
50	3	460	G
50	3	465	A
50	3	484	U
50	3	487	C
50	3	492	C
50	3	493	A
50	3	494	G
50	3	495	U
50	3	499	G
50	3	501	G
50	3	502	A

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Mol	Chain	Res	Type
50	3	509	G
50	3	511	U
50	3	514	A
50	3	515	A
50	3	517	G
50	3	519	A
50	3	528	U
50	3	539	U
50	3	540	A
50	3	543	U
50	3	544	U
50	3	545	C
50	3	546	U
50	3	553	A
50	3	557	G
50	3	562	C
50	3	563	A
50	3	564	A
50	3	565	C
50	3	566	G
50	3	568	G
50	3	573	A
50	3	579	U
50	3	583	U
50	3	584	G
50	3	589	A
50	3	595	U
50	3	596	G
50	3	598	G
50	3	601	U
50	3	605	A
50	3	606	G
50	3	608	A
50	3	609	U
50	3	612	G
50	3	620	G
50	3	623	A
50	3	636	U
50	3	637	U
50	3	638	A
50	3	641	U
50	3	656	G

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Mol	Chain	Res	Type
50	3	659	C
50	3	668	A
50	3	673	A
50	3	679	A
50	3	681	A
50	3	682	A
50	3	689	U
50	3	691	G
50	3	701	A
50	3	703	A
50	3	705	A
50	3	706	C
50	3	707	C
50	3	709	G
50	3	710	A
50	3	719	G
50	3	720	A
50	3	722	C
50	3	723	U
50	3	724	A
50	3	752	C
50	3	761	G
50	3	765	A
50	3	766	C
50	3	782	U
50	3	786	A
50	3	792	G
50	3	799	A
50	3	800	C
50	3	810	G
50	3	811	G
50	3	812	G
50	3	817	A
50	3	819	U
50	3	820	U
50	3	823	A
50	3	824	A
50	3	825	U
50	3	828	A
50	3	829	A
50	3	830	A
50	3	836	G

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Mol	Chain	Res	Type
50	3	837	A
50	3	840	G
50	3	841	C
50	3	847	C
50	3	854	A
50	3	855	A
50	3	862	U
50	3	863	U
50	3	868	C
50	3	880	C
50	3	882	C
50	3	883	A
50	3	885	A
50	3	893	A
50	3	894	G
50	3	902	U
50	3	904	C
50	3	906	G
50	3	932	U
50	3	933	A
50	3	936	G
50	3	944	U
50	3	947	A
50	3	949	C
50	3	951	C
50	3	952	U
50	3	953	G
50	3	954	A
50	3	968	U
50	3	969	A
50	3	970	U
50	3	977	A
50	3	981	A
50	3	982	G
50	3	993	A
50	3	995	A
50	3	997	G
50	3	998	C
50	3	1008	A
50	3	1009	A
50	3	1010	G
50	3	1011	A

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Mol	Chain	Res	Type
50	3	1013	G
50	3	1016	A
50	3	1017	A
50	3	1019	A
50	3	1021	C
50	3	1024	A
50	3	1026	A
50	3	1027	U
50	3	1032	A
50	3	1042	C
50	3	1045	A
50	3	1046	A
50	3	1049	U
50	3	1052	A
50	3	1055	A
50	3	1057	G
50	3	1061	A
50	3	1062	A
50	3	1068	U
50	3	1069	G
50	3	1080	A
50	3	1081	A
50	3	1083	A
50	3	1089	A
50	3	1101	U
50	3	1102	A
50	3	1105	A
50	3	1106	G
50	3	1107	C
50	3	1113	U
50	3	1115	G
50	3	1119	A
50	3	1123	A
50	3	1124	G
50	3	1125	U
50	3	1126	G
50	3	1132	C
50	3	1147	G
50	3	1148	U
50	3	1151	U
50	3	1154	U
50	3	1157	G

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Mol	Chain	Res	Type
50	3	1162	A
50	3	1163	G
50	3	1164	A
50	3	1165	U
50	3	1167	U
50	3	1168	A
50	3	1169	A
50	3	1170	C
50	3	1171	G
50	3	1174	G
50	3	1176	U
50	3	1177	A
50	3	1178	A
50	3	1179	G
50	3	1186	A
50	3	1191	A
50	3	1204	A
50	3	1208	A
50	3	1209	U
50	3	1210	A
50	3	1212	C
50	3	1216	U
50	3	1217	G
50	3	1234	U
50	3	1235	U
50	3	1236	G
50	3	1242	G
50	3	1250	A
50	3	1251	G
50	3	1253	G
50	3	1256	A
50	3	1257	G
50	3	1266	G
50	3	1268	U
50	3	1279	U
50	3	1280	G
50	3	1283	A
50	3	1284	A
50	3	1285	U
50	3	1286	G
50	3	1292	A
50	3	1295	A

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Mol	Chain	Res	Type
50	3	1297	U
50	3	1298	A
50	3	1301	G
50	3	1302	C
50	3	1322	A
50	3	1328	A
50	3	1329	U
50	3	1330	U
50	3	1338	G
50	3	1340	U
50	3	1342	C
50	3	1349	C
50	3	1353	G
50	3	1357	U
50	3	1360	U
50	3	1361	U
50	3	1370	A
50	3	1371	G
50	3	1378	C
50	3	1380	U
50	3	1393	A
50	3	1395	A
50	3	1396	A
50	3	1404	C
50	3	1406	A
50	3	1408	G
50	3	1412	A
50	3	1422	U
50	3	1423	A
50	3	1424	U
50	3	1431	A
50	3	1434	U
50	3	1437	A
50	3	1438	G
50	3	1444	C
50	3	1445	U
50	3	1448	U
50	3	1455	A
50	3	1456	C
50	3	1457	A
50	3	1463	G
50	3	1466	U

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Mol	Chain	Res	Type
50	3	1467	U
50	3	1470	C
50	3	1480	A
50	3	1481	U
50	3	1482	U
50	3	1483	G
50	3	1485	A
50	3	1487	U
50	3	1507	G
50	3	1508	G
50	3	1509	U
50	3	1510	A
50	3	1511	C
50	3	1515	A
50	3	1518	C
50	3	1519	A
50	3	1523	C
50	3	1527	U
50	3	1530	G
50	3	1532	A
50	3	1533	U
50	3	1534	A
50	3	1535	A
50	3	1541	A
50	3	1550	G
50	3	1557	G
50	3	1571	G
50	3	1581	U
50	3	1584	U
50	3	1587	U
50	3	1588	A
50	3	1589	A
50	3	1592	A
50	3	1600	A
50	3	1603	A
50	3	1612	U
50	3	1615	G
50	3	1616	G
50	3	1618	U
50	3	1619	A
50	3	1637	A
50	3	1640	G

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Mol	Chain	Res	Type
50	3	1641	A
50	3	1642	G
50	3	1643	A
50	3	1644	A
50	3	1651	C
50	3	1652	A
50	3	1653	C
50	3	1656	A
50	3	1667	G
50	3	1668	G
50	3	1681	G
50	3	1682	C
50	3	1693	U
50	3	1694	A
50	3	1697	C
50	3	1703	A
50	3	1706	C
50	3	1707	U
50	3	1708	G
50	3	1715	A
50	3	1716	A
50	3	1727	U
50	3	1728	A
50	3	1729	G
50	3	1733	G
50	3	1734	A
50	3	1737	G
50	3	1747	G
50	3	1748	U
50	3	1761	C
50	3	1762	A
50	3	1763	G
50	3	1764	U
50	3	1765	G
50	3	1768	G
50	3	1769	A
50	3	1770	A
50	3	1771	C
50	3	1780	A
50	3	1788	A
50	3	1789	C
50	3	1790	U

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Mol	Chain	Res	Type
50	3	1793	A
50	3	1794	A
50	3	1798	A
50	3	1807	C
50	3	1808	C
50	3	1809	A
50	3	1815	U
50	3	1821	G
50	3	1822	A
50	3	1823	U
50	3	1824	G
50	3	1828	A
50	3	1836	A
50	3	1842	G
50	3	1843	C
50	3	1855	A
50	3	1865	A
50	3	1866	G
50	3	1872	U
50	3	1873	A
50	3	1876	G
50	3	1878	A
50	3	1879	A
50	3	1880	G
50	3	1891	A
50	3	1906	G
50	3	1907	A
50	3	1908	A
50	3	1910	G
50	3	1913	G
50	3	1914	G
50	3	1920	A
50	3	1921	C
50	3	1922	U
50	3	1926	A
50	3	1934	A
50	3	1936	G
50	3	1937	G
50	3	1938	U
50	3	1944	A
50	3	1945	A
50	3	1951	A

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Mol	Chain	Res	Type
50	3	1952	G
50	3	1953	U
50	3	1961	A
50	3	1962	U
50	3	1970	C
50	3	1973	U
50	3	1977	A
50	3	1979	G
50	3	1988	A
50	3	1989	U
50	3	1998	U
50	3	1999	G
50	3	2000	U
50	3	2011	G
50	3	2012	A
50	3	2020	A
50	3	2028	G
50	3	2030	A
50	3	2037	A
50	3	2038	A
50	3	2040	A
50	3	2049	A
50	3	2050	G
50	3	2056	A
50	3	2059	G
50	3	2062	C
50	3	2063	G
50	3	2066	A
50	3	2067	A
50	3	2068	G
50	3	2075	U
50	3	2076	G
50	3	2080	C
50	3	2084	A
50	3	2100	G
50	3	2107	A
50	3	2108	C
50	3	2110	U
50	3	2111	U
50	3	2112	A
50	3	2114	C
50	3	2115	A

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Mol	Chain	Res	Type
50	3	2117	G
50	3	2118	U
50	3	2119	A
50	3	2123	A
50	3	2124	A
50	3	2125	U
50	3	2127	G
50	3	2131	G
50	3	2132	G
50	3	2133	A
50	3	2134	G
50	3	2138	U
50	3	2140	G
50	3	2154	A
50	3	2165	A
50	3	2166	U
50	3	2170	A
50	3	2171	A
50	3	2172	A
50	3	2180	U
50	3	2181	A
50	3	2184	A
50	3	2187	C
50	3	2193	U
50	3	2195	U
50	3	2197	U
50	3	2198	G
50	3	2200	U
50	3	2201	G
50	3	2202	U
50	3	2206	A
50	3	2207	A
50	3	2212	U
50	3	2219	U
50	3	2220	A
50	3	2222	C
50	3	2227	U
50	3	2228	U
50	3	2231	A
50	3	2233	A
50	3	2242	G
50	3	2246	G

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Mol	Chain	Res	Type
50	3	2247	G
50	3	2254	G
50	3	2257	U
50	3	2276	A
50	3	2285	G
50	3	2286	A
50	3	2287	G
50	3	2288	G
50	3	2291	U
50	3	2294	A
50	3	2295	A
50	3	2296	A
50	3	2305	C
50	3	2313	U
50	3	2315	G
50	3	2316	G
50	3	2317	A
50	3	2319	A
50	3	2320	U
50	3	2327	U
50	3	2328	A
50	3	2329	G
50	3	2333	G
50	3	2334	U
50	3	2335	A
50	3	2341	G
50	3	2342	U
50	3	2343	A
50	3	2344	A
50	3	2346	G
50	3	2351	U
50	3	2352	U
50	3	2353	G
50	3	2354	A
50	3	2355	C
50	3	2358	U
50	3	2362	A
50	3	2365	U
50	3	2369	G
50	3	2380	U
50	3	2391	G
50	3	2393	C

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Mol	Chain	Res	Type
50	3	2396	A
50	3	2398	U
50	3	2410	C
50	3	2414	U
50	3	2415	A
50	3	2418	G
50	3	2431	U
50	3	2435	C
50	3	2436	G
50	3	2437	G
50	3	2438	A
50	3	2439	U
50	3	2440	A
50	3	2442	A
50	3	2443	A
50	3	2449	U
50	3	2455	G
50	3	2456	A
50	3	2457	U
50	3	2458	A
50	3	2460	C
50	3	2467	A
50	3	2477	A
50	3	2480	G
50	3	2482	U
50	3	2483	C
50	3	2484	A
50	3	2488	C
50	3	2489	G
50	3	2497	U
50	3	2499	U
50	3	2500	U
50	3	2502	G
50	3	2503	G
50	3	2505	A
50	3	2507	C
50	3	2509	C
50	3	2511	A
50	3	2513	G
50	3	2514	U
50	3	2519	U
50	3	2521	A

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Mol	Chain	Res	Type
50	3	2527	U
50	3	2528	C
50	3	2538	A
50	3	2539	A
50	3	2542	A
50	3	2543	G
50	3	2544	G
50	3	2555	U
50	3	2570	U
50	3	2571	U
50	3	2572	A
50	3	2574	A
50	3	2575	G
50	3	2578	A
50	3	2580	A
50	3	2581	C
50	3	2582	G
50	3	2586	G
50	3	2596	A
50	3	2598	C
50	3	2605	G
50	3	2606	A
50	3	2610	A
50	3	2611	G
50	3	2618	C
50	3	2619	C
50	3	2621	U
50	3	2622	A
50	3	2623	U
50	3	2627	U
50	3	2629	G
50	3	2636	U
50	3	2637	A
50	3	2638	G
50	3	2643	A
50	3	2644	U
50	3	2647	A
50	3	2649	G
50	3	2653	G
50	3	2654	U
50	3	2664	U
50	3	2669	G

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Mol	Chain	Res	Type
50	3	2670	A
50	3	2681	G
50	3	2689	C
50	3	2690	U
50	3	2692	U
50	3	2694	A
50	3	2697	C
50	3	2698	U
50	3	2699	C
50	3	2715	C
50	3	2721	C
50	3	2722	G
50	3	2732	A
50	3	2733	A
50	3	2734	C
50	3	2737	G
50	3	2739	C
50	3	2741	A
50	3	2747	U
50	3	2749	A
50	3	2752	G
50	3	2756	A
50	3	2760	C
50	3	2765	A
50	3	2769	G
50	3	2773	A
50	3	2774	A
50	3	2779	C
50	3	2784	A
50	3	2786	A
50	3	2788	U
50	3	2790	A
50	3	2799	U
50	3	2800	U
50	3	2803	G
50	3	2805	A
50	3	2806	A
50	3	2808	A
50	3	2809	A
50	3	2810	A
50	3	2811	G
50	3	2813	A

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Mol	Chain	Res	Type
50	3	2815	G
50	3	2822	C
50	3	2824	A
50	3	2825	A
50	3	2828	C
50	3	2838	G
50	3	2839	A
50	3	2870	U
50	3	2871	G
50	3	2876	G
50	3	2878	G
50	3	2884	C
50	3	2888	U
50	3	2890	G
50	3	2897	G
50	3	2898	A
50	3	2899	C
51	4	5	G
51	4	8	C
51	4	9	C
51	4	10	C
51	4	11	A
51	4	13	G
51	4	22	G
51	4	23	A
51	4	25	A
51	4	27	A
51	4	28	C
51	4	31	G
51	4	33	U
51	4	35	C
51	4	38	U
51	4	39	U
51	4	40	U
51	4	41	C
51	4	42	G
51	4	45	C
51	4	46	C
51	4	48	A
51	4	51	A
51	4	54	U
51	4	55	A

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Mol	Chain	Res	Type
51	4	60	C
51	4	71	A
51	4	72	A
51	4	77	G
51	4	78	C
51	4	86	G
51	4	88	G
51	4	89	A
51	4	99	A
51	4	106	A
51	4	108	C
52	5	6	C
52	5	8	G
52	5	10	G
52	5	15	U
52	5	21	U
52	5	32	U
52	5	33	A
52	5	40	G
52	5	41	C
52	5	48	C
52	5	49	C
52	5	52	A
52	5	58	G
52	5	61	A
52	5	65	G
52	5	75	A
52	5	82	C
52	5	86	A
52	5	87	G
52	5	95	C
52	5	100	G
52	5	101	A
52	5	103	U
52	5	106	C
52	5	107	A
52	5	112	U
52	5	114	C
52	5	115	A
52	5	116	A
52	5	117	U
52	5	120	A

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Mol	Chain	Res	Type
52	5	130	G
52	5	132	G
52	5	134	G
52	5	136	U
52	5	137	A
52	5	149	G
52	5	159	U
52	5	163	G
52	5	167	A
52	5	169	G
52	5	187	A
52	5	197	A
52	5	198	A
52	5	202	A
52	5	203	C
52	5	212	G
52	5	220	U
52	5	223	G
52	5	230	G
52	5	236	C
52	5	240	U
52	5	241	C
52	5	242	A
52	5	243	G
52	5	247	G
52	5	262	G
52	5	269	A
52	5	277	G
52	5	285	G
52	5	303	A
52	5	324	C
52	5	325	A
52	5	326	C
52	5	328	G
52	5	340	A
52	5	342	G
52	5	343	G
52	5	348	C
52	5	352	A
52	5	361	U
52	5	363	U
52	5	368	C

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Mol	Chain	Res	Type
52	5	369	A
52	5	371	U
52	5	374	G
52	5	377	A
52	5	378	A
52	5	380	G
52	5	384	G
52	5	385	A
52	5	393	A
52	5	396	C
52	5	398	G
52	5	400	G
52	5	402	G
52	5	408	U
52	5	409	G
52	5	414	U
52	5	417	U
52	5	418	U
52	5	419	A
52	5	420	A
52	5	422	A
52	5	425	G
52	5	426	U
52	5	432	U
52	5	433	C
52	5	435	U
52	5	443	G
52	5	449	A
52	5	450	U
52	5	452	A
52	5	453	C
52	5	462	G
52	5	464	A
52	5	465	A
52	5	471	A
52	5	474	G
52	5	476	U
52	5	477	U
52	5	481	U
52	5	482	G
52	5	483	U
52	5	488	U

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Mol	Chain	Res	Type
52	5	489	U
52	5	493	A
52	5	494	A
52	5	503	G
52	5	508	A
52	5	509	C
52	5	510	U
52	5	515	G
52	5	516	C
52	5	525	G
52	5	530	A
52	5	532	U
52	5	545	A
52	5	547	C
52	5	549	U
52	5	557	A
52	5	561	A
52	5	562	U
52	5	567	C
52	5	568	G
52	5	569	U
52	5	570	A
52	5	571	A
52	5	574	C
52	5	575	A
52	5	577	G
52	5	578	C
52	5	586	G
52	5	592	A
52	5	594	A
52	5	605	A
52	5	618	U
52	5	627	U
52	5	628	A
52	5	637	A
52	5	638	A
52	5	639	A
52	5	642	A
52	5	647	U
52	5	650	A
52	5	653	G
52	5	657	G

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Mol	Chain	Res	Type
52	5	660	A
52	5	662	G
52	5	668	U
52	5	672	A
52	5	682	G
52	5	694	U
52	5	698	U
52	5	699	A
52	5	712	A
52	5	715	A
52	5	718	A
52	5	719	G
52	5	720	U
52	5	721	G
52	5	729	C
52	5	731	A
52	5	733	A
52	5	744	U
52	5	745	U
52	5	747	C
52	5	749	G
52	5	752	G
52	5	774	A
52	5	778	A
52	5	785	U
52	5	787	A
52	5	790	U
52	5	791	A
52	5	798	U
52	5	806	A
52	5	810	U
52	5	812	A
52	5	813	A
52	5	814	C
52	5	815	G
52	5	820	A
52	5	825	A
52	5	829	G
52	5	837	G
52	5	838	A
52	5	861	A
52	5	866	A

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Mol	Chain	Res	Type
52	5	867	A
52	5	868	G
52	5	870	A
52	5	877	C
52	5	883	A
52	5	885	U
52	5	895	A
52	5	896	G
52	5	907	A
52	5	908	A
52	5	910	C
52	5	911	G
52	5	921	G
52	5	922	G
52	5	929	C
52	5	934	G
52	5	935	U
52	5	953	A
52	5	955	U
52	5	963	U
52	5	964	A
52	5	965	C
52	5	966	A
52	5	970	A
52	5	972	A
52	5	973	A
52	5	974	C
52	5	975	C
52	5	976	U
52	5	977	U
52	5	984	A
52	5	985	C
52	5	987	U
52	5	988	G
52	5	999	C
52	5	1000	A
52	5	1001	A
52	5	1002	A
52	5	1012	A
52	5	1014	A
52	5	1015	U
52	5	1032	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	5	1034	G
52	5	1041	G
52	5	1044	G
52	5	1045	C
52	5	1047	U
52	5	1056	U
52	5	1072	G
52	5	1075	G
52	5	1077	U
52	5	1083	A
52	5	1085	G
52	5	1086	U
52	5	1092	A
52	5	1095	G
52	5	1115	G
52	5	1119	C
52	5	1121	U
52	5	1122	U
52	5	1125	C
52	5	1134	C
52	5	1135	U
52	5	1136	G
52	5	1141	U
52	5	1142	G
52	5	1154	A
52	5	1158	A
52	5	1159	A
52	5	1171	A
52	5	1172	A
52	5	1176	A
52	5	1187	U
52	5	1188	A
52	5	1200	G
52	5	1201	C
52	5	1203	A
52	5	1208	G
52	5	1211	A
52	5	1213	A
52	5	1215	U
52	5	1225	A
52	5	1232	C
52	5	1233	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	5	1235	C
52	5	1242	U
52	5	1254	A
52	5	1255	A
52	5	1256	U
52	5	1257	C
52	5	1260	U
52	5	1261	A
52	5	1271	U
52	5	1272	C
52	5	1273	A
52	5	1274	G
52	5	1276	U
52	5	1279	G
52	5	1292	A
52	5	1293	A
52	5	1294	U
52	5	1296	C
52	5	1310	C
52	5	1313	A
52	5	1314	A
52	5	1319	U
52	5	1320	A
52	5	1324	A
52	5	1327	G
52	5	1331	A
52	5	1333	C
52	5	1335	G
52	5	1337	U
52	5	1338	A
52	5	1340	G
52	5	1343	G
52	5	1352	A
52	5	1356	U
52	5	1369	A
52	5	1372	C
52	5	1373	A
52	5	1375	C
52	5	1385	A
52	5	1394	G
52	5	1397	G
52	5	1400	A

Continued on next page...

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Mol	Chain	Res	Type
52	5	1404	U
52	5	1415	G
52	5	1417	U
52	5	1421	A
52	5	1427	U
52	5	1428	A
52	5	1429	G
52	5	1433	G
52	5	1448	A
52	5	1450	C
52	5	1465	U
52	5	1466	U
52	5	1467	A
52	5	1468	A
52	5	1469	G
52	5	1472	G
52	5	1474	A
52	5	1476	C
52	5	1477	A
52	5	1478	A
52	5	1479	G
52	5	1481	U
52	5	1482	A
52	5	1492	G
52	5	1493	A
52	5	1495	C
52	5	1504	G
52	5	1505	G
53	6	3	G
53	6	5	C
53	6	10	A
53	6	11	G
53	6	17	U
53	6	18	C
53	6	20	G
53	6	21	U
53	6	22	A
53	6	28	A
53	6	34	U
53	6	36	A
53	6	43	G
53	6	44	U

Continued on next page...

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Mol	Chain	Res	Type
53	6	48	U
53	6	49	C
53	6	54	G
53	6	56	U
53	6	57	C
53	6	58	G
53	6	59	A
53	6	61	U
53	6	62	C
53	6	64	G
53	6	71	A
53	6	72	C
53	6	73	C
53	6	75	C
53	6	76	C
53	8	3	G
53	8	5	C
53	8	10	A
53	8	11	G
53	8	17	U
53	8	18	C
53	8	20	G
53	8	21	U
53	8	22	A
53	8	28	A
53	8	34	U
53	8	36	A
53	8	43	G
53	8	44	U
53	8	48	U
53	8	49	C
53	8	54	G
53	8	56	U
53	8	57	C
53	8	58	G
53	8	59	A
53	8	61	U
53	8	62	C
53	8	64	G
53	8	71	A
53	8	72	C
53	8	73	C

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Mol	Chain	Res	Type
53	8	75	C
53	8	76	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	3	296	U
50	3	311	G
50	3	402	A
50	3	410	G
50	3	425	U
50	3	500	U
50	3	514	A
50	3	688	U
50	3	881	A
50	3	903	A
50	3	967	U
50	3	996	A
50	3	1048	A
50	3	1082	A
50	3	1209	U
50	3	1211	U
50	3	1297	U
50	3	1507	G
50	3	1570	A
50	3	1583	G
50	3	1587	U
50	3	1588	A
50	3	1820	U
50	3	2132	G
50	3	2180	U
50	3	2342	U
50	3	2504	C
50	3	2506	C
50	3	2604	U
50	3	2635	G
50	3	2668	A
50	3	2764	U
50	3	2823	A
50	3	2897	G
51	4	10	C
51	4	54	U

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Mol	Chain	Res	Type
51	4	59	A
52	5	197	A
52	5	425	G
52	5	448	A
52	5	748	U
52	5	975	C
53	6	16	G
53	6	19	G
53	6	56	U
53	6	58	G
53	8	16	G
53	8	19	G
53	8	56	U
53	8	58	G

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](#)

There are no ligands in this entry.

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.

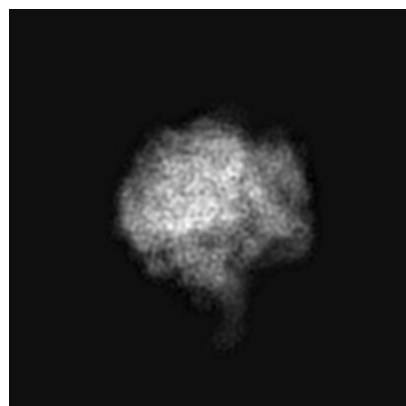
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13277. These allow visual inspection of the internal detail of the map and identification of artifacts.

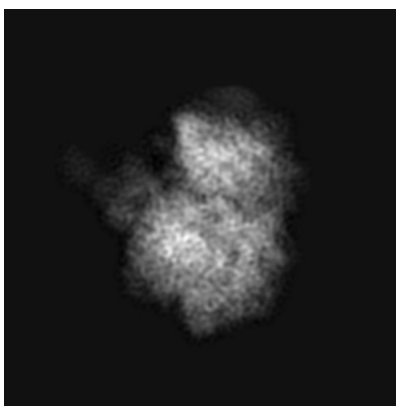
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

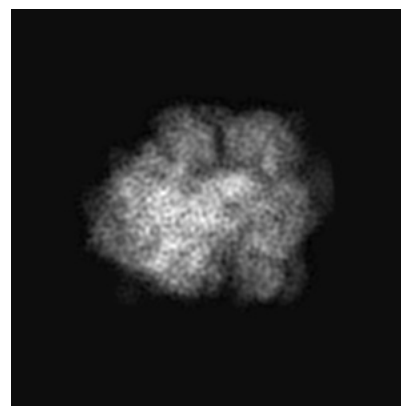
6.1.1 Primary map



X

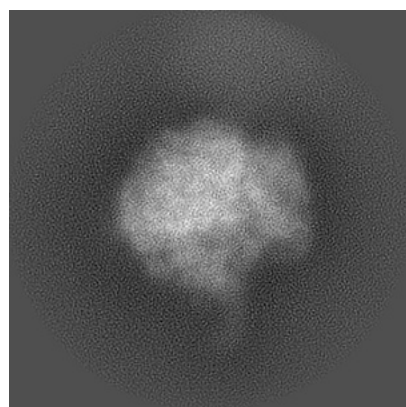


Y

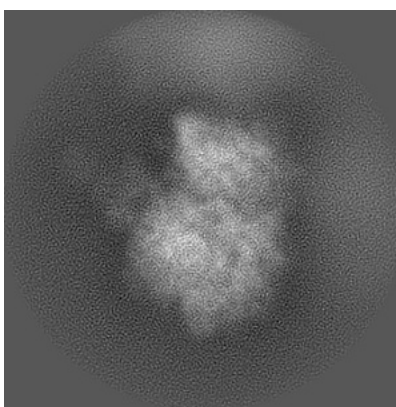


Z

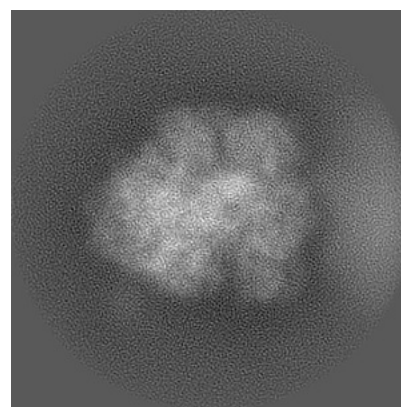
6.1.2 Raw map



X



Y

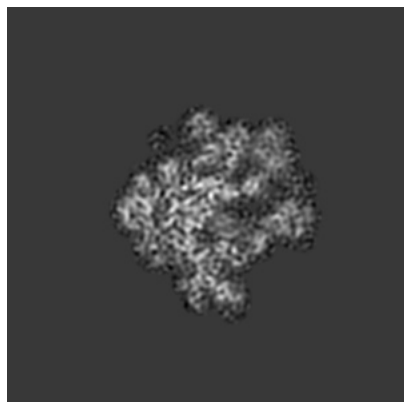


Z

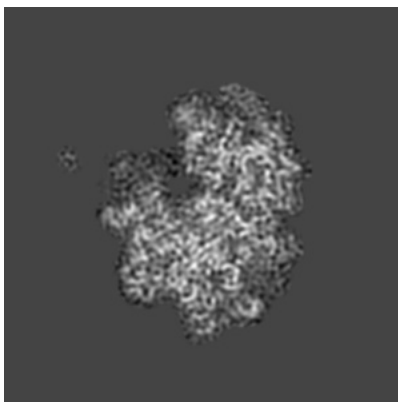
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

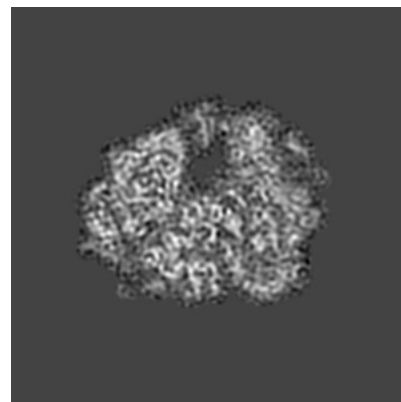
6.2.1 Primary map



X Index: 128

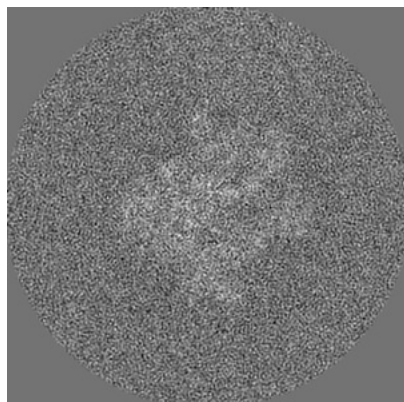


Y Index: 128

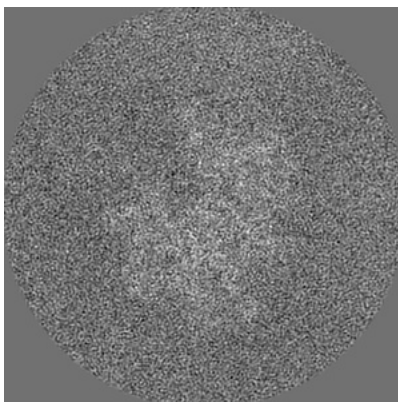


Z Index: 128

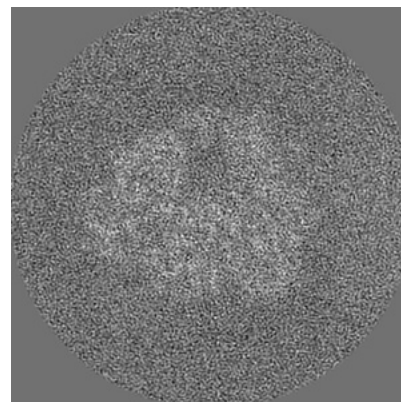
6.2.2 Raw map



X Index: 128



Y Index: 128

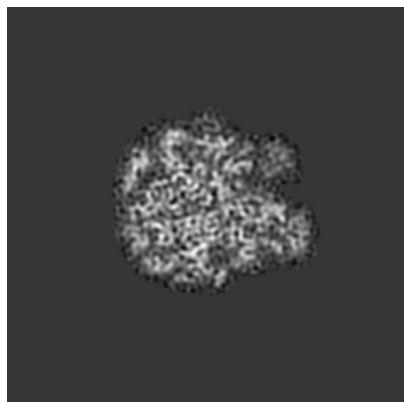


Z Index: 128

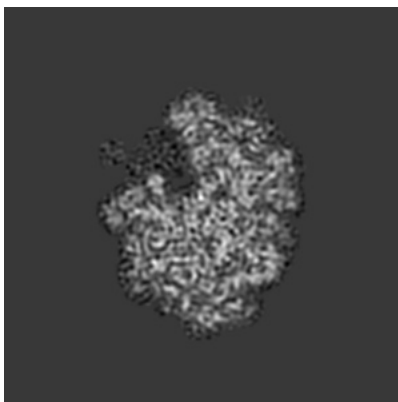
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

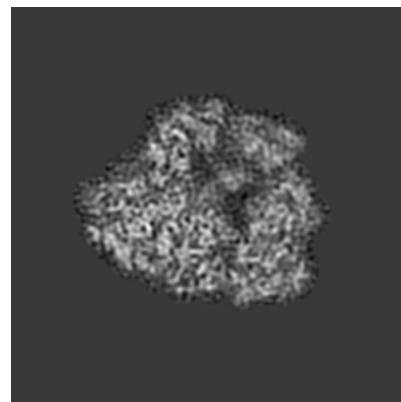
6.3.1 Primary map



X Index: 104

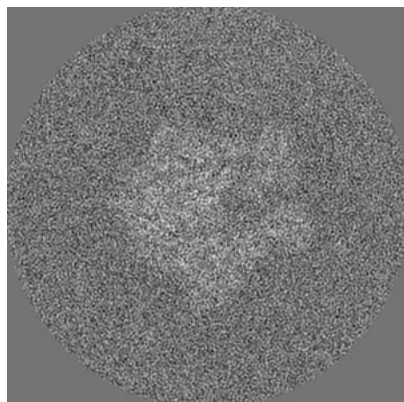


Y Index: 120

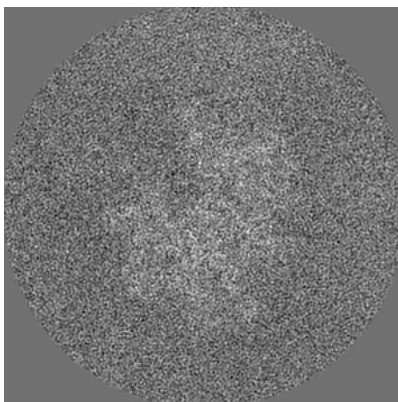


Z Index: 120

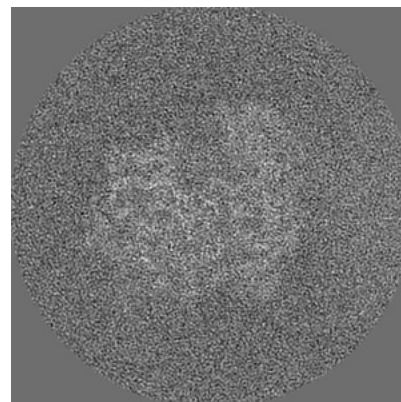
6.3.2 Raw map



X Index: 120



Y Index: 128

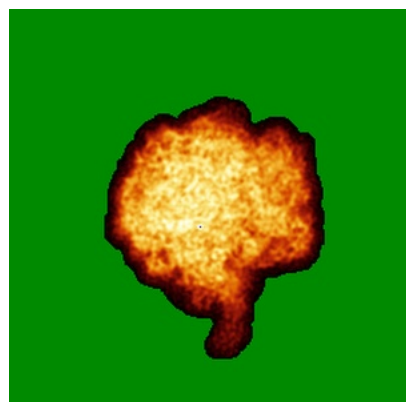


Z Index: 135

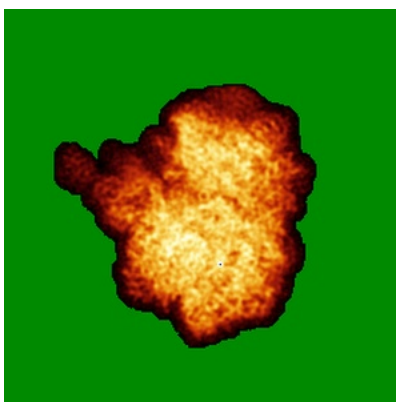
The images above show the largest variance slices of the map in three orthogonal directions.

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

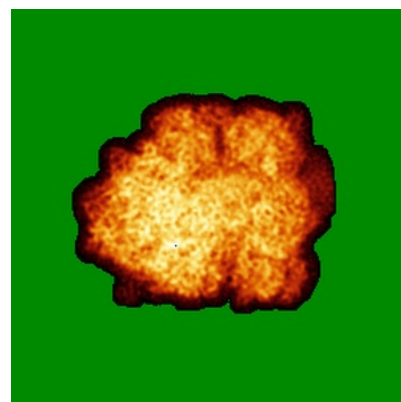
6.4.1 Primary map



X

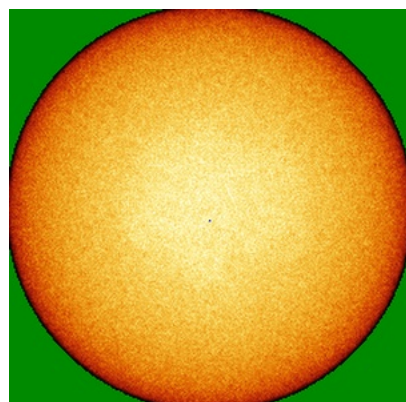


Y

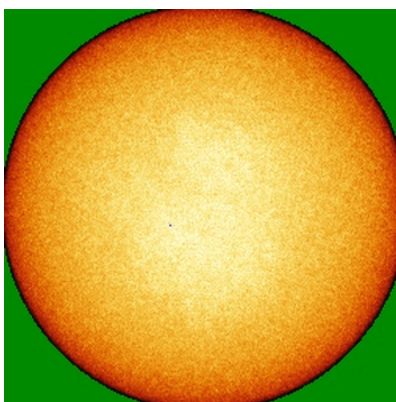


Z

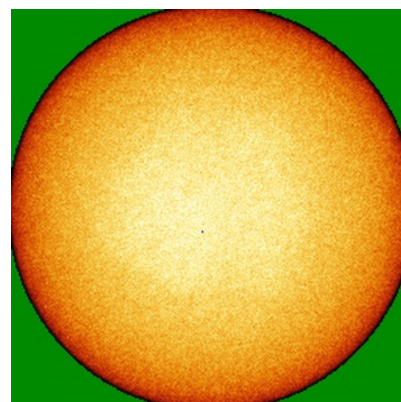
6.4.2 Raw map



X



Y



Z

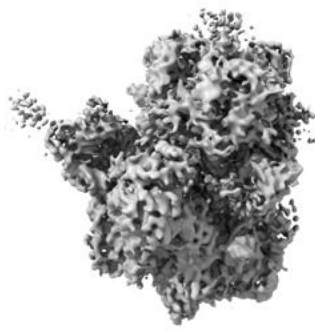
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



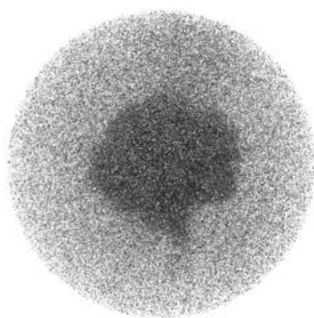
Y



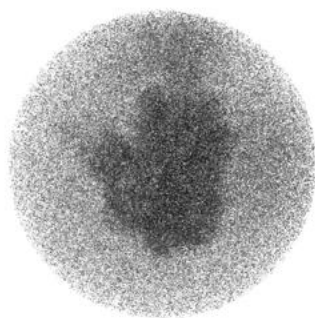
Z

The images above show the 3D surface view of the map at the recommended contour level 0.47. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

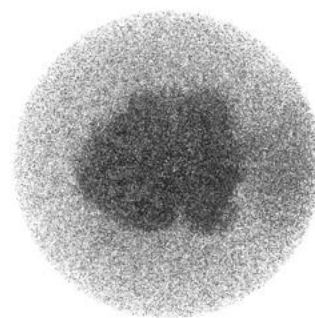
6.5.2 Raw map



X



Y



Z

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

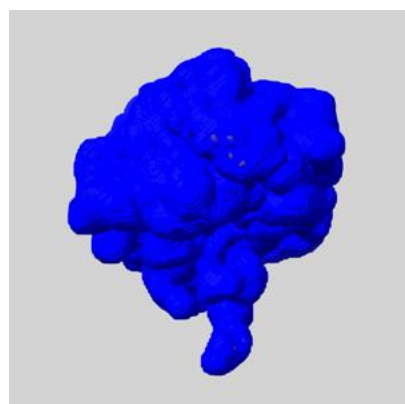
6.6 Mask visualisation [i](#)

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

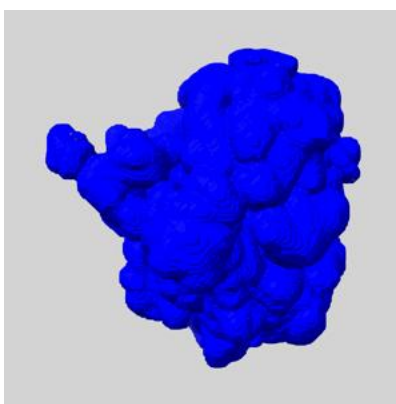
A mask typically either:

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

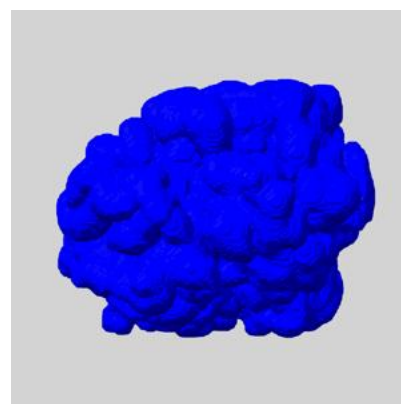
6.6.1 emd_13277_msk_1.map [i](#)



X



Y

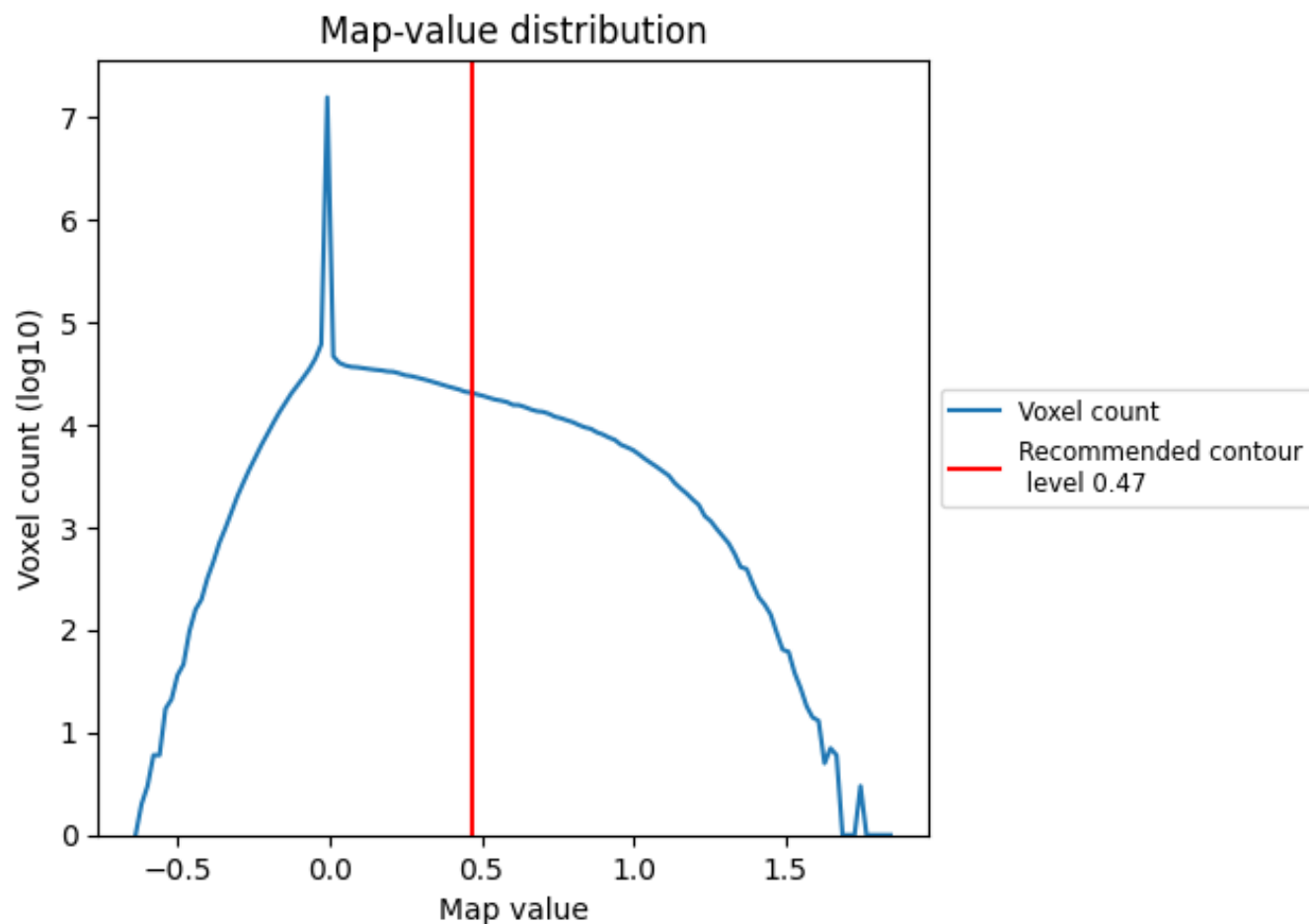


Z

7 Map analysis [i](#)

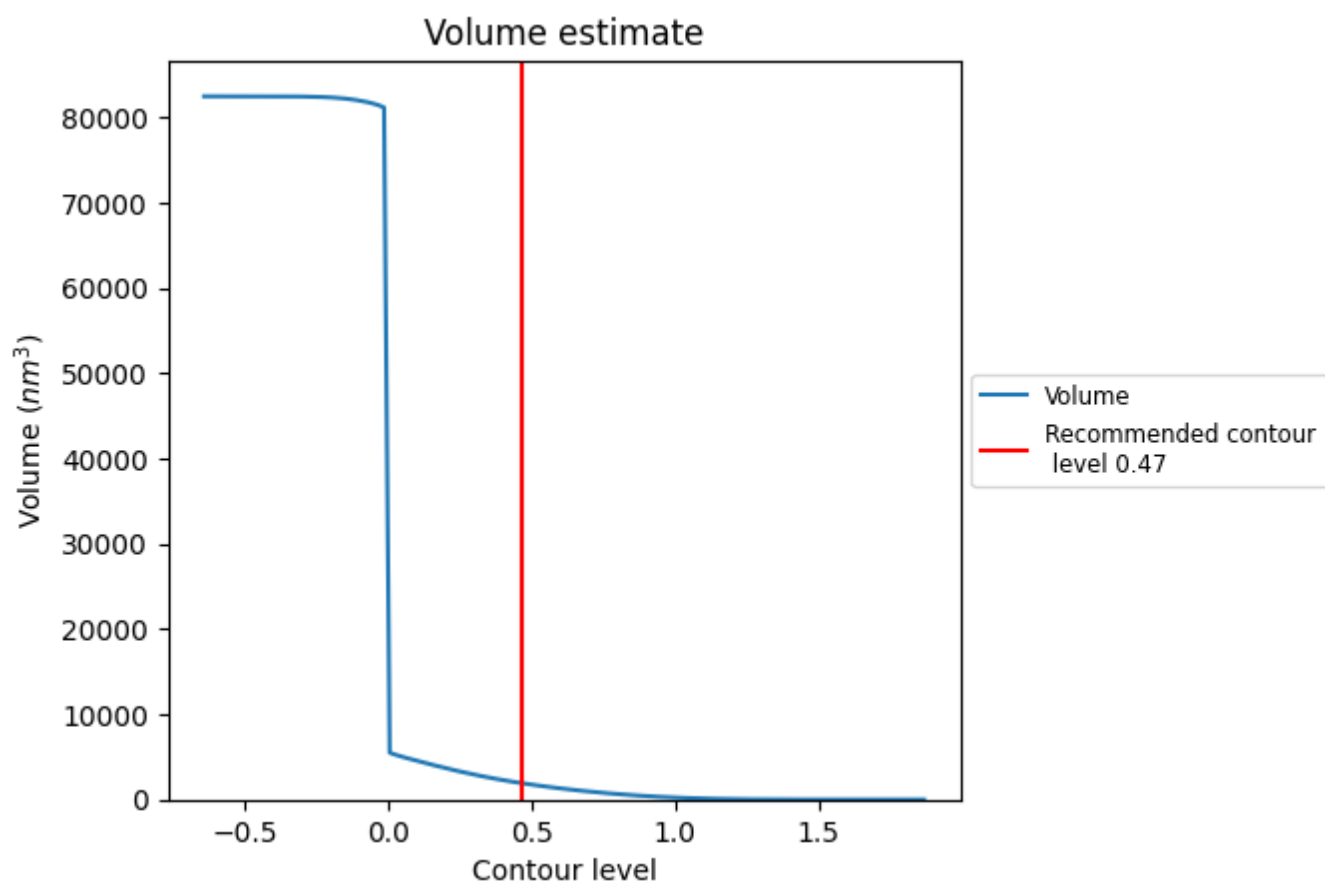
This section contains the results of statistical analysis of the map.

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.

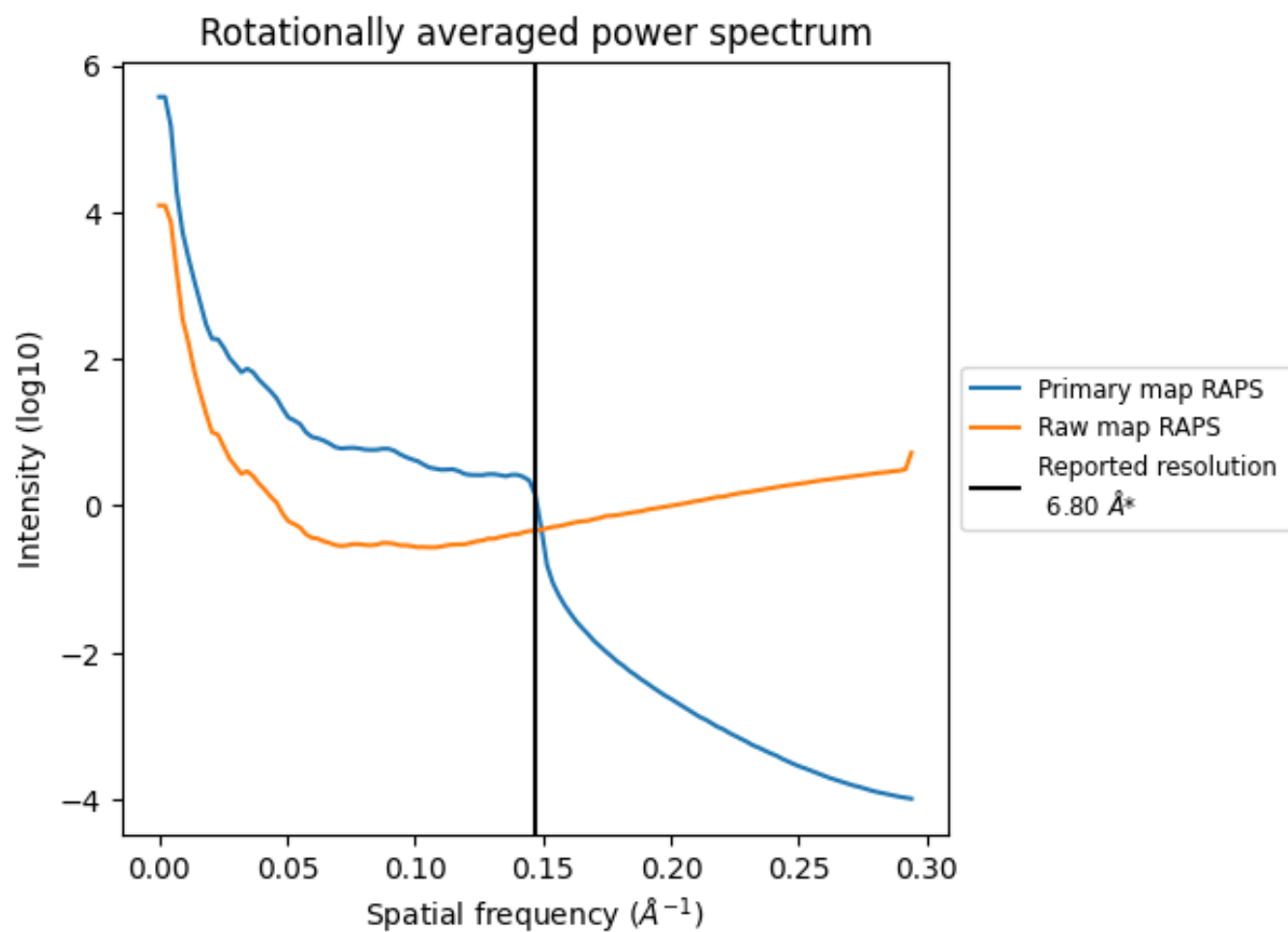
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1905 nm³; this corresponds to an approximate mass of 1721 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 ⓘ

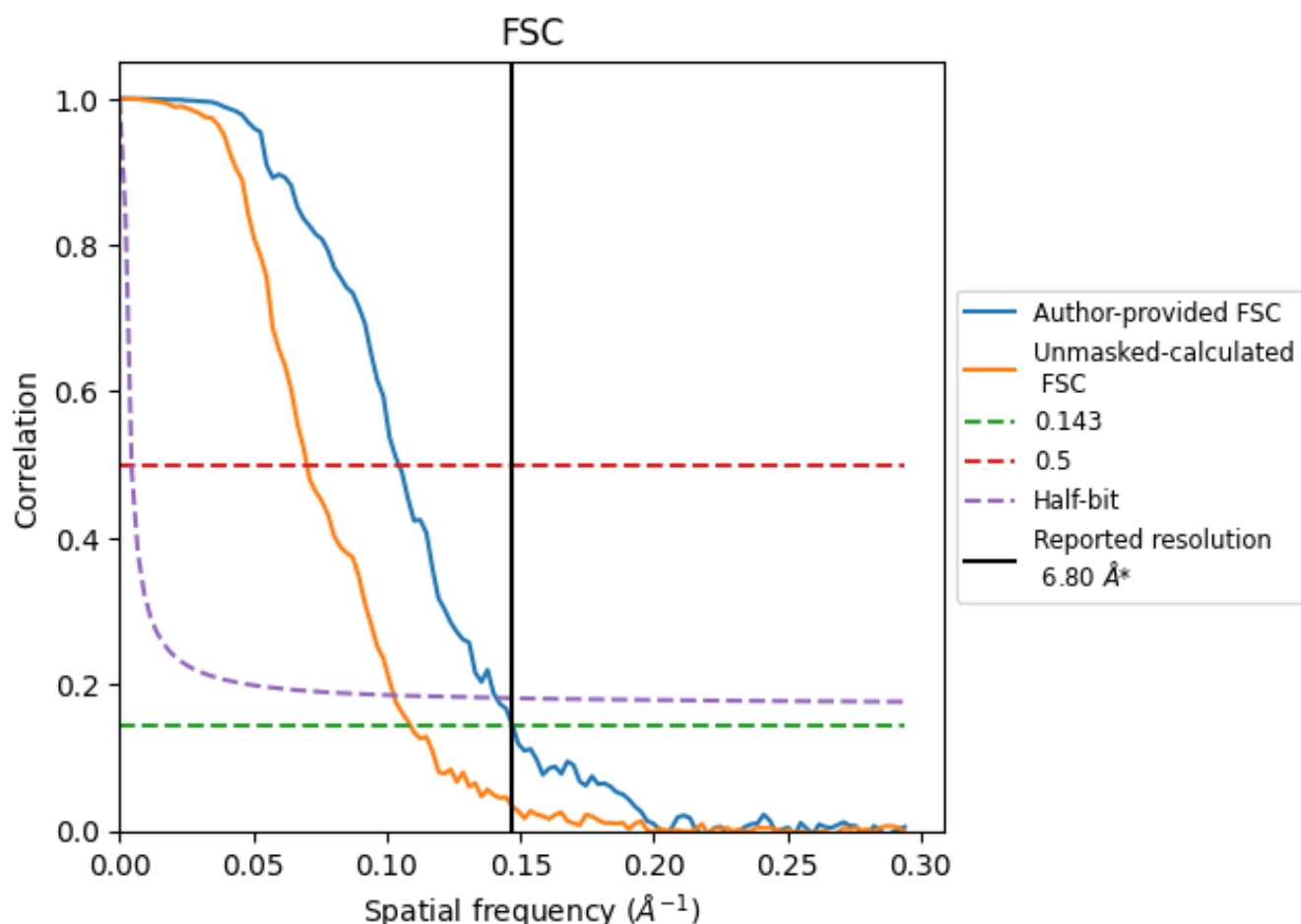


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

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 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

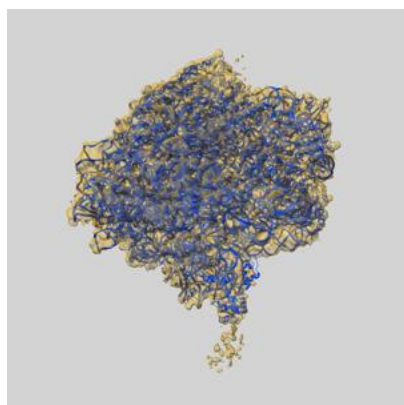
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.79	9.57	7.09
Unmasked-calculated*	9.17	14.27	9.74

*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 9.17 differs from the reported value 6.8 by more than 10 %

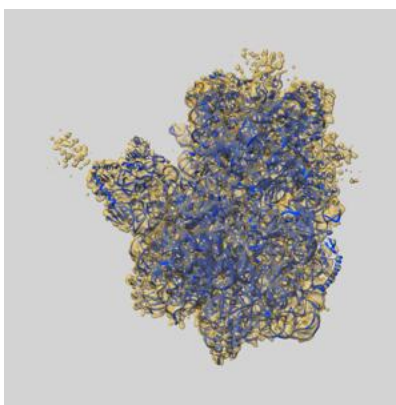
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13277 and PDB model 7PAM. Per-residue inclusion information can be found in section [3](#) on page [13](#).

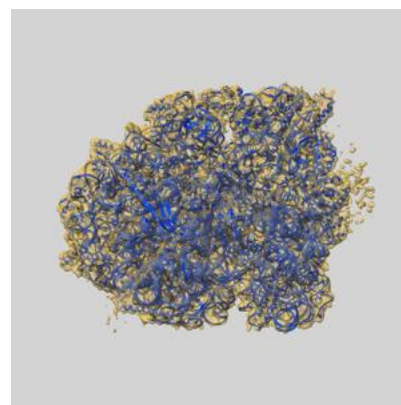
9.1 Map-model overlay [i](#)



X



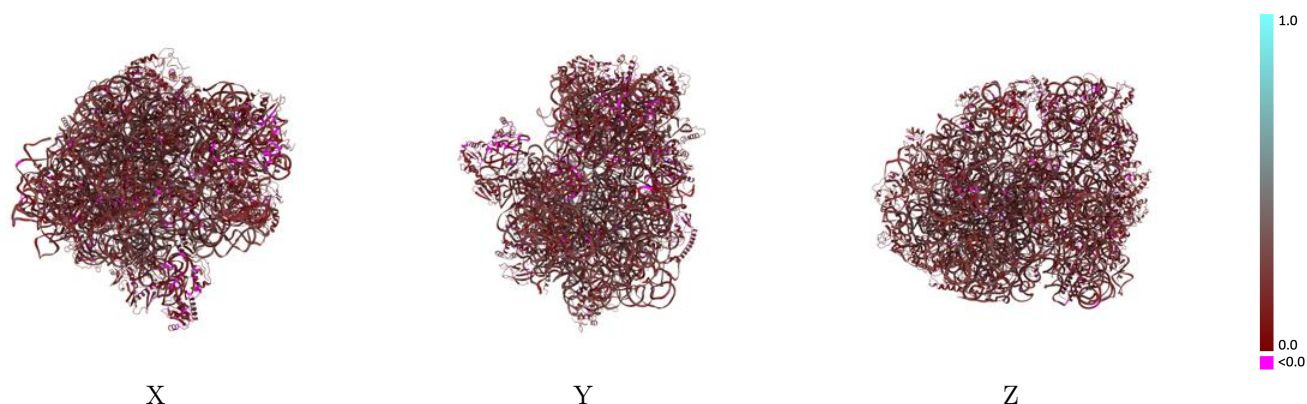
Y



Z

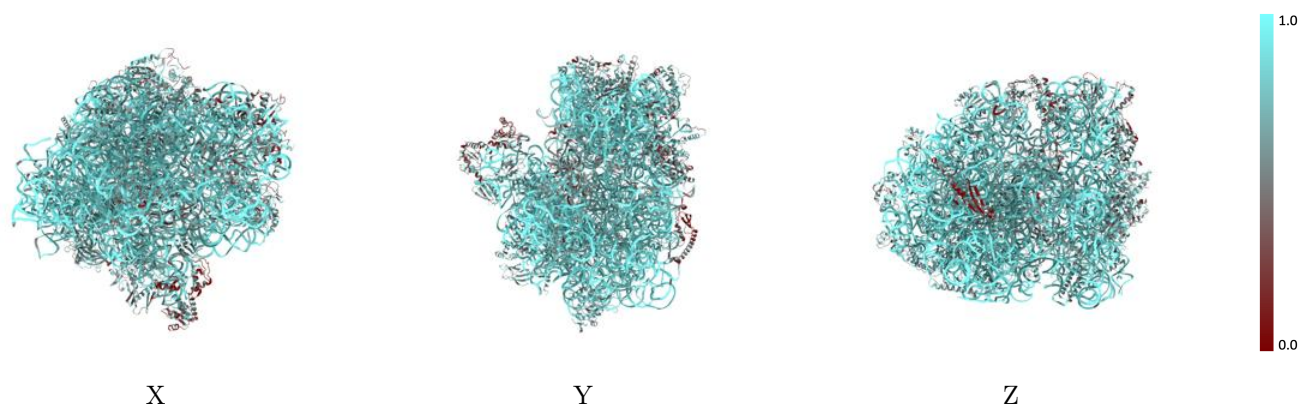
The images above show the 3D surface view of the map at the recommended contour level 0.47 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



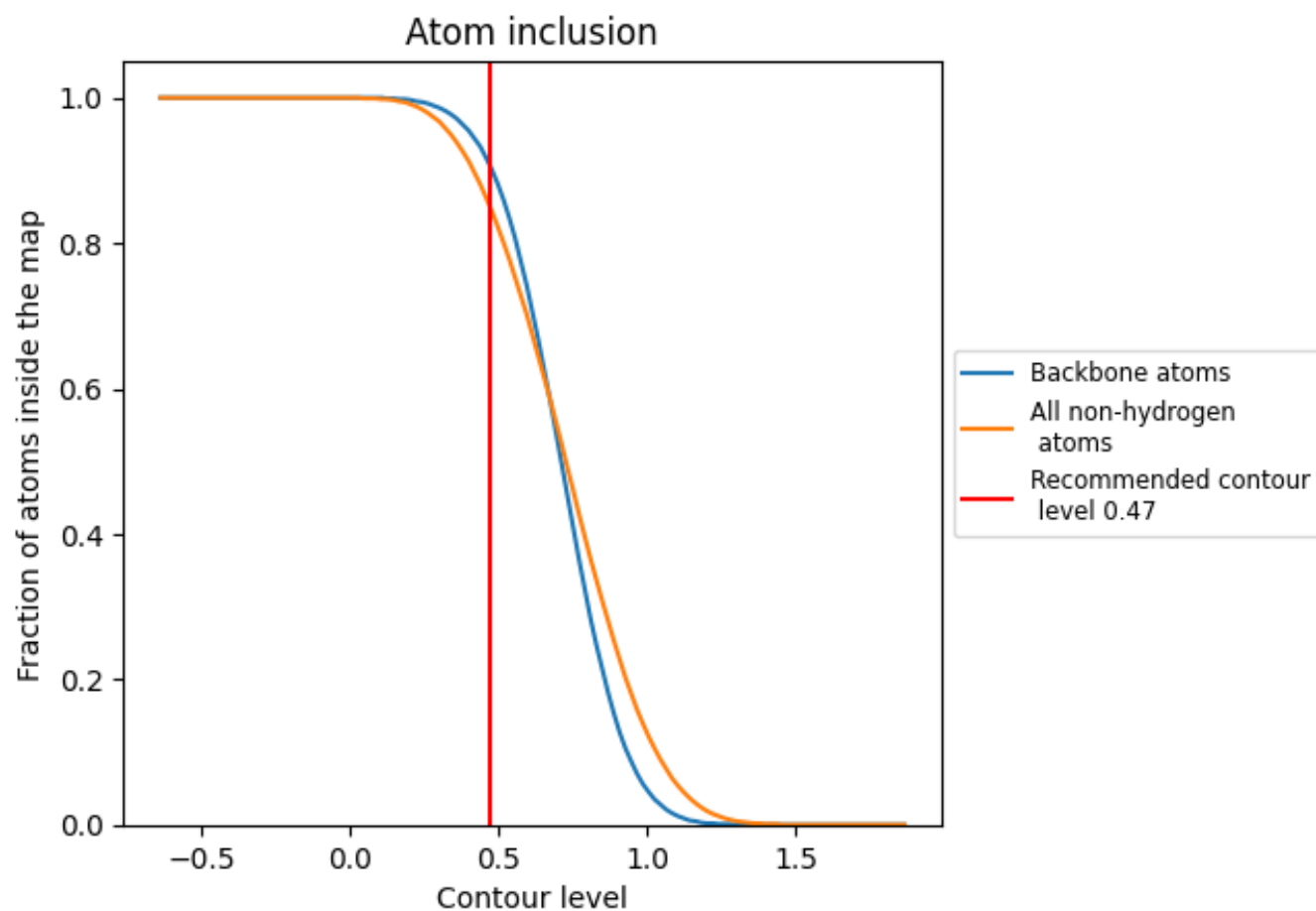
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.47).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.47) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.2070
0	 0.7780	 0.2020
1	 0.7360	 0.1820
2	 0.7740	 0.1920
3	 0.9510	 0.2250
4	 0.9400	 0.2230
5	 0.9430	 0.2100
6	 0.5790	 0.0940
8	 0.8780	 0.1940
A	 0.6320	 0.2010
B	 0.6220	 0.1920
C	 0.6310	 0.1730
D	 0.6790	 0.1900
E	 0.5970	 0.1960
F	 0.5620	 0.1730
G	 0.6620	 0.1780
H	 0.6080	 0.1660
I	 0.5900	 0.1650
J	 0.6780	 0.1820
K	 0.7140	 0.1950
L	 0.5620	 0.1710
M	 0.6860	 0.1500
N	 0.6370	 0.1840
O	 0.7680	 0.1960
P	 0.6930	 0.1740
Q	 0.6800	 0.1850
R	 0.5880	 0.1280
S	 0.7160	 0.1710
T	 0.6900	 0.1930
a	 0.7530	 0.1910
b	 0.6940	 0.1780
c	 0.7020	 0.2030
d	 0.6350	 0.1710
e	 0.6430	 0.2010
f	 0.2820	 0.1690



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Chain	Atom inclusion	Q-score
g	 0.4810	 0.1440
h	 0.3030	 0.1390
i	 0.7400	 0.1920
j	 0.6390	 0.1800
k	 0.7420	 0.1980
l	 0.7550	 0.2050
m	 0.7670	 0.1890
n	 0.7070	 0.2000
o	 0.6830	 0.2000
p	 0.7490	 0.1670
q	 0.7000	 0.1990
r	 0.7380	 0.2000
s	 0.7150	 0.2000
t	 0.5690	 0.1720
u	 0.6860	 0.1560
v	 0.7560	 0.1780
w	 0.6900	 0.2060
x	 0.5630	 0.1940
y	 0.7880	 0.2140
z	 0.7330	 0.1960