



wwPDB EM Validation Summary Report ⓘ

Dec 8, 2025 – 01:11 PM JST

PDB ID : 9KN5 / pdb_00009kn5
EMDB ID : EMD-62453
Title : Structure of the human 40S ribosome complexed with HCV IRES, eIF1A and eIF3
Authors : Iwasaki, W.; Kashiwagi, K.; Sakamoto, A.; Nishimoto, M.; Takahashi, M.; Machida, K.; Imataka, H.; Matsumoto, A.; Shichino, Y.; Iwasaki, S.; Imami, K.; Ito, T.
Deposited on : 2024-11-18
Resolution : 3.20 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

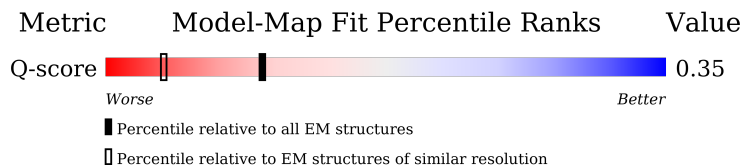
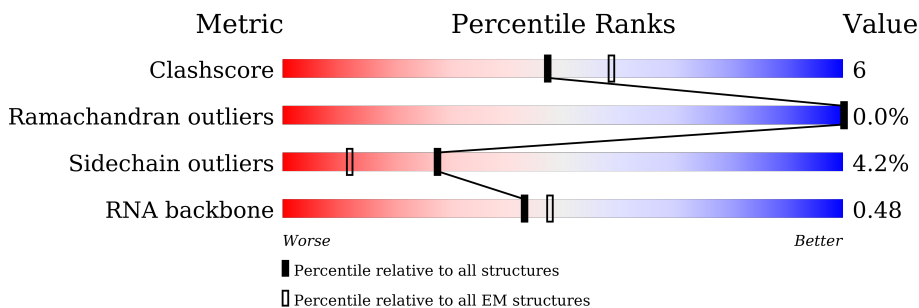
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











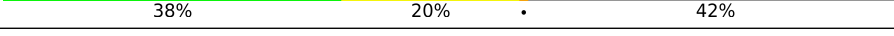

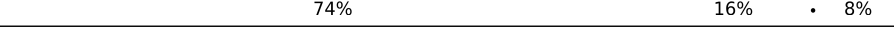
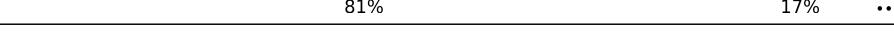

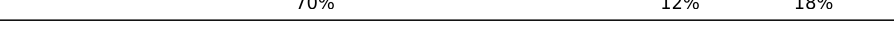


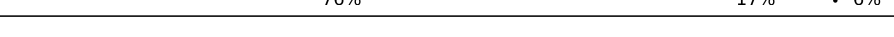

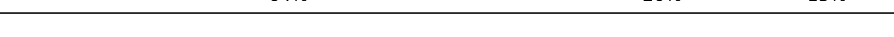






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1A	144	 49% 19% 32%
2	SA	295	 57% 15% 27%
3	SB	264	 67% 13% 20%









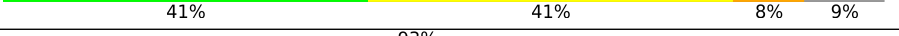
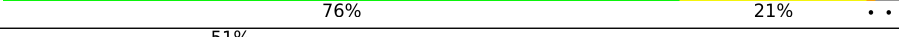
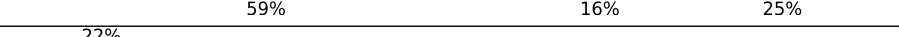


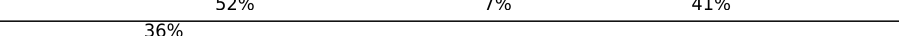

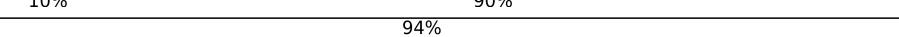


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Mol	Chain	Length	Quality of chain
4	SC	293	
5	SD	243	
6	SE	263	
7	SF	204	
8	SG	249	
9	SH	194	
10	SI	208	
11	SJ	194	
12	SK	165	
13	SL	158	
14	Sf	132	
15	SN	151	
16	SO	151	
17	SP	145	
18	SQ	146	
19	SR	135	
20	SS	152	
21	ST	145	
22	SU	119	
23	SV	83	
24	SW	130	
25	SX	143	
26	SY	133	
27	SZ	125	
28	Sa	115	

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Mol	Chain	Length	Quality of chain
29	Sb	84	 88% 11% .
30	Sc	69	 57% 32% . 10%
31	Sd	56	 79% 18% . .
32	Se	59	 76% 12% 12%
33	sh	156	 29% 11% . 59%
34	Sg	317	 79% 19% . .
35	Ln	25	 64% 32% .
36	S2	1869	 60% 31% . 6%
37	zz	332	 41% 41% 8% 9%
38	3m	374	 93% 76% 21% . .
39	3f	357	 51% 59% 16% 25%
40	3a	1382	 22% 35% 7% . 57%
41	3e	445	 83% 87% 9% .
42	3c	913	 38% 52% 7% 41%
43	3h	352	 36% 70% 20% 10%
44	3d	548	 7% 10% 90%
45	3k	218	 94% 85% 13% . .
46	3l	564	 86% 73% 18% . 8%

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 108797 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 Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	98	Total	C	N	O	S	0	0
			780	492	137	147	4		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SD	226	Total	C	N	O	S	0	0
			1756	1119	316	314	7		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SE	260	Total	C	N	O	S	0	0
			2065	1319	384	354	8		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	192	Total	C	N	O	S	0	0
			1518	948	287	276	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SH	187	Total	C	N	O	S	0	0
			1506	961	277	267	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SI	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 12 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SL	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Sf	121	Total	C	N	O	S	0	0
			935	586	165	175	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SO	135	Total	C	N	O	S	0	0
			1007	617	198	186	6		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SP	119	Total	C	N	O	S	0	0
			984	625	187	165	7		

- Molecule 18 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SS	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SZ	75	Total	C	N	O	S	0	0
			601	385	111	104	1		

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sa	100	Total	C	N	O	S	0	0
			803	501	166	131	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Sc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Se	52	Total	C	N	O	S	0	0
			417	259	92	65	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	sh	64	Total	C	N	O	S	0	0
			518	327	99	85	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 36 is a RNA chain called Chains: S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S2	1759	Total	C	N	O	P	6	0
			37669	16814	6767	12324	1764		

- Molecule 37 is a RNA chain called Chains: zz.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	zz	302	Total	C	N	O	P	0	0
			6443	2871	1148	2122	302		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3m	363	Total	C	N	O	S	0	0
			2639	1666	450	511	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3f	269	Total	C	N	O	S	0	0
			2063	1303	354	394	12		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3a	592	Total	C	N	O	S	0	0
			4475	2834	803	817	21		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3e	430	Total	C	N	O	S	0	0
			3224	2053	561	594	16		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3c	543	Total	C	N	O	S	0	0
			3924	2463	721	716	24		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3h	318	Total	C	N	O	S	0	0
			2520	1599	431	475	15		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3d	55	Total	C	N	O	S	0	0
			347	222	65	59	1		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3k	215	Total	C	N	O	S	0	0
			1475	932	251	282	10		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3l	520	Total	C	N	O	S	0	0
			4335	2808	715	793	19		

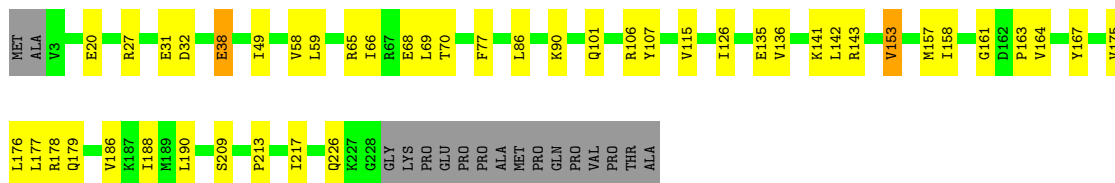
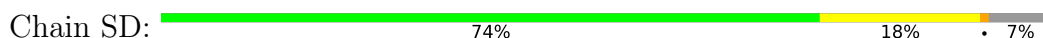
- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
47	Sa	1	Total	Zn	0
			1	1	
47	sh	1	Total	Zn	0
			1	1	

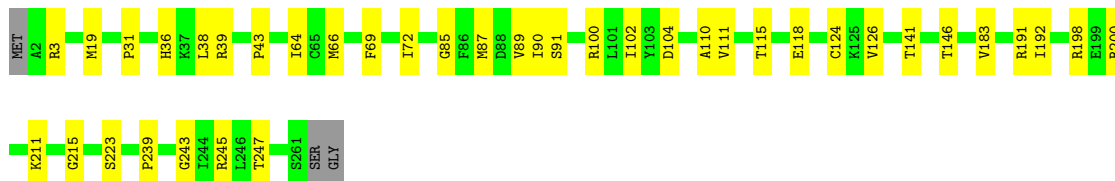
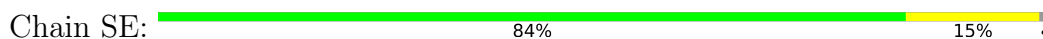
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	S2	8	Total	Mg	0
			8	8	

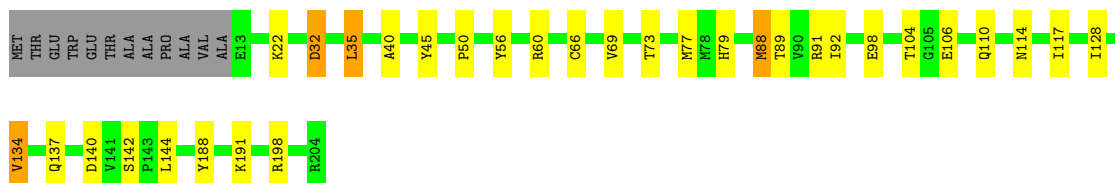
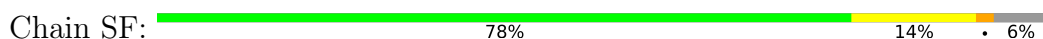
- Molecule 5: 40S ribosomal protein S3



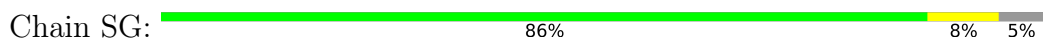
- Molecule 6: 40S ribosomal protein S4, X isoform



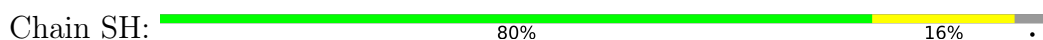
- Molecule 7: 40S ribosomal protein S5

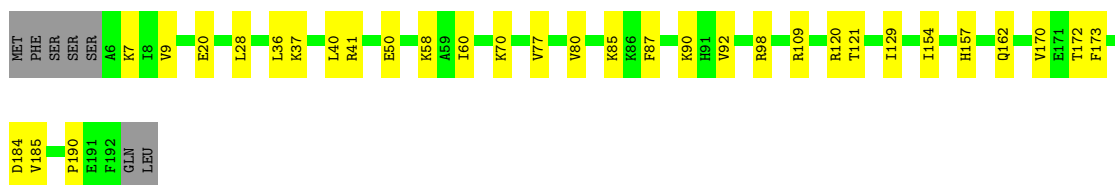


- Molecule 8: 40S ribosomal protein S6



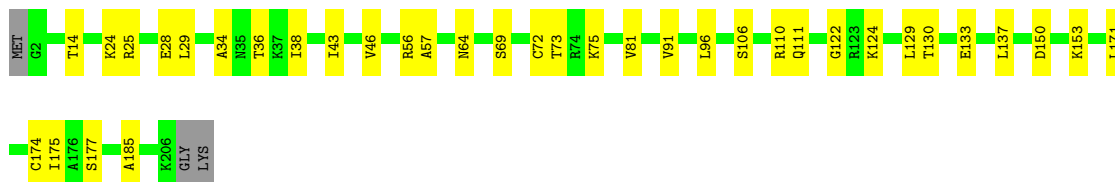
- Molecule 9: 40S ribosomal protein S7





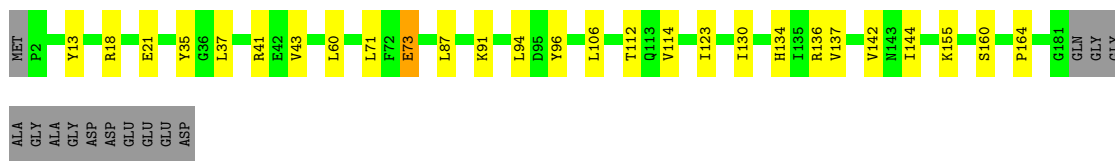
- Molecule 10: 40S ribosomal protein S8

Chain SI: 81% 17% .



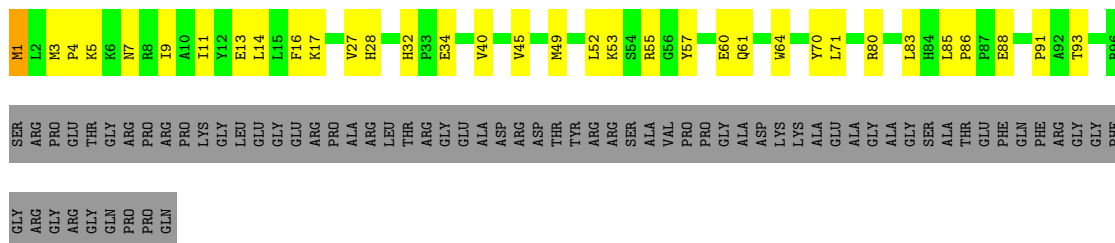
- Molecule 11: 40S ribosomal protein S9

Chain SJ: 79% 13% . 7%



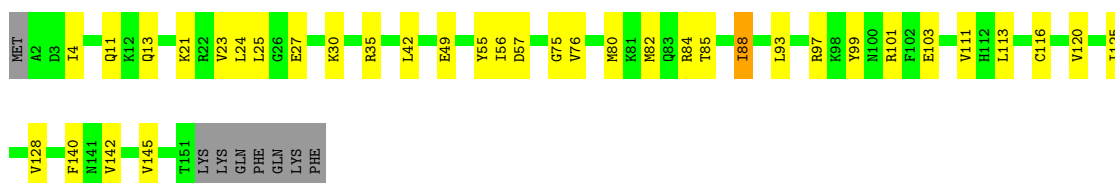
- Molecule 12: 40S ribosomal protein S10

Chain SK: 38% 20% . 42%

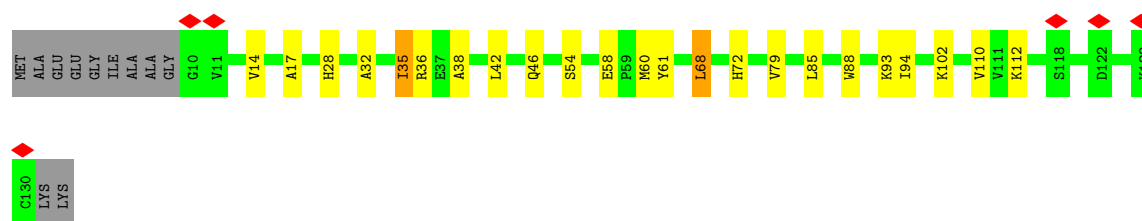
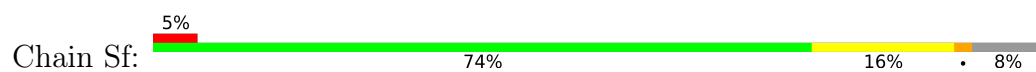


- Molecule 13: 40S ribosomal protein S11

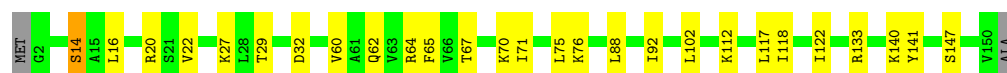
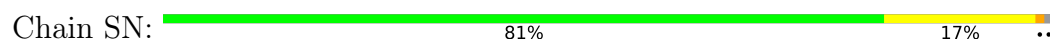
Chain SL: 72% 22% . 5%



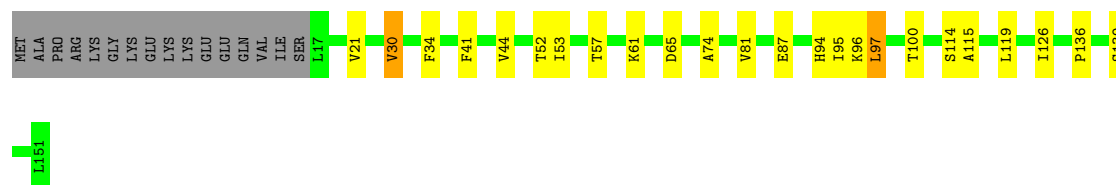
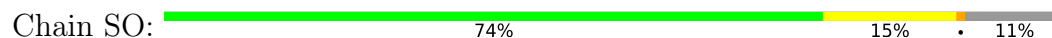
- Molecule 14: 40S ribosomal protein S12



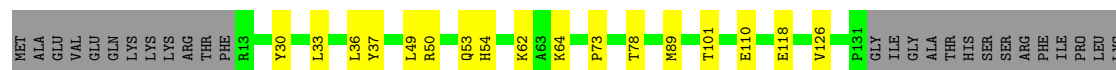
- Molecule 15: 40S ribosomal protein S13



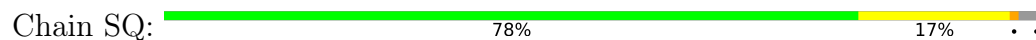
- Molecule 16: 40S ribosomal protein S14



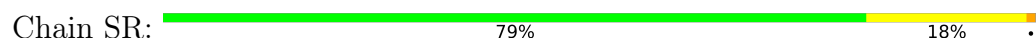
- Molecule 17: 40S ribosomal protein S15




- Molecule 18: 40S ribosomal protein S16

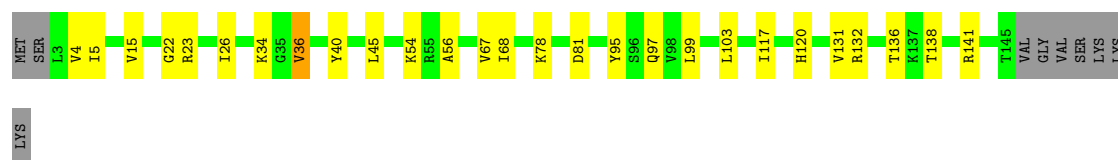


- Molecule 19: 40S ribosomal protein S17




- Molecule 20: 40S ribosomal protein S18

Chain SS:  76% 17% 6%



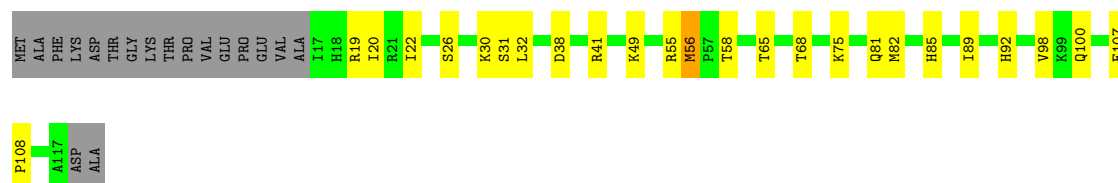
- Molecule 21: 40S ribosomal protein S19

Chain ST:  88% 10% 2%




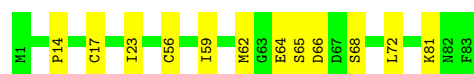
- Molecule 22: 40S ribosomal protein S20

Chain SU:  64% 20% 15%



- Molecule 23: 40S ribosomal protein S21

Chain SV:  86% 14%




- Molecule 24: 40S ribosomal protein S15a

Chain SW:  85% 12% 3%




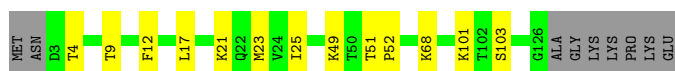
- Molecule 25: 40S ribosomal protein S23

Chain SX:  87% 11% 2%



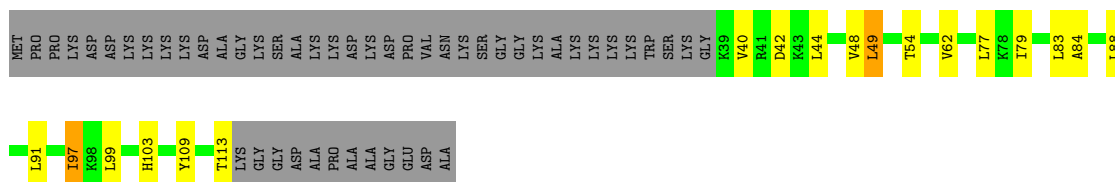
- Molecule 26: 40S ribosomal protein S24

Chain SY:  83% 10% 7%



- Molecule 27: 40S ribosomal protein S25

Chain SZ: 46% 13% 40%



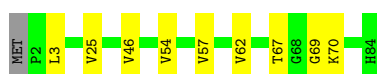
- Molecule 28: 40S ribosomal protein S26

Chain Sa: 77% 10% 13%



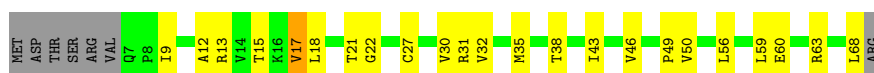
- Molecule 29: 40S ribosomal protein S27

Chain Sb: 88% 11%



- Molecule 30: 40S ribosomal protein S28

Chain Sc: 57% 32% 10%



- Molecule 31: 40S ribosomal protein S29

Chain Sd: 79% 18%



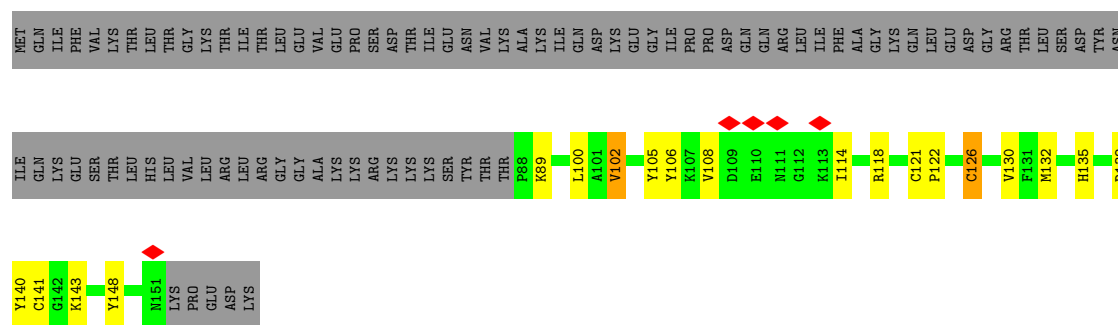
- Molecule 32: 40S ribosomal protein S30

Chain Se: 76% 12% 12%




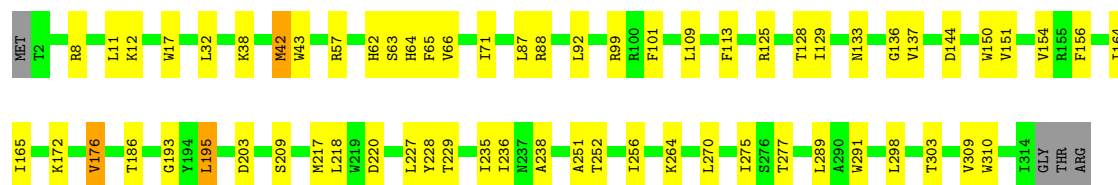
- Molecule 33: Ubiquitin-40S ribosomal protein S27a

Chain sh:  29% 11% 59%



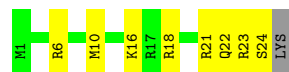
- Molecule 34: Receptor of activated protein C kinase 1

Chain Sg:  79% 19% 2%



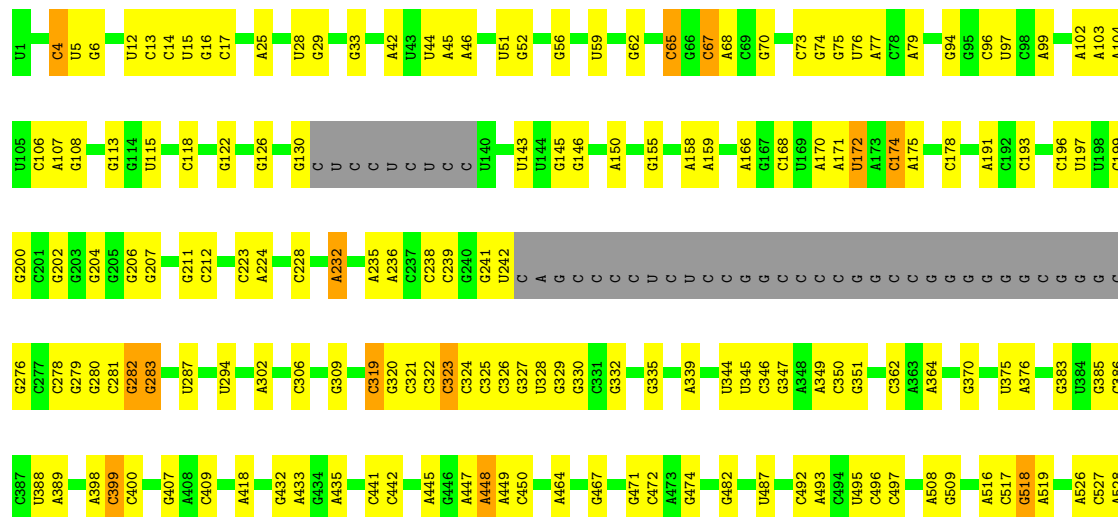
- Molecule 35: 60S ribosomal protein L41

Chain Ln:  64% 32% 4%



- Molecule 36: Chains: S2

Chain S2:  60% 31% 6%

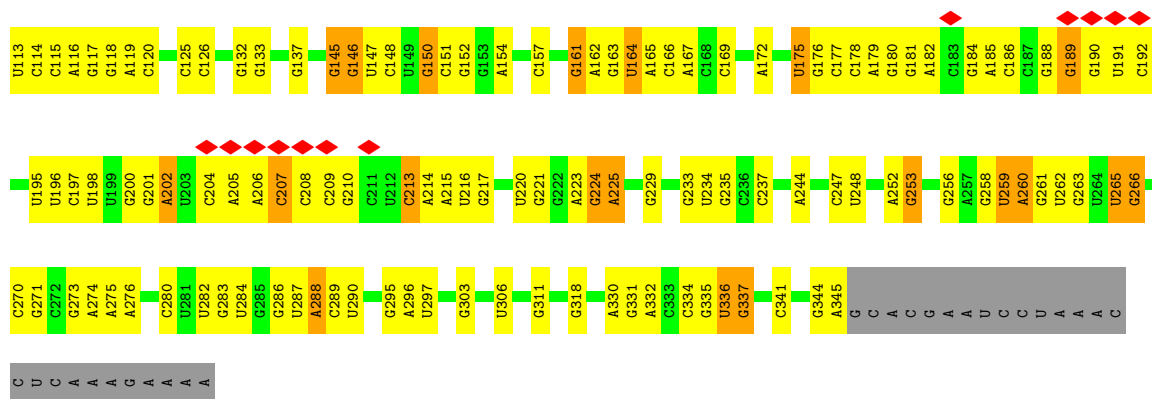


U1808	C1710	A1589	C1338	U1248	C1118	C974	G874	U	C	G835	A529
A1809	U1711	U1595	A1452	C1249	A1119	C975	A875	C	G	U530	
U1810	A1712	U1596	A1454	A1250	U1120	G975	C876	C	A	C639	
C1811	C1713	C1597	U1462	C1251	G1121		C877	C	G	A640	
A1813	A1715		U1463	A1253	A1133	A980	G878	C	C	A533	
G1814		A1601	U1463			A981		C	C	G534	
U1820	A1719	U1602	U1463	G1256	C1138	G982	U883	G786	A	G535	
U1821	G1722	G1603	A1489	U1257	C1139	A983	C884	A794	C	A536	
A1822	G1723	G1606	G1490	A1258	G1140	G984	U885	C790	C	U647	
A1823	A1724	C1609	U1492	A1259	A1144	G985	A886	C791	G	U538	
A1824	G1736	C1609	C1493	C1264	A1145	A990	U889	C792	C	U649	
A1825	G1737	C1618	U1494	G1274	A1149	G991	U890	C793	C	A650	
G1826			G1495	U1372		A992	A891	A795			
			U1496	G1275	C1153	A996	U892	G796		A655	
G1829	C1740	U1621	A1497	A1276	U1154	A997	G893	C797		G544	
	U1741	U1622	A1498	C1277			U894	G798		C660	
U1838	G1744	A1623		A1278	C1162	U1002	G895	U799		G546	
C1842	A1745	C1628	A1508	C1279	C1163	G1010	U896	U801		G547	
G1843		C1629	C1513	G1280	G1164	A1011	U897	U801		C663	
U1844	G1748	A1630	G1514	C1283			U898	C738		A669	
A1845			A1382		G1171	U1016	C900	U804		C550	
G1846	C1751	U1643	A1383	U1286	U1174	U1017	G901	U805		A671	
	C1752	C1644	A1522	A1287	U1175	U1018	U906			U551	
G1849	C1753	G1652	C1523	U1288			A908			A672	
A1850	G1754	U1653	A1531	A1291	A1189	A1023	U907	A825		G674	
A1851	C1755	G1654	C1532	A1295	A1190	U1025	A913	A826		G552	
	C1756		A1533	A1298	A1195	C1026	U914	A827		U553	
G1858	G1757	A1661	C1534	G1298		U1045		C834		A554	
A1859	U1758	A1664	U1535	A1301	G1198	U1061	U917	C		G559	
U1860	G1759	G1665	G1536	C1302	A1199	A1062	U918	G		A564	
G1861	U1761	C1666	A1537	G1303		U1081	A919	A		C568	
A1862	C1762	U1667	C1538	U1407	G1203	A1082	A920	G		A576	
U1864	G1763	U1668	G1540	A1408	A1204	A1083	G921	C		A693	
G1865	G1764	G1669	A1409	C1305	G1207	U1081	A922	C		A583	
			C1410	U1306		A1082					
A1869	A1768	U1670	C1411	U1307	G1207	A1084	G928	G841		A587	
	C1769	G1671	A1544	U1308	C1215	A1082	G929	C842		G888	
	G1770	U1672	G1546	C1309	A1216	C1085	C930	U844		G896	
				G1312	C1217		G931	U844		G897	
	U1775	C1673	G1550	U1317	A1217	C1098	G932	G845		C	
	G1776	A1679	C1553	G1318	C1218	G1099	G933	G846		U591	
	C1777	G1680	C1554	U1319	C1219	A1100		A847		C592	
	G1779		U1555	G1319	G1221	U1101	G942			C	
	U1780	C1683	C1554	U1318	C1222	G1102	U943	G852		U596	
	G1781		U1562	U1319	G1222	C1103				U596	
	A1782	C1689	C1562	G1420	A1228	U863	G952	U863		A604	
	C1783	U1690	G1563	G1320	G1105	A864	U954	U864		A605	
	G1784	G1691	C1421	G1321	G1229	C953	U954	A865		G606	
			G1422	G1322		U866		U866		U607	
	G1785	G1692	C1423			G1107					
	U1786	G1693	G1424	U1326	U1232	G1108	G958	G867		C614	
				G1327	G1233	C1109	G959	G868		C	
		A1579	C1434	U1332	U1242	U1114	U960	A869		G	
		A1580	C1435	A1332	U1243	U1115	A870	U871		G617	
	U1797	C1703	C1436	U1333	U1244	C1116	A963	A870		A	
	G1798	C1704	C1437	U1337		G1117	A964	A872		G629	
	G1799		A1588	C1327		C1117	U965	C872		C	

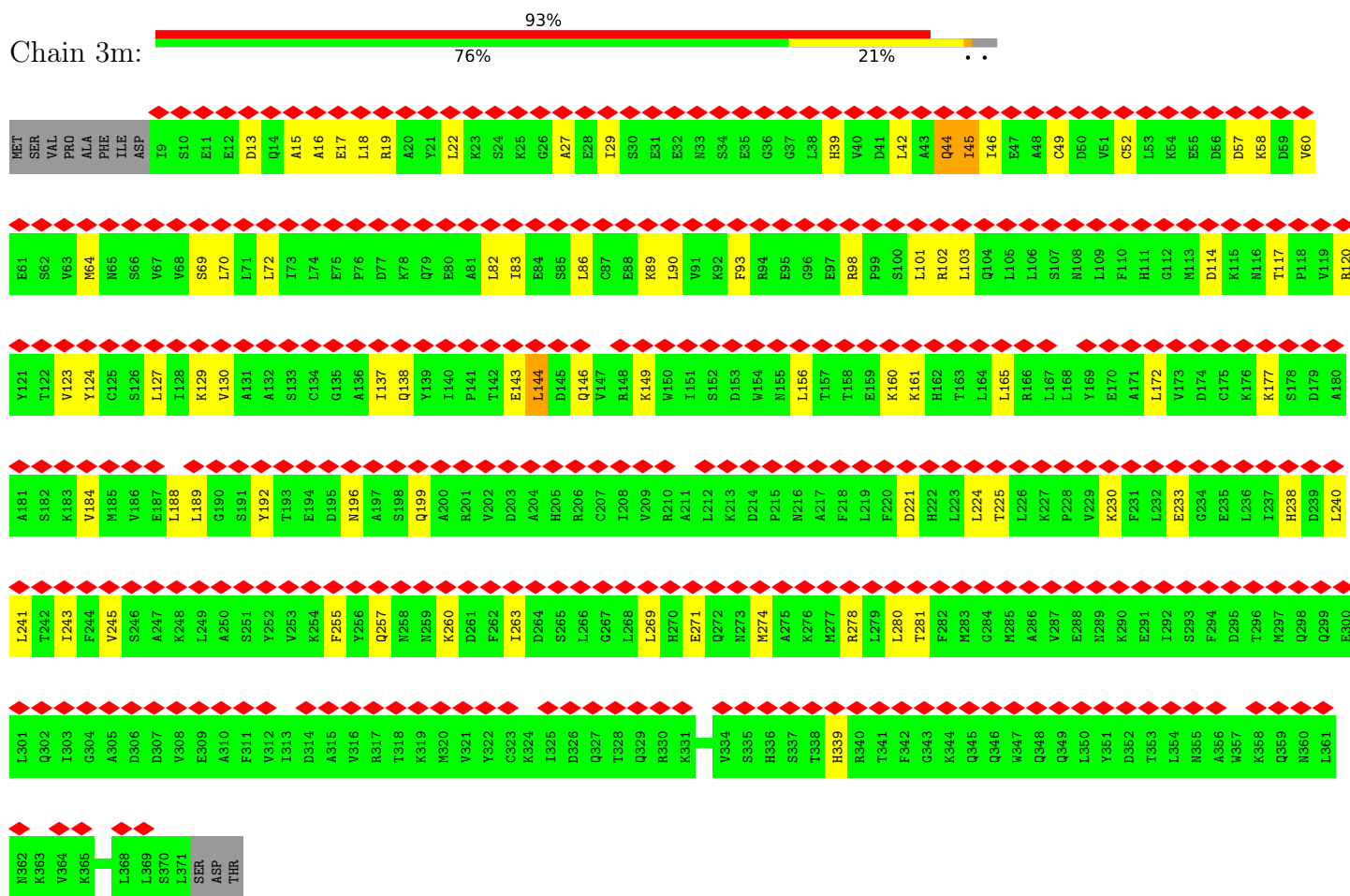
● Molecule 37: Chains: zz



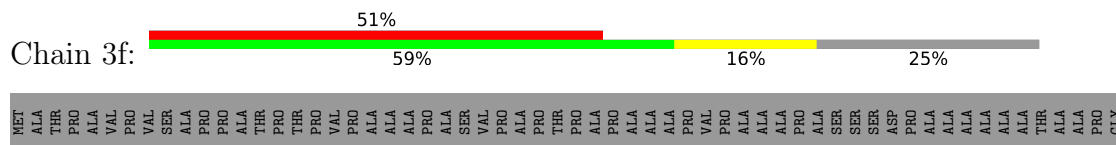
C	U	C	C	C44	C45	U46	U47	U48	G49	A50	G51	G52	A53	C54	C55	U56	C58	U59	G60	U61	C62	U63	U64	A70	A73	A74	U76	C79	U80	G81	G82	C83	C84	A85	U86	G87	G88	G94	U97	G98	A99	G102	U103	C104	G105	U106	G107	C108	A109	G110	C111	C112
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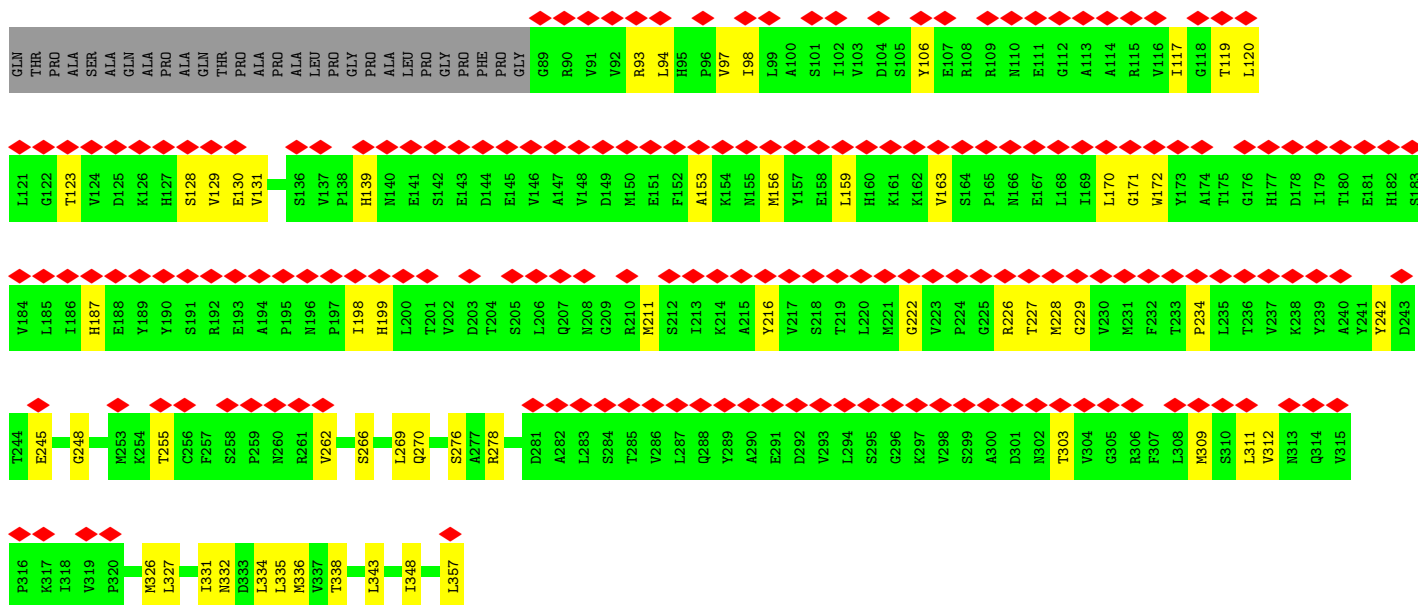


• Molecule 38: Eukaryotic translation initiation factor 3 subunit M

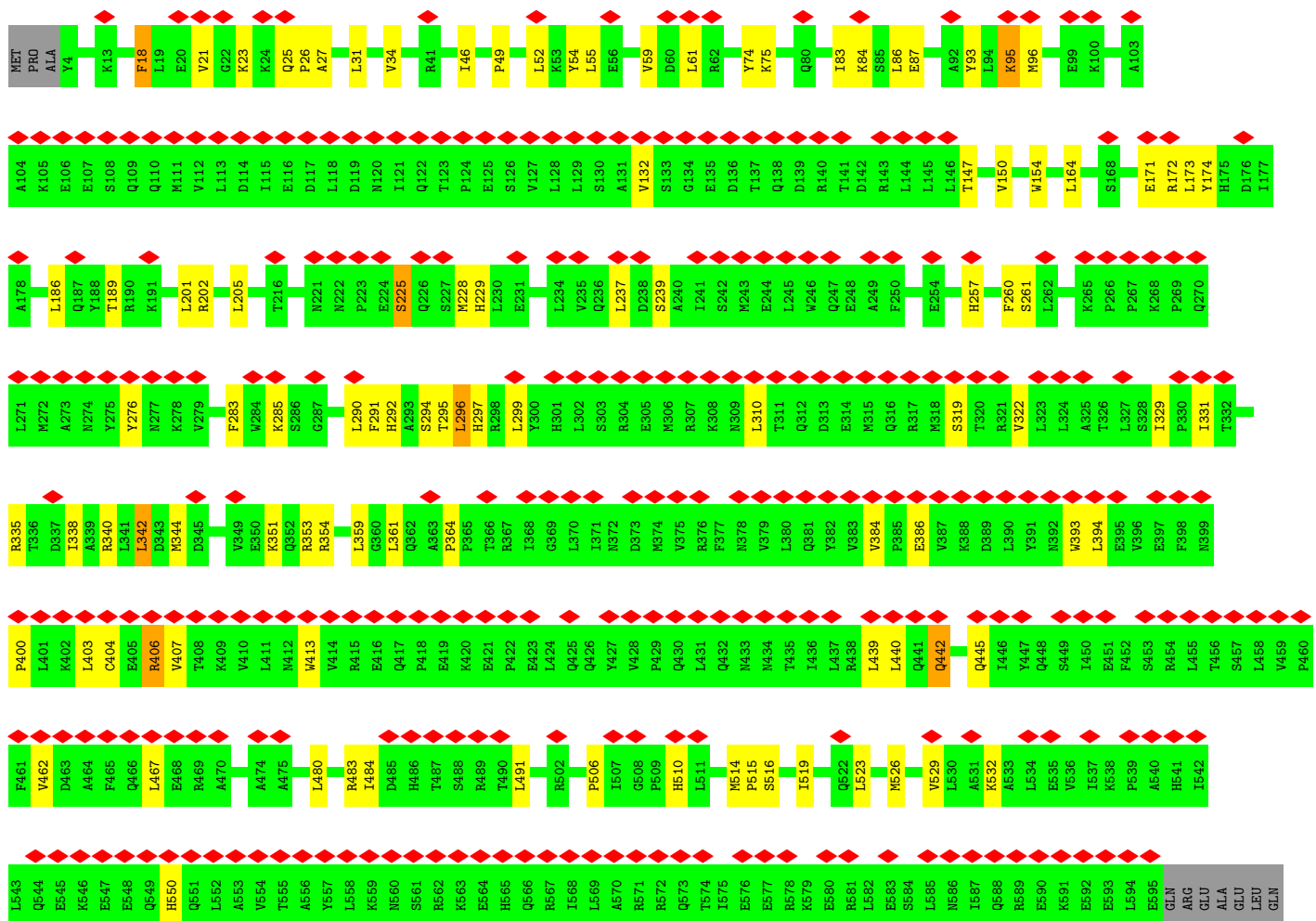
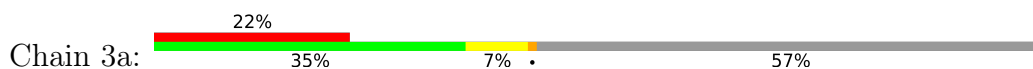


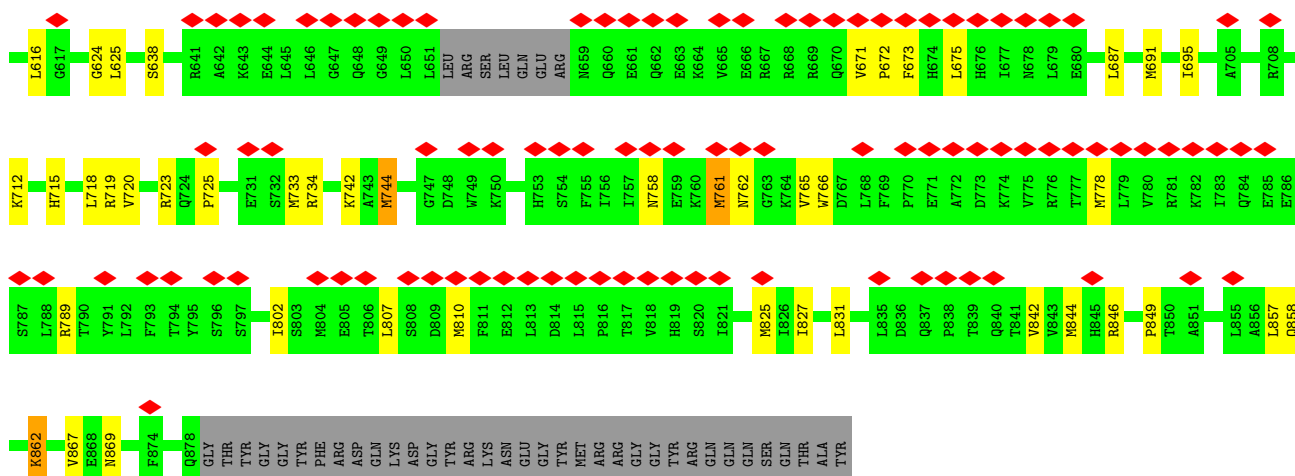
• Molecule 39: Eukaryotic translation initiation factor 3 subunit F



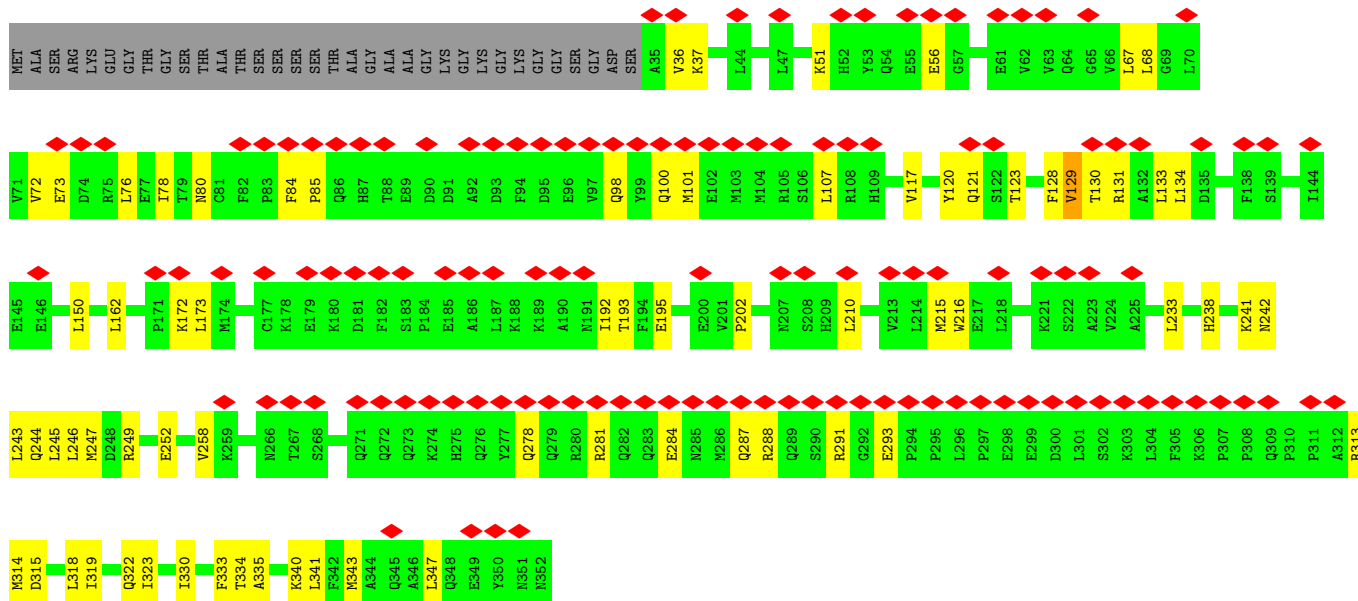


• Molecule 40: Eukaryotic translation initiation factor 3 subunit A

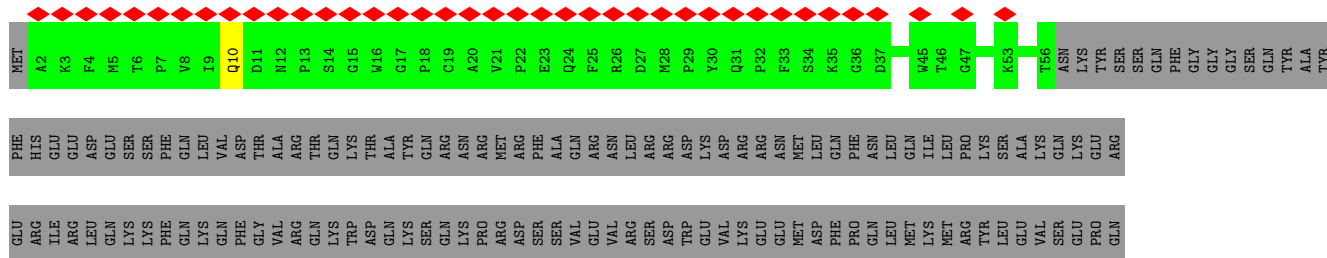


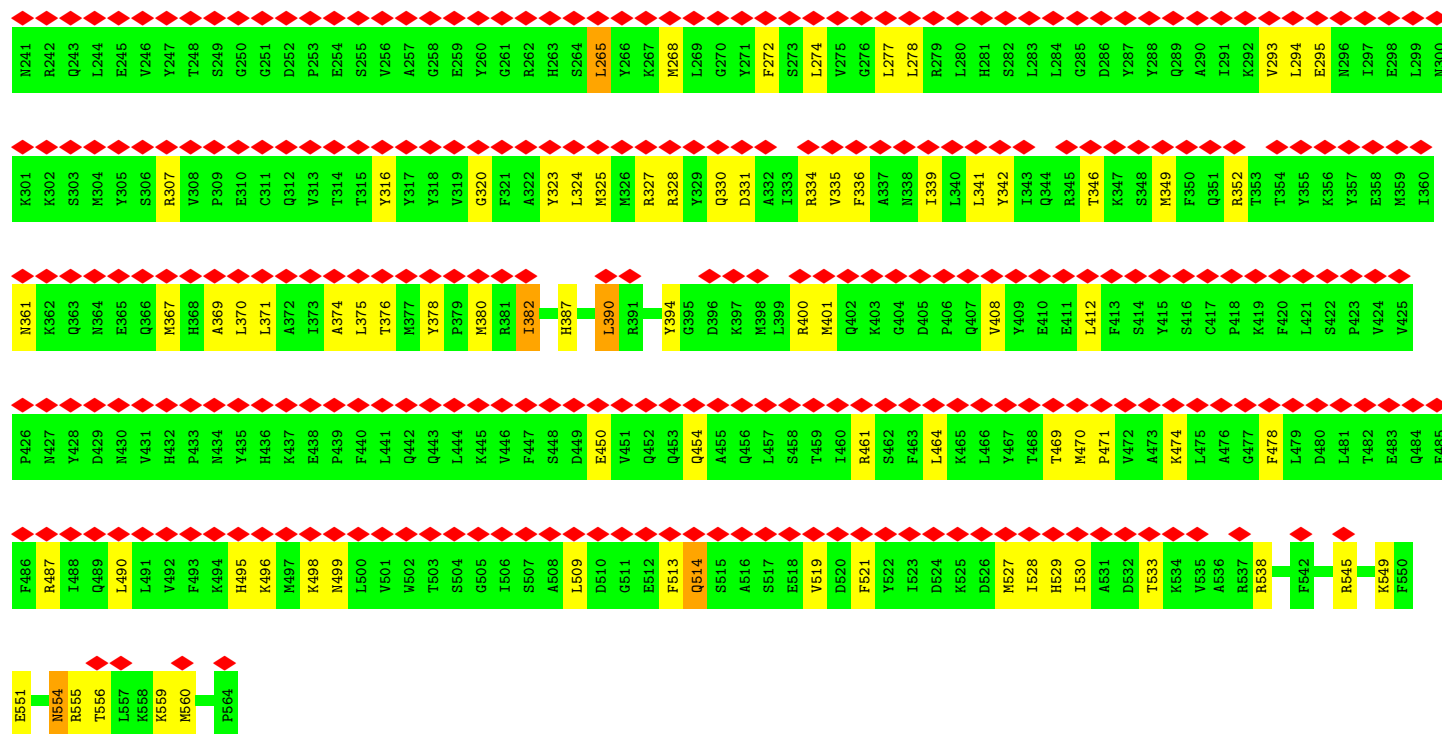


• Molecule 43: Eukaryotic translation initiation factor 3 subunit H



• Molecule 44: Eukaryotic translation initiation factor 3 subunit D





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	636.0, 636.0, 636.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.272, 1.272, 1.272	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.17	0/790	0.52	0/1058
2	SA	0.17	0/1742	0.42	0/2367
3	SB	0.16	0/1749	0.42	0/2340
4	SC	0.20	0/1737	0.52	0/2347
5	SD	0.15	0/1784	0.40	0/2402
6	SE	0.17	0/2107	0.45	0/2836
7	SF	0.18	0/1540	0.45	0/2071
8	SG	0.14	0/1946	0.41	0/2590
9	SH	0.19	0/1529	0.51	0/2048
10	SI	0.15	0/1711	0.39	0/2282
11	SJ	0.16	0/1524	0.41	0/2035
12	SK	0.27	0/834	0.74	0/1125
13	SL	0.20	0/1241	0.48	0/1662
14	Sf	0.16	0/945	0.49	0/1269
15	SN	0.18	0/1226	0.46	0/1649
16	SO	0.18	0/1020	0.43	0/1368
17	SP	0.23	0/1003	0.61	0/1340
18	SQ	0.20	0/1133	0.53	0/1517
19	SR	0.25	0/1082	0.64	0/1452
20	SS	0.19	0/1202	0.48	0/1610
21	ST	0.19	0/1122	0.51	0/1504
22	SU	0.20	0/813	0.54	0/1092
23	SV	0.21	0/643	0.53	0/860
24	SW	0.18	0/1051	0.45	0/1406
25	SX	0.17	0/1116	0.47	0/1490
26	SY	0.16	0/1031	0.38	0/1370
27	SZ	0.23	0/607	0.58	0/815
28	Sa	0.16	0/817	0.42	0/1095
29	Sb	0.20	0/665	0.43	0/891
30	Sc	0.19	0/490	0.50	0/656
31	Sd	0.22	0/470	0.56	0/623
32	Se	0.14	0/422	0.35	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	sh	0.16	0/529	0.42	0/701
34	Sg	0.14	0/2493	0.41	0/3394
35	Ln	0.19	0/231	0.64	1/294 (0.3%)
36	S2	0.14	0/42121	0.31	0/65651
37	zz	0.14	0/7199	0.34	0/11223
38	3m	0.15	0/2676	0.45	0/3635
39	3f	0.14	0/2099	0.36	0/2856
40	3a	0.13	0/4560	0.40	0/6207
41	3e	0.12	0/3288	0.35	0/4475
42	3c	0.13	0/3990	0.35	0/5424
43	3h	0.19	0/2571	0.39	0/3484
44	3d	0.11	0/358	0.30	0/493
45	3k	0.17	0/1502	0.44	0/2052
46	3l	0.13	0/4446	0.38	0/6013
All	All	0.16	0/115155	0.39	1/165627 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Ln	22	GLN	N-CA-C	-5.29	107.84	114.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	780	0	786	20	0
2	SA	1705	0	1706	26	0
3	SB	1722	0	1794	20	0
4	SC	1700	0	1784	28	0
5	SD	1756	0	1851	25	0
6	SE	2065	0	2169	22	0
7	SF	1518	0	1569	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	SG	1923	0	2089	14	0
9	SH	1506	0	1603	16	0
10	SI	1682	0	1769	17	0
11	SJ	1499	0	1618	17	0
12	SK	810	0	836	27	0
13	SL	1220	0	1289	22	0
14	Sf	935	0	964	14	0
15	SN	1202	0	1289	17	0
16	SO	1007	0	1032	13	0
17	SP	984	0	1033	11	0
18	SQ	1116	0	1185	13	0
19	SR	1068	0	1121	17	0
20	SS	1184	0	1244	18	0
21	ST	1103	0	1133	7	0
22	SU	803	0	873	14	0
23	SV	636	0	637	6	0
24	SW	1034	0	1080	8	0
25	SX	1098	0	1167	8	0
26	SY	1014	0	1082	7	0
27	SZ	601	0	662	12	0
28	Sa	803	0	850	6	0
29	Sb	651	0	672	6	0
30	Sc	488	0	514	14	0
31	Sd	459	0	452	9	0
32	Se	417	0	463	4	0
33	sh	518	0	527	9	0
34	Sg	2436	0	2393	34	0
35	Ln	230	0	276	2	0
36	S2	37669	0	19037	275	0
37	zz	6443	0	3259	60	0
38	3m	2639	0	2442	46	0
39	3f	2063	0	2054	39	0
40	3a	4475	0	4192	75	0
41	3e	3224	0	2925	24	0
42	3c	3924	0	3512	47	0
43	3h	2520	0	2445	52	0
44	3d	347	0	259	0	0
45	3k	1475	0	1239	21	0
46	3l	4335	0	4272	68	0
47	Sa	1	0	0	0	0
47	sh	1	0	0	0	0
48	S2	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	108797	0	87148	1128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:zz:61:U:H3	37:zz:107:G:H1	1.08	0.94
37:zz:52:G:N2	37:zz:111:C:O2	2.08	0.87
36:S2:197:U:H3	36:S2:202:G:H1	0.88	0.85
36:S2:1748:G:H1	36:S2:1786:U:H3	1.26	0.83
40:3a:276:TYR:HB3	40:3a:299:LEU:HD23	1.61	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	96/144 (67%)	88 (92%)	7 (7%)	1 (1%)	13	47
2	SA	214/295 (72%)	207 (97%)	7 (3%)	0	100	100
3	SB	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
4	SC	217/293 (74%)	209 (96%)	8 (4%)	0	100	100
5	SD	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
6	SE	258/263 (98%)	249 (96%)	9 (4%)	0	100	100
7	SF	190/204 (93%)	178 (94%)	12 (6%)	0	100	100
8	SG	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
9	SH	185/194 (95%)	177 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	SI	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
11	SJ	178/194 (92%)	177 (99%)	1 (1%)	0	100	100
12	SK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
13	SL	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
14	Sf	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
15	SN	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
16	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
17	SP	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
18	SQ	138/146 (94%)	135 (98%)	3 (2%)	0	100	100
19	SR	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
20	SS	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
21	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
22	SU	99/119 (83%)	99 (100%)	0	0	100	100
23	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
24	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
26	SY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
27	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
28	Sa	98/115 (85%)	95 (97%)	3 (3%)	0	100	100
29	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
30	Sc	60/69 (87%)	56 (93%)	4 (7%)	0	100	100
31	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	Se	50/59 (85%)	49 (98%)	1 (2%)	0	100	100
33	sh	62/156 (40%)	55 (89%)	7 (11%)	0	100	100
34	Sg	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
35	Ln	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
38	3m	361/374 (96%)	345 (96%)	16 (4%)	0	100	100
39	3f	267/357 (75%)	260 (97%)	7 (3%)	0	100	100
40	3a	590/1382 (43%)	568 (96%)	22 (4%)	0	100	100
41	3e	428/445 (96%)	418 (98%)	10 (2%)	0	100	100
42	3c	537/913 (59%)	521 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	3h	316/352 (90%)	306 (97%)	10 (3%)	0	100	100
44	3d	53/548 (10%)	50 (94%)	3 (6%)	0	100	100
45	3k	213/218 (98%)	204 (96%)	9 (4%)	0	100	100
46	3l	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
All	All	8178/10798 (76%)	7886 (96%)	291 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	112	HIS

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	1A	82/123 (67%)	79 (96%)	3 (4%)	29	62
2	SA	180/243 (74%)	172 (96%)	8 (4%)	24	57
3	SB	193/231 (84%)	186 (96%)	7 (4%)	30	62
4	SC	185/225 (82%)	175 (95%)	10 (5%)	18	51
5	SD	189/202 (94%)	181 (96%)	8 (4%)	25	58
6	SE	223/225 (99%)	216 (97%)	7 (3%)	35	66
7	SF	162/170 (95%)	154 (95%)	8 (5%)	21	54
8	SG	207/218 (95%)	204 (99%)	3 (1%)	62	82
9	SH	167/174 (96%)	160 (96%)	7 (4%)	25	58
10	SI	178/180 (99%)	166 (93%)	12 (7%)	13	44
11	SJ	160/168 (95%)	156 (98%)	4 (2%)	42	71
12	SK	87/136 (64%)	83 (95%)	4 (5%)	23	56
13	SL	134/142 (94%)	128 (96%)	6 (4%)	23	56
14	Sf	102/108 (94%)	97 (95%)	5 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	SN	130/131 (99%)	123 (95%)	7 (5%)	18	51
16	SO	104/119 (87%)	95 (91%)	9 (9%)	8	32
17	SP	107/130 (82%)	103 (96%)	4 (4%)	29	62
18	SQ	116/121 (96%)	110 (95%)	6 (5%)	19	52
19	SR	119/122 (98%)	110 (92%)	9 (8%)	11	39
20	SS	124/132 (94%)	118 (95%)	6 (5%)	21	55
21	ST	112/115 (97%)	108 (96%)	4 (4%)	30	62
22	SU	93/107 (87%)	87 (94%)	6 (6%)	14	45
23	SV	67/67 (100%)	64 (96%)	3 (4%)	23	56
24	SW	112/113 (99%)	105 (94%)	7 (6%)	15	46
25	SX	113/115 (98%)	105 (93%)	8 (7%)	12	42
26	SY	108/115 (94%)	103 (95%)	5 (5%)	23	56
27	SZ	67/103 (65%)	62 (92%)	5 (8%)	11	40
28	Sa	87/98 (89%)	84 (97%)	3 (3%)	32	63
29	Sb	75/76 (99%)	73 (97%)	2 (3%)	40	69
30	Sc	55/62 (89%)	52 (94%)	3 (6%)	18	51
31	Sd	48/49 (98%)	45 (94%)	3 (6%)	15	46
32	Se	42/48 (88%)	39 (93%)	3 (7%)	12	42
33	sh	56/140 (40%)	48 (86%)	8 (14%)	2	13
34	Sg	272/275 (99%)	261 (96%)	11 (4%)	27	59
35	Ln	23/24 (96%)	19 (83%)	4 (17%)	1	8
38	3m	252/335 (75%)	240 (95%)	12 (5%)	21	55
39	3f	229/289 (79%)	223 (97%)	6 (3%)	41	70
40	3a	434/1259 (34%)	418 (96%)	16 (4%)	29	62
41	3e	302/406 (74%)	295 (98%)	7 (2%)	45	72
42	3c	347/811 (43%)	341 (98%)	6 (2%)	56	78
43	3h	272/310 (88%)	266 (98%)	6 (2%)	47	73
44	3d	20/494 (4%)	19 (95%)	1 (5%)	20	54
45	3k	121/193 (63%)	115 (95%)	6 (5%)	20	54
46	3l	475/515 (92%)	461 (97%)	14 (3%)	37	67
All	All	6731/9419 (72%)	6449 (96%)	282 (4%)	27	58

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	3a	225	SER
40	3a	344	MET
43	3h	215	MET
15	SN	133	ARG
15	SN	60	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
46	3l	195	GLN
46	3l	232	HIS
34	Sg	62	HIS
34	Sg	26	GLN
46	3l	330	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	S2	1746/1869 (93%)	342 (19%)	6 (0%)
37	zz	301/332 (90%)	115 (38%)	0
All	All	2047/2201 (93%)	457 (22%)	6 (0%)

5 of 457 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
36	S2	4	C
36	S2	17	C
36	S2	25	A
36	S2	33	G
36	S2	42	A

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	S2	871	U
36	S2	1326	U
36	S2	1434	C
36	S2	517	C
36	S2	174	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

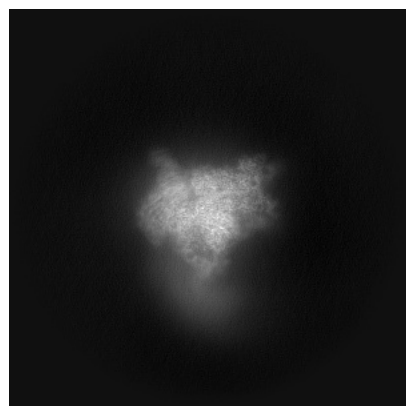
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62453. These allow visual inspection of the internal detail of the map and identification of artifacts.

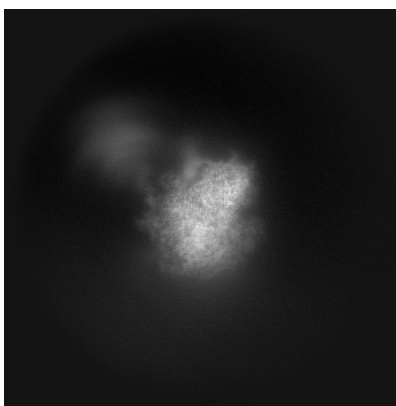
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

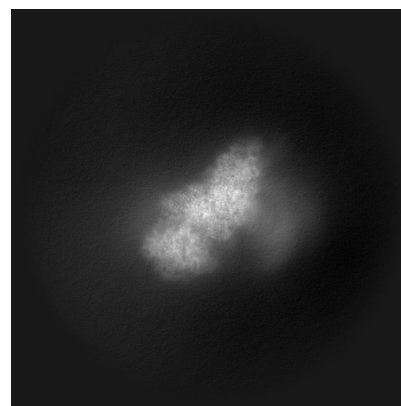
6.1.1 Primary map



X

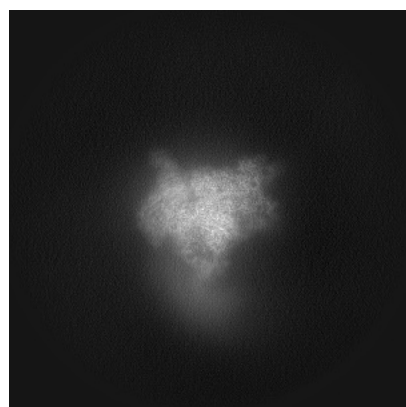


Y

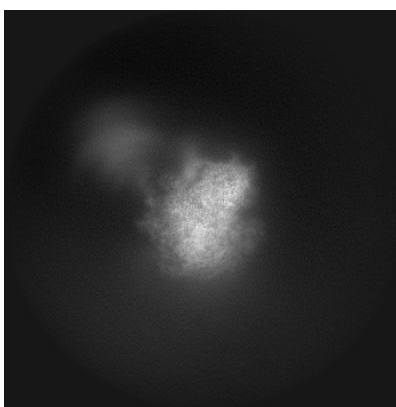


Z

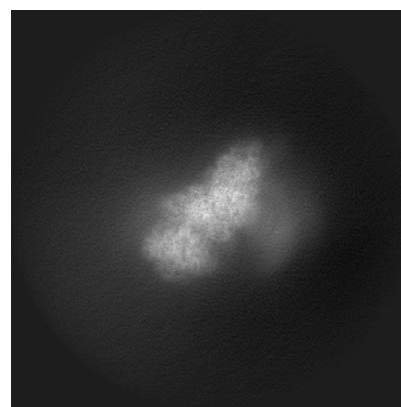
6.1.2 Raw map



X



Y

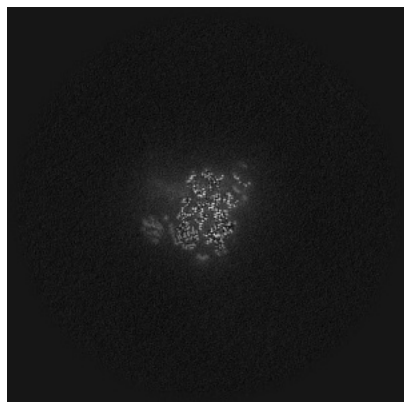


Z

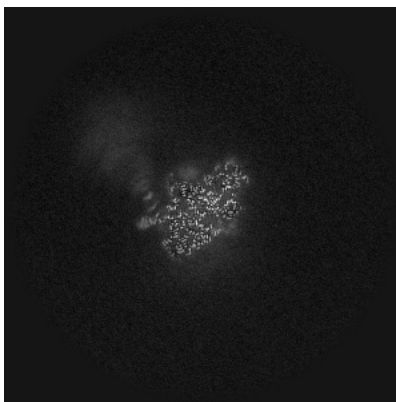
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

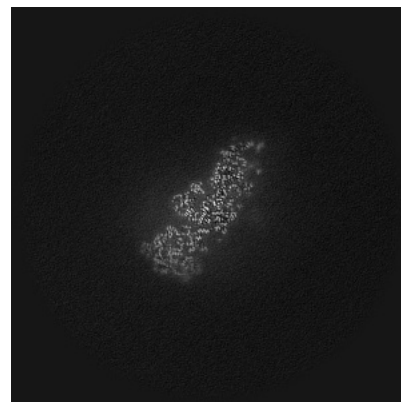
6.2.1 Primary map



X Index: 250

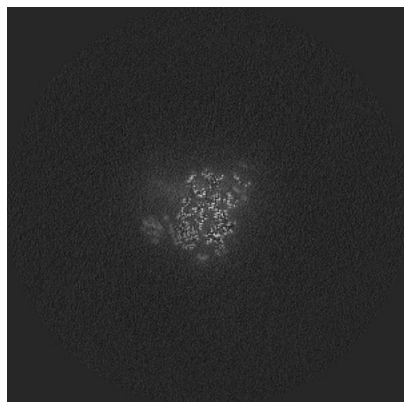


Y Index: 250

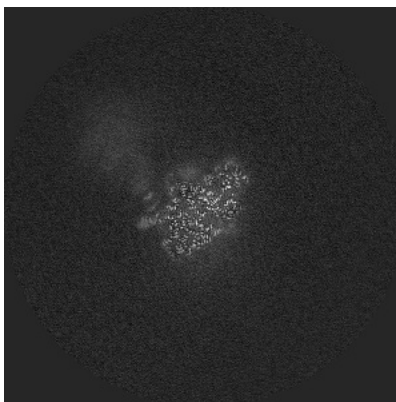


Z Index: 250

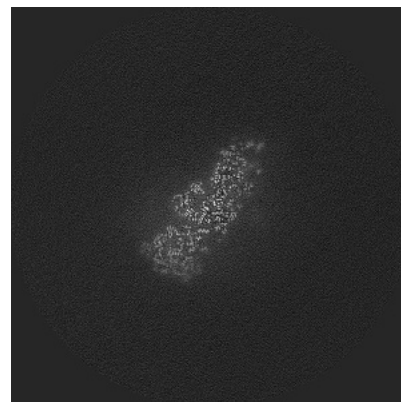
6.2.2 Raw map



X Index: 250



Y Index: 250

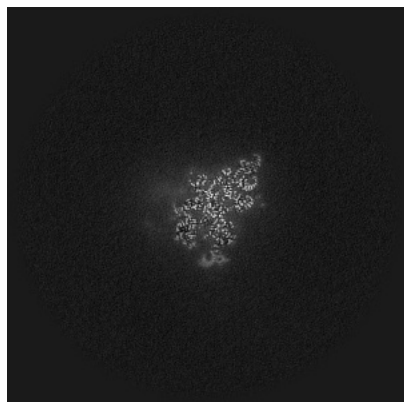


Z Index: 250

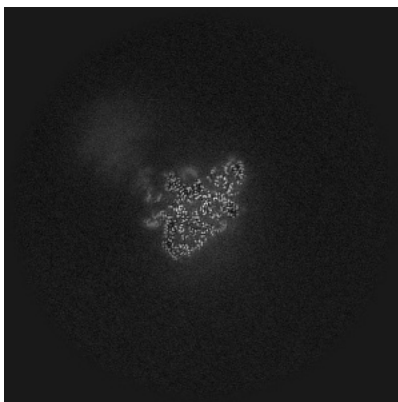
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

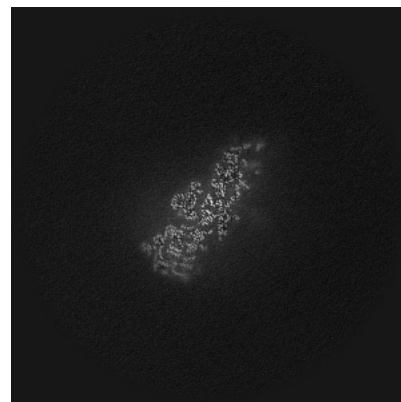
6.3.1 Primary map



X Index: 260

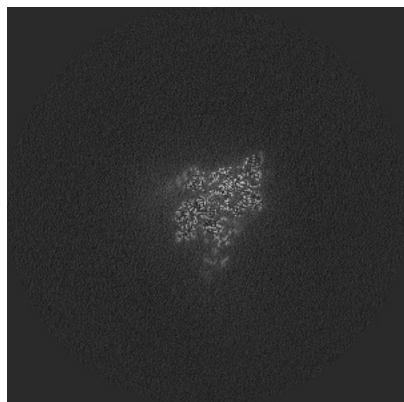


Y Index: 255

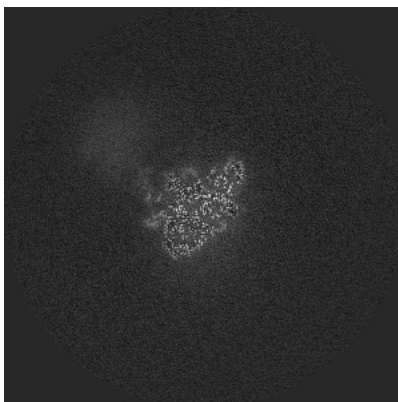


Z Index: 248

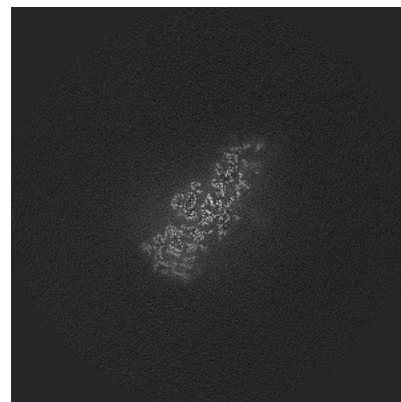
6.3.2 Raw map



X Index: 267



Y Index: 255

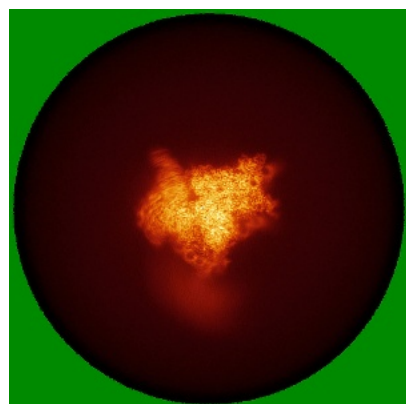


Z Index: 248

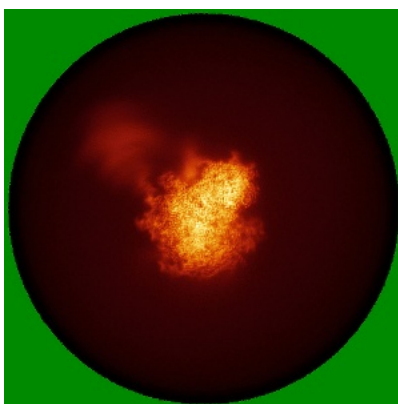
The images above show the largest variance slices of the map in three orthogonal directions.

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

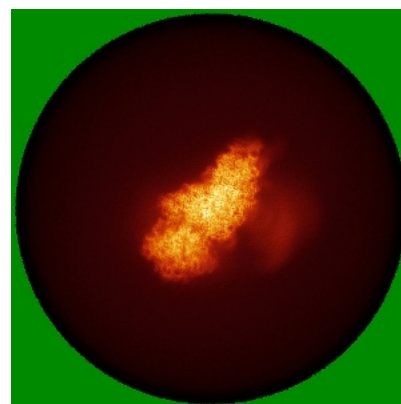
6.4.1 Primary map



X

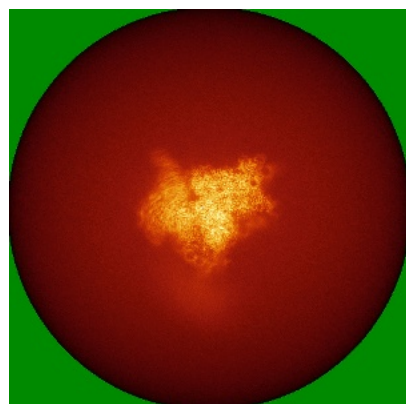


Y

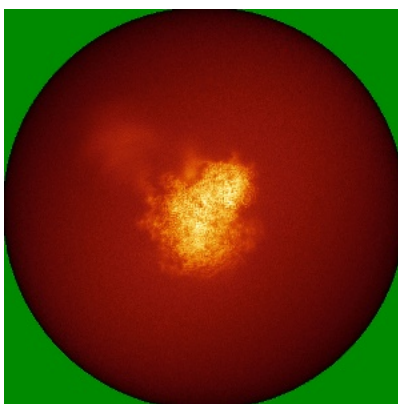


Z

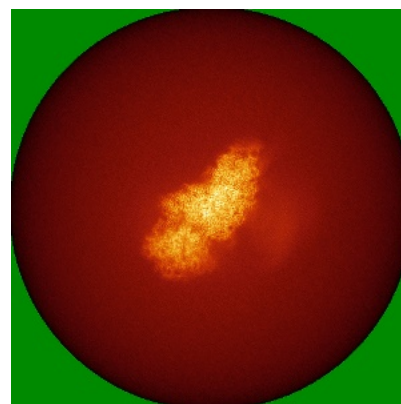
6.4.2 Raw map



X



Y

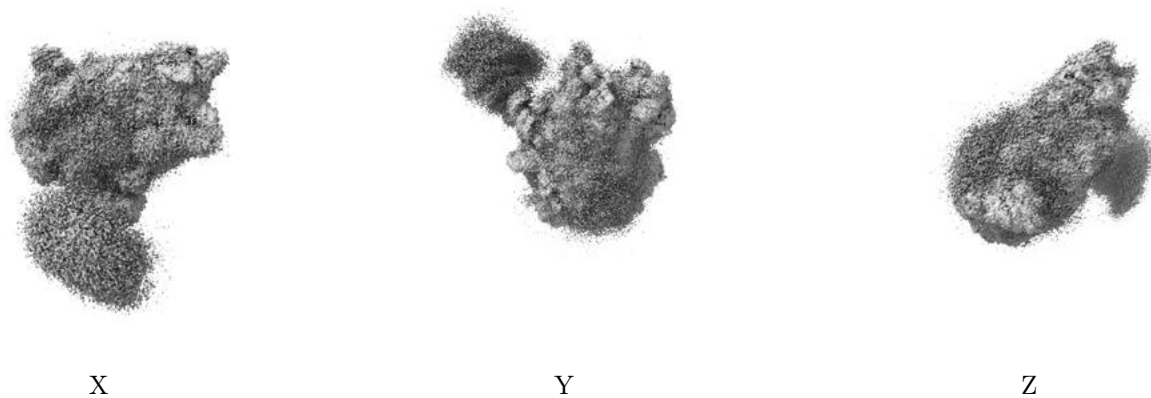


Z

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.

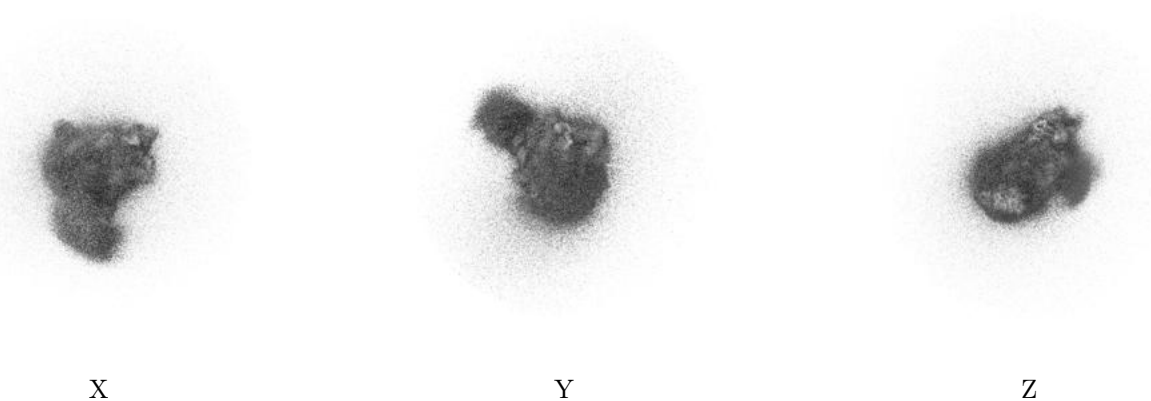
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

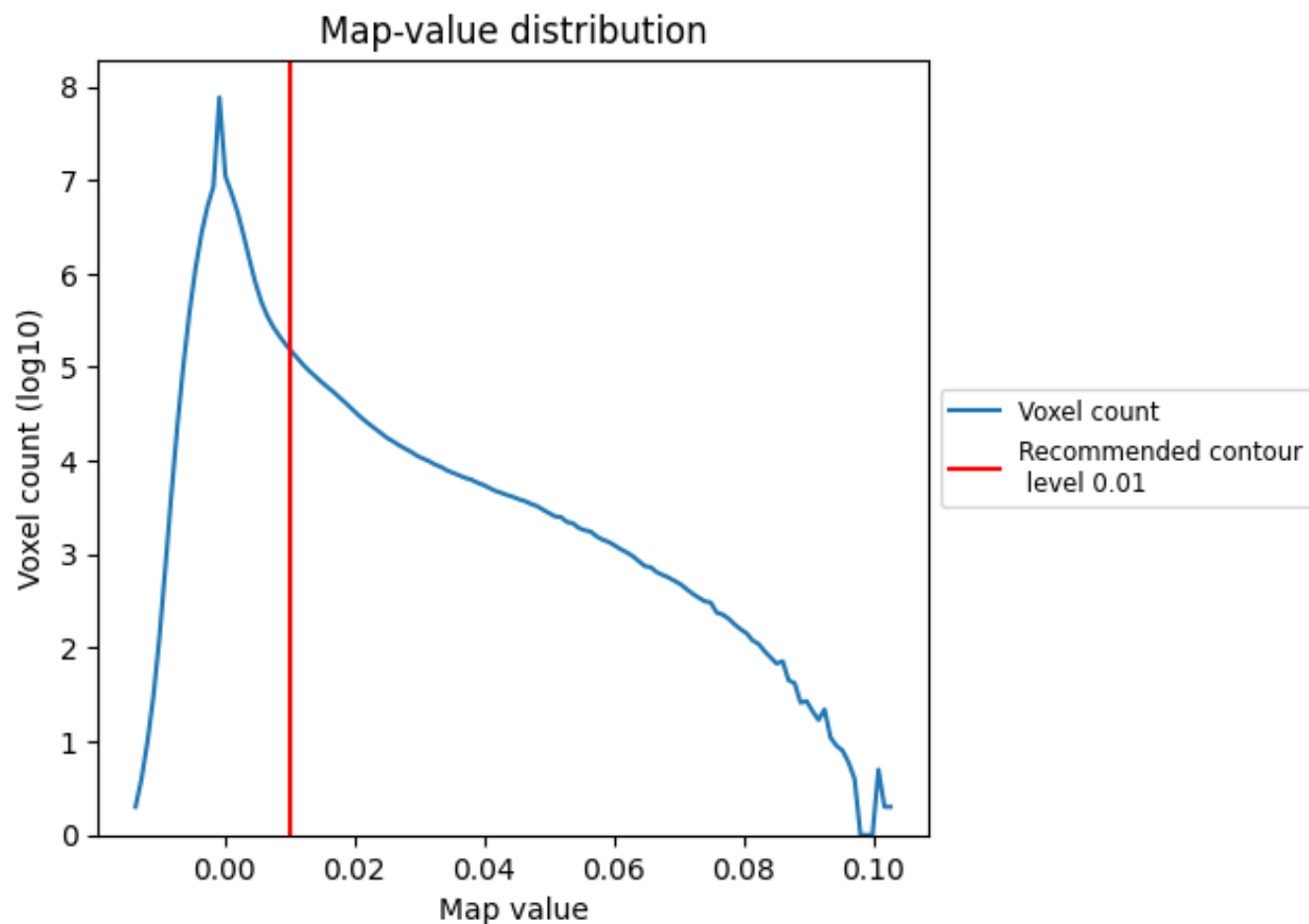
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

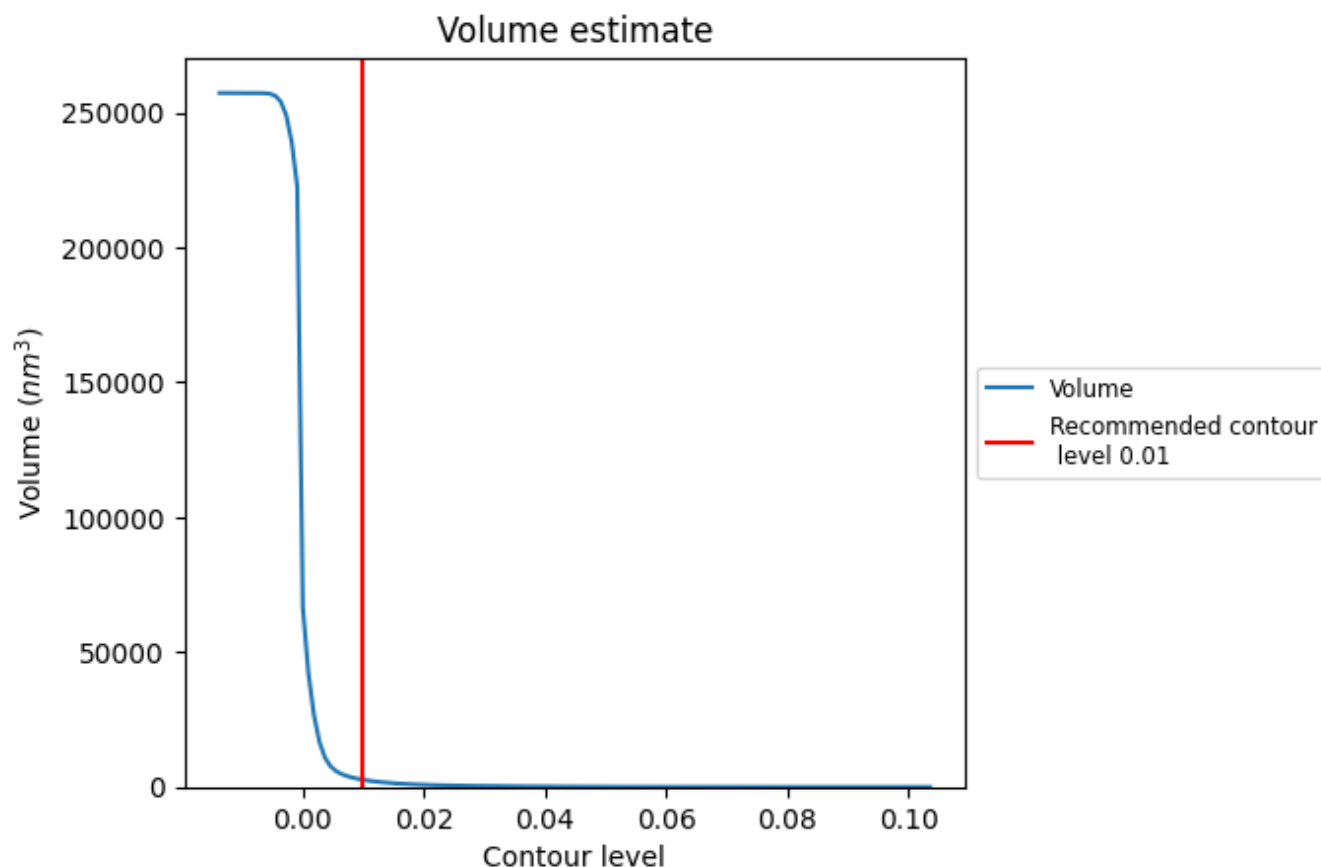
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

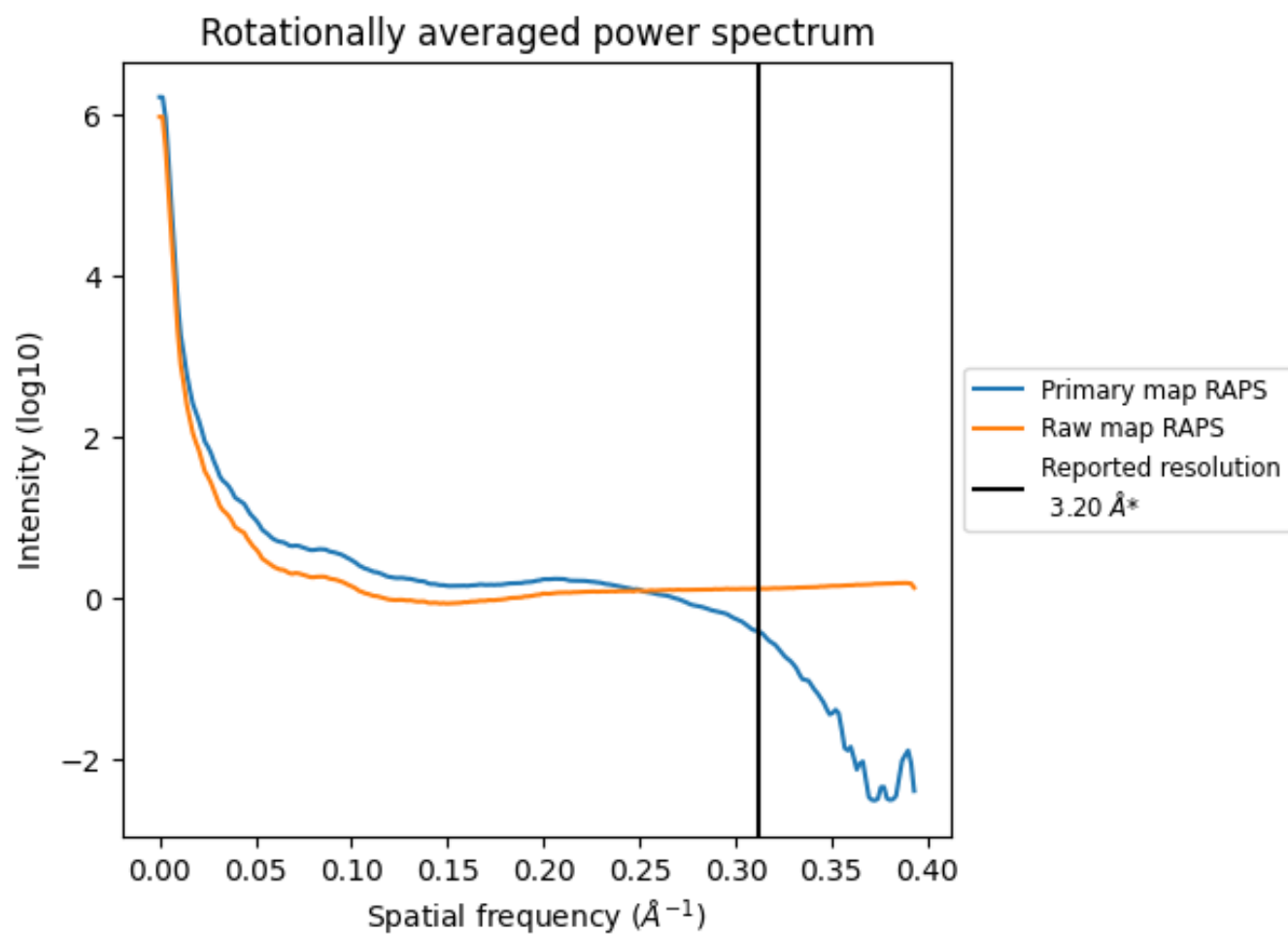
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2673 nm^3 ; this corresponds to an approximate mass of 2415 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 ⓘ

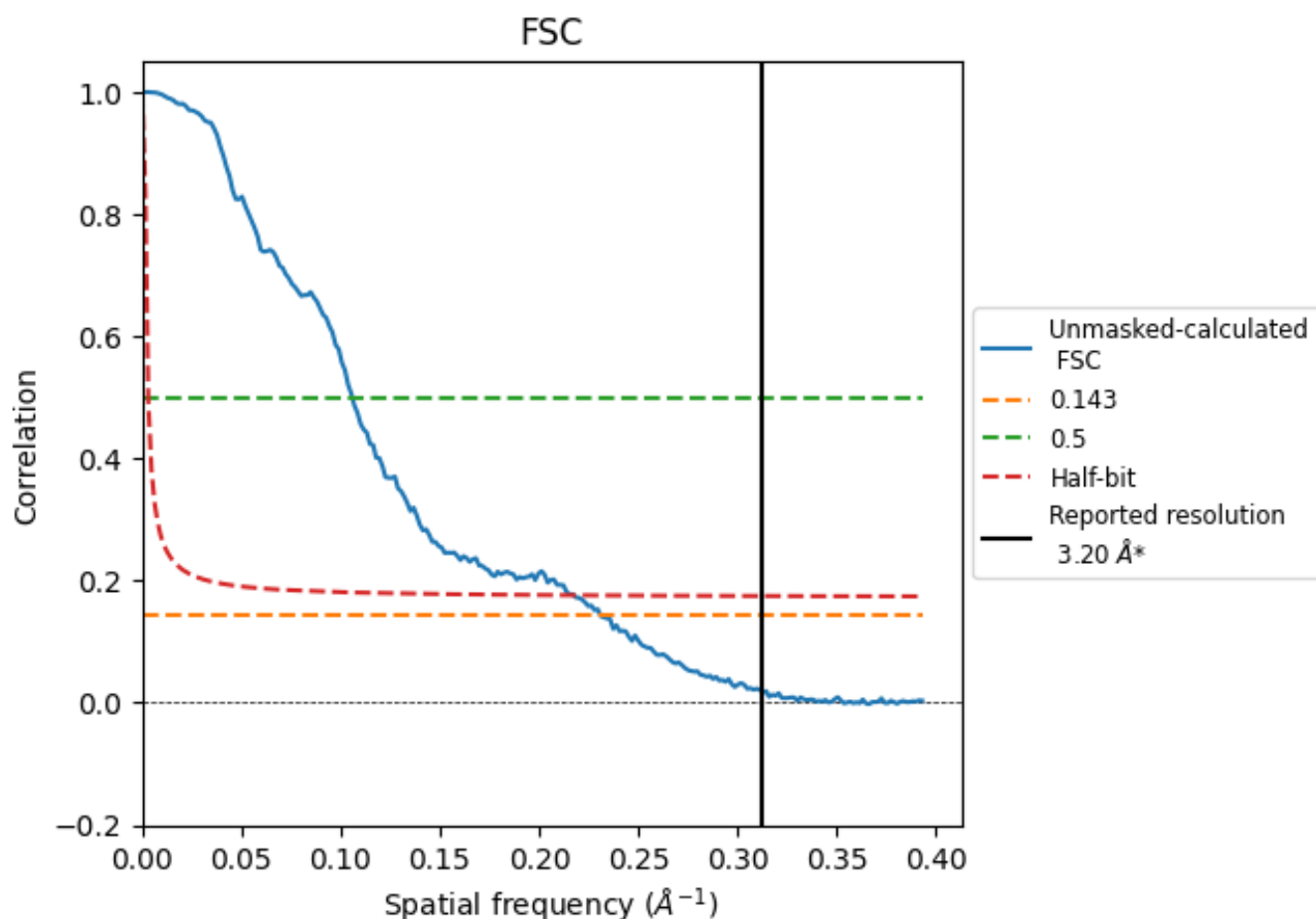


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

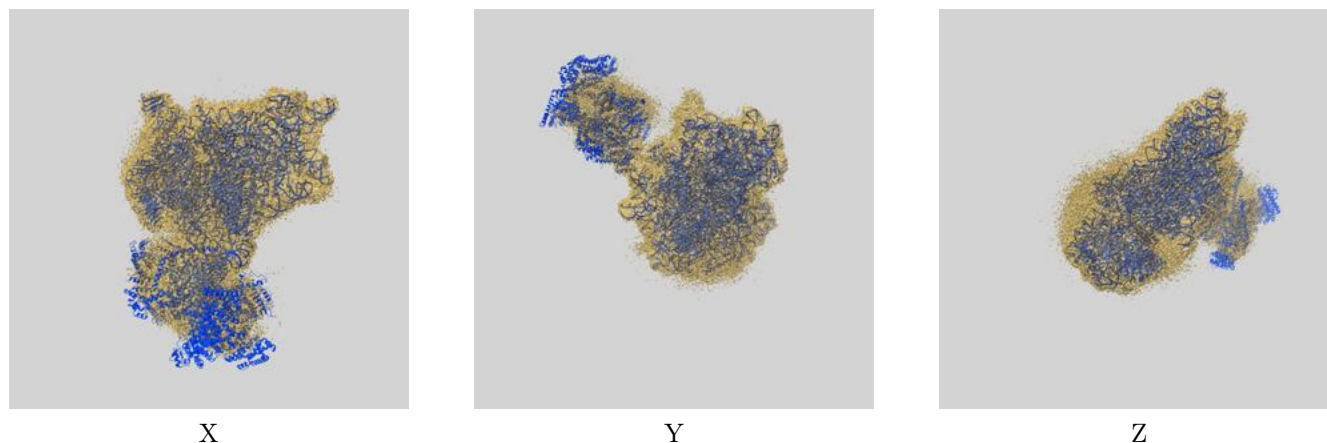
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	9.44	4.60

*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 4.33 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

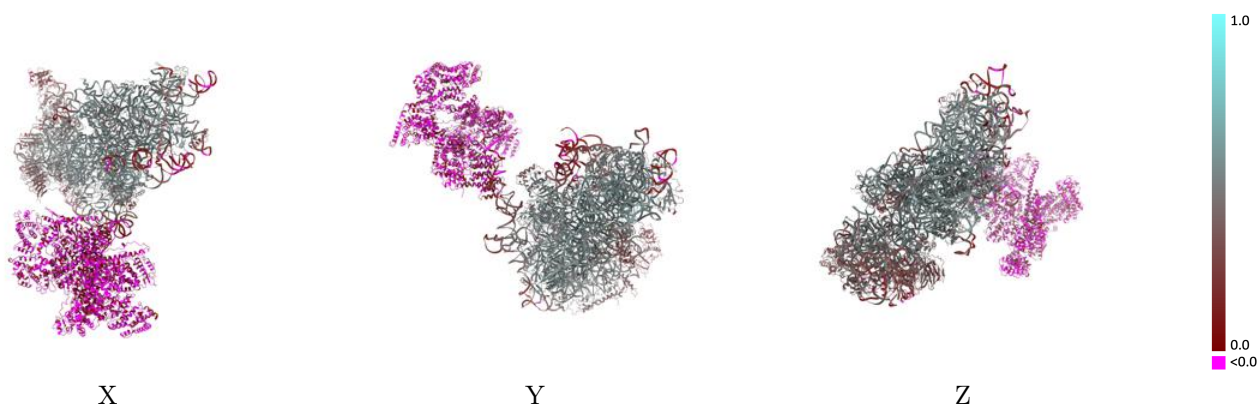
This section contains information regarding the fit between EMDB map EMD-62453 and PDB model 9KN5. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



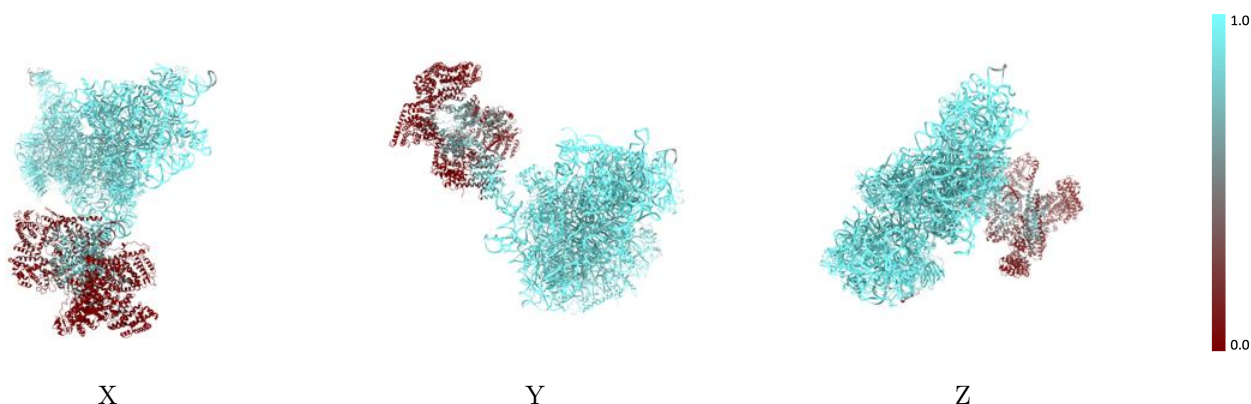
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



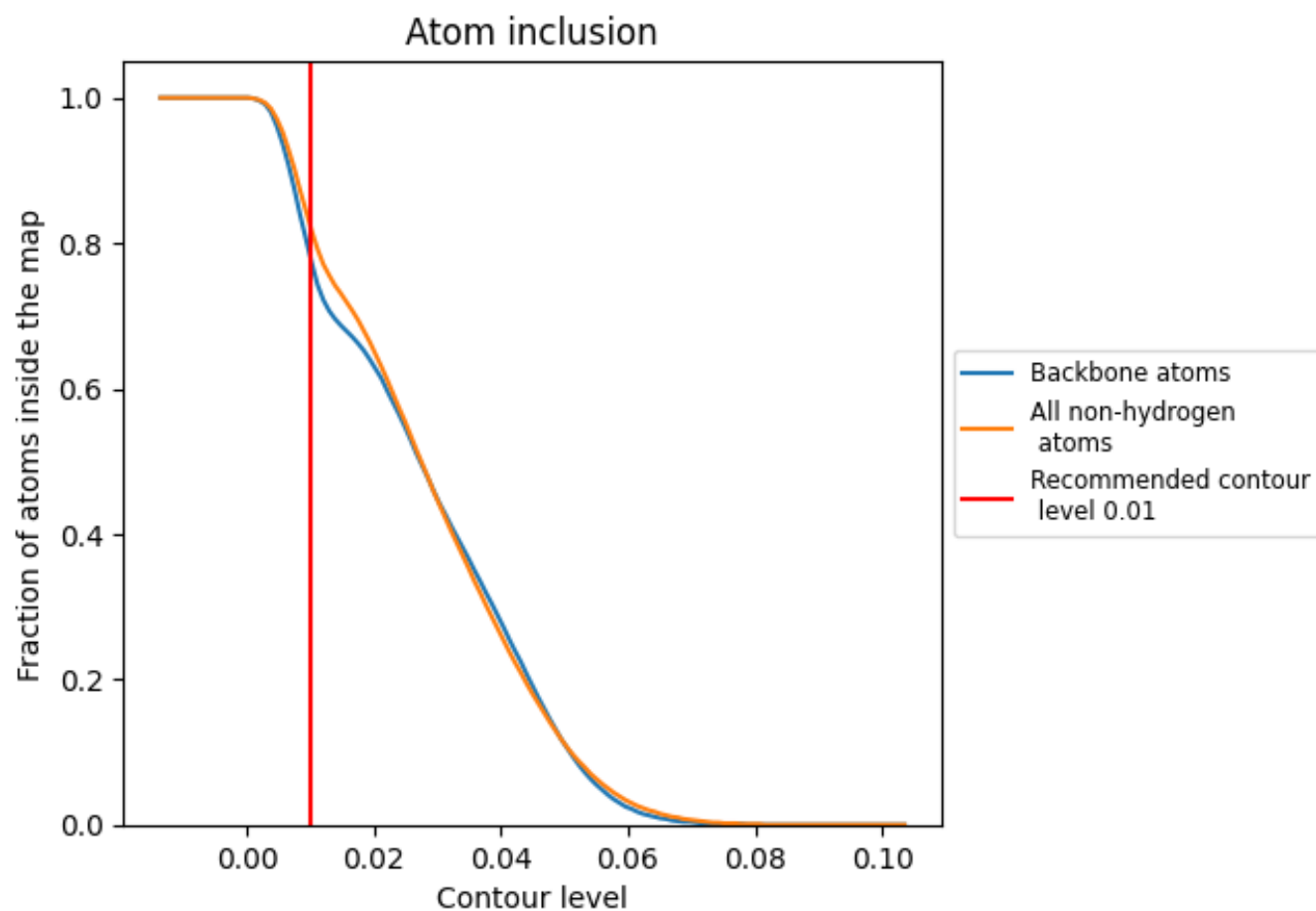
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 82% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.3500
1A	 0.9920	 0.2970
3a	 0.4480	 0.0310
3c	 0.3590	 0.0140
3d	 0.2760	 -0.0030
3e	 0.1610	 0.0060
3f	 0.3230	 0.0050
3h	 0.4970	 0.0100
3k	 0.0420	 -0.0100
3l	 0.0780	 0.0030
3m	 0.0540	 -0.0050
Ln	 1.0000	 0.4880
S2	 0.9970	 0.4720
SA	 0.9990	 0.5180
SB	 0.9920	 0.5170
SC	 0.9990	 0.5220
SD	 0.9970	 0.4180
SE	 0.9990	 0.5160
SF	 0.9990	 0.4910
SG	 0.9780	 0.4410
SH	 0.9910	 0.4550
SI	 0.9910	 0.5000
SJ	 0.9980	 0.5290
SK	 1.0000	 0.3610
SL	 0.9920	 0.5030
SN	 1.0000	 0.5200
SO	 0.9980	 0.5180
SP	 0.9880	 0.3580
SQ	 1.0000	 0.4440
SR	 0.9990	 0.4520
SS	 0.9890	 0.3960
ST	 0.9960	 0.4060
SU	 0.9960	 0.3880
SV	 0.9970	 0.5160
SW	 1.0000	 0.5210



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Chain	Atom inclusion	Q-score
SX	 1.0000	 0.5130
SY	 0.9980	 0.5080
SZ	 0.9970	 0.4360
Sa	 1.0000	 0.5370
Sb	 1.0000	 0.5140
Sc	 1.0000	 0.5220
Sd	 1.0000	 0.4420
Se	 1.0000	 0.4810
Sf	 0.8640	 0.1920
Sg	 0.9910	 0.3390
sh	 0.9050	 0.1990
zz	 0.9350	 0.3050