



# wwPDB EM Validation Summary Report ⓘ

Apr 22, 2024 – 03:16 PM JST

PDB ID : 8XXN  
EMDB ID : EMD-38754  
Title : Cryo-EM structure of the human 43S ribosome with PDCD4  
Authors : Ye, X.; Huang, Z.; Li, Y.; Wang, M.; Cheng, J.  
Deposited on : 2024-01-18  
Resolution : 3.60 Å (reported)  
Based on initial model : 7A09

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

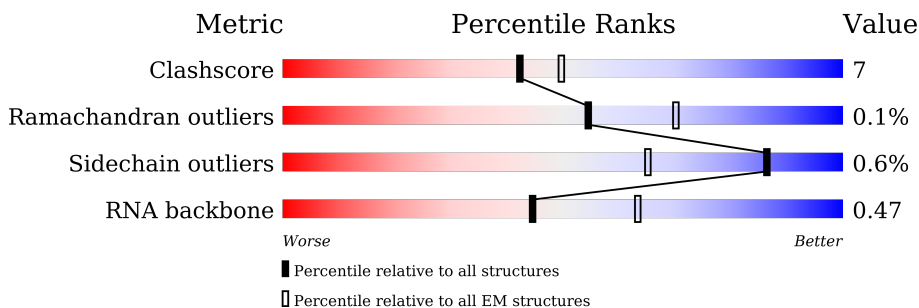
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	Ln	25	
2	S2	1869	
3	SA	295	
4	SB	264	
5	SD	243	
6	SE	263	
7	SF	204	

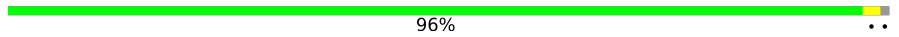
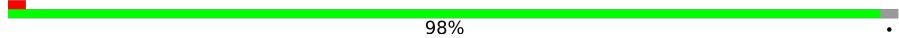








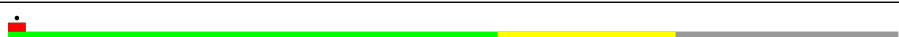



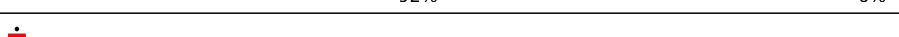
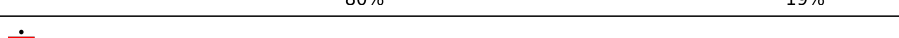

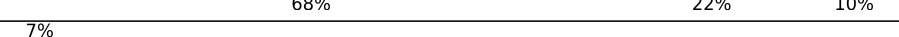
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Mol	Chain	Length	Quality of chain
8	SH	194	78% 17%
9	SI	208	75% 23%
10	SK	165	51% 8% 41%
11	SL	158	80% 16%
12	SP	145	61% 23% 17%
13	SQ	146	72% 27%
14	SR	135	78% 19%
15	SS	152	68% 27% 5%
16	ST	145	79% 20%
17	SU	119	62% 24% 13%
18	SV	83	81% 19%
19	SX	143	80% 18%
20	Sa	115	87% 11%
21	Sc	69	90% 7%
22	Sd	56	96%
23	Sg	317	99%
24	SC	293	62% 13% 24%
25	SG	249	70% 24% 5%
26	SJ	194	71% 24% 5%
27	SM	132	65% 27% 8%
28	SN	151	88% 11%
29	SO	151	74% 19% 7%
30	SW	130	85% 15%
31	SY	133	65% 32%
32	SZ	125	46% 14% 40%

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Mol	Chain	Length	Quality of chain
33	Sb	84	 96%
34	Se	59	 98%
35	Sf	156	 42% 57%
36	C1	113	 19% 78% 20%
37	4A	406	 82% 16%
38	CD	469	 73% 26%
39	3A	1382	 5% 41% 9% 50%
40	3B	814	 19% 62% 34%
41	3C	913	 54% 15% 32%
42	3E	445	 71% 22% 7%
43	3F	357	 55% 20% 25%
44	3G	320	 19% 8% 74%
45	3H	352	 59% 24% 16%
46	3I	325	 86% 92% 6%
47	3K	218	 80% 19%
48	3L	564	 50% 15% 34%
49	3M	374	 68% 22% 10%
50	3N	548	 7% 61% 21% 18%

## 2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 114565 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 60S ribosomal protein L41.

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

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	S2	1723	36535	16298	6533	11982	1722	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SA	221	1741	1106	305	322	8	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SB	214	1738	1103	310	311	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SD	227	1765	1125	317	315	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SE	262	2076	1324	386	358	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SF	189	1495	934	284	270	7	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SH	186	1497	956	274	266	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SI	206	1686	1058	332	291	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SK	98	827	539	148	134	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SL	153	1247	793	234	214	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SP	121	985	623	185	170	7	0	0

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SQ	144	1142	726	216	197	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SR	135	1090	685	202	198	5	0	0

- Molecule 15 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SS	145	1198	751	242	203	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	ST	143	1112	697	214	198	3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SU	103	817	511	155	147	4	0	0

- Molecule 18 is a protein called 40S ribosomal protein S21.

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

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Sa	102	821	512	171	133	5	0	0

- Molecule 21 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 22 is a protein called 40S ribosomal protein S29.

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

- Molecule 23 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 24 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 25 is a protein called 40S ribosomal protein S6.

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

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 28 is a protein called 40S ribosomal protein S13.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SN	150	1208	773	229	205	1	0	0

- Molecule 29 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SO	140	1049	642	204	197	6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SY	131	1065	673	209	178	5	0	0

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	SZ	75	598	382	111	104	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Se	58	459	284	100	74	1	0	0

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	C1	90	Total	C	N	O	0	0
			443	262	90	91		

- Molecule 37 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	4A	342	Total	C	N	O	0	0
			1691	1007	342	342		

- Molecule 38 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	CD	347	Total	C	N	O	0	0
			1841	1100	368	373		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3A	692	Total	C	N	O	S	0	0
			5379	3374	980	1003	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3C	625	Total	C	N	O	S	0	0
			5070	3204	898	933	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	3E	416	3437	2202	585	630	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	3F	269	2090	1317	356	405	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	3G	84	667	418	120	129	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	3H	295	2413	1532	417	449	15	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	3I	305	1497	887	305	305	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	3K	217	1750	1116	288	334	12	0	0

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	3L	372	3111	2011	520	563	17	0	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	3M	338	2705	1727	457	504	17	0	0

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	3N	447	3617	2279	625	691	22	0	0

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
51	S2	22	22	22	0
51	SG	1	1	1	0

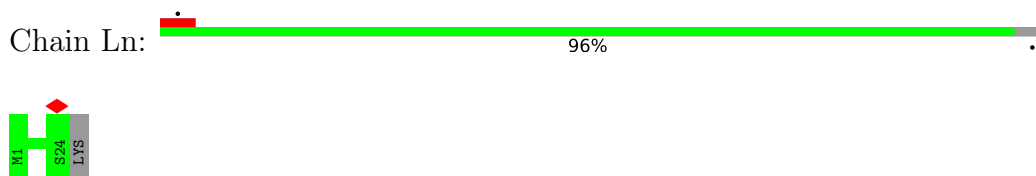
- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	Sa	1	1	1	0
52	Sd	1	1	1	0
52	Sf	1	1	1	0

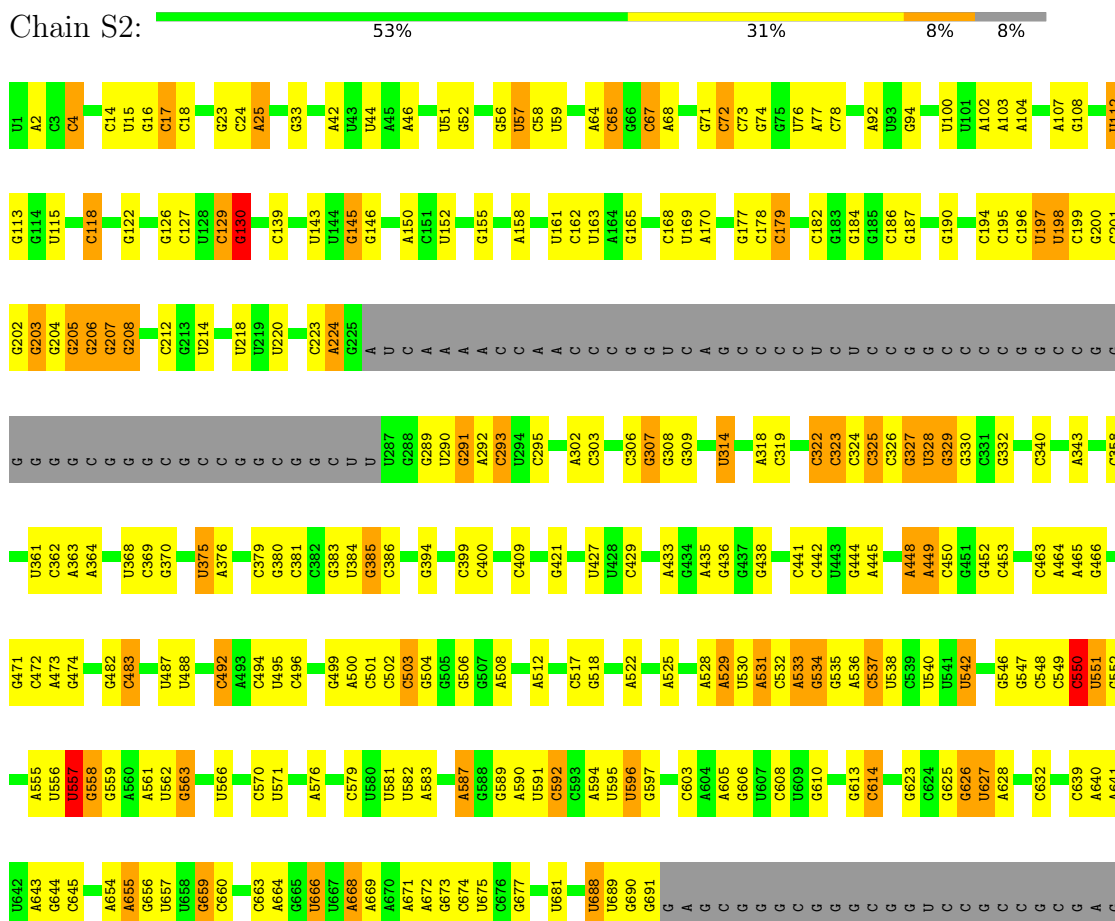
### 3 Residue-property plots [i](#)

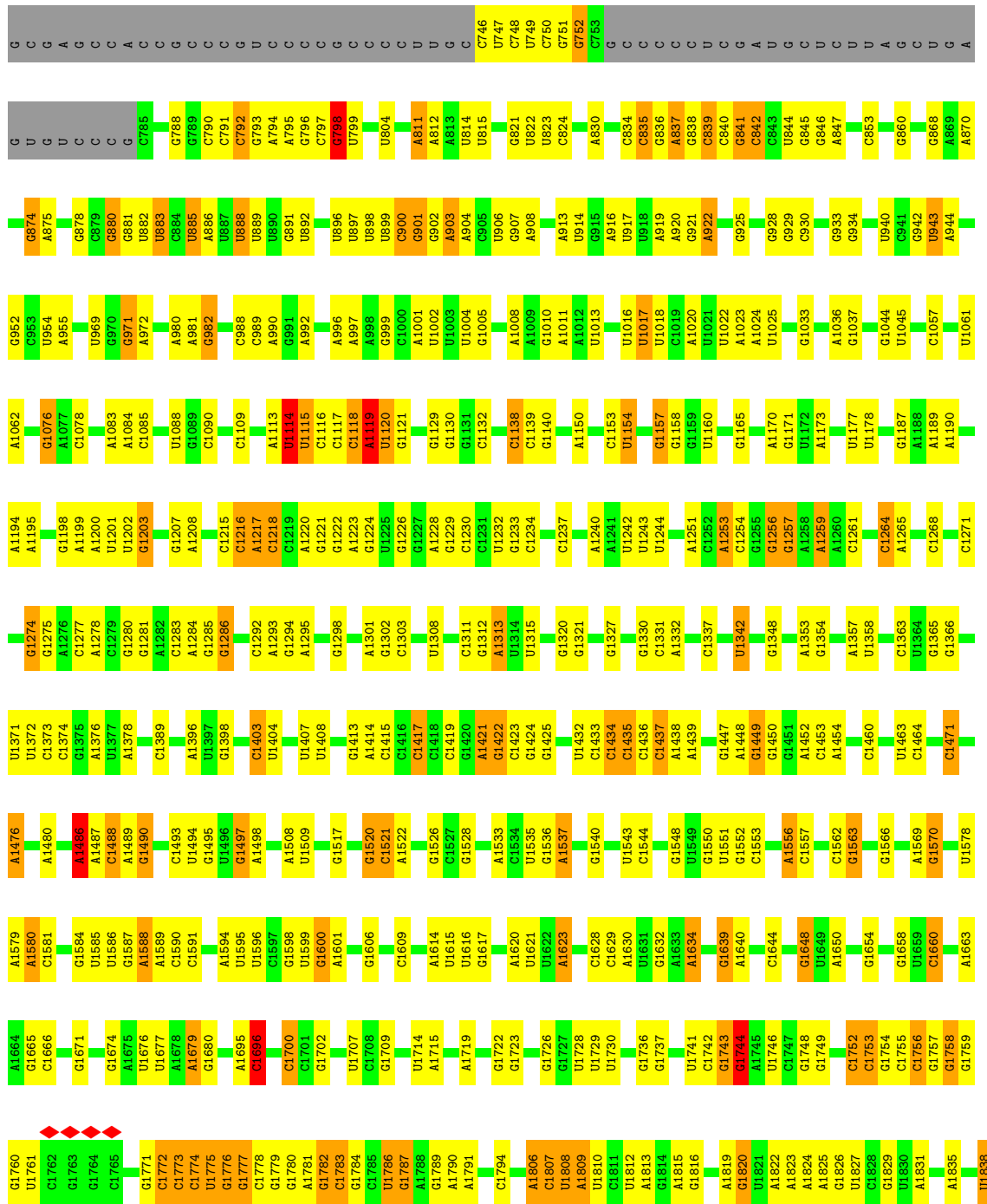
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 60S ribosomal protein L41



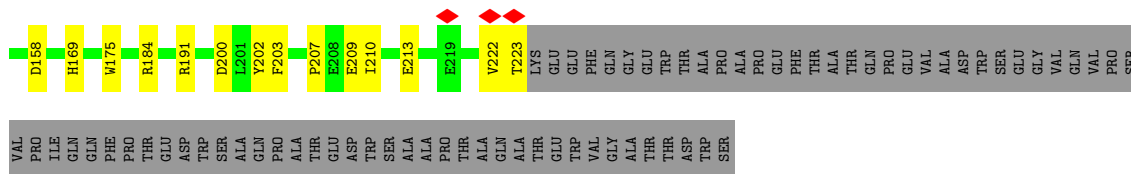
- Molecule 2: 18S rRNA



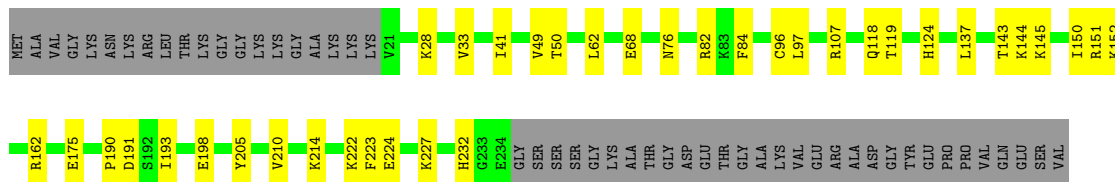


• Molecule 3: 40S ribosomal protein SA

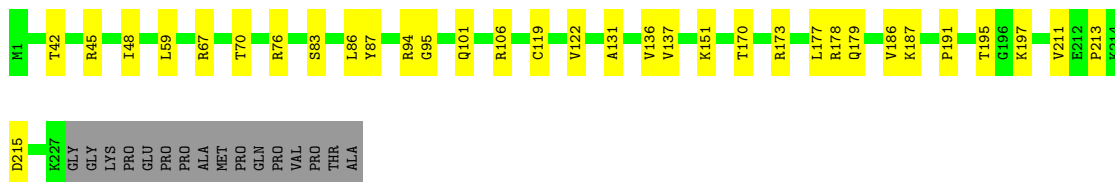
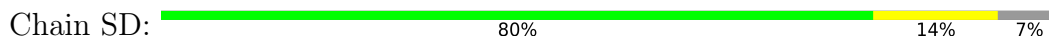




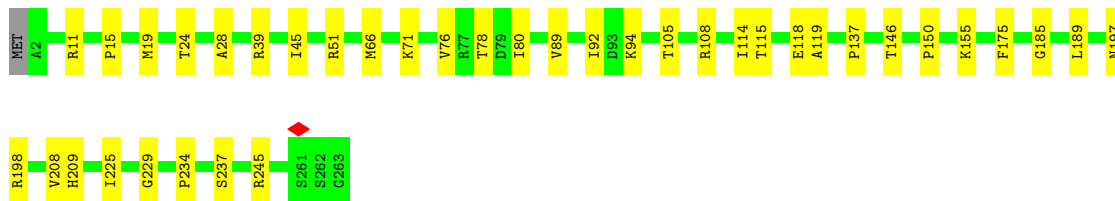
• Molecule 4: 40S ribosomal protein S3a



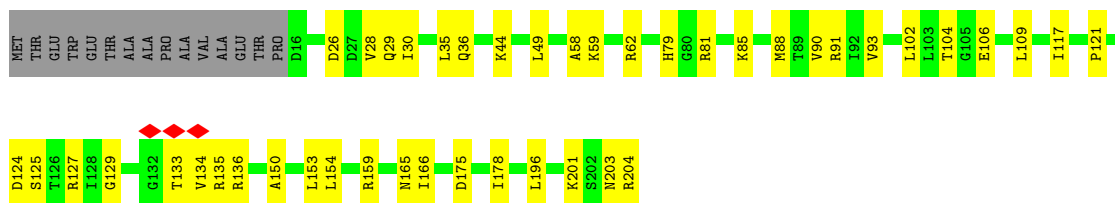
• Molecule 5: 40S ribosomal protein S3



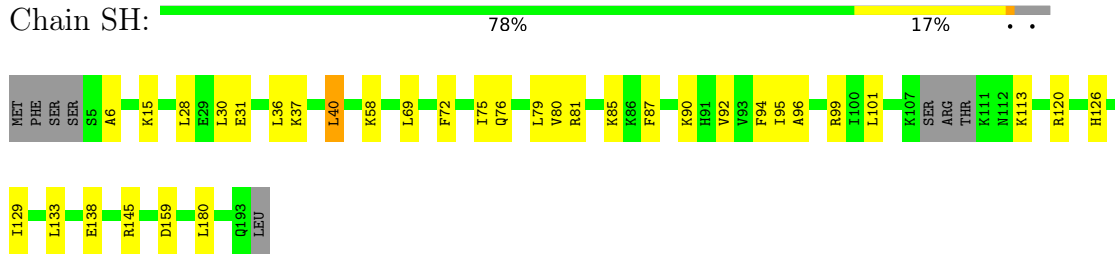
• Molecule 6: 40S ribosomal protein S4, X isoform



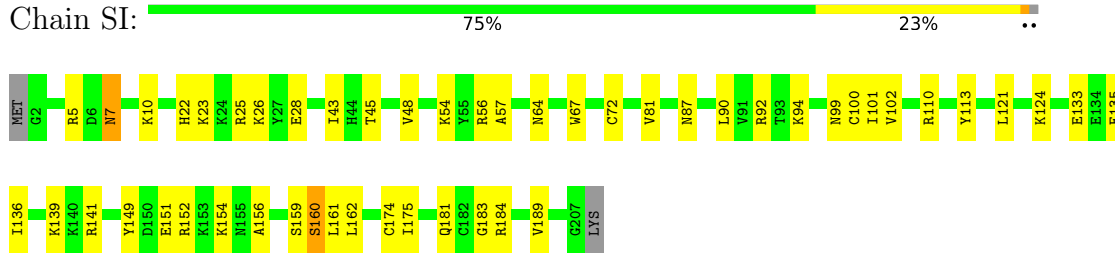
• Molecule 7: 40S ribosomal protein S5



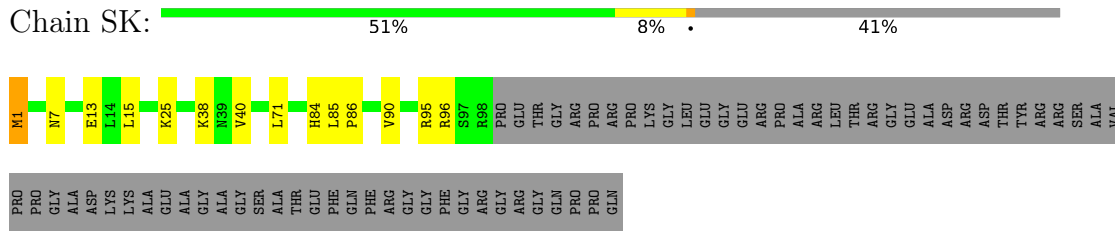
• Molecule 8: 40S ribosomal protein S7



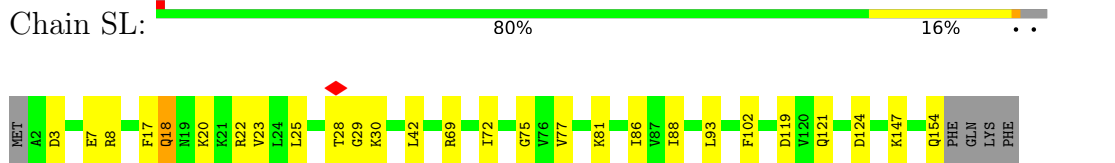
• Molecule 9: 40S ribosomal protein S8



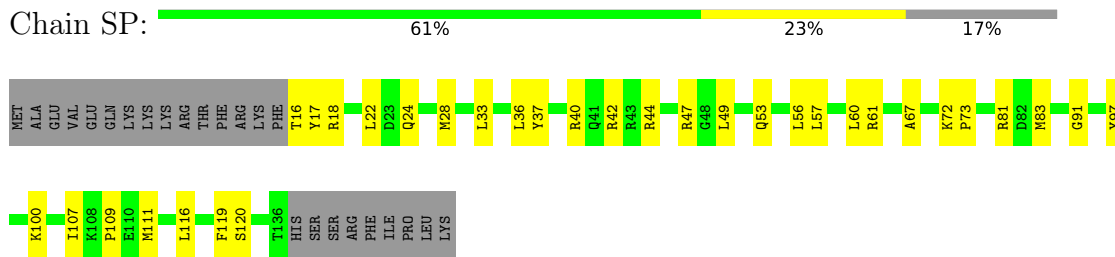
• Molecule 10: 40S ribosomal protein S10



• Molecule 11: 40S ribosomal protein S11



• Molecule 12: 40S ribosomal protein S15



• Molecule 13: 40S ribosomal protein S16

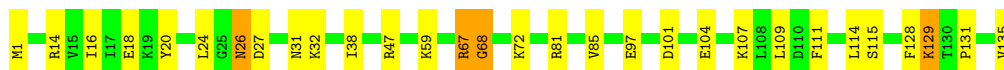






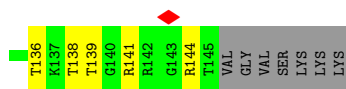
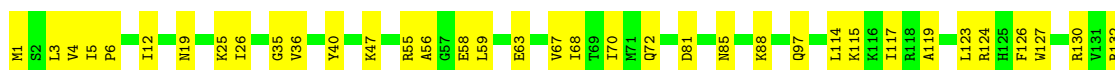
- Molecule 14: 40S ribosomal protein S17

Chain SR: 78% 19%



- Molecule 15: 40S ribosomal protein S18

Chain SS: 68% 27% 5%



- Molecule 16: 40S ribosomal protein S19

Chain ST: 79% 20%



- Molecule 17: 40S ribosomal protein S20

Chain SU: 62% 24% 13%



- Molecule 18: 40S ribosomal protein S21

Chain SV: 81% 19%

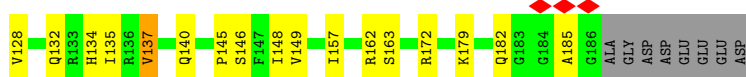


- Molecule 19: 40S ribosomal protein S23

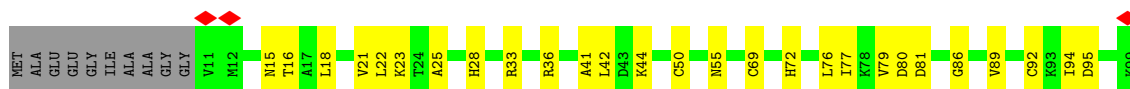




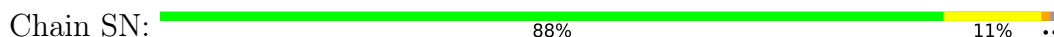
• Molecule 26: 40S ribosomal protein S9



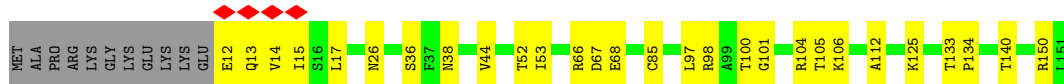
• Molecule 27: 40S ribosomal protein S12



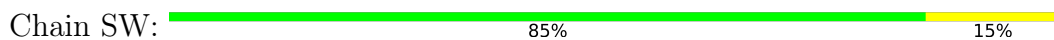
• Molecule 28: 40S ribosomal protein S13



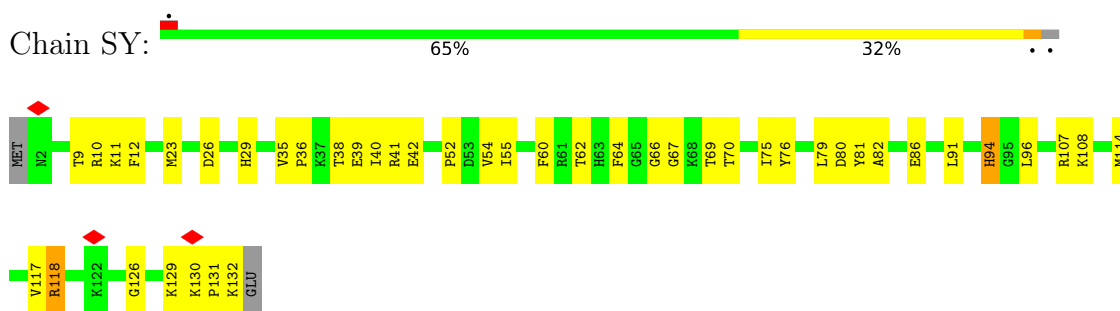
• Molecule 29: 40S ribosomal protein S14



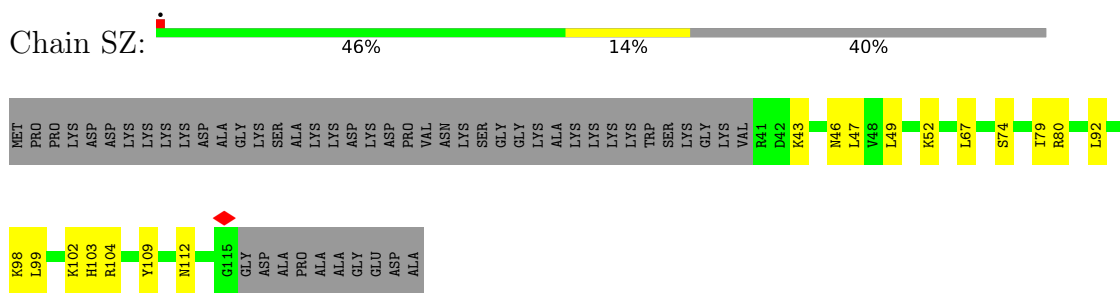
• Molecule 30: 40S ribosomal protein S15a



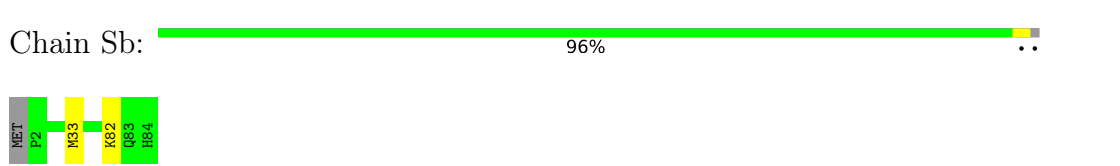
• Molecule 31: 40S ribosomal protein S24



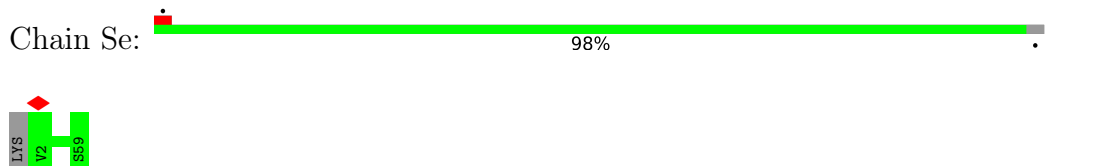
• Molecule 32: 40S ribosomal protein S25



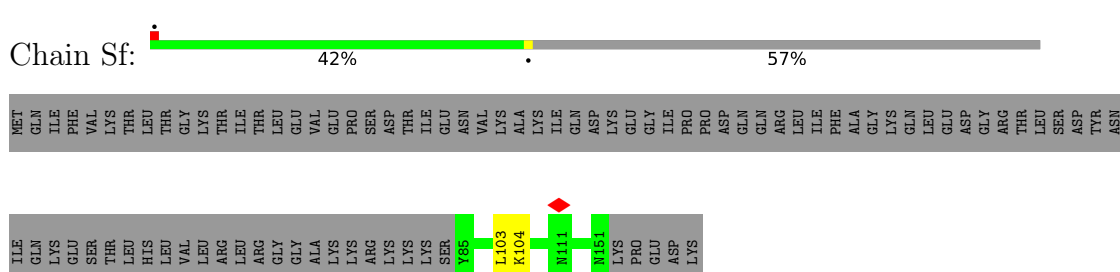
• Molecule 33: 40S ribosomal protein S27



• Molecule 34: 40S ribosomal protein S30



• Molecule 35: Ubiquitin-40S ribosomal protein S27a



• Molecule 36: Eukaryotic translation initiation factor 1



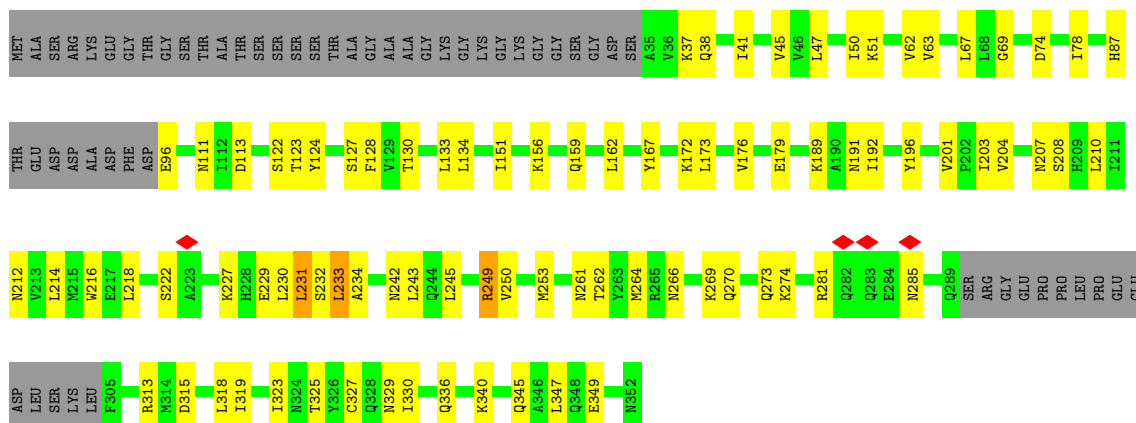




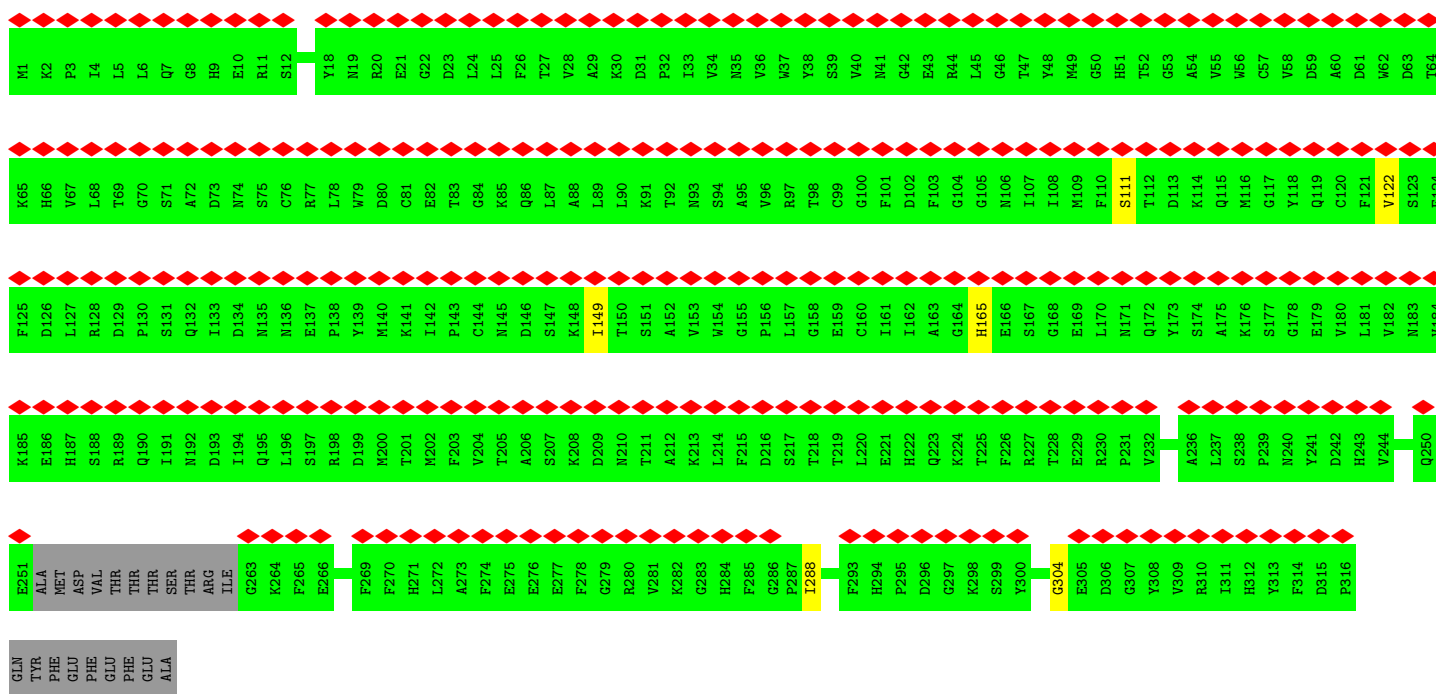
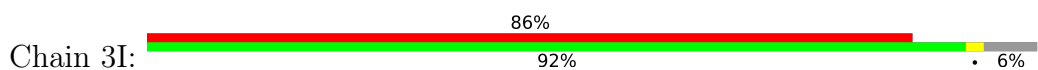




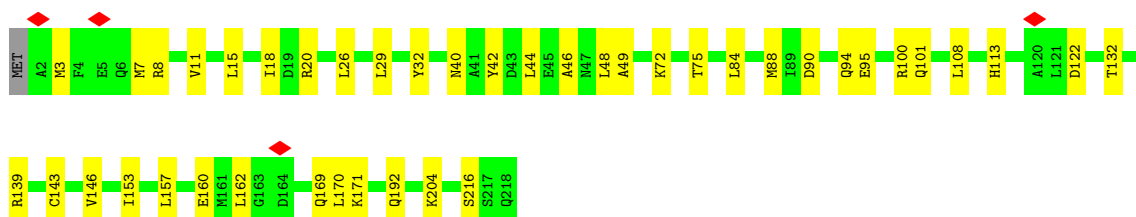
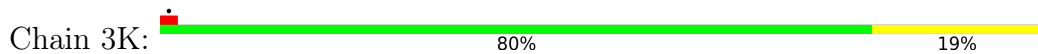




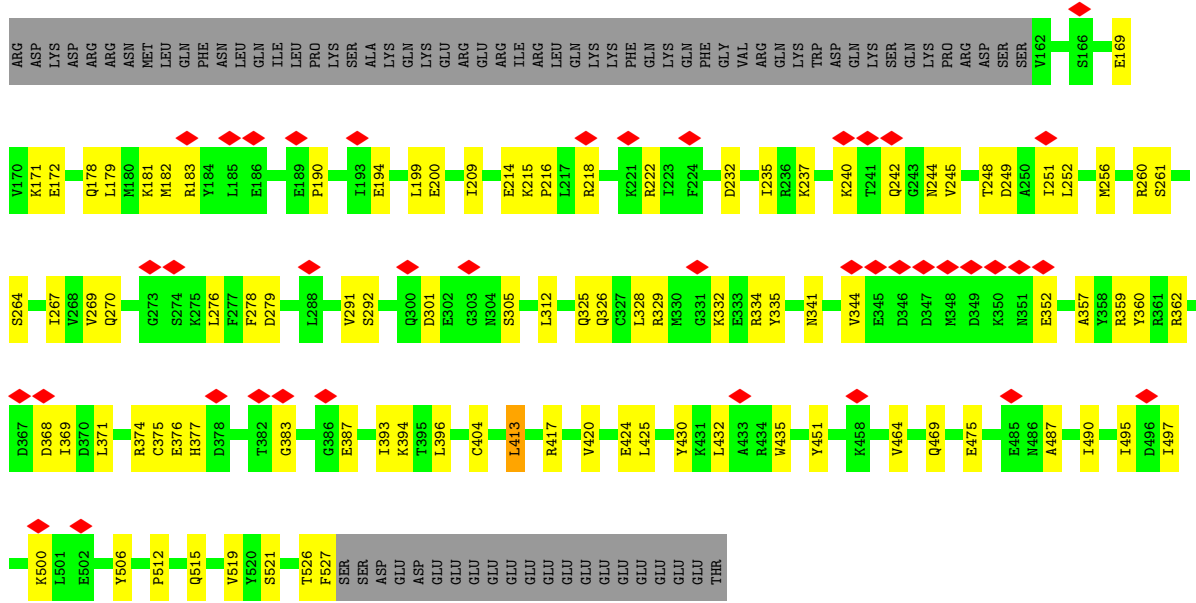
• Molecule 46: Eukaryotic translation initiation factor 3 subunit I



• Molecule 47: Eukaryotic translation initiation factor 3 subunit K







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12788	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	481.32, 481.32, 481.32	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	Ln	0.29	0/231	0.77	0/294
2	S2	0.60	0/40840	1.06	173/63635 (0.3%)
3	SA	0.39	0/1778	0.64	0/2416
4	SB	0.37	0/1765	0.68	0/2362
5	SD	0.39	0/1793	0.74	0/2414
6	SE	0.36	0/2118	0.65	0/2849
7	SF	0.35	0/1516	0.72	1/2037 (0.0%)
8	SH	0.34	0/1519	0.69	1/2033 (0.0%)
9	SI	0.36	0/1715	0.75	0/2287
10	SK	0.36	0/851	0.70	2/1147 (0.2%)
11	SL	0.39	0/1268	0.59	0/1696
12	SP	0.36	0/1003	0.80	0/1342
13	SQ	0.39	0/1160	0.76	2/1553 (0.1%)
14	SR	0.37	0/1105	0.75	1/1484 (0.1%)
15	SS	0.32	0/1216	0.72	0/1628
16	ST	0.34	0/1131	0.69	0/1515
17	SU	0.36	0/827	0.71	0/1110
18	SV	0.38	0/643	0.69	0/860
19	SX	0.43	0/1116	0.66	0/1490
20	Sa	0.40	0/836	0.73	0/1121
21	Sc	0.37	0/508	0.84	1/680 (0.1%)
22	Sd	0.43	0/470	0.74	0/623
23	Sg	0.30	0/2493	0.68	0/3394
24	SC	0.43	0/1762	0.68	1/2381 (0.0%)
25	SG	0.31	0/1946	0.71	1/2590 (0.0%)
26	SJ	0.40	0/1550	0.72	1/2069 (0.0%)
27	SM	0.34	0/950	0.75	0/1275
28	SN	0.37	0/1232	0.67	0/1656
29	SO	0.37	0/1062	0.67	0/1425
30	SW	0.39	0/1051	0.63	0/1406
31	SY	0.35	0/1083	0.72	0/1438
32	SZ	0.32	0/604	0.83	1/810 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Sb	0.36	0/665	0.69	0/891
34	Se	0.31	0/465	0.64	0/612
35	Sf	0.29	0/560	0.73	1/745 (0.1%)
36	C1	0.25	0/442	0.58	0/611
37	4A	0.25	0/1687	0.53	0/2344
38	CD	0.33	0/1846	0.53	0/2550
39	3A	0.28	0/5463	0.64	4/7394 (0.1%)
40	3B	0.27	0/2981	0.54	1/4115 (0.0%)
41	3C	0.31	0/5154	0.69	5/6942 (0.1%)
42	3E	0.29	0/3503	0.66	2/4728 (0.0%)
43	3F	0.29	0/2126	0.64	0/2890
44	3G	0.33	0/680	0.69	1/916 (0.1%)
45	3H	0.27	0/2458	0.65	2/3313 (0.1%)
46	3I	0.25	0/1495	0.48	0/2073
47	3K	0.26	0/1785	0.58	1/2414 (0.0%)
48	3L	0.29	0/3187	0.68	3/4299 (0.1%)
49	3M	0.28	0/2743	0.65	2/3697 (0.1%)
50	3N	0.29	0/3699	0.63	2/5001 (0.0%)
All	All	0.44	0/120081	0.83	209/170555 (0.1%)

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
7	SF	0	2
9	SI	0	1
14	SR	0	1
19	SX	0	5
21	Sc	0	1
26	SJ	0	1
32	SZ	0	1
33	Sb	0	2
43	3F	0	1
45	3H	0	1
48	3L	0	2
All	All	0	18

There are no bond length outliers.

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S2	1772	C	N3-C2-O2	-14.58	111.70	121.90
2	S2	1772	C	N1-C2-O2	14.18	127.41	118.90
2	S2	501	C	N1-C2-O2	13.09	126.75	118.90
2	S2	501	C	C2-N1-C1'	12.99	133.09	118.80
2	S2	293	C	N1-C2-O2	12.27	126.26	118.90

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	SF	133	THR	Peptide
7	SF	79	HIS	Peptide
9	SI	159	SER	Peptide
14	SR	67	ARG	Peptide
19	SX	86	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	Ln	230	0	276	0	0
2	S2	36535	0	18416	320	0
3	SA	1741	0	1746	32	0
4	SB	1738	0	1809	24	0
5	SD	1765	0	1865	23	0
6	SE	2076	0	2177	22	0
7	SF	1495	0	1549	26	0
8	SH	1497	0	1590	18	0
9	SI	1686	0	1772	40	0
10	SK	827	0	854	8	0
11	SL	1247	0	1323	20	0
12	SP	985	0	1031	25	0
13	SQ	1142	0	1213	25	0
14	SR	1090	0	1149	23	0
15	SS	1198	0	1261	30	0
16	ST	1112	0	1146	18	0
17	SU	817	0	882	18	0
18	SV	636	0	637	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	SX	1098	0	1167	14	0
20	Sa	821	0	870	0	0
21	Sc	506	0	536	0	0
22	Sd	459	0	448	0	0
23	Sg	2436	0	2393	0	0
24	SC	1725	0	1813	27	0
25	SG	1923	0	2088	42	0
26	SJ	1525	0	1640	34	0
27	SM	940	0	965	23	0
28	SN	1208	0	1294	14	0
29	SO	1049	0	1073	16	0
30	SW	1034	0	1080	13	0
31	SY	1065	0	1142	34	0
32	SZ	598	0	656	14	0
33	Sb	651	0	672	0	0
34	Se	459	0	503	0	0
35	Sf	548	0	555	0	0
36	C1	443	0	201	2	0
37	4A	1691	0	753	5	0
38	CD	1841	0	998	4	0
39	3A	5379	0	5155	83	0
40	3B	2966	0	1764	19	0
41	3C	5070	0	5110	91	0
42	3E	3437	0	3433	68	0
43	3F	2090	0	2092	56	0
44	3G	667	0	647	16	0
45	3H	2413	0	2411	69	0
46	3I	1497	0	676	3	0
47	3K	1750	0	1717	28	0
48	3L	3111	0	3085	59	0
49	3M	2705	0	2759	52	0
50	3N	3617	0	3495	71	0
51	S2	22	0	0	0	0
51	SG	1	0	0	0	0
52	Sa	1	0	0	0	0
52	Sd	1	0	0	0	0
52	Sf	1	0	0	0	0
All	All	114565	0	93887	1340	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 7.

The worst 5 of 1340 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)
41:3C:697:TYR:HH	41:3C:708:ARG:N	1.57	1.03
2:S2:886:A:N6	2:S2:901:G:C4	2.31	0.98
2:S2:885:U:H3	2:S2:901:G:H1	1.07	0.96
2:S2:1609:C:H42	2:S2:1630:A:H61	1.02	0.93
42:3E:99:GLU:O	42:3E:103:GLN:HB2	1.66	0.93

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	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SA	219/295 (74%)	205 (94%)	13 (6%)	1 (0%)	29	68
4	SB	212/264 (80%)	193 (91%)	19 (9%)	0	100	100
5	SD	225/243 (93%)	205 (91%)	19 (8%)	1 (0%)	34	71
6	SE	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
7	SF	187/204 (92%)	163 (87%)	24 (13%)	0	100	100
8	SH	182/194 (94%)	157 (86%)	23 (13%)	2 (1%)	14	53
9	SI	204/208 (98%)	179 (88%)	23 (11%)	2 (1%)	15	55
10	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
11	SL	151/158 (96%)	137 (91%)	14 (9%)	0	100	100
12	SP	119/145 (82%)	114 (96%)	5 (4%)	0	100	100
13	SQ	142/146 (97%)	126 (89%)	15 (11%)	1 (1%)	22	61
14	SR	133/135 (98%)	118 (89%)	14 (10%)	1 (1%)	19	59
15	SS	143/152 (94%)	129 (90%)	14 (10%)	0	100	100
16	ST	141/145 (97%)	127 (90%)	13 (9%)	1 (1%)	22	61
17	SU	101/119 (85%)	92 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
19	SX	139/143 (97%)	122 (88%)	16 (12%)	1 (1%)	22	61
20	Sa	100/115 (87%)	89 (89%)	10 (10%)	1 (1%)	15	55
21	Sc	62/69 (90%)	45 (73%)	17 (27%)	0	100	100
22	Sd	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
23	Sg	311/317 (98%)	267 (86%)	44 (14%)	0	100	100
24	SC	220/293 (75%)	204 (93%)	16 (7%)	0	100	100
25	SG	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
26	SJ	183/194 (94%)	169 (92%)	14 (8%)	0	100	100
27	SM	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
28	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
29	SO	138/151 (91%)	128 (93%)	9 (6%)	1 (1%)	22	61
30	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
31	SY	129/133 (97%)	117 (91%)	12 (9%)	0	100	100
32	SZ	73/125 (58%)	58 (80%)	15 (20%)	0	100	100
33	Sb	81/84 (96%)	67 (83%)	14 (17%)	0	100	100
34	Se	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
35	Sf	65/156 (42%)	54 (83%)	11 (17%)	0	100	100
36	C1	88/113 (78%)	80 (91%)	8 (9%)	0	100	100
37	4A	334/406 (82%)	319 (96%)	14 (4%)	1 (0%)	41	75
38	CD	343/469 (73%)	327 (95%)	16 (5%)	0	100	100
39	3A	682/1382 (49%)	658 (96%)	23 (3%)	1 (0%)	51	83
40	3B	528/814 (65%)	503 (95%)	25 (5%)	0	100	100
41	3C	615/913 (67%)	581 (94%)	34 (6%)	0	100	100
42	3E	406/445 (91%)	387 (95%)	19 (5%)	0	100	100
43	3F	267/357 (75%)	253 (95%)	14 (5%)	0	100	100
44	3G	82/320 (26%)	79 (96%)	3 (4%)	0	100	100
45	3H	289/352 (82%)	268 (93%)	21 (7%)	0	100	100
46	3I	301/325 (93%)	288 (96%)	13 (4%)	0	100	100
47	3K	215/218 (99%)	200 (93%)	15 (7%)	0	100	100
48	3L	370/564 (66%)	342 (92%)	28 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	3M	326/374 (87%)	316 (97%)	10 (3%)	0	100	100
50	3N	441/548 (80%)	420 (95%)	21 (5%)	0	100	100
All	All	10145/13101 (77%)	9404 (93%)	727 (7%)	14 (0%)	54	83

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SD	178	ARG
8	SH	15	LYS
9	SI	160	SER
37	4A	28	ASN
19	SX	127	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	183/243 (75%)	183 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100
5	SD	190/202 (94%)	189 (100%)	1 (0%)	88	95
6	SE	224/225 (100%)	224 (100%)	0	100	100
7	SF	159/170 (94%)	158 (99%)	1 (1%)	86	94
8	SH	166/174 (95%)	166 (100%)	0	100	100
9	SI	178/180 (99%)	177 (99%)	1 (1%)	86	94
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	137/142 (96%)	135 (98%)	2 (2%)	65	84
12	SP	107/130 (82%)	107 (100%)	0	100	100
13	SQ	119/121 (98%)	118 (99%)	1 (1%)	81	91
14	SR	122/122 (100%)	120 (98%)	2 (2%)	62	83
15	SS	126/132 (96%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	ST	113/115 (98%)	110 (97%)	3 (3%)	44	73
17	SU	94/107 (88%)	93 (99%)	1 (1%)	73	88
18	SV	67/67 (100%)	67 (100%)	0	100	100
19	SX	113/115 (98%)	113 (100%)	0	100	100
20	Sa	89/98 (91%)	88 (99%)	1 (1%)	73	88
21	Sc	57/62 (92%)	57 (100%)	0	100	100
22	Sd	48/49 (98%)	47 (98%)	1 (2%)	53	78
23	Sg	272/275 (99%)	272 (100%)	0	100	100
24	SC	188/225 (84%)	188 (100%)	0	100	100
25	SG	207/218 (95%)	206 (100%)	1 (0%)	88	95
26	SJ	161/168 (96%)	161 (100%)	0	100	100
27	SM	102/108 (94%)	100 (98%)	2 (2%)	55	79
28	SN	130/131 (99%)	128 (98%)	2 (2%)	65	84
29	SO	110/119 (92%)	106 (96%)	4 (4%)	35	67
30	SW	112/113 (99%)	112 (100%)	0	100	100
31	SY	113/115 (98%)	110 (97%)	3 (3%)	44	73
32	SZ	66/103 (64%)	65 (98%)	1 (2%)	65	84
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Se	47/48 (98%)	47 (100%)	0	100	100
35	Sf	60/140 (43%)	59 (98%)	1 (2%)	60	82
38	CD	37/404 (9%)	37 (100%)	0	100	100
39	3A	544/1259 (43%)	540 (99%)	4 (1%)	84	93
40	3B	90/702 (13%)	89 (99%)	1 (1%)	73	88
41	3C	553/811 (68%)	553 (100%)	0	100	100
42	3E	380/406 (94%)	378 (100%)	2 (0%)	88	95
43	3F	237/289 (82%)	236 (100%)	1 (0%)	91	97
44	3G	70/277 (25%)	70 (100%)	0	100	100
45	3H	269/310 (87%)	266 (99%)	3 (1%)	73	88
47	3K	192/193 (100%)	192 (100%)	0	100	100
48	3L	342/515 (66%)	337 (98%)	5 (2%)	65	84
49	3M	304/335 (91%)	303 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	3N	398/494 (81%)	396 (100%)	2 (0%)	88	95
All	All	7658/10679 (72%)	7611 (99%)	47 (1%)	86	94

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	3A	353	ARG
43	3F	126	LYS
39	3A	409	LYS
40	3B	497	GLN
45	3H	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
39	3A	512	GLN
49	3M	366	ASN
41	3C	869	ASN
48	3L	436	HIS
41	3C	637	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1701/1869 (91%)	433 (25%)	4 (0%)

5 of 433 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	2	A
2	S2	4	C
2	S2	17	C
2	S2	23	G
2	S2	25	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	112	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	S2	291	G
2	S2	688	U
2	S2	1434	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 monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 26 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.

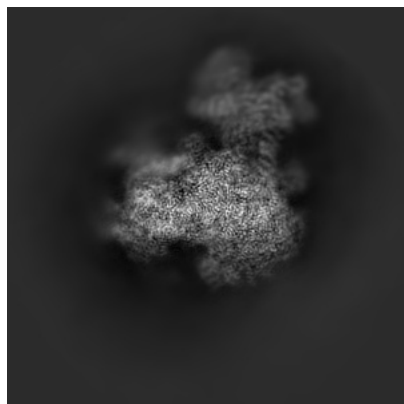
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38754. These allow visual inspection of the internal detail of the map and identification of artifacts.

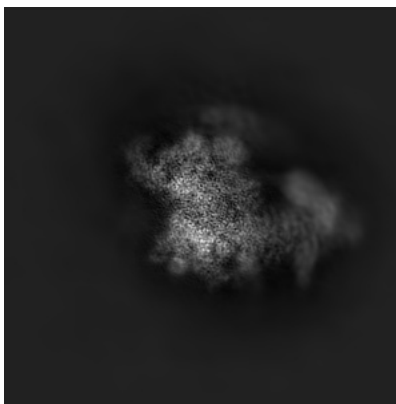
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

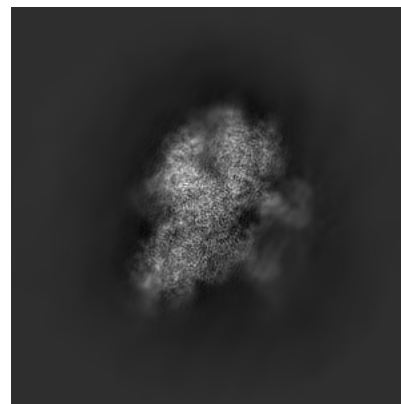
#### 6.1.1 Primary map



X

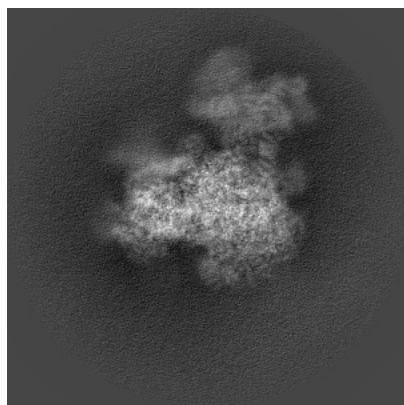


Y

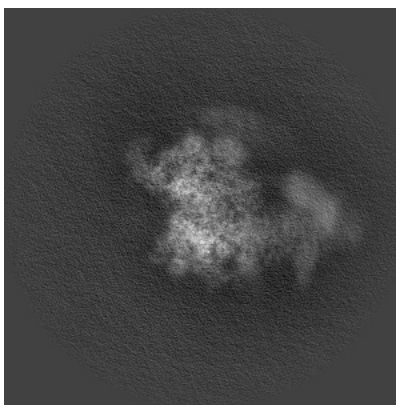


Z

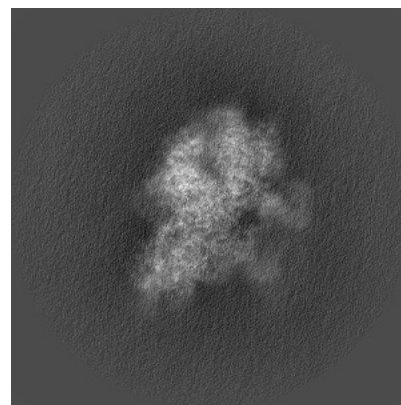
#### 6.1.2 Raw map



X



Y



Z

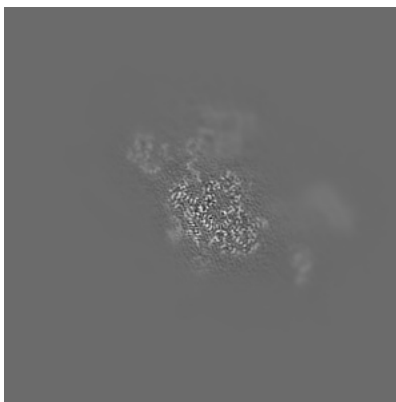
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

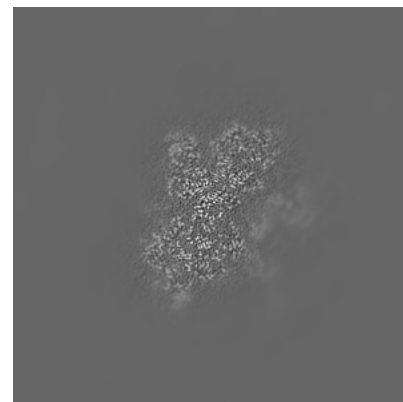
### 6.2.1 Primary map



X Index: 210

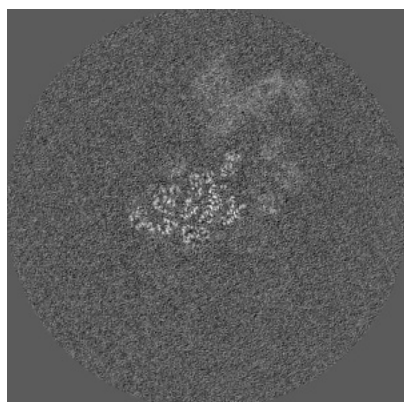


Y Index: 210

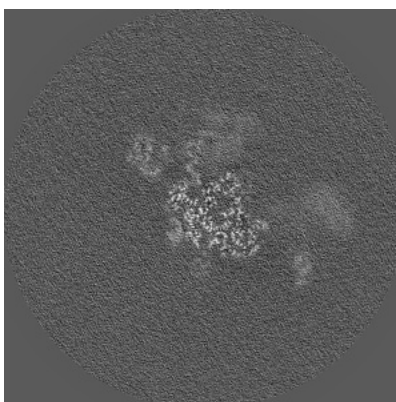


Z Index: 210

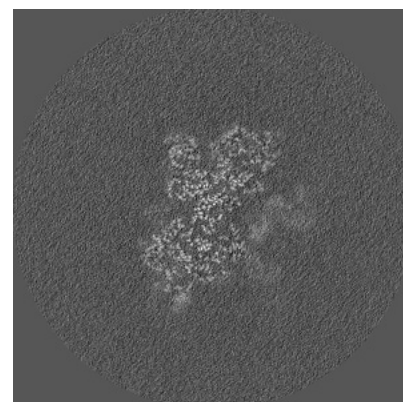
### 6.2.2 Raw map



X Index: 210



Y Index: 210



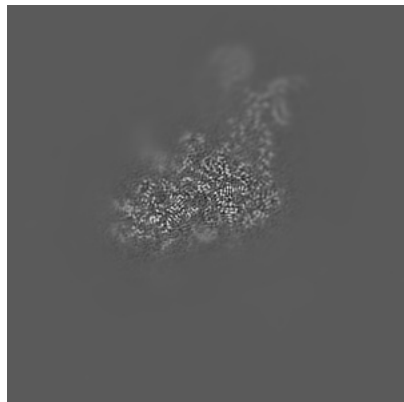
Z Index: 210

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

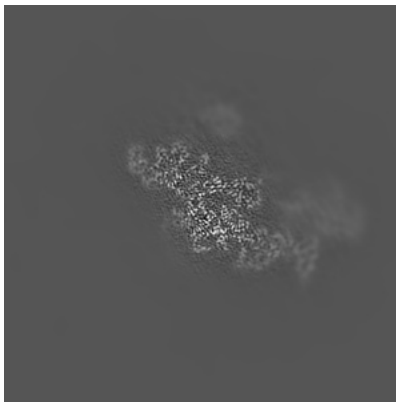


## 6.3 Largest variance slices [i](#)

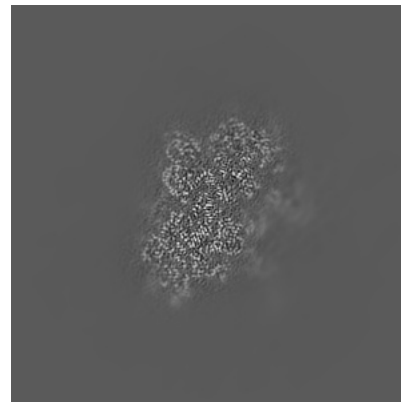
### 6.3.1 Primary map



X Index: 183

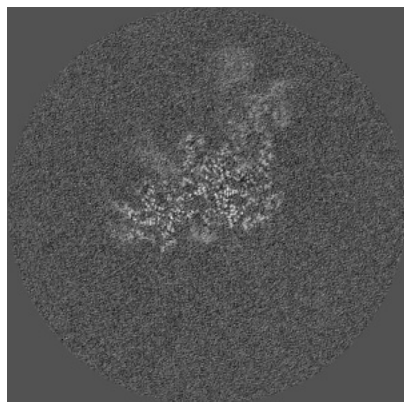


Y Index: 231

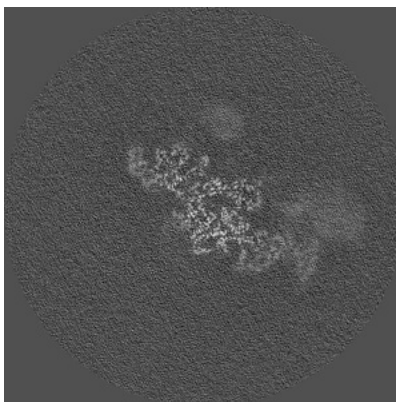


Z Index: 207

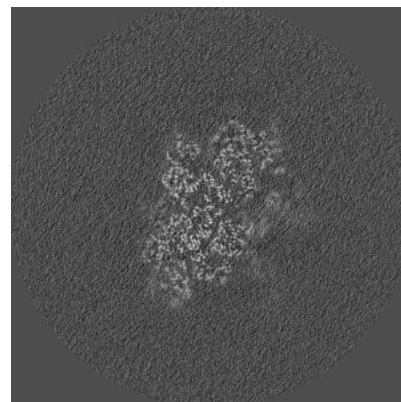
### 6.3.2 Raw map



X Index: 182



Y Index: 231

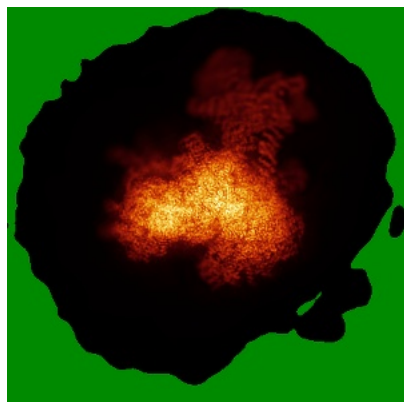


Z Index: 206

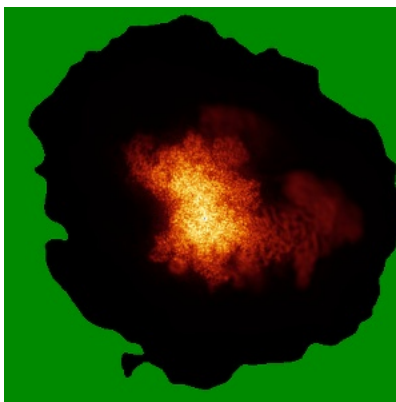
The images above show the largest variance slices of the map in three orthogonal directions.

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

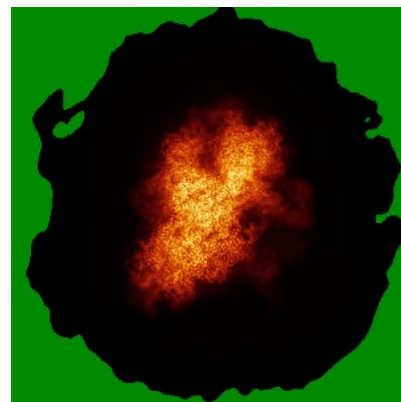
### 6.4.1 Primary map



X

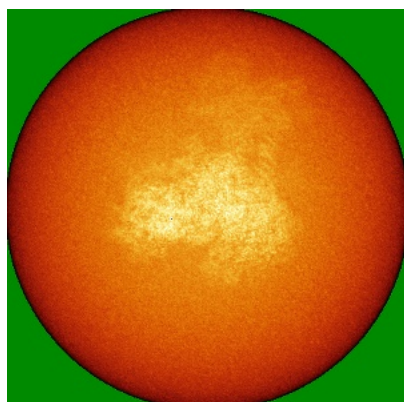


Y

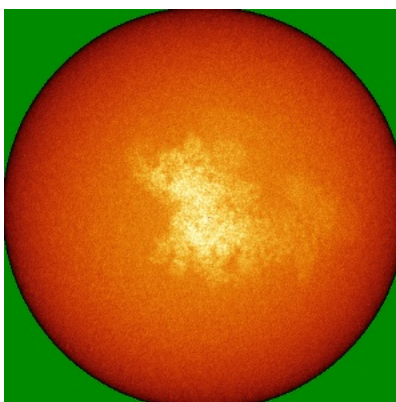


Z

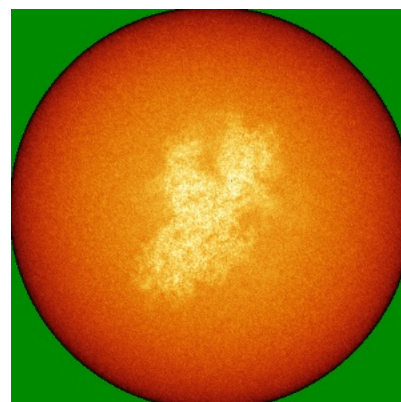
### 6.4.2 Raw map



X



Y

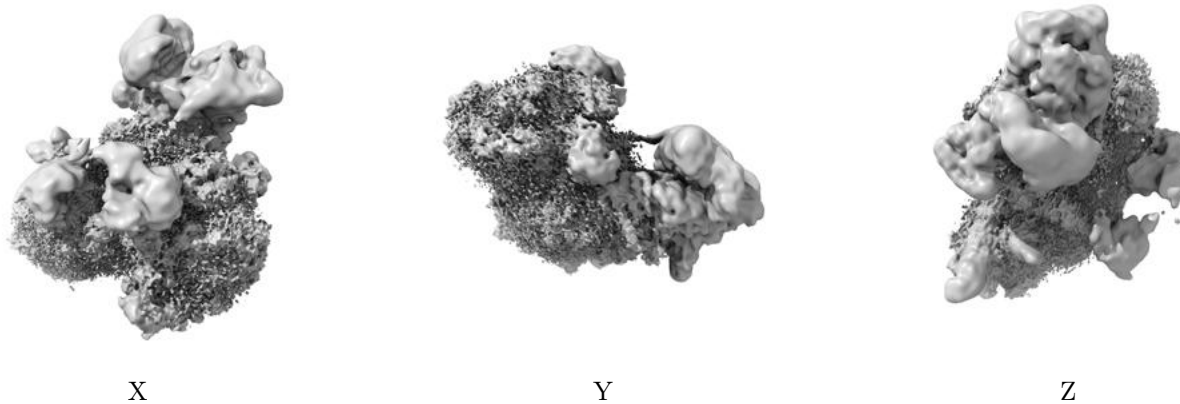


Z

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.

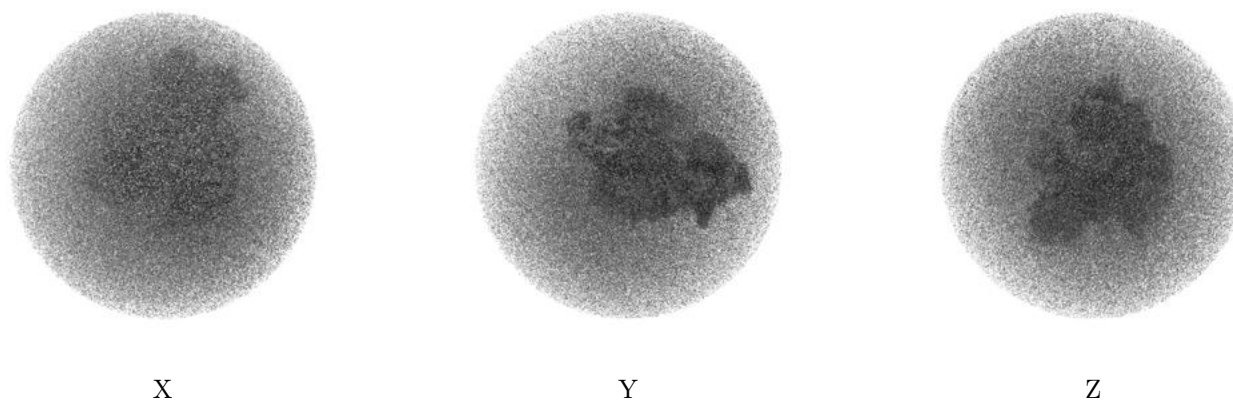
## 6.5 Orthogonal surface views [i](#)

### 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.

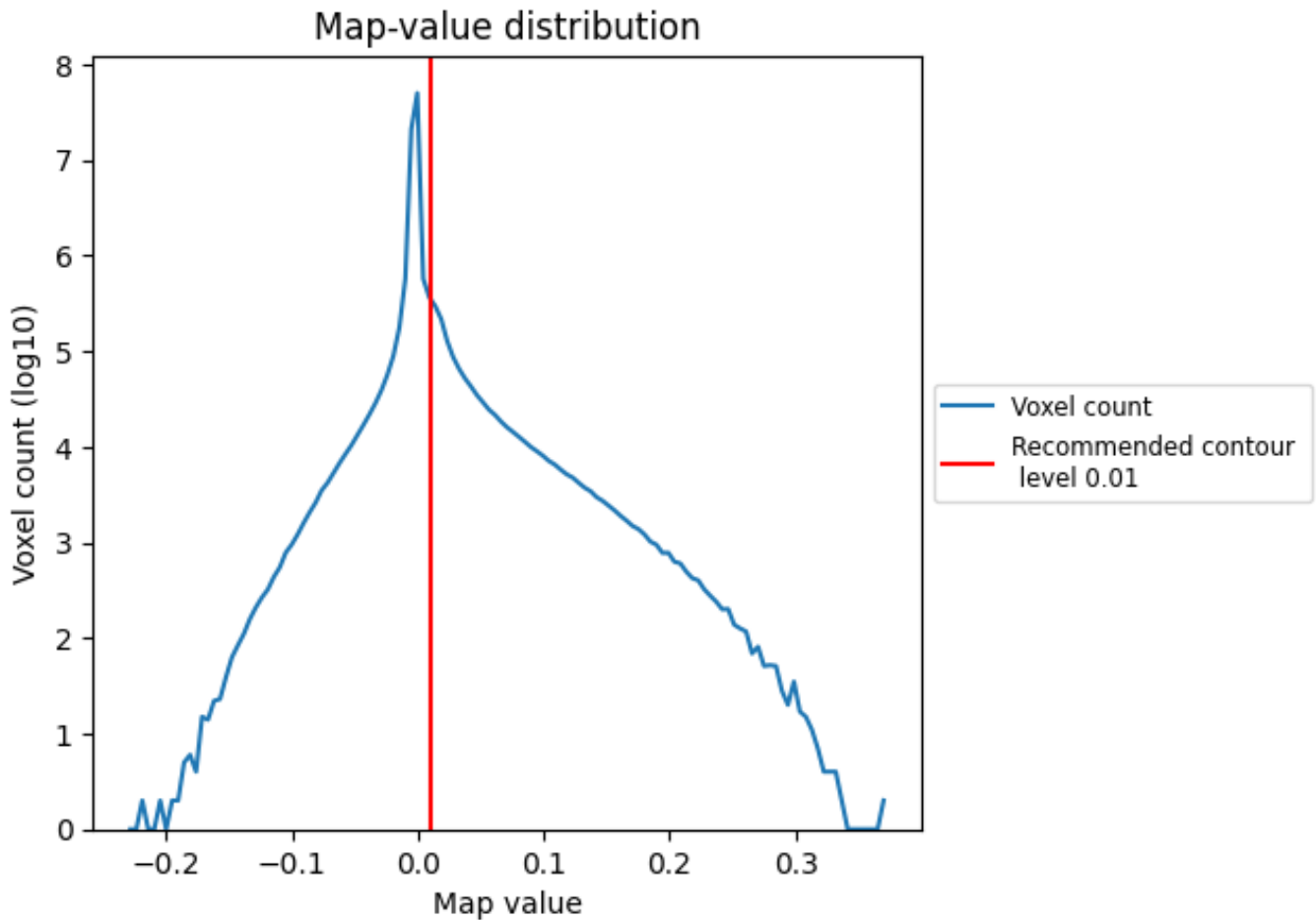
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

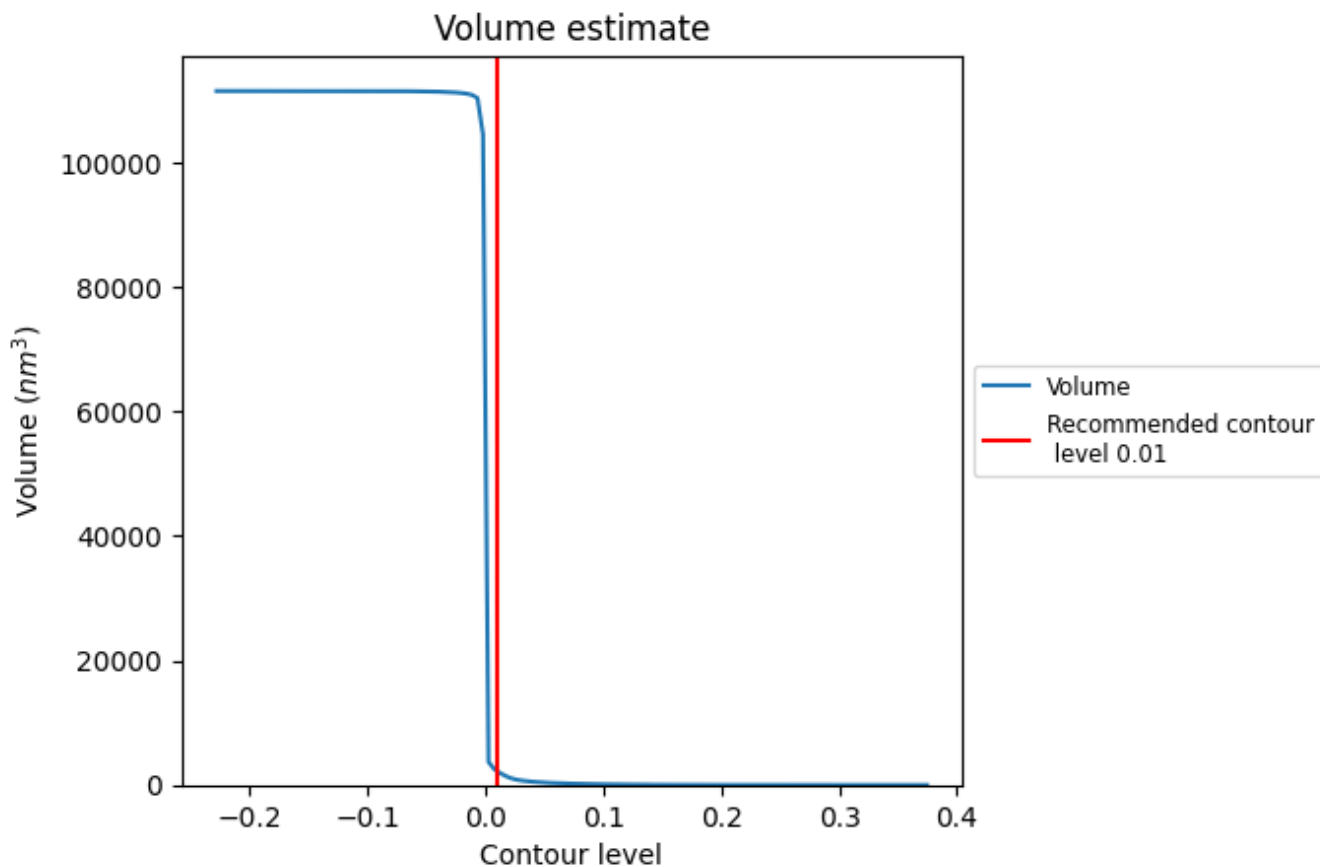
This section contains the results of statistical analysis of the map.

### 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.

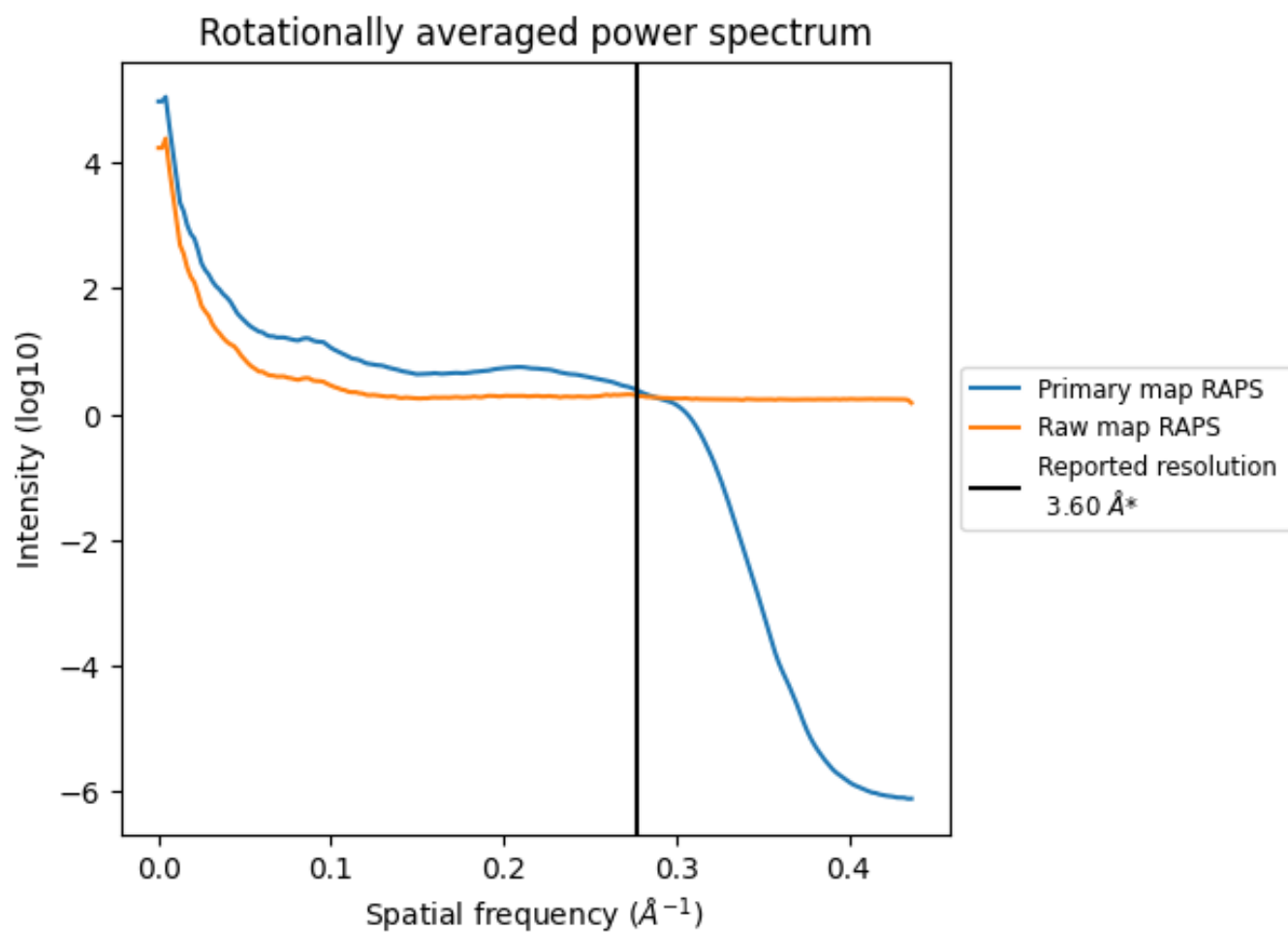
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2214  $\text{nm}^3$ ; this corresponds to an approximate mass of 2000 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

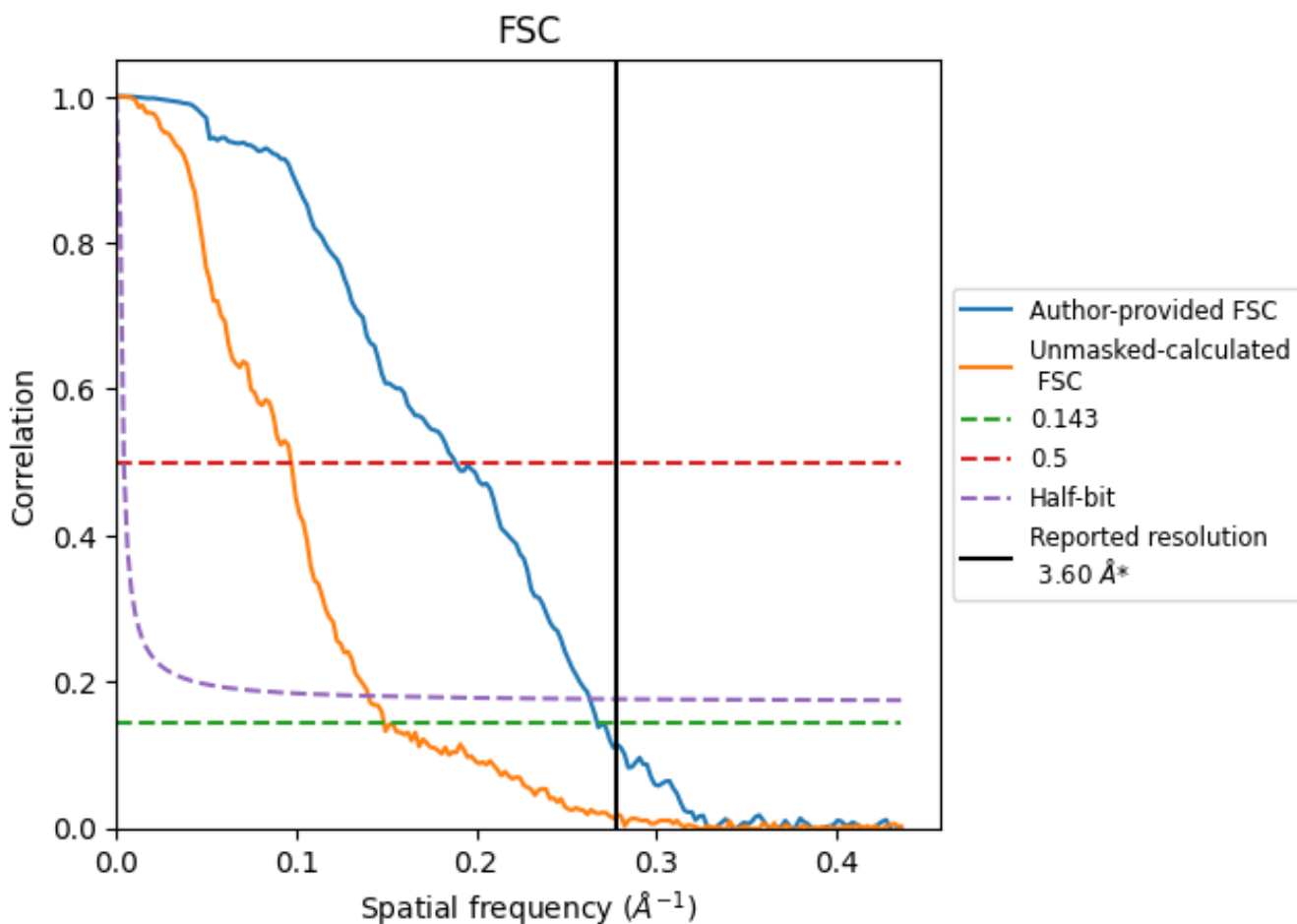


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	5.31	3.80
Unmasked-calculated*	6.72	10.29	7.13

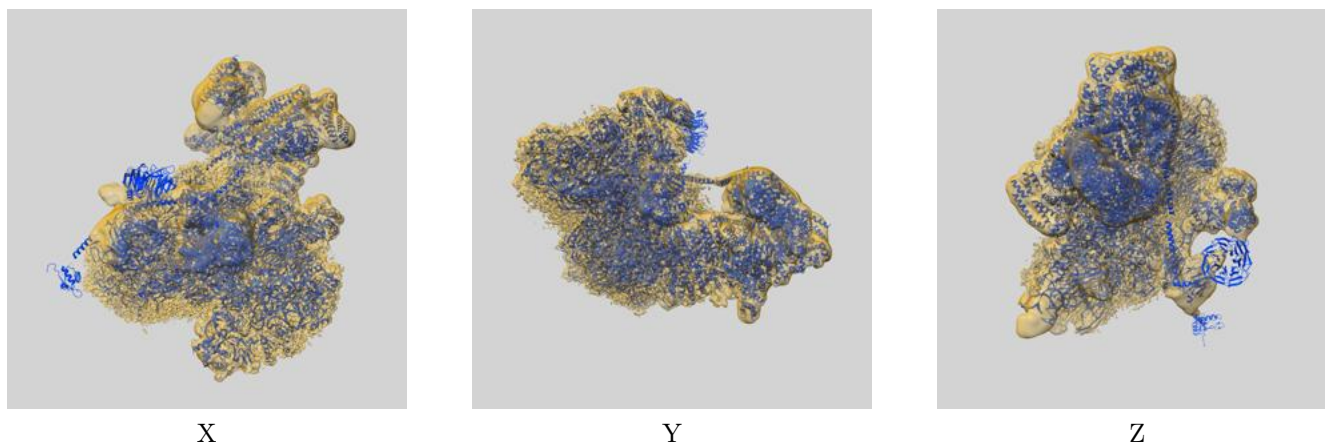
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.6 by more than 10 %



## 9 Map-model fit [i](#)

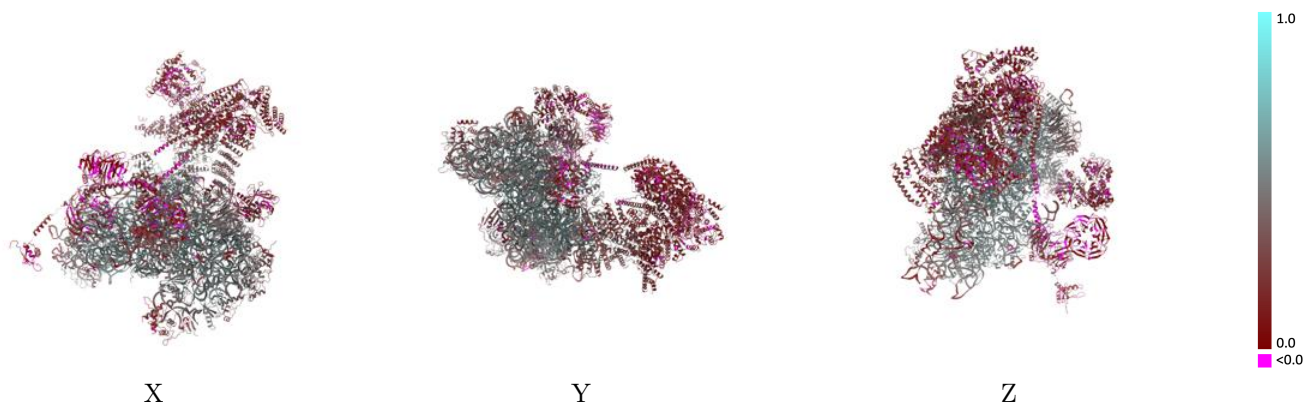
This section contains information regarding the fit between EMDB map EMD-38754 and PDB model 8XXN. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



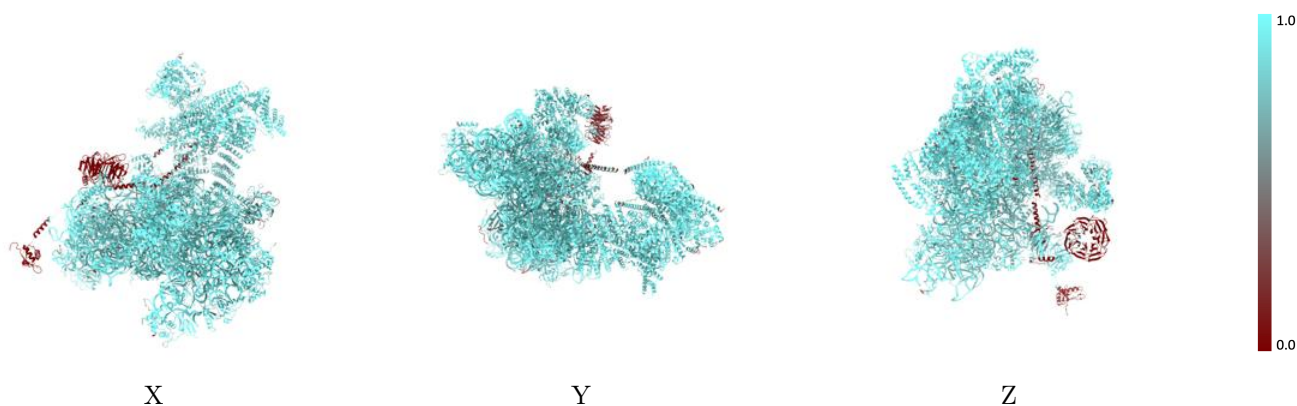
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



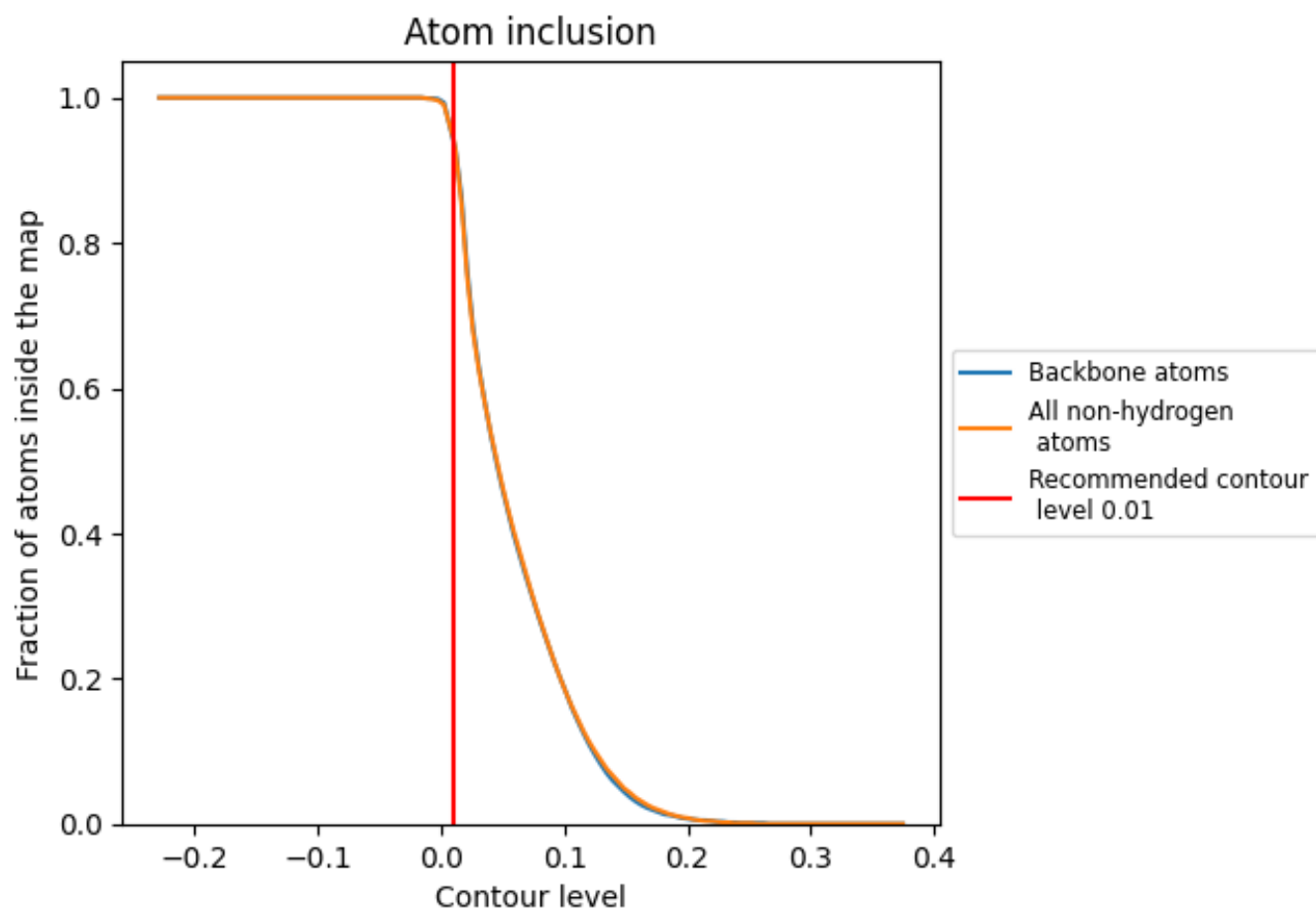
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 94% 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	 0.9450	 0.3740
3A	 0.9040	 0.2270
3B	 0.7020	 0.1290
3C	 0.9470	 0.3030
3E	 0.9700	 0.1700
3F	 0.9620	 0.1150
3G	 0.9830	 0.3040
3H	 0.9600	 0.1330
3I	 0.0760	 0.0340
3K	 0.9530	 0.1120
3L	 0.9440	 0.1020
3M	 0.9870	 0.1520
3N	 0.8220	 0.1860
4A	 0.9480	 0.1480
C1	 0.6820	 0.2590
CD	 0.9670	 0.2320
Ln	 0.8520	 0.3970
S2	 0.9900	 0.4850
SA	 0.9610	 0.4950
SB	 0.9770	 0.4800
SC	 0.9740	 0.5270
SD	 0.9720	 0.4950
SE	 0.9830	 0.5260
SF	 0.9510	 0.4530
SG	 0.9840	 0.4140
SH	 0.9690	 0.4300
SI	 0.9780	 0.4550
SJ	 0.9730	 0.5110
SK	 0.9790	 0.4530
SL	 0.9600	 0.5040
SM	 0.9200	 0.2250
SN	 0.9800	 0.5050
SO	 0.9430	 0.4670
SP	 0.9570	 0.4420
SQ	 0.9600	 0.4990



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Chain	Atom inclusion	Q-score
SR	 0.9500	 0.4640
SS	 0.9470	 0.4140
ST	 0.9690	 0.4540
SU	 0.9640	 0.4310
SV	 0.9840	 0.5070
SW	 0.9810	 0.5560
SX	 0.9800	 0.5370
SY	 0.9560	 0.4710
SZ	 0.9190	 0.3480
Sa	 0.9730	 0.5240
Sb	 0.9560	 0.4980
Sc	 0.9360	 0.4050
Sd	 0.9820	 0.5310
Se	 0.9370	 0.4670
Sf	 0.9480	 0.3020
Sg	 0.9820	 0.3780