wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 04:08 am BST

PDB ID	:	7PNV / pdb_00007pnv
EMDB ID	:	EMD-13553
Title	:	Assembly intermediate of mouse mitochondrial ribosome small subunit without mS37 in complex with RbfA and Mettl15
Authors	:	Itoh, Y.; Khawaja, A.; Laptev, I.; Sergiev, P.; Rorbach, J.; Amunts, A.
Deposited on	:	2021-09-08
Resolution	:	3.06 Å(reported)
Based on initial model	:	6RW4

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 (i) 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 (1)) were used in the production of this report:

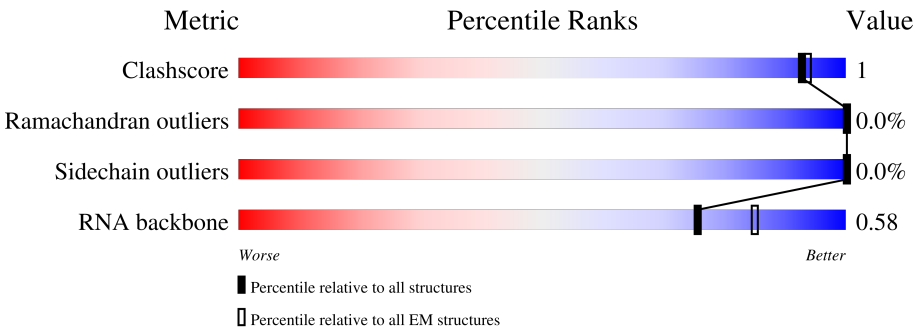
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

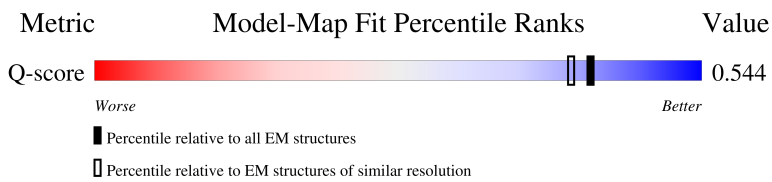
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13976 (2.56 - 3.56)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	956	82% 16%
2	B	291	73% 23%
3	C	167	74% 5% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	432	75% 5% 21%
5	E	125	90% 5% 5%
6	F	242	83% 14%
7	G	390	79% 17%
8	H	160	79% 8% 12%
9	I	191	69% 28%
10	J	139	75% 22%
11	K	128	71% 8% 21%
12	L	258	5% 66% 32%
13	M	135	7% 92% 7%
14	N	120	91% 6%
15	O	254	78% 22%
16	P	143	64% 32%
17	Q	86	97%
18	R	359	80% 18%
19	S	177	75% 23%
20	T	171	95%
21	U	200	87% 13%
22	V	415	86% 12%
23	W	186	52% 46%
24	X	391	87% 5% 9%
25	Y	384	7% 38% 61%
26	Z	106	7% 94% 5%
27	0	218	97%
28	1	320	85% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	3	200	36% 64%
30	4	685	17% 84% 14%
31	a	350	8% 53% 45%
32	b	406	57% 74% 5% 20%

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 131939 atoms, of which 60861 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	951	30430	9078	10223	3629	6549	951	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	223	3590	1142	1799	326	315	8	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2163	690	1091	197	180	5	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	343	5527	1716	2794	527	480	10	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	119	1916	599	968	171	175	3	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	208	3472	1096	1750	316	299	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	325	5304	1689	2630	480	491	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	140	2346	742	1193	200	207	4	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	137	2047	629	1038	191	184	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	181	5F0	ASN	conflict	UNP Q9DCA2

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	108	1749	528	903	172	141	5	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	101	1743	534	888	175	140	6	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	176	3041	930	1576	274	255	6	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	126	2004	623	1009	194	172	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	N	113	1839	575	951	160	150	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	197	3146	1014	1548	289	286	9	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	P	97	1610	505	818	140	139	8	0	0

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	86	1482	453	750	146	126	7	0	0

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	R	294	4816	1526	2416	418	449	7	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	S	136	2257	722	1133	199	201	2	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	T	170	2801	892	1413	238	246	12	0	0

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	U	174	2908	894	1459	283	270	2	0	0

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	V	365	5970	1911	2972	506	570	11	0	0

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	W	100	1606	503	813	141	146	3	0	0

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	X	357	5762	1834	2881	515	522	10	0	0

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	Y	149	2439	809	1193	201	233	3	0	0

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Z	101	1682	526	848	157	148	3	0	0

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	0	216	3649	1139	1838	355	313	4	0	0

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	1	277	4440	1397	2228	380	423	12	0	0

- Molecule 29 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	3	72	1371	414	728	135	93	1	0	0

- Molecule 30 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	4	589	9558	3064	4800	800	872	22	0	0

- Molecule 31 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	a	191	3129	977	1583	280	284	5	0	0

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	b	323	5114	1592	2595	454	462	11	0	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	A	46	46	46	0
33	B	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	Mg		
33	X	1	1	1		0
			Total	Mg		
33	3	1	1	1		0

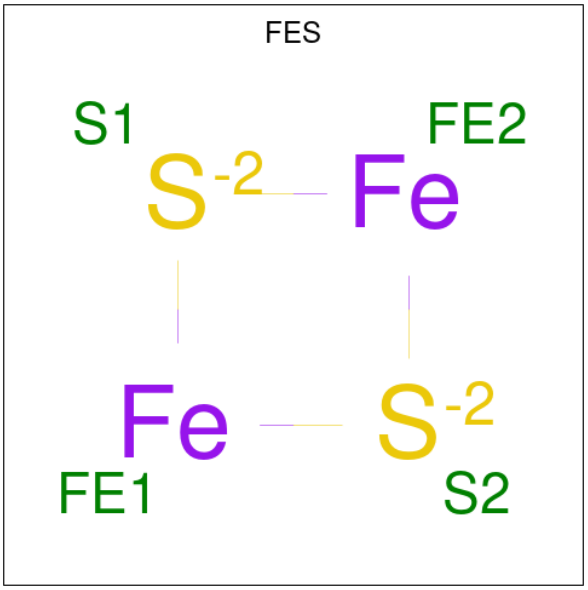
- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms			AltConf
			Total	K		
34	A	13	13	13		0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

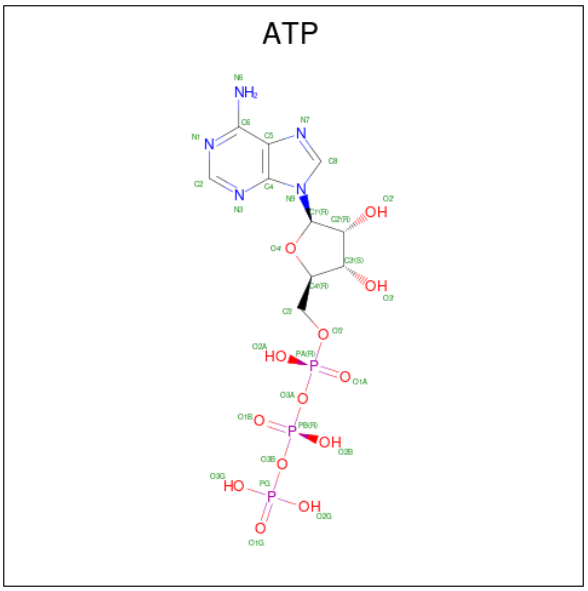
Mol	Chain	Residues	Atoms			AltConf
			Total	Zn		
35	O	1	1	1		0

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



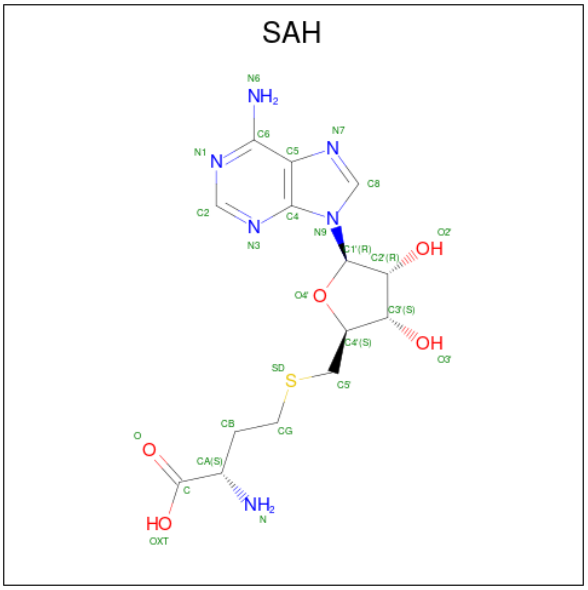
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
36	P	1	4	2	2	0
			Total	Fe	S	
36	T	1	4	2	2	0

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
37	X	1	43	10	12	5	13	3	0

- Molecule 38 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
38	b	1	46	14	20	6	5	1	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	A	549	549	549	0
39	B	23	23	23	0
39	C	19	19	19	0
39	D	34	34	34	0
39	E	2	2	2	0
39	F	7	7	7	0
39	G	10	10	10	0
39	H	19	19	19	0
39	I	5	5	5	0
39	J	14	14	14	0
39	K	25	25	25	0
39	L	6	6	6	0
39	M	16	16	16	0
39	N	8	8	8	0
39	O	25	25	25	0
39	P	3	3	3	0
39	Q	8	8	8	0
39	R	13	13	13	0
39	S	4	4	4	0
39	T	19	19	19	0
39	U	3	3	3	0
39	W	2	2	2	0

Continued on next page...

Continued from previous page...

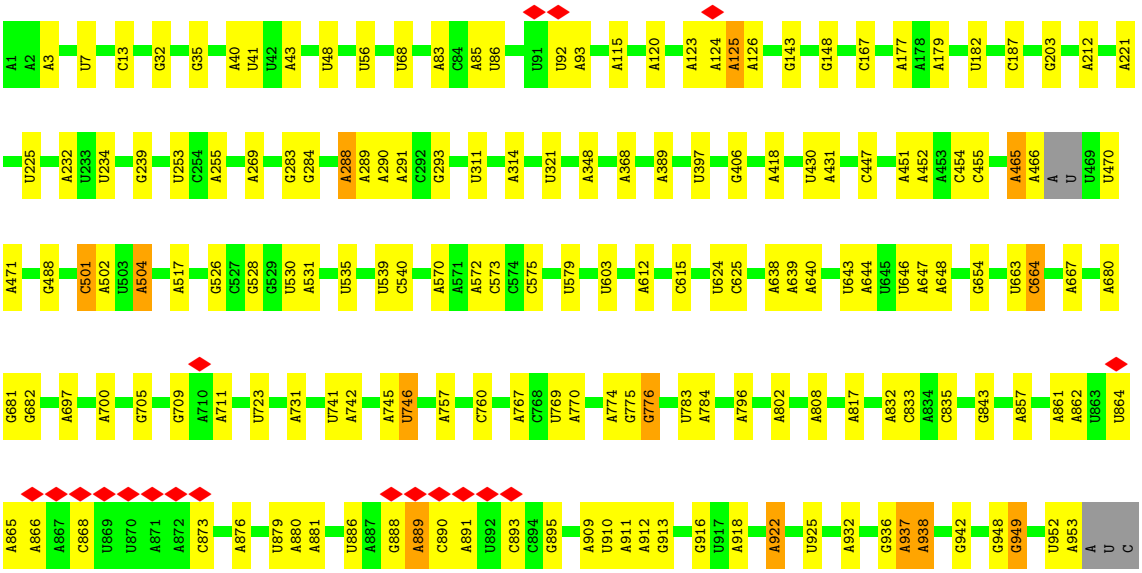
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	X	5	5	5	0
			Total	O	
39	Y	7	7	7	0
			Total	O	
39	Z	18	18	18	0
			Total	O	
39	0	7	7	7	0
			Total	O	
39	1	5	5	5	0
			Total	O	
39	3	7	7	7	0
			Total	O	
39	a	5	5	5	0

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.

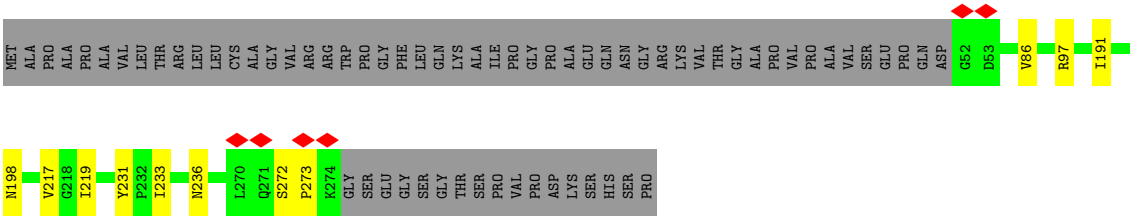
- Molecule 1: 12S mitochondrial rRNA

Chain A:



- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:

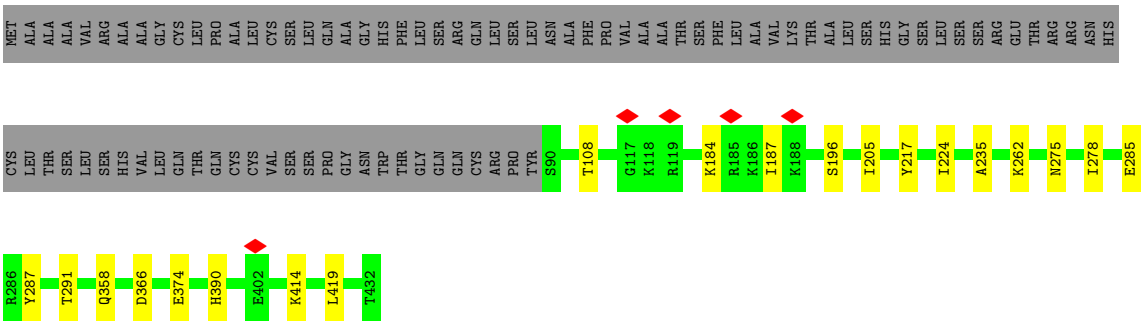


- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:

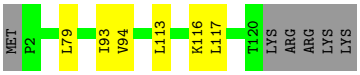
• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



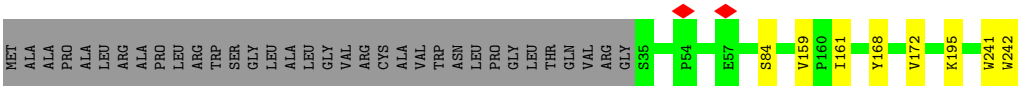
• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:



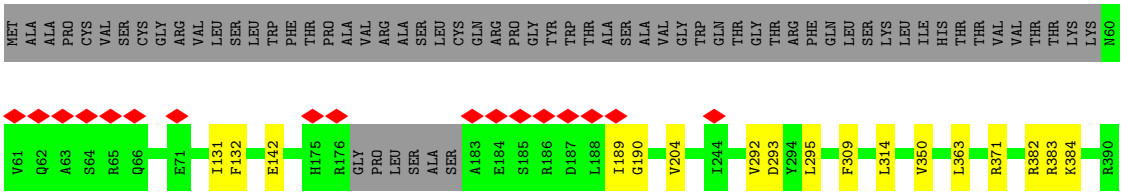
• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



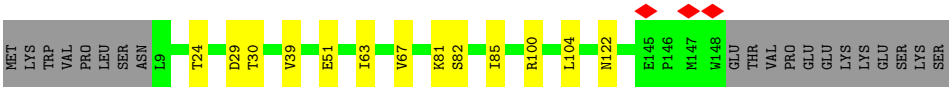
• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:



• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I: 69% 28%

MET GLN VAL LEU ARG ASN SER GLY SER TRP LEU LEU LEU SER TRP ALA GLY HIS GLY MET THR ARG PHE VAL GLY ILE ALA PRO ALA LYS ASN ILE HIS THR GLY ALA PRO ARG LEU GLU ASP SER ALA ALA ARG GLN ASN THR GLU ARG GLU ALA ALA PRO S55 V148 T173 D174

N175 T176 5F0181 L191

- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J: 75% 22%

MET SER TRP PRO GLY LEU LEU TYR GLY LEU THR THR SER LEU SER ARG GLY LEU ALA LEU ALA PRO GLN LEU TRP ALA ALA ARG SER MET A31 R78 P96 D117 R127 K138 LYS

- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K: 71% 8% 21%

MET ALA ALA SER VAL LEU GLY SER LEU LEU ARG THR PHE ARG GLN ALA VAL PRO PRO SER ALA SER GLY GLN VAL ARG GLY Y28 Y29 M34 D37 L38 K39 R40 K59 R80 S95 R108 R112 W128

- Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L: 5% 66% 32%

MET LEU ARG ALA ALA TRP ARG ALA LEU SER SER VAL ARG ALA GLN ALA VAL THR ARG ALA PRO VAL PRO ALA LEU ARG GLY GLY SER SER ALA SER LEU LEU SER ALA ARG CYS GLY LEU GLN PRO PRO SER LEU LEU ARG ALA ALA ARG ALA TYR ALA ALA VAL GLN LYS PRO VAL GLN

PRO K62 Q63 D64 P193 P194 R226 A227 L228 K229 A230 A231 A232 A233 A234 A235 K236 K237 GLU LYS ASN GLU GLY VAL PRO GLU ASN PRO SER ASN ALA VAL PRO GLU LYS THR GLN VAL ASN

- Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M: 7% 92% 7%

MET VAL GLN LEU THR THR ILE PHE CYS K10 D55 I104 E126 S127 E128 A129 K130 E131 T132 E133 A134 S135

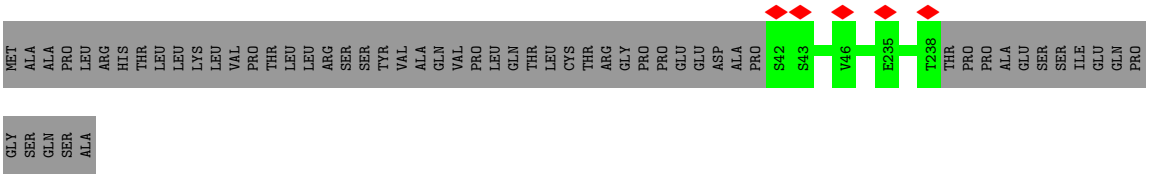
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N: 91% 6%

MET SER I3 V14 R73 V88 E112 P113 R114 E115 GLU LEU LYS VAL SER

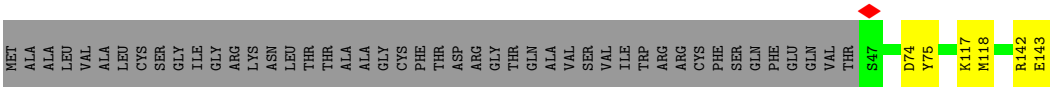
- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O: 78% 22%



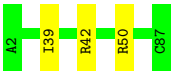
- Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain P: 64% 32%



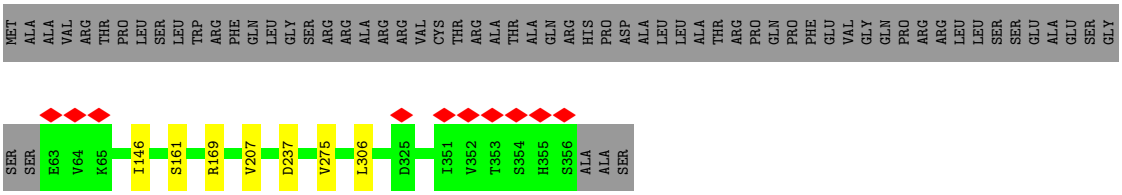
- Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain Q: 97%



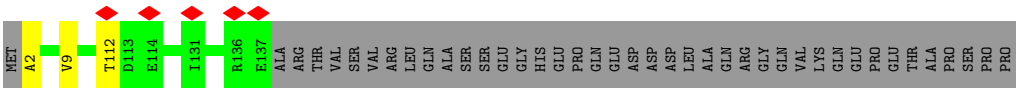
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R: 80% 18%



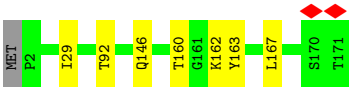
- Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S: 75% 23%



- Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T: 95%



- Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U: 87% 13%

MET LEU ARG ALA LEU ASN ARG LEU ALA ALA ARG PRO GLU THR ARG PRO PRO THR PRO LEU LEU LEU PRO VAL ARG GLY R27 N200

- Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V: 86% 12%

MET ALA ALA PRO MET VAL ARG CYS GLY MET LEU LEU ALA ARG ARG LEU ASP ALA SER ARG LEU CYS LEU ALA GLY LYS ARG CYS L29 V35 V175 P176 S177 L181 Y184 Y187 E195 D272 V279 S292 P293 D294 VAL GLN THR SER GLU ALA GLN PRO GLN

GLU GLY GLU ASP GLY LEU G310 S311 A312 L353 Q397 R398 E399 K400 A401 K402 Q403 E404 Y405 Q406 A407 L408 SER ALA ALA GLU LYS ALA ALA

- Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W: 52% 46%

MET ALA ALA LEU CYS ARG SER HIS ALA GLY THR ALA GLY SER ARG PHE LEU ARG ALA LEU VAL PHE SER LYS PRO LEU ARG ASN ALA SER THR GLU SER GLY SER GLU SER ALA THR HIS ASP SER SER ALA PRO ARG ALA ARG SER GLY GLY PHE ALA SER ALA LEU GLU ARG HIS SER

ASP LEU GLN ARG LYS ALA GLU LEU ARG LEU GLU SER PRO LYS PRO V76 K118 L153 T157 D158 R175 ASP SER LYS SER ARG GLU GLU GLN PRO SER LYS

- Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain X: 87% 5% 9%

MET LEU THR GLY ILE THR ARG LEU PHE SER ARG VAL GLN LYS LEU ASP PRO ARG CYS PHE LEU HIS MET SER VAL GLN ALA THR GLN ASN SER GLN VAL PRO A35 E36 R37 P38 R39 T40 V41 R116 E122 K127 L144 I145 L146 R159 E176 K205 E210

R225 V226 R227 L237 L240 T266 L267 K268 L274 I275 A276 L309 L330 E372 Q383 L391

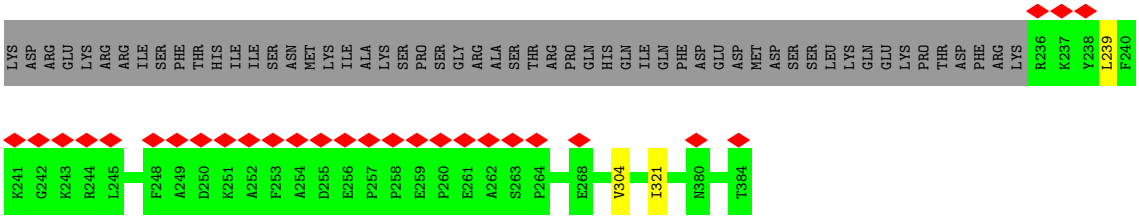
- Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain Y: 7% 38% 61%

MET LEU HIS ARG ILE PRO ALA PHE LEU ARG PRO ARG PRO PHE SER GLY LEU PRO LEU SER CYS GLY ASN ARG ASP VAL SER VAL ALA VAL LEU PRO ALA ALA GLN SER GLY ALA VAL ARG THR GLU ASN ASN ILE GLN ARG HIS PHE CYS THR SER ARG SER ILE CYS SER LYS LYS VAL

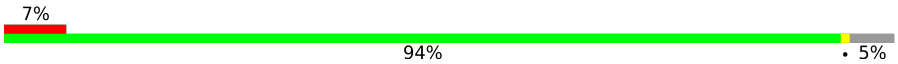
ASP GLN SER VAL PRO ALA ASN GLU ILE SER GLN LYS ALA ALA GLU SER GLN GLY ARG GLY LYS GLU THR LEU LYS LYS ASP LEU LEU ASP ILE ILE LYS ASP MET LYS VAL ASP LEU SER THR ALA ASN ASN VAL LYS THR PRO LYS PRO ARG GLY ARG LYS PRO SER ALA SER LEU GLU ALA

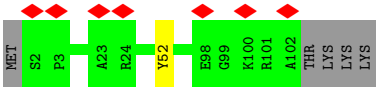
THR VAL ASP ARG LEU GLN LYS ALA PRO GLU ASP PRO PRO LYS LYS ARG ASN GLU PHE LEU SER PRO GLU LEU VAL ALA ALA SER ALA VAL ALA ASP SER LEU PRO PHE ASP LYS GLN THR THR LYS SER GLU LEU LEU ARG GLN LEU GLN GLN HIS GLU GLU GLU LEU ARG ALA GLN



• Molecule 26: 28S ribosomal protein S33, mitochondrial

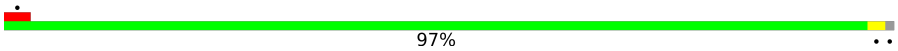
Chain Z:

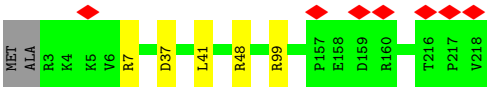




• Molecule 27: 28S ribosomal protein S34, mitochondrial

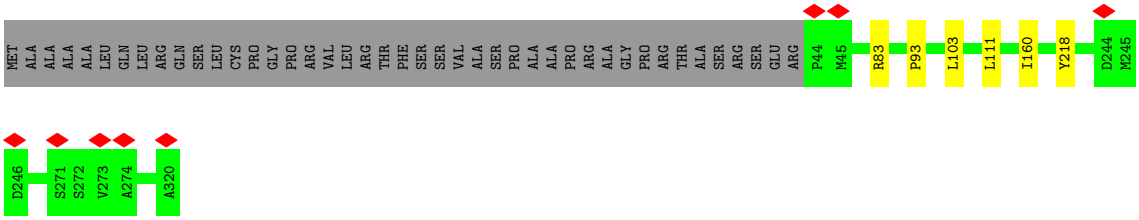
Chain 0:





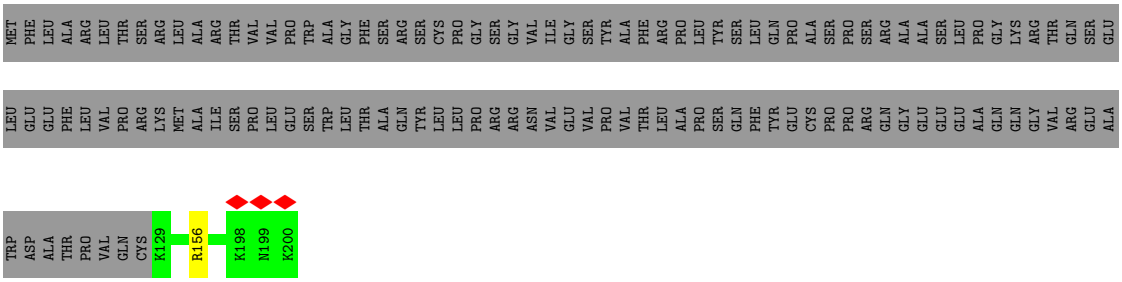
• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:



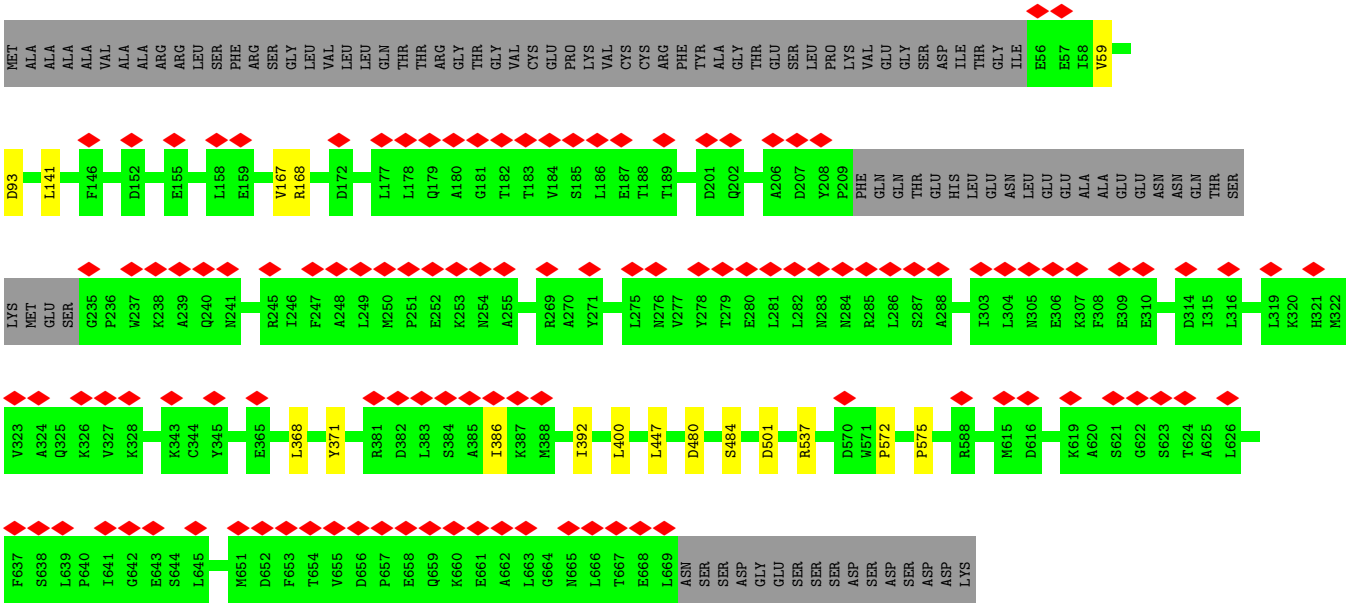
• Molecule 29: Aurora kinase A-interacting protein

Chain 3:



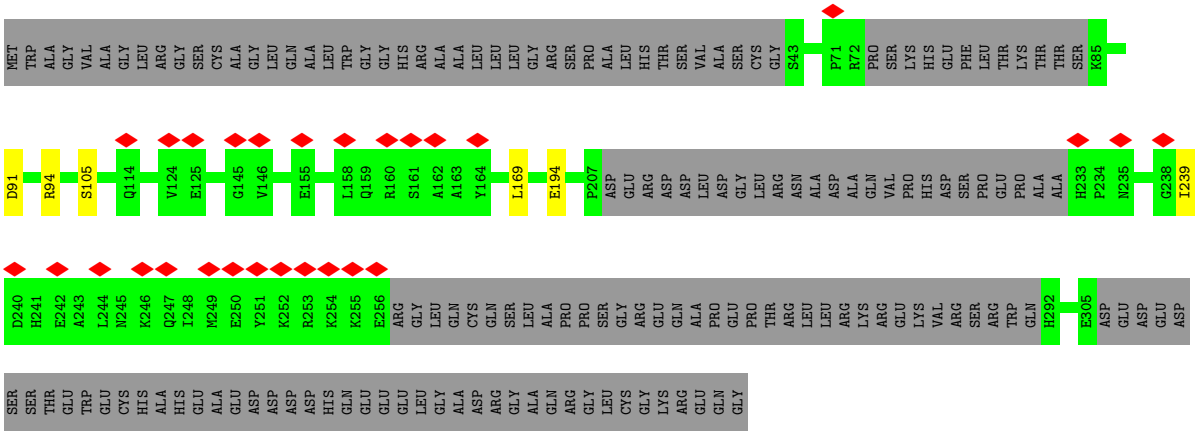
• Molecule 30: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



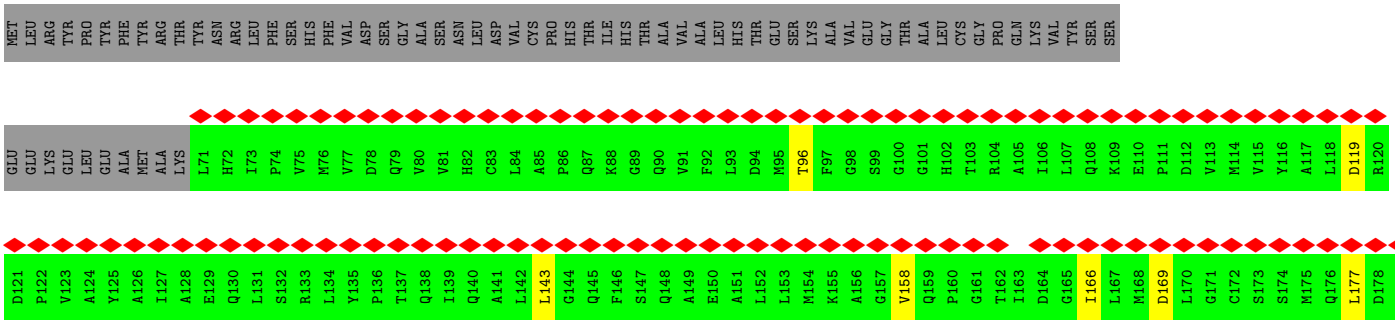
• Molecule 31: Putative ribosome-binding factor A, mitochondrial

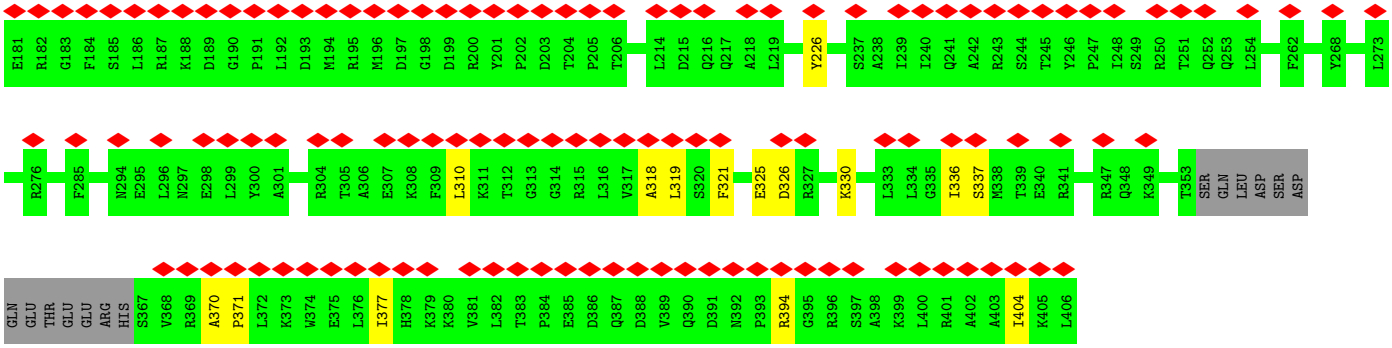
Chain a:



• Molecule 32: 12S rRNA N4-methylcytidine methyltransferase

Chain b:




E181
R182
G183
F184
S185
L186
R187
K188
D189
G190
P191
L192
D193
M194
R195
M196
D197
G198
D199
R200
Y201
P202
D203
T204
P205
T206
L214
D215
Q216
Q217
A218
L219
Y226
S237
A238
I239
I240
Q241
A242
R243
S244
T245
Y246
P247
I248
S249
R250
T251
Q252
Q253
L254
F262
Y268
L273
R276
F285
N294
E295
L296
N297
E298
L299
Y300
A301
R304
T305
A306
E307
K308
F309
L310
K311
T312
G313
G314
R315
L316
V317
A318
L319
S320
F321
E325
D326
R327
K330
L333
L334
G335
I336
S337
M338
T339
E340
R341
R347
Q348
K349
T353
SER
GLN
LEU
ASP
SER
ASP
GLN
GLU
THR
GLU
GLU
ARG
HIS
S367
V368
R369
A370
P371
L372
K373
W374
E375
L376
I377
H378
K379
K380
V381
L382
T383
P384
E385
D386
Q387
D388
V389
Q390
D391
N392
P393
R394
G395
R396
S397
A398
K399
L400
R401
A402
A403
I404
K405
L406

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59111	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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.795	Depositor
Minimum map value	-0.950	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.40192, 398.40192, 398.40192	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.69167, 0.69167, 0.69167	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5F0, AYA, MA6, ZN, SAH, 5MC, FES, ATP, MG, B8T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.11	0/22518	0.21	0/35045
2	B	0.13	0/1832	0.30	0/2479
3	C	0.13	0/1100	0.30	0/1485
4	D	0.13	0/2789	0.29	0/3739
5	E	0.12	0/966	0.30	0/1308
6	F	0.12	0/1763	0.29	0/2368
7	G	0.11	0/2734	0.31	0/3669
8	H	0.13	0/1179	0.28	0/1597
9	I	0.13	0/1018	0.31	0/1374
10	J	0.14	0/862	0.32	0/1155
11	K	0.15	0/871	0.34	0/1167
12	L	0.11	0/1485	0.26	0/1980
13	M	0.15	0/1017	0.32	0/1366
14	N	0.13	0/907	0.32	0/1228
15	O	0.11	0/1653	0.28	0/2254
16	P	0.12	0/809	0.30	0/1085
17	Q	0.13	0/735	0.31	0/980
18	R	0.11	0/2449	0.27	0/3311
19	S	0.12	0/1148	0.28	0/1541
20	T	0.11	0/1420	0.28	0/1903
21	U	0.12	0/1470	0.29	0/1976
22	V	0.09	0/3059	0.24	0/4135
23	W	0.12	0/805	0.30	0/1084
24	X	0.10	0/2952	0.26	0/3995
25	Y	0.10	0/1283	0.24	0/1730
26	Z	0.13	0/851	0.28	0/1133
27	0	0.13	0/1856	0.33	0/2511
28	1	0.11	0/2260	0.26	0/3063
29	3	0.13	0/654	0.32	0/860
30	4	0.09	0/4868	0.25	0/6597
31	a	0.10	0/1573	0.27	0/2115
32	b	0.10	0/2561	0.28	0/3457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.11	0/73447	0.26	0/103690

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	181	5F0	Mainchain

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	A	20207	10223	10209	43	0
2	B	1791	1799	1797	8	0
3	C	1072	1091	1087	7	0
4	D	2733	2794	2790	13	0
5	E	948	968	968	5	0
6	F	1722	1750	1748	8	0
7	G	2674	2630	2626	11	0
8	H	1153	1193	1190	10	0
9	I	1009	1038	1029	3	0
10	J	846	903	901	2	0
11	K	855	888	887	8	0
12	L	1465	1576	1574	3	0
13	M	995	1009	1006	2	0
14	N	888	951	947	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1598	1548	1547	0	0
16	P	792	818	817	5	0
17	Q	732	750	750	4	0
18	R	2400	2416	2415	6	0
19	S	1124	1133	1132	3	0
20	T	1388	1413	1413	5	0
21	U	1449	1459	1456	0	0
22	V	2998	2972	2967	8	0
23	W	793	813	811	3	0
24	X	2881	2881	2879	12	0
25	Y	1246	1193	1191	3	0
26	Z	834	848	847	1	0
27	0	1811	1838	1834	3	0
28	1	2212	2228	2226	5	0
29	3	643	728	726	1	0
30	4	4758	4800	4793	11	0
31	a	1546	1583	1579	4	0
32	b	2519	2595	2593	13	0
33	3	1	0	0	0	0
33	A	46	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	A	13	0	0	0	0
35	O	1	0	0	0	0
36	P	4	0	0	0	0
36	T	4	0	0	0	0
37	X	31	12	12	0	0
38	b	26	20	19	0	0
39	0	7	0	0	0	0
39	1	5	0	0	0	0
39	3	7	0	0	0	0
39	A	549	0	0	8	0
39	B	23	0	0	0	0
39	C	19	0	0	1	0
39	D	34	0	0	1	0
39	E	2	0	0	0	0
39	F	7	0	0	0	0
39	G	10	0	0	0	0
39	H	19	0	0	0	0
39	I	5	0	0	0	0
39	J	14	0	0	0	0
39	K	25	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	L	6	0	0	0	0
39	M	16	0	0	0	0
39	N	8	0	0	0	0
39	O	25	0	0	0	0
39	P	3	0	0	0	0
39	Q	8	0	0	0	0
39	R	13	0	0	0	0
39	S	4	0	0	0	0
39	T	19	0	0	0	0
39	U	3	0	0	0	0
39	W	2	0	0	0	0
39	X	5	0	0	0	0
39	Y	7	0	0	0	0
39	Z	18	0	0	0	0
39	a	5	0	0	0	0
All	All	71078	60861	60766	174	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 1.

The worst 5 of 174 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)
1:A:465:A:OP1	2:B:97:ARG:NH1	2.23	0.72
1:A:705:G:N7	39:A:1112:HOH:O	2.27	0.67
4:D:196:SER:O	39:D:501:HOH:O	2.13	0.65
1:A:942:G:O6	39:A:1102:HOH:O	2.12	0.64
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.31	0.64

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	
2	B	221/291 (76%)	217 (98%)	4 (2%)	0	100	100
3	C	130/167 (78%)	124 (95%)	6 (5%)	0	100	100
4	D	341/432 (79%)	336 (98%)	5 (2%)	0	100	100
5	E	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
6	F	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
7	G	321/390 (82%)	317 (99%)	4 (1%)	0	100	100
8	H	138/160 (86%)	135 (98%)	2 (1%)	1 (1%)	18	45
9	I	134/191 (70%)	129 (96%)	5 (4%)	0	100	100
10	J	106/139 (76%)	105 (99%)	1 (1%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	174/258 (67%)	173 (99%)	1 (1%)	0	100	100
13	M	124/135 (92%)	124 (100%)	0	0	100	100
14	N	111/120 (92%)	108 (97%)	3 (3%)	0	100	100
15	O	195/254 (77%)	193 (99%)	2 (1%)	0	100	100
16	P	95/143 (66%)	95 (100%)	0	0	100	100
17	Q	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
18	R	292/359 (81%)	283 (97%)	9 (3%)	0	100	100
19	S	134/177 (76%)	132 (98%)	2 (2%)	0	100	100
20	T	168/171 (98%)	167 (99%)	1 (1%)	0	100	100
21	U	172/200 (86%)	171 (99%)	1 (1%)	0	100	100
22	V	361/415 (87%)	356 (99%)	5 (1%)	0	100	100
23	W	98/186 (53%)	95 (97%)	3 (3%)	0	100	100
24	X	355/391 (91%)	349 (98%)	6 (2%)	0	100	100
25	Y	147/384 (38%)	145 (99%)	2 (1%)	0	100	100
26	Z	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
27	0	214/218 (98%)	209 (98%)	5 (2%)	0	100	100
28	1	275/320 (86%)	273 (99%)	2 (1%)	0	100	100
29	3	70/200 (35%)	70 (100%)	0	0	100	100
30	4	585/685 (85%)	580 (99%)	5 (1%)	0	100	100
31	a	183/350 (52%)	180 (98%)	3 (2%)	0	100	100
32	b	319/406 (79%)	310 (97%)	9 (3%)	0	100	100
All	All	6068/7829 (78%)	5973 (98%)	94 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	85	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	195/247 (79%)	195 (100%)	0	100	100
3	C	113/139 (81%)	113 (100%)	0	100	100
4	D	282/354 (80%)	282 (100%)	0	100	100
5	E	104/110 (94%)	104 (100%)	0	100	100
6	F	180/204 (88%)	180 (100%)	0	100	100
7	G	282/335 (84%)	282 (100%)	0	100	100
8	H	130/150 (87%)	130 (100%)	0	100	100
9	I	102/143 (71%)	102 (100%)	0	100	100
10	J	93/117 (80%)	93 (100%)	0	100	100
11	K	90/110 (82%)	90 (100%)	0	100	100
12	L	161/224 (72%)	161 (100%)	0	100	100
13	M	103/112 (92%)	103 (100%)	0	100	100
14	N	97/104 (93%)	97 (100%)	0	100	100
15	O	176/225 (78%)	176 (100%)	0	100	100
16	P	89/125 (71%)	89 (100%)	0	100	100
17	Q	77/77 (100%)	77 (100%)	0	100	100
18	R	261/313 (83%)	261 (100%)	0	100	100
19	S	117/152 (77%)	117 (100%)	0	100	100
20	T	153/154 (99%)	153 (100%)	0	100	100
21	U	149/171 (87%)	149 (100%)	0	100	100
22	V	326/362 (90%)	326 (100%)	0	100	100
23	W	87/156 (56%)	87 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X	314/346 (91%)	314 (100%)	0	100	100
25	Y	133/341 (39%)	133 (100%)	0	100	100
26	Z	88/93 (95%)	88 (100%)	0	100	100
27	0	190/191 (100%)	189 (100%)	1 (0%)	81	82
28	1	247/279 (88%)	247 (100%)	0	100	100
29	3	68/176 (39%)	68 (100%)	0	100	100
30	4	519/599 (87%)	519 (100%)	0	100	100
31	a	174/299 (58%)	174 (100%)	0	100	100
32	b	270/343 (79%)	270 (100%)	0	100	100
All	All	5370/6751 (80%)	5369 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	0	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	39	GLN
25	Y	379	ASN
22	V	145	ASN
24	X	228	ASN
27	0	45	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	949/956 (99%)	124 (13%)	0

5 of 124 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	7	U
1	A	32	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	A
1	A	41	U

There are no RNA pucker outliers to report.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	842	1	18,22,23	0.32	0	26,32,35	0.40	0
9	5F0	I	181	9	8,8,9	0.55	0	7,9,11	1.05	1 (14%)
1	MA6	A	937	1	23,26,27	0.30	0	34,38,41	0.58	1 (2%)
17	AYA	Q	2	17	6,7,8	0.77	0	5,8,10	0.57	0
1	MA6	A	938	1	23,26,27	0.30	0	34,38,41	0.57	1 (2%)
1	B8T	A	840	1	19,22,23	0.30	0	26,31,34	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	842	1	-	2/7/25/26	0/2/2/2
9	5F0	I	181	9	-	0/9/9/10	-
1	MA6	A	937	1	-	0/11/29/30	0/3/3/3
17	AYA	Q	2	17	-	0/4/6/8	-
1	MA6	A	938	1	-	1/11/29/30	0/3/3/3
1	B8T	A	840	1	-	0/7/27/28	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	181	5F0	O-C-CB	-2.44	118.31	125.43
1	A	937	MA6	C2-N1-C6	2.37	117.34	111.75
1	A	938	MA6	C2-N1-C6	2.36	117.34	111.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	938	MA6	C4'-C5'-O5'-P
1	A	842	5MC	O4'-C4'-C5'-O5'
1	A	842	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	937	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 63 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	FES	P	201	16,5	0,4,4	-	-	-		
38	SAH	b	501	-	27,28,28	0.40	0	38,40,40	0.44	0
37	ATP	X	401	33	29,33,33	0.49	0	44,52,52	0.51	0
36	FES	T	201	13,20	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	FES	P	201	16,5	-	-	0/1/1/1
38	SAH	b	501	-	-	3/15/31/31	0/3/3/3
37	ATP	X	401	33	-	0/22/38/38	0/3/3/3
36	FES	T	201	13,20	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

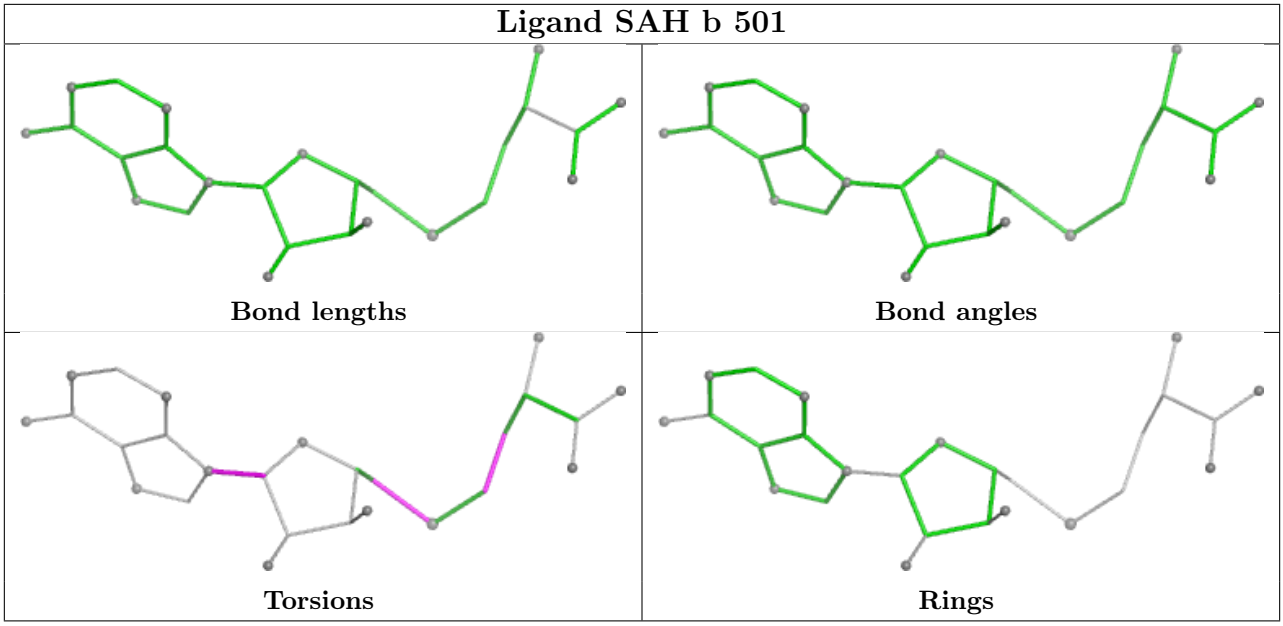
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	b	501	SAH	C4'-C5'-SD-CG
38	b	501	SAH	C2'-C1'-N9-C8
38	b	501	SAH	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

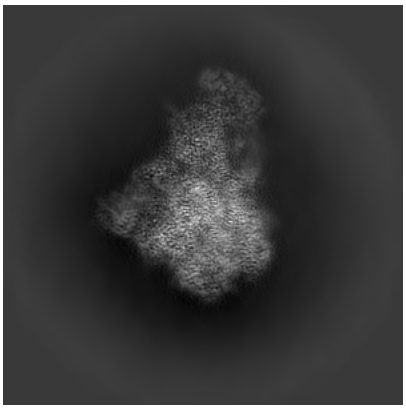
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13553. These allow visual inspection of the internal detail of the map and identification of artifacts.

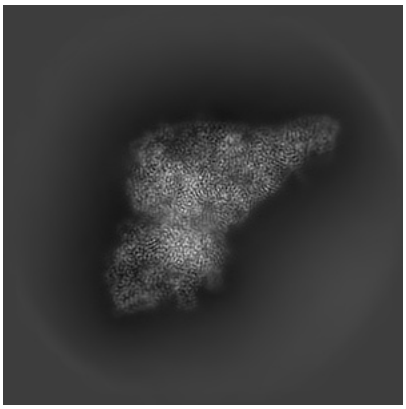
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

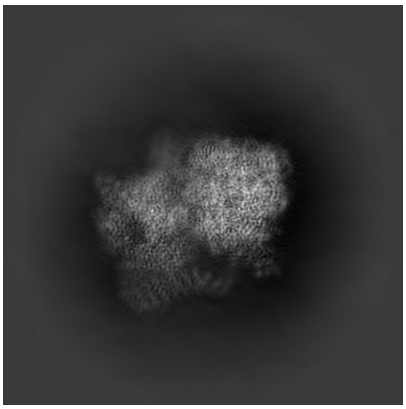
6.1.1 Primary map



X

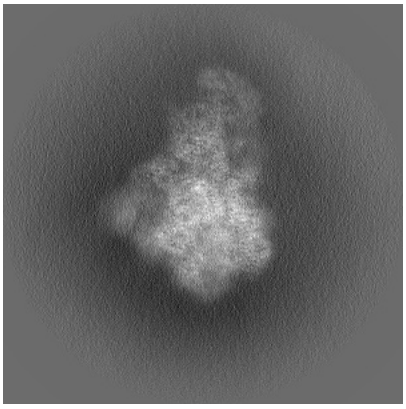


Y

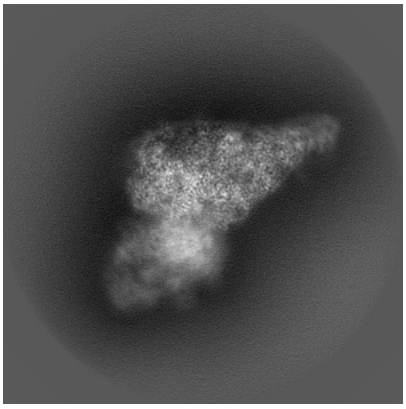


Z

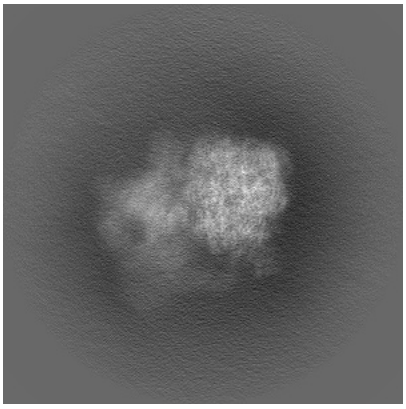
6.1.2 Raw map



X



Y



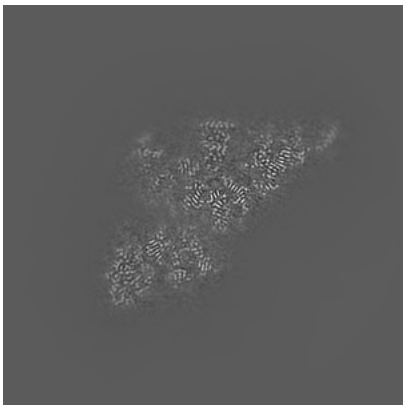
Z

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

6.2 Central slices (i)

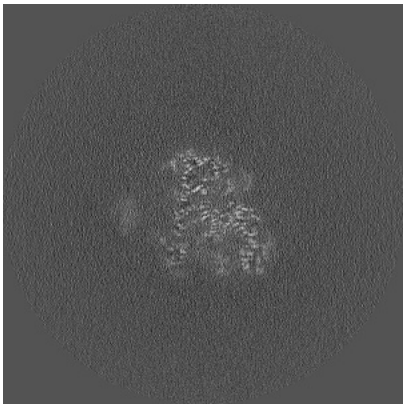
6.2.1 Primary map

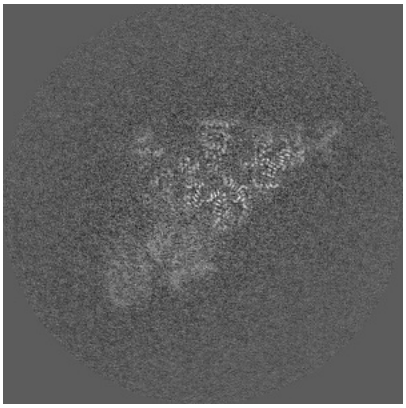
X Index: 288

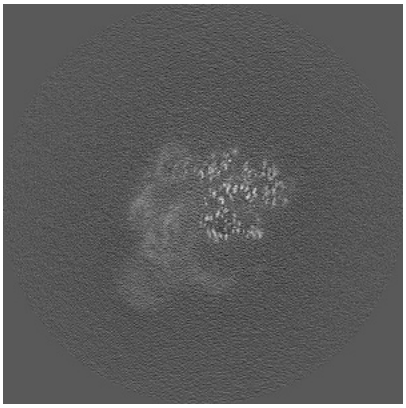

Y Index: 288

Z Index: 288

6.2.2 Raw map


X Index: 240

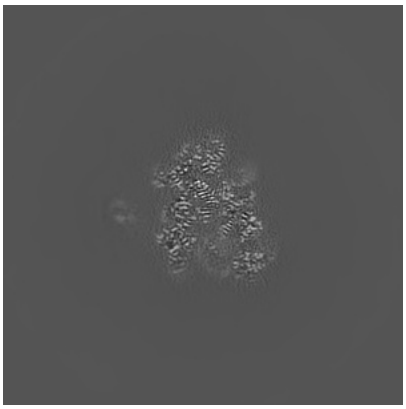

Y Index: 240


Z Index: 240

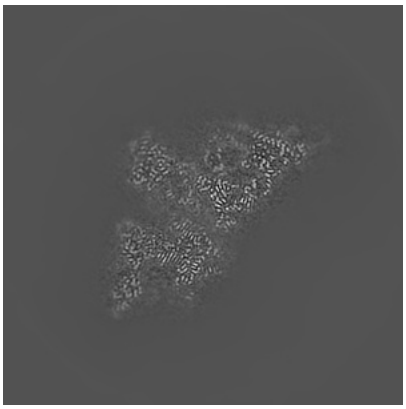
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

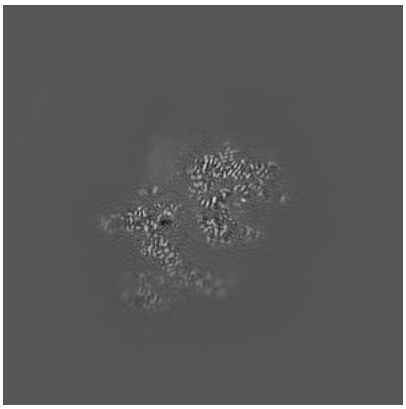
6.3.1 Primary map



X Index: 301

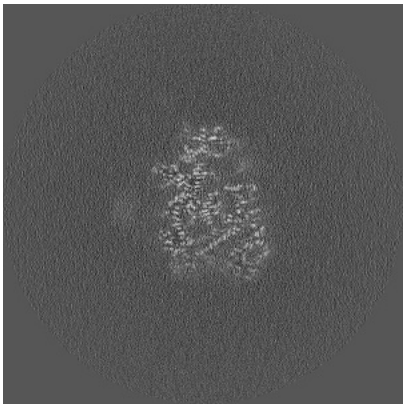


Y Index: 277

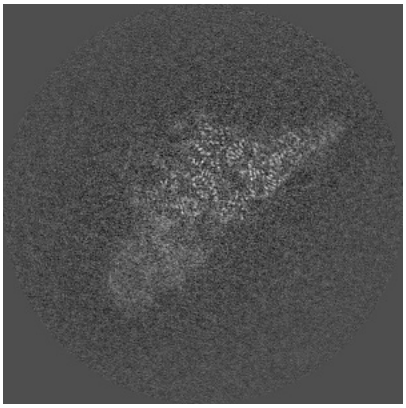


Z Index: 276

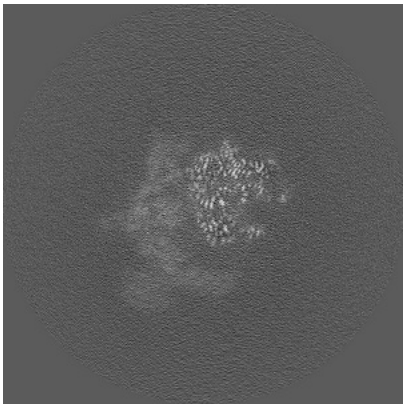
6.3.2 Raw map



X Index: 262



Y Index: 256

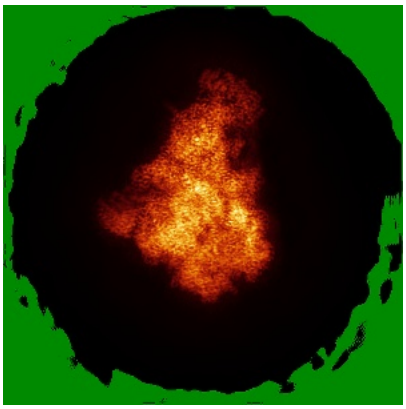


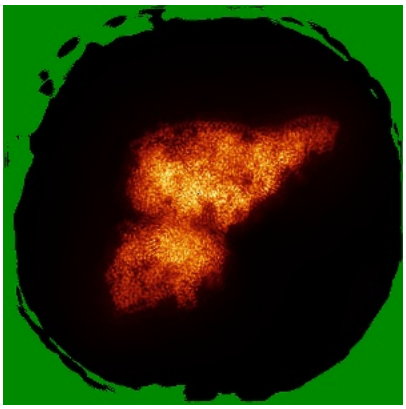
Z Index: 231

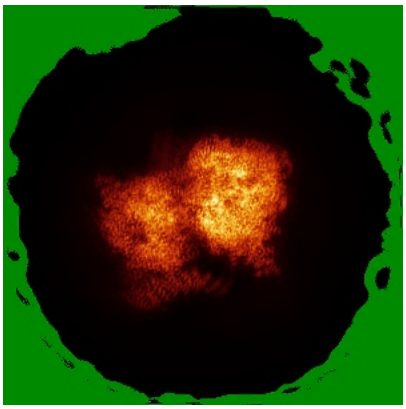
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

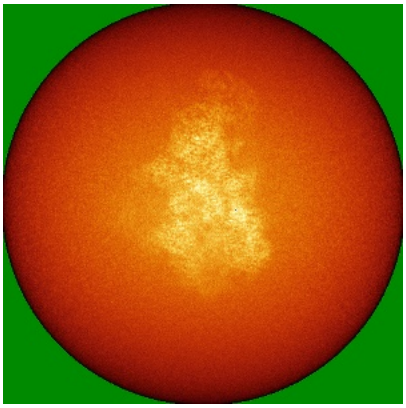
6.4.1 Primary map

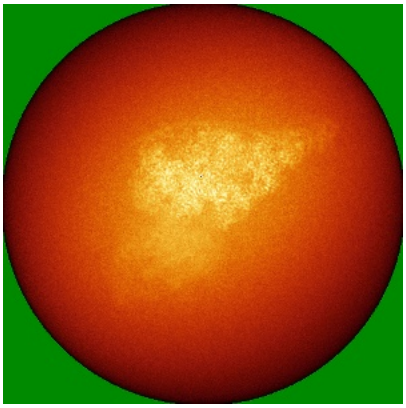

X

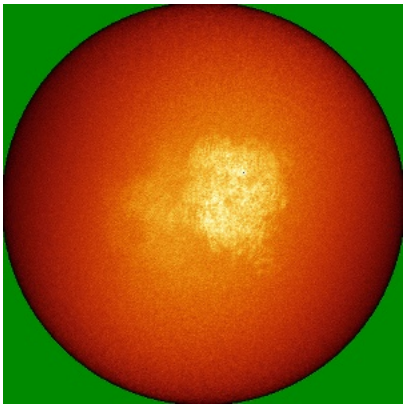

Y


Z

6.4.2 Raw map


X


Y


Z

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

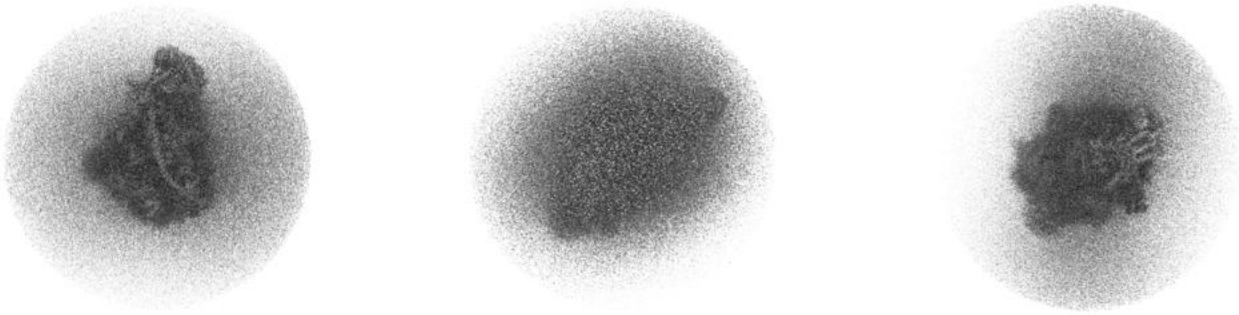
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

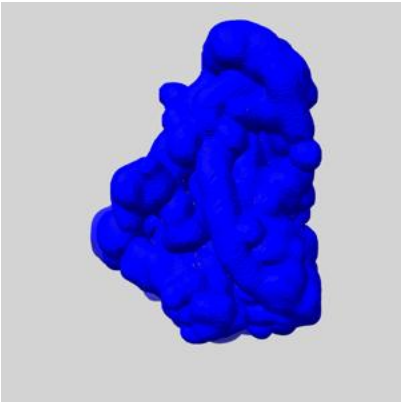
6.6 Mask visualisation (i)

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

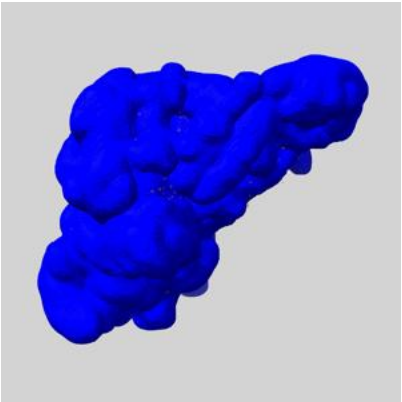
A mask typically either:

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

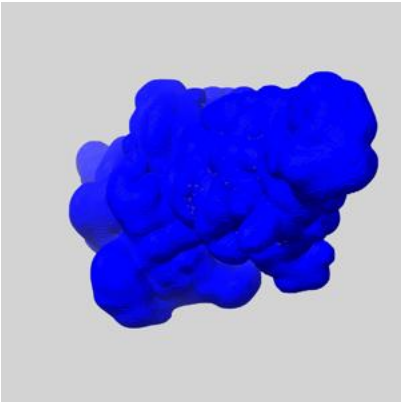
6.6.1 emd_13553_msk_1.map (i)



X



Y

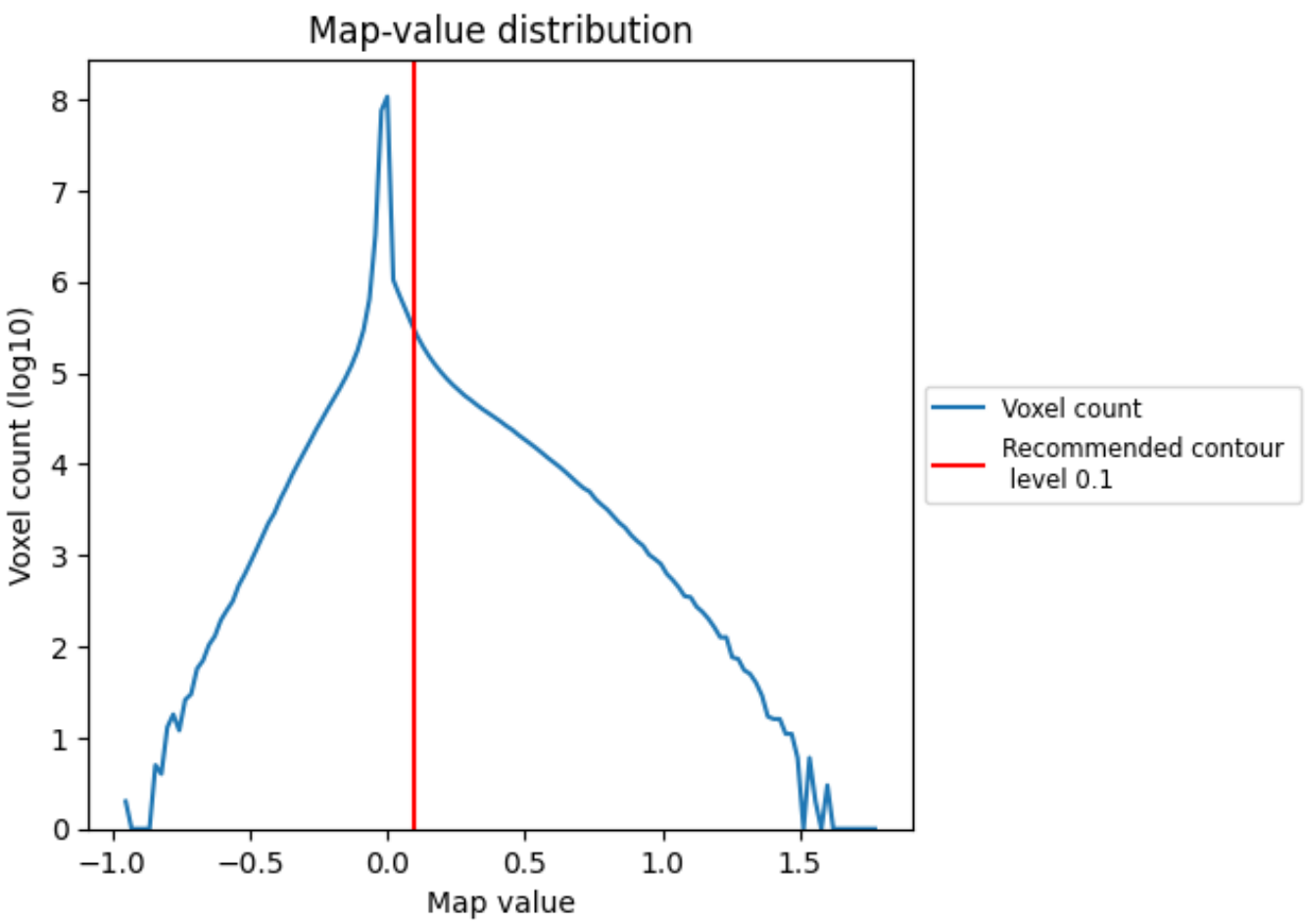


Z

7 Map analysis (i)

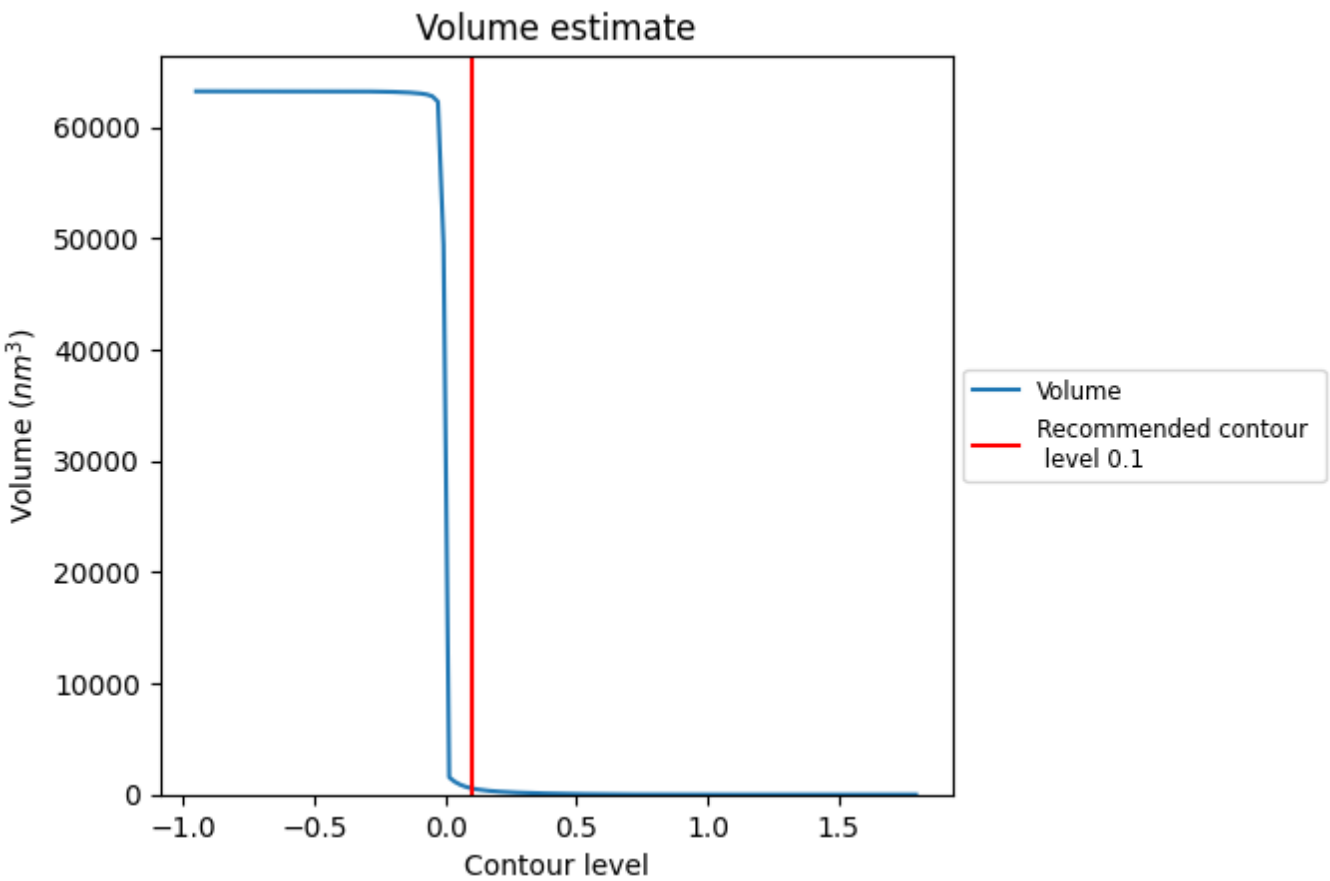
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

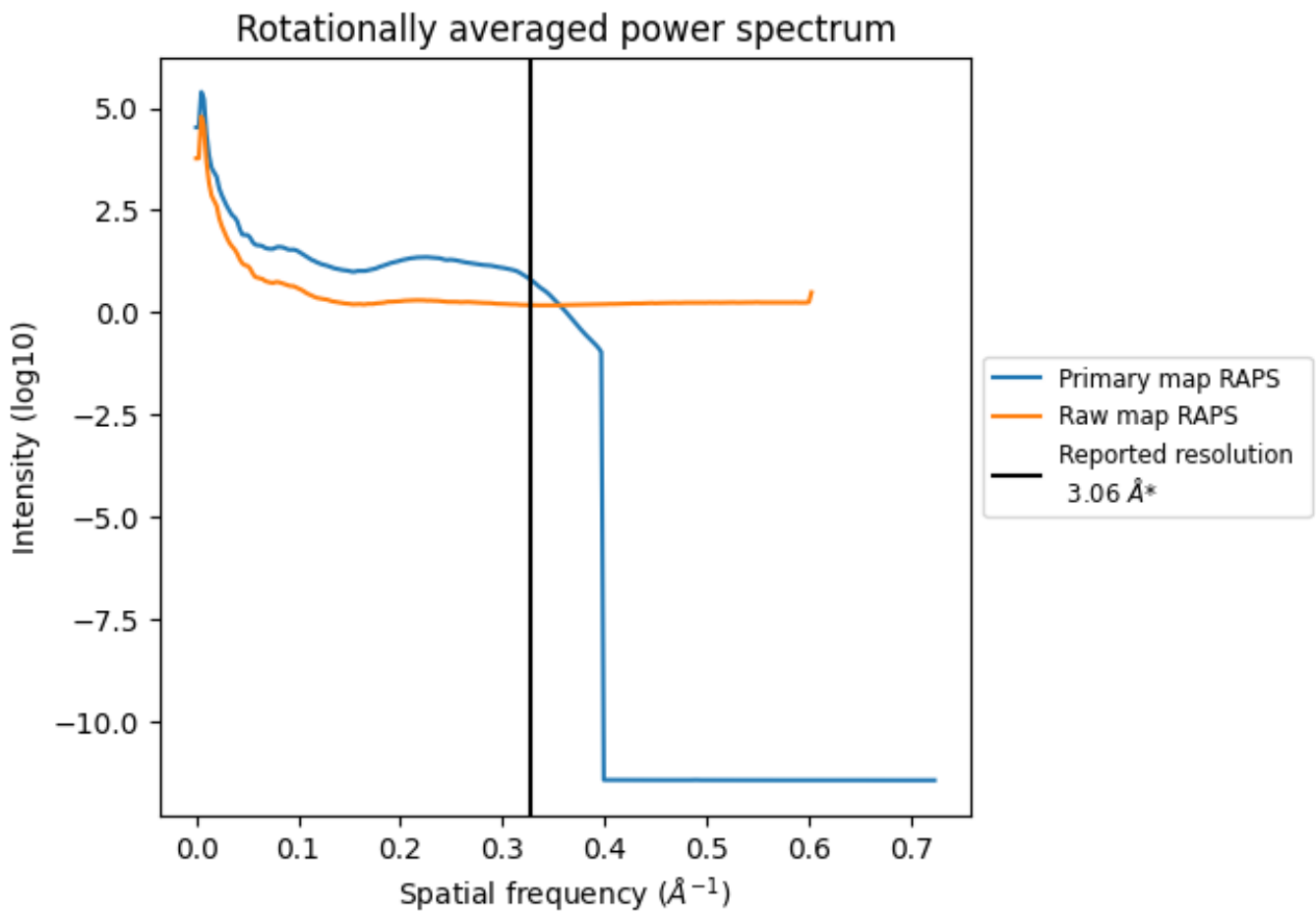
7.2 Volume estimate (i)



The volume at the recommended contour level is 564 nm^3; this corresponds to an approximate mass of 509 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)

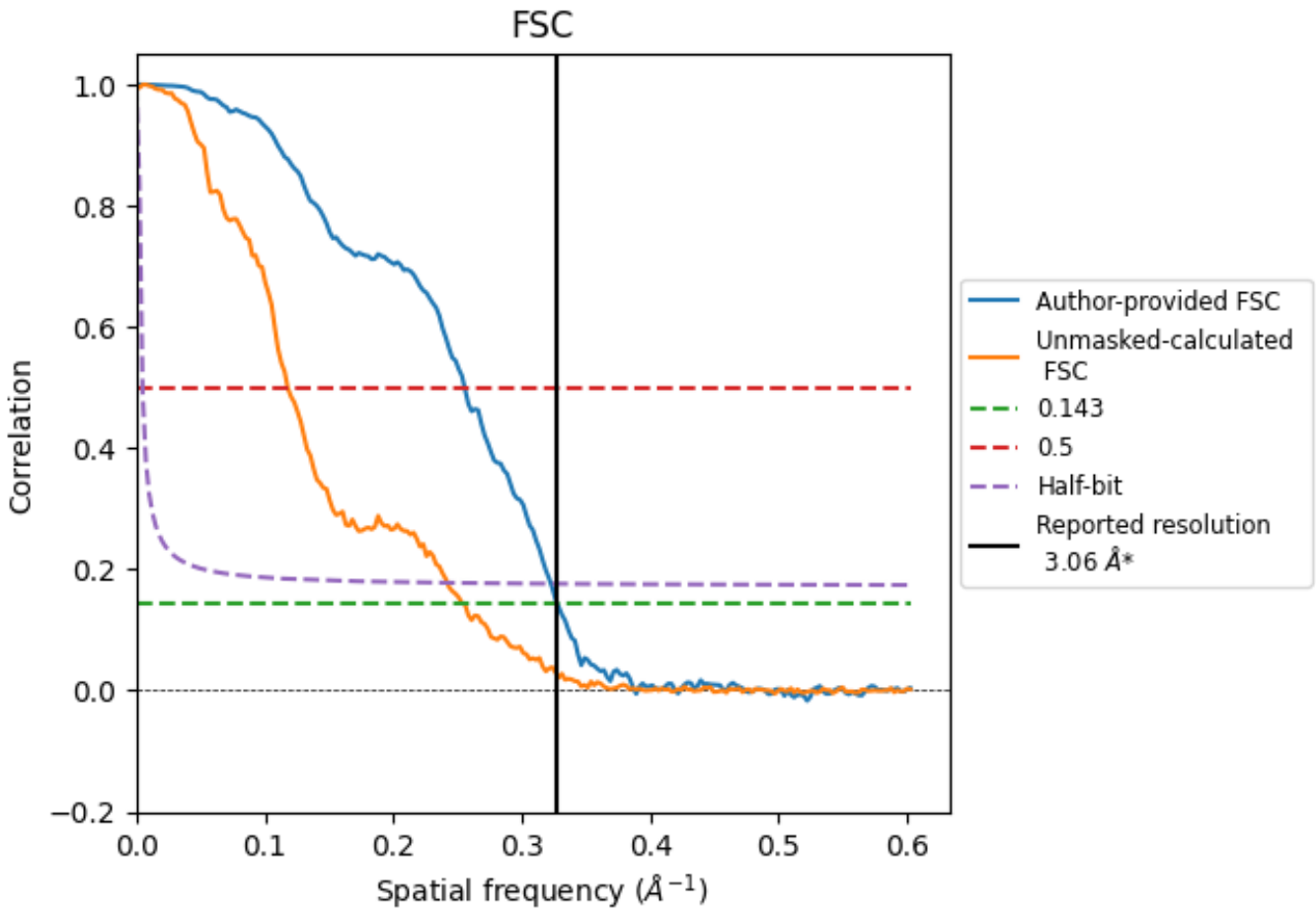


*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

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 0.327 Å^{-1}

8.2 Resolution estimates (i)

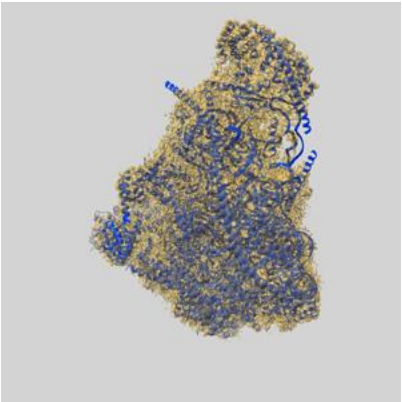
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.05	3.91	3.10
Unmasked-calculated*	3.93	8.48	4.13

*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 3.93 differs from the reported value 3.06 by more than 10 %

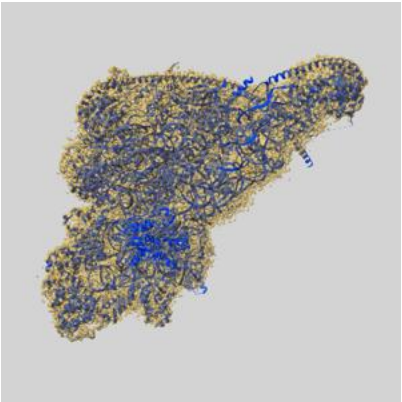
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13553 and PDB model 7PNV. Per-residue inclusion information can be found in section 3 on page 14.

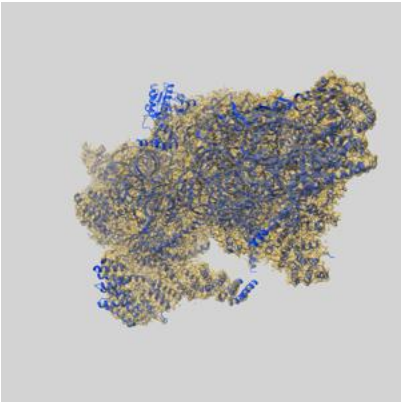
9.1 Map-model overlay (i)



X



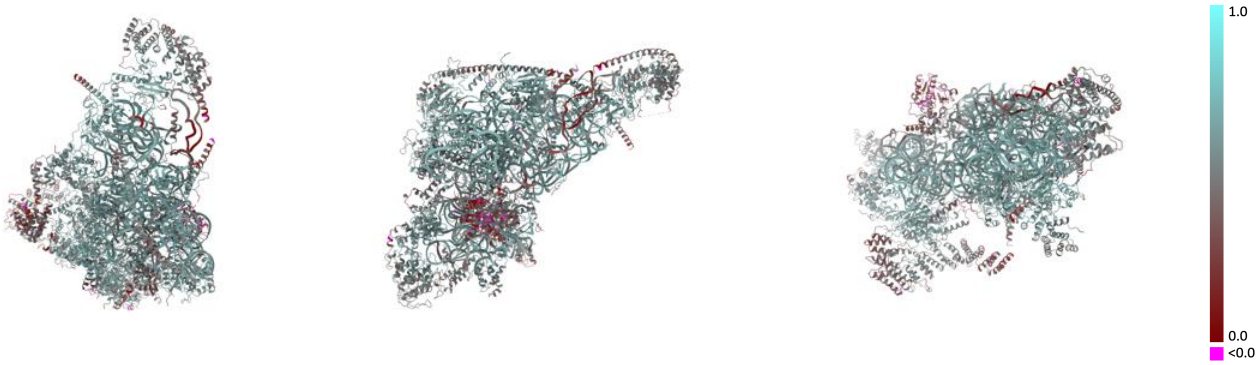
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

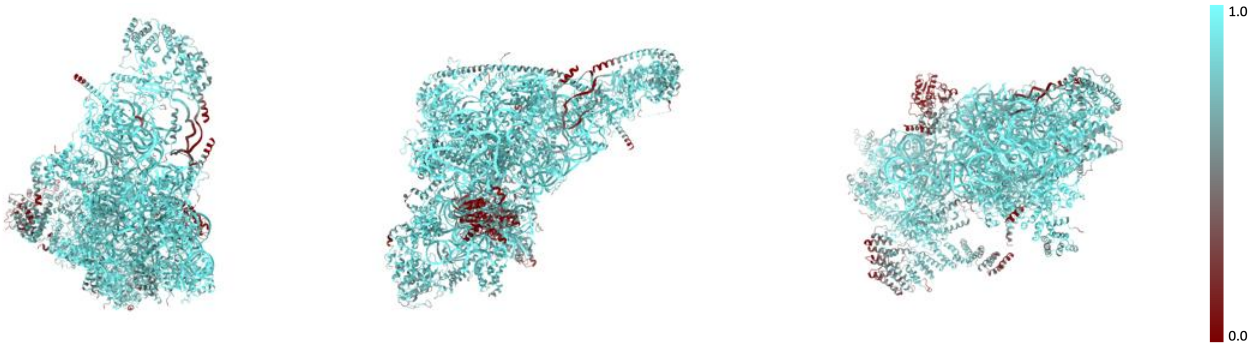
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

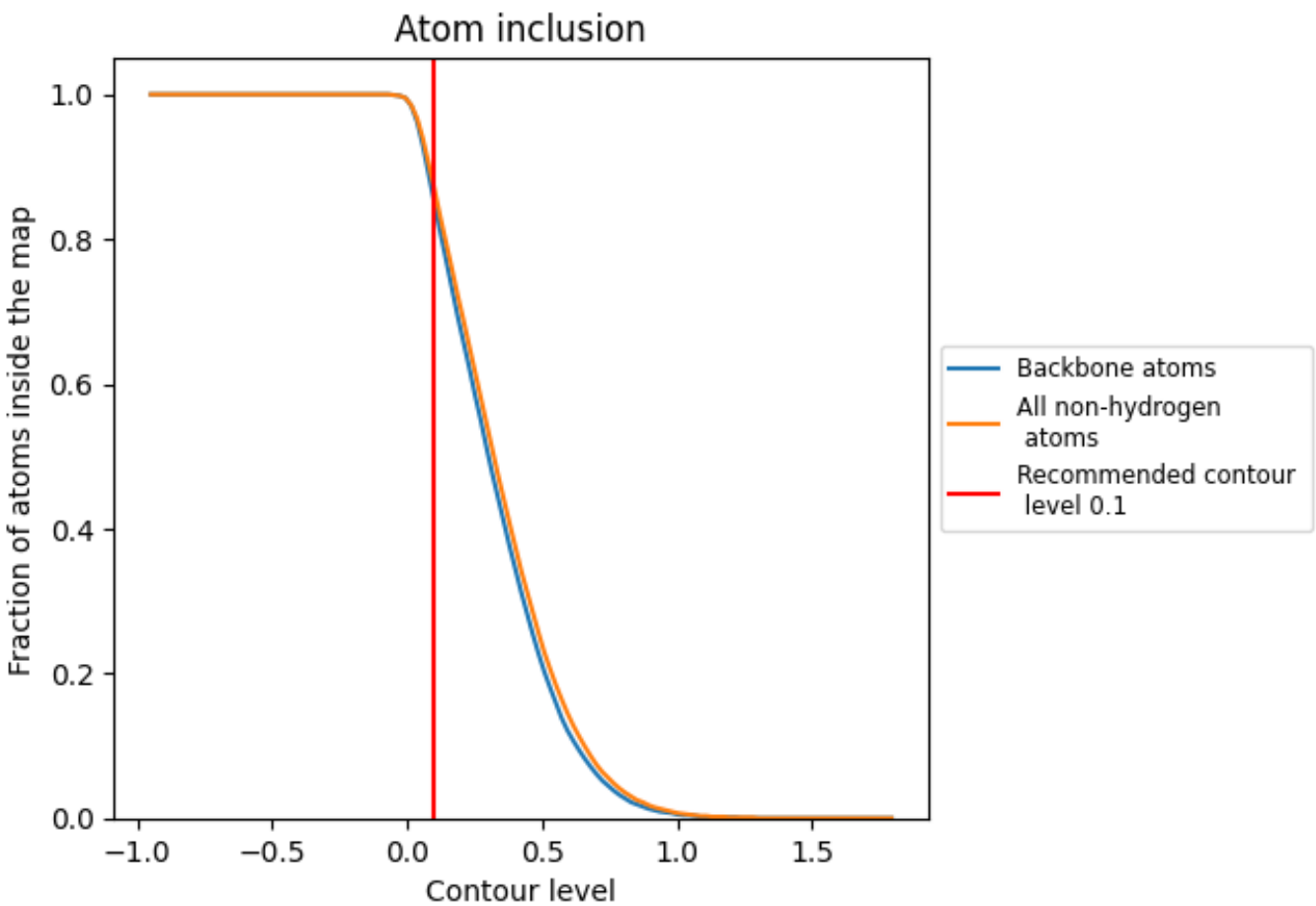
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.5440
0	0.8980	0.5550
1	0.8530	0.5440
3	0.8640	0.5440
4	0.6620	0.4290
A	0.9580	0.5940
B	0.9470	0.6110
C	0.9740	0.6360
D	0.9070	0.5720
E	0.9240	0.5700
F	0.9000	0.5420
G	0.8570	0.5340
H	0.9090	0.5860
I	0.9480	0.5800
J	0.9500	0.5900
K	0.9590	0.6300
L	0.8420	0.5400
M	0.9000	0.6030
N	0.9200	0.5940
O	0.9360	0.5950
P	0.9360	0.5840
Q	0.9700	0.6090
R	0.8850	0.5620
S	0.8390	0.5160
T	0.9200	0.5780
U	0.8310	0.5230
V	0.7750	0.4790
W	0.9260	0.5870
X	0.8480	0.5230
Y	0.7040	0.4890
Z	0.8660	0.5490
a	0.6750	0.4090
b	0.2530	0.2420