wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 04:25 pm BST

PDB ID	:	9RPF / pdb_00009rpf
EMDB ID	:	EMD-54163
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and mS37 (State M4)
Authors	:	Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.
Deposited on	:	2025-06-24
Resolution	:	4.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

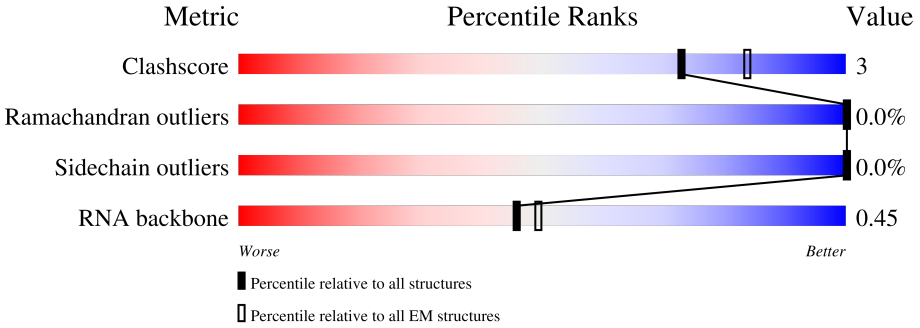
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

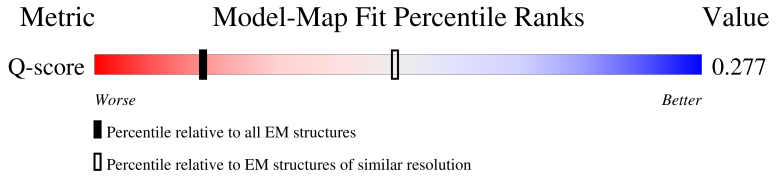
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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)	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	2407 (4.10 - 5.10)

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	0	218	6% 92% 7% •
2	1	323	6% 79% 7% 15%
3	2	118	35% 91% 9%

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Mol	Chain	Length	Quality of chain
4	3	199	31% 65%
5	B	296	74% 24%
6	C	167	77% 21%
7	D	430	5% 74% 5% 20%
8	E	125	9% 90% 8%
9	F	242	78% 8% 14%
10	H	201	66% 30%
11	I	194	64% 6% 29%
12	J	138	56% 20% 22%
13	K	128	71% 8% 21%
14	L	257	5% 63% 5% 32%
15	M	137	5% 81% 6% 13%
16	N	130	82% 15%
17	O	258	72% 25%
18	P	142	59% 9% 32%
19	Q	87	93% 7%
20	R	360	75% 7% 18%
21	S	190	67% 29%
22	T	173	92% 5%
23	U	205	80% 6% 14%
24	W	187	50% 47%
25	X	398	81% 8% 12%
26	Y	395	28% 69%
27	Z	106	81% 19%
28	A	955	72% 23%

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Mol	Chain	Length	Quality of chain
29	G	396	73% 9% 18%
30	V	414	81% 6% 13%
31	4	689	18% 78% 8% 15%
32	b	407	37% 54% 18% 29%

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 128691 atoms, of which 59624 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 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	215	3583	1130	1796	339	313	5	0	0

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	276	4507	1419	2269	381	427	11	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	118	1903	579	968	182	166	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 4 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	3	70	1324	401	699	134	89	1	0	0

- Molecule 5 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	B	225	3643	1164	1815	331	323	10	0	0

- Molecule 6 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	C	132	2171	699	1088	195	185	4	0	0

- Molecule 7 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	D	343	5533	1713	2802	518	487	13	0	0

- Molecule 8 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	E	122	1973	614	1001	177	177	4	0	0

- Molecule 9 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	F	208	3494	1104	1769	312	298	11	0	0

- Molecule 10 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	H	140	2335	745	1183	194	210	3	0	0

- Molecule 11 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	I	137	2080	642	1060	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 12 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	J	108	1723	521	884	169	143	6	0	0

- Molecule 13 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	K	101	1747	537	885	179	141	5	0	0

- Molecule 14 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	L	174	2993	925	1540	270	251	7	0	0

- Molecule 15 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	M	119	1907	594	965	185	157	6	0	0

- Molecule 16 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	N	110	1796	562	928	156	147	3	0	0

- Molecule 17 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	O	194	3164	1019	1565	295	278	7	0	0

- Molecule 18 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	P	97	1588	501	807	134	138	8	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	Q	87	1501	460	757	150	126	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 20 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	R	295	4837	1533	2428	413	455	8	0	0

- Molecule 21 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	S	135	2226	716	1115	198	196	1	0	0

- Molecule 22 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	T	168	2764	877	1393	239	244	11	0	0

- Molecule 23 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	U	176	2987	916	1499	301	267	4	0	0

- Molecule 24 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	W	100	1589	498	800	141	146	4	0	0

- Molecule 25 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	X	352	5693	1822	2844	499	517	11	0	0

- Molecule 26 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Y	122	2004	665	975	169	193	2	0	0

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	Z	86	1464	468	734	128	130	4	0	0

- Molecule 28 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
28	A	955	30584	9098	10302	3652	6577	955	0	0

- Molecule 29 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	G	324	5304	1684	2650	473	483	14	0	0

- Molecule 30 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	V	362	5931	1904	2962	495	558	12	0	0

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	4	588	9534	3053	4766	808	879	28	0	0

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	b	290	4599	1440	2327	406	415	11	0	0

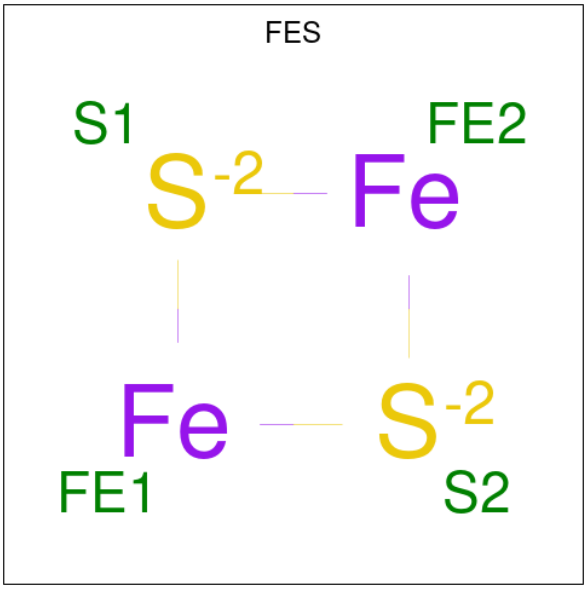
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	3	1	1	1	0
33	B	1	1	1	0
33	A	44	44	44	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

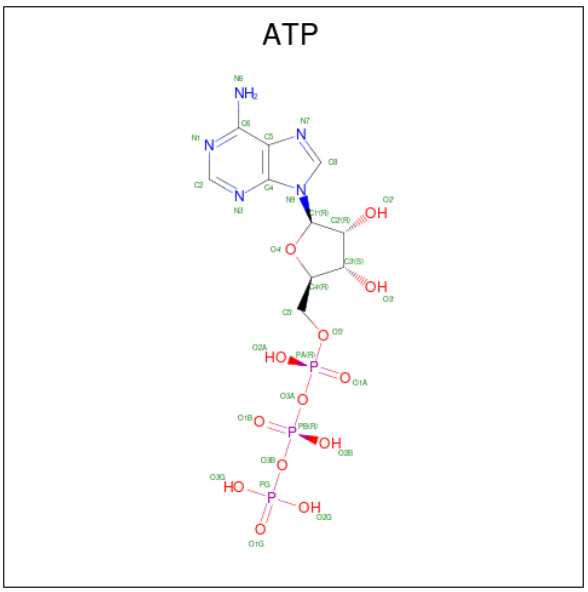
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	O	1	1	1	0

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



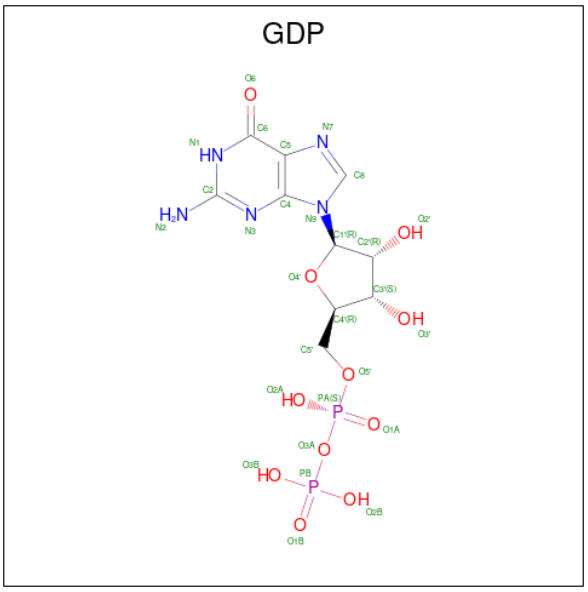
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
35	P	1	4	2	2	0
35	T	1	4	2	2	0

- Molecule 36 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	
36	X	1	43	10	12	5	13	3	0

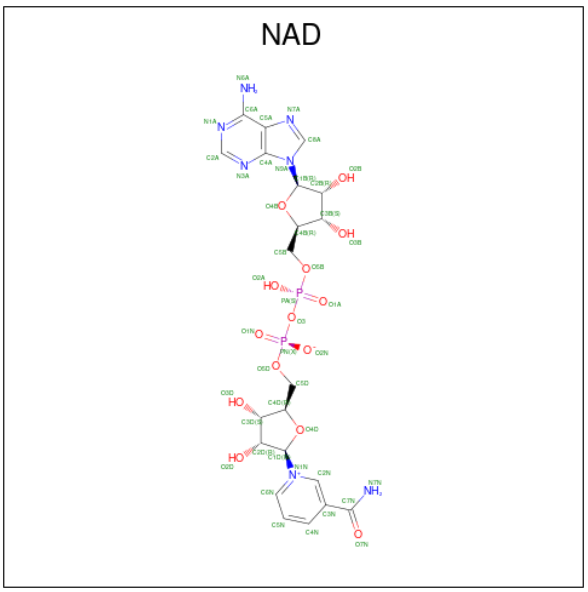
- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
37	X	1	38	10	10	5	11	2	0

- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

$C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
38	A	1	70	21	26	7	14	2	0

- Molecule 39 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
39	A	3	3	3	0

- Molecule 40 is water.

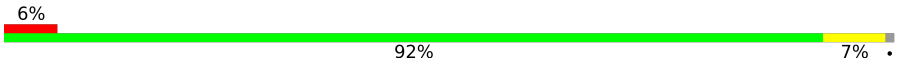
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
40	T	1	1	1	0

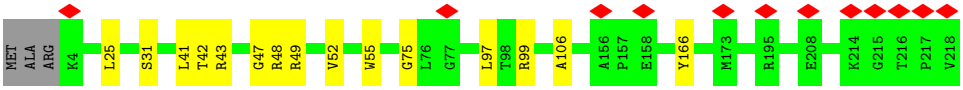
3 Residue-property plots (i)

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: 28S ribosomal protein S34, mitochondrial

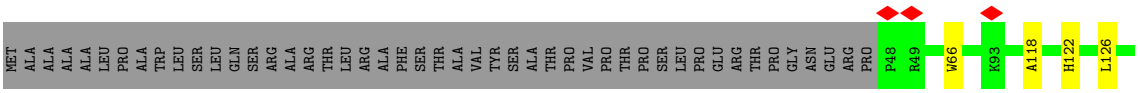
Chain 0:

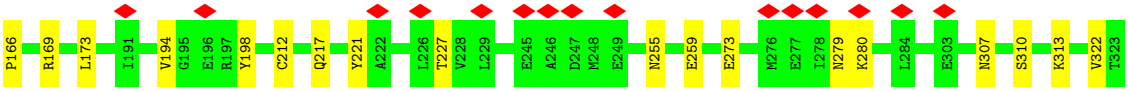




- Molecule 2: 28S ribosomal protein S35, mitochondrial

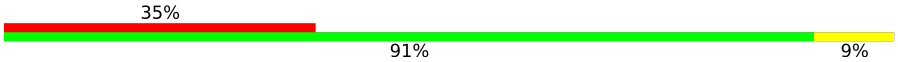
Chain 1:

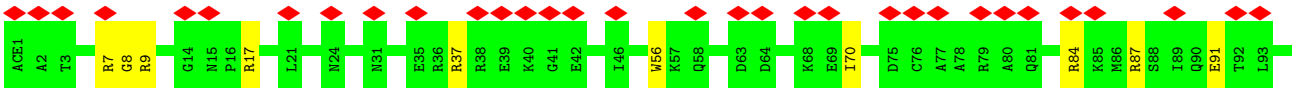


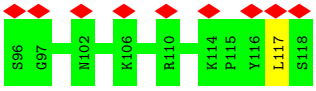


- Molecule 3: Small ribosomal subunit protein mS37

Chain 2:

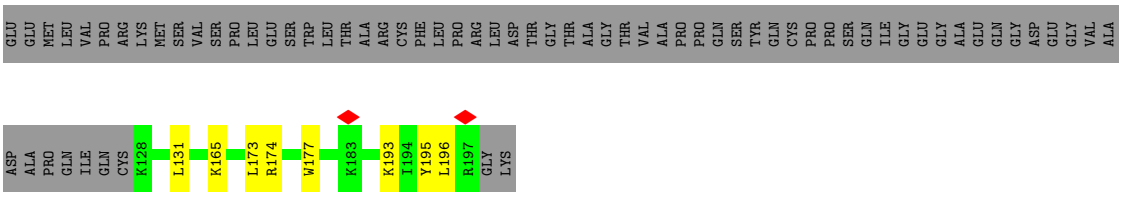






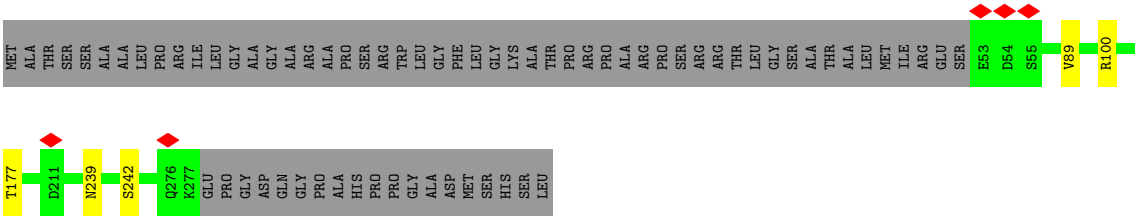
- Molecule 4: Aurora kinase A-interacting protein

Chain 3:



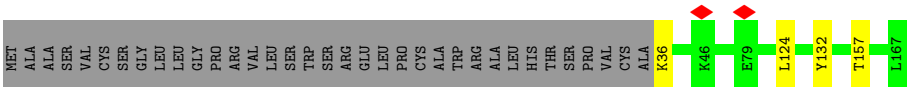
• Molecule 5: 28S ribosomal protein S2, mitochondrial

Chain B:



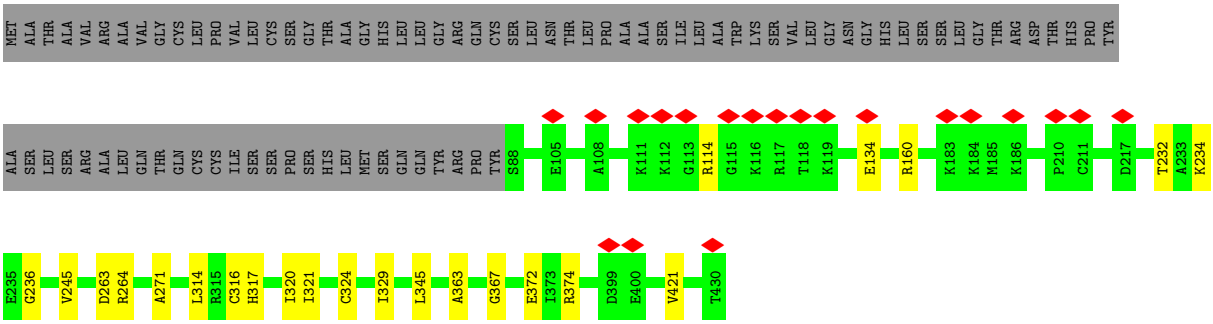
• Molecule 6: 28S ribosomal protein S24, mitochondrial

Chain C:



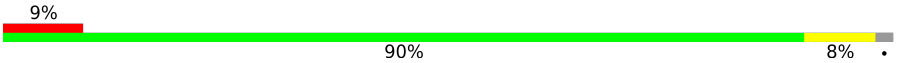
• Molecule 7: 28S ribosomal protein S5, mitochondrial

Chain D:



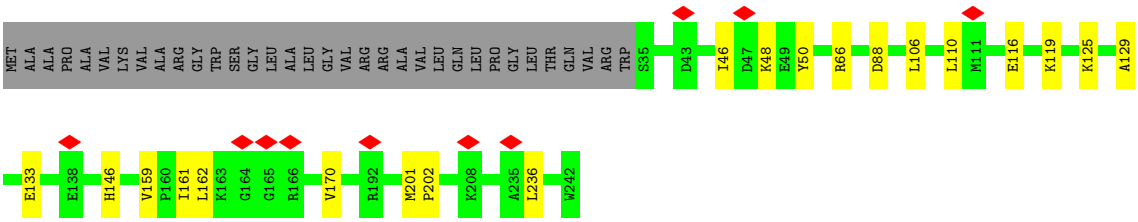
• Molecule 8: 28S ribosomal protein S6, mitochondrial

Chain E:



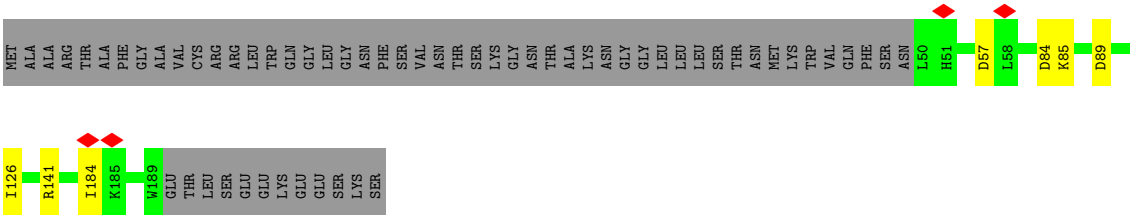
• Molecule 9: 28S ribosomal protein S7, mitochondrial

Chain F:



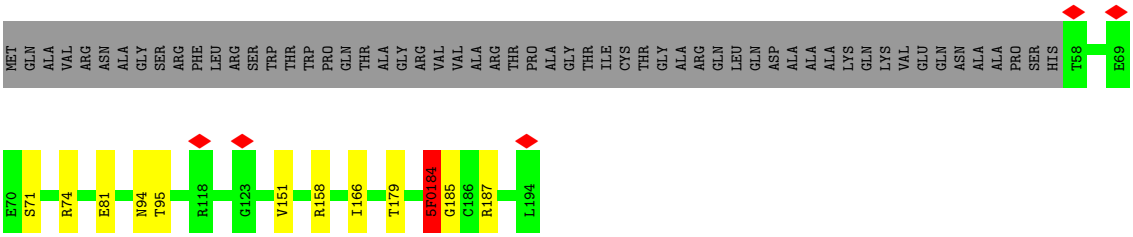
• Molecule 10: 28S ribosomal protein S10, mitochondrial

Chain H:



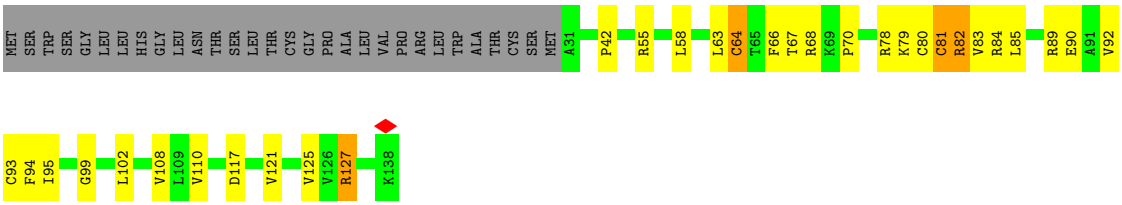
• Molecule 11: 28S ribosomal protein S11, mitochondrial

Chain I:



• Molecule 12: 28S ribosomal protein S12, mitochondrial

Chain J:

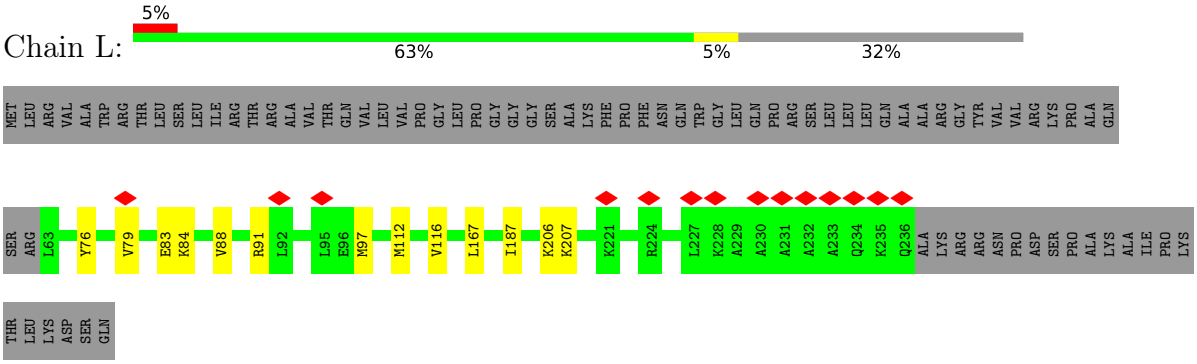


• Molecule 13: 28S ribosomal protein S14, mitochondrial

Chain K:

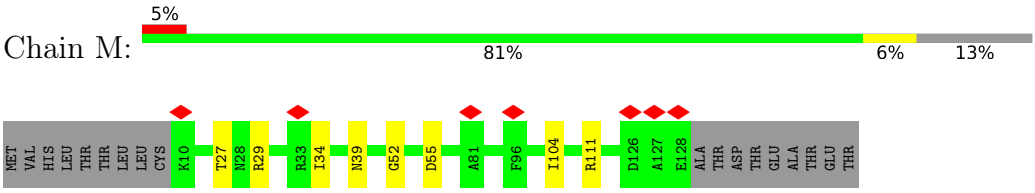
• Molecule 14: 28S ribosomal protein S15, mitochondrial

Chain L:



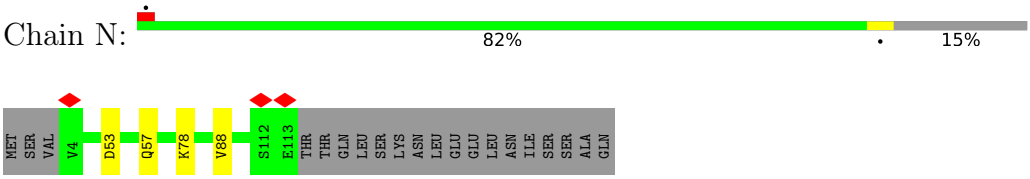
- Molecule 15: 28S ribosomal protein S16, mitochondrial

Chain M:



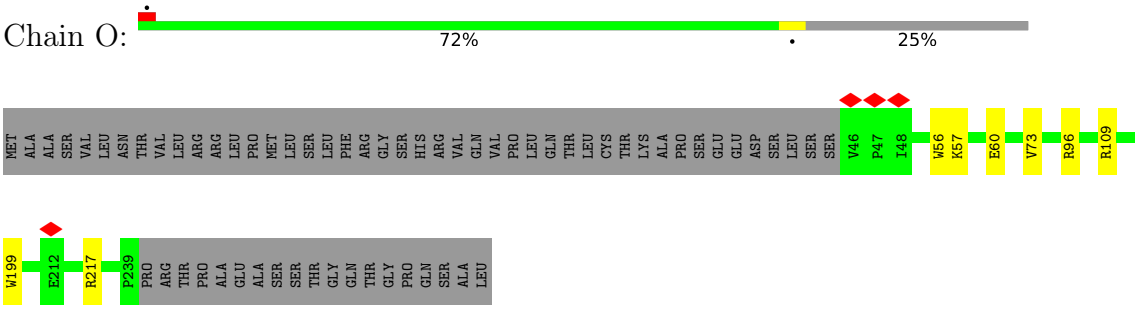
- Molecule 16: 28S ribosomal protein S17, mitochondrial

Chain N:



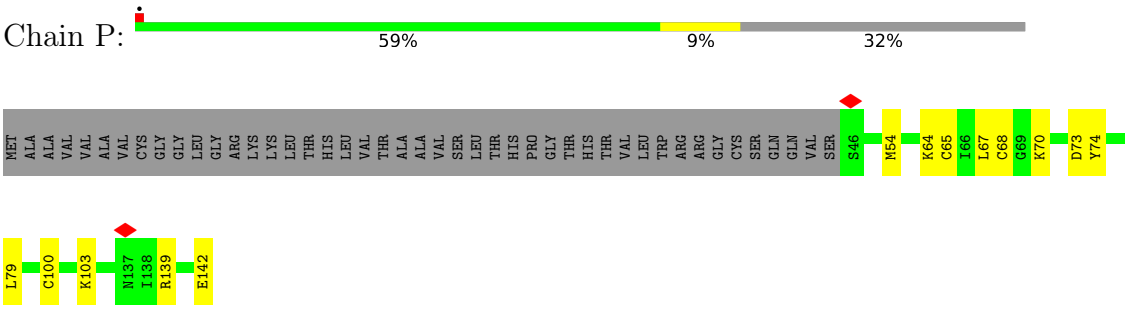
- Molecule 17: 28S ribosomal protein S18b, mitochondrial

Chain O:



- Molecule 18: 28S ribosomal protein S18c, mitochondrial

Chain P:



- Molecule 19: Small ribosomal subunit protein bS21m

Chain Q: 93% 7%

ACE1 V19 M32 I39 C49 R50 R77 R80 C87

• Molecule 20: 28S ribosomal protein S22, mitochondrial

Chain R: 75% 7% 18%

MET ALA PRO LEU GLY THR THR VAL LEU LEU TRP SER LEU LEU ARG SER SER PRO GLY VAL GLU ARG VAL CYS PHE ARG ALA ARG ILE GLN PRO TRP HIS GLY GLY LEU LEU GLN PRO LEU PRO CYS SER PHE GLU MET GLY LEU PRO ARG ARG ARG PHE SER SER GLU ALA ALA GLU SER

GLY SER PRO E64 T66 T69 D72 M82 K146 I147 S162 I165 R191 V195 I204 E212 Y219 K248 R256 L262 T265 V276 I281 L300 L307 A317 A321 Q347 E351 H356 S357 A358 ALA SER

• Molecule 21: 28S ribosomal protein S23, mitochondrial

Chain S: 67% 29%

MET A2 E7 V51 R52 Y65 Y75 G79 S80 R98 E128 R133 G136 GLU ALA ARG THR GLN HIS GLY GLY SER HIS VAL SER ARG LYS SER GLU HIS LEU SER VAL ARG PRO GLN THR ALA LEU GLU GLU ASN GLU THR GLN LYS GLU VAL PRO GLN ASP

GLN HIS LEU GLU ALA PRO ALA ASP GLN SER LYS GLY LEU LEU PRO PRO

• Molecule 22: 28S ribosomal protein S25, mitochondrial

Chain T: 92% 5%

MET P2 M3 K4 R11 T92 P131 R132 L136 R137 E138 C141 Q146 L167 K168 A169 ASP ALA GLN ASP

• Molecule 23: 28S ribosomal protein S26, mitochondrial

Chain U: 80% 6% 14%

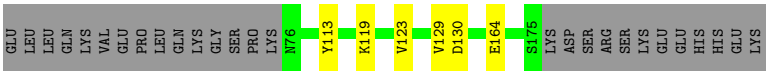
MET LEU ARG ALA LEU SER ARG LEU GLY ALA GLY THR PRO CYS ARG PRO ARG ALA PRO LEU VAL LEU PRO ALA ARG GLY R27 M44 R80 E84 D98 E127 E130 Q131 R134 L137 R141 W149 Q161 V164 R170 L173 D182 I191

R202 ARG ASP SER

• Molecule 24: 28S ribosomal protein S28, mitochondrial

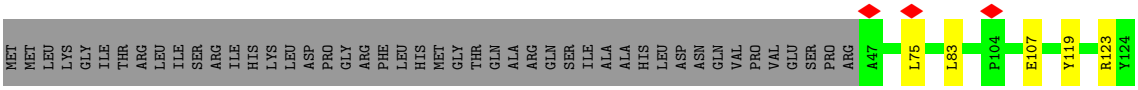
Chain W: 50% 47%

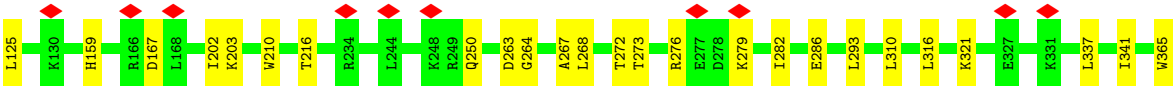
MET ALA ALA LEU CYS ARG THR ARG ALA VAL ALA ALA GLU SER HIS PHE LEU ARG VAL PHE LEU PHE PHE ARG PRO PHE ARG GLY VAL GLY THR GLU SER GLY SER GLU SER GLY SER SER ASN ALA LYS GLU PRO LYS THR ARG ALA GLY GLY PHE ALA SER ALA LEU GLU ARG HIS SER

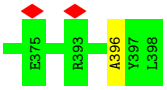


• Molecule 25: 28S ribosomal protein S29, mitochondrial

Chain X:

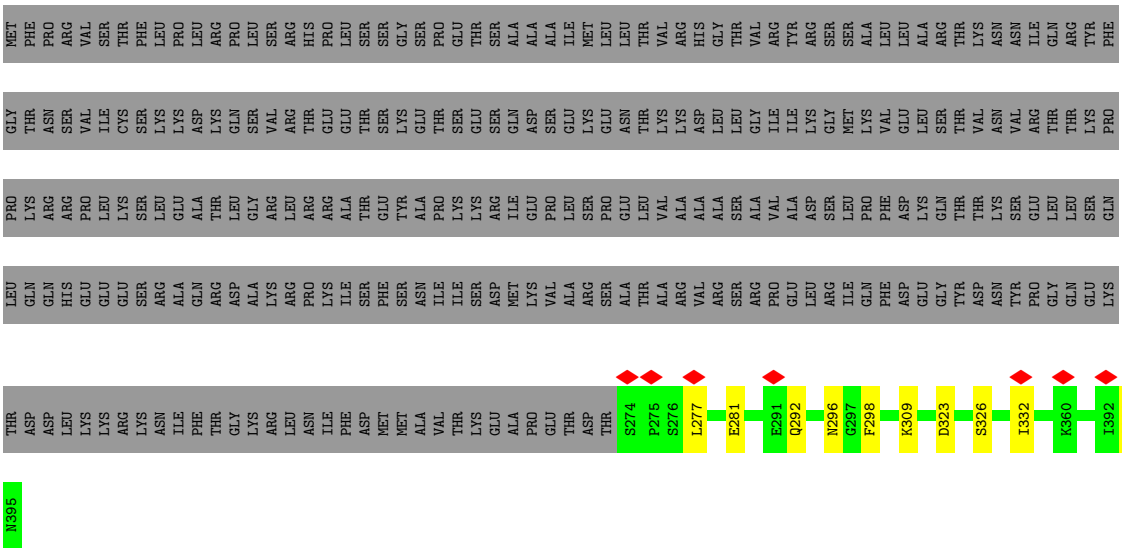






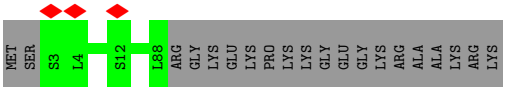
• Molecule 26: 28S ribosomal protein S31, mitochondrial

Chain Y:



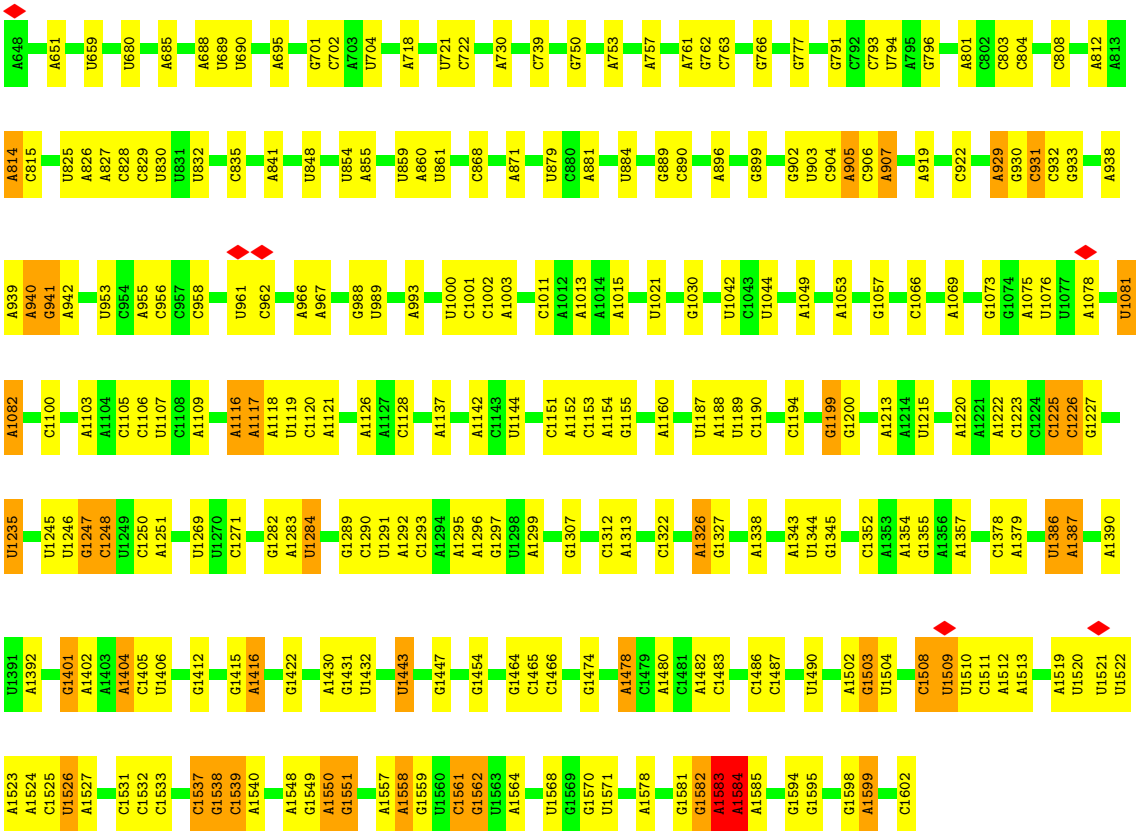
• Molecule 27: 28S ribosomal protein S33, mitochondrial

Chain Z:



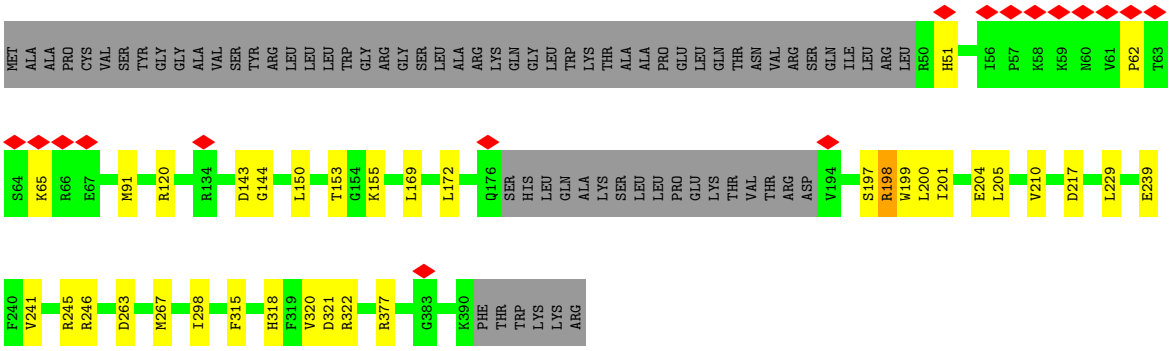
• Molecule 28: 12S mitochondrial rRNA

Chain A:



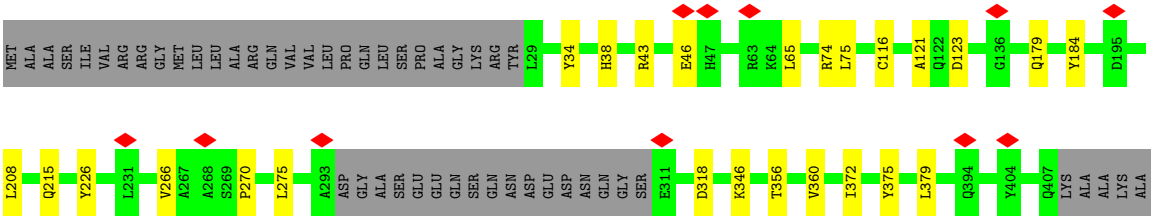
• Molecule 29: 28S ribosomal protein S9, mitochondrial

Chain G:



• Molecule 30: 28S ribosomal protein S27, mitochondrial

Chain V:



SER
ALA

- Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:

MET ALA VAL VAL SER ALA VAL ARG TRP LEU GLY LEU ARG SER ARG LEU GLY GLN PRO LEU THR GLY ARG ARG ALA GLY LEU CYS GLU GLN ALA ARG SER CYS ARG PHE TYR SER GLY SER ALA THR LEU SER LYS VAL GLU GLY THR ASP VAL THR GLY ILE E55 V58 I59 L74

D91 D92 L1140 F145 Q148 I149 K150 I161 E162 L163 R164 K165 V166 K167 A168 S169 V170 D171 G180 T181 T182 V183 E186 L194 L195 C196 Y197 Y198 G199 D200 Q201 E202 P203 S204 T205 D206 Y207 H208 PHE GLN GLN THR GLY GLN SER GLU ALA LEU GLU GLU GLU ASN

ASP GLU THR SER ARG ARG LYS ALA GLY HIS Q233 F234 G235 V236 T237 W238 R239 A240 K241 N242 N243 A244 E245 R246 I247 M251 Y259 V267 K268 H269 R270 Y279 L282 N285 R286 L287 H288 A289 N296 A296 L297 I298 E299 A300 T301 V302 C303 A304 I305 N306 K312 W313

I316 L320 V324 K327 V328 K329 N336 R344 F345 H346 V347 F348 A349 R350 S351 P352 A353 L357 M360 E366 P367 S368 L369 A370 T371 Y372 I376 R377 L378 P382 G383 D384 P385 L386 K387 R388 I393 L400 F405 D411 D412 D413 K414 F415 F416

R427 K440 T441 D451 R454 Y458 L467 Q470 I471 D472 L481 A485 M493 D501 E507 V508 E518 R537 D550 E560 S561 Q562 P563 I564 R565 Q566 T567 A568 I579 K594 M595 L610 E613 S617 A618 K619 V620 S621 N622

S625 Q626 E629 V630 V631 E632 L633 A636 I641 C642 E643 T646 M650 S651 D652 F653 A654 I655 N656 Q657 E658 E661 A662 L663 S664 N665 L666 THR ALA LEU THR SER ASP SER ASP THR ASP SER SER SER ASP SER ASP SER ASP THR SER GLU GLY LYS

- Molecule 32: 12S rRNA N4-methylcytidine (m4C) methyltransferase

Chain b:

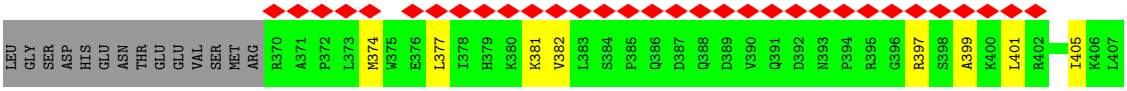
MET LEU ARG TYR PRO TYR PHE CYS ARG MET TYR LYS GLU CYS LEU SER CYS TRP LEU GLU SER GLY ILE PRO ASN LEU GLY VAL TRP PRO ASN ARG ILE HIS THR THR ALA GLU LYS TYR ARG GLU TYR GLU ALA ARG GLU GLN THR ASP GLN THR GLN ALA GLN GLU LEU HIS ARG SER

GLN ASP ARG ASP PHE GLU THR MET ALA LYS L71 H72 I73 P74 V75 M76 V77 D78 E79 V80 V81 H82 C83 P86 Q87 K88 F92 L93 D94 M95 T96 F97 H102 T103 K104 A105 I106 L107 E110 S111 D112 I113 Y116 A117 L118 D119 R120 A124 L127 A128 E129 H130 L131

S132 E133 L134 Y135 I139 G144 Q145 F146 S147 Q148 A149 E150 A151 LEU LEU MET LYS ALA GLY VAL GLN PRO GLY T162 V166 L167 M168 D169 L170 G171 C172 S173 S174 M175 Q176 L177 D178 F184 S185 L186 R187 LYS ASP GLY PRO LEU ASP MET R195 M196 D197 R200 Y201 P202 D203

T206 A207 V210 V211 N212 A213 L214 D215 Q216 Q217 A218 L219 A220 S221 T222 L223 R224 T225 Y226 G227 E228 E229 K230 H231 A232 K233 K234 I235 A236 S237 A238 I239 V240 Q241 A242 R243 S244 I245 I248 T251 L254 A255 Y258 A259 G260 A261 F262 A266 R270 K271 D272 L273

L274 Q275 I280 A281 T282 K283 T284 F285 Q286 A287 L288 R289 I290 F291 V292 N293 N294 E295 L296 N297 E298 L299 Y300 G313 L316 V317 A318 L319 S323 L324 E325 D326 R327 I328 L333 S337 M338 T339 GLU ARG PHE ASN LEU SER VAL ARG GLN GLN VAL MET LYS THR SER GLN


LEU
GLY
SER
ASP
HIS
GLU
ASN
THR
GLU
GLU
VAL
SER
MET
ARG
R370
A371
P372
L373
M374
W375
E376
L377
I378
H379
K380
K381
V382
L383
S384
P385
Q386
D387
Q388
D389
V390
Q391
D392
N393
P394
R395
G396
R397
S398
A399
K400
L401
R402
I405
K406
L407

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	495.0, 495.0, 495.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, K, ZN, 5MU, FES, 5F0, MA6, ACE, GDP, NAD, B8T, ATP, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	0	0.09	0/1834	0.25	0/2484
2	1	0.08	0/2285	0.24	0/3090
3	2	0.24	0/947	0.39	0/1266
4	3	0.24	0/636	0.41	0/839
5	B	0.08	0/1871	0.23	0/2531
6	C	0.08	0/1113	0.23	0/1505
7	D	0.09	0/2783	0.24	0/3724
8	E	0.08	0/989	0.23	0/1335
9	F	0.08	0/1767	0.23	0/2373
10	H	0.08	0/1178	0.23	0/1598
11	I	0.09	0/1030	0.26	0/1386
12	J	0.87	0/855	0.97	2/1148 (0.2%)
13	K	0.07	0/880	0.22	0/1182
14	L	0.08	0/1477	0.22	0/1974
15	M	0.08	0/963	0.24	0/1295
16	N	0.08	0/886	0.22	0/1199
17	O	0.21	0/1655	0.35	0/2254
18	P	0.09	0/798	0.25	0/1070
19	Q	0.07	0/754	0.22	0/1003
20	R	0.07	0/2456	0.22	0/3317
21	S	0.07	0/1138	0.19	0/1533
22	T	0.08	0/1402	0.24	0/1883
23	U	0.07	0/1510	0.21	0/2025
24	W	0.11	0/801	0.28	0/1079
25	X	0.08	0/2921	0.24	0/3954
26	Y	0.08	0/1060	0.26	0/1430
27	Z	0.08	0/747	0.22	0/1000
28	A	0.10	0/22562	0.23	0/35124
29	G	0.26	0/2710	0.45	2/3635 (0.1%)
30	V	0.22	0/3030	0.40	0/4093
31	4	0.08	0/4877	0.25	0/6598
32	b	0.16	0/2311	0.32	0/3116

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.15	0/72226	0.28	4/102043 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
11	I	0	1
12	J	0	4
17	O	0	1
30	V	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	J	64	CYS	N-CA-C	6.42	118.27	108.52
12	J	64	CYS	N-CA-CB	-6.16	101.44	111.24
29	G	239	GLU	N-CA-C	-5.26	105.22	111.69
29	G	198	ARG	N-CA-CB	-5.02	104.32	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	37	ARG	Sidechain
11	I	184	5F0	Mainchain
12	J	68	ARG	Sidechain
12	J	82	ARG	Sidechain
12	J	89	ARG	Sidechain

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	0	1787	1796	1796	10	0
2	1	2238	2269	2269	18	0
3	2	935	968	969	8	0
4	3	625	699	699	5	0
5	B	1828	1815	1815	5	0
6	C	1083	1088	1088	3	0
7	D	2731	2802	2802	18	0
8	E	972	1001	1000	9	0
9	F	1725	1769	1769	15	0
10	H	1152	1183	1183	6	0
11	I	1020	1060	1052	10	0
12	J	839	884	886	43	0
13	K	862	885	885	8	0
14	L	1453	1540	1540	10	0
15	M	942	965	966	7	0
16	N	868	928	928	3	0
17	O	1599	1565	1565	5	0
18	P	781	807	806	10	0
19	Q	744	757	758	7	0
20	R	2409	2428	2428	15	0
21	S	1111	1115	1115	7	0
22	T	1371	1393	1394	7	0
23	U	1488	1499	1499	8	0
24	W	789	800	800	5	0
25	X	2849	2844	2844	22	0
26	Y	1029	975	974	11	0
27	Z	730	734	734	0	0
28	A	20282	10302	10300	82	0
29	G	2654	2650	2649	35	0
30	V	2969	2962	2961	15	0
31	4	4768	4766	4766	36	0
32	b	2272	2327	2325	54	0
33	3	1	0	0	0	0
33	A	44	0	0	0	0
33	B	1	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	1	0
35	T	4	0	0	0	0
36	X	31	12	12	0	0
37	X	28	10	12	0	0
38	A	44	26	26	0	0
39	A	3	0	0	0	0
40	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	69067	59624	59615	414	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 3.

The worst 5 of 414 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)
12:J:80:CYS:SG	12:J:94:PHE:HA	1.18	1.69
12:J:80:CYS:SG	12:J:94:PHE:CA	2.04	1.42
12:J:64:CYS:SG	12:J:82:ARG:O	2.14	1.05
29:G:200:LEU:HD23	29:G:201:ILE:O	1.58	1.03
29:G:200:LEU:CD2	29:G:201:ILE:O	2.08	1.01

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	0	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
2	1	274/323 (85%)	263 (96%)	11 (4%)	0	100	100
3	2	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
4	3	68/199 (34%)	68 (100%)	0	0	100	100
5	B	223/296 (75%)	215 (96%)	8 (4%)	0	100	100
6	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
7	D	341/430 (79%)	328 (96%)	13 (4%)	0	100	100
8	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
9	F	206/242 (85%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	138/201 (69%)	136 (99%)	2 (1%)	0	100	100
11	I	134/194 (69%)	123 (92%)	10 (8%)	1 (1%)	18	55
12	J	106/138 (77%)	95 (90%)	10 (9%)	1 (1%)	14	49
13	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
14	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
15	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
16	N	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
17	O	192/258 (74%)	185 (96%)	7 (4%)	0	100	100
18	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
19	Q	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
20	R	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
21	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
22	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
23	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
24	W	98/187 (52%)	94 (96%)	4 (4%)	0	100	100
25	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
26	Y	120/395 (30%)	119 (99%)	1 (1%)	0	100	100
27	Z	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
29	G	320/396 (81%)	300 (94%)	20 (6%)	0	100	100
30	V	358/414 (86%)	353 (99%)	5 (1%)	0	100	100
31	4	584/689 (85%)	570 (98%)	14 (2%)	0	100	100
32	b	282/407 (69%)	271 (96%)	11 (4%)	0	100	100
All	All	5899/7710 (76%)	5735 (97%)	162 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	J	81	CYS
11	I	185	GLY

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	0	188/190 (99%)	188 (100%)	0	100	100
2	1	254/291 (87%)	254 (100%)	0	100	100
3	2	100/100 (100%)	100 (100%)	0	100	100
4	3	65/166 (39%)	65 (100%)	0	100	100
5	B	198/249 (80%)	198 (100%)	0	100	100
6	C	115/143 (80%)	115 (100%)	0	100	100
7	D	286/357 (80%)	286 (100%)	0	100	100
8	E	104/107 (97%)	104 (100%)	0	100	100
9	F	185/209 (88%)	185 (100%)	0	100	100
10	H	130/180 (72%)	130 (100%)	0	100	100
11	I	104/146 (71%)	104 (100%)	0	100	100
12	J	93/118 (79%)	92 (99%)	1 (1%)	65	74
13	K	91/113 (80%)	91 (100%)	0	100	100
14	L	158/226 (70%)	158 (100%)	0	100	100
15	M	97/113 (86%)	97 (100%)	0	100	100
16	N	96/115 (84%)	96 (100%)	0	100	100
17	O	175/230 (76%)	175 (100%)	0	100	100
18	P	88/123 (72%)	88 (100%)	0	100	100
19	Q	78/78 (100%)	78 (100%)	0	100	100
20	R	264/318 (83%)	264 (100%)	0	100	100
21	S	116/164 (71%)	116 (100%)	0	100	100
22	T	153/157 (98%)	153 (100%)	0	100	100
23	U	152/174 (87%)	152 (100%)	0	100	100
24	W	87/158 (55%)	87 (100%)	0	100	100
25	X	311/351 (89%)	311 (100%)	0	100	100
26	Y	113/357 (32%)	113 (100%)	0	100	100
27	Z	80/95 (84%)	80 (100%)	0	100	100
29	G	282/342 (82%)	282 (100%)	0	100	100
30	V	325/364 (89%)	324 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	4	526/609 (86%)	526 (100%)	0	100	100
32	b	244/350 (70%)	244 (100%)	0	100	100
All	All	5258/6693 (79%)	5256 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	108	VAL
30	V	38	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
29	G	261	GLN
31	4	274	GLN
29	G	288	HIS
30	V	245	HIS
31	4	373	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	A	954/955 (99%)	208 (21%)	9 (0%)

5 of 208 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	A	651	A
28	A	659	U
28	A	680	U
28	A	688	A
28	A	689	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1537	C
28	A	1550	A
28	A	1502	A

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Mol	Chain	Res	Type
28	A	1508	C
28	A	1513	A

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	$\#\|Z\| > 2$
28	MA6	A	1583	28	23,26,27	1.27	3 (13%)	34,38,41	3.27	14 (41%)
28	5MC	A	1488	28	18,22,23	0.54	0	26,32,35	0.49	0
11	5F0	I	184	11	8,8,9	0.58	0	7,9,11	1.17	1 (14%)
28	5MU	A	1076	28	19,22,23	0.40	0	28,32,35	0.49	0
28	MA6	A	1584	28	23,26,27	1.28	3 (13%)	34,38,41	3.10	11 (32%)
28	B8T	A	1486	28	19,22,23	3.32	8 (42%)	26,31,34	0.84	1 (3%)

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
28	MA6	A	1583	28	-	3/11/29/30	0/3/3/3
28	5MC	A	1488	28	-	0/7/25/26	0/2/2/2
11	5F0	I	184	11	-	2/9/9/10	-
28	5MU	A	1076	28	-	0/7/25/26	0/2/2/2
28	MA6	A	1584	28	-	0/11/29/30	0/3/3/3
28	B8T	A	1486	28	-	0/7/27/28	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	1486	B8T	C4-N3	7.63	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	1486	B8T	C6-C5	5.99	1.49	1.35
28	A	1486	B8T	C2-N3	5.97	1.48	1.36
28	A	1486	B8T	C4-N4	4.85	1.45	1.35
28	A	1486	B8T	C2-N1	4.56	1.49	1.40

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	1583	MA6	N1-C6-N6	-12.64	103.26	117.08
28	A	1584	MA6	N1-C6-N6	-11.87	104.10	117.08
28	A	1583	MA6	C5-C6-N6	6.61	136.82	125.30
28	A	1584	MA6	C5-C6-N6	5.91	135.59	125.30
28	A	1584	MA6	N1-C2-N3	-5.37	120.20	128.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	1583	MA6	O4'-C4'-C5'-O5'
11	I	184	5F0	OD1-C1-CA-CB
28	A	1583	MA6	C4'-C5'-O5'-P
28	A	1583	MA6	C3'-C4'-C5'-O5'
11	I	184	5F0	O-C-CB-CA

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	1583	MA6	5	0
11	I	184	5F0	2	0
28	A	1076	5MU	1	0
28	A	1584	MA6	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 50 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
35	FES	P	201	8,18	0,4,4	-	-	-		
36	ATP	X	501	-	29,33,33	0.29	0	44,52,52	0.67	1 (2%)
37	GDP	X	502	-	28,30,30	1.13	3 (10%)	44,47,47	1.83	8 (18%)
38	NAD	A	1701	33	45,48,48	0.73	1 (2%)	63,73,73	0.74	2 (3%)
35	FES	T	201	22	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
35	FES	P	201	8,18	-	-	0/1/1/1
37	GDP	X	502	-	-	4/16/32/32	0/3/3/3
36	ATP	X	501	-	-	5/22/38/38	0/3/3/3
38	NAD	A	1701	33	-	3/30/62/62	0/5/5/5
35	FES	T	201	22	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	502	GDP	C5-C4	3.06	1.47	1.38
37	X	502	GDP	C6-N1	-2.44	1.34	1.38
38	A	1701	NAD	O4D-C1D	-2.29	1.37	1.41
37	X	502	GDP	C5-N7	-2.18	1.34	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	502	GDP	C5-C4-N3	-6.17	118.45	128.46
37	X	502	GDP	C2-N3-C4	4.91	121.05	112.30
37	X	502	GDP	N9-C4-N3	4.69	135.36	125.94
37	X	502	GDP	PA-O3A-PB	-3.70	120.12	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	502	GDP	C6-C5-N7	3.19	136.19	130.25

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	X	501	ATP	C5'-O5'-PA-O2A
36	X	501	ATP	C5'-O5'-PA-O3A
37	X	502	GDP	C5'-O5'-PA-O3A
38	A	1701	NAD	C5B-O5B-PA-O1A
38	A	1701	NAD	C5B-O5B-PA-O3

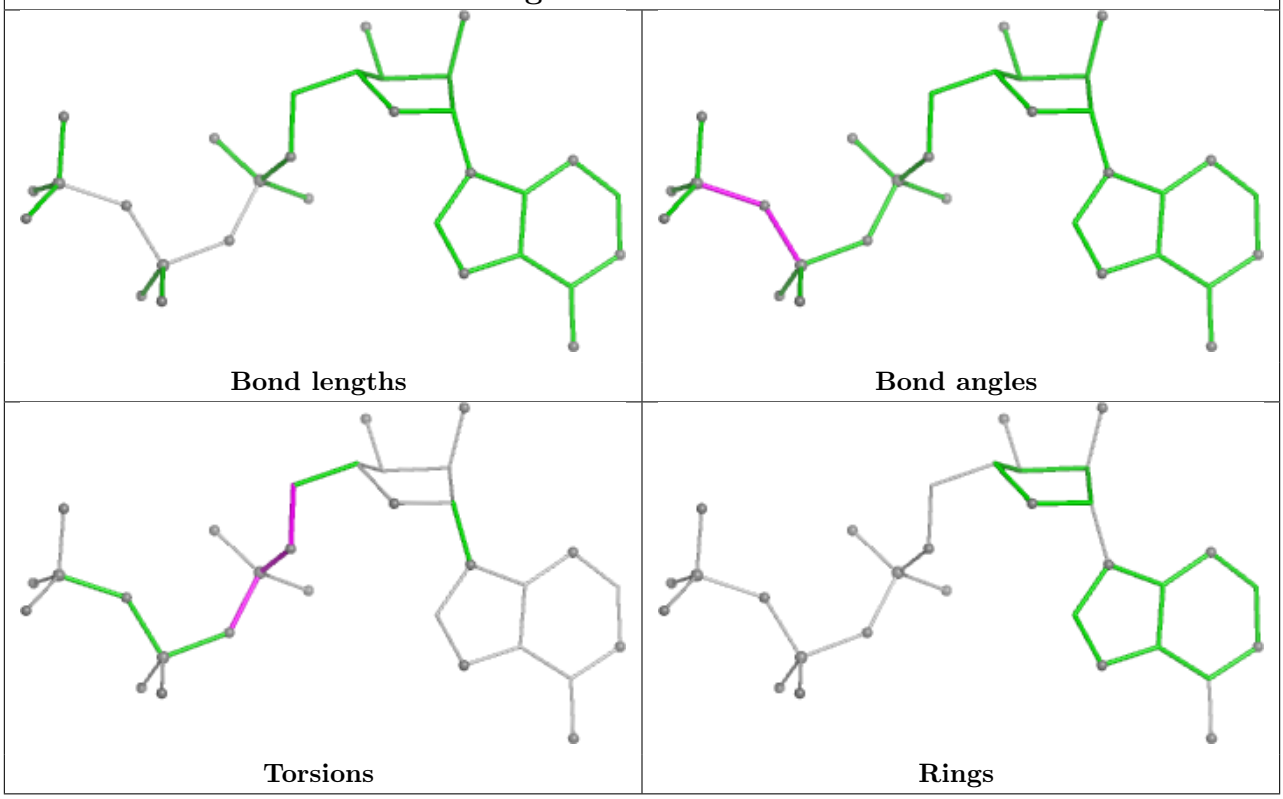
There are no ring outliers.

1 monomer is involved in 1 short contact:

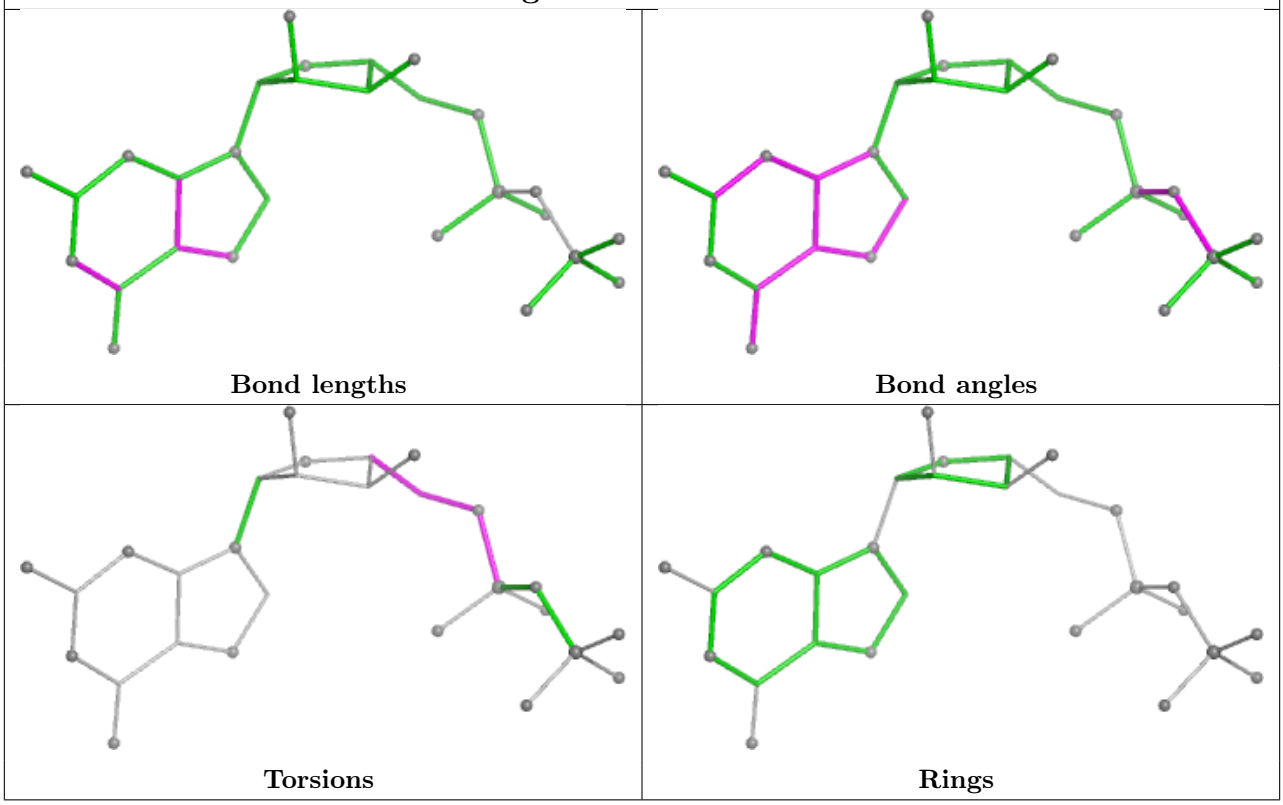
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	P	201	FES	1	0

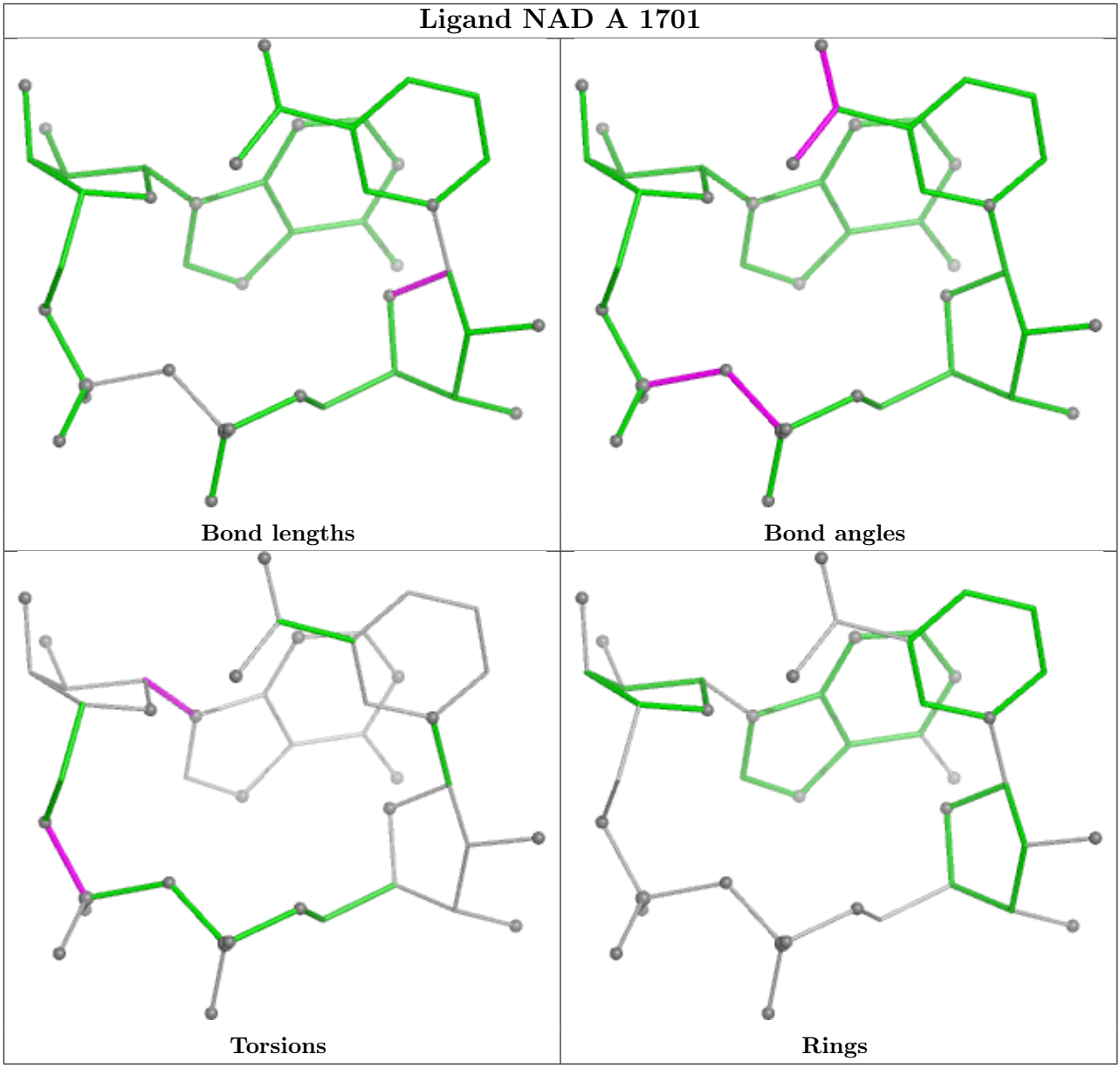
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand ATP X 501



Ligand GDP X 502





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1486:B8T	O3'	1487:C	P	3.07

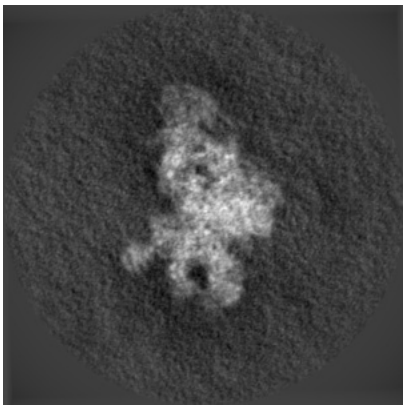
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54163. These allow visual inspection of the internal detail of the map and identification of artifacts.

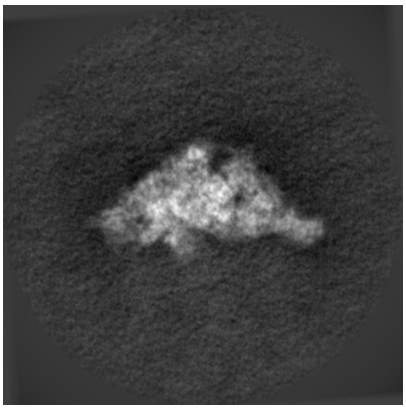
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

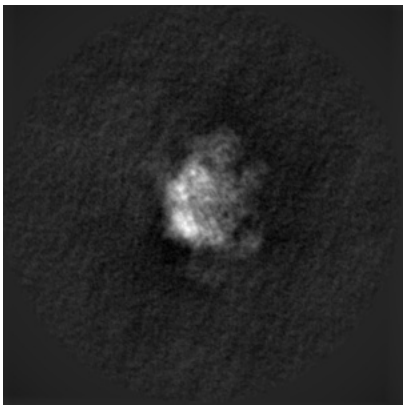
6.1.1 Primary map



X

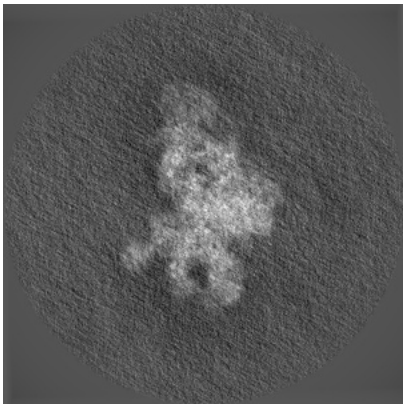


Y

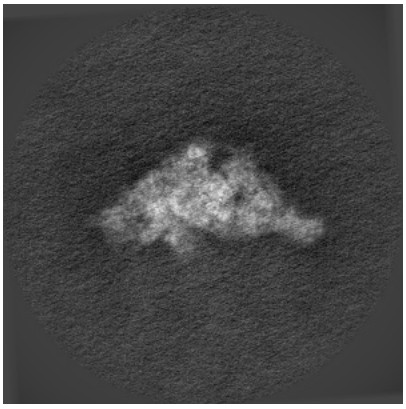


Z

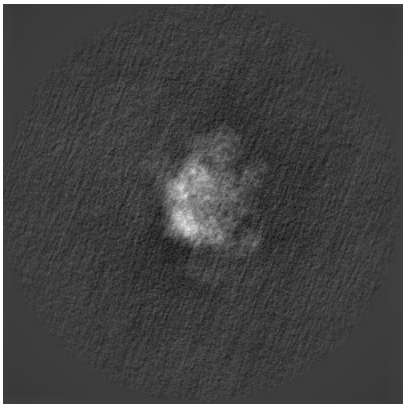
6.1.2 Raw map



X



Y

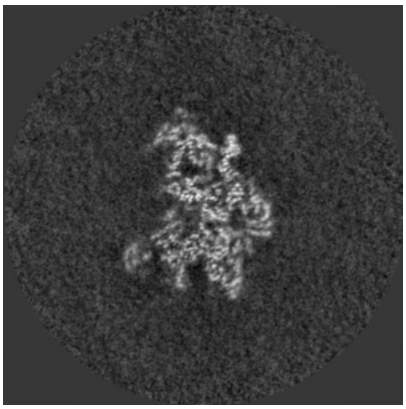


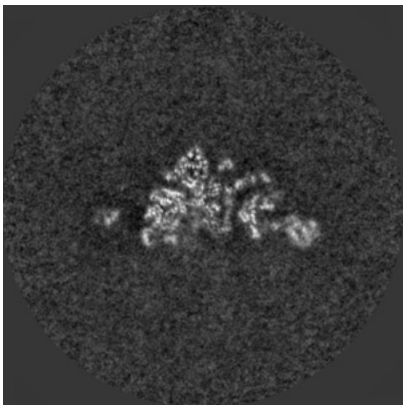
Z

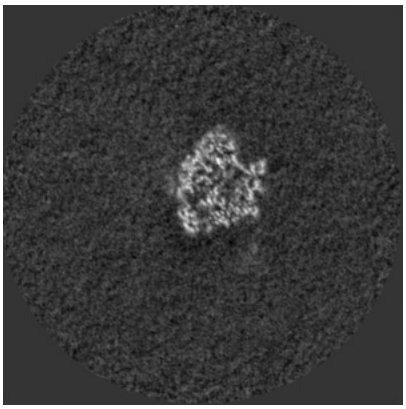
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

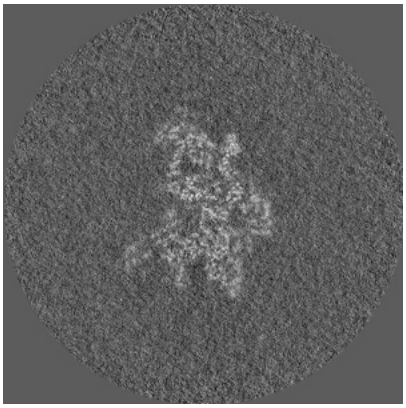
6.2.1 Primary map

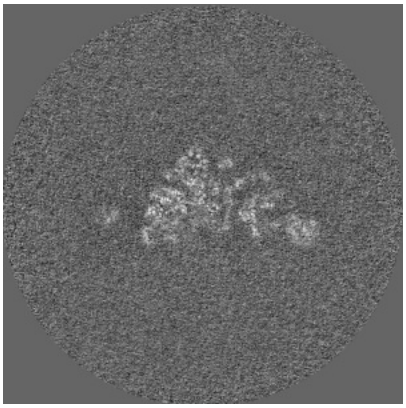

X Index: 300


Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300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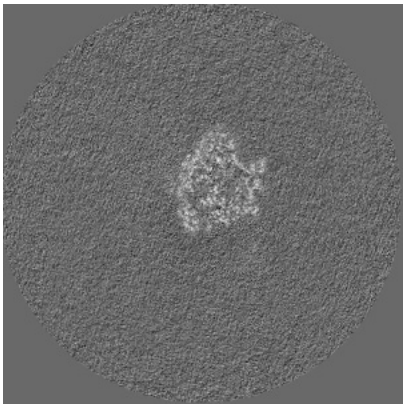
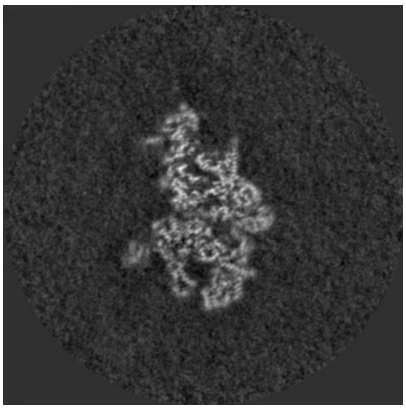
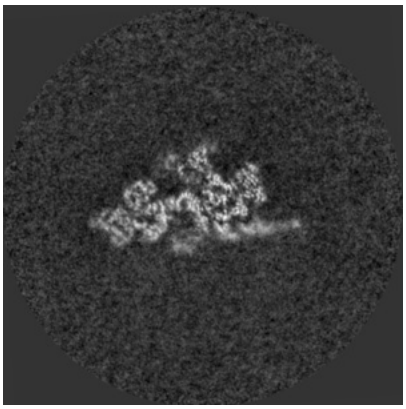

Z Index: 300

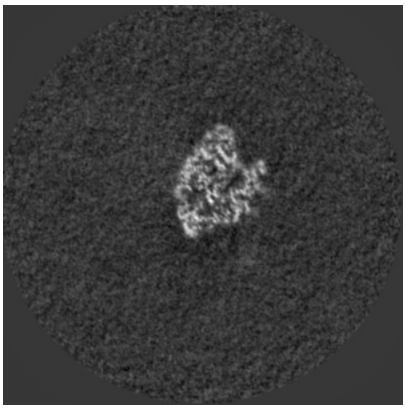
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

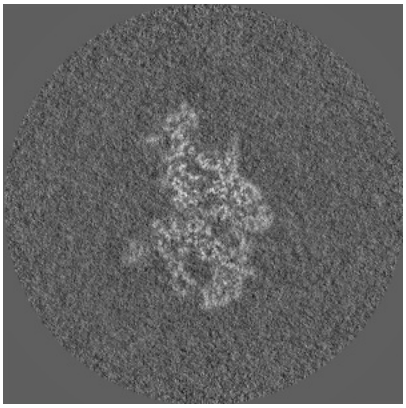
6.3.1 Primary map

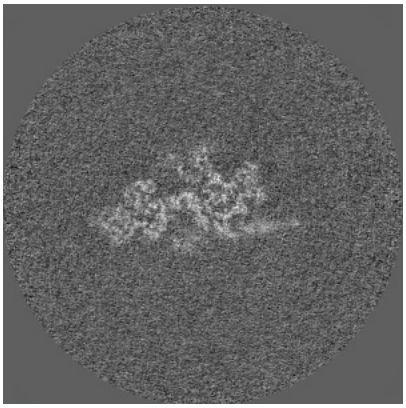

X Index: 287

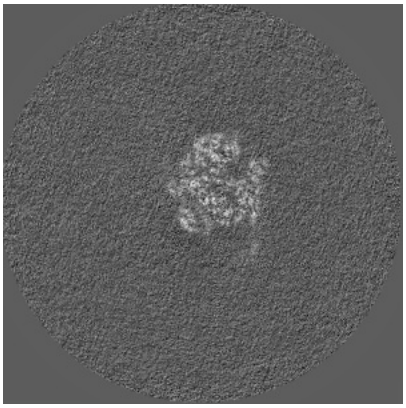

Y Index: 325


Z Index: 304

6.3.2 Raw map


X Index: 287

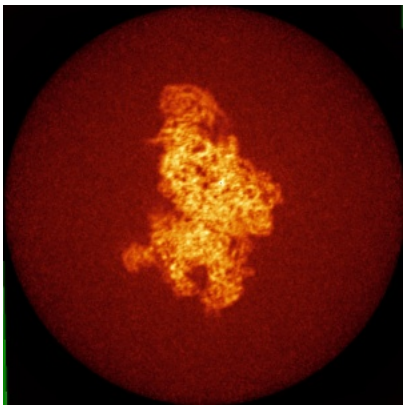

Y Index: 326

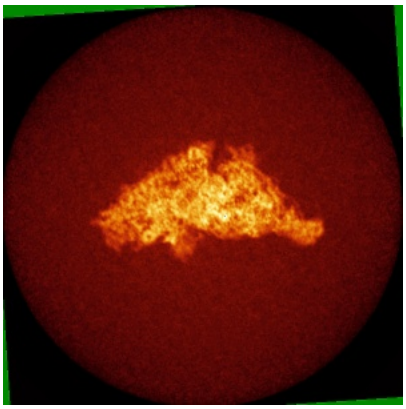

Z Index: 295

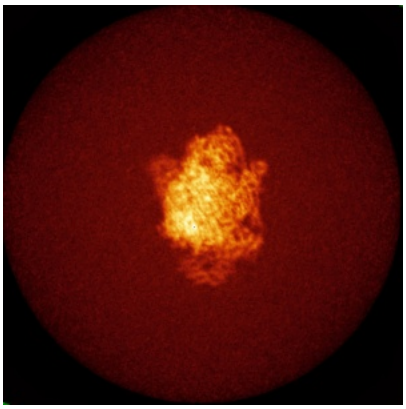
The images above show the largest variance slices of the map in three orthogonal directions.

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

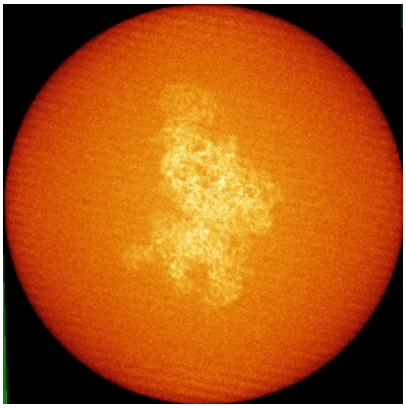
6.4.1 Primary map

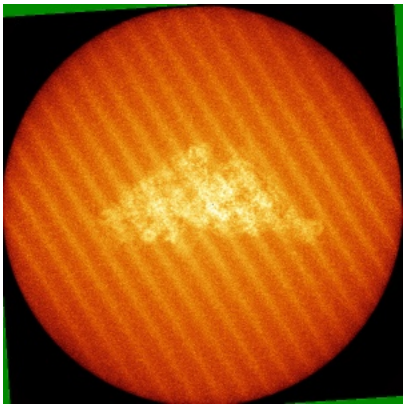

X

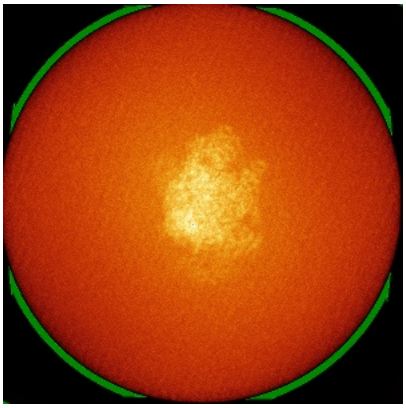

Y


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.

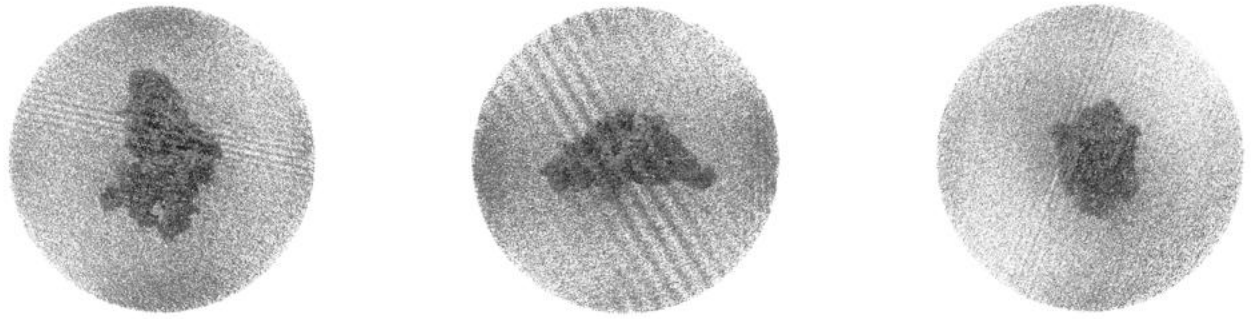
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

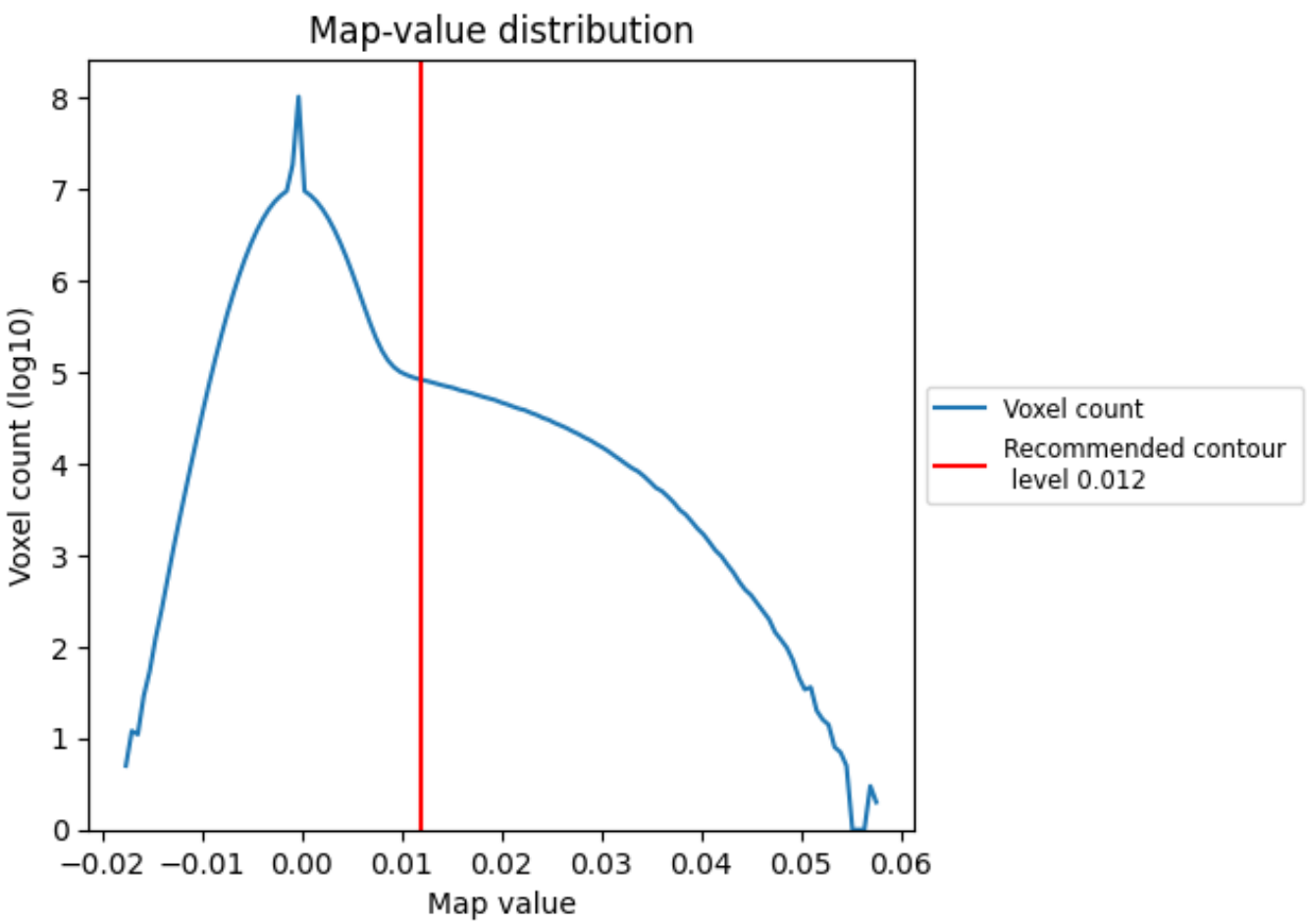
6.6 Mask visualisation (i)

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

7 Map analysis (i)

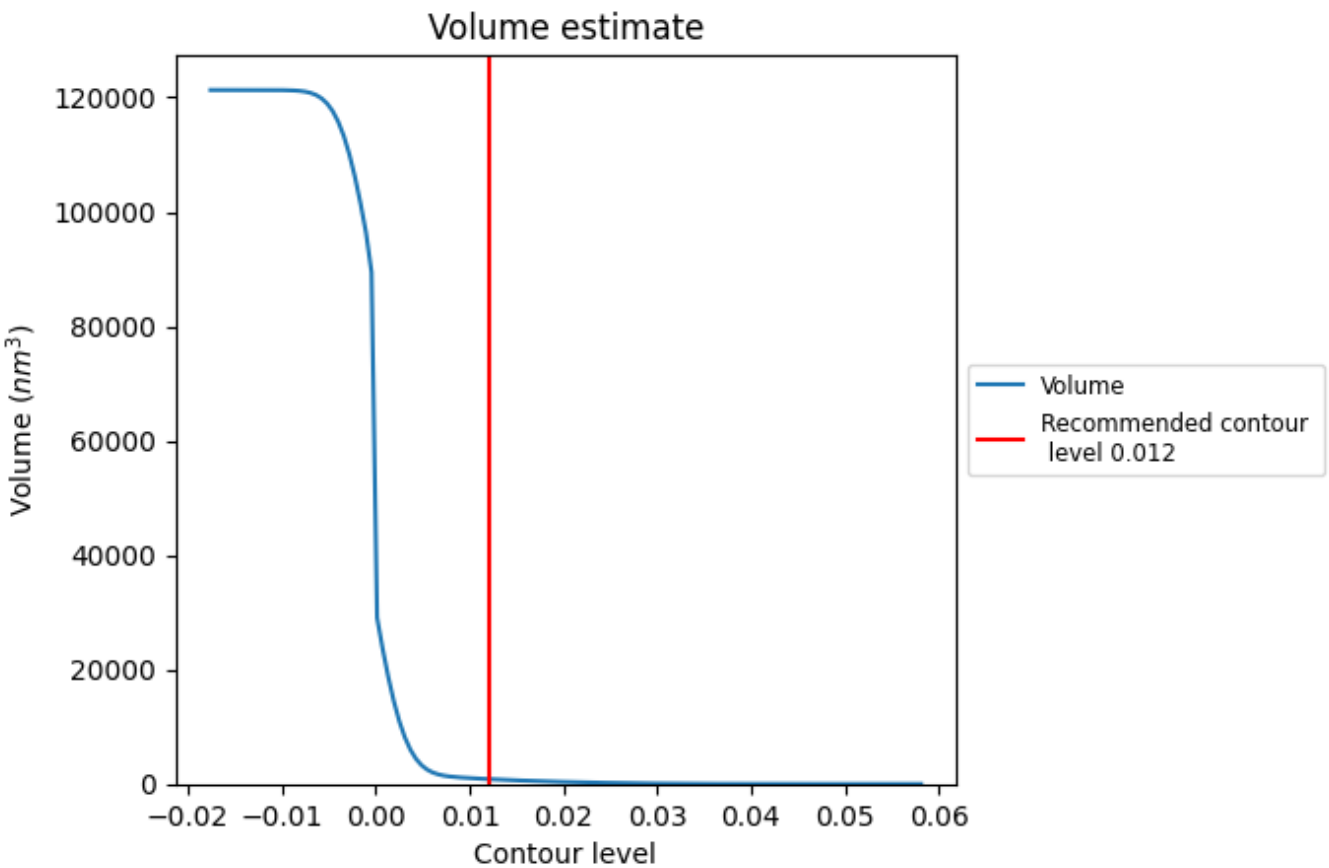
This section contains the results of statistical analysis of the map.

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.

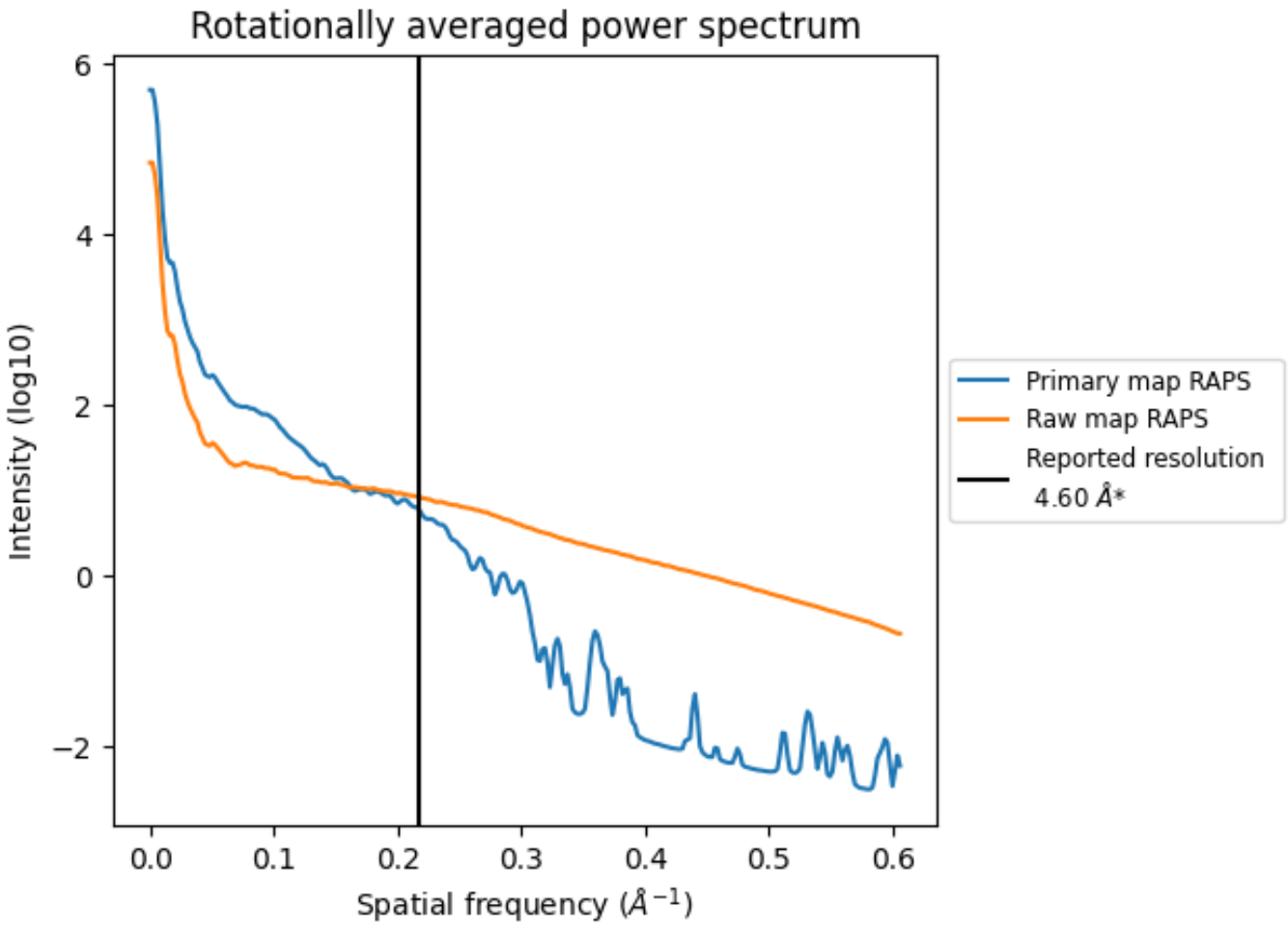
7.2 Volume estimate (i)



The volume at the recommended contour level is 850 nm^3; this corresponds to an approximate mass of 768 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)

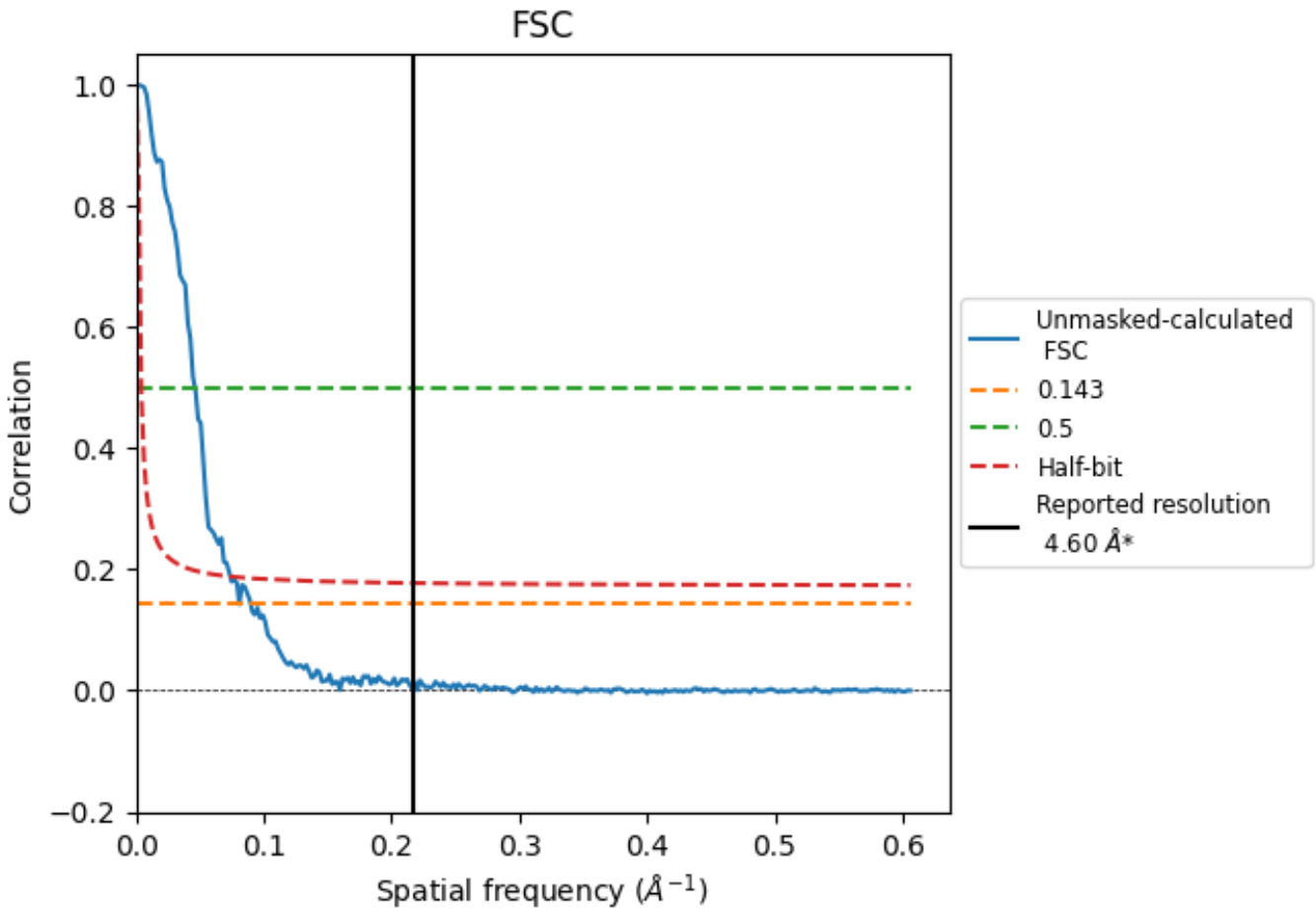


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

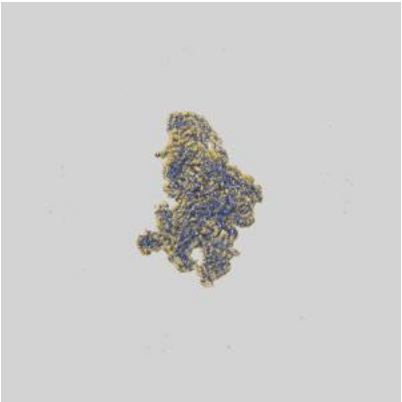
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	12.38	21.79	13.57

*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 12.38 differs from the reported value 4.6 by more than 10 %

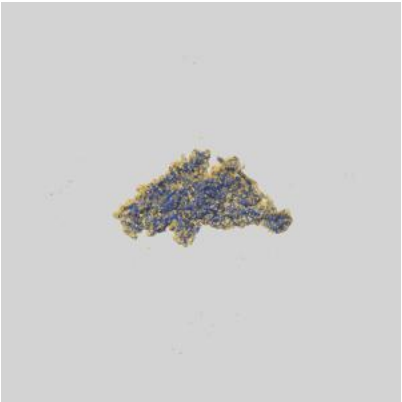
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54163 and PDB model 9RPF. Per-residue inclusion information can be found in section 3 on page 13.

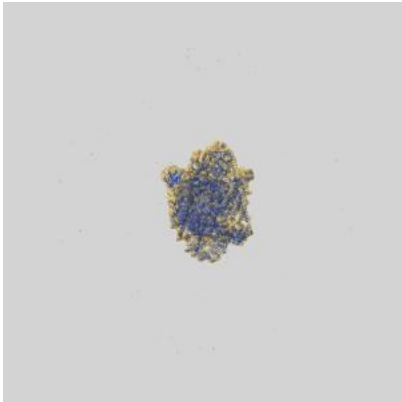
9.1 Map-model overlay (i)



X



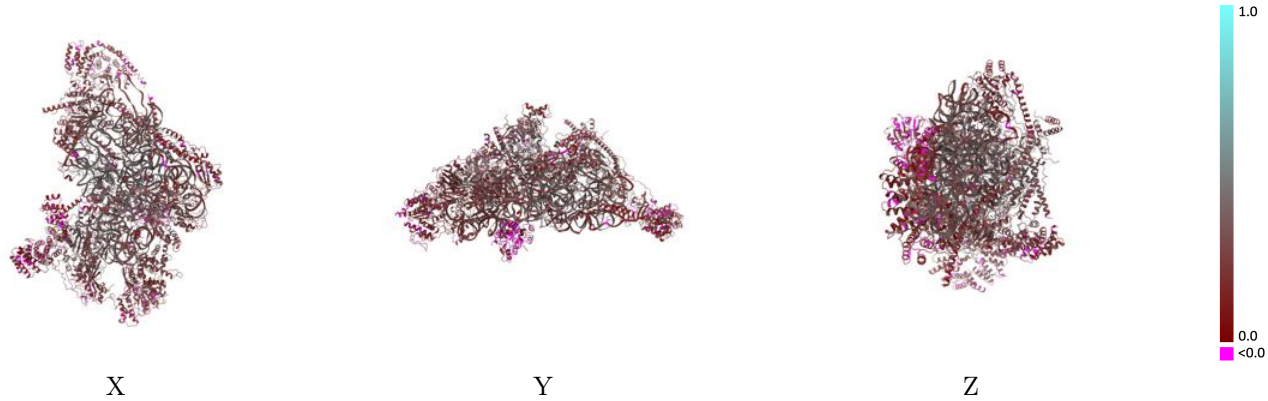
Y



Z

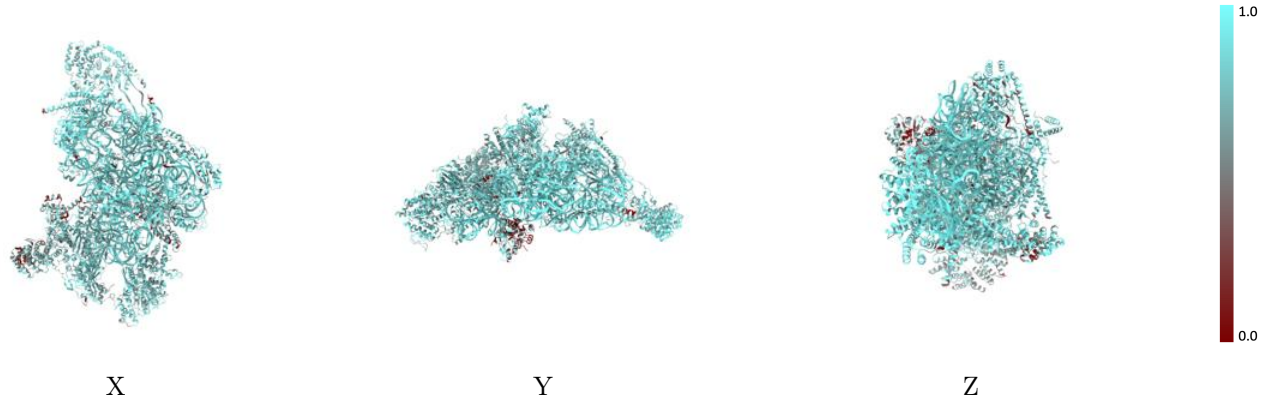
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



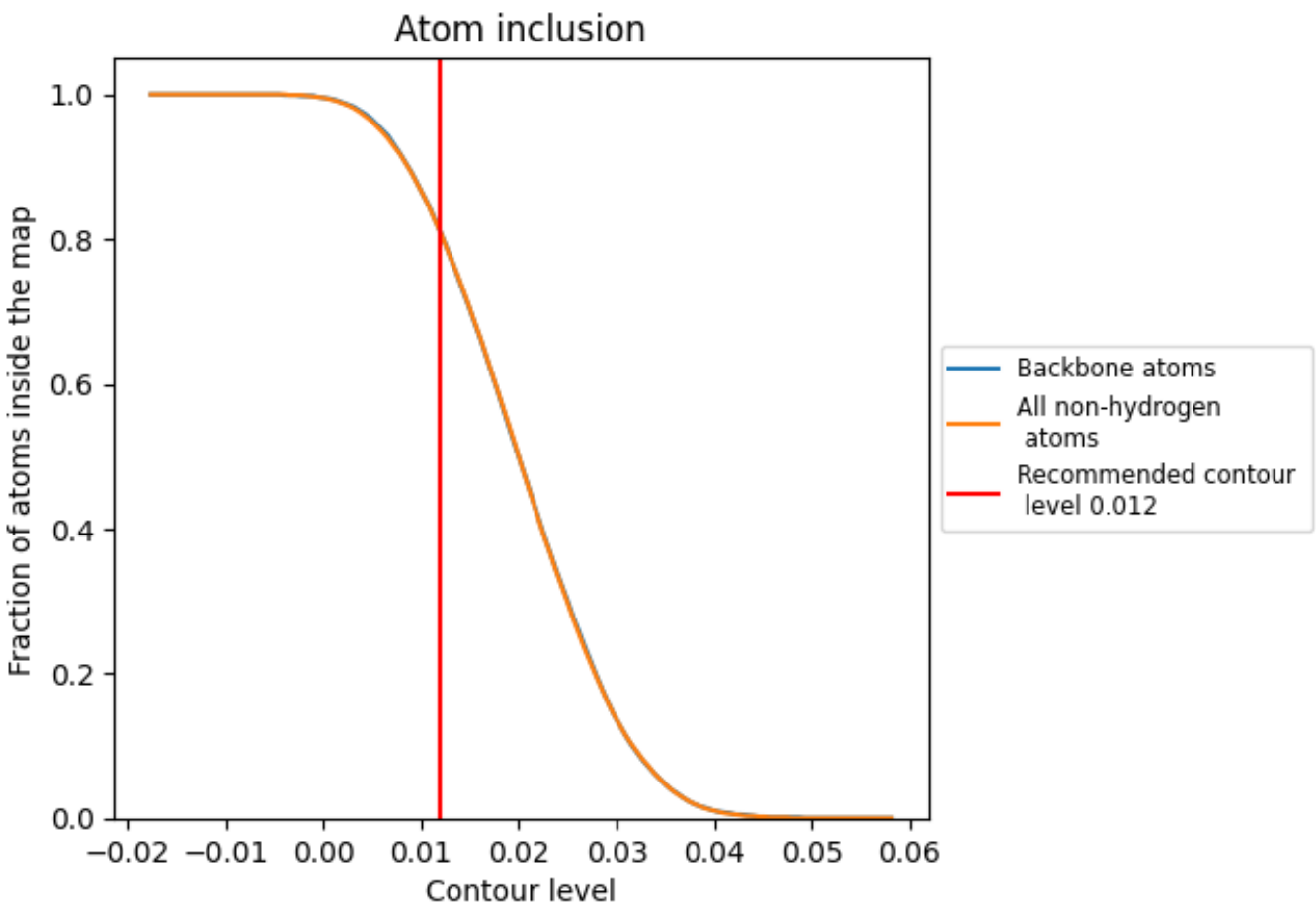
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.2770
0	0.7950	0.2330
1	0.7640	0.2340
2	0.5320	0.2330
3	0.7770	0.2700
4	0.6250	0.1530
A	0.9510	0.3420
B	0.8360	0.3560
C	0.7960	0.3520
D	0.7690	0.3390
E	0.7490	0.2410
F	0.7470	0.2530
G	0.7770	0.2690
H	0.7790	0.2930
I	0.8280	0.2720
J	0.8260	0.3590
K	0.8430	0.3030
L	0.7560	0.2380
M	0.8300	0.2910
N	0.8380	0.3400
O	0.8490	0.3110
P	0.8090	0.2990
Q	0.8020	0.3130
R	0.8500	0.2910
S	0.8240	0.3230
T	0.8310	0.3430
U	0.7770	0.2270
V	0.8260	0.1640
W	0.8550	0.3490
X	0.7730	0.1910
Y	0.7000	0.2080
Z	0.7760	0.2930
b	0.4220	0.0530