Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 01:51 am BST

PDB ID	:	7PNW / pdb_00007pnw
EMDB ID	:	EMD-13554
Title	:	Mouse mitochondrial ribosome small subunit lacking m5U modification
Authors	:	Itoh, Y.; Khawaja, A.; Laptev, I.; Sergiev, P.; Rorbach, J.; Amunts, A.
Deposited on	:	2021-09-08
Resolution	:	3.09 Å(reported)
Based on initial model	:	6RW4

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

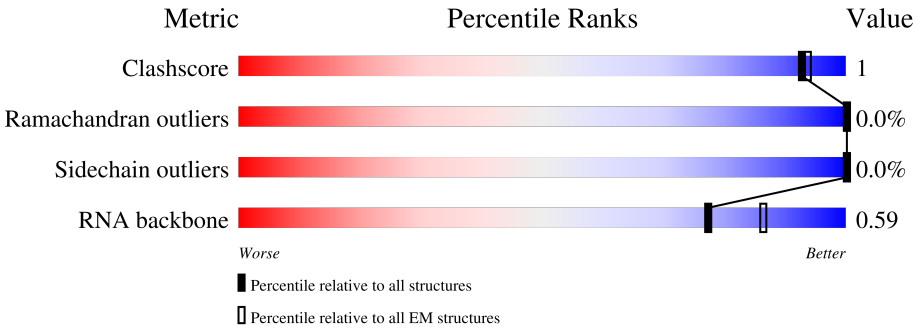
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

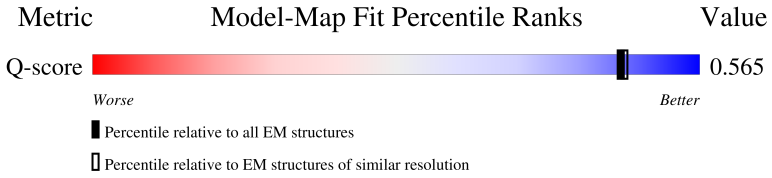
1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	81% 16%
2	B	291	74% 23%
3	C	167	77% 21%

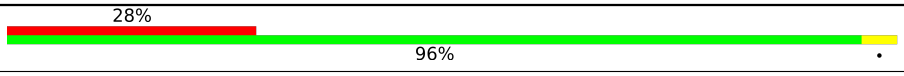
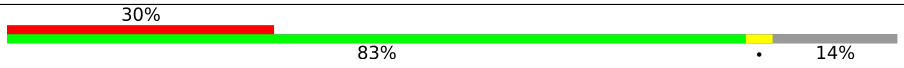
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Mol	Chain	Length	Quality of chain
4	D	432	6% 75% 22%
5	E	125	94%
6	F	242	5% 84% 14%
7	G	390	8% 80% 17%
8	H	160	81% 6% 12%
9	I	191	69% 28%
10	J	139	74% 22%
11	K	128	76% 21%
12	L	258	7% 67% 32%
13	M	135	8% 90% 7%
14	N	120	5% 92% 6%
15	O	254	76% 22%
16	P	143	63% 5% 32%
17	Q	86	94% 6%
18	R	359	79% 18%
19	S	177	6% 75% 23%
20	T	171	95% 5%
21	U	200	85% 13%
22	V	415	11% 86% 12%
23	W	186	51% 46%
24	X	391	7% 86% 5% 9%
25	Y	384	9% 38% 61%
26	Z	106	7% 95% 5%
27	0	218	5% 94% 6%
28	1	320	86% 13%

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Mol	Chain	Length	Quality of chain
29	2	117	
30	3	200	
31	4	685	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 125573 atoms, of which 57662 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	954	30524	9106	10255	3639	6570	954	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	339	5460	1698	2758	519	475	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	122	1986	617	1007	181	178	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
7	G	325	Total	C	H	N	O	S	0	0
			5304	1689	2630	480	491	14		

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

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

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

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

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
10	J	108	Total	C	H	N	O	S	0	0
			1749	528	903	172	141	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	117	Total	C	H	N	O	S	0	0
			1906	580	964	183	169	10		

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	72	Total	C	H	N	O	S	0	0
			1371	414	728	135	93	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	589	Total	C	H	N	O	S	0	0
			9558	3064	4800	800	872	22		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	54	Total	Mg	0
			54	54	
32	B	1	Total	Mg	0
			1	1	
32	X	1	Total	Mg	0
			1	1	
32	3	1	Total	Mg	0
			1	1	

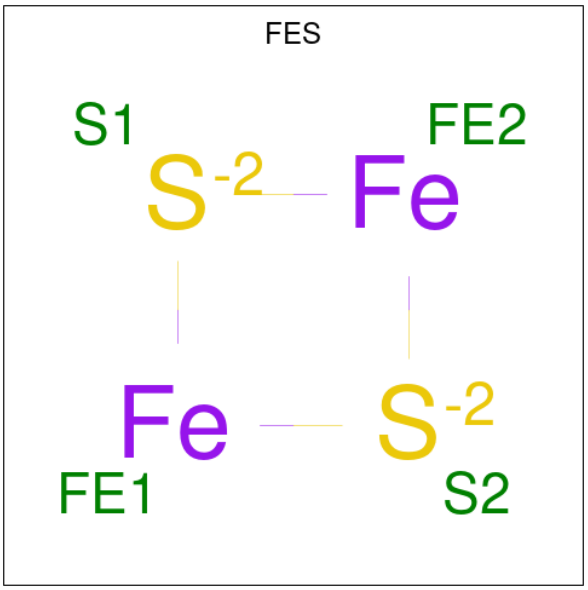
- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
33	A	10	Total K 10 10	0

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

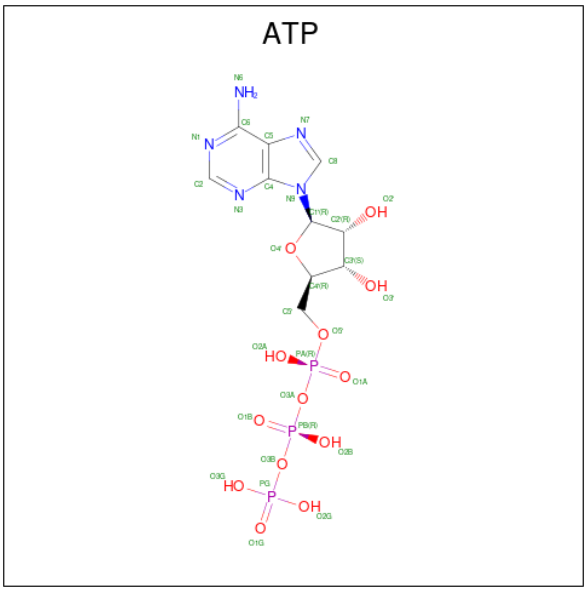
Mol	Chain	Residues	Atoms	AltConf
34	O	1	Total Zn 1 1	0

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	P	1	Total Fe S 4 2 2	0
35	T	1	Total Fe S 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
36	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	A	521	Total	O	0
			521	521	
37	B	18	Total	O	0
			18	18	
37	C	23	Total	O	0
			23	23	
37	D	40	Total	O	0
			40	40	
37	E	1	Total	O	0
			1	1	
37	F	4	Total	O	0
			4	4	
37	G	13	Total	O	0
			13	13	
37	H	20	Total	O	0
			20	20	
37	I	7	Total	O	0
			7	7	
37	J	5	Total	O	0
			5	5	
37	K	20	Total	O	0
			20	20	

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Mol	Chain	Residues	Atoms	AltConf
37	L	3	Total O 3 3	0
37	M	12	Total O 12 12	0
37	N	1	Total O 1 1	0
37	O	20	Total O 20 20	0
37	P	2	Total O 2 2	0
37	Q	5	Total O 5 5	0
37	R	5	Total O 5 5	0
37	S	4	Total O 4 4	0
37	T	6	Total O 6 6	0
37	U	3	Total O 3 3	0
37	W	3	Total O 3 3	0
37	X	5	Total O 5 5	0
37	Y	5	Total O 5 5	0
37	Z	11	Total O 11 11	0
37	0	4	Total O 4 4	0
37	1	12	Total O 12 12	0
37	2	4	Total O 4 4	0
37	3	5	Total O 5 5	0
37	4	1	Total O 1 1	0

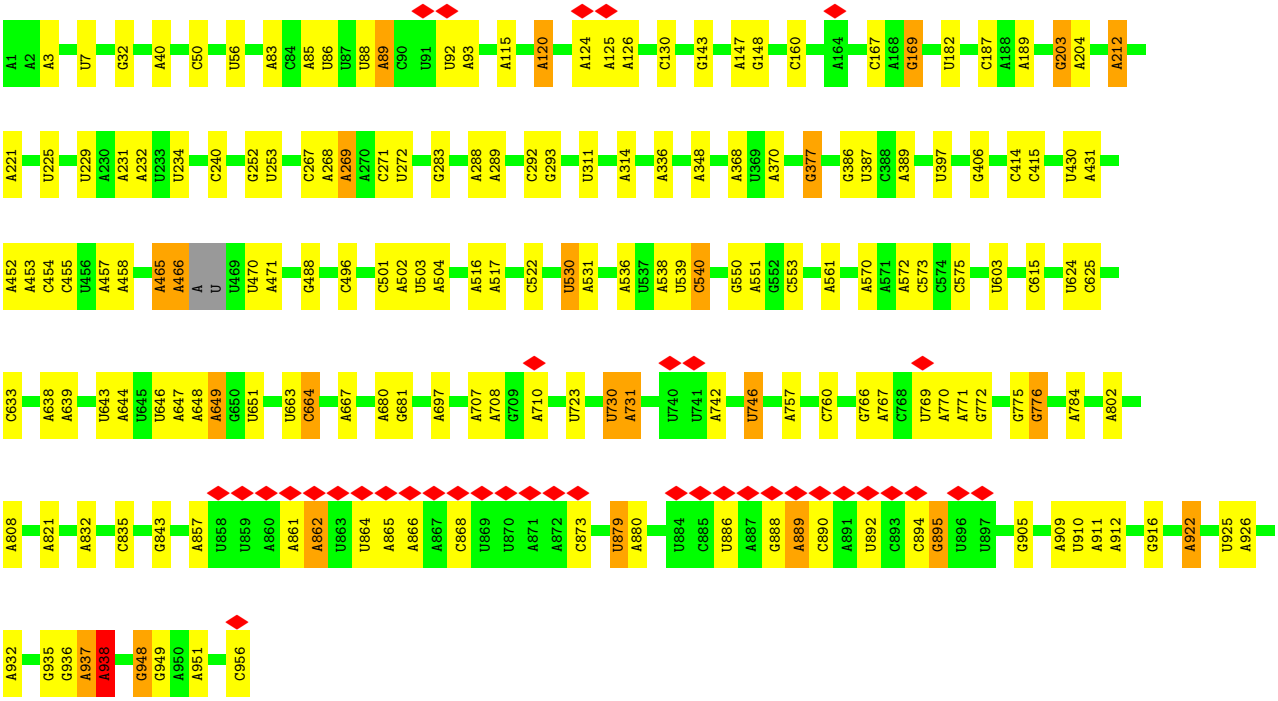
3 Residue-property plots (i)

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: 12S mitochondrial rRNA

Chain A:

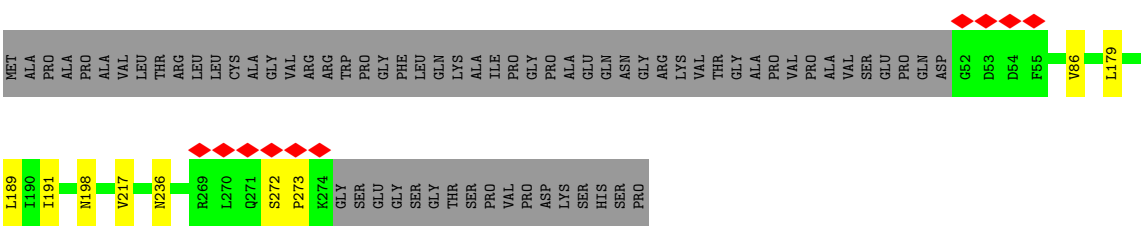




• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:





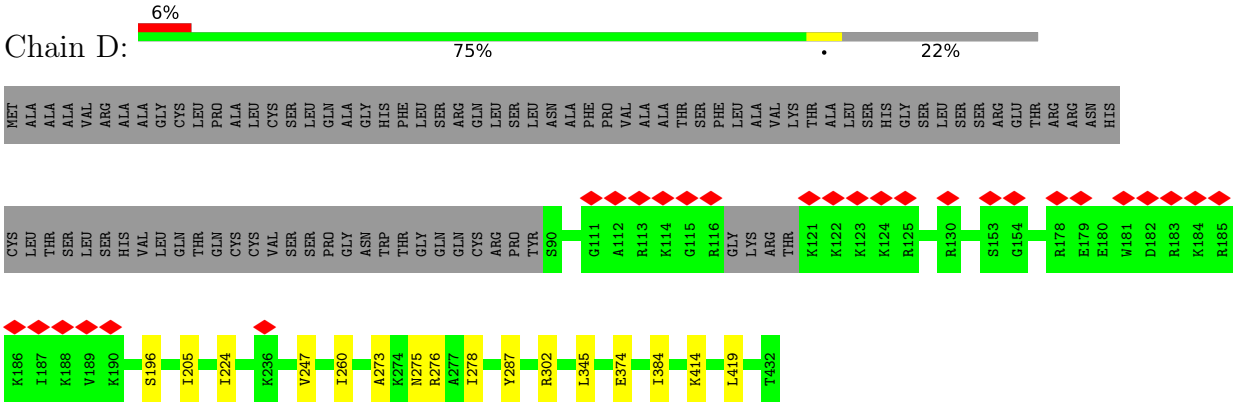
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



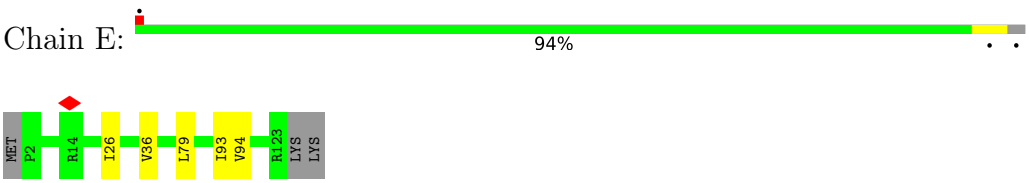
• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



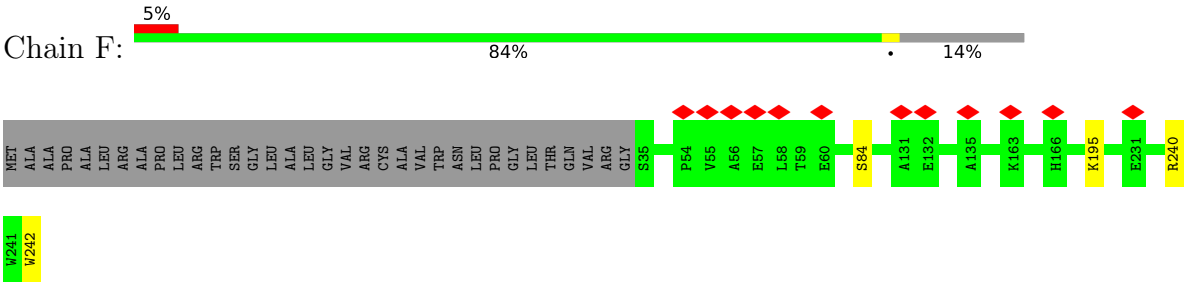
• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:



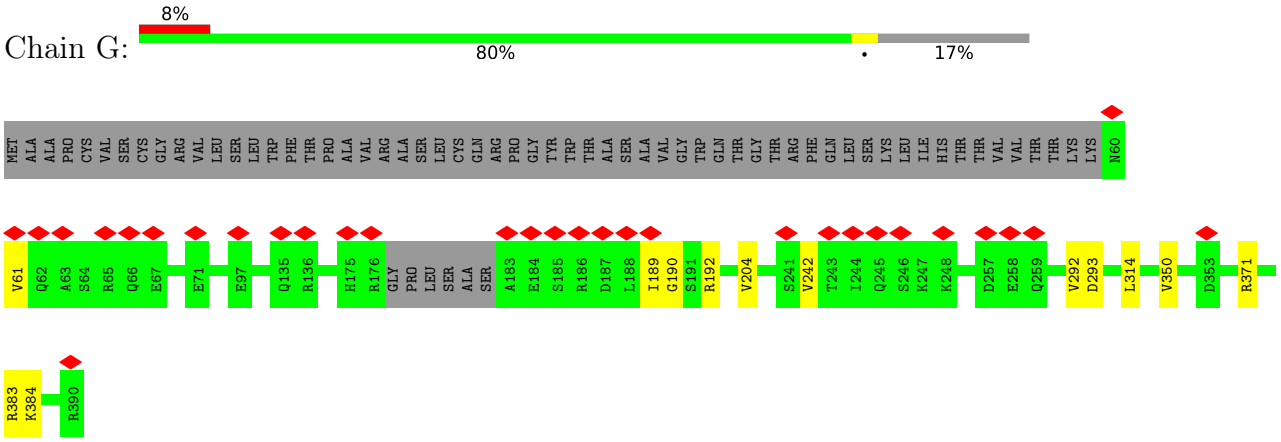
• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



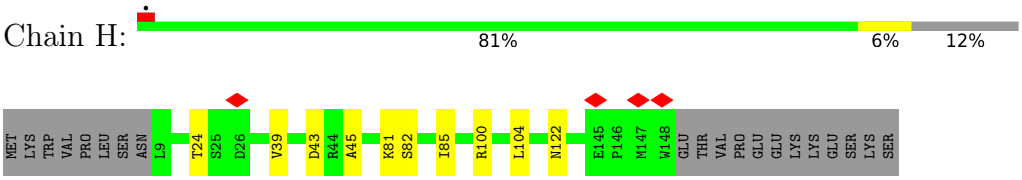
• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:



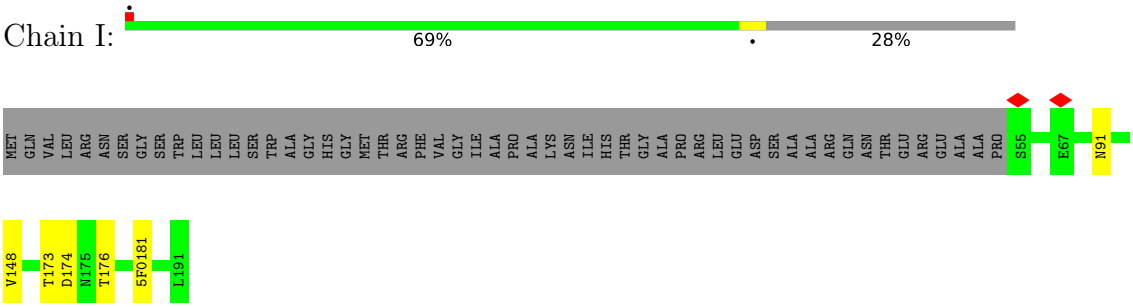
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



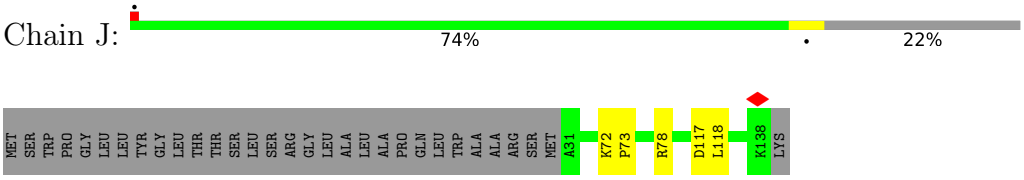
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



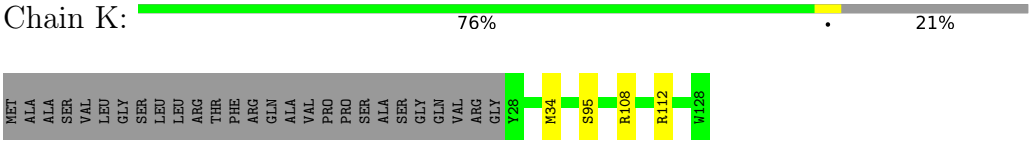
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



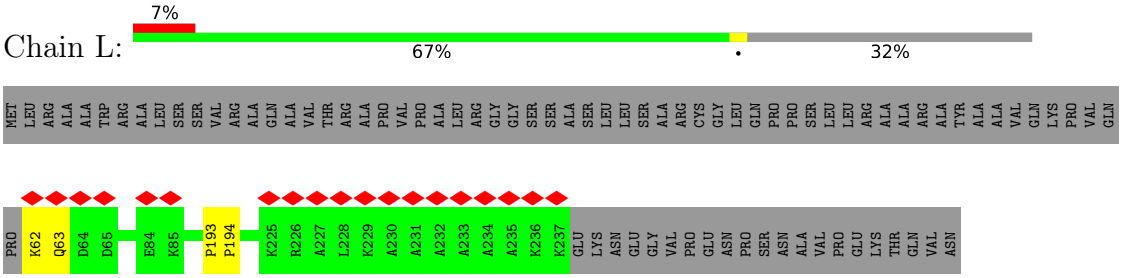
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



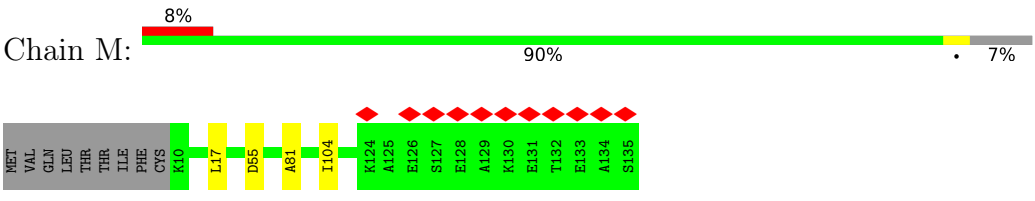
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



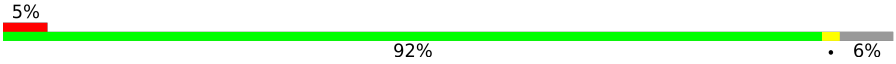
• Molecule 13: 28S ribosomal protein S16, mitochondrial

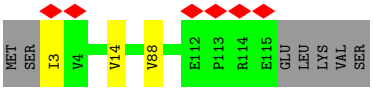
Chain M:



• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:

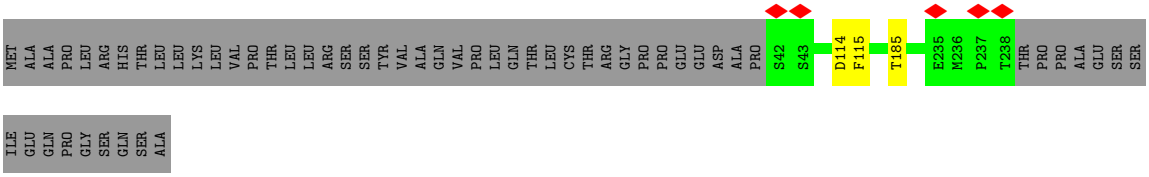




• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:

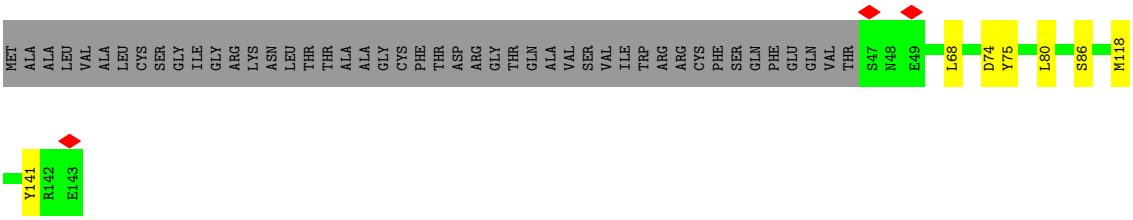




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

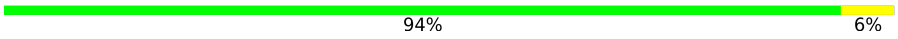
Chain P:

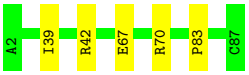




• Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain Q:

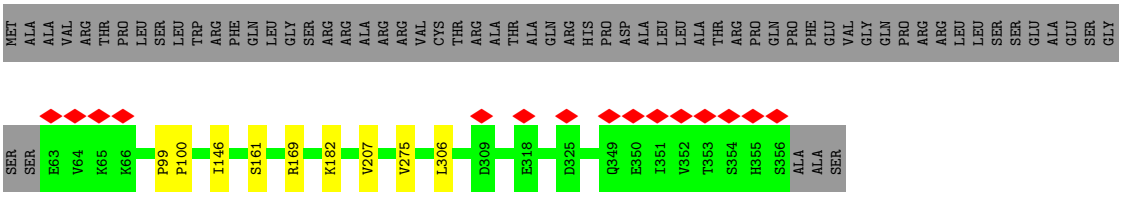




• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:

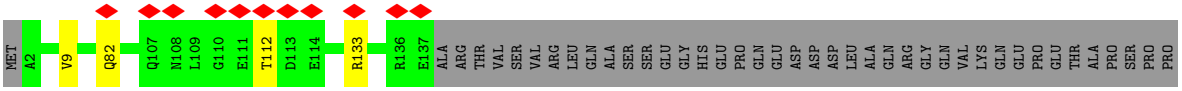




• Molecule 19: 28S ribosomal protein S23, mitochondrial

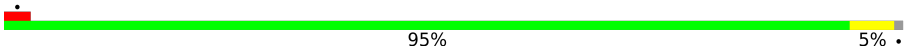
Chain S:

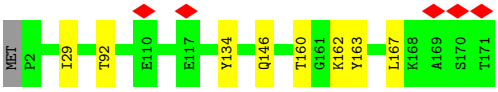




• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:

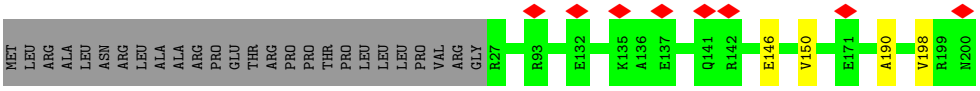




• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:

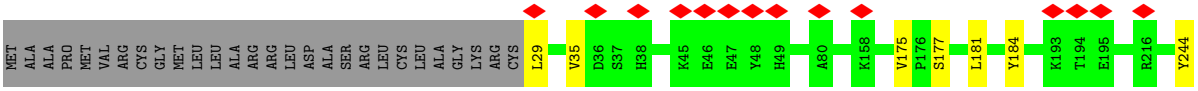


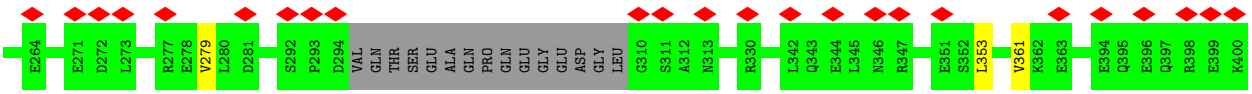


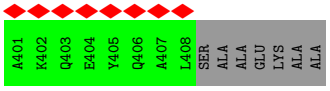
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:





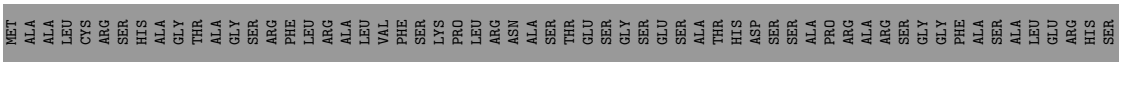


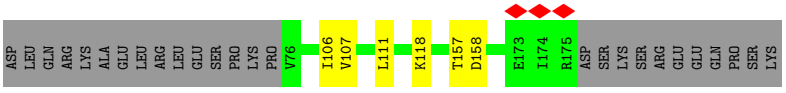


• Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W:



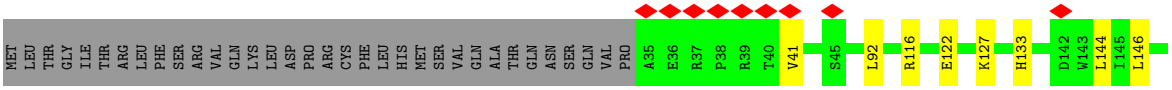


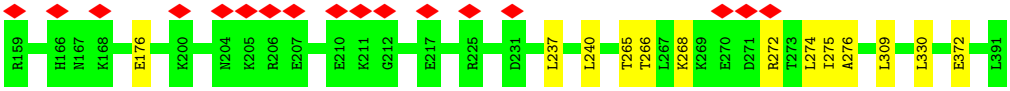


• Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain X:

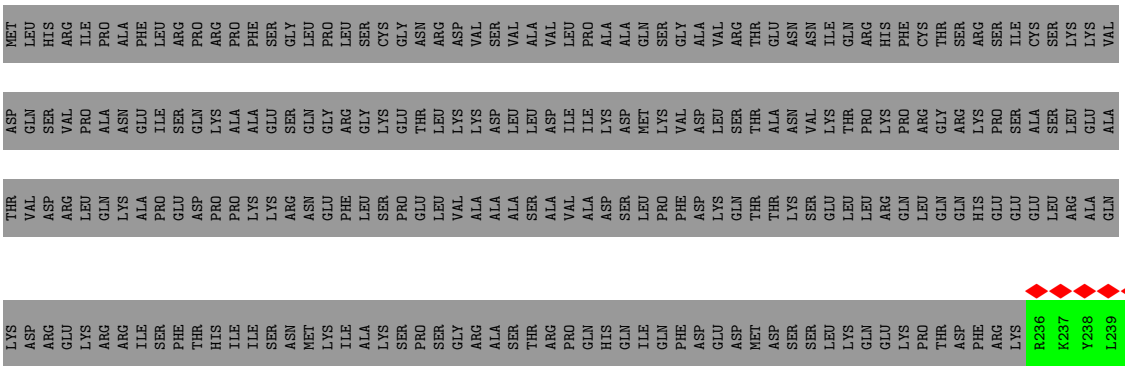




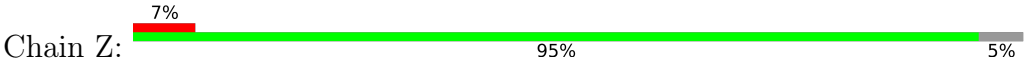


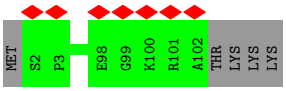
• Molecule 25: 28S ribosomal protein S31, mitochondrial



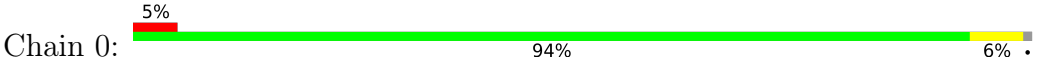


• Molecule 26: 28S ribosomal protein S33, mitochondrial



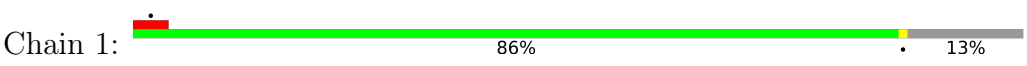


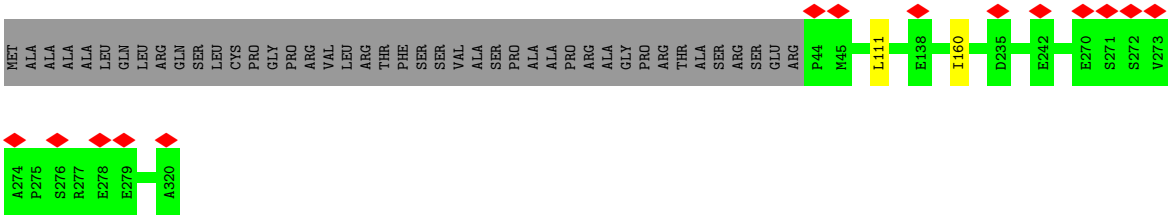
• Molecule 27: 28S ribosomal protein S34, mitochondrial





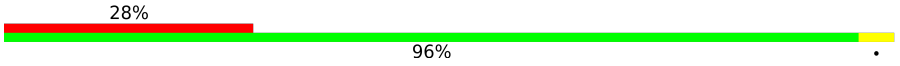
• Molecule 28: 28S ribosomal protein S35, mitochondrial

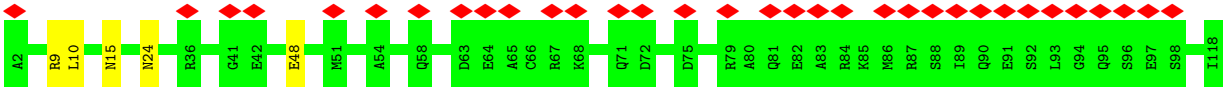




• Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain 2:

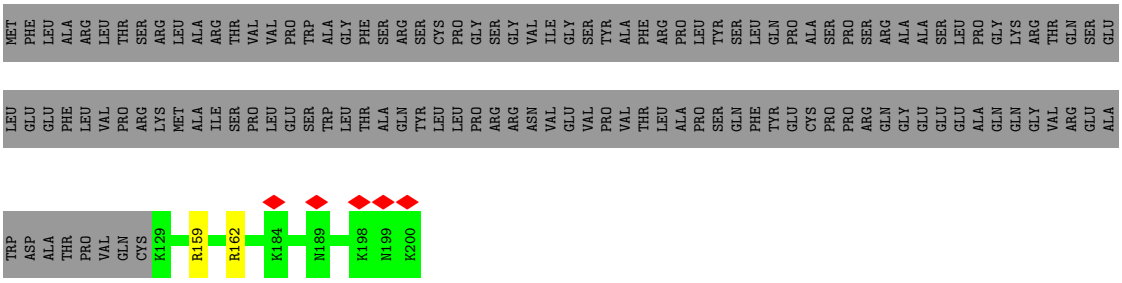




• Molecule 30: Aurora kinase A-interacting protein

Chain 3:

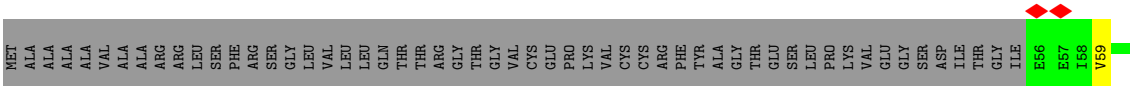


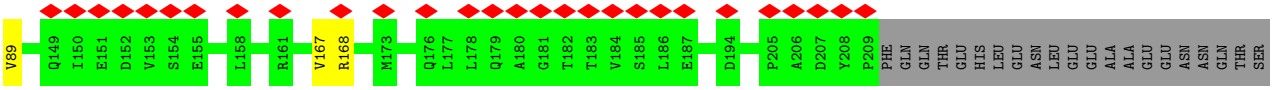


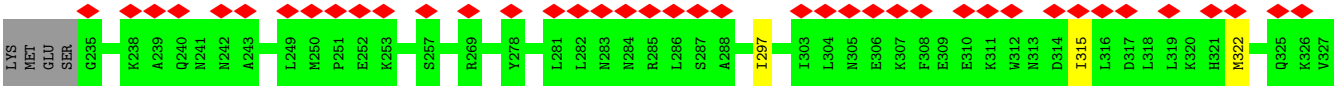
• Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

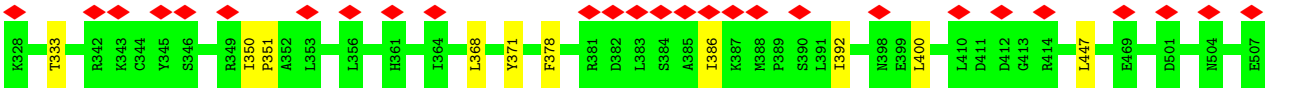
Chain 4:

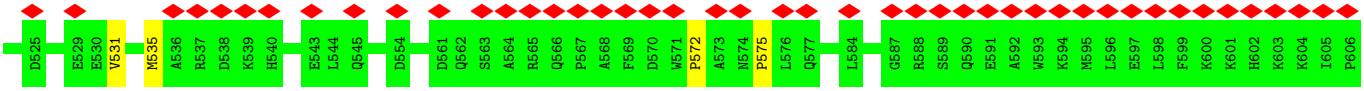


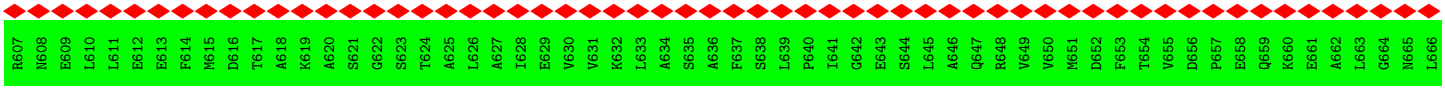


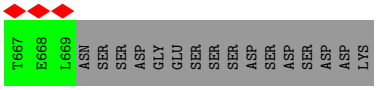












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44121	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	1.762	Depositor
Minimum map value	-0.939	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.14	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, MG, 5F0, 5MC, ATP, AYA, B8T, MA6, ZN, FES

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	0/22587	0.19	0/35152
2	B	0.13	0/1832	0.31	0/2479
3	C	0.13	0/1100	0.28	0/1485
4	D	0.13	0/2757	0.30	0/3696
5	E	0.12	0/997	0.32	0/1347
6	F	0.11	0/1763	0.29	0/2368
7	G	0.11	0/2734	0.30	0/3669
8	H	0.13	0/1179	0.28	0/1597
9	I	0.12	0/1018	0.31	0/1374
10	J	0.14	0/862	0.35	0/1155
11	K	0.15	0/871	0.35	0/1167
12	L	0.10	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	0.28	0/1085
17	Q	0.12	0/735	0.31	0/980
18	R	0.11	0/2449	0.27	0/3311
19	S	0.12	0/1148	0.29	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	0.27	0/3995
25	Y	0.10	0/1283	0.25	0/1730
26	Z	0.13	0/851	0.29	0/1133
27	0	0.12	0/1856	0.33	0/2511
28	1	0.10	0/2260	0.26	0/3063
29	2	0.10	0/949	0.28	0/1264
30	3	0.12	0/654	0.31	0/860
31	4	0.09	0/4868	0.25	0/6597
All	All	0.11	0/70330	0.26	0/99485

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	20269	10255	10242	52	0
2	B	1791	1799	1797	7	0
3	C	1072	1091	1087	3	0
4	D	2702	2758	2753	10	0
5	E	979	1007	1007	4	0
6	F	1722	1750	1748	3	0
7	G	2674	2630	2626	8	0
8	H	1153	1193	1190	7	0
9	I	1009	1038	1029	4	0
10	J	846	903	901	3	0
11	K	855	888	887	3	0
12	L	1465	1576	1574	2	0
13	M	995	1009	1006	3	0
14	N	888	951	947	3	0
15	O	1598	1548	1547	2	0
16	P	792	818	817	5	0
17	Q	732	750	750	4	0
18	R	2400	2416	2415	7	0
19	S	1124	1133	1132	3	0
20	T	1388	1413	1413	6	0
21	U	1449	1459	1456	2	0
22	V	2998	2972	2967	9	0
23	W	793	813	811	4	0
24	X	2881	2881	2879	14	0
25	Y	1246	1193	1191	2	0
26	Z	834	848	847	0	0
27	0	1811	1838	1834	8	0
28	1	2212	2228	2226	2	0
29	2	942	964	963	4	0
30	3	643	728	726	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	4758	4800	4793	12	0
32	3	1	0	0	0	0
32	A	54	0	0	0	0
32	B	1	0	0	0	0
32	X	1	0	0	0	0
33	A	10	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	0	0
35	T	4	0	0	0	0
36	X	31	12	12	0	0
37	0	4	0	0	0	0
37	1	12	0	0	0	0
37	2	4	0	0	0	0
37	3	5	0	0	0	0
37	4	1	0	0	0	0
37	A	521	0	0	7	0
37	B	18	0	0	0	0
37	C	23	0	0	0	0
37	D	40	0	0	2	0
37	E	1	0	0	0	0
37	F	4	0	0	0	0
37	G	13	0	0	0	0
37	H	20	0	0	0	0
37	I	7	0	0	0	0
37	J	5	0	0	0	0
37	K	20	0	0	0	0
37	L	3	0	0	0	0
37	M	12	0	0	0	0
37	N	1	0	0	0	0
37	O	20	0	0	0	0
37	P	2	0	0	0	0
37	Q	5	0	0	0	0
37	R	5	0	0	0	0
37	S	4	0	0	0	0
37	T	6	0	0	0	0
37	U	3	0	0	0	0
37	W	3	0	0	0	0
37	X	5	0	0	0	0
37	Y	5	0	0	0	0
37	Z	11	0	0	0	0
All	All	67911	57662	57573	169	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.

All (169) 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:370:A:OP2	29:2:9:ARG:NH2	2.09	0.85
29:2:10:LEU:O	29:2:15:ASN:ND2	2.14	0.80
1:A:862:A:N6	1:A:895:G:O6	2.23	0.71
6:F:84:SER:OG	24:X:372:GLU:OE2	2.07	0.71
1:A:647:A:OP1	2:B:198:ASN:ND2	2.24	0.70
1:A:272:U:OP2	37:A:1101:HOH:O	2.12	0.67
1:A:453:A:OP2	37:A:1102:HOH:O	2.13	0.66
22:V:279:VAL:HG23	22:V:353:LEU:HD11	1.79	0.65
20:T:92:THR:HG22	20:T:92:THR:O	1.99	0.62
1:A:551:A:HO2'	1:A:771:A:HO2'	1.47	0.61
5:E:79:LEU:HG	5:E:93:ILE:HD12	1.83	0.61
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.33	0.61
13:M:104:ILE:HG23	18:R:146:ILE:HG12	1.82	0.60
1:A:723:U:OP1	6:F:195:LYS:NZ	2.34	0.60
1:A:746:U:O2'	1:A:802:A:N6	2.35	0.60
14:N:3:ILE:HG22	14:N:3:ILE:O	2.03	0.58
22:V:279:VAL:CG2	22:V:353:LEU:HD11	2.33	0.58
24:X:268:LYS:HG2	24:X:274:LEU:HD23	1.86	0.58
1:A:550:G:N2	1:A:772:G:O2'	2.37	0.57
1:A:240:C:O2'	1:A:252:G:N2	2.37	0.57
5:E:94:VAL:CG1	16:P:118:MET:HE1	2.35	0.57
7:G:204:VAL:HG12	7:G:204:VAL:O	2.04	0.56
22:V:29:LEU:HD12	22:V:181:LEU:HD23	1.86	0.56
1:A:267:C:O2'	1:A:271:C:OP1	2.21	0.56
6:F:240:ARG:NH2	6:F:242:TRP:O	2.39	0.56
4:D:276:ARG:NH1	37:D:502:HOH:O	2.36	0.56
8:H:81:LYS:O	11:K:112:ARG:NH1	2.37	0.56
3:C:119:ILE:HB	3:C:153:LEU:HD12	1.88	0.55
1:A:808:A:OP2	7:G:371:ARG:NH2	2.39	0.55
17:Q:67:GLU:OE2	17:Q:70:ARG:NH1	2.40	0.54
24:X:176:GLU:N	24:X:176:GLU:OE2	2.41	0.54
22:V:35:VAL:HG12	22:V:35:VAL:O	2.08	0.54
1:A:503:U:O4'	30:3:159:ARG:NH2	2.40	0.54
1:A:888:G:O2'	1:A:889:A:O4'	2.25	0.54
7:G:383:ARG:NH2	7:G:384:LYS:O	2.41	0.54
24:X:122:GLU:O	24:X:127:LYS:NZ	2.41	0.54
9:I:148:VAL:HG13	9:I:148:VAL:O	2.07	0.52
24:X:275:ILE:HG22	24:X:276:ALA:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:C:O2'	1:A:649:A:N1	2.39	0.51
1:A:951:A:OP2	29:2:24:ASN:ND2	2.44	0.51
1:A:386:G:N2	1:A:387:U:O4	2.44	0.51
5:E:94:VAL:HG11	16:P:118:MET:HE1	1.91	0.51
29:2:48:GLU:N	29:2:48:GLU:OE1	2.43	0.51
1:A:377:G:OP2	37:A:1104:HOH:O	2.20	0.51
2:B:86:VAL:HG12	2:B:86:VAL:O	2.10	0.51
1:A:212:A:N7	1:A:269:A:O2'	2.41	0.50
1:A:336:A:OP1	9:I:91:ASN:ND2	2.42	0.50
1:A:746:U:HO2'	1:A:802:A:N6	2.10	0.50
4:D:205:ILE:HG21	4:D:224:ILE:HD11	1.93	0.50
27:0:54:ALA:O	27:0:58:VAL:HG23	2.12	0.50
1:A:651:U:O2'	2:B:179:LEU:HD23	2.12	0.50
1:A:766:G:OP1	24:X:272:ARG:NH2	2.43	0.50
31:4:531:VAL:HG12	31:4:535:MET:HE2	1.94	0.50
24:X:41:VAL:HG12	24:X:41:VAL:O	2.11	0.49
24:X:146:LEU:HD21	24:X:237:LEU:HD22	1.95	0.48
2:B:272:SER:HB3	2:B:273:PRO:HD3	1.94	0.48
31:4:386:ILE:O	31:4:386:ILE:HG22	2.14	0.48
7:G:292:VAL:HG12	7:G:293:ASP:N	2.29	0.48
16:P:74:ASP:OD1	16:P:75:TYR:N	2.47	0.48
18:R:161:SER:O	18:R:169:ARG:NH1	2.44	0.48
1:A:540:C:O2'	1:A:821:A:N1	2.47	0.48
16:P:86:SER:HG	16:P:141:TYR:HH	1.60	0.48
2:B:236:ASN:OD1	23:W:118:LYS:NZ	2.47	0.48
14:N:88:VAL:HG13	14:N:88:VAL:O	2.14	0.48
24:X:144:LEU:CD2	24:X:240:LEU:HD22	2.44	0.47
24:X:116:ARG:NH2	24:X:330:LEU:O	2.47	0.47
4:D:302:ARG:NH1	37:D:504:HOH:O	2.38	0.47
25:Y:304:VAL:HG13	28:1:160:ILE:HD11	1.95	0.47
1:A:561:A:O2'	1:A:707:A:N1	2.48	0.47
10:J:72:LYS:CG	10:J:73:PRO:HA	2.45	0.47
31:4:59:VAL:O	31:4:59:VAL:HG23	2.14	0.47
1:A:948:G:OP1	37:A:1105:HOH:O	2.21	0.46
20:T:160:THR:HG22	20:T:162:LYS:H	1.81	0.46
10:J:78:ARG:NE	10:J:117:ASP:OD2	2.49	0.46
1:A:225:U:O2'	1:A:232:A:N1	2.45	0.46
1:A:160:C:OP1	27:0:19:ARG:NH2	2.49	0.46
11:K:34:MET:HE3	11:K:95:SER:HB2	1.98	0.46
18:R:275:VAL:HG11	18:R:306:LEU:HD12	1.98	0.46
19:S:9:VAL:O	19:S:9:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:368:LEU:HD12	31:4:447:LEU:HD13	1.99	0.45
1:A:730:U:H2'	1:A:731:A:O4'	2.15	0.45
7:G:314:LEU:HD13	7:G:350:VAL:HG11	1.97	0.45
1:A:406:G:H4'	1:A:932:A:H4'	1.99	0.45
2:B:191:ILE:HA	2:B:217:VAL:O	2.17	0.45
4:D:275:ASN:O	4:D:278:ILE:HG22	2.17	0.45
22:V:29:LEU:HD11	22:V:184:TYR:CG	2.53	0.44
7:G:192:ARG:HG2	7:G:242:VAL:HG22	1.99	0.44
4:D:414:LYS:HG3	4:D:419:LEU:HD22	2.00	0.44
8:H:104:LEU:HD12	8:H:104:LEU:N	2.32	0.44
24:X:266:THR:HG23	24:X:309:LEU:HD13	1.99	0.44
8:H:39:VAL:HG22	8:H:100:ARG:O	2.17	0.44
22:V:175:VAL:HG12	22:V:177:SER:H	1.83	0.44
3:C:136:VAL:HG22	3:C:153:LEU:HD23	2.00	0.44
27:0:71:LEU:HD11	27:0:141:LEU:HD22	1.98	0.44
12:L:62:LYS:HG2	12:L:63:GLN:H	1.82	0.44
21:U:146:GLU:O	21:U:150:VAL:HG23	2.17	0.44
23:W:106:ILE:HG23	23:W:111:LEU:HD23	1.99	0.44
3:C:87:LEU:HD13	3:C:87:LEU:O	2.17	0.44
23:W:157:THR:HG22	23:W:158:ASP:N	2.33	0.44
25:Y:282:PRO:HB2	31:4:89:VAL:CG1	2.48	0.44
7:G:61:VAL:HG13	7:G:61:VAL:O	2.17	0.43
1:A:120:A:OP1	1:A:130:C:O2'	2.30	0.43
24:X:92:LEU:HD21	24:X:133:HIS:HB2	2.00	0.43
17:Q:42:ARG:O	17:Q:42:ARG:HG3	2.17	0.43
12:L:193:PRO:HA	12:L:194:PRO:HD3	1.95	0.43
14:N:14:VAL:HG23	20:T:29:ILE:HD13	1.99	0.43
9:I:173:THR:HG22	9:I:174:ASP:N	2.34	0.43
27:0:37:ASP:O	27:0:41:LEU:N	2.52	0.43
1:A:147:A:OP2	20:T:134:TYR:OH	2.35	0.43
4:D:374:GLU:N	4:D:384:ILE:O	2.46	0.43
15:O:114:ASP:OD1	15:O:115:PHE:N	2.52	0.43
27:0:103:ASP:N	27:0:111:HIS:O	2.49	0.43
7:G:189:ILE:HG22	7:G:190:GLY:N	2.34	0.43
20:T:163:TYR:CE2	20:T:167:LEU:HD11	2.54	0.43
1:A:221:A:N1	1:A:268:A:O2'	2.51	0.42
15:O:185:THR:OG1	18:R:182:LYS:NZ	2.41	0.42
16:P:68:LEU:HD21	16:P:80:LEU:HD11	2.01	0.42
1:A:465:A:O2'	1:A:466:A:O5'	2.35	0.42
8:H:82:SER:O	11:K:108:ARG:NH2	2.52	0.42
5:E:26:ILE:HG23	5:E:36:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:THR:O	8:H:24:THR:HG23	2.19	0.42
1:A:229:U:OP1	4:D:196:SER:OG	2.31	0.42
1:A:663:U:H3'	1:A:664:C:H5'	2.00	0.42
27:0:41:LEU:HD22	27:0:58:VAL:HG11	2.02	0.42
1:A:88:U:H2'	1:A:89:A:O4'	2.20	0.42
1:A:457:A:H4'	1:A:458:A:OP2	2.19	0.42
1:A:926:A:OP2	37:A:1106:HOH:O	2.21	0.42
21:U:190:ALA:O	21:U:198:VAL:N	2.52	0.42
31:4:167:VAL:HG23	31:4:168:ARG:N	2.35	0.42
1:A:775:G:H5"	1:A:776:G:OP1	2.20	0.42
1:A:879:U:H2'	27:0:99:ARG:HD3	2.02	0.42
19:S:112:THR:HG22	19:S:112:THR:O	2.20	0.41
1:A:730:U:O4'	1:A:730:U:OP2	2.37	0.41
4:D:247:VAL:HG22	4:D:273:ALA:HB1	2.01	0.41
1:A:50:C:O2'	1:A:203:G:N7	2.44	0.41
19:S:82:GLN:OE1	19:S:133:ARG:NH2	2.53	0.41
22:V:29:LEU:HD11	22:V:184:TYR:CD2	2.55	0.41
8:H:122:ASN:HB3	28:1:111:LEU:HD11	2.03	0.41
1:A:530:U:O2'	1:A:922:A:N7	2.40	0.41
1:A:937:MA6:H93	1:A:938:MA6:N6	2.36	0.41
1:A:909:A:H2'	1:A:910:U:O4'	2.20	0.41
10:J:117:ASP:OD1	10:J:118:LEU:N	2.54	0.41
31:4:350:ILE:HB	31:4:351:PRO:HD3	2.02	0.41
18:R:207:VAL:O	18:R:207:VAL:HG12	2.21	0.41
22:V:244:TYR:CD1	22:V:244:TYR:C	2.99	0.41
1:A:496:C:OP1	30:3:162:ARG:NH1	2.43	0.41
4:D:287:TYR:OH	4:D:374:GLU:OE2	2.36	0.41
24:X:265:THR:OG1	24:X:275:ILE:O	2.39	0.41
1:A:169:G:O2'	1:A:204:A:OP1	2.39	0.41
1:A:414:C:H2'	1:A:415:C:O4'	2.21	0.41
13:M:17:LEU:HD23	13:M:81:ALA:HB2	2.03	0.41
17:Q:83:PRO:HA	23:W:107:VAL:HG21	2.02	0.41
18:R:99:PRO:HA	18:R:100:PRO:HD3	1.98	0.41
4:D:260:ILE:HD11	4:D:345:LEU:HD13	2.03	0.41
18:R:207:VAL:O	18:R:207:VAL:CG1	2.69	0.41
31:4:322:MET:HE1	31:4:333:THR:HG21	2.03	0.41
8:H:43:ASP:OD1	8:H:45:ALA:N	2.52	0.40
31:4:378:PHE:CD2	31:4:392:ILE:HD12	2.56	0.40
22:V:29:LEU:HD13	22:V:361:VAL:HG11	2.02	0.40
24:X:275:ILE:HG22	24:X:276:ALA:H	1.86	0.40
27:0:110:ASP:OD1	27:0:110:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:A:OP1	37:A:1107:HOH:O	2.22	0.40
2:B:189:LEU:HD11	2:B:217:VAL:HG23	2.03	0.40
31:4:297:ILE:HG23	31:4:315:ILE:HG23	2.03	0.40
31:4:572:PRO:HB2	31:4:575:PRO:HD2	2.02	0.40
1:A:935:G:H2'	1:A:937:MA6:OP2	2.22	0.40
1:A:516:A:O2'	37:A:1103:HOH:O	2.19	0.40
9:I:176:THR:HG21	17:Q:39:ILE:HD13	2.02	0.40
31:4:371:TYR:CE2	31:4:400:LEU:HD21	2.57	0.40

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%)	219 (99%)	2 (1%)	0	100	100
3	C	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
4	D	335/432 (78%)	331 (99%)	4 (1%)	0	100	100
5	E	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
6	F	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
7	G	321/390 (82%)	316 (98%)	5 (2%)	0	100	100
8	H	138/160 (86%)	134 (97%)	3 (2%)	1 (1%)	18	49
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	195/254 (77%)	192 (98%)	3 (2%)	0	100	100
16	P	95/143 (66%)	94 (99%)	1 (1%)	0	100	100
17	Q	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
18	R	292/359 (81%)	284 (97%)	8 (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%)	170 (99%)	2 (1%)	0	100	100
22	V	361/415 (87%)	355 (98%)	6 (2%)	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%)	210 (98%)	4 (2%)	0	100	100
28	1	275/320 (86%)	273 (99%)	2 (1%)	0	100	100
29	2	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
30	3	70/200 (35%)	70 (100%)	0	0	100	100
31	4	585/685 (85%)	580 (99%)	5 (1%)	0	100	100
All	All	5678/7190 (79%)	5594 (98%)	83 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	113/139 (81%)	113 (100%)	0	100	100
4	D	279/354 (79%)	279 (100%)	0	100	100
5	E	107/110 (97%)	107 (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
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	85
28	1	247/279 (88%)	247 (100%)	0	100	100
29	2	103/103 (100%)	103 (100%)	0	100	100
30	3	68/176 (39%)	68 (100%)	0	100	100
31	4	519/599 (87%)	519 (100%)	0	100	100
All	All	5029/6212 (81%)	5028 (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. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	HIS
3	C	81	HIS
4	D	177	GLN
4	D	229	ASN
4	D	353	HIS
5	E	100	GLN
7	G	87	HIS
7	G	156	GLN
7	G	288	HIS
7	G	378	GLN
8	H	42	HIS
8	H	84	HIS
9	I	84	HIS
9	I	95	GLN
10	J	105	HIS
11	K	124	GLN
12	L	119	ASN
12	L	196	HIS
12	L	219	GLN
13	M	61	HIS
13	M	75	HIS
14	N	9	HIS
14	N	57	GLN
15	O	63	HIS
16	P	96	HIS
17	Q	53	GLN
18	R	95	GLN
18	R	109	GLN
19	S	91	ASN
22	V	156	ASN
22	V	224	GLN
23	W	105	HIS
24	X	136	HIS
24	X	228	ASN
25	Y	370	ASN
25	Y	379	ASN
26	Z	54	ASN
27	0	111	HIS

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Mol	Chain	Res	Type
27	0	137	HIS
28	1	182	HIS
30	3	142	HIS
31	4	190	ASN
31	4	372	HIS
31	4	376	HIS
31	4	521	HIS
31	4	577	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	952/956 (99%)	125 (13%)	0

All (125) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	7	U
1	A	32	G
1	A	40	A
1	A	56	U
1	A	83	A
1	A	85	A
1	A	86	U
1	A	89	A
1	A	92	U
1	A	93	A
1	A	115	A
1	A	120	A
1	A	124	A
1	A	125	A
1	A	126	A
1	A	143	G
1	A	148	G
1	A	167	C
1	A	169	G
1	A	182	U
1	A	187	C
1	A	203	G
1	A	212	A

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Mol	Chain	Res	Type
1	A	231	A
1	A	234	U
1	A	253	U
1	A	269	A
1	A	283	G
1	A	288	A
1	A	289	A
1	A	292	C
1	A	293	G
1	A	311	U
1	A	314	A
1	A	348	A
1	A	368	A
1	A	377	G
1	A	389	A
1	A	397	U
1	A	430	U
1	A	431	A
1	A	452	A
1	A	454	C
1	A	455	C
1	A	465	A
1	A	466	A
1	A	470	U
1	A	471	A
1	A	488	G
1	A	501	C
1	A	502	A
1	A	504	A
1	A	517	A
1	A	522	C
1	A	530	U
1	A	531	A
1	A	536	A
1	A	538	A
1	A	539	U
1	A	540	C
1	A	553	C
1	A	570	A
1	A	572	A
1	A	573	C
1	A	575	C

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Mol	Chain	Res	Type
1	A	603	U
1	A	615	C
1	A	624	U
1	A	625	C
1	A	638	A
1	A	639	A
1	A	643	U
1	A	644	A
1	A	646	U
1	A	648	A
1	A	649	A
1	A	664	C
1	A	667	A
1	A	680	A
1	A	681	G
1	A	697	A
1	A	708	A
1	A	710	A
1	A	730	U
1	A	731	A
1	A	742	A
1	A	746	U
1	A	757	A
1	A	760	C
1	A	767	A
1	A	769	U
1	A	770	A
1	A	776	G
1	A	784	A
1	A	832	A
1	A	835	C
1	A	843	G
1	A	857	A
1	A	861	A
1	A	862	A
1	A	864	U
1	A	865	A
1	A	866	A
1	A	868	C
1	A	873	C
1	A	879	U
1	A	880	A

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Mol	Chain	Res	Type
1	A	886	U
1	A	889	A
1	A	890	C
1	A	892	U
1	A	894	C
1	A	895	G
1	A	905	G
1	A	911	A
1	A	912	A
1	A	916	G
1	A	922	A
1	A	925	U
1	A	936	G
1	A	938	MA6
1	A	948	G
1	A	949	G
1	A	956	C

There are no RNA pucker outliers to report.

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

7 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	$\#\|Z\| > 2$
17	AYA	Q	2	17	6,7,8	0.76	0	5,8,10	0.52	0
1	MA6	A	937	1	23,26,27	0.31	0	34,38,41	0.57	1 (2%)
1	MA6	A	938	1	23,26,27	0.30	0	34,38,41	0.57	1 (2%)
29	AYA	2	2	29	6,7,8	0.80	0	5,8,10	0.54	0
1	B8T	A	840	1	19,22,23	0.31	0	26,31,34	0.33	0
1	5MC	A	842	1	18,22,23	0.32	0	26,32,35	0.44	0
9	5F0	I	181	9	8,8,9	0.57	0	7,9,11	1.07	1 (14%)

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

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	-2.46	118.25	125.43
1	A	938	MA6	C2-N1-C6	2.35	117.29	111.75
1	A	937	MA6	C2-N1-C6	2.34	117.28	111.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	938	MA6	C4'-C5'-O5'-P
1	A	840	B8T	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	937	MA6	2	0
1	A	938	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 71 ligands modelled in this entry, 68 are monoatomic - leaving 3 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	T	201	13,20	0,4,4	-	-	-		
36	ATP	X	401	32	29,33,33	0.50	0	44,52,52	0.51	0
35	FES	P	201	16,5	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	ATP	X	401	32	-	0/22/38/38	0/3/3/3
35	FES	P	201	16,5	-	-	0/1/1/1
35	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.

There are no torsion outliers.

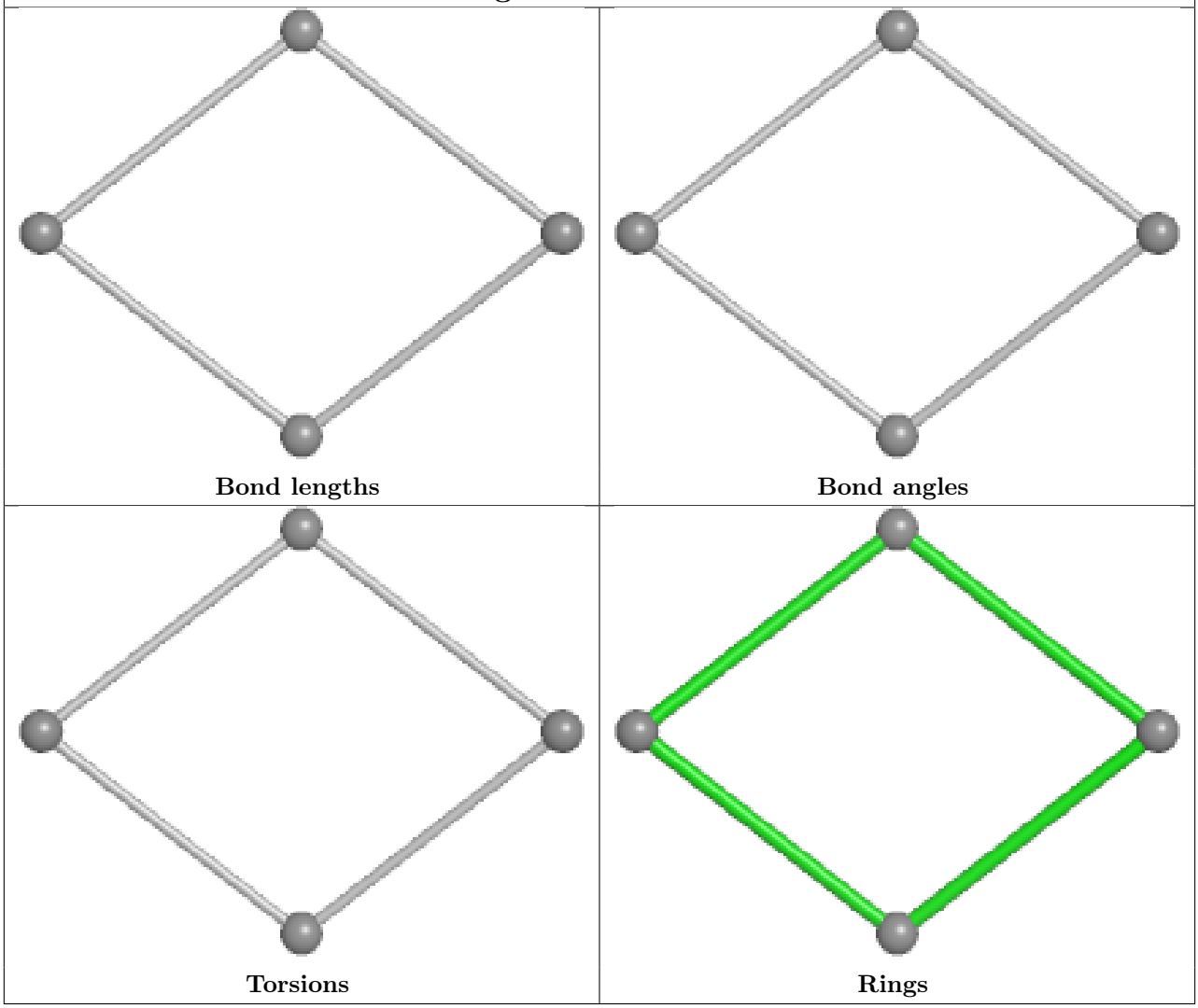
There are no ring outliers.

No monomer is involved in short contacts.

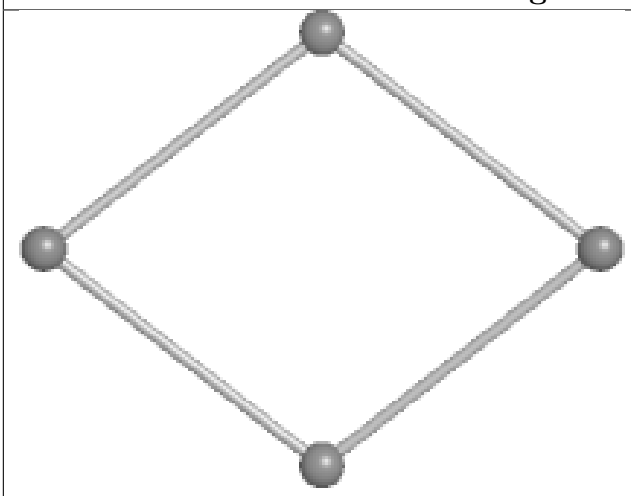
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

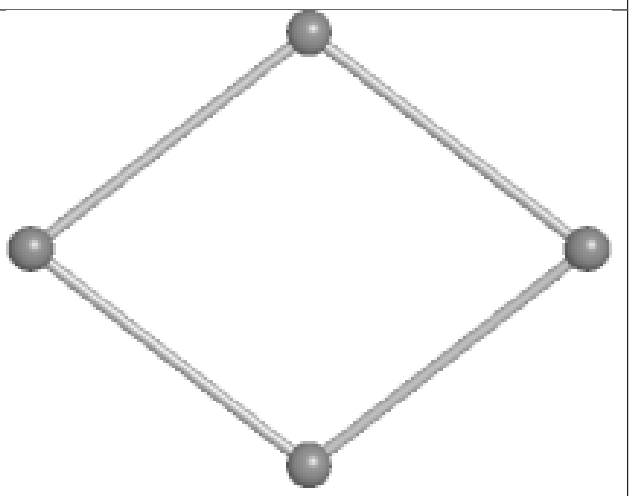
Ligand FES T 201



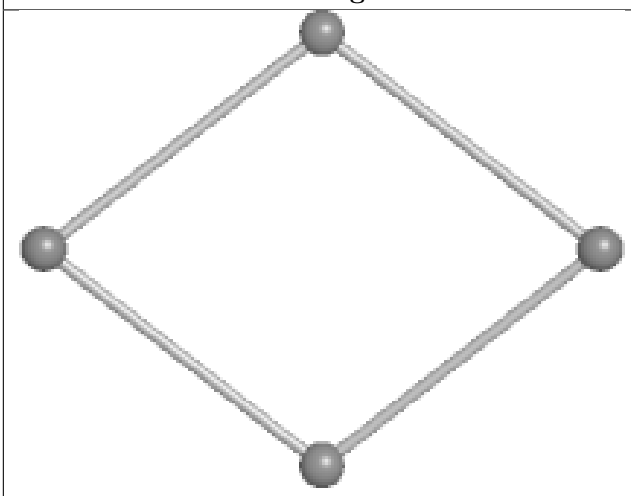
Ligand FES P 201



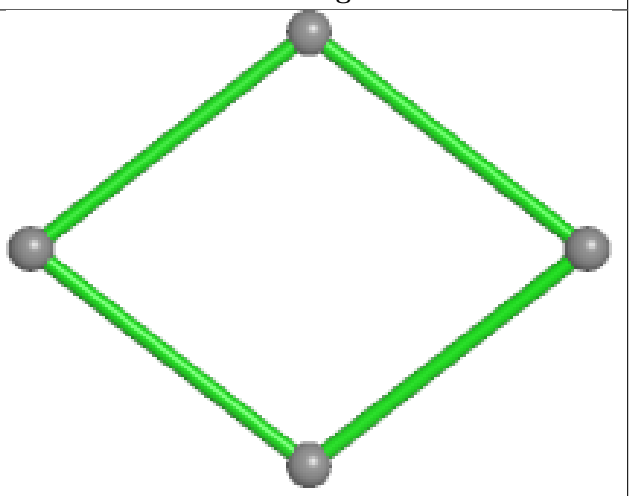
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

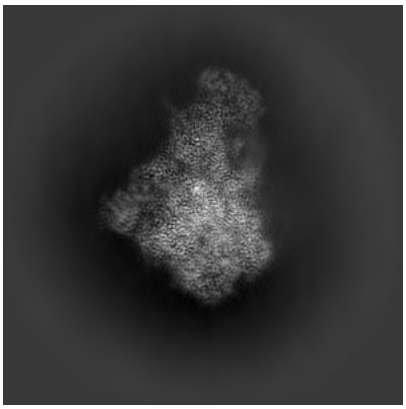
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13554. These allow visual inspection of the internal detail of the map and identification of artifacts.

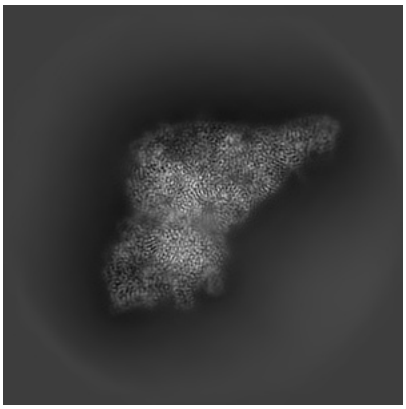
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

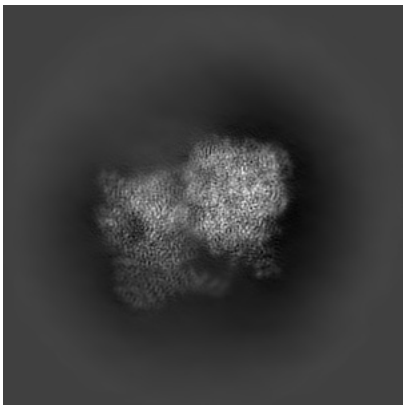
6.1.1 Primary map



X

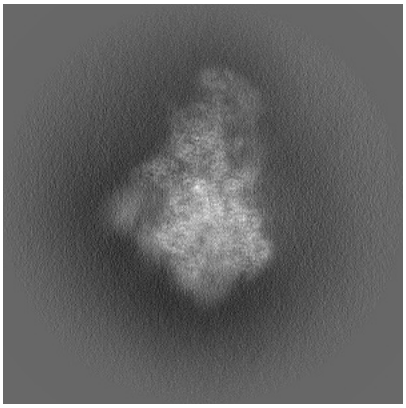


Y

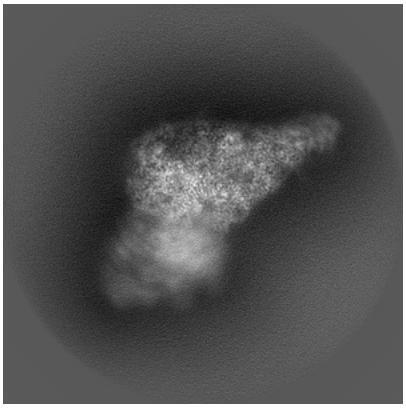


Z

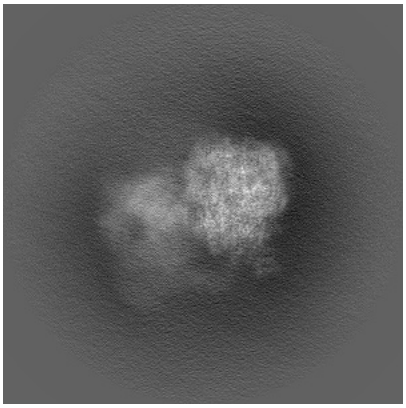
6.1.2 Raw map



X



Y

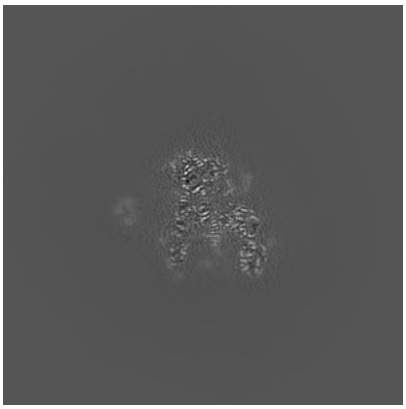


Z

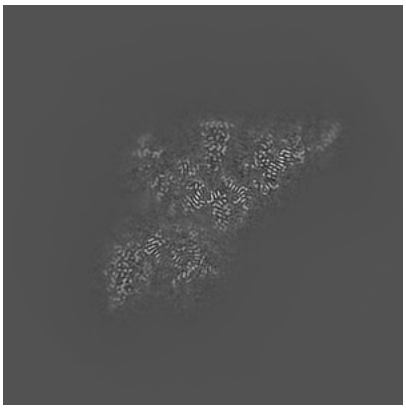
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 288

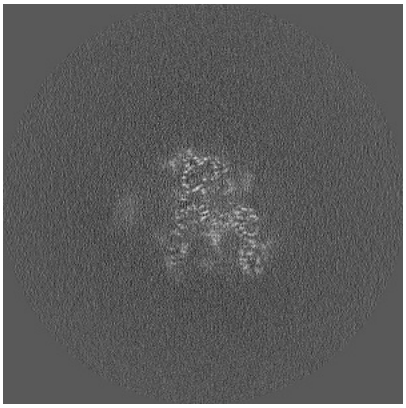


Y Index: 288

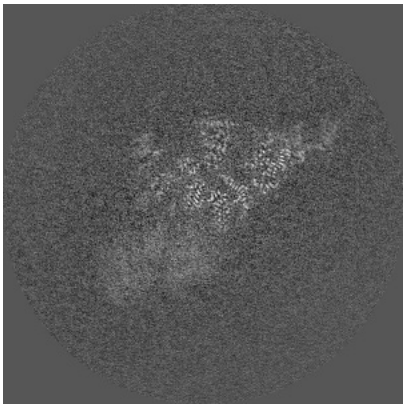


Z Index: 288

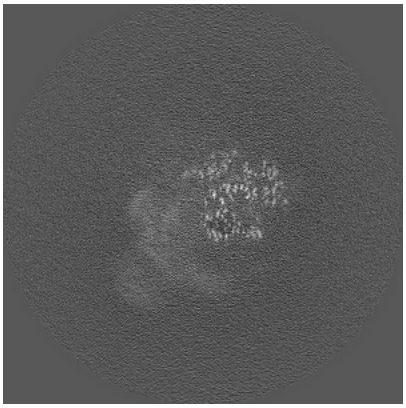
6.2.2 Raw map



X Index: 240



Y Index: 240

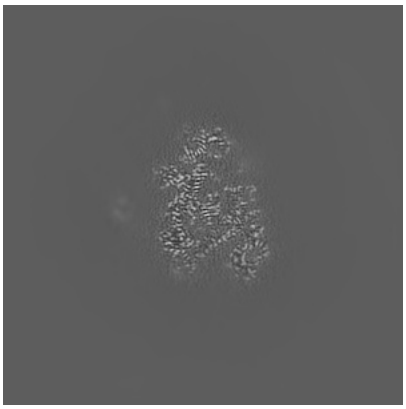


Z Index: 240

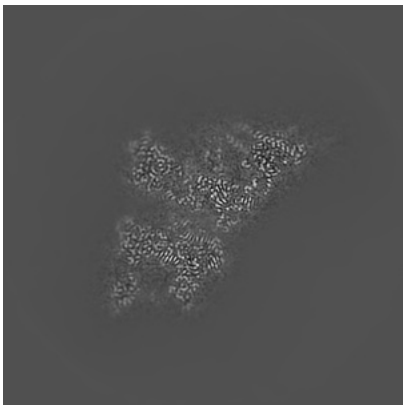
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 314

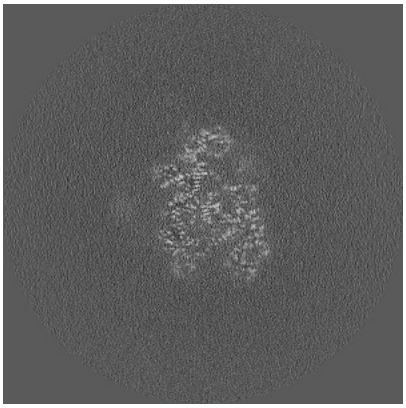


Y Index: 276

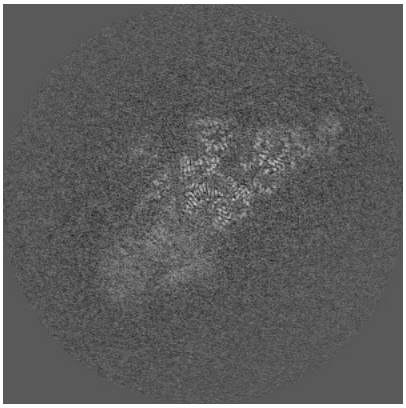


Z Index: 278

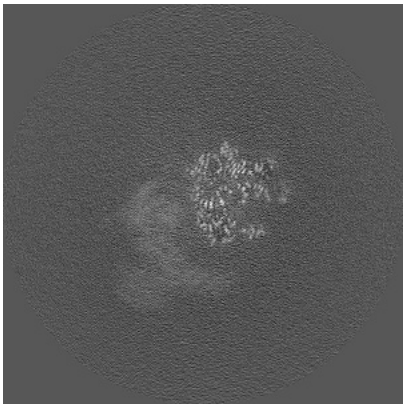
6.3.2 Raw map



X Index: 261



Y Index: 243

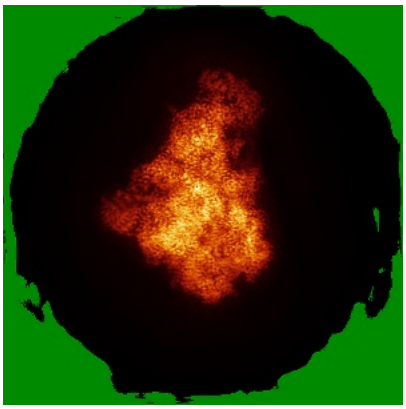


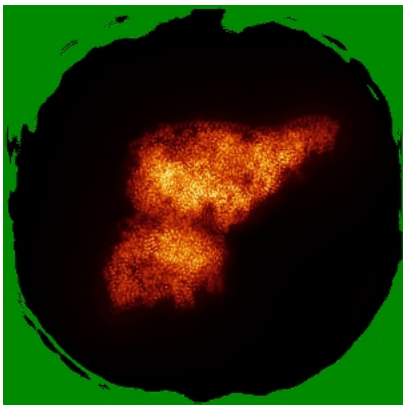
Z Index: 232

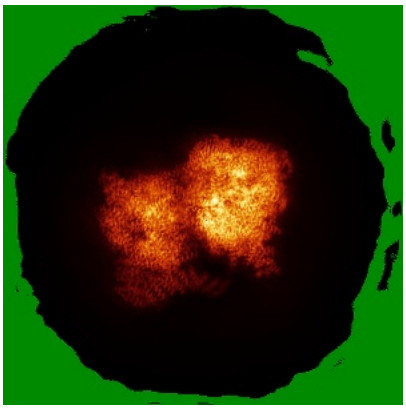
The images above show the largest variance slices of the map in three orthogonal directions.

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

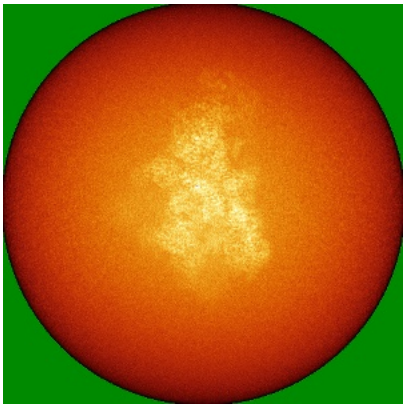
6.4.1 Primary map

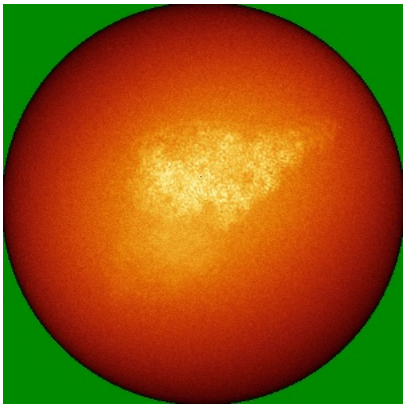

X

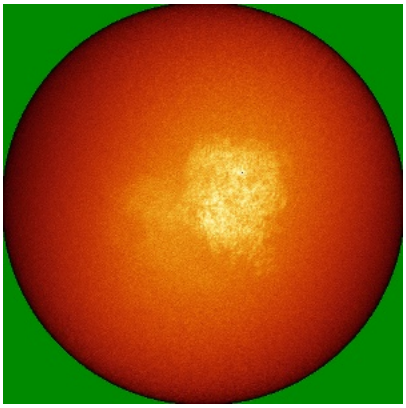

Y


Z

6.4.2 Raw map


X

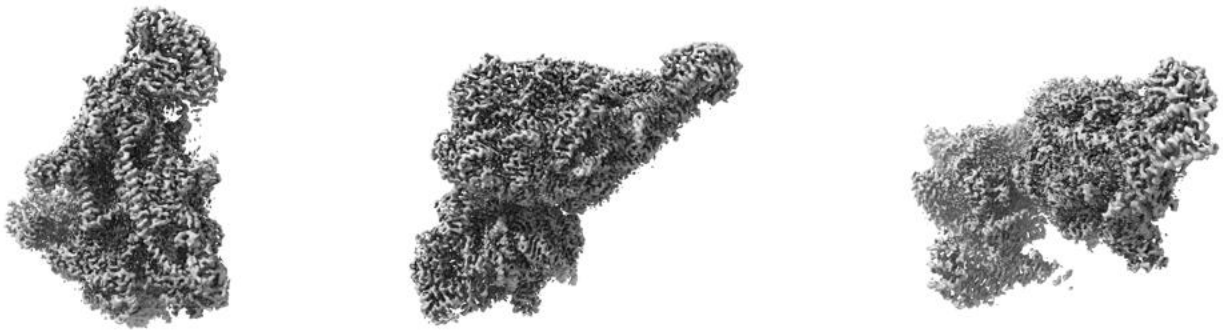

Y


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)

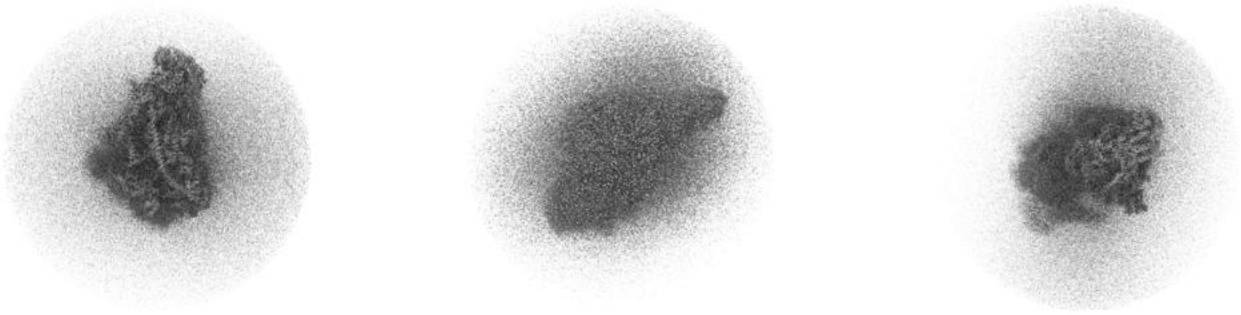
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

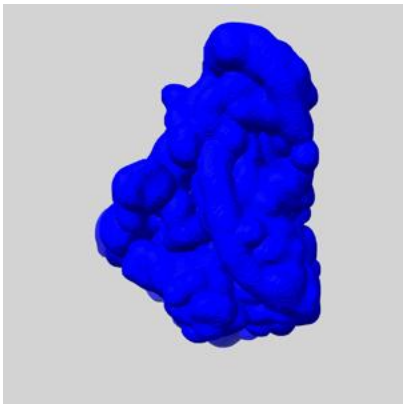
6.6 Mask visualisation

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

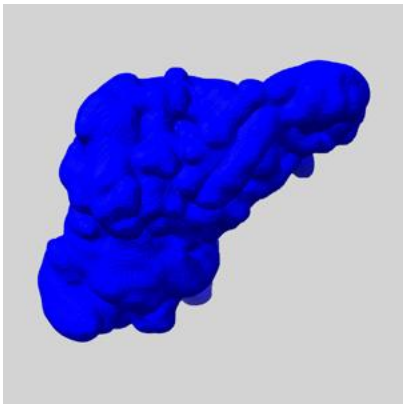
A mask typically either:

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

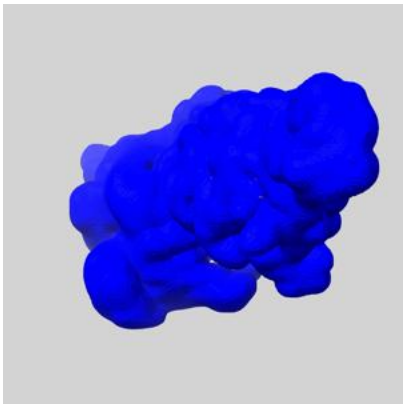
6.6.1 emd_13554_msk_1.map



X



Y

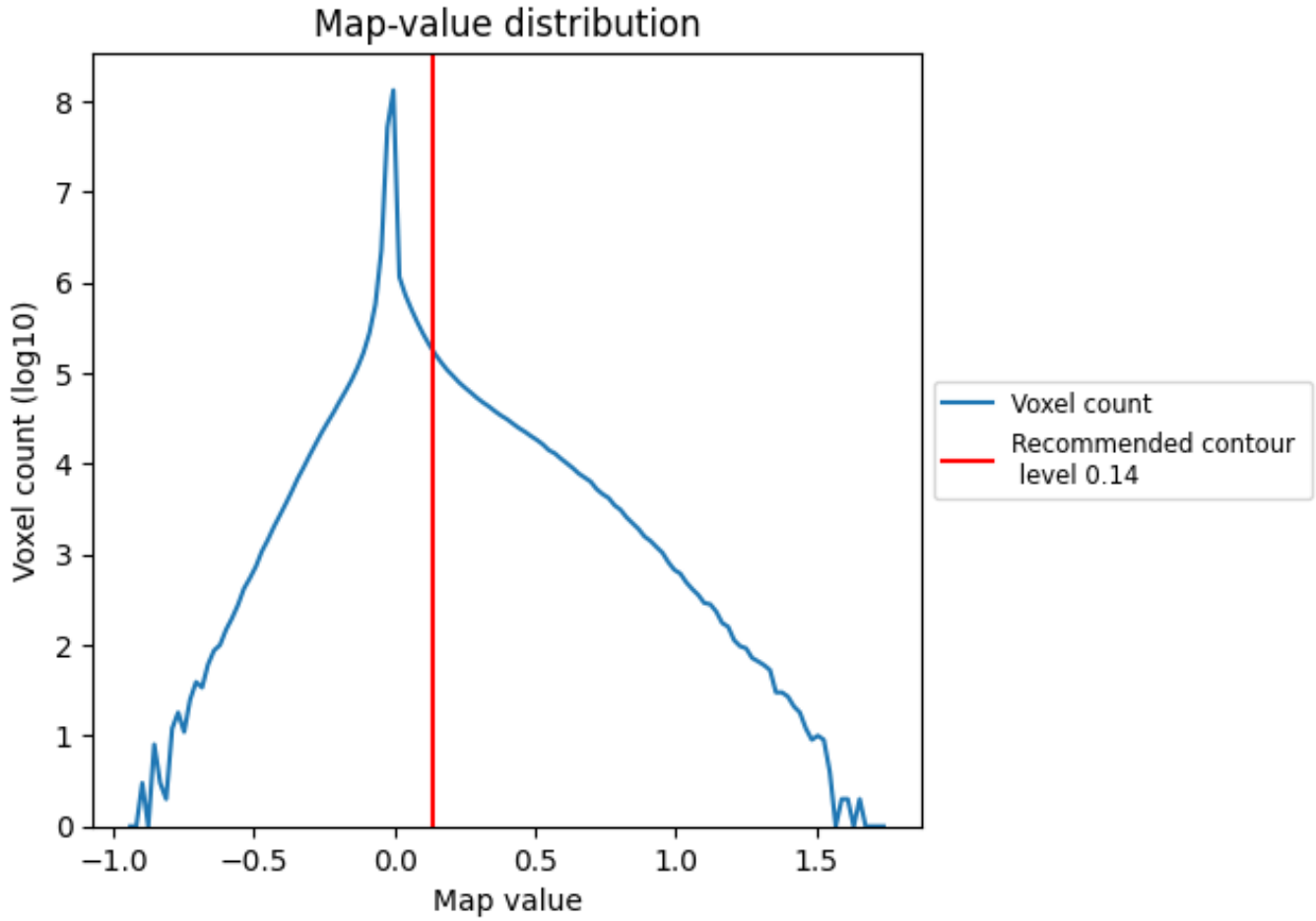


Z

7 Map analysis

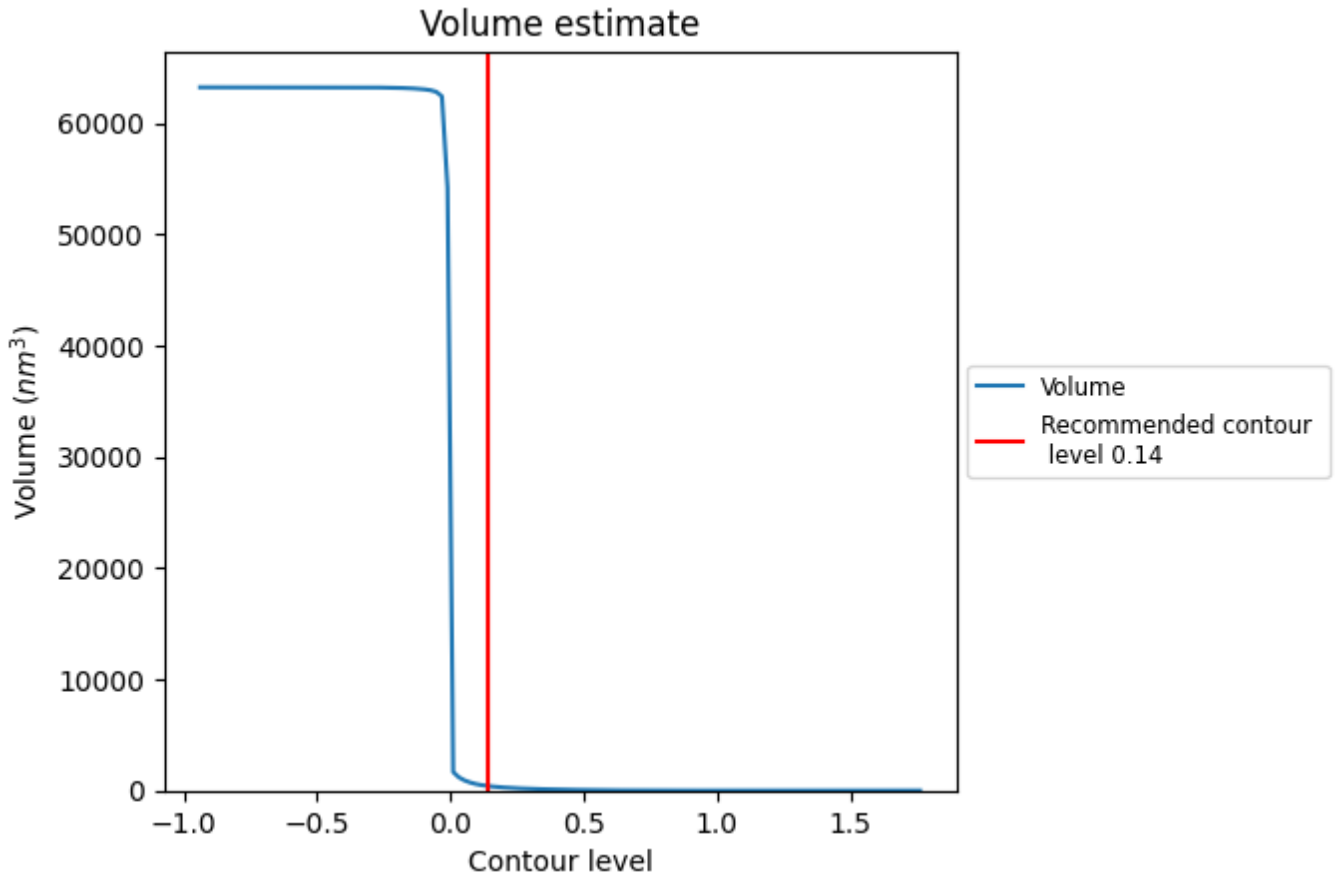
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

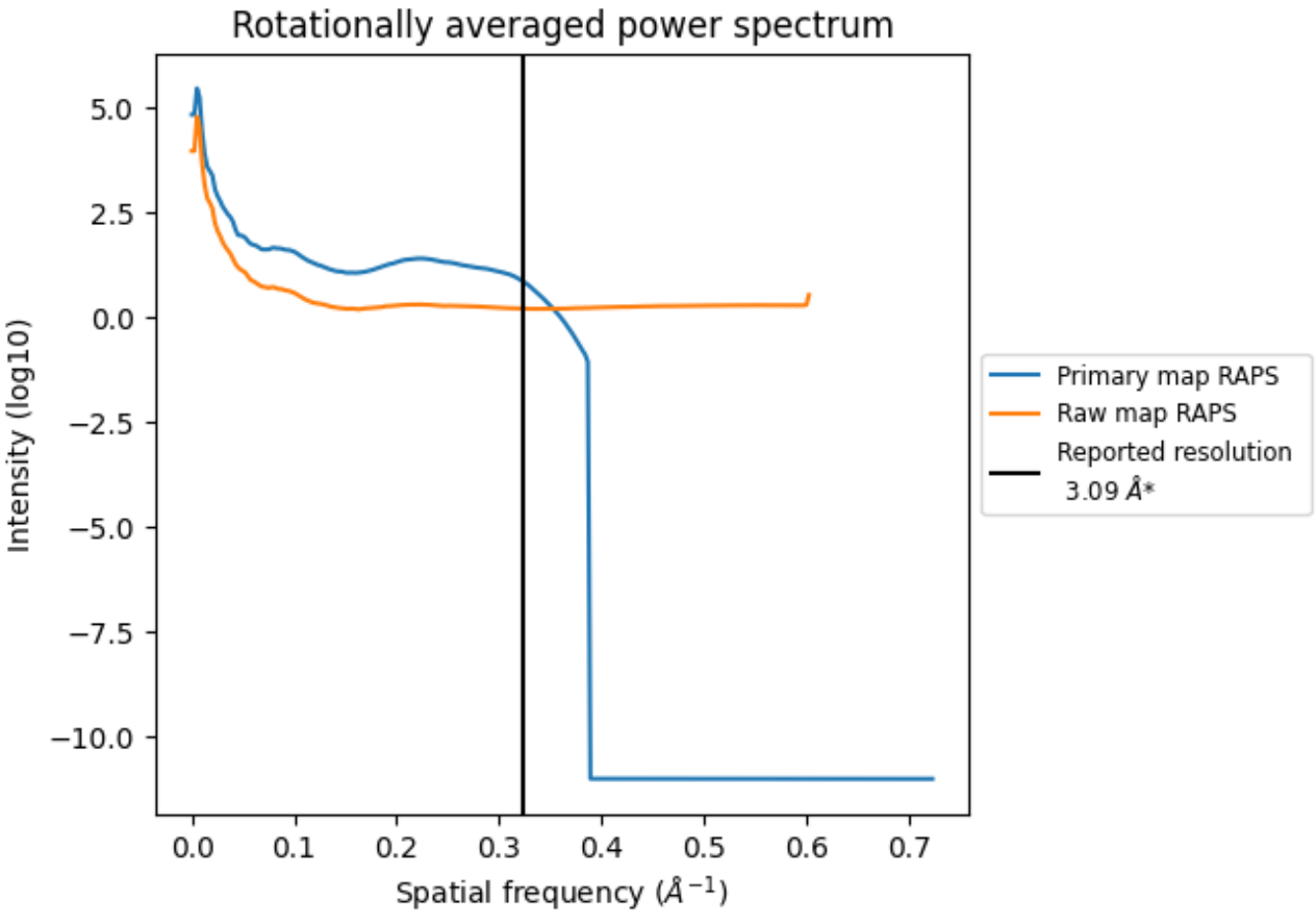
7.2 Volume estimate



The volume at the recommended contour level is 413 nm^3; this corresponds to an approximate mass of 373 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)

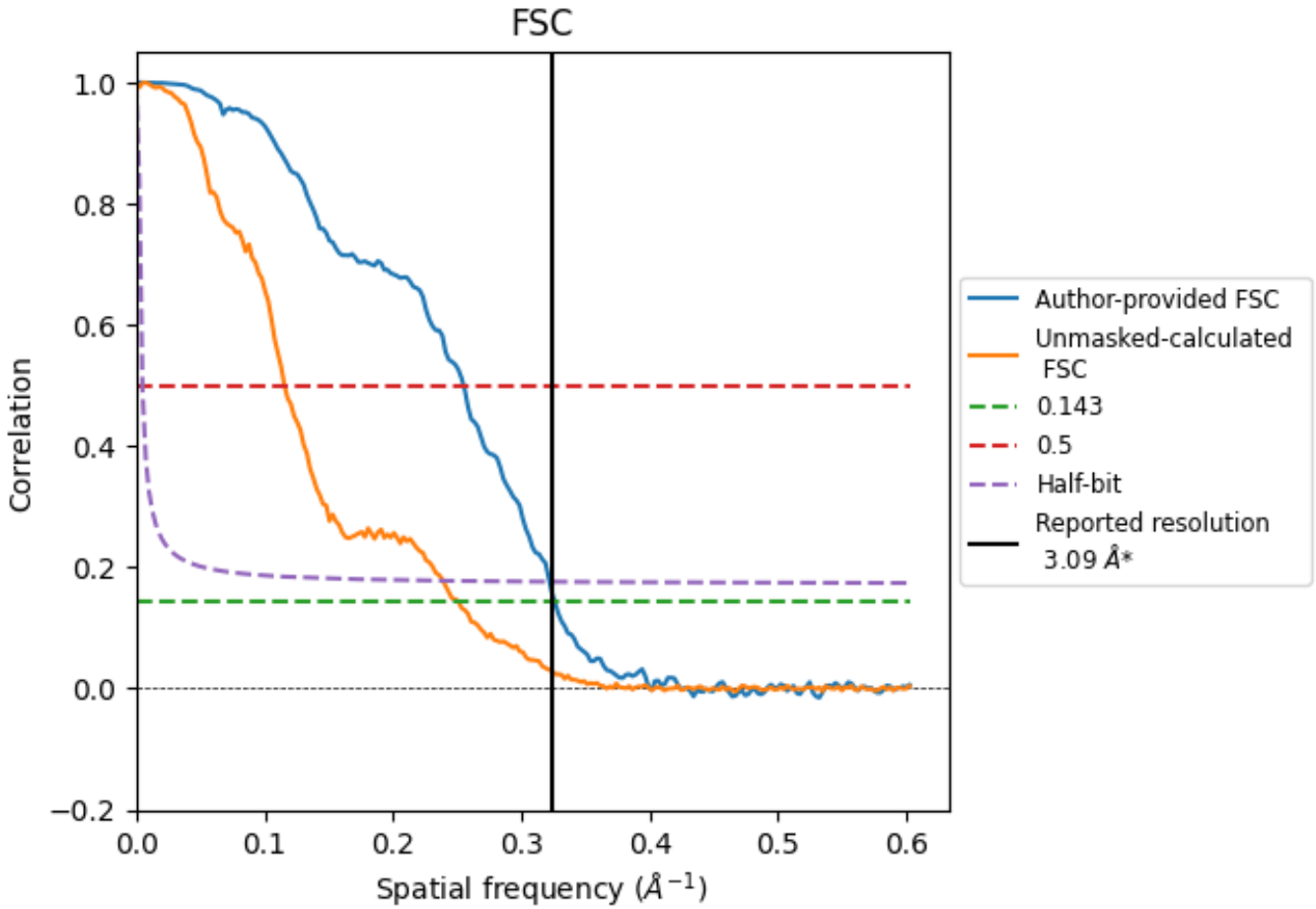


*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8.2 Resolution estimates (i)

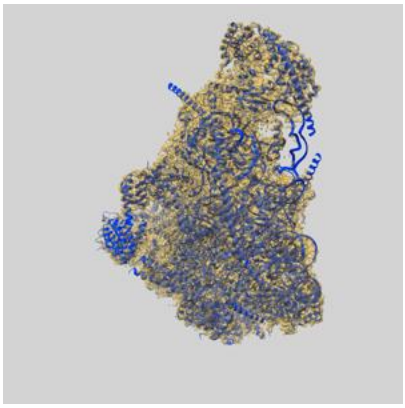
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.07	3.92	3.11
Unmasked-calculated*	3.98	8.66	4.19

*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 3.98 differs from the reported value 3.09 by more than 10 %

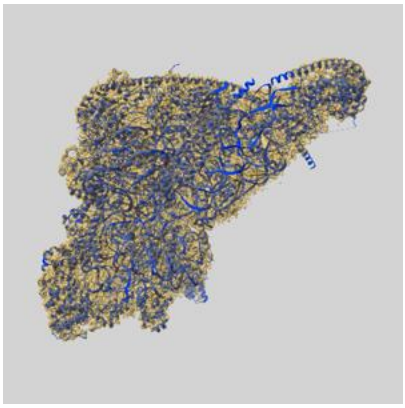
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13554 and PDB model 7PNW. Per-residue inclusion information can be found in section 3 on page 13.

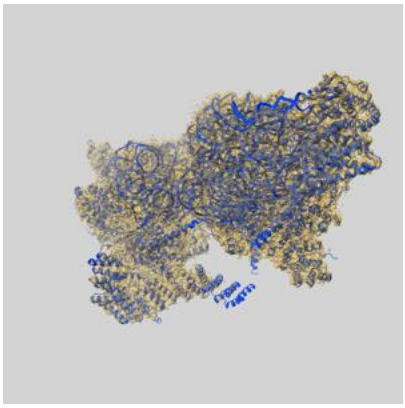
9.1 Map-model overlay



X



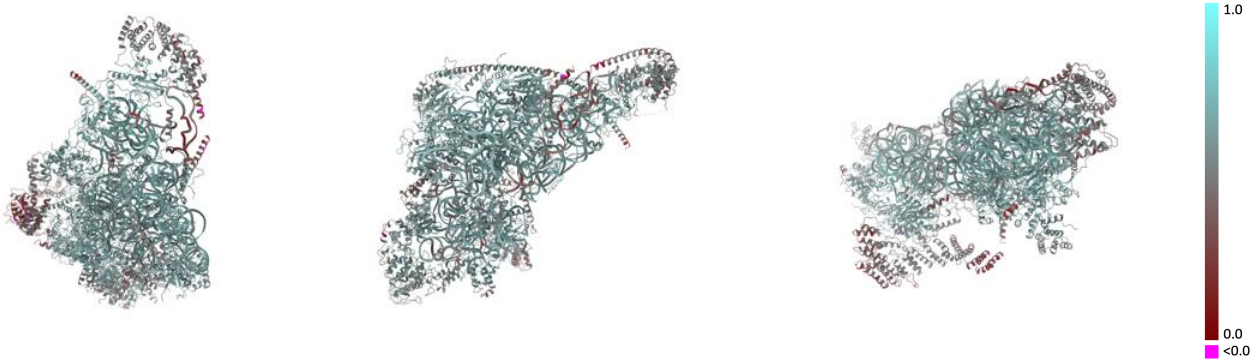
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

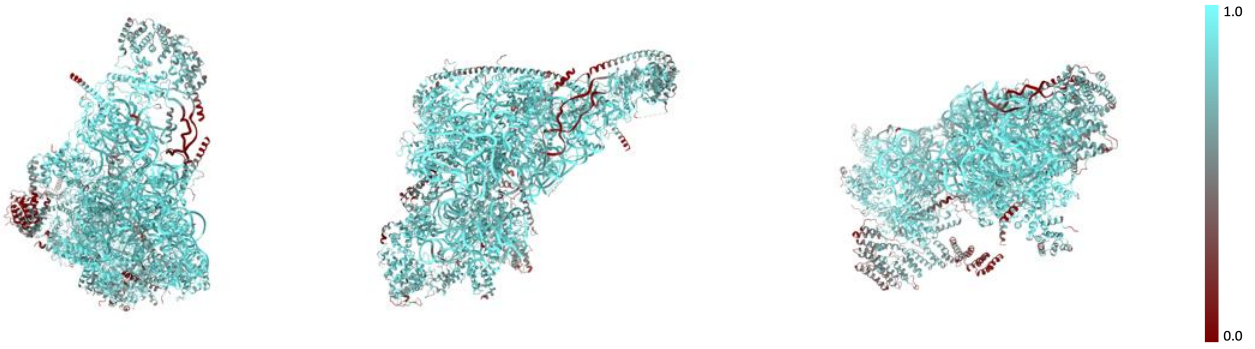
9.2 Q-score mapped to coordinate model



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.

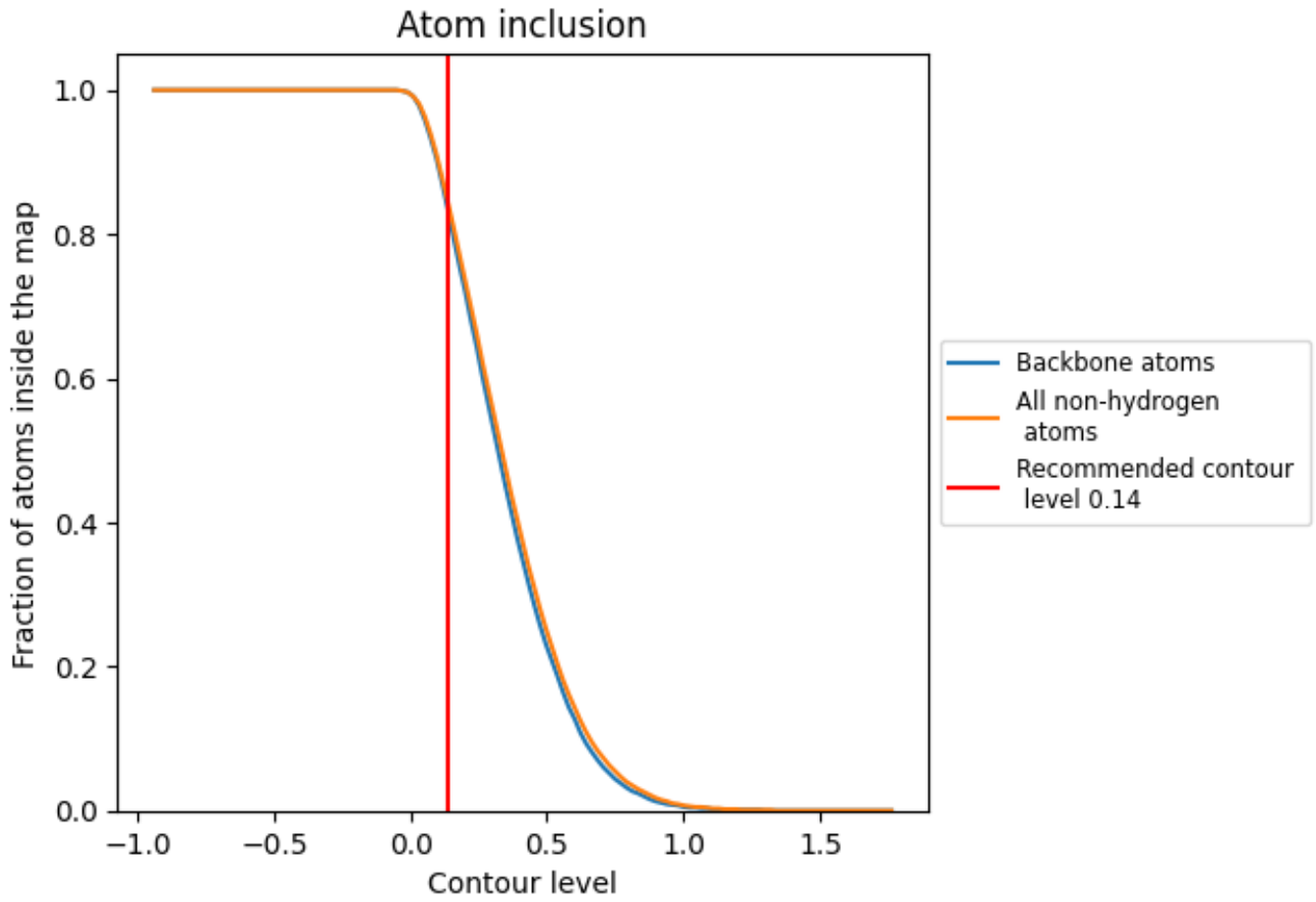
9.3 Atom inclusion mapped to coordinate model



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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5650
0	0.8550	0.5750
1	0.7910	0.5520
2	0.6240	0.4990
3	0.8170	0.5800
4	0.5170	0.4190
A	0.9240	0.5970
B	0.9240	0.6120
C	0.9550	0.6260
D	0.8510	0.5800
E	0.8750	0.5820
F	0.8020	0.5460
G	0.7830	0.5480
H	0.8620	0.5890
I	0.9030	0.5910
J	0.9150	0.5970
K	0.9560	0.6410
L	0.7980	0.5680
M	0.8870	0.6080
N	0.8980	0.6160
O	0.9010	0.6010
P	0.9160	0.6040
Q	0.9400	0.6140
R	0.8350	0.5740
S	0.7880	0.5440
T	0.8830	0.5850
U	0.7680	0.5540
V	0.6640	0.4720
W	0.8870	0.5860
X	0.7920	0.5480
Y	0.6460	0.4820
Z	0.8390	0.5740

