



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:37 PM UTC

PDB ID : 6YWV / pdb_00006ywv
EMDB ID : EMD-10977
Title : The structure of the Atp25 bound assembly intermediate of the mitoribosome from *Neurospora crassa*
Authors : Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on : 2020-04-30
Resolution : 3.03 Å(reported)

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:

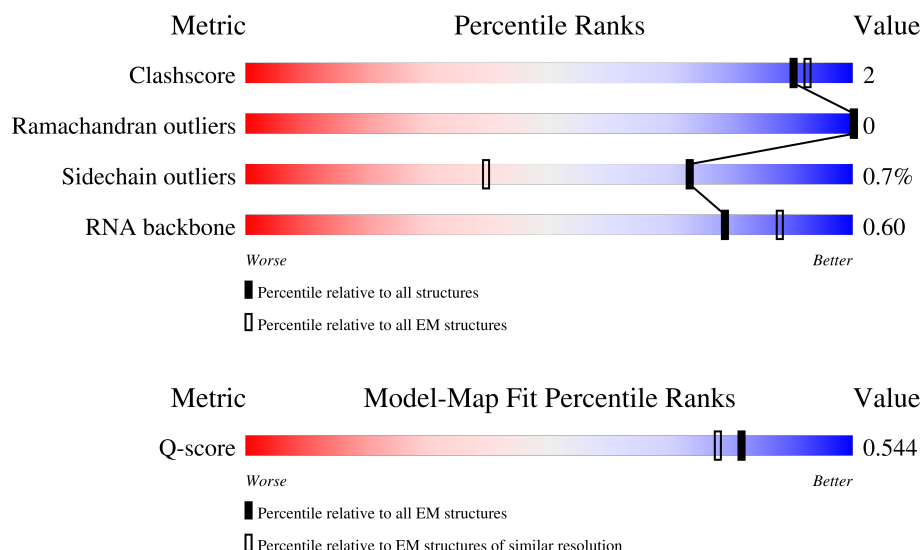
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.03 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.



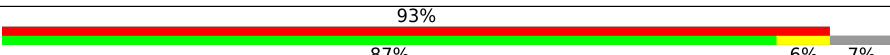
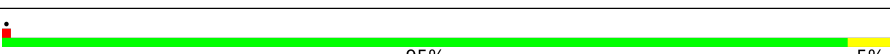
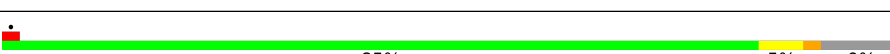
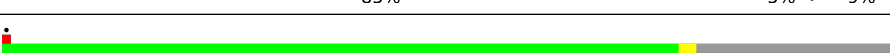
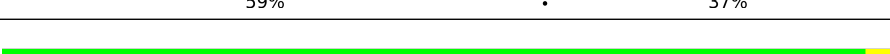
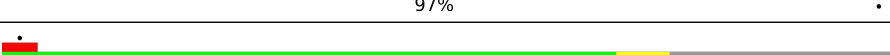
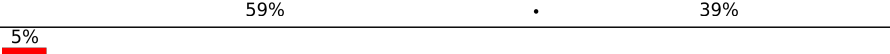
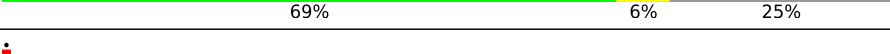
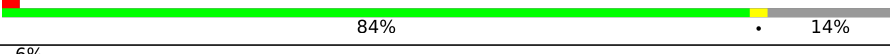
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13929 (2.53 - 3.53)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3464	
2	B	383	
3	C	384	

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Mol	Chain	Length	Quality of chain
4	D	325	
5	E	352	
6	F	255	
7	f	347	
8	g	158	
9	H	183	
10	I	131	
11	J	312	
12	K	249	
13	L	193	
14	M	258	
15	N	217	
16	O	364	
17	P	228	
18	Q	396	
19	R	447	
20	S	274	
21	T	263	
22	U	161	
23	V	219	
24	W	129	
25	X	59	
26	Y	140	
27	0	124	
28	1	449	

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Mol	Chain	Length	Quality of chain
29	2	370	
30	3	103	
31	4	138	
32	5	439	
33	6	368	
34	7	165	
35	8	443	
36	h	98	
37	i	218	
38	9	267	
39	a	225	
40	b	162	
41	c	110	
42	d	292	
43	n	699	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 207611 atoms, of which 91129 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 23 S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2529	Total	C	H	N	O	P	0	0
			81042	24198	27083	9701	17531	2529		

- Molecule 2 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	317	Total	C	H	N	O	S	0	0
			4997	1541	2519	497	425	15		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	307	Total	C	H	N	O	S	0	0
			4759	1468	2423	447	413	8		

- Molecule 4 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	254	Total	C	H	N	O	S	0	0
			4068	1280	2040	372	371	5		

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	309	Total	C	H	N	O	S	0	0
			4910	1558	2461	436	443	12		

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	201	Total	C	H	N	O	S	0	0
			3253	1022	1645	290	288	8		

- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	f	245	Total	C	H	N	O	S	0	0
			3801	1202	1925	325	346	3		

- Molecule 8 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	147	Total	C	H	N	O	S	0	0
			2257	700	1154	203	196	4		

- Molecule 9 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	183	Total	C	H	N	O	S	0	0
			2885	899	1459	268	251	8		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	119	Total	C	H	N	O	S	0	0
			1898	564	985	182	159	8		

- Molecule 11 is a protein called 50S ribosomal subunit protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	243	Total	C	H	N	O	S	0	0
			3827	1198	1939	346	343	1		

- Molecule 12 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	157	Total	C	H	N	O	S	0	0
			2591	805	1319	246	217	4		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	192	Total	C	H	N	O	S	0	0
			3135	960	1590	294	285	6		

- Molecule 14 is a protein called Mitochondrial ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	194	Total	C	H	N	O	S	0	0
			3164	981	1628	292	253	10		

- Molecule 15 is a protein called Aconitate hydratase.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	N	133	Total	C	H	N	O	S	0	0
			2176	673	1120	195	182	6		

- Molecule 16 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	O	272	Total	C	H	N	O	S	0	0
			4532	1392	2323	424	387	6		

- Molecule 17 is a protein called Mitochondrial ribosomal protein subunit L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	180	Total	C	H	N	O	S	0	0
			2975	953	1494	270	254	4		

- Molecule 18 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Q	353	Total	C	H	N	O	S	0	0
			5829	1786	2961	547	524	11		

- Molecule 19 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	R	231	Total	C	H	N	O	S	0	0
			3851	1184	1968	372	323	4		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	S	179	Total	C	H	N	O	S	0	0
			2979	937	1507	281	252	2		

- Molecule 21 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	T	171	Total	C	H	N	O	S	0	0
			2782	886	1366	260	267	3		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	U	138	Total	C	H	N	O	S	0	0
			2263	698	1164	213	185	3		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	V	56	Total	C	H	N	O	S	0	0
			921	291	462	85	82	1		

- Molecule 24 is a protein called Mitochondrial ribosomal protein subunit L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	W	59	Total	C	H	N	O	S	0	0
			950	282	490	98	72	8		

- Molecule 25 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	X	48	Total	C	H	N	O	S	0	0
			836	263	433	71	65	4		

- Molecule 26 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Y	46	Total	C	H	N	O	S	0	0
			777	224	412	84	56	1		

- Molecule 27 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	46	Total	C	H	N	O	S	0	0
			797	240	409	86	58	4		

- Molecule 28 is a protein called Mitochondrial large ribosomal subunit YmL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	367	Total	C	H	N	O	S	0	0
			6014	1899	3029	547	531	8		

- Molecule 29 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	123	Total	C	H	N	O	S	0	0
			2101	660	1055	211	171	4		

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	95	Total	C	H	N	O	S	0	0
			1536	489	773	135	137	2		

- Molecule 31 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	137	Total	C	H	N	O	S	0	0
			2139	671	1087	192	183	6		

- Molecule 32 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	5	350	Total	C	H	N	O	S	0	0
			5429	1740	2710	477	493	9		

- Molecule 33 is a protein called 50S ribosomal subunit L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	6	273	Total	C	H	N	O	S	0	0
			4474	1418	2248	399	401	8		

- Molecule 34 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	84	Total	C	H	N	O	0	0
			1383	431	709	130	113		

- Molecule 35 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	8	331	Total	C	H	N	O	S	0	0
			5374	1683	2714	480	489	8		

- Molecule 36 is a protein called Mitochondrial ribosomal protein L44.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	h	94	Total	C	H	N	O	S	0	0
			1525	474	774	134	139	4		

- Molecule 37 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	i	121	Total	C	H	N	O	S	0	0
			1949	599	995	177	174	4		

- Molecule 38 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	9	206	Total	C	H	N	O	S	0	0
			3341	1051	1698	295	290	7		

- Molecule 39 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	a	161	Total	C	H	N	O	S	0	0
			2671	837	1340	253	235	6		

- Molecule 40 is a protein called Mitochondrial 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	b	161	Total	C	H	N	O	S	0	0
			2693	840	1379	249	221	4		

- Molecule 41 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	c	98	Total	C	H	N	O	S	0	0
			1700	528	873	162	134	3		

- Molecule 42 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	d	235	Total	C	H	N	O	S	0	0
			3797	1180	1909	363	339	6		

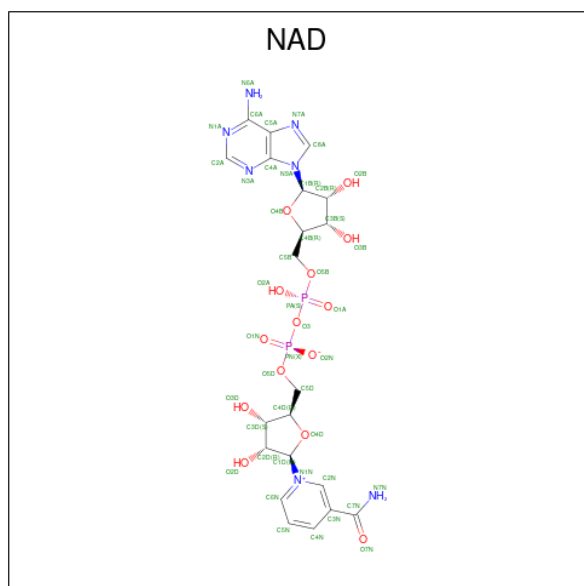
- Molecule 43 is a protein called ATPase synthesis protein 25, mitochondrial.

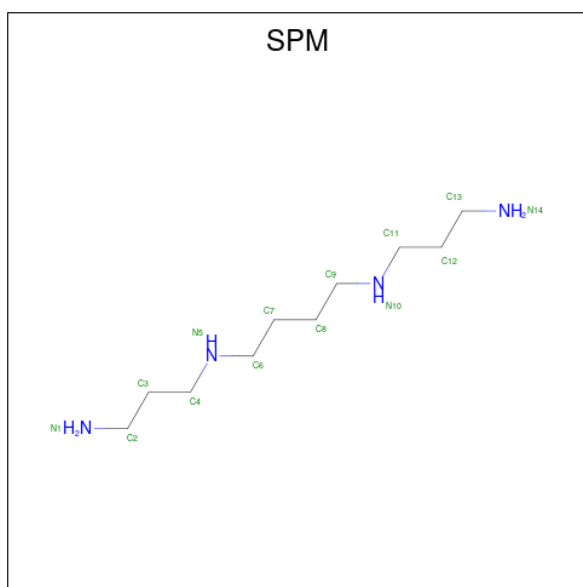
Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	186	Total	C	H	N	O	S	0	0
			2951	913	1505	261	265	7		

- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	142	Total	Mg	0
			142	142	
44	K	1	Total	Mg	0
			1	1	
44	c	1	Total	Mg	0
			1	1	

- Molecule 45 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
46	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 47 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
47	A	23	Total	K	0
			23	23	

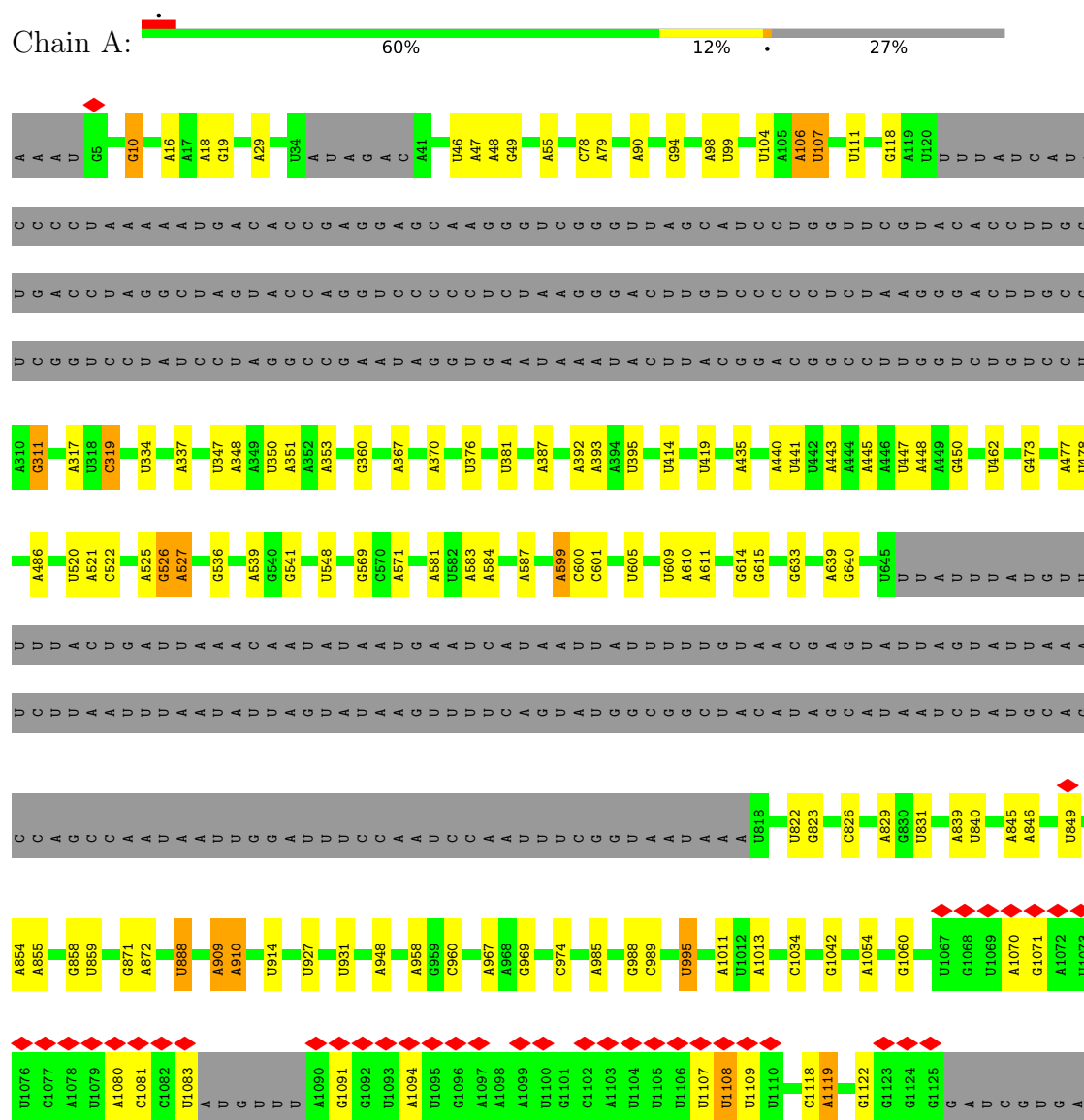
- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	W	1	Total	Zn	0
			1	1	
48	0	1	Total	Zn	0
			1	1	

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: 23 S rRNA





Chain D:  73% 5% 22%

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

PRO T62 T63 S71 L75 E81 A85 S129 P130 Q131 K132 G133 T134 R138 D160 F161 S162 R181 K210 K235 E236 A237 G238 R239 L275 T278 R285 V300 T301 R302 VAL ALA VAL GLN LEU ARG GLN LYS G312 R324 TTR

• Molecule 5: 50S ribosomal protein L5

Chain E:  13% 83% 5% 12%

MET ALA SER LEU ARG GLY VAL SER ARG SER ALA ARG ALA LEU GLN PRO PHE SER ALA GLN PHE ALA VAL ARG ARG CYS ALA SER THR GLN THR GLY ALA GLY ALA ALA THR PRO LYS SER ASN I44 P45 D46 L47 A48 E49 T52 R53 A58 P61 S62 E63 E64 D65

E68 D77 R78 K79 A80 R81 K93 R96 G97 H100 Q103 S108 D109 K151 K152 E153 R157 E162 P183 E186 R187 D188 K211 D214 Q242 Q243 Q244 L245 Q246 K249 K278 D279 V280 K281 G282 D289 E301 D302 E308 V309

E310 D314 H315 Y316 P317 A318 K319 M320 T331 D335 R336 Q337 L345 N352

• Molecule 6: 60S ribosomal protein L6

Chain F:  76% 21%

MET PHE ALA PRO SER ARG ARG ARG VAL LEU GLU ALA VAL ALA SER SER SER SER PRO VAL VAL THR LEU PRO GLY PHE LEU VAL PRO ALA PHE GLN THR THR ALA ALA ALA ARG ARG ASN PHE SER GLN THR THR THR ARG PRO S52 E113 M123 Q129 R169

V161 E192 Q251 K252 LYS ILE LYS

• Molecule 7: Uncharacterized protein

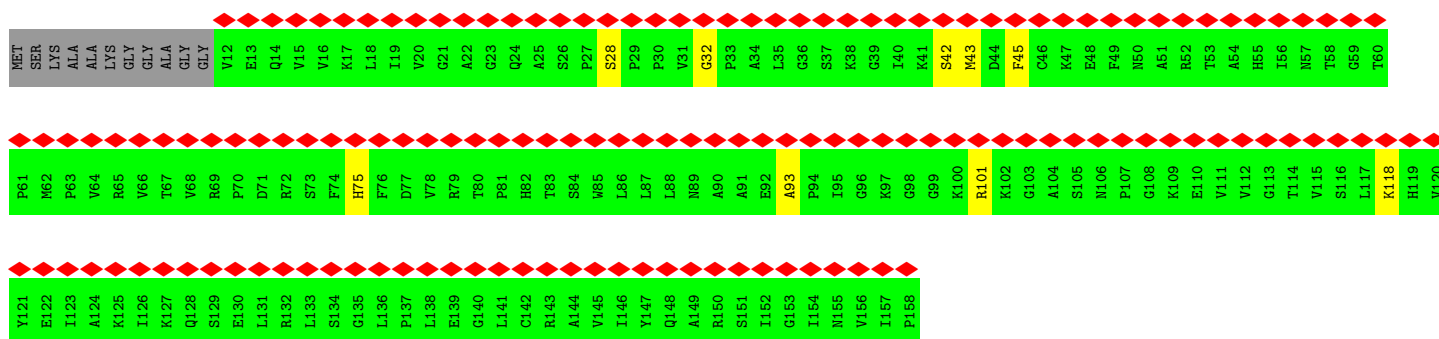
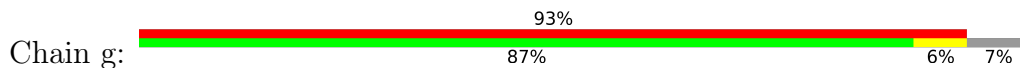
Chain f:  67% 68% 29%

MET SER ARG LEU SER ARG ARG PRO ALA VAL ARG GLY LEU GLY GLY ALA ILE LYS SER SER ARG ILE SER SER ARG SER SER ALA LEU VAL M85 M86 R87 S88 T89 P90 PHE L91 M92 L93 I94 F95 S155 Q96 H97 N98 N99 L100 T101 A102 A103 E104 W105 A106 A107 T108 R109 R110 E111 L112 S113 L114 A115 N116 S117 N118 V119 P120

P61 P62 T63 Q64 P65 P66 S67 A68 R69 P70 V71 D72 T73 R74 K75 S76 Q77 L78 L79 R80 T81 Y82 D143 T83 S84 M85 L86 R87 S88 T89 P90 PHE L91 M92 L93 I94 F95 S155 Q96 H97 N98 N99 L100 T101 A102 A103 E104 W105 A106 A107 T108 R109 R110 E111 L112 S113 L114 A115 N116 S117 N118 V119 P120

V121 P122 E123 G124 A125 P126 D127 I128 T129 S130 K131 I132 H133 L134 Q135 V136 V137 R138 T139 R140 I141 F142 D143 V144 A145 L146 K147 T148 V149 E150 F151 F152 D153 P154 S155 T156 V157 E158 P159 T160 T161 A162 T163 T164 A165 T166 G167 T168 K169 V170 P171 A172 T173 Y174 N175 H176 D177 L178 H181

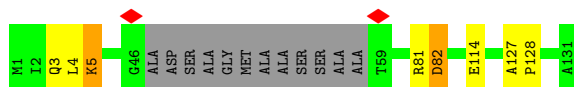
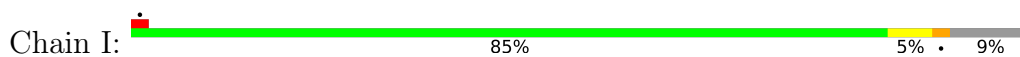
- Molecule 8: 60S ribosomal protein L19



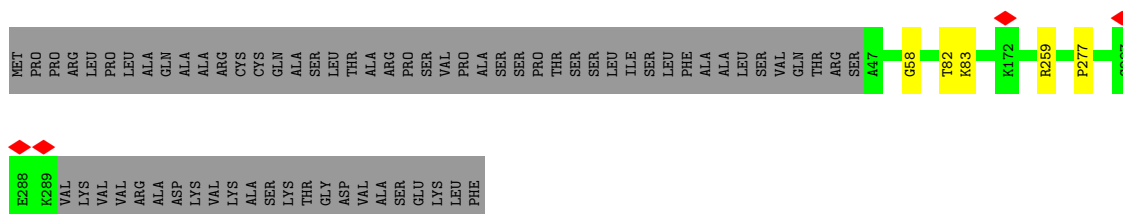
- Molecule 9: Ribosomal protein L13



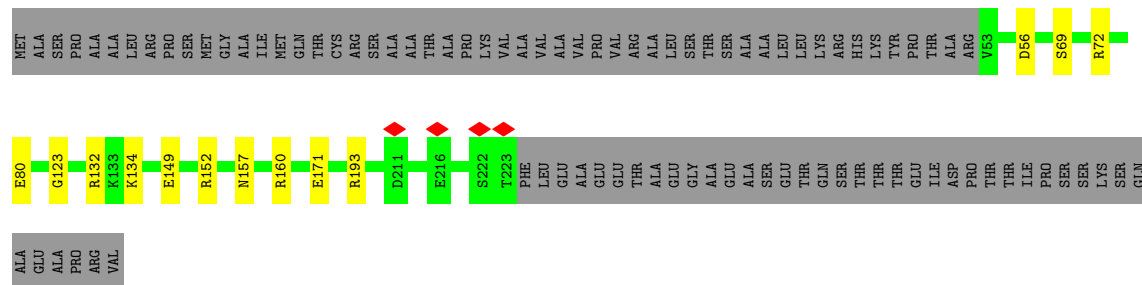
- Molecule 10: 50S ribosomal protein L14



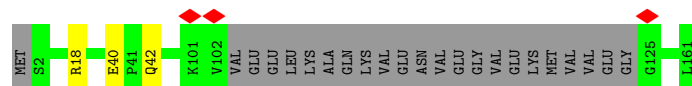
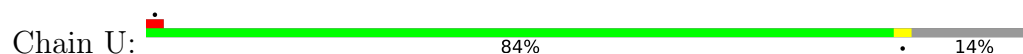
- Molecule 11: 50S ribosomal subunit protein L15



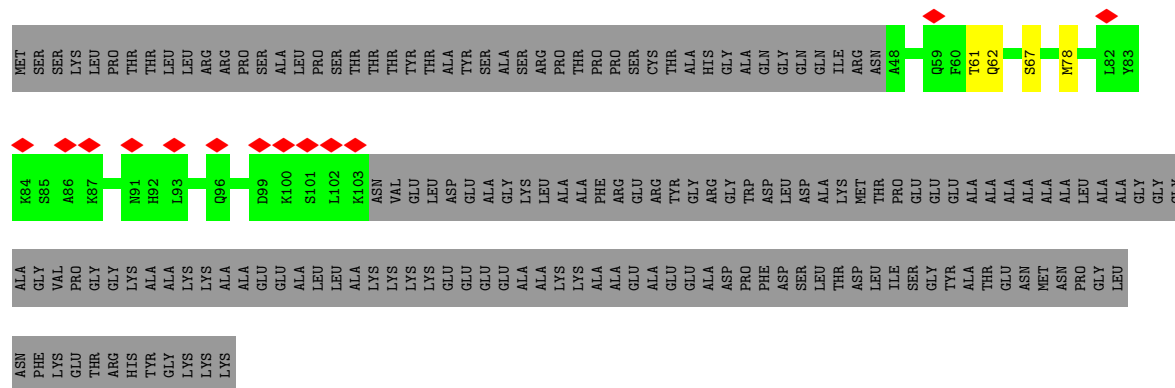
- Molecule 21: 54S ribosomal protein L4, mitochondrial



- Molecule 22: 50S ribosomal protein L30

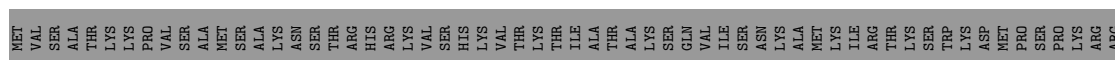


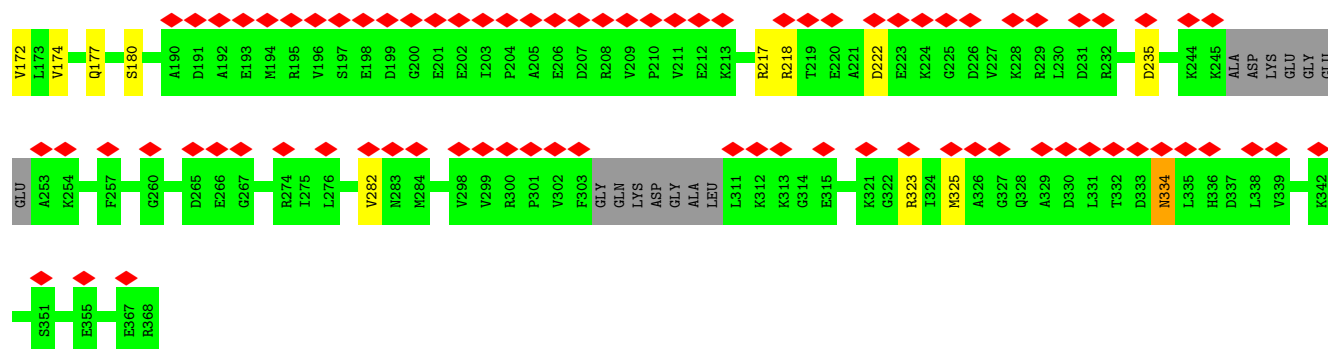
- Molecule 23: Uncharacterized protein



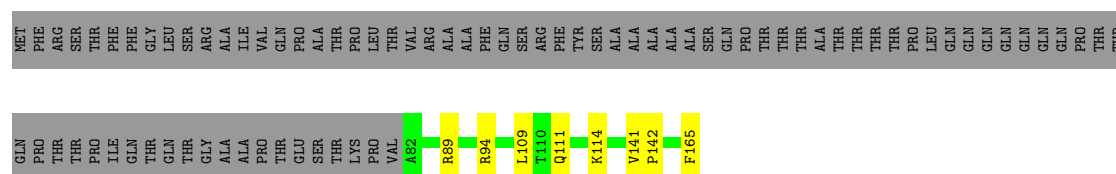
- Molecule 24: Mitochondrial ribosomal protein subunit L32



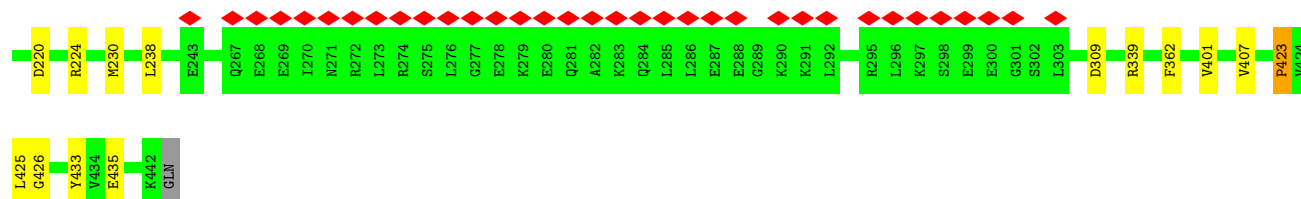
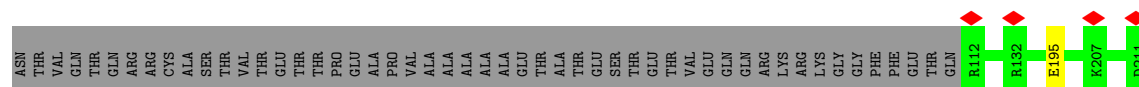
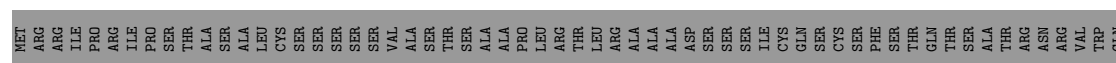




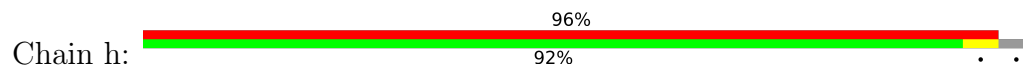
- Molecule 34: Uncharacterized protein



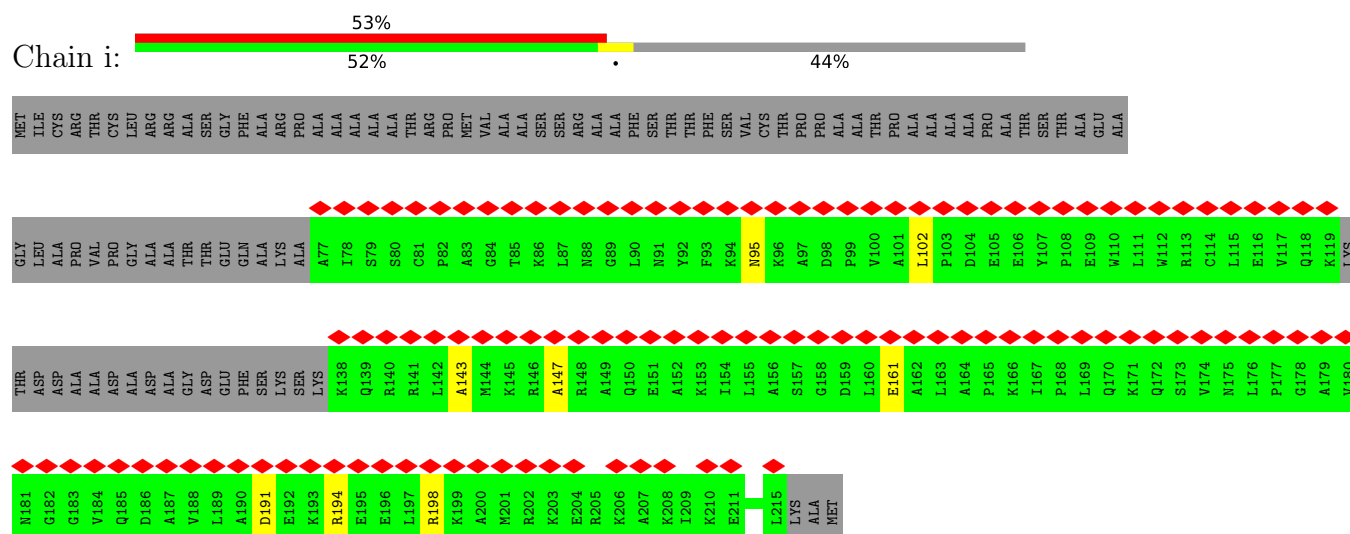
- Molecule 35: Uncharacterized protein



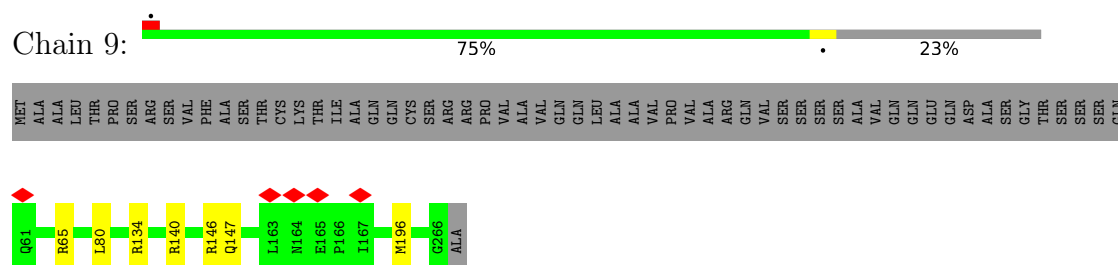
- Molecule 36: Mitochondrial ribosomal protein L44



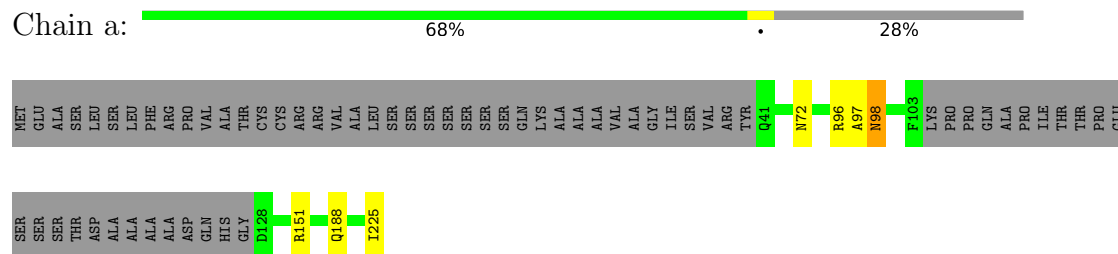
- Molecule 37: Uncharacterized protein



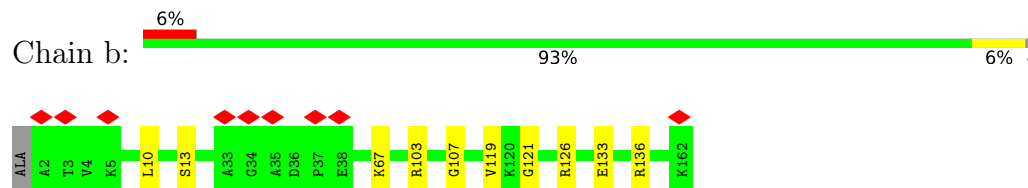
- Molecule 38: RNase III domain-containing protein



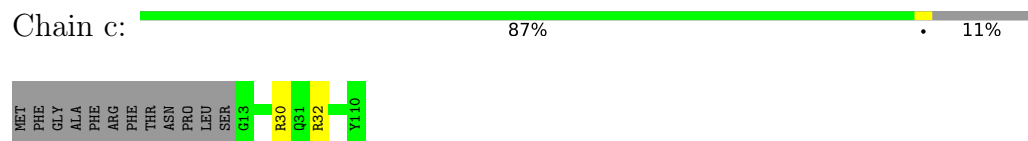
- Molecule 39: 60S ribosomal protein L20



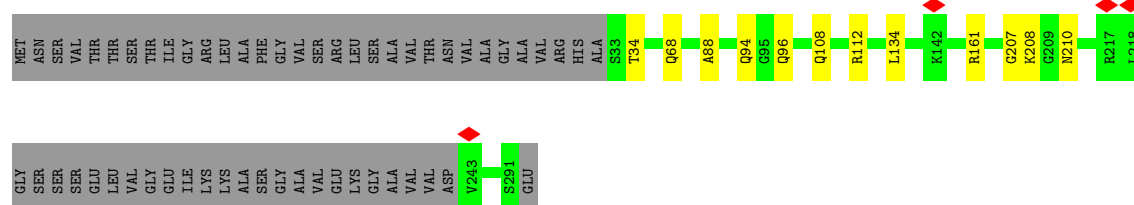
- Molecule 40: Mitochondrial 60S ribosomal protein L25



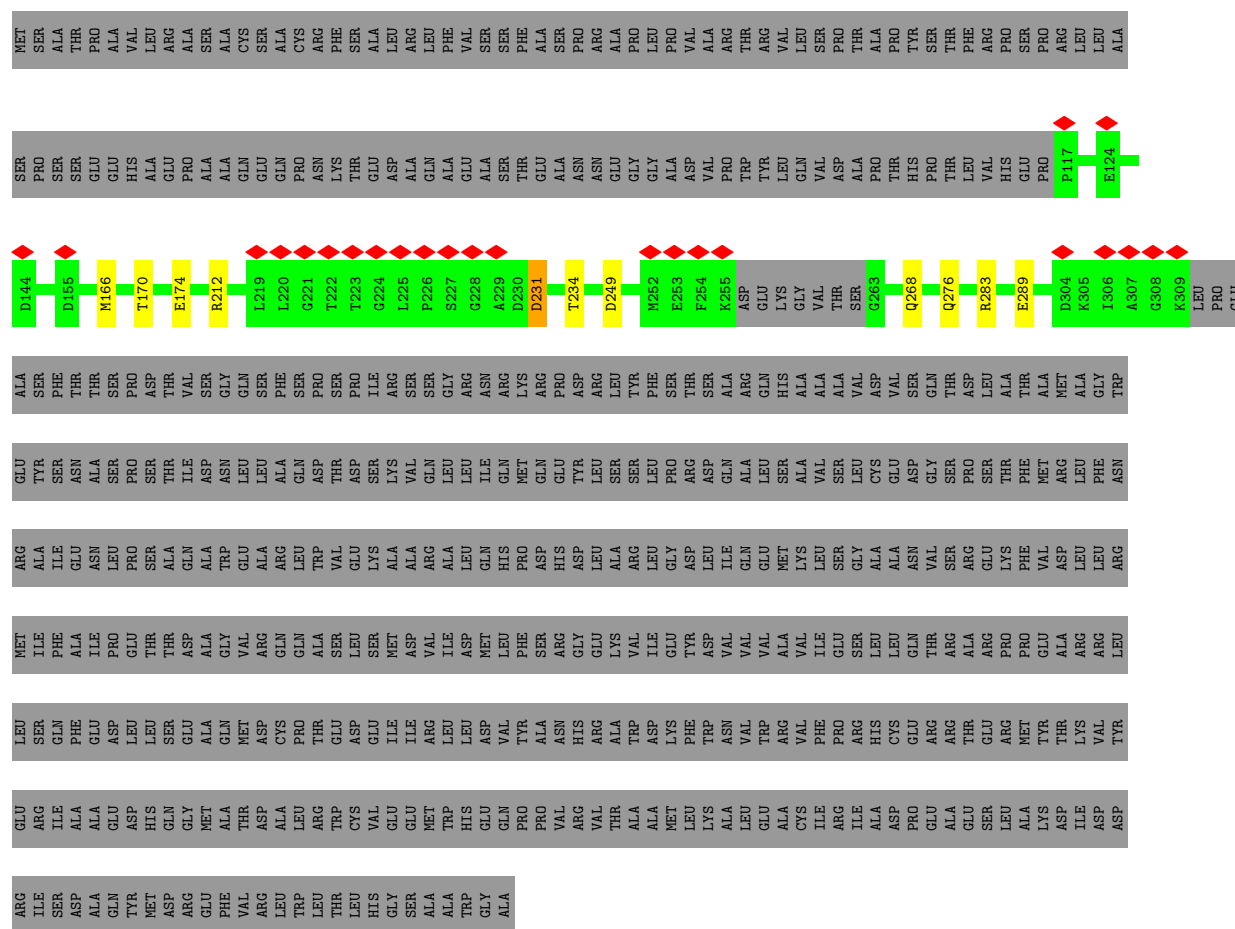
- Molecule 41: 54S ribosomal protein L31, mitochondrial



Chain d: 76% 20%



Chain n:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.282	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0292	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.10	0/60430	0.19	0/94085
2	B	0.11	0/2536	0.31	0/3421
3	C	0.11	0/2380	0.30	0/3209
4	D	0.10	0/2072	0.28	0/2794
5	E	0.10	0/2518	0.27	0/3427
6	F	0.09	0/1644	0.24	0/2218
7	f	0.09	0/1923	0.25	0/2631
8	g	0.10	0/1126	0.27	0/1525
9	H	0.12	0/1460	0.28	0/1975
10	I	0.12	0/918	0.34	0/1225
11	J	0.11	0/1931	0.29	0/2597
12	K	0.10	0/1297	0.27	0/1740
13	L	0.11	0/1569	0.30	0/2106
14	M	0.11	0/1572	0.29	0/2117
15	N	0.11	0/1077	0.29	0/1452
16	O	0.11	0/2248	0.29	0/3015
17	P	0.11	0/1523	0.25	0/2058
18	Q	0.11	0/2916	0.28	0/3927
19	R	0.11	0/1918	0.29	0/2573
20	S	0.11	0/1510	0.30	0/2042
21	T	0.10	0/1454	0.27	0/1974
22	U	0.10	0/1117	0.29	0/1496
23	V	0.09	0/471	0.27	0/638
24	W	0.12	0/467	0.33	0/616
25	X	0.11	0/411	0.30	0/551
26	Y	0.14	0/368	0.35	0/485
27	0	0.12	0/395	0.30	0/523
28	1	0.10	0/3053	0.27	0/4108
29	2	0.11	0/1074	0.31	0/1449
30	3	0.11	0/783	0.28	0/1056
31	4	0.11	0/1077	0.29	0/1453
32	5	0.11	0/2790	0.29	0/3794

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.09	0/2274	0.27	0/3062
34	7	0.10	0/686	0.31	0/919
35	8	0.10	0/2714	0.27	0/3657
36	h	0.10	0/763	0.26	0/1027
37	i	0.11	0/967	0.28	0/1296
38	9	0.10	0/1678	0.29	0/2267
39	a	0.12	0/1364	0.29	0/1842
40	b	0.10	0/1348	0.27	0/1816
41	c	0.12	0/846	0.29	0/1134
42	d	0.10	0/1930	0.27	0/2597
43	n	0.09	0/1470	0.26	0/1980
All	All	0.10	0/124068	0.24	0/179877

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 ⓘ

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	53959	27083	27083	124	0
2	B	2478	2519	2519	11	0
3	C	2336	2423	2420	11	0
4	D	2028	2040	2040	12	0
5	E	2449	2461	2461	8	0
6	F	1608	1645	1645	3	0
7	f	1876	1925	1925	6	0
8	g	1103	1154	1154	6	0
9	H	1426	1459	1459	8	0
10	I	913	985	985	4	0
11	J	1888	1939	1939	3	0
12	K	1272	1319	1319	9	0
13	L	1545	1590	1590	3	0
14	M	1536	1628	1628	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1056	1120	1120	6	0
16	O	2209	2323	2323	14	0
17	P	1481	1494	1494	2	0
18	Q	2868	2961	2961	17	0
19	R	1883	1968	1968	6	0
20	S	1472	1507	1507	8	0
21	T	1416	1366	1366	10	0
22	U	1099	1164	1164	3	0
23	V	459	462	462	3	0
24	W	460	490	489	4	0
25	X	403	433	433	4	0
26	Y	365	412	412	6	0
27	0	388	409	409	0	0
28	1	2985	3029	3029	11	0
29	2	1046	1055	1055	6	0
30	3	763	773	773	4	0
31	4	1052	1087	1087	7	0
32	5	2719	2710	2710	12	0
33	6	2226	2248	2248	15	0
34	7	674	709	709	3	0
35	8	2660	2714	2714	9	0
36	h	751	774	774	2	0
37	i	954	995	995	6	0
38	9	1643	1698	1698	6	0
39	a	1331	1340	1340	7	0
40	b	1314	1379	1379	5	0
41	c	827	873	873	2	0
42	d	1888	1909	1909	7	0
43	n	1446	1505	1505	6	0
44	A	142	0	0	0	0
44	K	1	0	0	0	0
44	c	1	0	0	0	0
45	A	44	26	26	3	0
46	A	14	26	26	0	0
47	A	23	0	0	0	0
48	0	1	0	0	0	0
48	W	1	0	0	0	0
All	All	116482	91129	91125	321	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 2.

All (321) 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)
40:b:121:GLY:O	40:b:126:ARG:NH2	2.13	0.82
1:A:445:A:OP2	18:Q:324:ARG:NH2	2.14	0.80
13:L:136:ARG:NH1	24:W:95:PRO:O	2.16	0.77
1:A:1307:G:N2	1:A:1315:A:OP1	2.19	0.75
16:O:364:TRP:O	31:4:125:ARG:NH1	2.20	0.75
29:2:276:ARG:NH1	33:6:170:ASP:OD2	2.20	0.74
1:A:2797:C:OP1	25:X:39:LYS:NZ	2.20	0.74
1:A:3363:A:O2'	1:A:3365:A:OP2	2.07	0.72
7:f:92:MET:SD	7:f:268:ARG:NH2	2.63	0.72
1:A:2925:A:OP2	1:A:2926:C:N4	2.23	0.70
1:A:3033:G:N2	1:A:3033:G:OP2	2.23	0.70
18:Q:248:ASP:OD1	21:T:123:GLY:N	2.25	0.69
21:T:56:ASP:OD1	21:T:72:ARG:NH2	2.25	0.69
37:i:191:ASP:OD1	37:i:194:ARG:NH2	2.25	0.69
11:J:259:ARG:NH2	11:J:277:PRO:O	2.26	0.68
28:1:267:ASP:OD2	28:1:271:ARG:NH2	2.27	0.68
2:B:280:ARG:NH2	2:B:364:LYS:O	2.26	0.68
1:A:311:G:O6	18:Q:219:ARG:NH1	2.27	0.68
1:A:1083:U:O2	1:A:1091:G:N1	2.27	0.67
29:2:350:TYR:OH	33:6:323:ARG:NH2	2.28	0.67
1:A:3033:G:O2'	1:A:3062:U:O4	2.13	0.67
3:C:100:ARG:O	3:C:104:THR:OG1	2.13	0.66
21:T:80:GLU:O	42:d:161:ARG:NH2	2.27	0.66
1:A:2008:U:OP2	1:A:2013:A:N6	2.29	0.66
1:A:3452:A:OP2	32:5:218:ARG:NH1	2.29	0.65
18:Q:75:THR:OG1	18:Q:78:ASN:OD1	2.15	0.65
42:d:108:GLN:OE1	42:d:112:ARG:NH2	2.30	0.65
9:H:9:ARG:NH2	39:a:225:ILE:O	2.30	0.64
43:n:166:MET:SD	43:n:276:GLN:NE2	2.70	0.64
3:C:206:ASP:OD2	3:C:335:ARG:NH2	2.31	0.64
1:A:1152:U:O2'	12:K:134:ARG:NH2	2.30	0.64
38:9:80:LEU:O	39:a:151:ARG:NH2	2.31	0.63
14:M:145:ARG:NH2	14:M:187:ASN:OD1	2.32	0.63
1:A:2028:G:OP1	2:B:357:ARG:NH1	2.29	0.63
1:A:1201:G:O6	12:K:76:LYS:NZ	2.30	0.63
1:A:2758:U:O2'	1:A:2759:U:OP1	2.17	0.63
18:Q:72:ASP:OD1	18:Q:73:GLU:N	2.32	0.62
42:d:94:GLN:OE1	42:d:96:GLN:NE2	2.32	0.62
21:T:157:ASN:OD1	21:T:160:ARG:NH1	2.32	0.62
32:5:204:TYR:OH	38:9:196:MET:O	2.16	0.62
28:1:269:GLY:O	28:1:271:ARG:NH2	2.33	0.62
1:A:473:G:N7	20:S:147:ARG:NH2	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:93:ALA:O	8:g:101:ARG:NH1	2.33	0.61
18:Q:196:GLU:OE2	18:Q:197:TYR:N	2.33	0.61
1:A:3094:A:OP1	9:H:94:ARG:NH1	2.33	0.61
2:B:172:ASP:N	2:B:291:ILE:O	2.34	0.61
4:D:160:ASP:OD2	4:D:162:SER:OG	2.18	0.60
1:A:822:U:N3	1:A:823:G:O6	2.35	0.60
23:V:62:GLN:NE2	23:V:78:MET:SD	2.74	0.60
12:K:103:ASP:OD2	12:K:106:ARG:NH1	2.32	0.60
1:A:831:U:OP1	1:A:854:A:O2'	2.17	0.60
16:O:206:ARG:NH1	24:W:80:MET:SD	2.73	0.60
1:A:2785:A:O2'	1:A:2786:A:OP2	2.19	0.59
32:5:106:THR:O	32:5:120:ASN:ND2	2.35	0.59
18:Q:147:GLU:OE1	18:Q:177:ARG:NH1	2.36	0.59
1:A:2958:C:O2	1:A:3034:G:N2	2.33	0.59
1:A:599:A:OP2	15:N:187:ARG:NH1	2.34	0.59
1:A:536:G:N2	1:A:539:A:OP2	2.36	0.58
1:A:1537:G:OP1	24:W:78:ARG:NH1	2.32	0.58
1:A:615:G:O2'	1:A:2254:G:OP1	2.22	0.58
29:2:326:GLU:OE2	29:2:326:GLU:N	2.32	0.58
28:1:219:PHE:O	28:1:340:ARG:NH1	2.36	0.58
12:K:101:MET:O	12:K:167:ASN:N	2.36	0.58
1:A:3024:A:OP1	3:C:256:SER:OG	2.23	0.57
10:I:82:ASP:OD1	10:I:82:ASP:N	2.37	0.57
19:R:284:ARG:O	40:b:136:ARG:NH1	2.38	0.57
1:A:3007:U:O2'	1:A:3008:C:O4'	2.21	0.57
26:Y:137:ARG:NE	26:Y:140:ALA:O	2.37	0.57
4:D:81:GLU:OE2	4:D:285:ARG:NE	2.37	0.57
18:Q:110:SER:HB2	18:Q:111:PRO:HD2	1.88	0.56
23:V:67:SER:O	29:2:361:ARG:NH2	2.39	0.56
32:5:313:LYS:NZ	32:5:417:ASP:OD1	2.38	0.56
1:A:3389:G:O2'	1:A:3409:A:N6	2.39	0.56
32:5:346:ARG:O	38:9:65:ARG:NH2	2.38	0.56
1:A:1247:G:N7	41:c:30:ARG:NH1	2.53	0.56
1:A:1916:U:OP2	1:A:1917:A:N6	2.39	0.56
9:H:3:GLN:NE2	16:O:359:ARG:O	2.38	0.56
1:A:1229:G:OP2	1:A:1229:G:N2	2.39	0.55
21:T:132:ARG:NH1	30:3:77:ASP:OD1	2.40	0.55
32:5:146:LEU:O	38:9:140:ARG:NH2	2.40	0.55
1:A:1108:U:OP2	1:A:1119:A:O2'	2.24	0.55
1:A:2955:U:O2'	1:A:3037:U:OP2	2.25	0.55
31:4:81:ARG:NH1	31:4:107:GLY:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:d:68:GLN:NE2	42:d:210:ASN:O	2.40	0.55
21:T:171:GLU:OE1	21:T:171:GLU:N	2.40	0.54
1:A:888:U:OP1	26:Y:111:ARG:NH1	2.40	0.54
1:A:2310:U:OP2	1:A:2440:G:O2'	2.24	0.54
1:A:2759:U:O2	45:A:3607:NAD:N7N	2.40	0.54
1:A:319:C:O2	18:Q:219:ARG:NH2	2.41	0.54
1:A:614:G:OP1	1:A:1528:U:O2'	2.24	0.54
16:O:296:PHE:O	16:O:317:THR:HG22	2.08	0.54
33:6:149:ARG:NH2	33:6:152:VAL:O	2.39	0.54
14:M:170:ASN:OD1	14:M:171:HIS:N	2.41	0.54
16:O:184:GLU:OE2	16:O:332:ARG:NE	2.36	0.54
1:A:1034:C:O2'	22:U:42:GLN:O	2.26	0.53
8:g:118:LYS:NZ	37:i:102:LEU:O	2.40	0.53
10:I:114:GLU:N	10:I:114:GLU:OE2	2.41	0.53
20:S:93:THR:OG1	20:S:140:ARG:NH1	2.38	0.53
11:J:82:THR:HG22	11:J:83:LYS:HG2	1.89	0.53
1:A:3047:G:N2	1:A:3050:A:OP2	2.39	0.53
1:A:1865:G:N2	1:A:1868:A:OP2	2.38	0.53
1:A:927:U:O2'	1:A:1895:U:OP1	2.26	0.53
31:4:125:ARG:NH2	39:a:72:ASN:O	2.40	0.53
33:6:282:VAL:HG12	33:6:282:VAL:O	2.09	0.53
14:M:46:ASN:O	14:M:64:VAL:N	2.41	0.52
42:d:88:ALA:O	42:d:134:LEU:N	2.37	0.52
28:1:105:GLU:O	28:1:116:ARG:NH1	2.42	0.52
32:5:119:ASN:OD1	32:5:119:ASN:C	2.52	0.52
33:6:217:ARG:NH2	33:6:235:ASP:OD2	2.44	0.51
1:A:450:G:OP2	20:S:166:ARG:NH2	2.43	0.51
1:A:3313:G:OP1	1:A:3313:G:N2	2.43	0.51
1:A:600:C:OP2	15:N:187:ARG:NH2	2.43	0.51
1:A:2251:U:O2'	24:W:66:PRO:O	2.27	0.51
1:A:2488:U:OP1	25:X:8:ARG:NH2	2.40	0.51
1:A:2582:G:OP2	19:R:356:ARG:NH2	2.43	0.51
1:A:605:U:O4'	1:A:1191:G:O2'	2.28	0.51
9:H:2:SER:O	31:4:123:SER:OG	2.25	0.51
18:Q:208:ARG:N	18:Q:222:ARG:O	2.43	0.51
1:A:3372:G:OP1	3:C:162:ARG:NH1	2.39	0.51
18:Q:34:GLN:NE2	18:Q:95:GLU:OE1	2.43	0.51
43:n:231:ASP:OD1	43:n:231:ASP:N	2.43	0.51
15:N:157:ALA:HB3	15:N:158:PRO:CD	2.41	0.50
5:E:62:SER:OG	5:E:63:GLU:N	2.44	0.50
1:A:1203:U:OP1	12:K:107:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:143:ALA:O	37:i:147:ALA:N	2.43	0.50
1:A:94:G:O2'	30:3:16:ARG:NH2	2.44	0.50
1:A:2900:A:H3'	1:A:2901:A:H5''	1.93	0.50
32:5:208:GLU:N	32:5:208:GLU:OE1	2.45	0.50
1:A:2689:G:O6	28:1:367:GLU:N	2.42	0.50
4:D:300:VAL:HG23	4:D:300:VAL:O	2.12	0.50
1:A:2851:G:O2'	25:X:21:GLY:O	2.26	0.50
1:A:3334:C:OP1	3:C:217:ARG:NH1	2.44	0.50
5:E:186:GLU:OE2	5:E:337:GLN:NE2	2.44	0.50
18:Q:164:GLN:NE2	18:Q:169:LYS:O	2.45	0.50
19:R:174:GLU:N	19:R:174:GLU:OE1	2.45	0.49
35:8:195:GLU:OE1	35:8:339:ARG:NE	2.45	0.49
1:A:1352:U:OP1	7:f:74:ARG:NH1	2.43	0.49
20:S:42:TYR:OH	20:S:93:THR:O	2.26	0.49
35:8:238:LEU:O	35:8:238:LEU:HG	2.12	0.49
1:A:995:U:O2'	1:A:1496:U:O2	2.29	0.49
1:A:2925:A:O2'	1:A:2926:C:O4'	2.29	0.49
2:B:373:ASN:ND2	2:B:376:VAL:O	2.45	0.49
1:A:2684:U:O4	1:A:2685:A:N6	2.46	0.49
37:i:95:ASN:ND2	37:i:95:ASN:O	2.45	0.49
33:6:325:MET:SD	33:6:325:MET:N	2.86	0.48
1:A:2952:C:O2'	1:A:2954:A:N1	2.43	0.48
1:A:2040:U:O2'	1:A:2041:A:OP2	2.26	0.48
19:R:336:THR:O	19:R:340:GLY:N	2.44	0.48
1:A:1199:A:OP2	12:K:78:ARG:NH1	2.46	0.48
4:D:181:ARG:NH2	4:D:275:LEU:O	2.43	0.48
1:A:601:C:OP1	15:N:185:LYS:NZ	2.40	0.48
16:O:154:ARG:NH2	35:8:426:GLY:O	2.45	0.48
1:A:526:G:O2'	1:A:527:A:P	2.72	0.48
1:A:3033:G:O2'	1:A:3035:G:N7	2.46	0.48
17:P:160:LYS:NZ	18:Q:168:ASP:O	2.42	0.48
26:Y:117:ARG:NH1	26:Y:138:LEU:O	2.47	0.48
7:f:148:THR:O	7:f:152:PHE:HB3	2.14	0.47
9:H:8:THR:N	16:O:352:ASP:OD1	2.47	0.47
12:K:87:THR:O	12:K:87:THR:OG1	2.30	0.47
36:h:25:LEU:O	36:h:28:SER:OG	2.31	0.47
1:A:2883:A:O2'	1:A:2884:A:O5'	2.32	0.47
18:Q:105:VAL:HG12	18:Q:105:VAL:O	2.13	0.47
19:R:287:ARG:NH1	40:b:133:GLU:OE2	2.47	0.47
21:T:80:GLU:OE2	42:d:207:GLY:N	2.47	0.47
33:6:170:ASP:OD1	33:6:170:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:A:N6	1:A:1373:A:O4'	2.48	0.47
8:g:43:MET:SD	8:g:43:MET:N	2.88	0.47
17:P:159:THR:OG1	17:P:161:ASP:OD1	2.27	0.47
1:A:640:G:OP1	34:7:94:ARG:NH2	2.47	0.47
1:A:1251:C:O2'	9:H:127:MET:O	2.33	0.47
4:D:235:LYS:NZ	4:D:236:GLU:OE2	2.46	0.47
5:E:308:GLU:N	5:E:308:GLU:OE2	2.45	0.47
2:B:295:ILE:HG13	2:B:296:MET:HG2	1.97	0.46
8:g:28:SER:O	8:g:32:GLY:N	2.41	0.46
8:g:42:SER:O	8:g:45:PHE:N	2.49	0.46
1:A:989:C:O2	1:A:2894:A:O2'	2.32	0.46
33:6:156:ASP:OD1	33:6:156:ASP:N	2.49	0.46
33:6:177:GLN:O	33:6:180:SER:OG	2.30	0.46
40:b:103:ARG:O	40:b:107:GLY:N	2.48	0.46
4:D:238:GLY:O	4:D:239:ARG:HG3	2.15	0.46
28:1:267:ASP:OD2	28:1:267:ASP:C	2.59	0.46
29:2:357:GLU:OE1	33:6:101:THR:OG1	2.34	0.46
37:i:161:GLU:OE1	37:i:161:GLU:N	2.49	0.46
20:S:106:ASN:N	20:S:115:THR:O	2.43	0.46
1:A:1388:U:H4'	1:A:1389:A:O4'	2.16	0.46
1:A:1726:A:O2'	1:A:1727:U:O5'	2.29	0.46
4:D:63:THR:O	4:D:85:ALA:N	2.46	0.46
1:A:2758:U:C2'	1:A:2759:U:OP1	2.63	0.46
7:f:58:ASP:OD2	7:f:58:ASP:N	2.49	0.46
35:8:220:ASP:OD2	35:8:224:ARG:NE	2.47	0.46
1:A:1930:U:O2'	2:B:76:ARG:NH1	2.48	0.45
1:A:3037:U:O2'	1:A:3038:A:O4'	2.26	0.45
4:D:181:ARG:NH2	4:D:278:THR:O	2.40	0.45
5:E:97:GLY:O	5:E:103:GLN:NE2	2.42	0.45
16:O:293:ASN:O	16:O:318:THR:OG1	2.25	0.45
16:O:257:ALA:O	16:O:261:GLU:N	2.49	0.45
2:B:253:GLU:N	2:B:253:GLU:OE1	2.49	0.45
14:M:188:VAL:HG23	14:M:188:VAL:O	2.17	0.45
1:A:909:A:O2'	1:A:910:A:P	2.75	0.45
1:A:2026:U:O2'	2:B:356:THR:OG1	2.31	0.45
22:U:40:GLU:OE2	22:U:42:GLN:NE2	2.48	0.45
15:N:119:THR:OG1	31:4:121:ASN:ND2	2.49	0.45
1:A:525:A:O2'	1:A:526:G:H3'	2.17	0.45
1:A:2584:U:O4	1:A:2585:A:N6	2.50	0.45
14:M:219:VAL:HG12	14:M:219:VAL:O	2.16	0.45
1:A:541:G:N7	26:Y:135:ARG:NH1	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2924:U:O4	1:A:2925:A:N6	2.49	0.44
1:A:3004:U:H3'	1:A:3005:G:C5'	2.46	0.44
21:T:149:GLU:OE1	21:T:152:ARG:NH2	2.50	0.44
1:A:1330:A:OP2	37:i:198:ARG:NH2	2.47	0.44
1:A:826:C:O2'	1:A:859:U:OP1	2.34	0.44
1:A:2963:U:H2'	1:A:2964:G:O4'	2.18	0.44
45:A:3607:NAD:H8A	45:A:3607:NAD:PA	2.58	0.44
12:K:91:THR:O	12:K:134:ARG:NH1	2.51	0.44
14:M:74:LEU:HD12	14:M:75:PRO:O	2.18	0.44
1:A:1396:A:OP2	41:c:32:ARG:NH2	2.45	0.44
1:A:1689:G:OP2	2:B:92:TYR:OH	2.33	0.44
1:A:111:U:OP1	30:3:78:GLN:O	2.36	0.44
4:D:71:SER:O	4:D:75:LEU:N	2.44	0.44
14:M:178:GLU:OE2	14:M:210:ARG:NE	2.51	0.44
25:X:7:SER:O	25:X:30:ARG:NH2	2.50	0.44
40:b:10:LEU:O	40:b:13:SER:OG	2.35	0.44
1:A:381:U:OP1	26:Y:125:LYS:NZ	2.43	0.43
1:A:2883:A:HO2'	1:A:2884:A:C5'	2.32	0.43
6:F:123:ASN:N	6:F:129:GLN:OE1	2.51	0.43
26:Y:118:VAL:O	26:Y:124:GLN:NE2	2.50	0.43
28:1:251:ASP:OD1	28:1:252:SER:N	2.50	0.43
35:8:309:ASP:OD2	35:8:309:ASP:N	2.49	0.43
3:C:118:THR:OG1	3:C:119:VAL:N	2.50	0.43
1:A:1458:G:N2	1:A:1459:U:O4	2.51	0.43
1:A:3345:U:OP1	3:C:350:HIS:NE2	2.46	0.43
3:C:91:SER:OG	9:H:113:LYS:O	2.34	0.43
30:3:73:ARG:HH11	30:3:73:ARG:HG3	1.84	0.43
8:g:75:HIS:O	8:g:75:HIS:CG	2.71	0.43
16:O:241:LYS:NZ	18:Q:72:ASP:OD1	2.49	0.43
21:T:69:SER:O	42:d:34:THR:OG1	2.31	0.43
35:8:401:VAL:HG21	35:8:425:LEU:HD21	2.00	0.43
39:a:98:ASN:OD1	39:a:98:ASN:N	2.33	0.43
1:A:1514:A:HO2'	31:4:37:SER:HG	1.59	0.43
32:5:229:ASP:OD1	32:5:229:ASP:C	2.60	0.43
1:A:55:A:H2	1:A:3079:A:H2'	1.83	0.42
1:A:633:G:O2'	11:J:58:GLY:O	2.30	0.42
1:A:2829:U:OP1	5:E:100:HIS:ND1	2.47	0.42
1:A:2883:A:O2'	1:A:2884:A:P	2.77	0.42
33:6:334:ASN:HD22	33:6:334:ASN:C	2.25	0.42
39:a:97:ALA:O	39:a:98:ASN:C	2.63	0.42
2:B:61:ASP:OD1	2:B:66:ARG:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:8:433:TYR:CZ	35:8:435:GLU:HB2	2.54	0.42
1:A:2895:G:OP1	4:D:138:ARG:NH1	2.44	0.42
4:D:210:LYS:N	4:D:210:LYS:HD2	2.34	0.42
12:K:144:SER:O	12:K:144:SER:OG	2.33	0.42
32:5:228:ASP:O	38:9:146:ARG:NH1	2.50	0.42
1:A:2758:U:O2'	1:A:2759:U:P	2.78	0.42
1:A:2967:U:O4	1:A:2968:A:N6	2.52	0.42
3:C:213:VAL:HG21	3:C:317:LYS:HG3	2.01	0.42
1:A:1247:G:H2'	1:A:1248:G:O4'	2.19	0.42
2:B:243:ALA:HB1	2:B:294:ASN:O	2.19	0.42
34:7:141:VAL:N	34:7:142:PRO:CD	2.82	0.42
1:A:360:G:OP2	20:S:116:ARG:NH2	2.49	0.42
1:A:3111:G:N2	1:A:3114:A:OP2	2.50	0.42
13:L:36:HIS:O	13:L:105:LYS:NZ	2.49	0.42
9:H:108:ASP:OD1	9:H:109:ALA:N	2.53	0.42
43:n:283:ARG:NE	43:n:289:GLU:OE2	2.52	0.42
16:O:153:VAL:HG13	35:8:423:PRO:HD3	2.02	0.41
28:1:398:GLU:OE2	28:1:402:ARG:NH1	2.52	0.41
39:a:96:ARG:NH2	39:a:96:ARG:HB2	2.35	0.41
1:A:16:A:O3'	38:9:134:ARG:NH1	2.53	0.41
1:A:1221:G:O2'	1:A:1402:A:O2'	2.36	0.41
4:D:210:LYS:H	4:D:210:LYS:CD	2.33	0.41
7:f:129:THR:O	7:f:129:THR:HG22	2.20	0.41
16:O:139:ASP:OD2	18:Q:152:LYS:NZ	2.53	0.41
21:T:134:LYS:O	21:T:193:ARG:NH1	2.50	0.41
28:1:167:GLU:OE2	28:1:170:LYS:NZ	2.53	0.41
32:5:117:GLN:O	32:5:118:PHE:HB2	2.20	0.41
33:6:171:GLU:H	33:6:171:GLU:CD	2.28	0.41
33:6:218:ARG:NE	33:6:222:ASP:OD2	2.53	0.41
5:E:157:ARG:NH2	5:E:183:PRO:O	2.52	0.41
10:I:127:ALA:N	10:I:128:PRO:CD	2.83	0.41
29:2:248:ASP:N	29:2:249:PRO:CD	2.83	0.41
1:A:106:A:H5'	1:A:107:U:C5'	2.50	0.41
16:O:50:LYS:O	16:O:50:LYS:CG	2.69	0.41
20:S:108:SER:OG	20:S:112:GLU:N	2.54	0.41
31:4:49:LEU:N	31:4:50:PRO:CD	2.84	0.41
43:n:174:GLU:OE1	43:n:234:THR:OG1	2.38	0.41
43:n:249:ASP:OD2	43:n:268:GLN:NE2	2.54	0.41
19:R:105:TRP:O	19:R:119:ILE:HD11	2.20	0.41
1:A:520:U:H4'	1:A:521:A:H5'	2.03	0.41
1:A:871:G:H2'	1:A:872:A:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:A:OP2	22:U:18:ARG:NH1	2.54	0.41
1:A:3016:A:OP2	43:n:212:ARG:NH2	2.54	0.41
1:A:3107:G:O2'	1:A:3116:G:O6	2.36	0.41
5:E:331:THR:O	5:E:331:THR:HG22	2.21	0.41
7:f:109:ARG:NH2	7:f:134:LEU:O	2.54	0.41
10:I:4:LEU:O	10:I:5:LYS:HB2	2.21	0.41
18:Q:191:ASP:O	18:Q:195:GLY:N	2.46	0.41
1:A:49:G:OP1	3:C:78:ARG:NH2	2.53	0.41
1:A:3124:G:O6	3:C:317:LYS:NZ	2.45	0.41
1:A:2896:G:H2'	1:A:2897:G:O4'	2.22	0.40
15:N:157:ALA:HB3	15:N:158:PRO:HD3	2.03	0.40
32:5:177:ALA:H	35:8:407:VAL:HG12	1.85	0.40
34:7:89:ARG:NH2	34:7:165:PHE:O	2.49	0.40
1:A:1150:U:N3	5:E:162:GLU:O	2.51	0.40
1:A:2900:A:H3'	1:A:2901:A:C5'	2.51	0.40
14:M:151:ALA:O	14:M:170:ASN:ND2	2.47	0.40
23:V:61:THR:OG1	33:6:156:ASP:OD2	2.39	0.40
28:1:205:ARG:HA	28:1:209:TYR:HB3	2.04	0.40
36:h:35:ARG:NH1	36:h:39:MET:O	2.54	0.40
1:A:1484:A:O2'	1:A:1511:G:N2	2.52	0.40
1:A:1726:A:O2'	1:A:1727:U:C6	2.75	0.40
6:F:169:ARG:NE	6:F:192:GLU:OE1	2.53	0.40
6:F:181:VAL:HG13	6:F:181:VAL:O	2.21	0.40
13:L:58:ARG:O	13:L:86:ARG:NH1	2.54	0.40
1:A:909:A:H4'	1:A:910:A:OP1	2.22	0.40
1:A:2807:A:N6	28:1:422:PRO:O	2.47	0.40
16:O:258:ALA:O	16:O:262:THR:OG1	2.33	0.40
1:A:10:G:N1	39:a:188:GLN:OE1	2.44	0.40
1:A:2883:A:N1	20:S:111:ASN:ND2	2.64	0.40
1:A:2956:G:N2	1:A:3006:U:O2'	2.54	0.40
45:A:3607:NAD:H8A	45:A:3607:NAD:O2A	2.21	0.40
14:M:142:THR:O	14:M:189:ALA:N	2.50	0.40
33:6:171:GLU:CD	33:6:171:GLU:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	313/383 (82%)	310 (99%)	3 (1%)	0	100	100
3	C	305/384 (79%)	298 (98%)	7 (2%)	0	100	100
4	D	250/325 (77%)	246 (98%)	4 (2%)	0	100	100
5	E	307/352 (87%)	306 (100%)	1 (0%)	0	100	100
6	F	199/255 (78%)	196 (98%)	3 (2%)	0	100	100
7	f	243/347 (70%)	238 (98%)	5 (2%)	0	100	100
8	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
9	H	181/183 (99%)	178 (98%)	3 (2%)	0	100	100
10	I	115/131 (88%)	111 (96%)	4 (4%)	0	100	100
11	J	241/312 (77%)	235 (98%)	6 (2%)	0	100	100
12	K	153/249 (61%)	151 (99%)	2 (1%)	0	100	100
13	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
14	M	192/258 (74%)	187 (97%)	5 (3%)	0	100	100
15	N	131/217 (60%)	126 (96%)	5 (4%)	0	100	100
16	O	268/364 (74%)	262 (98%)	6 (2%)	0	100	100
17	P	178/228 (78%)	178 (100%)	0	0	100	100
18	Q	351/396 (89%)	349 (99%)	2 (1%)	0	100	100
19	R	227/447 (51%)	223 (98%)	4 (2%)	0	100	100
20	S	175/274 (64%)	172 (98%)	3 (2%)	0	100	100
21	T	169/263 (64%)	167 (99%)	2 (1%)	0	100	100
22	U	134/161 (83%)	134 (100%)	0	0	100	100
23	V	54/219 (25%)	54 (100%)	0	0	100	100
24	W	57/129 (44%)	55 (96%)	2 (4%)	0	100	100
25	X	46/59 (78%)	46 (100%)	0	0	100	100
26	Y	44/140 (31%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	44/124 (36%)	44 (100%)	0	0	100	100
28	1	365/449 (81%)	360 (99%)	5 (1%)	0	100	100
29	2	121/370 (33%)	120 (99%)	1 (1%)	0	100	100
30	3	93/103 (90%)	90 (97%)	3 (3%)	0	100	100
31	4	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
32	5	346/439 (79%)	343 (99%)	3 (1%)	0	100	100
33	6	267/368 (73%)	263 (98%)	4 (2%)	0	100	100
34	7	82/165 (50%)	80 (98%)	2 (2%)	0	100	100
35	8	329/443 (74%)	325 (99%)	4 (1%)	0	100	100
36	h	92/98 (94%)	91 (99%)	1 (1%)	0	100	100
37	i	117/218 (54%)	111 (95%)	6 (5%)	0	100	100
38	9	204/267 (76%)	199 (98%)	5 (2%)	0	100	100
39	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
40	b	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
41	c	96/110 (87%)	94 (98%)	2 (2%)	0	100	100
42	d	231/292 (79%)	230 (100%)	1 (0%)	0	100	100
43	n	182/699 (26%)	175 (96%)	7 (4%)	0	100	100
All	All	7688/11097 (69%)	7568 (98%)	120 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	261/312 (84%)	260 (100%)	1 (0%)	84	87
3	C	242/303 (80%)	241 (100%)	1 (0%)	84	87
4	D	216/274 (79%)	215 (100%)	1 (0%)	81	86
5	E	267/296 (90%)	263 (98%)	4 (2%)	57	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	173/216 (80%)	172 (99%)	1 (1%)	78	85
7	f	206/287 (72%)	206 (100%)	0	100	100
8	g	120/124 (97%)	120 (100%)	0	100	100
9	H	149/149 (100%)	149 (100%)	0	100	100
10	I	100/105 (95%)	96 (96%)	4 (4%)	28	59
11	J	198/255 (78%)	198 (100%)	0	100	100
12	K	135/205 (66%)	134 (99%)	1 (1%)	76	84
13	L	164/165 (99%)	164 (100%)	0	100	100
14	M	164/209 (78%)	163 (99%)	1 (1%)	78	85
15	N	119/188 (63%)	119 (100%)	0	100	100
16	O	235/315 (75%)	232 (99%)	3 (1%)	61	79
17	P	158/196 (81%)	157 (99%)	1 (1%)	78	85
18	Q	312/347 (90%)	311 (100%)	1 (0%)	86	88
19	R	196/359 (55%)	192 (98%)	4 (2%)	48	73
20	S	159/242 (66%)	158 (99%)	1 (1%)	78	85
21	T	153/224 (68%)	153 (100%)	0	100	100
22	U	118/138 (86%)	118 (100%)	0	100	100
23	V	52/170 (31%)	52 (100%)	0	100	100
24	W	50/102 (49%)	50 (100%)	0	100	100
25	X	46/54 (85%)	46 (100%)	0	100	100
26	Y	38/116 (33%)	38 (100%)	0	100	100
27	0	41/108 (38%)	41 (100%)	0	100	100
28	1	316/384 (82%)	314 (99%)	2 (1%)	78	85
29	2	109/317 (34%)	109 (100%)	0	100	100
30	3	83/91 (91%)	80 (96%)	3 (4%)	31	62
31	4	113/114 (99%)	113 (100%)	0	100	100
32	5	279/351 (80%)	276 (99%)	3 (1%)	65	80
33	6	238/310 (77%)	234 (98%)	4 (2%)	53	75
34	7	69/136 (51%)	66 (96%)	3 (4%)	26	57
35	8	285/378 (75%)	282 (99%)	3 (1%)	65	80
36	h	85/88 (97%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	i	99/162 (61%)	99 (100%)	0	100	100
38	9	176/225 (78%)	175 (99%)	1 (1%)	78	85
39	a	146/196 (74%)	145 (99%)	1 (1%)	76	84
40	b	141/141 (100%)	139 (99%)	2 (1%)	59	78
41	c	86/96 (90%)	86 (100%)	0	100	100
42	d	201/243 (83%)	200 (100%)	1 (0%)	81	86
43	n	157/590 (27%)	155 (99%)	2 (1%)	61	79
All	All	6655/9281 (72%)	6606 (99%)	49 (1%)	73	84

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	109	HIS
3	C	285	ILE
4	D	210	LYS
5	E	93	LYS
5	E	96	ARG
5	E	108	SER
5	E	109	ASP
6	F	251	GLN
10	I	3	GLN
10	I	5	LYS
10	I	81	ARG
10	I	82	ASP
12	K	87	THR
14	M	81	THR
16	O	53	VAL
16	O	356	THR
16	O	357	SER
17	P	53	PHE
18	Q	116	ILE
19	R	111	THR
19	R	190	VAL
19	R	292	MET
19	R	296	SER
20	S	52	ILE
28	1	271	ARG
28	1	427	ARG
30	3	10	LEU
30	3	69	SER

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Mol	Chain	Res	Type
30	3	71	THR
32	5	153	SER
32	5	371	VAL
32	5	433	MET
33	6	171	GLU
33	6	172	VAL
33	6	174	VAL
33	6	334	ASN
34	7	109	LEU
34	7	111	GLN
34	7	114	LYS
35	8	230	MET
35	8	362	PHE
35	8	423	PRO
38	9	147	GLN
39	a	98	ASN
40	b	67	LYS
40	b	119	VAL
42	d	208	LYS
43	n	170	THR
43	n	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	83	ASN
3	C	149	ASN
3	C	155	GLN
3	C	232	HIS
3	C	237	GLN
3	C	246	ASN
4	D	89	HIS
4	D	125	HIS
6	F	251	GLN
9	H	85	HIS
9	H	114	HIS
10	I	3	GLN
11	J	113	ASN
11	J	228	HIS
13	L	24	ASN
14	M	45	HIS
15	N	112	HIS

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Mol	Chain	Res	Type
17	P	29	HIS
17	P	78	ASN
17	P	98	GLN
18	Q	140	ASN
18	Q	143	ASN
18	Q	161	GLN
18	Q	332	GLN
19	R	193	HIS
19	R	266	ASN
20	S	162	HIS
21	T	122	HIS
21	T	178	ASN
22	U	94	GLN
23	V	59	GLN
25	X	11	ASN
25	X	53	GLN
28	1	287	HIS
28	1	295	HIS
28	1	348	GLN
28	1	362	HIS
29	2	284	HIS
29	2	306	HIS
31	4	30	HIS
32	5	189	GLN
33	6	84	GLN
33	6	296	HIS
33	6	334	ASN
35	8	218	ASN
35	8	242	ASN
35	8	378	GLN
36	h	92	GLN
39	a	141	ASN
39	a	187	HIS
39	a	201	ASN
42	d	114	GLN
43	n	178	HIS
43	n	268	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2505/3464 (72%)	349 (13%)	12 (0%)

All (349) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A
1	A	48	A
1	A	78	C
1	A	79	A
1	A	90	A
1	A	98	A
1	A	99	U
1	A	104	U
1	A	106	A
1	A	107	U
1	A	118	G
1	A	311	G
1	A	317	A
1	A	319	C
1	A	334	U
1	A	337	A
1	A	347	U
1	A	348	A
1	A	350	U
1	A	351	A
1	A	353	A
1	A	367	A
1	A	370	A
1	A	376	U
1	A	387	A
1	A	392	A
1	A	393	A
1	A	395	U
1	A	414	U
1	A	419	U
1	A	435	A

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Mol	Chain	Res	Type
1	A	440	A
1	A	441	U
1	A	443	A
1	A	447	U
1	A	448	A
1	A	462	U
1	A	477	A
1	A	478	U
1	A	486	A
1	A	522	C
1	A	526	G
1	A	527	A
1	A	548	U
1	A	569	G
1	A	571	A
1	A	581	A
1	A	583	A
1	A	584	A
1	A	587	A
1	A	599	A
1	A	609	U
1	A	610	A
1	A	611	A
1	A	639	A
1	A	829	A
1	A	839	A
1	A	840	U
1	A	845	A
1	A	846	A
1	A	849	U
1	A	855	A
1	A	858	G
1	A	888	U
1	A	909	A
1	A	910	A
1	A	914	U
1	A	931	U
1	A	948	A
1	A	958	A
1	A	960	C
1	A	967	A
1	A	969	G

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Mol	Chain	Res	Type
1	A	974	C
1	A	985	A
1	A	988	G
1	A	995	U
1	A	1011	A
1	A	1013	A
1	A	1042	G
1	A	1054	A
1	A	1060	G
1	A	1070	A
1	A	1071	G
1	A	1080	A
1	A	1081	C
1	A	1094	A
1	A	1107	U
1	A	1108	U
1	A	1109	U
1	A	1118	C
1	A	1119	A
1	A	1122	G
1	A	1140	U
1	A	1141	A
1	A	1160	C
1	A	1190	A
1	A	1206	G
1	A	1219	A
1	A	1235	A
1	A	1242	G
1	A	1248	G
1	A	1254	A
1	A	1257	U
1	A	1258	U
1	A	1267	G
1	A	1268	U
1	A	1271	A
1	A	1280	A
1	A	1287	A
1	A	1289	A
1	A	1292	A
1	A	1303	A
1	A	1307	G
1	A	1316	A

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Mol	Chain	Res	Type
1	A	1331	A
1	A	1333	G
1	A	1334	A
1	A	1358	A
1	A	1377	U
1	A	1379	U
1	A	1380	A
1	A	1381	A
1	A	1382	C
1	A	1389	A
1	A	1415	A
1	A	1431	A
1	A	1452	G
1	A	1453	A
1	A	1457	G
1	A	1484	A
1	A	1487	U
1	A	1494	U
1	A	1495	A
1	A	1496	U
1	A	1509	A
1	A	1522	U
1	A	1526	A
1	A	1529	G
1	A	1546	A
1	A	1565	A
1	A	1566	A
1	A	1567	A
1	A	1568	A
1	A	1578	G
1	A	1589	A
1	A	1590	A
1	A	1591	A
1	A	1595	U
1	A	1604	G
1	A	1605	U
1	A	1613	C
1	A	1620	U
1	A	1626	U
1	A	1627	A
1	A	1634	G
1	A	1648	U

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Mol	Chain	Res	Type
1	A	1695	A
1	A	1703	A
1	A	1719	A
1	A	1722	A
1	A	1726	A
1	A	1727	U
1	A	1842	A
1	A	1843	A
1	A	1844	U
1	A	1852	A
1	A	1866	A
1	A	1880	U
1	A	1884	U
1	A	1910	G
1	A	1917	A
1	A	1921	A
1	A	1922	C
1	A	1923	C
1	A	1924	G
1	A	1935	A
1	A	1936	U
1	A	1982	G
1	A	1986	G
1	A	1992	U
1	A	1993	U
1	A	2002	A
1	A	2020	A
1	A	2029	C
1	A	2030	A
1	A	2039	A
1	A	2041	A
1	A	2048	A
1	A	2051	A
1	A	2052	U
1	A	2226	U
1	A	2227	G
1	A	2228	U
1	A	2258	A
1	A	2265	C
1	A	2266	A
1	A	2268	A
1	A	2278	C

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Mol	Chain	Res	Type
1	A	2287	A
1	A	2290	C
1	A	2291	G
1	A	2295	A
1	A	2304	G
1	A	2327	U
1	A	2409	U
1	A	2411	A
1	A	2418	A
1	A	2419	A
1	A	2420	U
1	A	2421	U
1	A	2427	A
1	A	2439	A
1	A	2440	G
1	A	2441	A
1	A	2477	A
1	A	2478	U
1	A	2481	G
1	A	2482	U
1	A	2485	G
1	A	2486	U
1	A	2491	A
1	A	2506	G
1	A	2509	U
1	A	2511	C
1	A	2541	A
1	A	2543	C
1	A	2547	A
1	A	2548	U
1	A	2582	G
1	A	2592	A
1	A	2595	A
1	A	2596	A
1	A	2631	A
1	A	2638	A
1	A	2656	A
1	A	2658	A
1	A	2659	G
1	A	2663	U
1	A	2666	G
1	A	2685	A

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Mol	Chain	Res	Type
1	A	2686	U
1	A	2690	G
1	A	2694	G
1	A	2710	U
1	A	2711	U
1	A	2719	U
1	A	2720	U
1	A	2721	U
1	A	2722	U
1	A	2758	U
1	A	2759	U
1	A	2775	U
1	A	2784	U
1	A	2786	A
1	A	2795	U
1	A	2797	C
1	A	2806	U
1	A	2808	A
1	A	2810	A
1	A	2811	A
1	A	2836	G
1	A	2838	C
1	A	2843	G
1	A	2852	A
1	A	2858	A
1	A	2875	U
1	A	2880	G
1	A	2881	G
1	A	2882	A
1	A	2884	A
1	A	2891	G
1	A	2897	G
1	A	2898	A
1	A	2899	U
1	A	2900	A
1	A	2901	A
1	A	2909	A
1	A	2912	U
1	A	2914	C
1	A	2927	A
1	A	2942	U
1	A	2945	G

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Mol	Chain	Res	Type
1	A	2949	C
1	A	2951	U
1	A	2954	A
1	A	2955	U
1	A	2956	G
1	A	2957	U
1	A	2958	C
1	A	2969	A
1	A	2971	C
1	A	2980	U
1	A	2994	A
1	A	3005	G
1	A	3006	U
1	A	3007	U
1	A	3009	G
1	A	3018	A
1	A	3019	A
1	A	3025	C
1	A	3030	G
1	A	3034	G
1	A	3035	G
1	A	3037	U
1	A	3053	C
1	A	3054	A
1	A	3055	G
1	A	3061	U
1	A	3062	U
1	A	3063	U
1	A	3065	U
1	A	3079	A
1	A	3081	U
1	A	3082	U
1	A	3107	G
1	A	3115	G
1	A	3124	G
1	A	3125	G
1	A	3135	U
1	A	3137	U
1	A	3156	U
1	A	3169	G
1	A	3259	A
1	A	3260	C

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Mol	Chain	Res	Type
1	A	3261	A
1	A	3262	A
1	A	3263	U
1	A	3276	G
1	A	3288	A
1	A	3296	A
1	A	3310	A
1	A	3345	U
1	A	3349	A
1	A	3359	A
1	A	3413	A
1	A	3420	A
1	A	3424	A
1	A	3425	U
1	A	3428	U
1	A	3429	A
1	A	3447	A
1	A	3448	A
1	A	3449	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	526	G
1	A	909	A
1	A	1205	A
1	A	1567	A
1	A	2051	A
1	A	2482	U
1	A	2720	U
1	A	2758	U
1	A	2883	A
1	A	2890	C
1	A	2955	U
1	A	2957	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 171 ligands modelled in this entry, 169 are monoatomic - leaving 2 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
46	SPM	A	3644	-	13,13,13	0.35	0	12,12,12	0.76	0
45	NAD	A	3607	-	46,48,48	0.88	1 (2%)	64,73,73	1.38	7 (10%)

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
46	SPM	A	3644	-	-	4/11/11/11	-
45	NAD	A	3607	-	-	3/30/62/62	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	3607	NAD	C2N-N1N	-2.25	1.32	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	3607	NAD	C5A-C4A-N3A	-5.74	118.81	126.72
45	A	3607	NAD	N3A-C4A-N9A	4.42	134.69	127.17
45	A	3607	NAD	C5A-N7A-C8A	3.15	108.40	103.45
45	A	3607	NAD	C2A-N3A-C4A	3.01	119.18	111.83
45	A	3607	NAD	N9A-C8A-N7A	-2.93	109.79	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	3607	NAD	N3A-C2A-N1A	-2.66	124.56	128.58
45	A	3607	NAD	C4A-C5A-N7A	-2.61	107.59	110.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

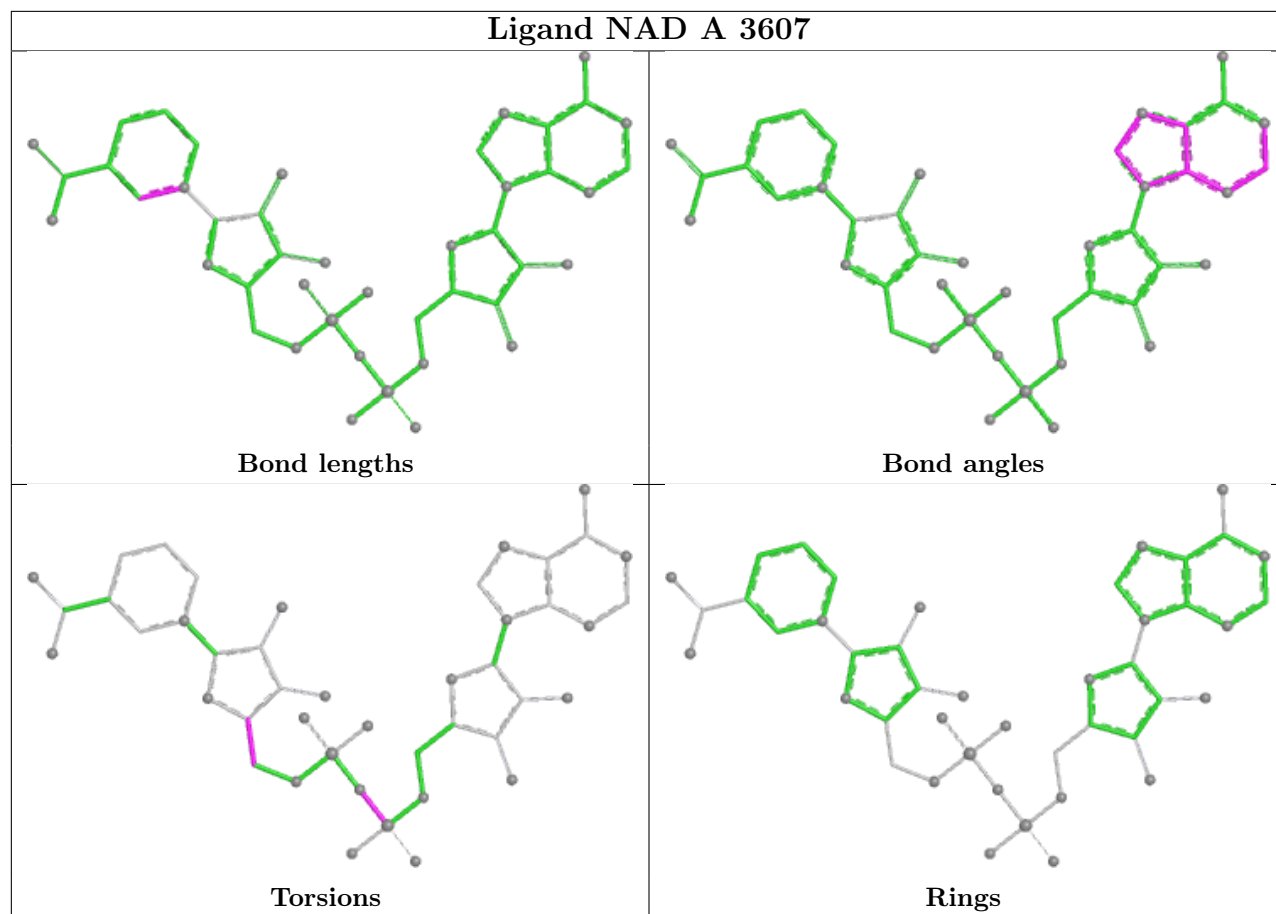
Mol	Chain	Res	Type	Atoms
46	A	3644	SPM	C7-C8-C9-N10
45	A	3607	NAD	O4D-C4D-C5D-O5D
46	A	3644	SPM	C2-C3-C4-N5
46	A	3644	SPM	C7-C6-N5-C4
45	A	3607	NAD	C3D-C4D-C5D-O5D
45	A	3607	NAD	PN-O3-PA-O1A
46	A	3644	SPM	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	3607	NAD	3	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

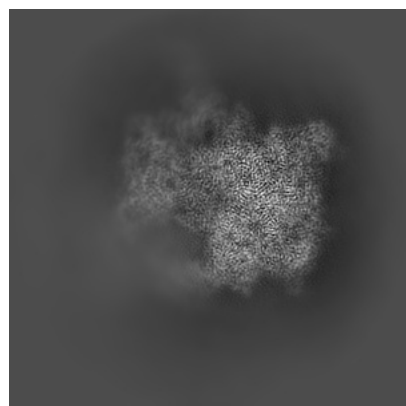
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10977. These allow visual inspection of the internal detail of the map and identification of artifacts.

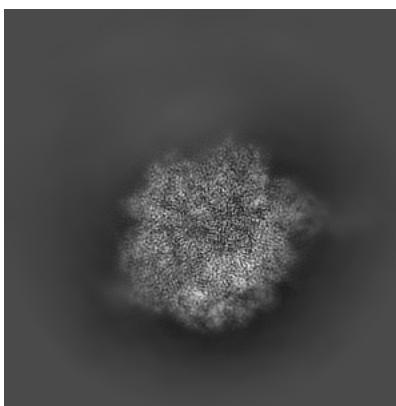
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

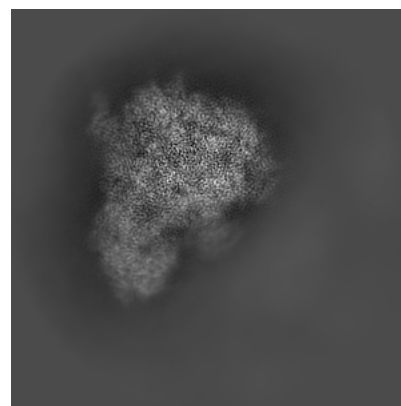
6.1.1 Primary map



X

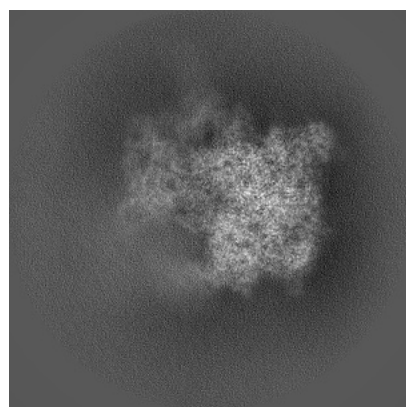


Y

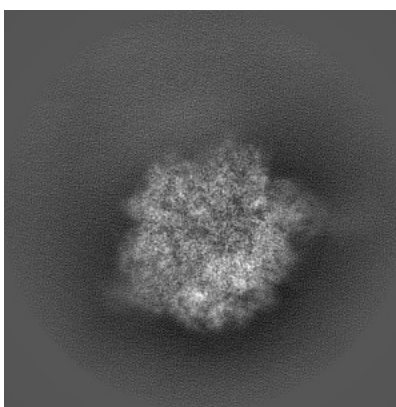


Z

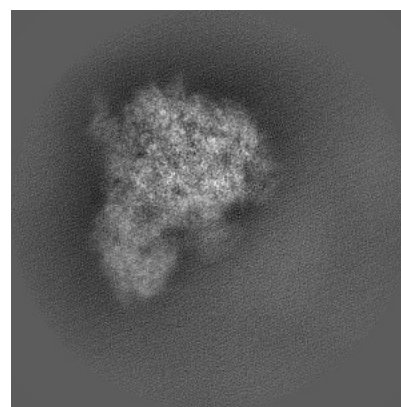
6.1.2 Raw map



X



Y

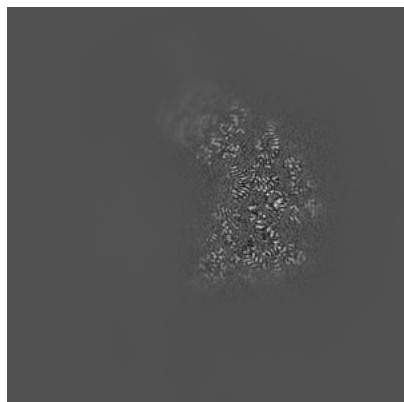


Z

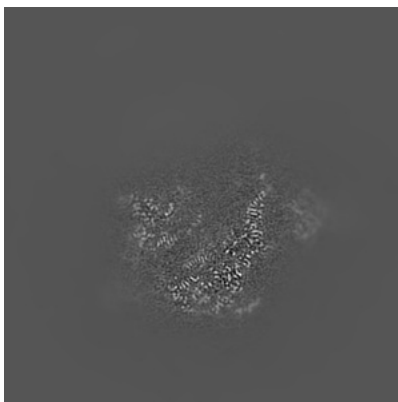
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

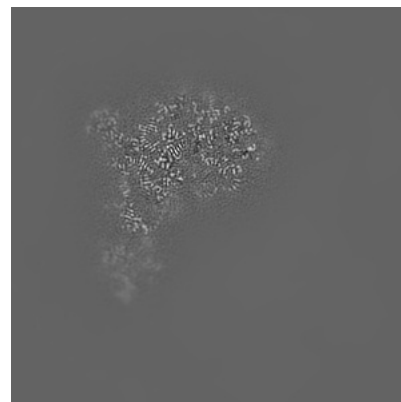
6.2.1 Primary map



X Index: 200

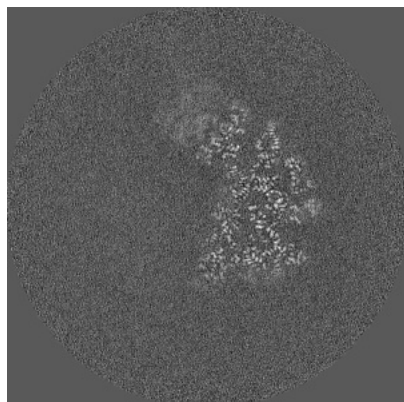


Y Index: 200

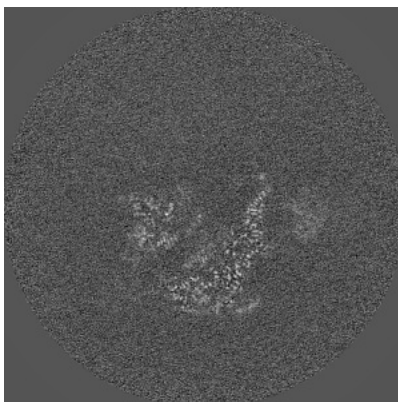


Z Index: 200

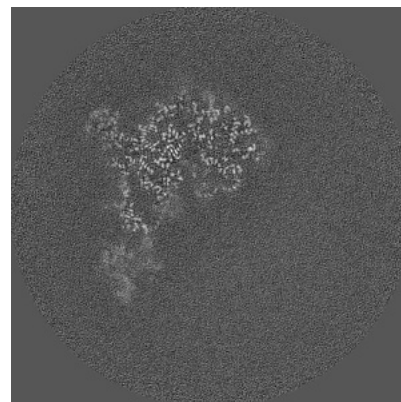
6.2.2 Raw map



X Index: 200



Y Index: 200

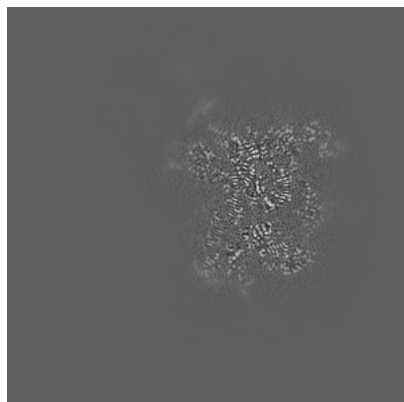


Z Index: 200

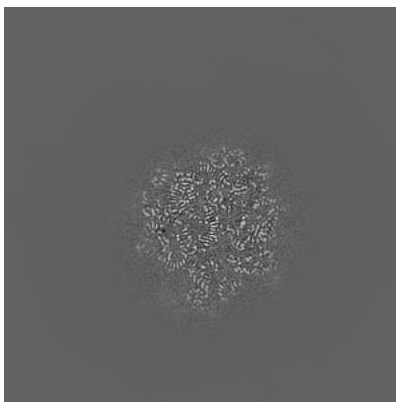
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

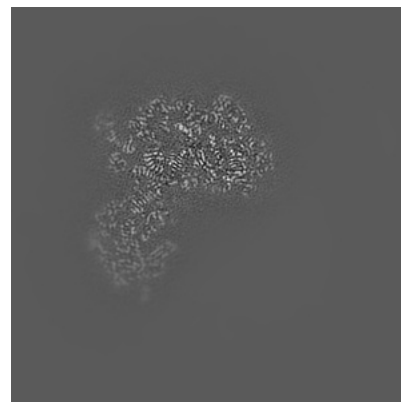
6.3.1 Primary map



X Index: 171

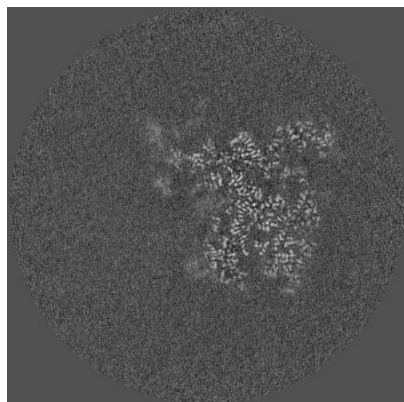


Y Index: 259

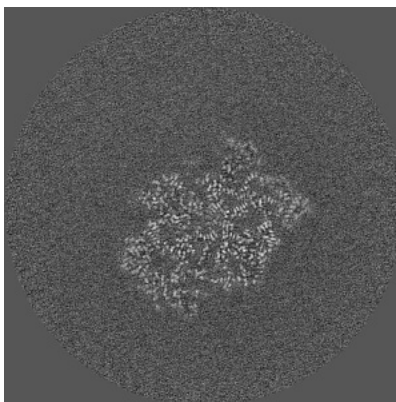


Z Index: 215

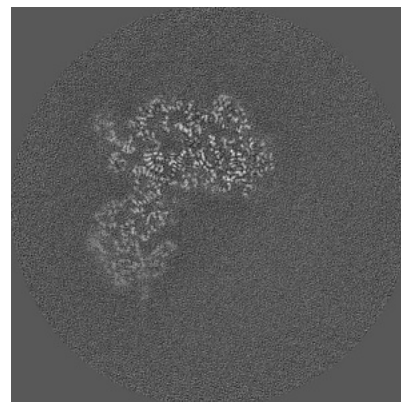
6.3.2 Raw map



X Index: 161



Y Index: 228

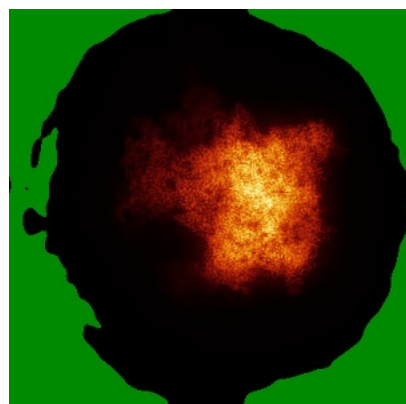


Z Index: 215

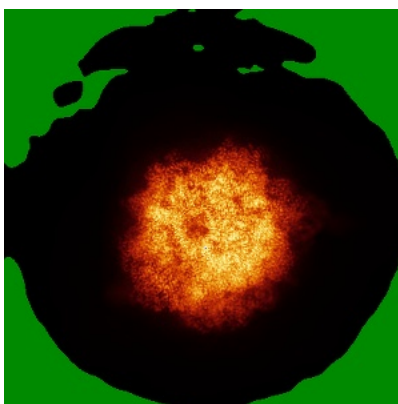
The images above show the largest variance slices of the map in three orthogonal directions.

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

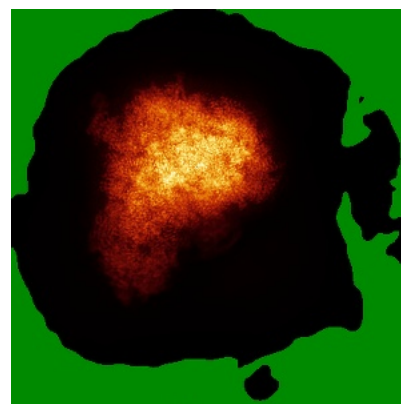
6.4.1 Primary map



X

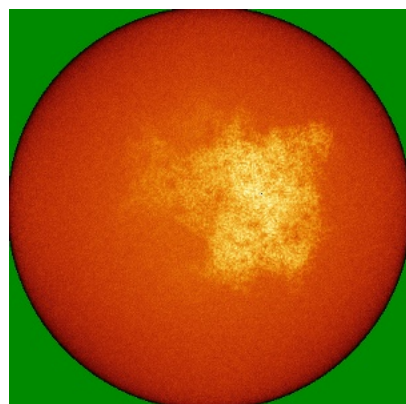


Y

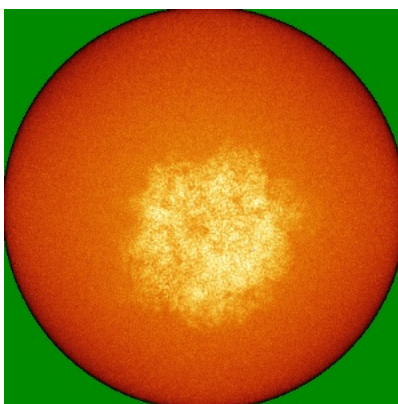


Z

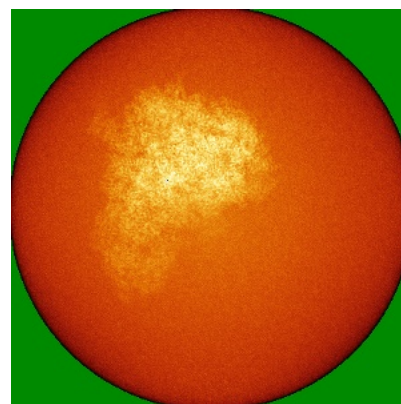
6.4.2 Raw map



X



Y

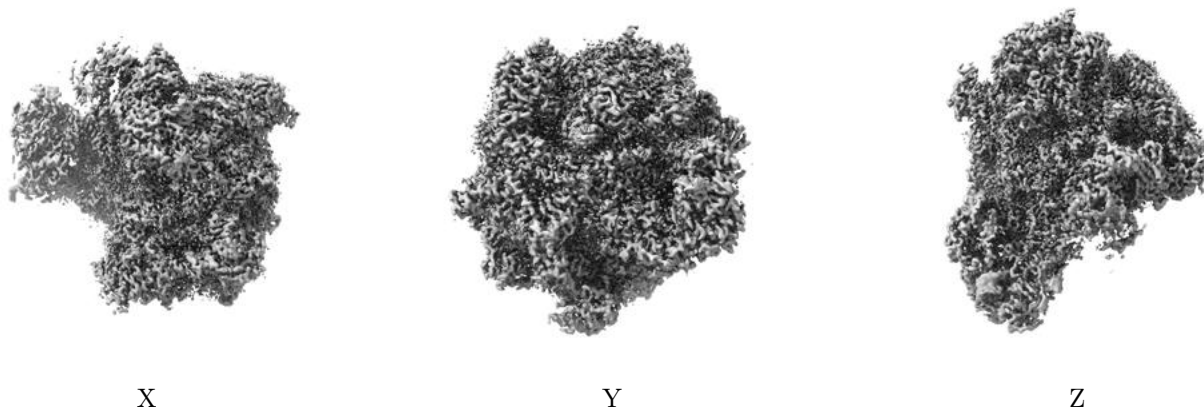


Z

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

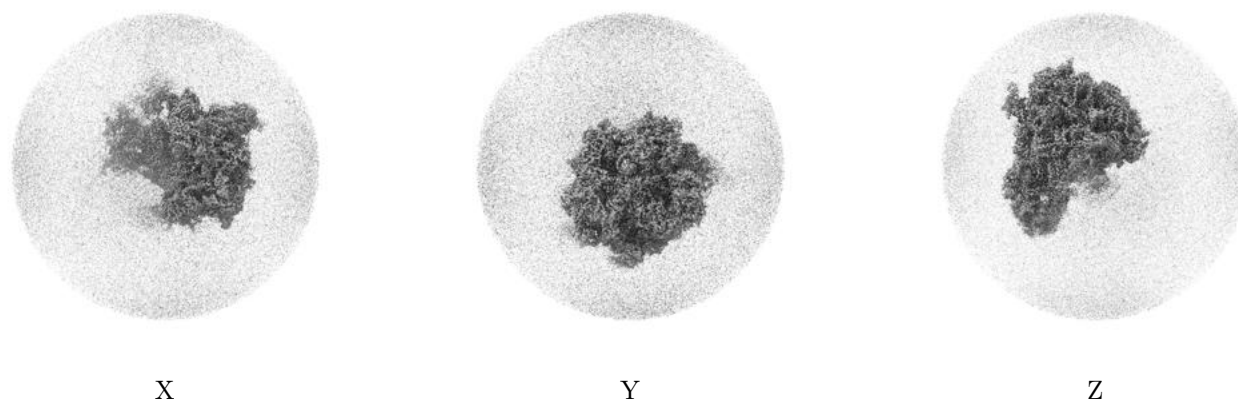
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

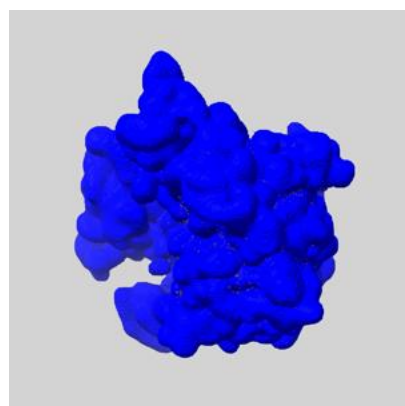
6.6 Mask visualisation [i](#)

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

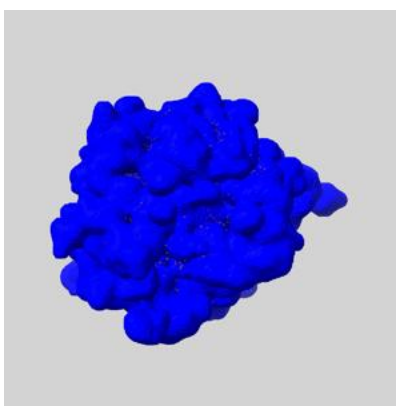
A mask typically either:

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

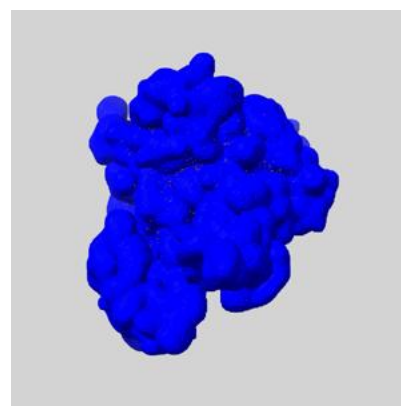
6.6.1 emd_10977_msk_1.map [i](#)



X



Y

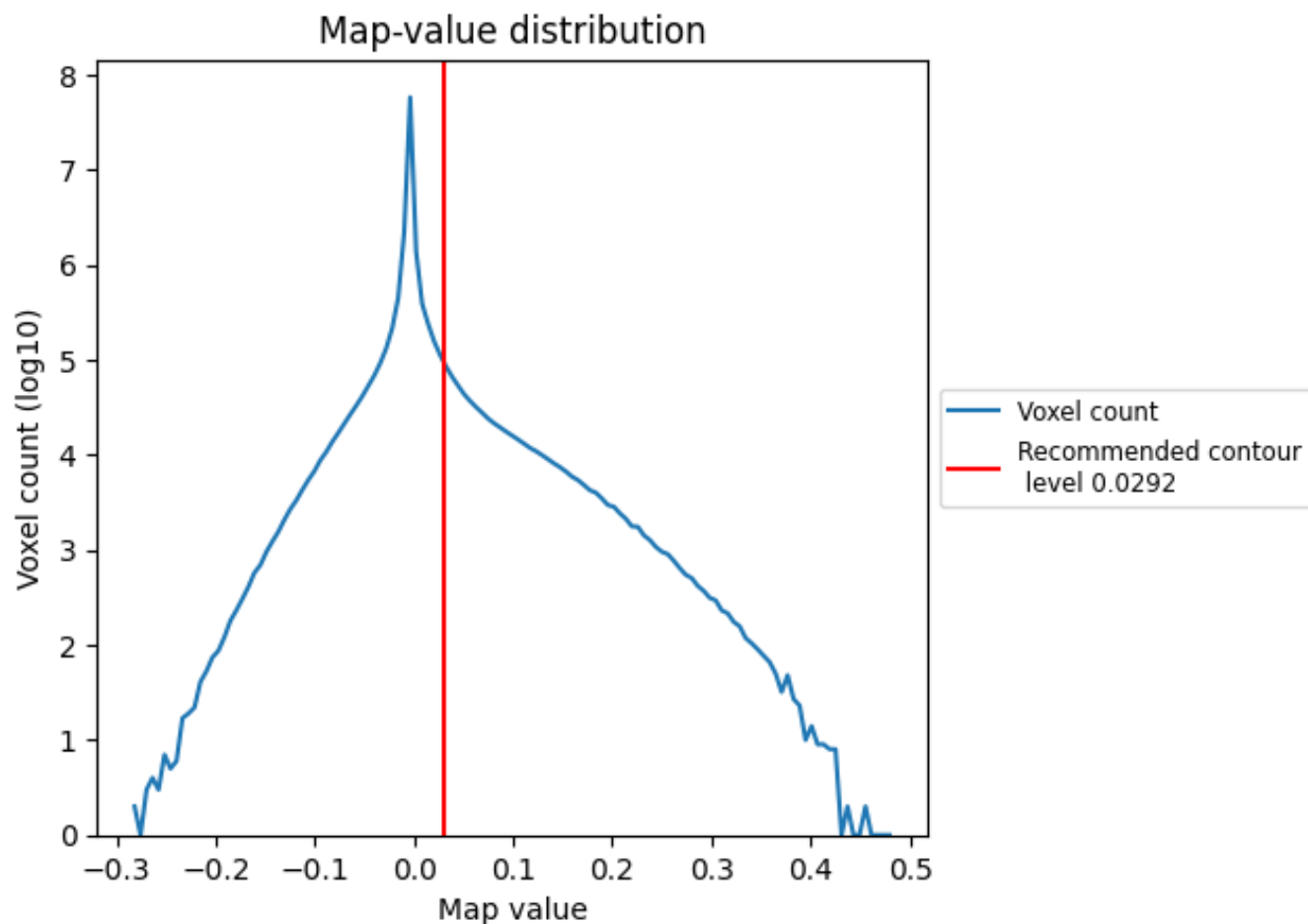


Z

7 Map analysis [i](#)

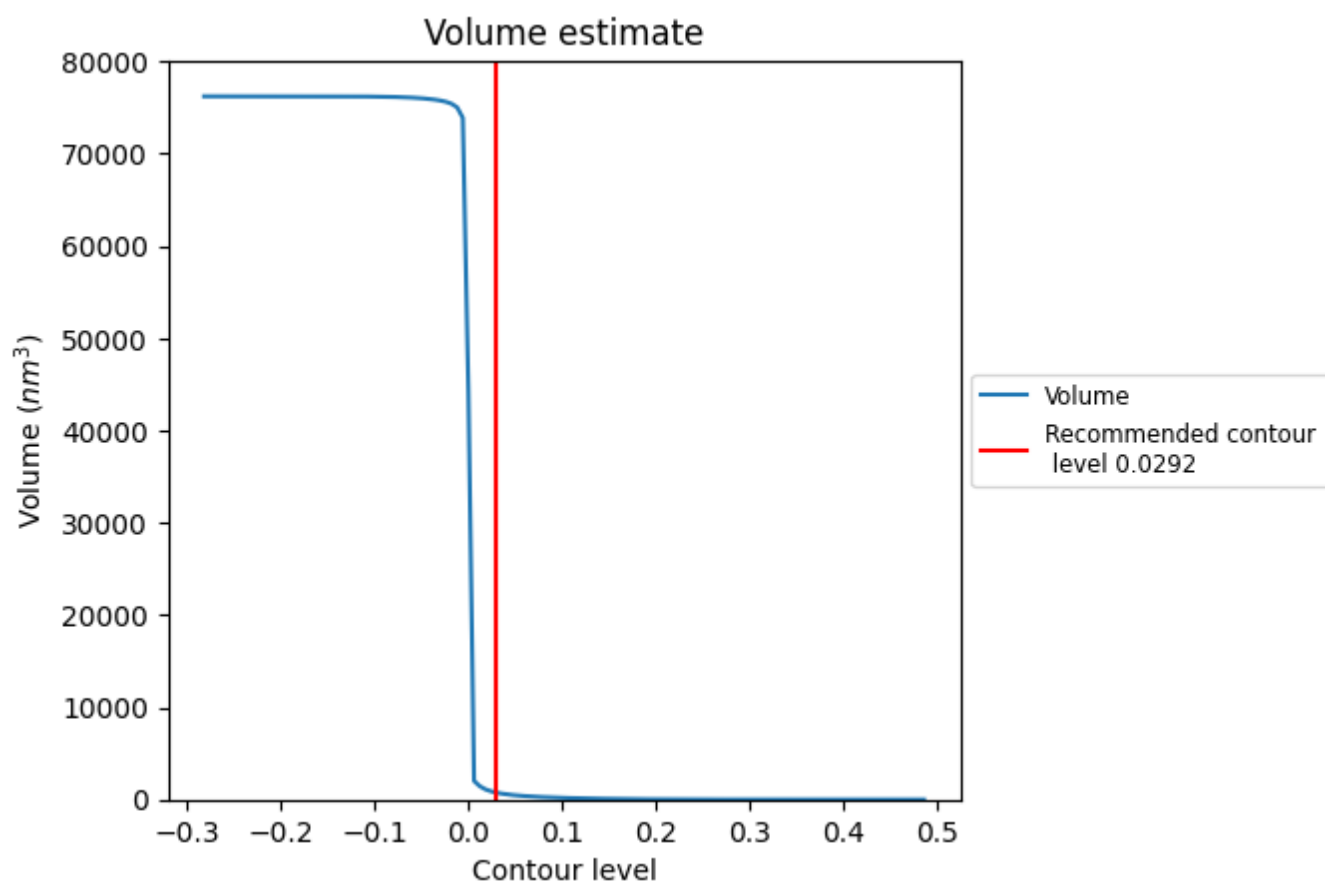
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

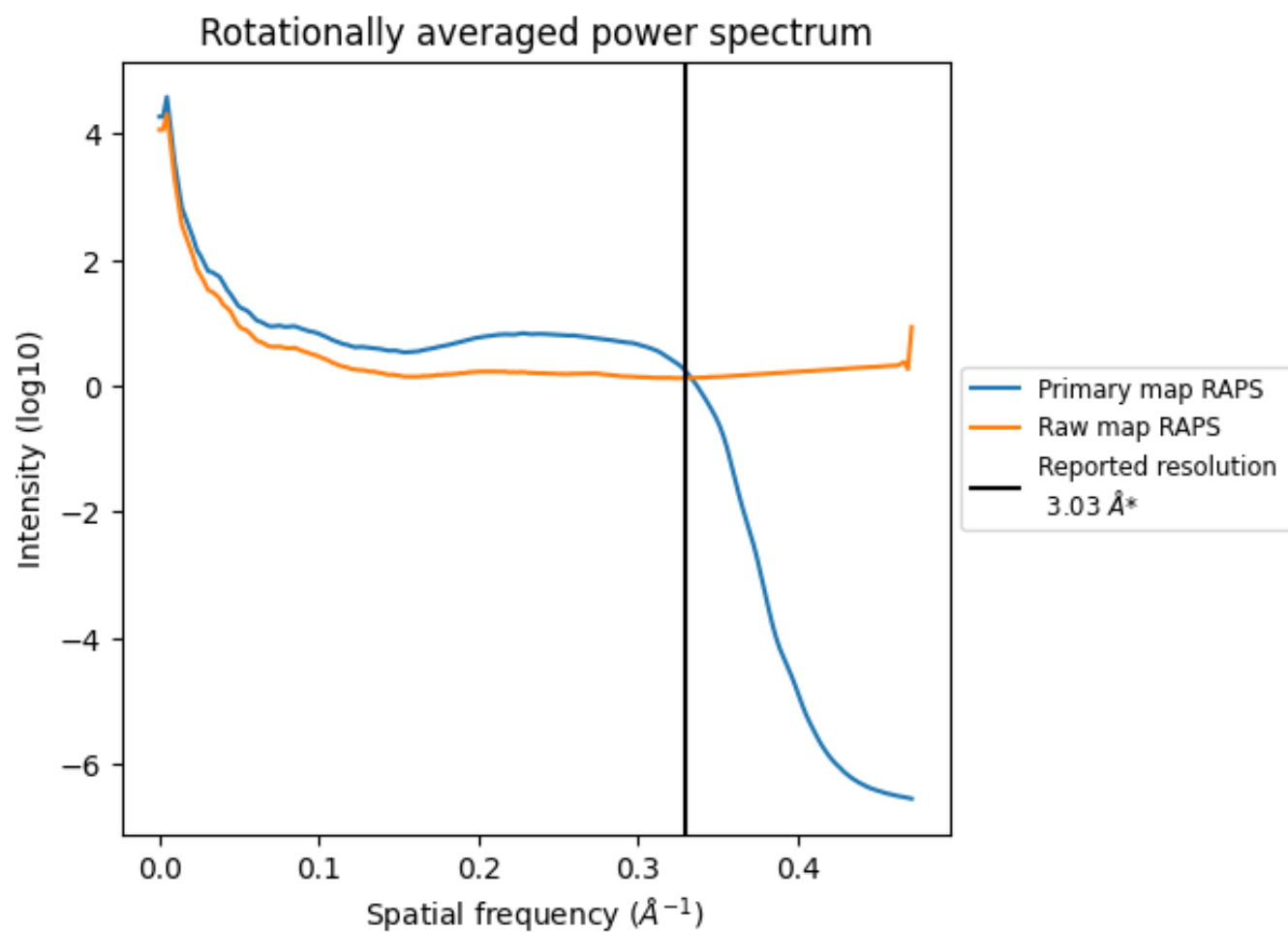
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 766 nm³; this corresponds to an approximate mass of 692 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

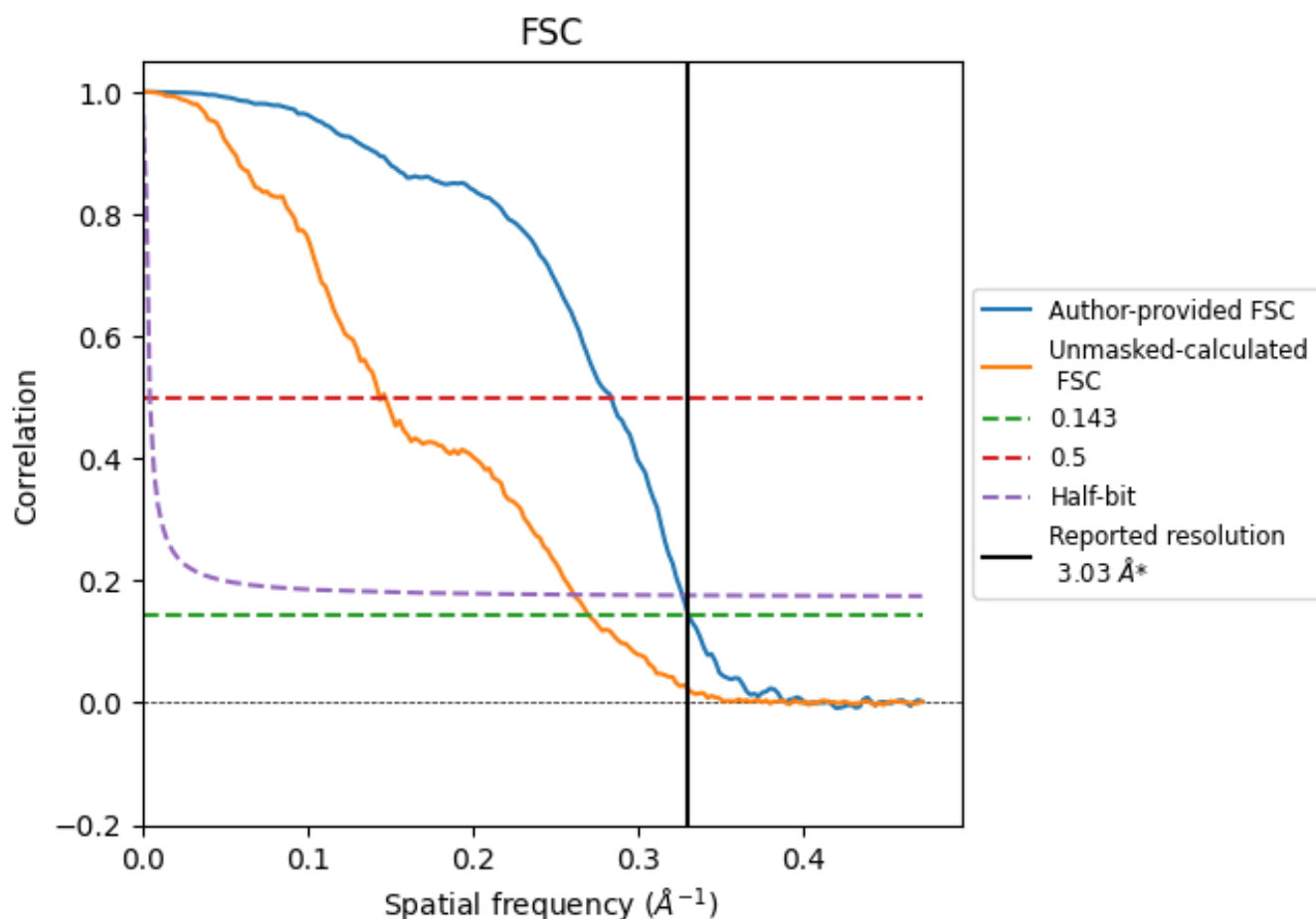


*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

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 $0.330 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

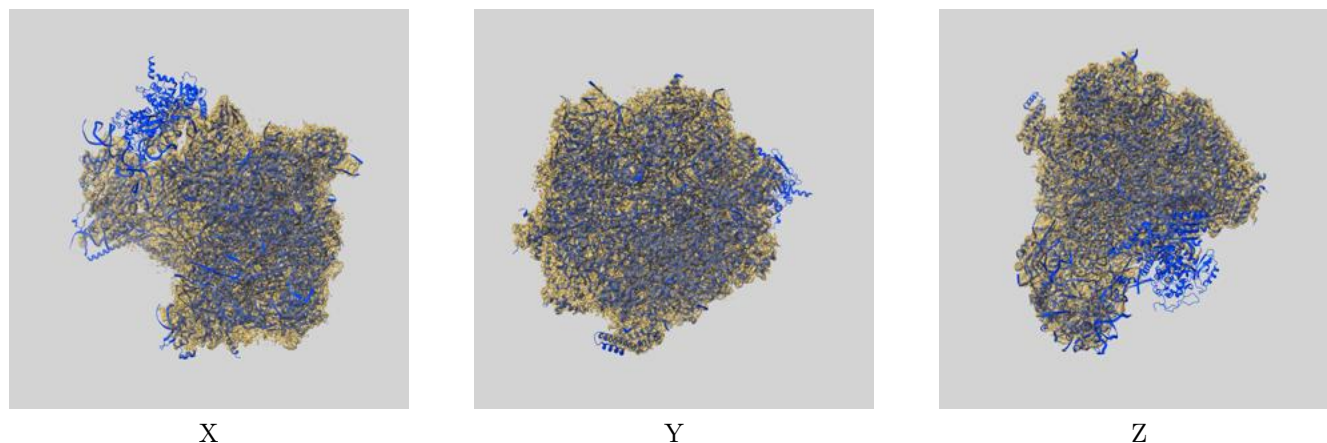
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.53	3.06
Unmasked-calculated*	3.70	6.97	3.83

*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 3.70 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

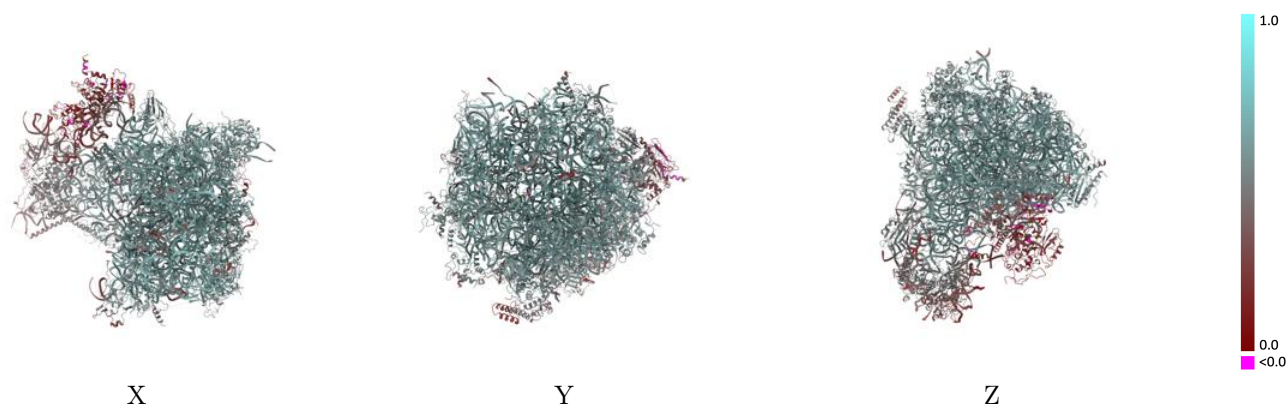
This section contains information regarding the fit between EMDB map EMD-10977 and PDB model 6YWV. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



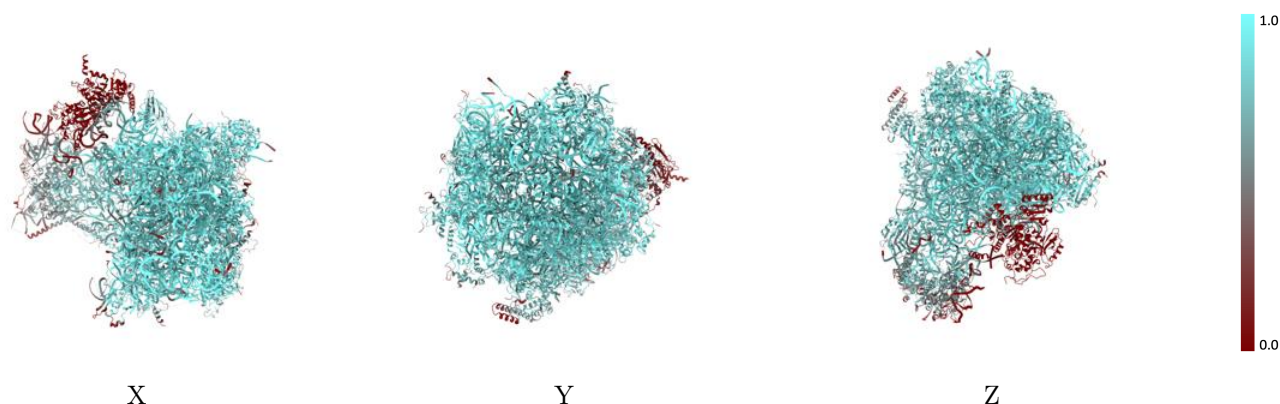
The images above show the 3D surface view of the map at the recommended contour level 0.0292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



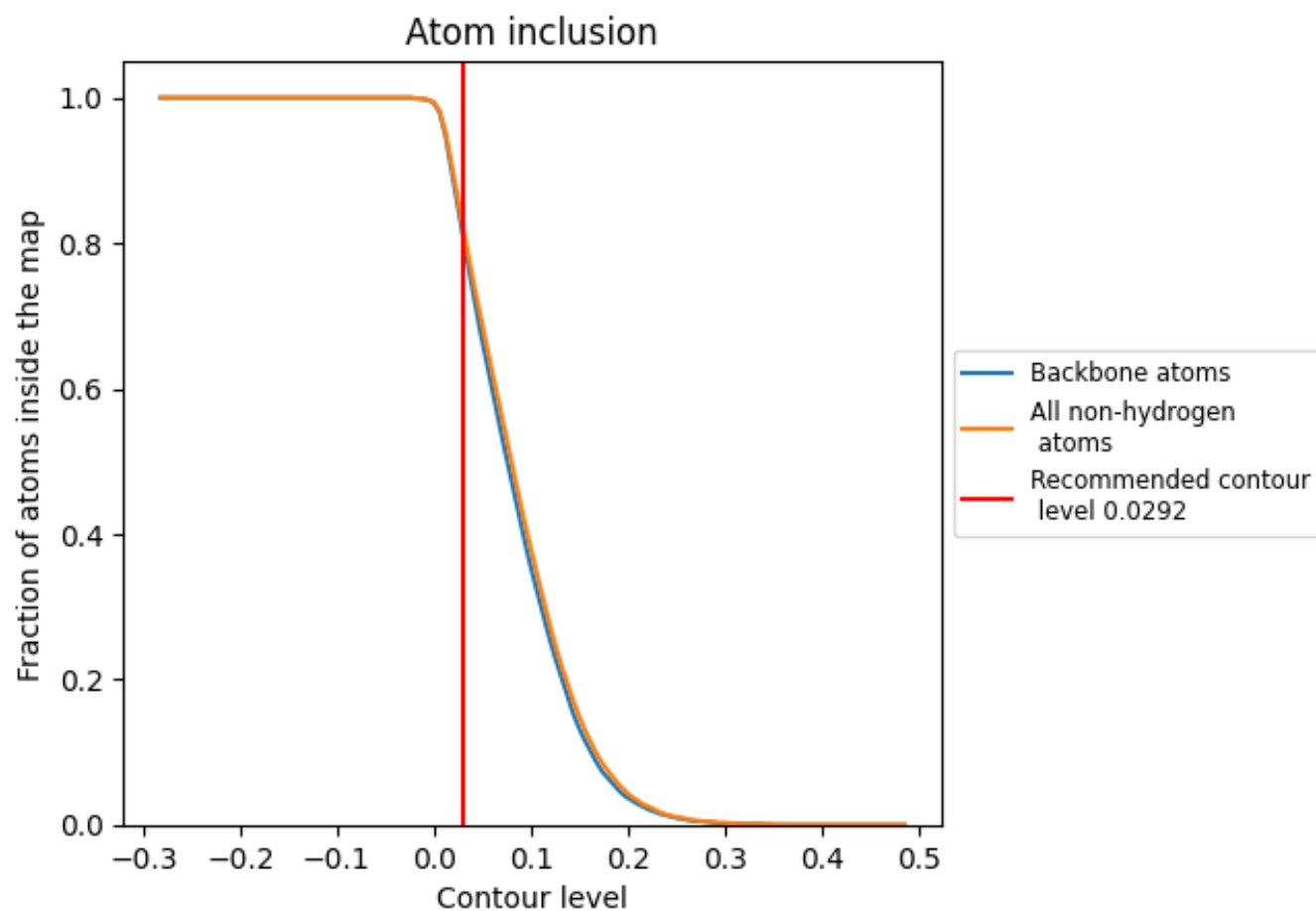
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0292).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.0292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5440
0	 0.9700	 0.6220
1	 0.7340	 0.5000
2	 0.6160	 0.4440
3	 0.9030	 0.5780
4	 0.9400	 0.6120
5	 0.8810	 0.5710
6	 0.4600	 0.3880
7	 0.8850	 0.5760
8	 0.6840	 0.4810
9	 0.8060	 0.5320
A	 0.9010	 0.5690
B	 0.8030	 0.5510
C	 0.9320	 0.6080
D	 0.8650	 0.5660
E	 0.6240	 0.4630
F	 0.8160	 0.5350
H	 0.9500	 0.6160
I	 0.9040	 0.5910
J	 0.8720	 0.5730
K	 0.8740	 0.5800
L	 0.9130	 0.5920
M	 0.8490	 0.5580
N	 0.9030	 0.5910
O	 0.8590	 0.5750
P	 0.9140	 0.5880
Q	 0.8420	 0.5530
R	 0.7140	 0.5000
S	 0.8580	 0.5630
T	 0.8790	 0.5750
U	 0.8820	 0.5790
V	 0.5470	 0.4340
W	 0.9490	 0.6040
X	 0.8940	 0.5700
Y	 0.9650	 0.6270



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Chain	Atom inclusion	Q-score
a	 0.8700	 0.5570
b	 0.8110	 0.5370
c	 0.9500	 0.6170
d	 0.8810	 0.5810
f	 0.0670	 0.2410
g	 0.0060	 0.1910
h	 0.0000	 0.1860
i	 0.0460	 0.2230
n	 0.7310	 0.5220