



## Full wwPDB EM Validation Report ⓘ

Jan 21, 2024 – 08:50 am GMT

PDB ID : 8OM3  
EMDB ID : EMD-16967  
Title : Small subunit of yeast mitochondrial ribosome in complex with IF3/Aim23.  
Authors : Itoh, Y.; Chicherin, I.; Kamenski, P.; Amunts, A.  
Deposited on : 2023-03-31  
Resolution : 2.87 Å (reported)  
Based on initial model : 5MRC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

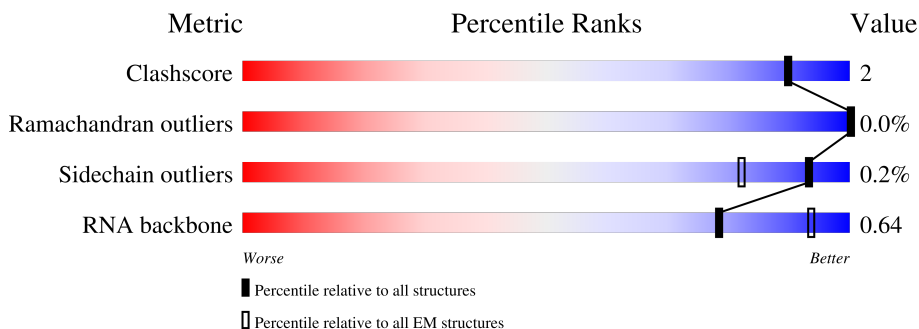
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	344	
2	B	394	
3	C	398	
4	D	486	
5	E	307	
6	F	131	
7	G	247	

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Mol	Chain	Length	Quality of chain
8	H	155	
9	I	278	
10	J	203	
11	K	217	
12	L	153	
13	M	143	
14	N	115	
15	O	286	
16	P	121	
17	Q	237	
18	R	138	
19	S	91	
20	T	177	
21	U	264	
22	V	318	
23	W	450	
24	X	110	
25	Y	319	
26	Z	95	
27	1	111	
28	2	130	
29	3	266	
30	4	321	
31	5	339	
32	6	345	

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Mol	Chain	Length	Quality of chain
33	8	500	
34	r	1647	
35	d	364	

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 166687 atoms, of which 75300 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	300	4908	1552	2481	427	441	7	1	0

- Molecule 2 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	342	5436	1709	2722	467	535	3	0	0

- Molecule 3 is a protein called Ribosomal protein VAR1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	372	6181	1930	3091	553	574	33	0	0

- Molecule 4 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	341	5729	1842	2896	499	487	5	0	0

- Molecule 5 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	294	4708	1494	2360	418	428	8	0	0

- Molecule 6 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	131	2184	671	1129	189	191	4	0	0

- Molecule 7 is a protein called 37S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	203	3272	1019	1660	289	299	5	0	0

- Molecule 8 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	155	2509	774	1286	219	221	9	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ACE	-	acetylation	UNP Q03799

- Molecule 9 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	231	3783	1181	1925	334	338	5	1	0

- Molecule 10 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	162	2655	853	1334	227	237	4	0	0

- Molecule 11 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	151	2475	775	1266	213	215	6	1	0

- Molecule 12 is a protein called 37S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	123	1932	579	993	192	164	4	0	0

- Molecule 13 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	119	1937	591	1002	178	160	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	41	LEU	PHE	variant	UNP P53937

- Molecule 14 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	N	113	1917	596	986	179	152	4	0	0

- Molecule 15 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	223	3668	1134	1853	334	339	8	0	0

- Molecule 16 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	P	120	1963	604	1011	178	168	2	0	0

- Molecule 17 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	235	3944	1208	2014	356	361	5	1	0

- Molecule 18 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	R	101	1671	507	853	162	145	4	0	0

- Molecule 19 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	79	1277	404	648	114	109	2	0	0

- Molecule 20 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	92	1569	483	800	150	131	5	1	0

- Molecule 21 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	237	3868	1228	1929	339	365	7	0	0

- Molecule 22 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	V	286	4692	1450	2398	406	434	4	0	0

- Molecule 23 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	W	402	6555	2078	3329	542	598	8	0	0

- Molecule 24 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	X	98	1619	503	832	142	139	3	0	0

- Molecule 25 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	Y	272	4514	1436	2241	408	425	4	0	0

- Molecule 26 is a protein called 37S ribosomal protein MRP10, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	Z	92	1487	459	758	137	127	6	0	0

- Molecule 27 is a protein called Mitochondrial mRNA-processing protein COX24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	1	31	613	170	334	68	39	2	0	0

- Molecule 28 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	2	102	1724	544	866	161	152	1	0	0

- Molecule 29 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	3	257	4103	1326	2040	349	383	5	0	0

- Molecule 30 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	4	303	4859	1538	2423	422	466	10	0	0

- Molecule 31 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	5	291	4770	1524	2409	404	429	4	0	0

- Molecule 32 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	6	319	5208	1646	2615	467	474	6	0	0

- Molecule 33 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	8	467	7371	2341	3681	621	708	20	0	0

- Molecule 34 is a RNA chain called 15S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
34	r	1487	47450	14212	15844	5580	10326	1488	1	0

- Molecule 35 is a protein called Altered inheritance of mitochondria protein 23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	d	144	2449	750	1254	218	222	5	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	357	LEU	-	expression tag	UNP P47015
d	358	GLU	-	expression tag	UNP P47015
d	359	HIS	-	expression tag	UNP P47015
d	360	HIS	-	expression tag	UNP P47015
d	361	HIS	-	expression tag	UNP P47015
d	362	HIS	-	expression tag	UNP P47015
d	363	HIS	-	expression tag	UNP P47015
d	364	HIS	-	expression tag	UNP P47015

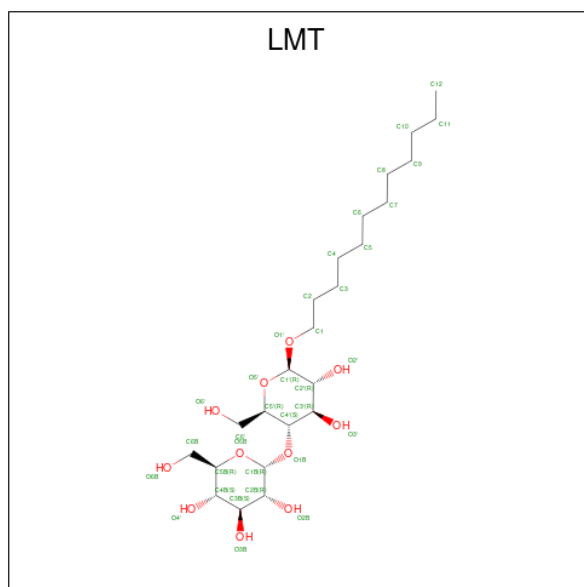
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	B	1	Total	Mg	0
			1	1	
36	K	1	Total	Mg	0
			1	1	
36	W	1	Total	Mg	0
			1	1	
36	r	93	Total	Mg	0
			93	93	

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
37	M	1	Total K 1 1	0
37	r	25	Total K 25 25	0

- Molecule 38 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms	AltConf
38	O	1	Total C H O 38 12 25 1	0

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms		AltConf
40	M	1	Total 1	O 1	0
40	N	28	Total 28	O 28	0
40	O	18	Total 18	O 18	0
40	P	25	Total 25	O 25	0
40	S	2	Total 2	O 2	0
40	T	9	Total 9	O 9	0
40	U	8	Total 8	O 8	0
40	V	5	Total 5	O 5	0
40	W	22	Total 22	O 22	0
40	X	8	Total 8	O 8	0
40	Y	18	Total 18	O 18	0
40	Z	5	Total 5	O 5	0
40	1	3	Total 3	O 3	0
40	2	4	Total 4	O 4	0
40	3	1	Total 1	O 1	0
40	6	12	Total 12	O 12	0
40	8	2	Total 2	O 2	0
40	r	1140	Total 1140	O 1140	0




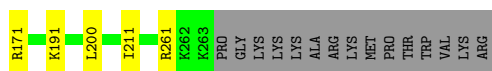
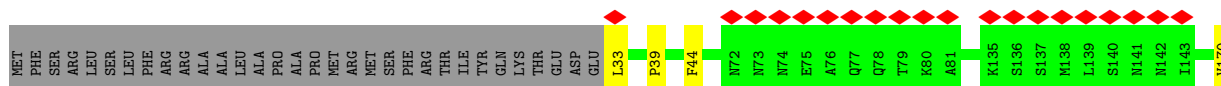


Chain H:  94% 6%




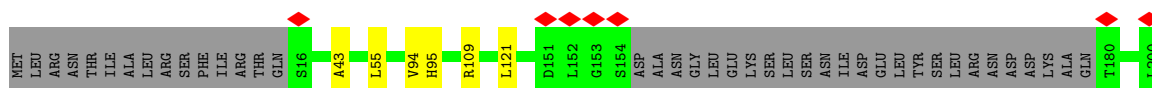
• Molecule 9: 37S ribosomal protein S9, mitochondrial

Chain I:  7% 80% 17%



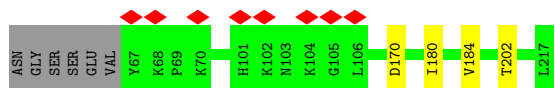
• Molecule 10: 37S ribosomal protein S10, mitochondrial

Chain J:  77% 20%




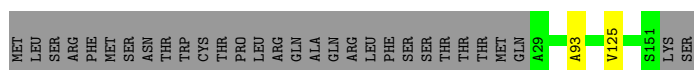
• Molecule 11: 37S ribosomal protein S18, mitochondrial

Chain K:  68% 30%




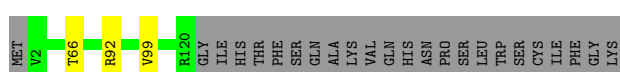
• Molecule 12: 37S ribosomal protein S12, mitochondrial

Chain L:  79% 20%



• Molecule 13: 37S ribosomal protein SWS2, mitochondrial

Chain M:  81% 17%





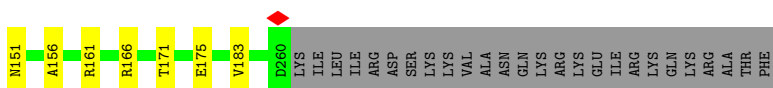
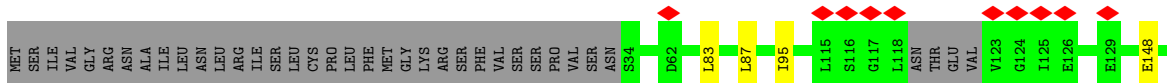
- Molecule 14: 37S ribosomal protein MRP2, mitochondrial

Chain N:  97%



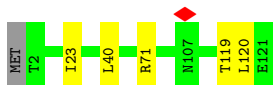
- Molecule 15: 37S ribosomal protein S28, mitochondrial

Chain O:  74%





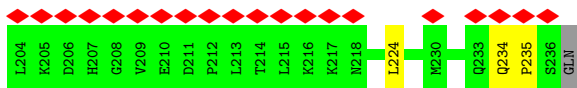
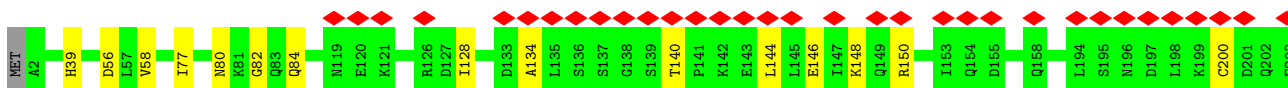
- Molecule 16: 37S ribosomal protein S16, mitochondrial

Chain P:  95%



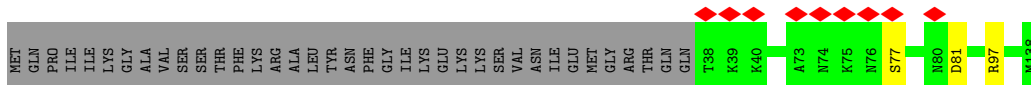
- Molecule 17: 37S ribosomal protein S17, mitochondrial

Chain Q:  22%  92%  8%





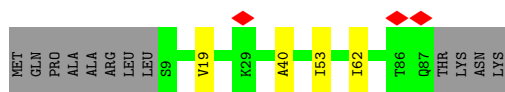
- Molecule 18: 37S ribosomal protein RSM18, mitochondrial

Chain R:  7%  71%  27%

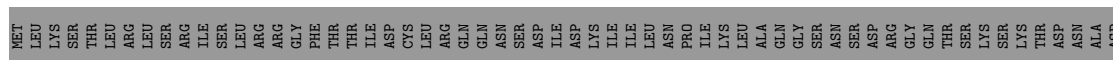


- Molecule 19: 37S ribosomal protein S19, mitochondrial

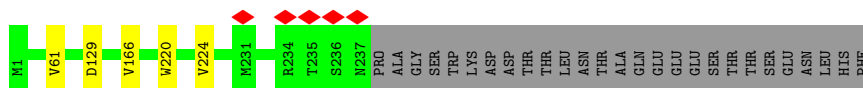
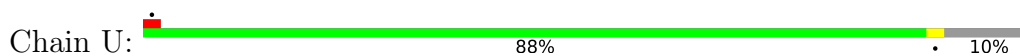
Chain S:  82%  13%



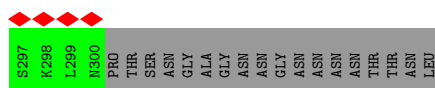
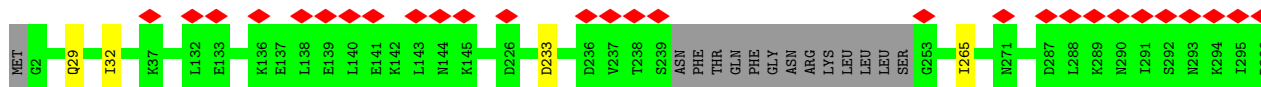
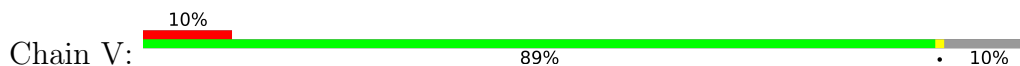
• Molecule 20: 37S ribosomal protein MRP21, mitochondrial



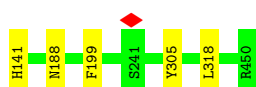
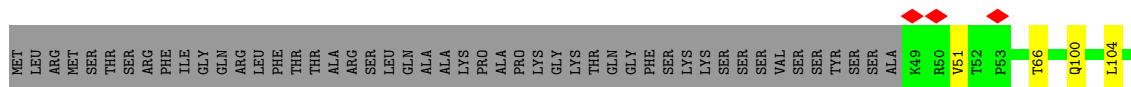
• Molecule 21: 37S ribosomal protein S25, mitochondrial



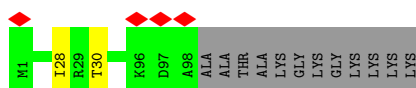
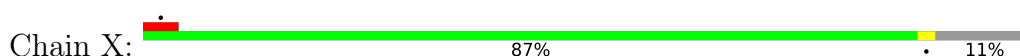
• Molecule 22: 37S ribosomal protein PET123, mitochondrial



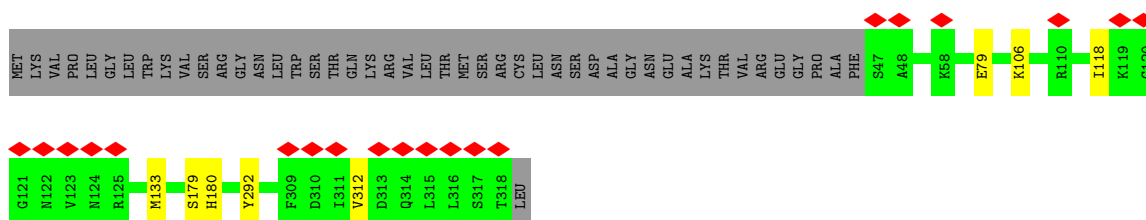
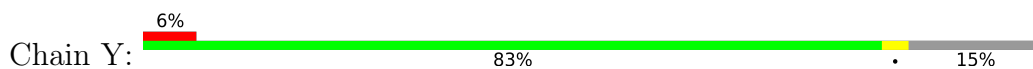
• Molecule 23: 37S ribosomal protein S23, mitochondrial



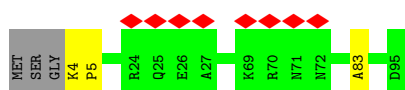
• Molecule 24: Mitochondrial 37S ribosomal protein S27



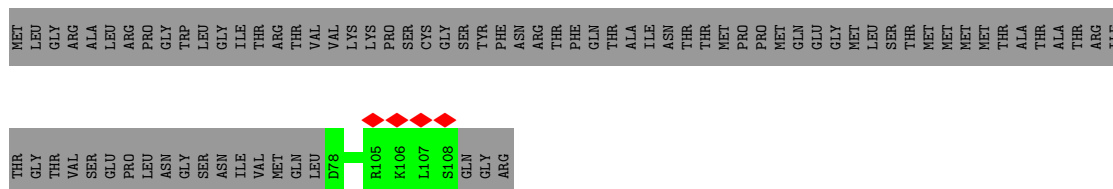
- Molecule 25: 37S ribosomal protein S24, mitochondrial



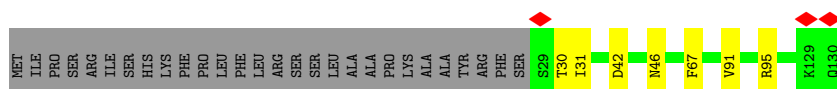
- Molecule 26: 37S ribosomal protein MRP10, mitochondrial



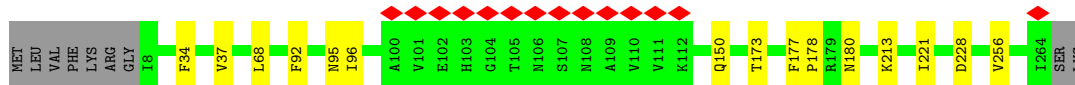
- Molecule 27: Mitochondrial mRNA-processing protein COX24



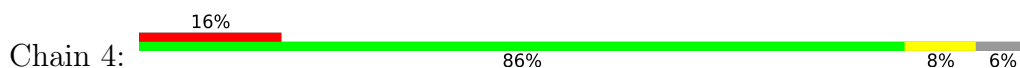
- Molecule 28: Protein FYV4, mitochondrial

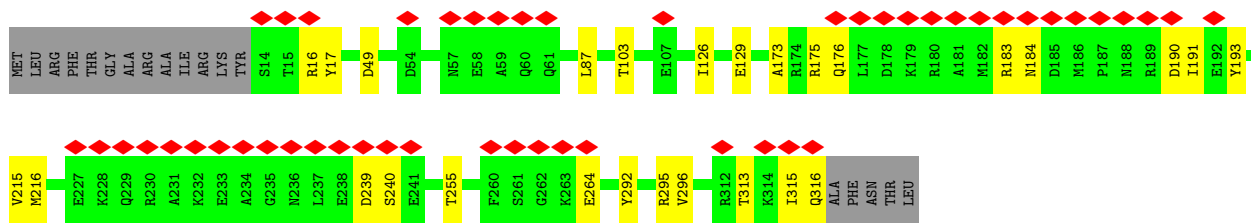


- Molecule 29: 37S ribosomal protein S26, mitochondrial

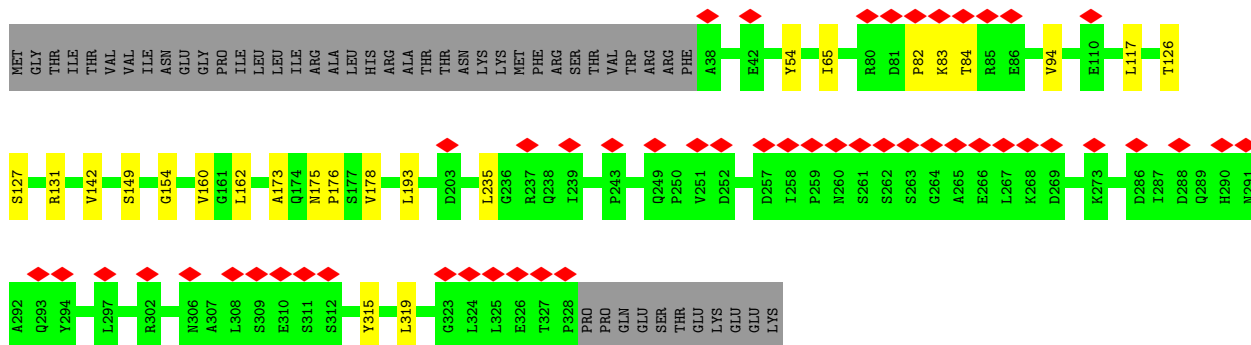
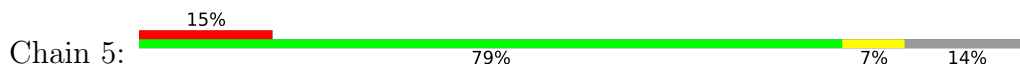


- Molecule 30: 37S ribosomal protein MRP1, mitochondrial

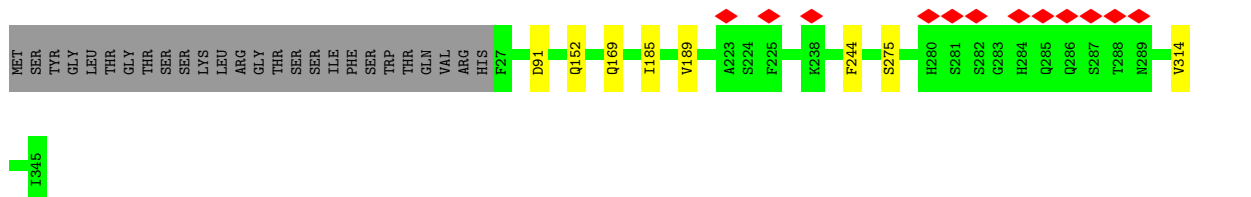




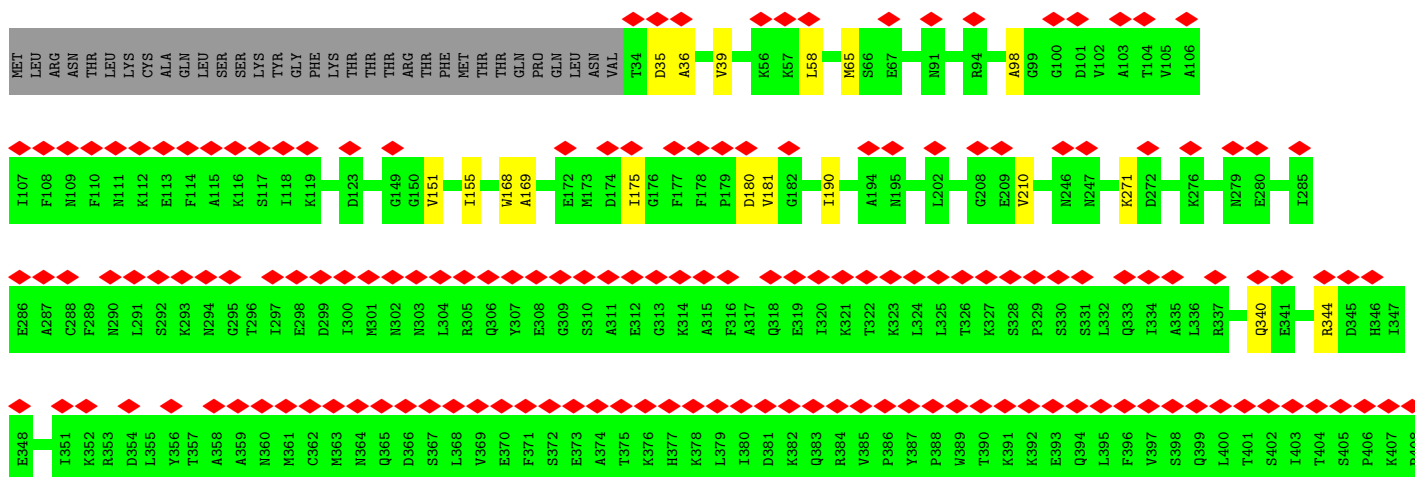
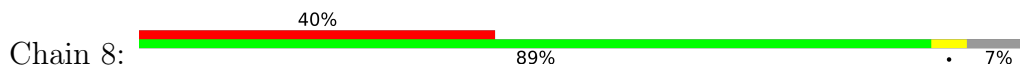
• Molecule 31: 37S ribosomal protein MRP13, mitochondrial

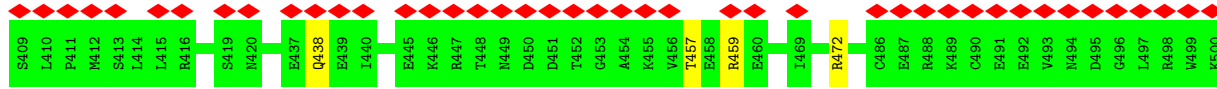


• Molecule 32: 37S ribosomal protein S35, mitochondrial

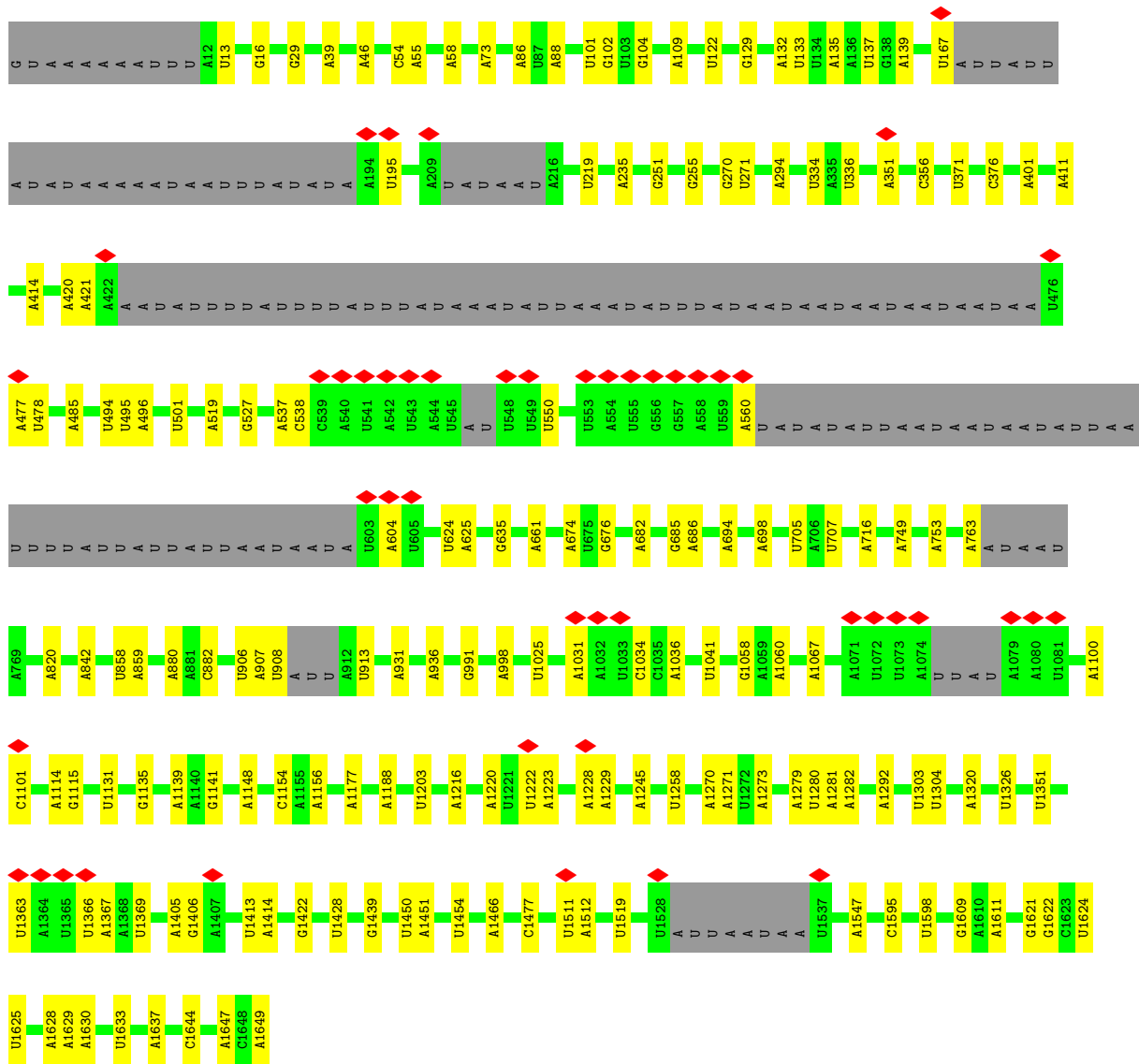
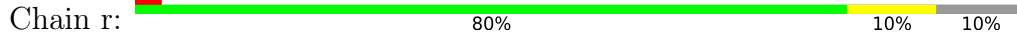


• Molecule 33: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

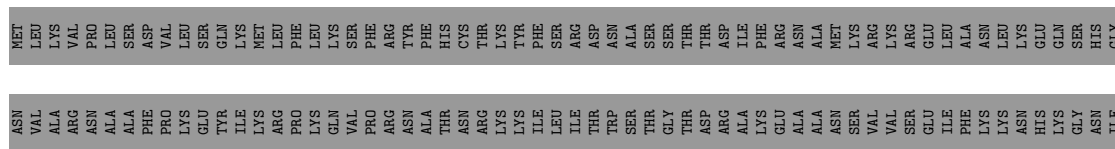




• Molecule 34: 15S mitochondrial rRNA



• Molecule 35: Altered inheritance of mitochondria protein 23, mitochondrial



LYS	VAL	VAL	VAL	ASP	PRO	THR	THR	HIS	ARG	ILE	GLU	ALA	SER	ASN	ILE	ARG	TYR	PHE	ALA	LYS	GLY	ILE	ASP	LEU	LEU	ILE	VAL	ASN	ASN	VAL	GLU	GLN	ILE	ASP	ASN	GLU	ASN	GLN	ILE	PRO	LEU	VAL	LYS	ILE	GLU	SER	ARG	VAL	ALA	LEU	LYS	TYR	SER	ASP
PHE	LEU	ALA	LYS	LYS	GLU	LYS	GLU	LEU	MET	GLU	LEU	GLY	VAL	LEU	ASN	LYS	SER	TYR	LYS	ASN	LEU	VAL	THR	ASP	LYS	K208	E209	D210	N211	N257	N258	N259	L260	E264	E265	L266	ASP	ARG	SER	GLN	LYS	G272	E273	P274	P275	R276	L277	Q283	E298	D302	N310			
D321	N322	K323	P324	Q325	N326	N327	D328	K329	R330	A331	L332	K333	E334	L335	R336	K337	K338	E339	R340	Q341	E342	K343	L344	Q345	K346	R347	I348	K351	K352	K353	N354	E355	N356	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS													

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53922	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.792	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	398.4, 398.4, 398.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.664, 0.664, 0.664	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, K, MG, LMT, ACE

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	0.25	0/2483	0.46	0/3345
2	B	0.24	0/2764	0.45	0/3746
3	C	0.24	0/3133	0.41	0/4215
4	D	0.25	0/2913	0.46	0/3923
5	E	0.25	0/2403	0.47	0/3237
6	F	0.24	0/1068	0.48	0/1430
7	G	0.23	0/1641	0.45	0/2216
8	H	0.24	0/1244	0.46	0/1677
9	I	0.24	0/1895	0.46	0/2552
10	J	0.25	0/1355	0.46	0/1834
11	K	0.25	0/1232	0.46	0/1642
12	L	0.25	0/954	0.54	0/1281
13	M	0.24	0/949	0.50	0/1267
14	N	0.26	0/948	0.51	0/1267
15	O	0.24	0/1837	0.48	0/2457
16	P	0.26	0/968	0.55	0/1307
17	Q	0.24	0/1953	0.48	0/2609
18	R	0.25	0/830	0.52	0/1106
19	S	0.26	0/645	0.50	0/872
20	T	0.25	0/784	0.50	0/1035
21	U	0.24	0/1982	0.45	0/2679
22	V	0.24	0/2325	0.42	0/3112
23	W	0.25	0/3292	0.42	0/4449
24	X	0.26	0/801	0.46	0/1070
25	Y	0.24	0/2329	0.47	0/3142
26	Z	0.24	0/745	0.46	0/1004
27	1	0.23	0/279	0.62	0/355
28	2	0.24	0/877	0.45	0/1173
29	3	0.25	0/2114	0.44	0/2872
30	4	0.25	0/2485	0.46	0/3354
31	5	0.24	0/2417	0.43	0/3275
32	6	0.25	0/2655	0.47	0/3583



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	8	0.24	0/3766	0.45	0/5099
34	r	0.23	0/35392	0.68	0/55064
35	d	0.24	0/1209	0.43	0/1613
All	All	0.24	0/94667	0.56	0/134862

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	2427	2481	2480	17	0
2	B	2714	2722	2721	11	0
3	C	3090	3091	3085	14	0
4	D	2833	2896	2895	8	0
5	E	2348	2360	2359	7	0
6	F	1055	1129	1129	2	0
7	G	1612	1660	1658	14	0
8	H	1223	1286	1288	5	0
9	I	1858	1925	1925	6	0
10	J	1321	1334	1332	3	0
11	K	1209	1266	1266	2	0
12	L	939	993	992	1	0
13	M	935	1002	1000	2	0
14	N	931	986	985	0	0
15	O	1815	1853	1851	6	0
16	P	952	1011	1010	3	0
17	Q	1930	2014	2014	10	0
18	R	818	853	852	2	0
19	S	629	648	647	2	0
20	T	769	800	800	3	0
21	U	1939	1929	1929	5	0
22	V	2294	2398	2396	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	W	3226	3329	3327	5	0
24	X	787	832	832	1	0
25	Y	2273	2241	2240	6	0
26	Z	729	758	757	2	0
27	1	279	334	333	0	0
28	2	858	866	865	4	0
29	3	2063	2040	2039	7	0
30	4	2436	2423	2422	14	0
31	5	2361	2409	2408	13	0
32	6	2593	2615	2613	6	0
33	8	3690	3681	3680	14	0
34	r	31606	15844	15850	0	0
35	d	1195	1254	1252	0	0
36	B	1	0	0	0	0
36	K	1	0	0	0	0
36	W	1	0	0	0	0
36	r	93	0	0	0	0
37	M	1	0	0	0	0
37	r	25	0	0	0	0
38	O	13	25	25	1	0
39	W	31	12	12	0	0
40	1	3	0	0	0	0
40	2	4	0	0	0	0
40	3	1	0	0	0	0
40	6	12	0	0	0	0
40	8	2	0	0	0	0
40	A	8	0	0	0	0
40	B	32	0	0	2	0
40	C	8	0	0	0	0
40	D	22	0	0	0	0
40	E	23	0	0	0	0
40	G	7	0	0	0	0
40	H	15	0	0	1	0
40	I	27	0	0	1	0
40	J	18	0	0	0	0
40	K	7	0	0	0	0
40	L	6	0	0	0	0
40	M	1	0	0	0	0
40	N	28	0	0	0	0
40	O	18	0	0	0	0
40	P	25	0	0	0	0
40	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	T	9	0	0	0	0
40	U	8	0	0	0	0
40	V	5	0	0	0	0
40	W	22	0	0	0	0
40	X	8	0	0	0	0
40	Y	18	0	0	0	0
40	Z	5	0	0	1	0
40	r	1140	0	0	0	0
All	All	91387	75300	75269	176	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 (176) 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)
2:B:349:ASP:OD1	40:B:501:HOH:O	2.09	0.71
7:G:70:PRO:HD3	7:G:76:VAL:HG22	1.73	0.70
2:B:355:VAL:O	40:B:502:HOH:O	2.11	0.67
3:C:255:ASN:OD1	3:C:256:ILE:N	2.30	0.65
9:I:200:LEU:HD11	9:I:211:ILE:HD11	1.78	0.65
7:G:204:VAL:HG21	23:W:51:VAL:HG22	1.80	0.64
18:R:77:SER:O	18:R:81:ASP:N	2.32	0.63
23:W:188:ASN:OD1	23:W:305:TYR:OH	2.16	0.63
15:O:183:VAL:HG22	38:O:301:LMT:H111	1.82	0.62
2:B:89:LEU:HD12	7:G:43:VAL:HG13	1.82	0.61
7:G:168:THR:HG22	7:G:178:VAL:HG22	1.83	0.61
29:3:68:LEU:O	29:3:213:LYS:NZ	2.34	0.61
1:A:298:LEU:HD13	30:4:255:THR:HG21	1.83	0.60
31:5:84:THR:HG22	31:5:84:THR:O	2.02	0.59
1:A:195:LYS:CG	21:U:166:VAL:HG21	2.32	0.59
4:D:172:LEU:HD21	4:D:391:LEU:CD1	2.33	0.58
3:C:48:LYS:HG3	25:Y:312:VAL:HG11	1.86	0.58
6:F:17:PRO:HB2	6:F:47:ILE:HD11	1.86	0.58
8:H:98:ARG:O	40:H:201:HOH:O	2.17	0.58
26:Z:83:ALA:O	40:Z:101:HOH:O	2.17	0.58
5:E:112:LEU:HD12	5:E:113:PRO:HD2	1.86	0.57
28:2:67:PHE:O	28:2:95:ARG:NH2	2.37	0.57
16:P:71:ARG:HG2	32:6:314:VAL:HG21	1.87	0.57
33:8:155:ILE:HD11	33:8:190:ILE:HD11	1.87	0.57
3:C:43:LEU:HD21	7:G:76:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:8:180:ASP:O	33:8:181:VAL:HG22	2.06	0.56
21:U:220:TRP:O	21:U:224:VAL:HG23	2.06	0.55
33:8:35:ASP:OD1	33:8:36:ALA:N	2.39	0.55
13:M:66:THR:O	13:M:66:THR:HG23	2.07	0.55
1:A:195:LYS:HG3	21:U:166:VAL:HG21	1.88	0.54
31:5:315:TYR:CE2	31:5:319:LEU:HD11	2.43	0.54
33:8:169:ALA:HB2	33:8:210:VAL:HG22	1.89	0.54
2:B:85:LYS:O	7:G:43:VAL:HG11	2.09	0.53
7:G:246:LEU:O	7:G:247:LYS:CB	2.57	0.52
29:3:173:THR:O	29:3:180:ASN:ND2	2.43	0.52
30:4:190:ASP:OD1	30:4:191:ILE:N	2.44	0.51
20:T:115:GLU:OE2	20:T:119:ARG:NE	2.43	0.51
29:3:150:GLN:NE2	29:3:228:ASP:OD2	2.43	0.51
7:G:63:LEU:HD12	7:G:64:PRO:HD2	1.93	0.51
33:8:175:ILE:O	33:8:175:ILE:HG22	2.11	0.50
30:4:176:GLN:HG2	30:4:313:THR:HG21	1.92	0.50
30:4:292:TYR:O	30:4:296:VAL:HG23	2.11	0.50
29:3:34:PHE:HA	29:3:37:VAL:HG12	1.94	0.49
28:2:30:THR:HG22	28:2:31:ILE:N	2.26	0.49
1:A:161:LEU:HD21	1:A:176:LEU:HD22	1.95	0.48
2:B:89:LEU:CD1	7:G:43:VAL:HG13	2.43	0.48
1:A:234:VAL:O	1:A:234:VAL:HG22	2.13	0.48
3:C:206:GLU:HG3	3:C:206:GLU:O	2.13	0.48
17:Q:200:CYS:SG	17:Q:224:LEU:HD11	2.54	0.48
1:A:206:LEU:CD2	1:A:291:VAL:HG21	2.43	0.48
15:O:83:LEU:HD11	15:O:156:ALA:HB2	1.95	0.48
10:J:43:ALA:HB2	10:J:121:LEU:HD21	1.94	0.48
18:R:97:ARG:NH1	22:V:233:ASP:OD1	2.46	0.48
1:A:157:PHE:CE2	1:A:161:LEU:HD22	2.49	0.47
2:B:257:ARG:NH2	2:B:261:GLU:OE2	2.47	0.47
4:D:221:LEU:HD13	4:D:370:LEU:HD22	1.95	0.47
5:E:172:VAL:HG22	5:E:201:ALA:HB1	1.95	0.47
15:O:166:ARG:NE	15:O:175:GLU:OE2	2.45	0.47
17:Q:146:GLU:OE2	17:Q:150:ARG:NH2	2.47	0.47
31:5:131:ARG:NH2	31:5:173:ALA:O	2.47	0.47
8:H:91:LEU:HD23	8:H:152:CYS:HB3	1.96	0.47
32:6:91:ASP:OD1	32:6:91:ASP:N	2.45	0.47
19:S:19:VAL:HG21	19:S:40:ALA:HB2	1.97	0.47
20:T:128:ASN:ND2	20:T:132:ASP:OD1	2.48	0.47
21:U:61:VAL:O	21:U:61:VAL:HG13	2.14	0.47
4:D:386:ILE:HG23	4:D:391:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:67:PHE:CD1	28:2:91:VAL:HG13	2.50	0.47
1:A:184:LEU:HD11	22:V:265:ILE:HD11	1.97	0.46
1:A:168:GLU:OE1	1:A:168:GLU:N	2.45	0.46
31:5:160:VAL:HG12	31:5:160:VAL:O	2.14	0.46
8:H:99:ILE:HG21	8:H:118:ILE:HD11	1.97	0.46
13:M:92:ARG:HB2	13:M:99:VAL:HG12	1.97	0.46
32:6:169:GLN:NE2	32:6:275:SER:OG	2.48	0.46
2:B:344:ALA:HB3	2:B:355:VAL:HG11	1.98	0.46
15:O:87:LEU:HD13	15:O:95:ILE:HD13	1.98	0.46
15:O:148:GLU:OE1	15:O:151:ASN:ND2	2.45	0.46
3:C:45:MET:HG2	25:Y:312:VAL:HG13	1.98	0.45
10:J:55:LEU:HD21	10:J:109:ARG:HG2	1.97	0.45
19:S:53:ILE:HD12	19:S:62:ILE:HD12	1.97	0.45
1:A:279:GLU:HB2	1:A:298:LEU:HD11	1.99	0.45
30:4:175:ARG:NH2	30:4:184:ASN:OD1	2.49	0.45
31:5:149:SER:O	31:5:154:GLY:N	2.50	0.45
17:Q:144:LEU:O	17:Q:148:LYS:N	2.44	0.45
15:O:161:ARG:HD2	15:O:171:THR:HG22	1.98	0.45
17:Q:140:THR:HA	17:Q:144:LEU:HD12	1.99	0.45
29:3:177:PHE:CG	29:3:178:PRO:HD3	2.51	0.45
30:4:16:ARG:NH2	30:4:49:ASP:OD1	2.50	0.45
16:P:119:THR:OG1	16:P:120:LEU:N	2.50	0.45
17:Q:80:ASN:OD1	17:Q:84:GLN:NE2	2.50	0.45
1:A:43:LEU:HD22	1:A:61:ARG:HG2	1.99	0.45
17:Q:234:GLN:HB2	17:Q:235:PRO:HD3	1.98	0.45
2:B:252:ARG:NH1	2:B:363:ASP:O	2.50	0.45
23:W:66:THR:O	23:W:66:THR:HG22	2.17	0.45
25:Y:179:SER:OG	25:Y:180:HIS:ND1	2.49	0.45
4:D:478:TYR:CE2	4:D:482:LEU:HD11	2.52	0.44
9:I:200:LEU:HD11	9:I:211:ILE:CD1	2.44	0.44
5:E:112:LEU:HD11	25:Y:133:MET:SD	2.58	0.44
33:8:340:GLN:O	33:8:344:ARG:NH1	2.50	0.44
2:B:297:SER:HG	9:I:33:LEU:N	2.16	0.44
31:5:65:ILE:HG22	31:5:65:ILE:O	2.17	0.44
5:E:286:LEU:HD11	32:6:244:PHE:CE2	2.53	0.44
7:G:246:LEU:O	7:G:247:LYS:HB2	2.18	0.44
29:3:221:ILE:HG22	29:3:256:VAL:HG13	2.00	0.43
7:G:247:LYS:OXT	7:G:247:LYS:HG2	2.18	0.43
30:4:103:THR:O	30:4:295:ARG:NH2	2.43	0.43
16:P:23:ILE:O	16:P:40:LEU:N	2.48	0.43
1:A:234:VAL:HB	1:A:268:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:56:ASP:OD1	17:Q:82:GLY:N	2.51	0.43
1:A:238:ASN:O	1:A:239:ASN:HB2	2.19	0.43
2:B:58:LEU:HD21	3:C:12:MET:SD	2.59	0.43
3:C:179:LEU:O	3:C:182:ILE:HG13	2.19	0.43
1:A:63:LEU:C	1:A:63:LEU:HD12	2.37	0.43
6:F:40:ARG:NE	6:F:72:ASP:OD2	2.51	0.43
17:Q:134:ALA:CB	17:Q:144:LEU:HD11	2.49	0.43
1:A:172:ASN:OD1	1:A:173:SER:N	2.52	0.43
3:C:34:LYS:HD3	7:G:46:TRP:CD2	2.54	0.43
8:H:86:LEU:CD1	8:H:154:VAL:HG13	2.49	0.43
30:4:215:VAL:HG13	30:4:216:MET:N	2.34	0.43
4:D:395:GLU:N	4:D:396:PRO:HD2	2.34	0.42
3:C:236:ILE:HG13	3:C:236:ILE:O	2.19	0.42
20:T:95:ASN:O	20:T:99:ARG:N	2.52	0.42
29:3:92:PHE:CZ	29:3:96:ILE:HD13	2.54	0.42
1:A:121:LYS:HB2	1:A:181:VAL:HG21	2.01	0.42
4:D:432:SER:N	4:D:433:PRO:HD2	2.34	0.42
7:G:65:GLU:O	7:G:76:VAL:N	2.53	0.42
9:I:261:ARG:NH1	40:I:307:HOH:O	2.51	0.42
21:U:129:ASP:OD1	33:8:271:LYS:NZ	2.53	0.42
3:C:367:LYS:N	3:C:371:ILE:O	2.51	0.42
17:Q:58:VAL:HG12	17:Q:77:ILE:HD13	2.01	0.42
31:5:54:TYR:HB2	31:5:94:VAL:HG21	2.01	0.42
31:5:193:LEU:HD21	31:5:235:LEU:HA	2.01	0.42
33:8:457:THR:HG22	33:8:459:ARG:H	1.84	0.42
28:2:42:ASP:O	28:2:46:ASN:ND2	2.52	0.42
30:4:126:ILE:HG21	30:4:129:GLU:OE2	2.20	0.42
33:8:39:VAL:HG23	33:8:65:MET:HG2	2.01	0.42
22:V:29:GLN:OE1	22:V:32:ILE:HD12	2.20	0.42
31:5:82:PRO:O	31:5:83:LYS:HB2	2.20	0.42
10:J:94:VAL:O	10:J:95:HIS:HB2	2.20	0.42
33:8:438:GLN:OE1	33:8:438:GLN:N	2.51	0.42
23:W:100:GLN:O	23:W:104:LEU:HD13	2.19	0.41
30:4:315:ILE:O	30:4:316:GLN:C	2.58	0.41
5:E:208:ILE:HG13	5:E:208:ILE:O	2.20	0.41
9:I:39:PRO:HB3	9:I:44:PHE:CG	2.55	0.41
31:5:117:LEU:HD23	31:5:162:LEU:HD12	2.02	0.41
31:5:175:ASN:N	31:5:176:PRO:HD3	2.35	0.41
33:8:151:VAL:HG13	33:8:168:TRP:HE1	1.85	0.41
3:C:160:ILE:O	3:C:160:ILE:HG22	2.20	0.41
3:C:169:ASN:O	5:E:91:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:199:PHE:HB2	23:W:318:LEU:HD23	2.01	0.41
24:X:28:ILE:O	24:X:30:THR:HG23	2.21	0.41
30:4:183:ARG:NH1	30:4:264:GLU:OE1	2.53	0.41
33:8:180:ASP:O	33:8:181:VAL:CG2	2.68	0.41
9:I:170:VAL:HG22	9:I:171:ARG:N	2.35	0.41
17:Q:128:ILE:O	17:Q:128:ILE:HG22	2.20	0.41
33:8:58:LEU:HB3	33:8:98:ALA:HB2	2.02	0.41
3:C:188:ASN:ND2	25:Y:79:GLU:OE2	2.52	0.41
11:K:170:ASP:O	11:K:202:THR:HA	2.21	0.41
33:8:169:ALA:CB	33:8:210:VAL:HG22	2.49	0.41
11:K:180:ILE:O	11:K:184:VAL:HG22	2.20	0.41
3:C:3:LEU:O	3:C:7:ASN:N	2.40	0.41
5:E:21:LEU:HD13	5:E:33:ILE:HG21	2.03	0.41
31:5:126:THR:HG22	31:5:127:SER:N	2.36	0.41
30:4:17:TYR:CD2	30:4:87:LEU:HD21	2.56	0.41
31:5:142:VAL:HG11	31:5:178:VAL:CG1	2.50	0.41
4:D:172:LEU:HD11	4:D:391:LEU:CD1	2.51	0.40
26:Z:4:LYS:N	26:Z:5:PRO:CD	2.84	0.40
12:L:93:ALA:HB1	12:L:125:VAL:HG13	2.04	0.40
25:Y:106:LYS:HD2	25:Y:118:ILE:HD11	2.04	0.40
30:4:173:ALA:HB1	30:4:193:TYR:HB2	2.03	0.40
30:4:239:ASP:OD1	30:4:240:SER:N	2.54	0.40
1:A:113:ARG:HB3	1:A:114:PRO:HD2	2.02	0.40
2:B:85:LYS:C	7:G:43:VAL:HG11	2.42	0.40
8:H:1:ACE:H1	8:H:31:LEU:HD22	2.03	0.40
32:6:185:ILE:O	32:6:189:VAL:HG23	2.21	0.40
4:D:166:PRO:HB2	4:D:171:ALA:HB2	2.04	0.40
32:6:152:GLN:N	32:6:152:GLN:OE1	2.54	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	
1	A	299/344 (87%)	287 (96%)	12 (4%)	0	100	100
2	B	338/394 (86%)	329 (97%)	9 (3%)	0	100	100
3	C	362/398 (91%)	354 (98%)	8 (2%)	0	100	100
4	D	337/486 (69%)	335 (99%)	2 (1%)	0	100	100
5	E	292/307 (95%)	285 (98%)	6 (2%)	1 (0%)	41	70
6	F	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
7	G	199/247 (81%)	197 (99%)	2 (1%)	0	100	100
8	H	154/155 (99%)	152 (99%)	2 (1%)	0	100	100
9	I	230/278 (83%)	226 (98%)	4 (2%)	0	100	100
10	J	158/203 (78%)	152 (96%)	6 (4%)	0	100	100
11	K	150/217 (69%)	148 (99%)	2 (1%)	0	100	100
12	L	121/153 (79%)	120 (99%)	1 (1%)	0	100	100
13	M	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
14	N	111/115 (96%)	111 (100%)	0	0	100	100
15	O	219/286 (77%)	217 (99%)	2 (1%)	0	100	100
16	P	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
17	Q	234/237 (99%)	232 (99%)	2 (1%)	0	100	100
18	R	99/138 (72%)	98 (99%)	1 (1%)	0	100	100
19	S	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
20	T	91/177 (51%)	90 (99%)	1 (1%)	0	100	100
21	U	235/264 (89%)	230 (98%)	5 (2%)	0	100	100
22	V	282/318 (89%)	279 (99%)	3 (1%)	0	100	100
23	W	400/450 (89%)	390 (98%)	10 (2%)	0	100	100
24	X	96/110 (87%)	96 (100%)	0	0	100	100
25	Y	270/319 (85%)	266 (98%)	4 (2%)	0	100	100
26	Z	90/95 (95%)	88 (98%)	2 (2%)	0	100	100
27	1	29/111 (26%)	29 (100%)	0	0	100	100
28	2	100/130 (77%)	98 (98%)	2 (2%)	0	100	100
29	3	255/266 (96%)	247 (97%)	8 (3%)	0	100	100
30	4	301/321 (94%)	289 (96%)	12 (4%)	0	100	100
31	5	289/339 (85%)	283 (98%)	6 (2%)	0	100	100
32	6	317/345 (92%)	311 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	8	465/500 (93%)	451 (97%)	14 (3%)	0	100	100
35	d	140/364 (38%)	132 (94%)	8 (6%)	0	100	100
All	All	7104/8553 (83%)	6953 (98%)	150 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	264	LYS

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/309 (87%)	270 (100%)	0	100	100
2	B	307/350 (88%)	307 (100%)	0	100	100
3	C	361/385 (94%)	361 (100%)	0	100	100
4	D	306/437 (70%)	304 (99%)	2 (1%)	84	94
5	E	253/266 (95%)	252 (100%)	1 (0%)	91	97
6	F	120/120 (100%)	120 (100%)	0	100	100
7	G	174/211 (82%)	172 (99%)	2 (1%)	73	90
8	H	142/141 (101%)	142 (100%)	0	100	100
9	I	205/245 (84%)	204 (100%)	1 (0%)	88	96
10	J	146/183 (80%)	146 (100%)	0	100	100
11	K	131/192 (68%)	131 (100%)	0	100	100
12	L	102/131 (78%)	102 (100%)	0	100	100
13	M	100/121 (83%)	100 (100%)	0	100	100
14	N	101/103 (98%)	100 (99%)	1 (1%)	76	91
15	O	192/250 (77%)	192 (100%)	0	100	100
16	P	105/106 (99%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	217/218 (100%)	215 (99%)	2 (1%)	78	92
18	R	89/121 (74%)	89 (100%)	0	100	100
19	S	68/78 (87%)	68 (100%)	0	100	100
20	T	82/159 (52%)	82 (100%)	0	100	100
21	U	212/236 (90%)	212 (100%)	0	100	100
22	V	260/287 (91%)	260 (100%)	0	100	100
23	W	369/409 (90%)	368 (100%)	1 (0%)	92	97
24	X	85/92 (92%)	85 (100%)	0	100	100
25	Y	249/289 (86%)	248 (100%)	1 (0%)	91	97
26	Z	83/85 (98%)	83 (100%)	0	100	100
27	1	30/98 (31%)	30 (100%)	0	100	100
28	2	93/117 (80%)	93 (100%)	0	100	100
29	3	232/240 (97%)	231 (100%)	1 (0%)	91	97
30	4	267/281 (95%)	267 (100%)	0	100	100
31	5	259/303 (86%)	259 (100%)	0	100	100
32	6	289/312 (93%)	289 (100%)	0	100	100
33	8	413/444 (93%)	412 (100%)	1 (0%)	93	98
35	d	136/336 (40%)	136 (100%)	0	100	100
All	All	6448/7655 (84%)	6435 (100%)	13 (0%)	93	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	391	LEU
4	D	484	ASN
5	E	15	HIS
7	G	77	ASP
7	G	164	MET
9	I	191	LYS
14	N	86	PHE
17	Q	39[A]	HIS
17	Q	39[B]	HIS
23	W	141	HIS
25	Y	292	TYR
29	3	95	ASN
33	8	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	227	ASN
10	J	105	HIS
13	M	48	HIS
15	O	54	GLN
15	O	195	HIS
15	O	201	ASN
25	Y	246	GLN
29	3	180	ASN
30	4	69	HIS
32	6	169	GLN
33	8	128	ASN
35	d	354	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	r	1476/1647 (89%)	166 (11%)	0

All (166) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	r	13	U
34	r	16	G
34	r	29	G
34	r	39	A
34	r	46	A
34	r	54	C
34	r	55	A
34	r	58	A
34	r	73	A
34	r	86	A
34	r	88	A
34	r	101	U
34	r	102	G
34	r	104	G
34	r	109	A
34	r	122	U
34	r	129	G
34	r	132	A
34	r	133	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	r	135	A
34	r	137	U
34	r	139	A
34	r	167	U
34	r	195	U
34	r	219	U
34	r	235	A
34	r	251	G
34	r	255	G
34	r	270	G
34	r	271	U
34	r	294	A
34	r	334	U
34	r	336	U
34	r	351	A
34	r	356	C
34	r	371	U
34	r	376	C
34	r	401	A
34	r	411	A
34	r	414	A
34	r	420	A
34	r	421	A
34	r	477	A
34	r	478	U
34	r	485	A
34	r	494	U
34	r	495	U
34	r	496	A
34	r	501	U
34	r	519	A
34	r	527	G
34	r	537	A
34	r	538	C
34	r	550	U
34	r	560	A
34	r	604	A
34	r	624	U
34	r	625	A
34	r	635	G
34	r	661	A
34	r	674	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	r	676	G
34	r	682	A
34	r	685	G
34	r	686	A
34	r	694	A
34	r	698	A
34	r	705	U
34	r	707	U
34	r	716	A
34	r	749	A
34	r	753	A
34	r	763	A
34	r	820	A
34	r	842	A
34	r	858	U
34	r	859	A
34	r	880	A
34	r	882	C
34	r	906	U
34	r	907	A
34	r	908	U
34	r	913	U
34	r	931	A
34	r	936	A
34	r	991	G
34	r	998	A
34	r	1025	U
34	r	1031	A
34	r	1034	C
34	r	1036	A
34	r	1041	U
34	r	1058	G
34	r	1060	A
34	r	1067	A
34	r	1100	A
34	r	1101	C
34	r	1114	A
34	r	1115	G
34	r	1131	U
34	r	1135	G
34	r	1139	A
34	r	1141	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	r	1148	A
34	r	1154	C
34	r	1156	A
34	r	1177	A
34	r	1188	A
34	r	1203	U
34	r	1216	A
34	r	1220	A
34	r	1222	U
34	r	1223	A
34	r	1228	A
34	r	1229	A
34	r	1245	A
34	r	1258	U
34	r	1270	A
34	r	1271	A
34	r	1273	A
34	r	1279	A
34	r	1280	U
34	r	1281	A
34	r	1282	A
34	r	1292	A
34	r	1303	U
34	r	1304	U
34	r	1320	A
34	r	1326	U
34	r	1351	U
34	r	1363	U
34	r	1366	U
34	r	1367	A
34	r	1369	U
34	r	1405	A
34	r	1406	G
34	r	1413	U
34	r	1414	A
34	r	1422	G
34	r	1428	U
34	r	1439	G
34	r	1450	U
34	r	1451	A
34	r	1454	U
34	r	1466	A

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Mol	Chain	Res	Type
34	r	1477	C
34	r	1511	U
34	r	1512	A
34	r	1519	U
34	r	1547	A
34	r	1595	C
34	r	1598	U
34	r	1609	G
34	r	1611	A
34	r	1621	G
34	r	1622	G
34	r	1624	U
34	r	1625	U
34	r	1628	A
34	r	1629	A
34	r	1630	A
34	r	1633	U
34	r	1637	A
34	r	1644	C
34	r	1647	A
34	r	1649	A

There are no RNA pucker outliers to report.

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 124 ligands modelled in this entry, 122 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	$\# Z  > 2$
38	LMT	O	301	-	12,12,36	0.16	0	11,11,47	0.20	0
39	ATP	W	501	36	26,33,33	0.75	0	31,52,52	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMT	O	301	-	-	0/10/10/61	-
39	ATP	W	501	36	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

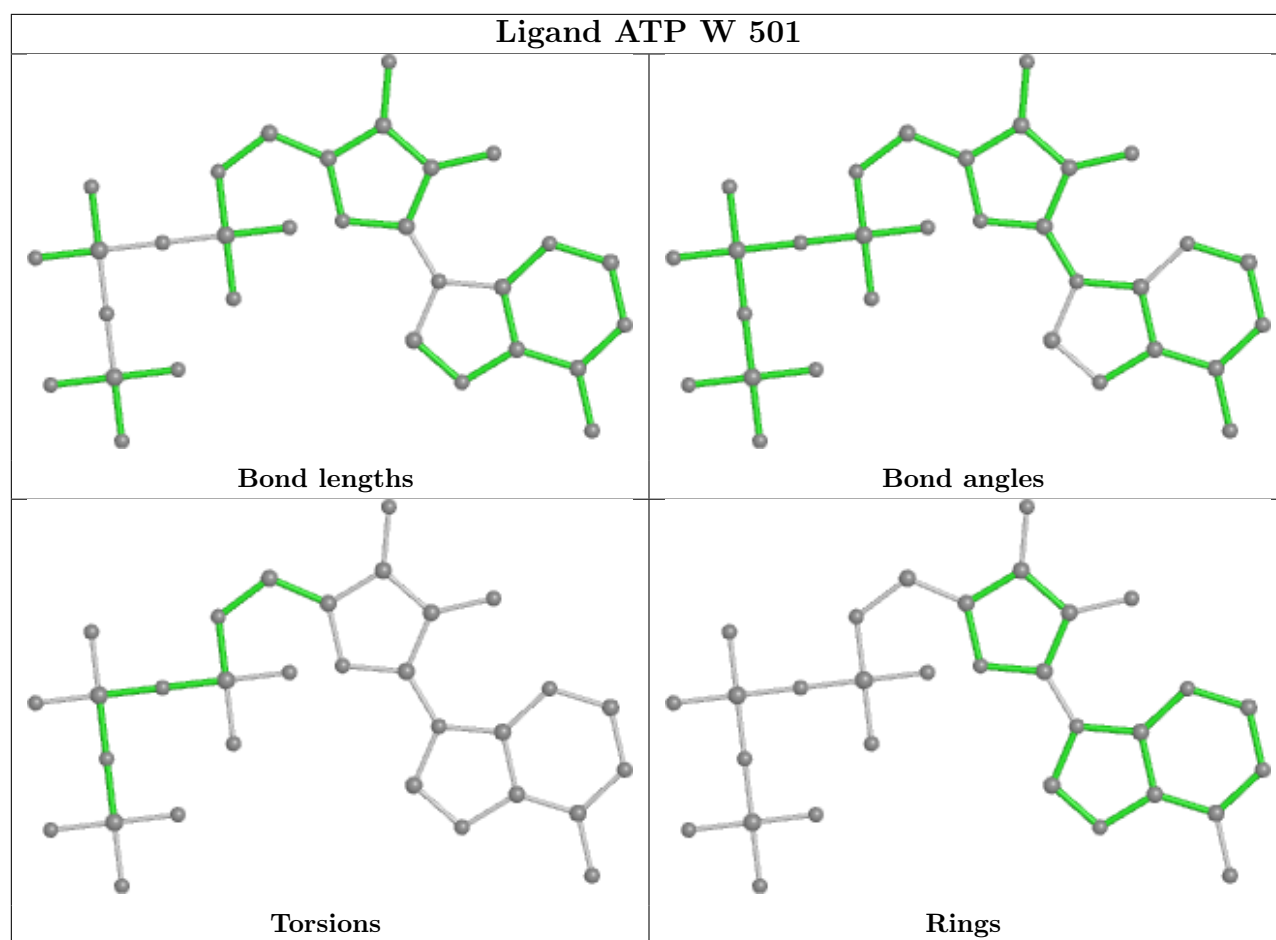
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	O	301	LMT	1	0

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

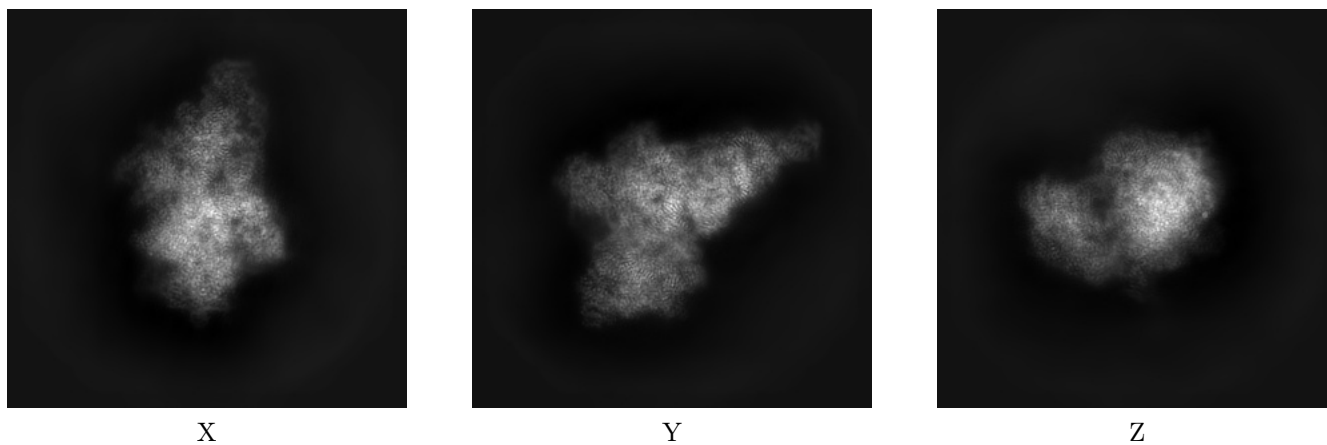
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16967. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

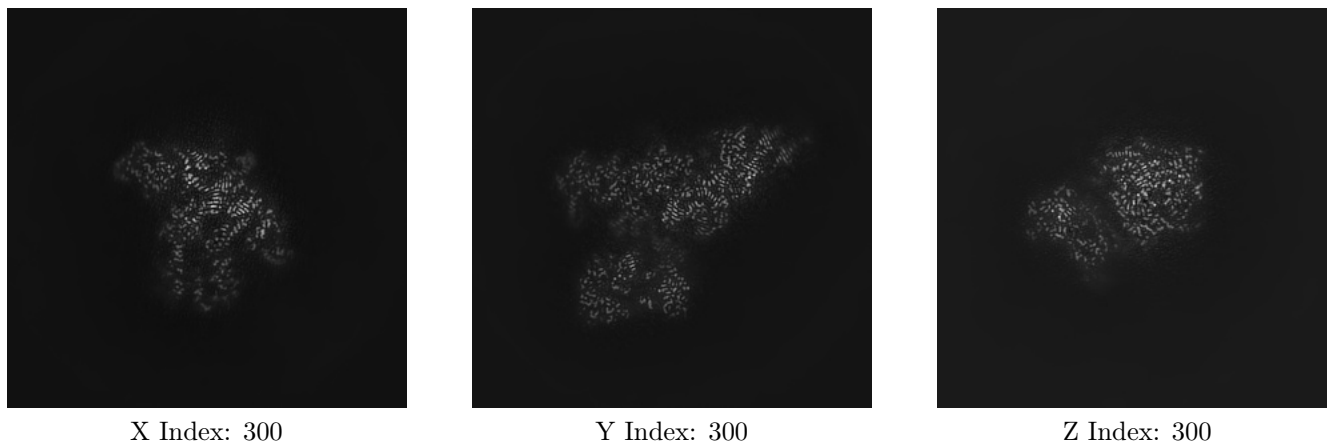
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

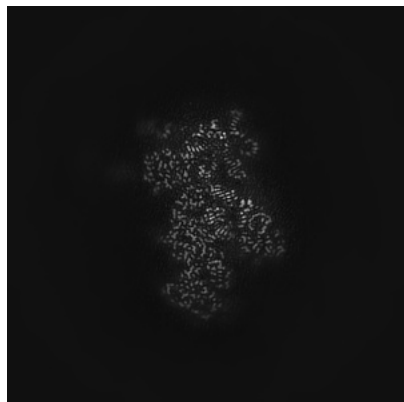
#### 6.2.1 Primary map



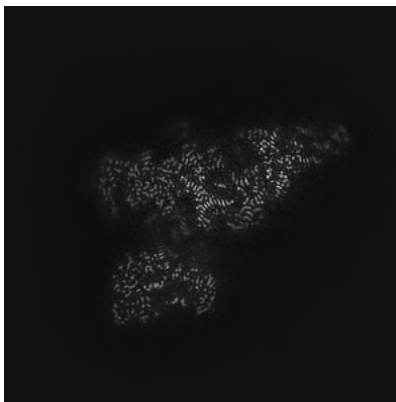
The images above show central slices of the map in three orthogonal directions.

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

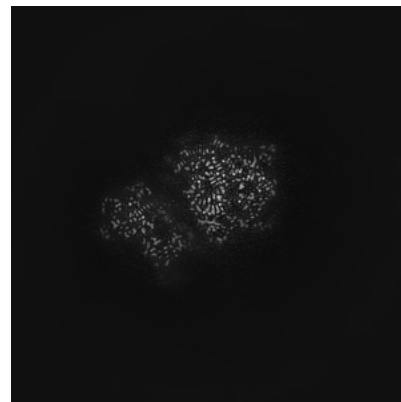
### 6.3.1 Primary map



X Index: 330



Y Index: 307

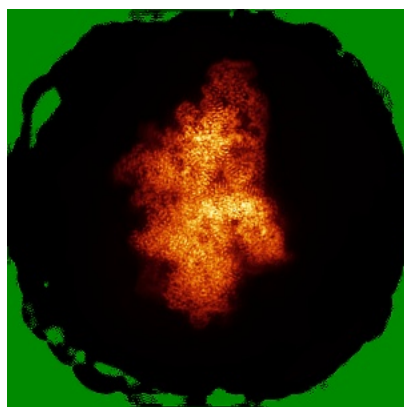


Z Index: 298

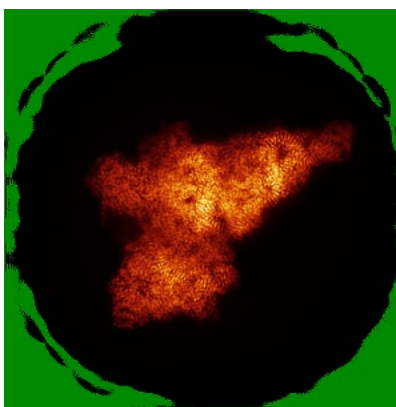
The images above show the largest variance slices of the map in three orthogonal directions.

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

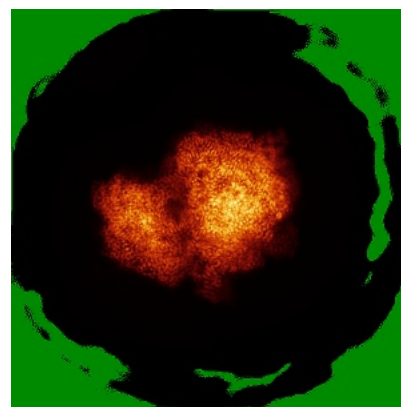
### 6.4.1 Primary map



X



Y

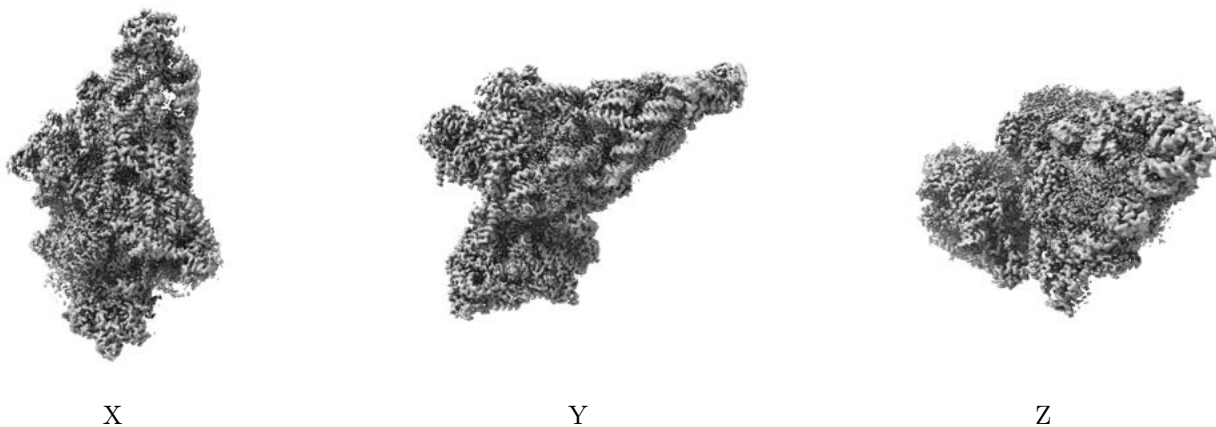


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

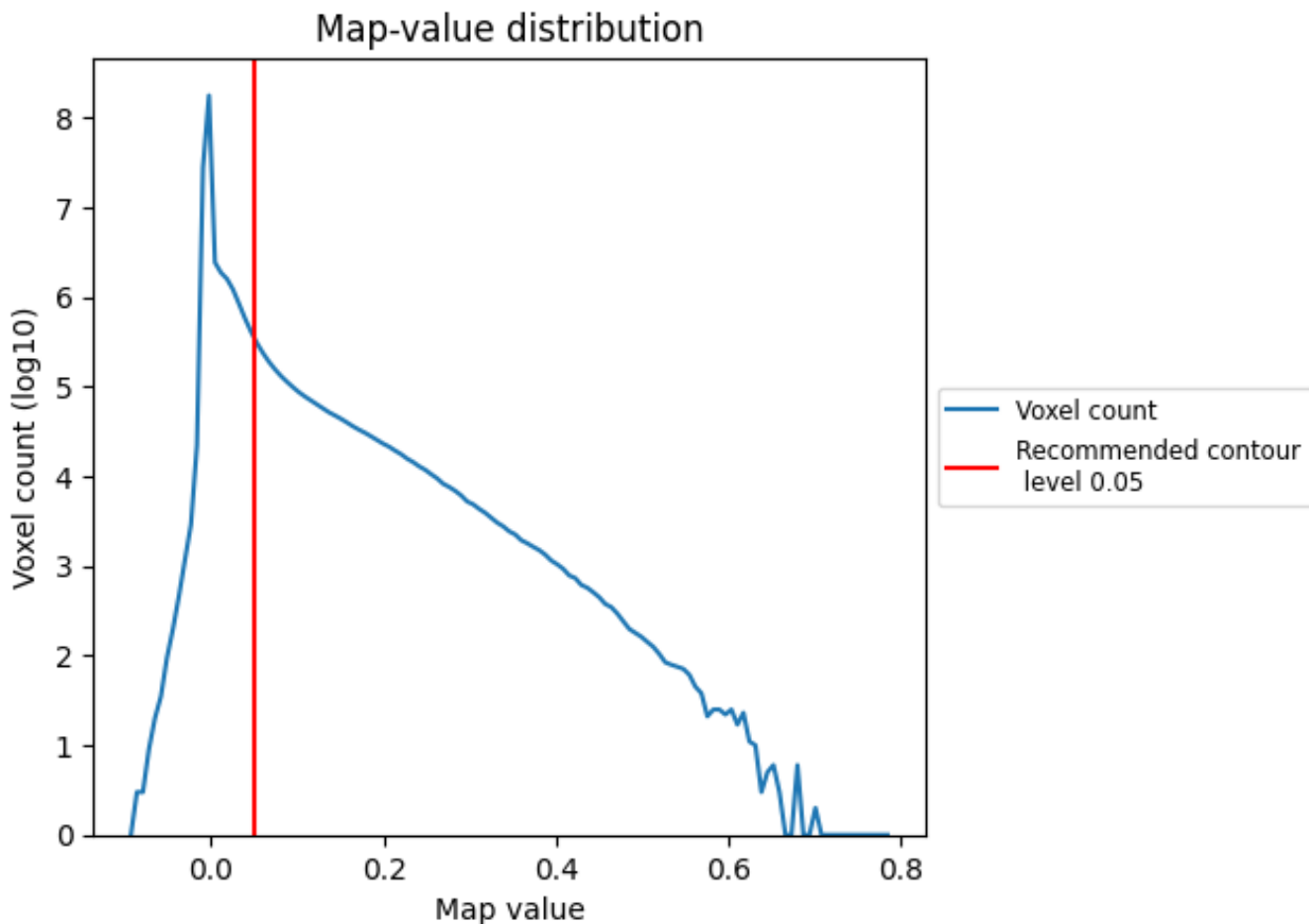
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

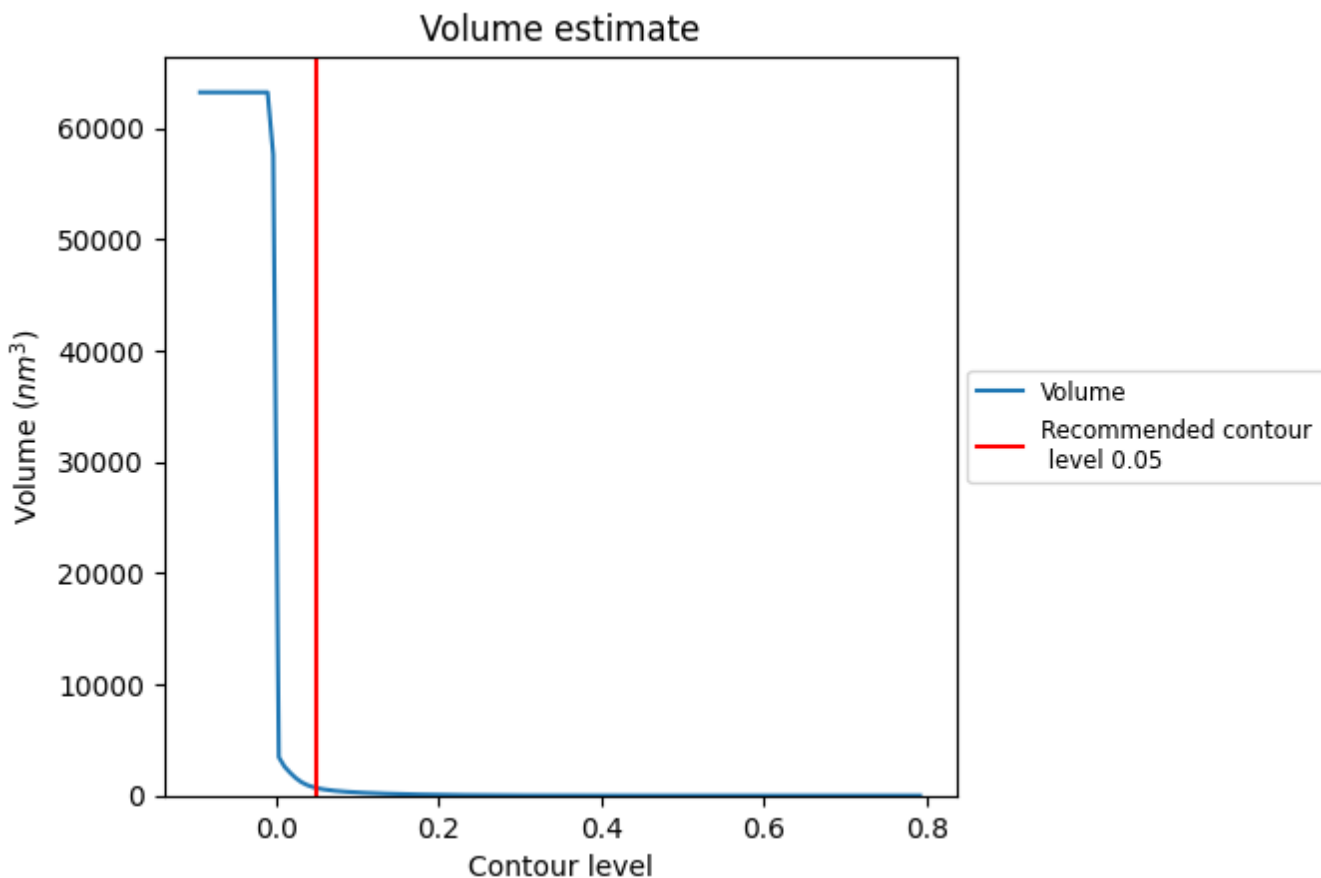
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

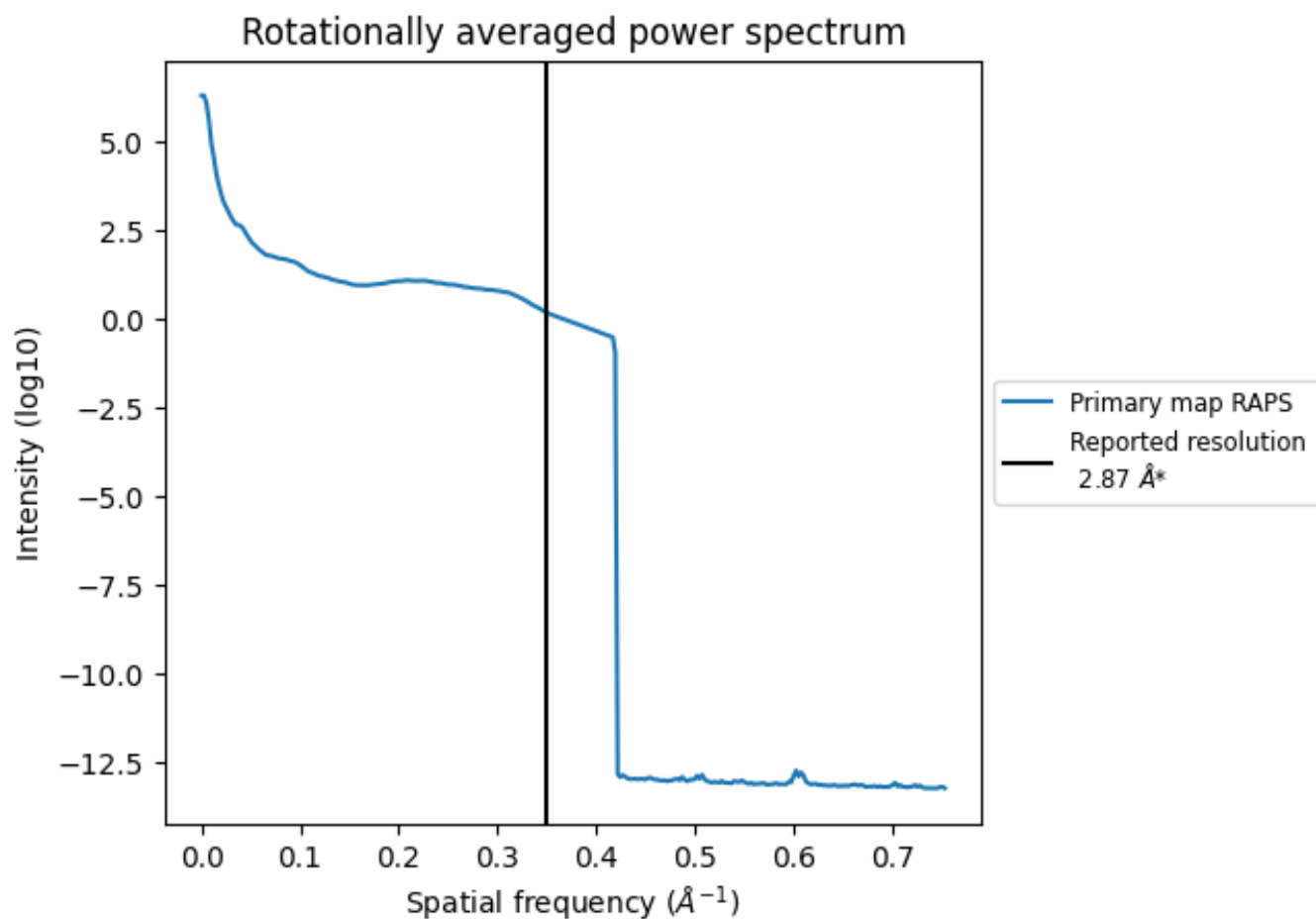
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 686 nm<sup>3</sup>; this corresponds to an approximate mass of 620 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 0.348 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

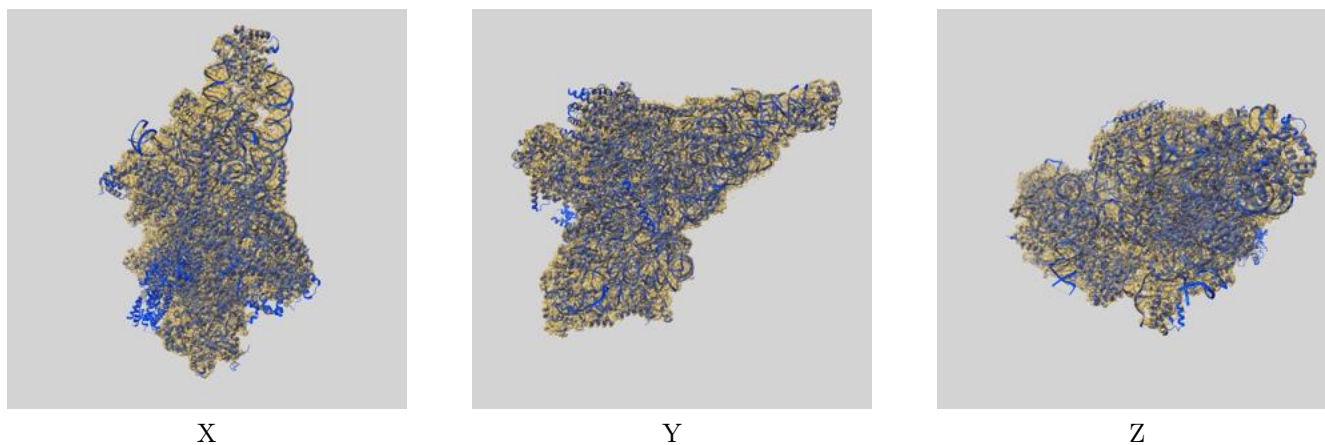
This section was not generated. No FSC curve or half-maps provided.



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

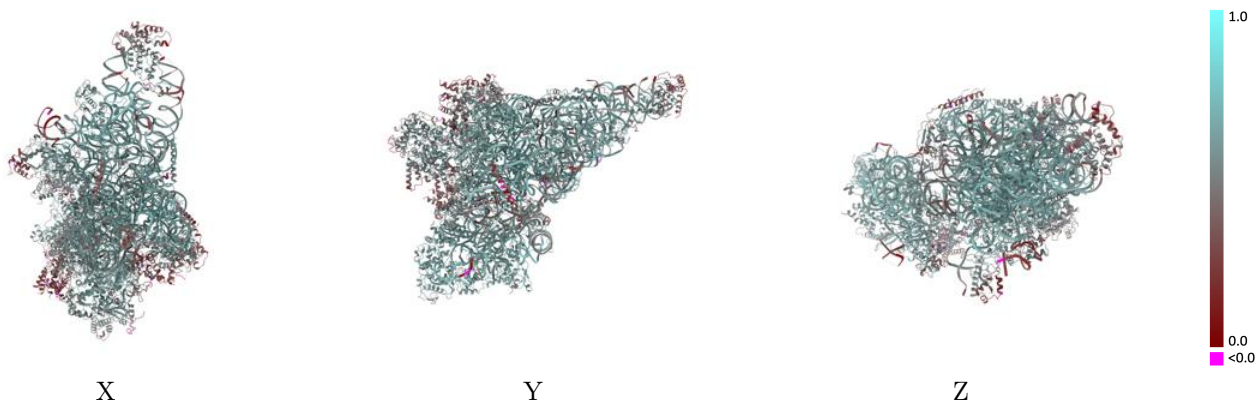
This section contains information regarding the fit between EMDB map EMD-16967 and PDB model 8OM3. Per-residue inclusion information can be found in section 3 on page 14.

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



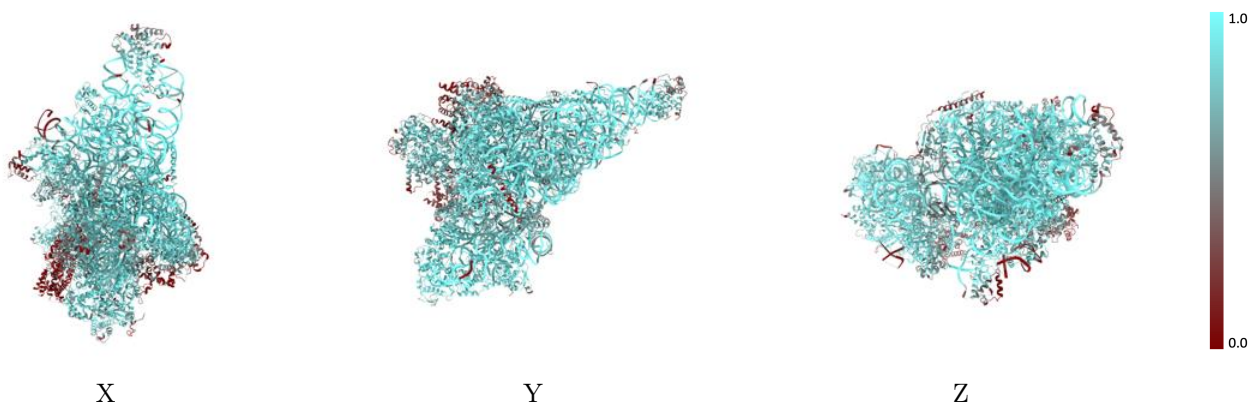
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



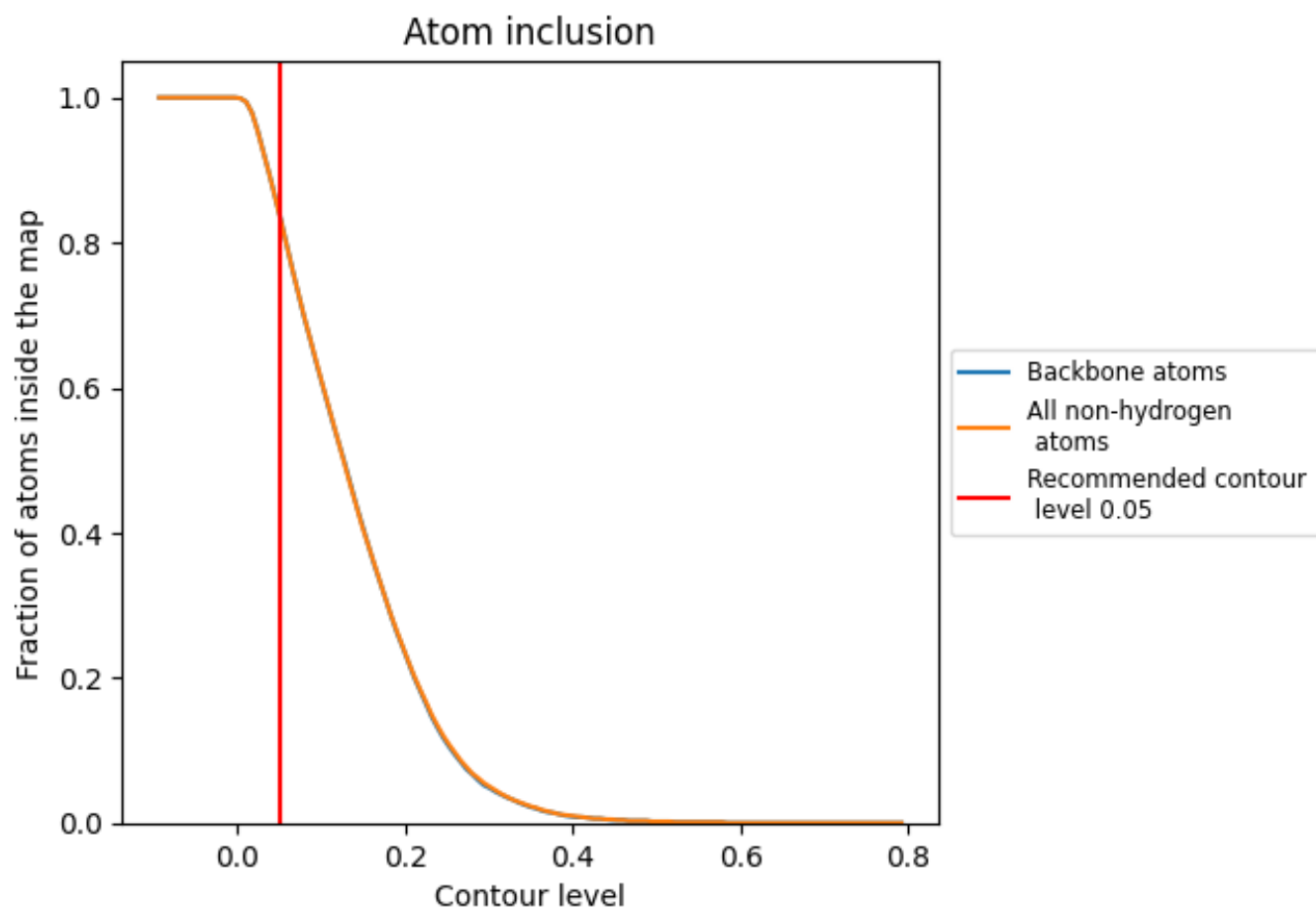
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.5640
1	 0.8330	 0.5500
2	 0.8970	 0.5880
3	 0.8520	 0.5580
4	 0.7010	 0.4840
5	 0.6860	 0.4470
6	 0.8600	 0.5680
8	 0.4680	 0.5100
A	 0.6600	 0.4710
B	 0.7430	 0.5420
C	 0.6500	 0.4730
D	 0.8190	 0.5560
E	 0.9010	 0.6020
F	 0.8860	 0.5770
G	 0.6710	 0.5000
H	 0.9660	 0.6480
I	 0.8700	 0.5780
J	 0.8950	 0.6060
K	 0.8560	 0.5690
L	 0.9590	 0.6260
M	 0.9170	 0.6130
N	 0.9610	 0.6480
O	 0.8860	 0.5920
P	 0.9310	 0.6140
Q	 0.6830	 0.4890
R	 0.8610	 0.5690
S	 0.8660	 0.6040
T	 0.8350	 0.5420
U	 0.9120	 0.6000
V	 0.7650	 0.5210
W	 0.9040	 0.6080
X	 0.8640	 0.5780
Y	 0.8100	 0.5550
Z	 0.7780	 0.5240
d	 0.5050	 0.3880
r	 0.9400	 0.5970

