



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 09:32 PM EST

PDB ID : 6NF8
EMDB ID : EMD-9362
Title : Structure of human mitochondrial translation initiation factor 3 bound to the small ribosomal subunit -Class I
Authors : Sharma, M.; Koripella, R.; Agrawal, R.
Deposited on : 2018-12-19
Resolution : 3.48 Å (reported)
Based on initial model : 3JD5

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:

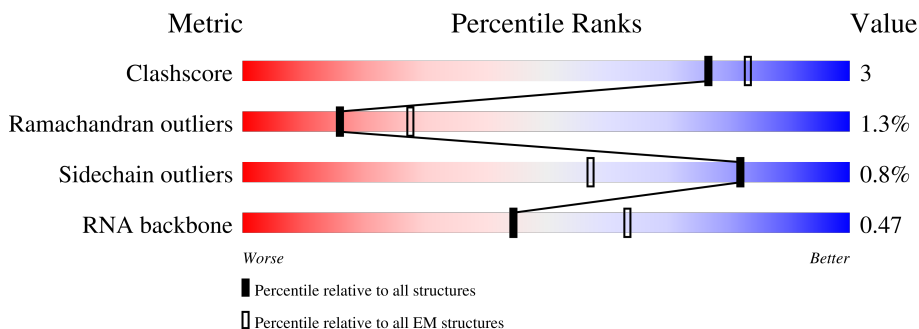
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.48 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.



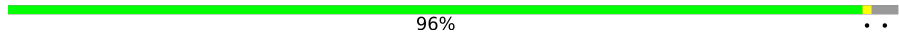


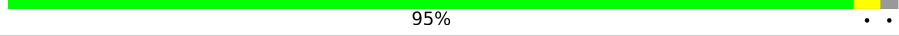




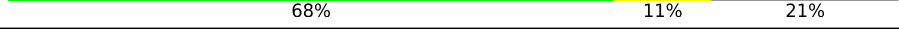
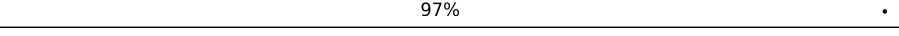
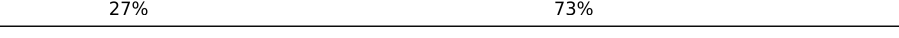
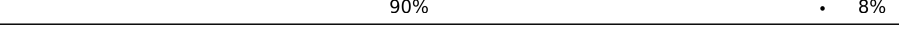

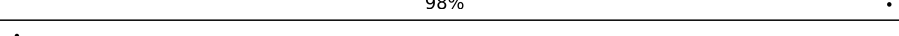


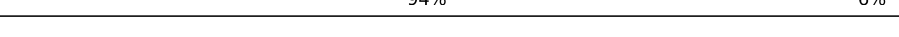

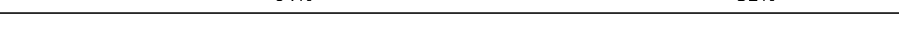






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 ≥ 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	955	
2	C	167	
3	E	430	
4	L	139	
5	P	135	
6	Q	130	
7	a	359	

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Mol	Chain	Length	Quality of chain
8	c	173	 96%
9	d	205	 85% 14%
10	e	415	 83% 14%
11	j	218	 95%
12	p	258	 71% 28%
13	G	242	 79% 7% 14%
14	I	396	 70% 9% 21%
15	J	201	 58% 5% 36%
16	N	128	 68% 11% 21%
17	g	351	 97%
18	h	386	 27% 73%
19	i	106	 90% 8%
20	k	325	 83% 15%
21	m	118	 98%
22	o	575	 79% 20%
23	B	293	 71% 26%
24	F	124	 94% 6%
25	K	197	 63% 6% 31%
26	O	256	 64% 32%
27	R	143	 62% 6% 32%
28	U	87	 87% 10%
29	b	190	 70% 29%
30	f	189	 52% 48%
31	n	199	 34% 64%
32	z	247	 17% 81% 16%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 65776 atoms, of which 0 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 28S ribosomal RNA, mitochondria.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	952	20256	9090	3685	6529	952	0	0

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	123	998	648	177	169	4	0	0

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	309	2464	1535	472	446	11	0	0

- Molecule 4 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	109	853	534	175	140	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	116	916	580	180	151	5	0	0

- Molecule 6 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	109	857	555	153	145	4	0	0

- Molecule 7 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	289	2356	1505	400	443	8	0	0

- Molecule 8 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	c	168	1374	878	246	241	9	0	0

- Molecule 9 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	d	176	1463	899	290	272	2	0	0

- Molecule 10 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	e	358	2950	1886	496	554	14	0	0

- Molecule 11 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	j	213	1792	1132	346	309	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	p	187	1531	968	288	267	8	0	0

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	208	1721	1093	313	302	13	0	0

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	311	2541	1608	454	467	12	0	0

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	J	128	1049	676	180	190	3	0	0

- Molecule 16 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	101	861	538	178	140	5	0	0

- Molecule 17 is a protein called DAP3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	g	351	2855	1835	502	508	10	0	0

- Molecule 18 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	h	103	871	566	141	161	3	0	0

- Molecule 19 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	i	98	818	519	153	143	3	0	0

- Molecule 20 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	k	275	2227	1418	377	421	11	0	0

- Molecule 21 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	118	Total	C	N	O	S	0	0
			945	587	185	164	9		

- Molecule 22 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	461	Total	C	N	O	S	0	0
			3273	2082	573	605	13		

- Molecule 23 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	217	Total	C	N	O	S	0	0
			1726	1102	319	298	7		

- Molecule 24 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	124	Total	C	N	O	S	0	0
			991	627	179	179	6		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	136	Total	C	N	O	S	0	0
			1001	628	193	177	3		

- Molecule 26 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	173	Total	C	N	O	S	0	0
			1421	904	258	250	9		

- Molecule 27 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	97	Total	C	N	O	S	0	0
			788	507	136	138	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	86	Total	C	N	O	S	0	0
			737	457	148	124	8		

- Molecule 29 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	135	Total	C	N	O	S	0	0
			1108	717	195	194	2		

- Molecule 30 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	98	Total	C	N	O	S	0	0
			775	493	135	143	4		

- Molecule 31 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	72	Total	C	N	O	S	0	0
			642	409	142	89	2		

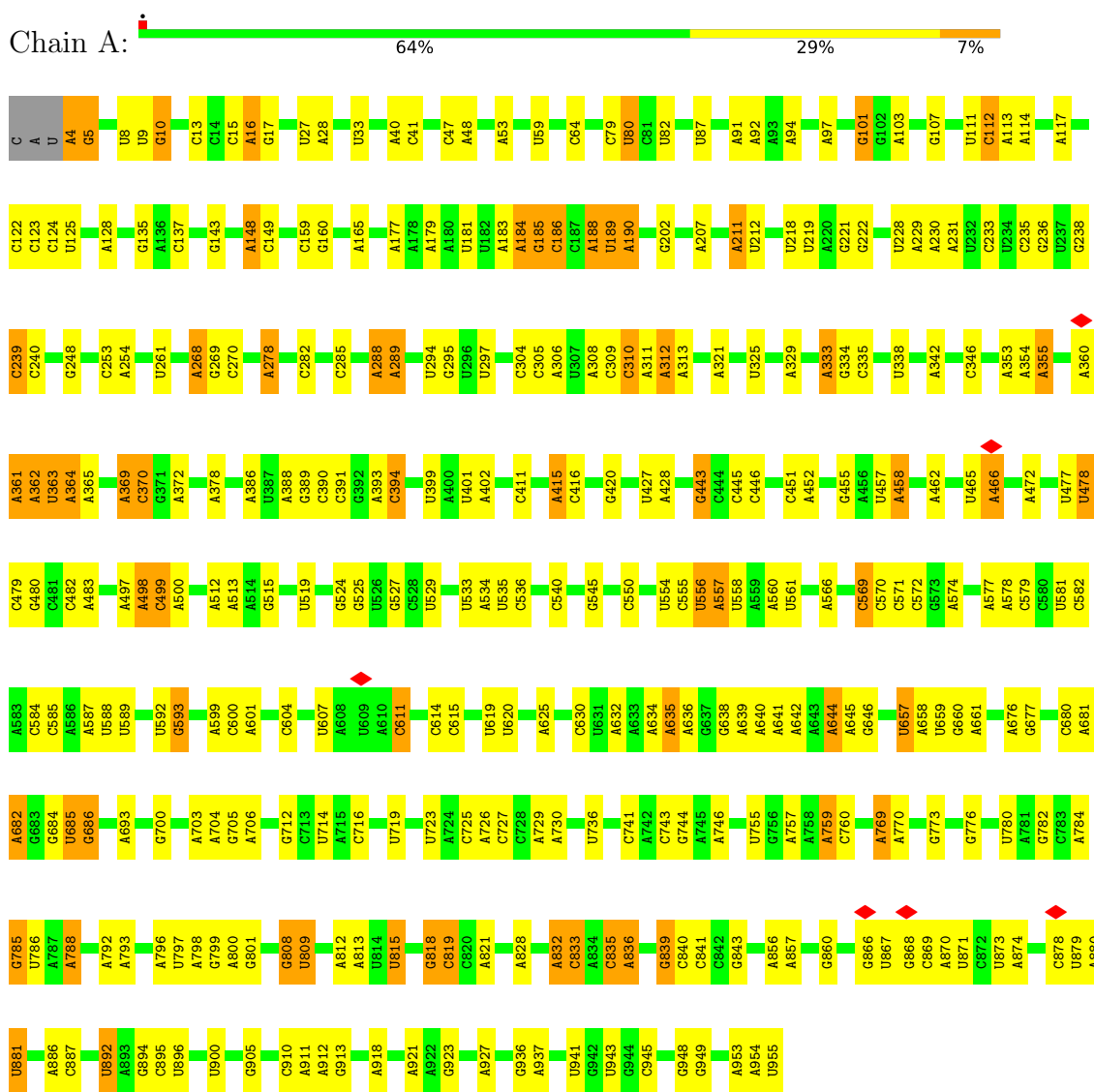
- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	207	Total	C	N	O	S	0	0
			1616	998	305	305	8		

3 Residue-property plots i

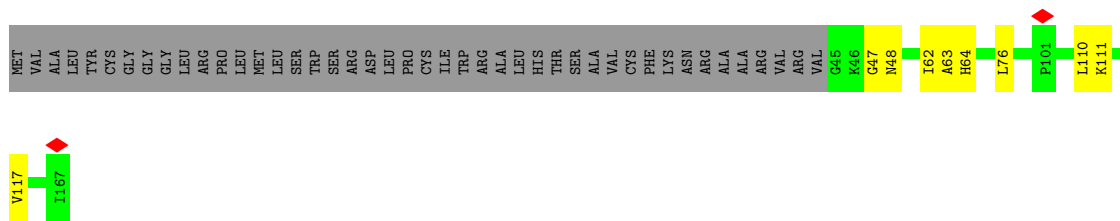
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 28S ribosomal RNA, mitochondria

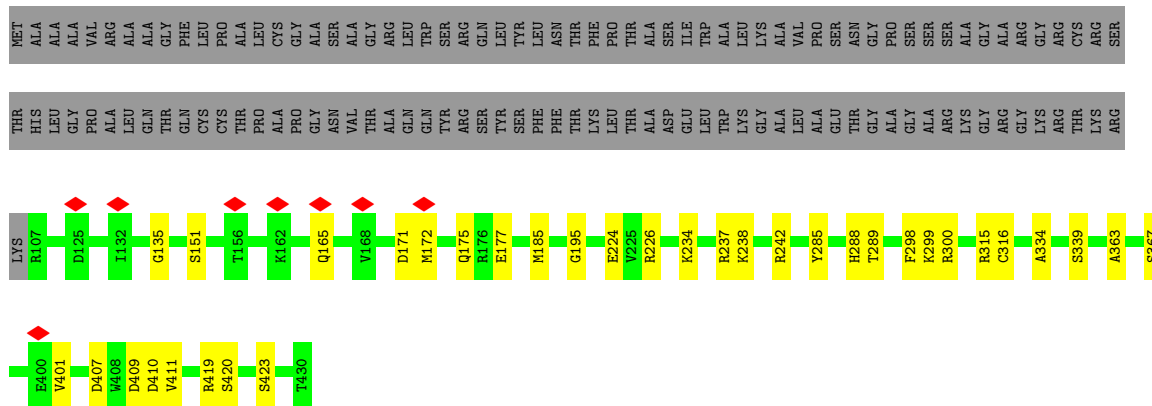


- Molecule 2: 28S ribosomal protein S24, mitochondrial

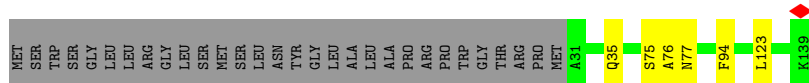




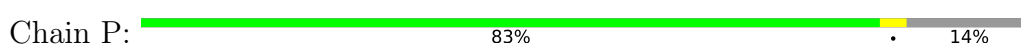
• Molecule 3: 28S ribosomal protein S5, mitochondrial



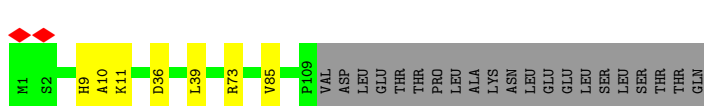
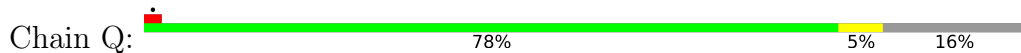
• Molecule 4: 28S ribosomal protein S12, mitochondrial



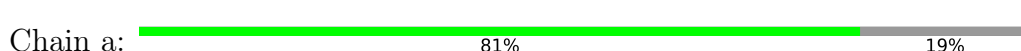
• Molecule 5: 28S ribosomal protein S16, mitochondrial



• Molecule 6: 28S ribosomal protein S17, mitochondrial



• Molecule 7: 28S ribosomal protein S22, mitochondrial



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


SER PRO LYS ILE K65 K133 SER SER ALA ALA ALA SER

- Molecule 8: 28S ribosomal protein S25, mitochondrial

Chain c:  96%


MET P2 K133 G145 A169 GLY ALA GLN ASP

- Molecule 9: 28S ribosomal protein S26, mitochondrial

Chain d:  85%

MET LEU ARG ALA MET SER THR LEU ALA ARG ALA ARG PRO PRO GLN PHE LEU LEU ALA ARG GLY R27 T169 H202 LYS GLY SER

- Molecule 10: 28S ribosomal protein S27, mitochondrial

Chain e:  83%

MET ALA PRO MET VAL ARG ARG ALA ILE PHE LEU ALA ARG ASN VAL LEU PRO GLN LEU SER ALA ARG ALA LYS ARG Y28 D47 G120 D123 M131 D140 K193 L209 G212 R241 Y244 S269 P270 R277 T291 ALA PRO ALA GLN GLU

SER PRO GLU GLN PRO GLN GLU GLU PHE LEU PRO ALA SER SER E313 E322 E406 ALA ARG ALA ALA LYS ALA ALA

- Molecule 11: 28S ribosomal protein S34, mitochondrial

Chain j:  95%

H1 R4 R5 R25 R26 R27 H137 H145 Y166 I196 T213 LYS GLY THR ALA VAL

- Molecule 12: 28S ribosomal protein S18b, mitochondrial

Chain p:  71%

MET ALA SER VAL ASN VAL LEU ARG ARG ALA PRO TYR PHE SER PRO PHE ARG GLY TYR GLY VAL GLN VAL PRO LEU THR LEU CYS THR LYS ALA PRO PRO GLU ASP ASP LEU PRO PRO ILE PRO VAL SER PRO Y51 L113 G229 N235 P236 K237 VAL

PRO LEU THR PRO ASN PRO GLU THR SER THR GLU GLN ALA GLY PRO PRO GLN SER SER ALA LEU

- Molecule 13: 28S ribosomal protein S7, mitochondrial

LEU
THR
ALA
ASP
PHE
THR
LEU
SER
GLN
GLU
GLN
LYS
GLU
ALA
LEU
GLY
ASP
GLY
THR
ALA
LEU
THR
SER
SER
SER
GLU
SER
ASP
SER
SER
ASP
THR
SER
LYS
ASP
LYS

- Molecule 23: 28S ribosomal protein S2, mitochondrial

Chain B:  71% 26%

MET
ALA
THR
GLY
ALA
VAL
LEU
PRO
ARG
GLY
LEU
GLY
ALA
GLY
VAL
HIS
PRO
ALA
ALA
PRO
ARG
ALA
GLY
ALA
GLN
ARG
GLY
THR
LEU
GLY
SER
SER
ALA
GLY
ALA
ALA
HIS
SER
PRO
ARG
GLU
GLU
PRO
GLU
ARG
ASP
SER
SER
ASP
R47
A84
R87
H88
R89
G101
Q115
M119

F126
R136
V191
R253
Q263
GLY
ALA
PRO
GLY
PRO
HIS
PRO
ALA
ASN
PRO
ALA
ALA
GLY
ALA
PRO
SER
PRO
GLY
GLN
ALA
LEU
MET
GLY
HIS
SER
PRO

- Molecule 24: 28S ribosomal protein S6, mitochondrial

Chain F:  94% 6%

M1
P2
E5
A12
Y63
P71
V94
T99
V111
K124

- Molecule 25: 28S ribosomal protein S11, mitochondrial

Chain K:  63% 6% 31%

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

S62
I88
N96
N97
T98
V103
R151
V153
R161
D180
P185
H186
N187
L197

- Molecule 26: 28S ribosomal protein S15, mitochondrial

Chain O:  64% 6% 32%

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

SER
GLN
E83
G80
K147
D148
H151
K152
R153
R170
Y194
H195
Q217
A230
A231
A232
A233
Q234
K235
GLN
GLY
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ARG
ASN
PRO
GLU
SER
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THR
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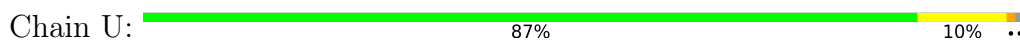
- Molecule 27: 28S ribosomal protein S18c, mitochondrial

Chain R:  62% 6% 32%

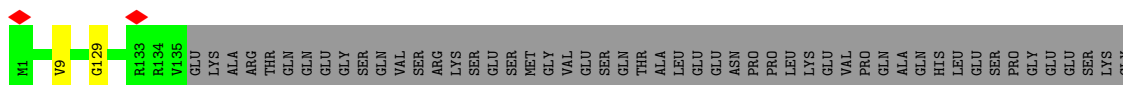
MET
ALA
VAL
LEU
LEU
CYS
GLY
GLY
GLY
LYS
ARG
PHE
THR
ARG
PHE
PRO
THR
ALA
PHE
VAL
CYS
LEU
THR
SER
GLY
THR
ARG
VAL
LEU
TRP
ARG
SER
CYS
SER
GLN
CYS
LYS
GLN
VAL
THR
S47
Q83
F84
I85
F88
I92
G102
R106

G119
P134
E143

- Molecule 28: 28S ribosomal protein S21, mitochondrial

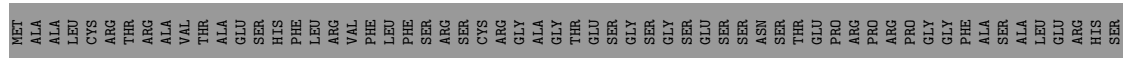
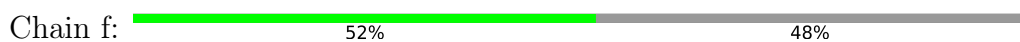


- Molecule 29: 28S ribosomal protein S23, mitochondrial

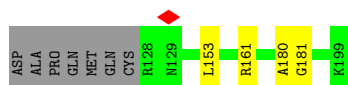
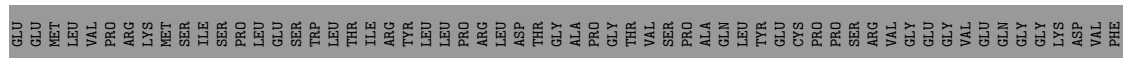
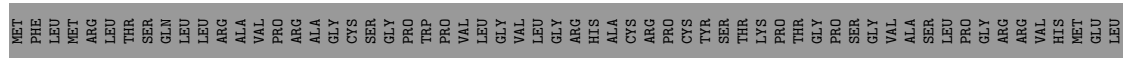


LEU
SER
PRO
PRO

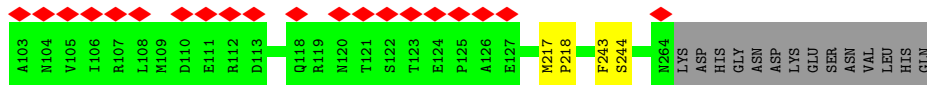
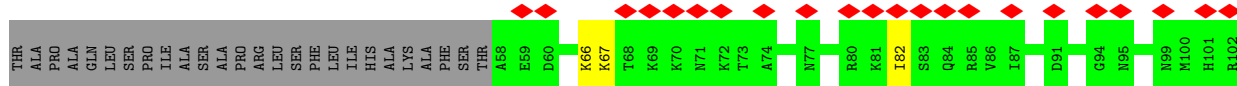
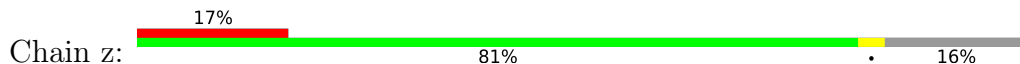
- Molecule 30: 28S ribosomal protein S28, mitochondrial



- Molecule 31: Aurora kinase A interacting protein 1



- Molecule 32: Translation initiation factor IF-3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.256	Depositor
Minimum map value	-1.205	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/22681	0.70	3/35318 (0.0%)
2	C	0.23	0/1026	0.37	0/1389
3	E	0.23	0/2511	0.39	0/3369
4	L	0.23	0/872	0.40	0/1171
5	P	0.23	0/937	0.37	0/1262
6	Q	0.23	0/874	0.39	0/1183
7	a	0.23	0/2403	0.36	0/3246
8	c	0.23	0/1406	0.38	0/1894
9	d	0.22	0/1489	0.34	0/2008
10	e	0.23	0/3011	0.35	0/4066
11	j	0.22	0/1841	0.37	0/2493
12	p	0.23	0/1583	0.36	0/2149
13	G	0.25	0/1761	0.37	0/2366
14	I	0.24	0/2597	0.37	0/3487
15	J	0.22	0/1071	0.37	0/1447
16	N	0.21	0/878	0.35	0/1179
17	g	0.24	0/2923	0.38	0/3956
18	h	0.24	0/899	0.33	0/1209
19	i	0.23	0/834	0.34	0/1112
20	k	0.22	0/2275	0.35	0/3075
21	m	0.23	0/961	0.35	0/1284
22	o	0.23	0/2605	0.35	0/3526
23	B	0.24	0/1766	0.37	0/2392
24	F	0.23	0/1009	0.39	0/1362
25	K	0.23	0/1021	0.40	0/1380
26	O	0.23	0/1443	0.33	0/1927
27	R	0.23	0/805	0.37	0/1082
28	U	0.23	0/748	0.34	0/995
29	b	0.24	0/1135	0.35	0/1528
30	f	0.23	0/787	0.40	0/1059
31	n	0.22	0/654	0.34	0/862
32	z	0.23	0/1633	0.38	0/2191
All	All	0.20	0/68439	0.51	3/96967 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	569	C	OP1-P-O3'	-10.62	81.83	105.20
1	A	569	C	OP2-P-O3'	-10.59	81.90	105.20
1	A	570	C	OP1-P-OP2	7.31	130.56	119.60

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	20256	0	10258	132	0
2	C	998	0	1005	5	0
3	E	2464	0	2489	20	0
4	L	853	0	904	4	0
5	P	916	0	944	2	0
6	Q	857	0	920	4	0
7	a	2356	0	2371	0	0
8	c	1374	0	1395	0	0
9	d	1463	0	1438	0	0
10	e	2950	0	2940	0	0
11	j	1792	0	1810	0	0
12	p	1531	0	1495	0	0
13	G	1721	0	1751	11	0
14	I	2541	0	2498	22	0
15	J	1049	0	1088	7	0
16	N	861	0	890	9	0
17	g	2855	0	2894	0	0
18	h	871	0	814	0	0
19	i	818	0	845	0	0
20	k	2227	0	2267	0	0
21	m	945	0	984	0	0
22	o	3273	0	2705	0	0
23	B	1726	0	1747	6	0
24	F	991	0	1034	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	K	1001	0	1041	7	0
26	O	1421	0	1526	5	0
27	R	788	0	823	6	0
28	U	737	0	759	6	0
29	b	1108	0	1124	0	0
30	f	775	0	793	0	0
31	n	642	0	718	0	0
32	z	1616	0	1600	0	0
All	All	65776	0	55870	205	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:G:O2'	1:A:786:U:O2	1.93	0.87
1:A:607:U:O2	1:A:686:G:O6	1.92	0.86
1:A:363:U:O2'	1:A:364:A:OP1	1.93	0.86
1:A:391:C:O2'	1:A:478:U:O2	1.92	0.86
1:A:188:A:O2'	1:A:189:U:O5'	1.96	0.83
1:A:755:U:O2'	1:A:798:A:N3	2.10	0.83
1:A:222:G:O2'	1:A:270:C:O2	1.96	0.82
1:A:17:G:N2	1:A:512:A:O2'	2.14	0.81
1:A:843:G:O2'	1:A:937:A:O2'	1.99	0.80
1:A:288:A:HO2'	1:A:515:G:HO2'	1.23	0.80
1:A:4:A:O2'	1:A:5:G:OP1	2.00	0.80
1:A:519:U:HO2'	1:A:636:A:HO2'	1.26	0.80
1:A:579:C:O2	16:N:86:ARG:NE	2.15	0.80
1:A:585:C:O2	1:A:700:G:N2	2.12	0.80
1:A:519:U:O2'	1:A:636:A:O2'	1.99	0.79
1:A:310:C:O2'	27:R:106:ARG:NH1	2.16	0.79
1:A:297:U:O2	1:A:393:A:N7	2.19	0.76
1:A:759:A:N6	1:A:799:G:N2	2.34	0.76
1:A:8:U:O2	1:A:17:G:O6	2.04	0.76
1:A:113:A:N6	1:A:135:G:C2	2.54	0.76
1:A:736:U:OP1	13:G:197:ARG:NE	2.18	0.76
1:A:635:A:OP2	3:E:242:ARG:NH1	2.20	0.75
1:A:186:C:N4	1:A:202:G:OP2	2.20	0.74
1:A:808:G:O2'	1:A:809:U:OP1	2.05	0.73
1:A:812:A:O2'	1:A:813:A:O4'	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:102:GLY:O	27:R:106:ARG:NH1	2.22	0.73
1:A:235:C:N4	1:A:236:G:O6	2.22	0.72
1:A:401:U:O3'	1:A:943:U:O2'	2.07	0.72
1:A:808:G:HO2'	1:A:809:U:P	2.12	0.72
1:A:122:C:N4	6:Q:73:ARG:O	2.23	0.72
1:A:556:U:O2'	1:A:557:A:O5'	2.06	0.72
5:P:20:ARG:NH2	5:P:41:CYS:SG	2.63	0.72
1:A:309:C:O2'	1:A:369:A:N3	2.23	0.71
1:A:401:U:O2'	1:A:943:U:O2	2.07	0.71
1:A:211:A:N7	1:A:268:A:O2'	2.22	0.71
1:A:335:C:OP1	25:K:97:ASN:ND2	2.22	0.71
14:I:202:LYS:NZ	14:I:215:ASP:OD1	2.23	0.71
15:J:85:LYS:NZ	15:J:110:GLU:OE2	2.24	0.71
2:C:76:LEU:O	16:N:103:ARG:NH2	2.25	0.70
5:P:20:ARG:NH2	5:P:42:PRO:O	2.23	0.70
3:E:135:GLY:O	3:E:165:GLN:NE2	2.26	0.69
14:I:378:GLU:OE1	14:I:381:LYS:NZ	2.25	0.69
1:A:122:C:OP2	6:Q:73:ARG:NH2	2.26	0.68
1:A:228:U:OP2	1:A:229:A:O2'	2.10	0.68
1:A:545:G:N1	1:A:776:G:OP2	2.27	0.68
1:A:759:A:C6	1:A:799:G:N2	2.61	0.68
1:A:638:G:O2'	1:A:646:G:OP2	2.08	0.68
16:N:96:ARG:NH1	16:N:98:ARG:O	2.26	0.68
1:A:607:U:C2	1:A:686:G:O6	2.46	0.67
1:A:361:A:O2'	1:A:378:A:O4'	2.12	0.67
1:A:657:U:O4	14:I:122:ARG:NH1	2.29	0.65
27:R:83:GLN:NE2	27:R:134:PRO:O	2.30	0.64
16:N:116:ASP:OD1	16:N:125:ARG:NH2	2.30	0.64
1:A:399:U:N3	1:A:446:C:O2'	2.30	0.64
1:A:945:C:OP2	28:U:49:CYS:N	2.31	0.63
23:B:115:GLN:OE1	23:B:119:ASN:ND2	2.32	0.63
1:A:867:U:O4	1:A:892:U:N3	2.31	0.63
1:A:792:A:O2'	1:A:793:A:O4'	2.09	0.63
1:A:785:G:N2	14:I:377:ARG:O	2.22	0.62
13:G:36:ARG:NH1	14:I:374:PRO:O	2.32	0.62
1:A:338:U:OP2	25:K:96:ASN:ND2	2.32	0.62
1:A:945:C:OP1	28:U:52:ARG:NH2	2.33	0.62
1:A:527:G:O6	1:A:828:A:N6	2.33	0.62
14:I:155:LYS:NZ	14:I:217:ASP:OD2	2.32	0.62
1:A:759:A:N6	1:A:799:G:C2	2.68	0.61
24:F:5:GLU:N	24:F:94:VAL:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:C:O5'	1:A:839:G:N2	2.34	0.61
14:I:260:LEU:N	14:I:269:PHE:O	2.33	0.61
1:A:289:A:N3	1:A:482:C:O2'	2.28	0.61
1:A:415:A:O2'	1:A:941:U:O2	2.17	0.61
1:A:9:U:O4	1:A:16:A:N7	2.34	0.60
14:I:237:GLU:N	14:I:237:GLU:OE1	2.34	0.60
1:A:184:A:O2'	1:A:185:G:O5'	2.15	0.60
1:A:818:G:O2'	1:A:819:C:O5'	2.13	0.60
1:A:342:A:O2'	1:A:420:G:O3'	2.19	0.59
3:E:300:ARG:O	3:E:339:SER:OG	2.19	0.59
14:I:231:LEU:O	14:I:233:CYS:N	2.35	0.59
1:A:394:C:O2'	26:O:195:HIS:O	2.21	0.59
1:A:10:G:N2	1:A:13:C:OP2	2.36	0.59
1:A:27:U:O4	1:A:28:A:N6	2.35	0.59
15:J:117:ARG:NH2	16:N:128:TRP:O	2.36	0.59
1:A:815:U:OP2	13:G:177:ARG:NH2	2.35	0.58
1:A:443:G:OP2	26:O:147:LYS:NZ	2.37	0.58
1:A:295:G:O2'	26:O:153:ARG:NH2	2.37	0.57
1:A:585:C:N3	1:A:700:G:N1	2.45	0.57
1:A:843:G:HO2'	1:A:937:A:HO2'	1.31	0.57
1:A:87:U:O4	1:A:94:A:N6	2.38	0.56
3:E:285:TYR:N	3:E:289:THR:O	2.37	0.56
1:A:113:A:N6	1:A:135:G:N2	2.54	0.55
25:K:88:ILE:N	25:K:103:VAL:O	2.39	0.55
1:A:835:C:OP1	3:E:237:ARG:NH2	2.38	0.55
1:A:498:A:O2'	1:A:499:C:O5'	2.25	0.55
1:A:278:A:OP1	3:E:419:ARG:NH1	2.40	0.55
1:A:607:U:O2	1:A:686:G:C6	2.60	0.55
3:E:171:ASP:OD1	3:E:172:MET:N	2.40	0.55
14:I:304:PHE:O	14:I:310:ARG:NH1	2.40	0.54
6:Q:36:ASP:OD2	6:Q:39:LEU:N	2.40	0.54
13:G:68:LEU:HD21	14:I:366:GLN:HB2	1.89	0.54
1:A:554:U:O4	1:A:555:C:N4	2.40	0.54
14:I:330:CYS:SG	14:I:331:THR:N	2.82	0.53
1:A:818:G:HO2'	1:A:819:C:P	2.31	0.53
1:A:780:U:O2'	14:I:392:THR:HG22	2.08	0.53
3:E:316:CYS:SG	3:E:334:ALA:N	2.79	0.53
1:A:953:A:O2'	28:U:61:ARG:NH1	2.42	0.53
15:J:104:ILE:O	15:J:105:SER:OG	2.22	0.53
1:A:786:U:OP1	14:I:388:ARG:NH2	2.42	0.52
1:A:15:C:OP1	3:E:339:SER:OG	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:U:O2'	1:A:177:A:N3	2.42	0.52
1:A:743:C:OP2	1:A:769:A:N6	2.43	0.52
26:O:148:ASP:OD2	26:O:151:HIS:ND1	2.42	0.52
1:A:611:C:N3	1:A:685:U:N3	2.59	0.52
3:E:410:ASP:OD1	3:E:411:VAL:N	2.41	0.51
1:A:113:A:C6	1:A:135:G:N2	2.79	0.51
14:I:135:GLN:OE1	14:I:136:ARG:N	2.43	0.51
3:E:420:SER:OG	3:E:423:SER:OG	2.27	0.51
16:N:91:CYS:SG	16:N:92:VAL:N	2.83	0.51
1:A:188:A:HO2'	1:A:189:U:C5'	2.16	0.51
1:A:128:A:N6	26:O:217:GLN:OE1	2.44	0.51
4:L:77:ASN:N	4:L:77:ASN:OD1	2.45	0.50
28:U:48:PRO:O	28:U:52:ARG:NE	2.44	0.50
1:A:233:C:N4	1:A:261:U:O4	2.45	0.50
1:A:625:A:OP1	3:E:234:LYS:NZ	2.43	0.50
23:B:126:PHE:O	23:B:253:ARG:NH1	2.39	0.50
1:A:354:A:O2'	1:A:355:A:O4'	2.21	0.50
1:A:312:A:N6	1:A:369:A:OP2	2.45	0.49
13:G:203:GLU:OE2	13:G:207:GLN:NE2	2.44	0.49
1:A:462:A:OP1	23:B:89:ARG:NH2	2.44	0.49
1:A:540:C:O3'	13:G:185:LYS:NZ	2.25	0.49
24:F:63:TYR:OH	27:R:119:GLY:O	2.19	0.49
1:A:785:G:O2'	14:I:378:GLU:OE2	2.30	0.49
1:A:285:C:OP1	1:A:466:A:N6	2.44	0.49
23:B:84:ALA:N	23:B:101:GLY:O	2.46	0.49
2:C:110:LEU:HD23	2:C:111:LYS:N	2.28	0.48
24:F:2:PRO:O	24:F:99:THR:OG1	2.32	0.48
3:E:224:GLU:OE2	3:E:226:ARG:NH2	2.47	0.48
2:C:62:ILE:O	2:C:63:ALA:HB3	2.13	0.48
1:A:80:U:O4	1:A:101:G:N1	2.47	0.48
27:R:85:ILE:HG22	27:R:92:ILE:HG22	1.96	0.47
15:J:123:SER:OG	15:J:124:VAL:N	2.46	0.47
1:A:477:U:H2'	1:A:478:U:C6	2.49	0.47
1:A:797:U:OP1	16:N:102:ARG:NH1	2.42	0.47
1:A:558:U:HO2'	1:A:560:A:N6	2.12	0.47
13:G:37:TYR:OH	14:I:373:ASP:OD1	2.32	0.47
14:I:214:SER:OG	14:I:215:ASP:N	2.48	0.46
1:A:4:A:HO2'	1:A:5:G:P	2.33	0.46
1:A:704:A:N6	1:A:705:G:O6	2.49	0.46
3:E:172:MET:SD	3:E:175:GLN:NE2	2.88	0.46
3:E:298:PHE:O	3:E:300:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:U:OP2	1:A:582:C:O2'	2.29	0.46
1:A:189:U:O3'	1:A:190:A:O4'	2.34	0.46
1:A:362:A:O5'	25:K:187:ASN:ND2	2.48	0.46
1:A:593:G:P	1:A:593:G:H21	2.38	0.46
1:A:832:A:O2'	1:A:839:G:N2	2.49	0.46
1:A:333:A:N1	1:A:346:C:O2'	2.35	0.46
14:I:72:ASP:OD1	14:I:73:PHE:N	2.49	0.45
1:A:297:U:C2	1:A:393:A:N7	2.85	0.45
1:A:239:C:O2'	4:L:75:SER:OG	2.35	0.45
3:E:401:VAL:HG22	3:E:401:VAL:O	2.16	0.45
13:G:70:LYS:HE3	14:I:248:VAL:HG11	1.97	0.45
1:A:188:A:C2'	1:A:189:U:O5'	2.65	0.45
2:C:64:HIS:NE2	16:N:124:GLN:OE1	2.50	0.44
25:K:161:ARG:NH2	25:K:180:ASP:OD1	2.50	0.44
13:G:59:THR:HG23	13:G:60:GLU:N	2.32	0.44
25:K:97:ASN:OD1	25:K:98:THR:N	2.49	0.44
1:A:577:A:N3	1:A:582:C:N4	2.61	0.44
24:F:111:VAL:HG13	24:F:111:VAL:O	2.17	0.44
1:A:644:A:OP2	23:B:136:ARG:NH2	2.50	0.44
1:A:880:A:H3'	1:A:881:U:C5'	2.48	0.44
1:A:457:U:O4	1:A:458:A:N6	2.51	0.43
1:A:788:A:OP1	14:I:389:ARG:NE	2.51	0.43
3:E:315:ARG:NH1	3:E:423:SER:O	2.51	0.43
15:J:181:PRO:O	15:J:183:HIS:N	2.49	0.43
15:J:79:LEU:O	15:J:171:GLU:N	2.46	0.43
1:A:840:C:HO2'	1:A:841:C:H6	1.64	0.43
3:E:363:ALA:O	3:E:367:SER:N	2.49	0.43
25:K:185:PRO:O	25:K:187:ASN:N	2.52	0.43
27:R:88:PHE:O	28:U:10:ARG:N	2.49	0.43
1:A:8:U:C2	1:A:17:G:O6	2.72	0.43
1:A:288:A:O2'	1:A:515:G:O2'	2.05	0.43
1:A:716:C:O2'	1:A:773:G:O4'	2.37	0.43
16:N:94:THR:O	16:N:95:SER:OG	2.30	0.43
1:A:111:U:H4'	1:A:112:C:C5'	2.49	0.42
3:E:409:ASP:OD1	3:E:410:ASP:N	2.52	0.42
1:A:744:G:N1	1:A:770:A:OP2	2.46	0.42
4:L:94:PHE:N	4:L:123:LEU:O	2.47	0.42
1:A:288:A:HO2'	1:A:515:G:C2'	2.28	0.42
3:E:420:SER:HG	3:E:423:SER:HG	1.62	0.42
1:A:577:A:OP2	1:A:800:A:N6	2.45	0.42
1:A:402:A:H61	1:A:445:C:H42	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:C:HO2'	1:A:836:A:P	2.43	0.42
2:C:110:LEU:HD21	2:C:117:VAL:HG13	2.02	0.42
1:A:369:A:H3'	1:A:370:C:H5''	2.01	0.42
1:A:148:A:C2	1:A:149:C:C5	3.07	0.41
1:A:294:U:O2'	1:A:372:A:N3	2.40	0.41
1:A:881:U:O2	1:A:881:U:O4'	2.37	0.41
1:A:480:G:N7	4:L:35:GLN:NE2	2.68	0.41
28:U:5:LEU:HB2	28:U:8:ILE:HD11	2.02	0.41
6:Q:9:HIS:O	6:Q:11:LYS:N	2.54	0.41
13:G:68:LEU:HD22	14:I:362:GLU:HG3	2.02	0.41
23:B:191:VAL:HG12	23:B:191:VAL:O	2.20	0.41
1:A:363:U:HO2'	1:A:364:A:P	2.33	0.41
1:A:813:A:HO2'	13:G:181:PHE:HE1	1.65	0.41
1:A:682:A:N6	15:J:124:VAL:HG13	2.36	0.40
1:A:47:C:HO2'	1:A:48:A:C5'	2.33	0.40
1:A:269:G:H2'	1:A:270:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	121/167 (72%)	102 (84%)	17 (14%)	2 (2%)	9	40
3	E	307/430 (71%)	257 (84%)	44 (14%)	6 (2%)	7	37
4	L	107/139 (77%)	93 (87%)	13 (12%)	1 (1%)	17	54
5	P	114/135 (84%)	103 (90%)	10 (9%)	1 (1%)	17	54
6	Q	107/130 (82%)	93 (87%)	12 (11%)	2 (2%)	8	37
7	a	287/359 (80%)	258 (90%)	29 (10%)	0	100	100
8	c	166/173 (96%)	152 (92%)	12 (7%)	2 (1%)	13	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	d	174/205 (85%)	167 (96%)	7 (4%)	0	100	100
10	e	354/415 (85%)	316 (89%)	31 (9%)	7 (2%)	7	37
11	j	211/218 (97%)	172 (82%)	35 (17%)	4 (2%)	8	37
12	p	185/258 (72%)	161 (87%)	22 (12%)	2 (1%)	14	50
13	G	206/242 (85%)	187 (91%)	18 (9%)	1 (0%)	29	66
14	I	307/396 (78%)	283 (92%)	22 (7%)	2 (1%)	22	60
15	J	126/201 (63%)	109 (86%)	16 (13%)	1 (1%)	19	57
16	N	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
17	g	349/351 (99%)	316 (90%)	28 (8%)	5 (1%)	11	43
18	h	101/386 (26%)	94 (93%)	7 (7%)	0	100	100
19	i	96/106 (91%)	83 (86%)	11 (12%)	2 (2%)	7	35
20	k	273/325 (84%)	239 (88%)	28 (10%)	6 (2%)	6	35
21	m	116/118 (98%)	95 (82%)	19 (16%)	2 (2%)	9	40
22	o	306/575 (53%)	260 (85%)	39 (13%)	7 (2%)	6	34
23	B	215/293 (73%)	190 (88%)	25 (12%)	0	100	100
24	F	122/124 (98%)	114 (93%)	6 (5%)	2 (2%)	9	41
25	K	134/197 (68%)	110 (82%)	23 (17%)	1 (1%)	22	60
26	O	171/256 (67%)	150 (88%)	19 (11%)	2 (1%)	13	47
27	R	95/143 (66%)	82 (86%)	13 (14%)	0	100	100
28	U	84/87 (97%)	76 (90%)	6 (7%)	2 (2%)	6	33
29	b	133/190 (70%)	118 (89%)	13 (10%)	2 (2%)	10	42
30	f	96/189 (51%)	90 (94%)	6 (6%)	0	100	100
31	n	70/199 (35%)	64 (91%)	3 (4%)	3 (4%)	2	21
32	z	205/247 (83%)	171 (83%)	28 (14%)	6 (3%)	4	29
All	All	5437/7382 (74%)	4800 (88%)	566 (10%)	71 (1%)	16	45

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	e	270	PRO
11	j	145	HIS
19	i	96	LYS
20	k	98	PRO
3	E	185	MET

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Mol	Chain	Res	Type
3	E	288	HIS
3	E	299	LYS
10	e	120	GLY
10	e	212	GLY
17	g	298	ASN
21	m	27	LEU
22	o	487	SER
26	O	80	GLY
28	U	84	TRP
29	b	9	VAL
29	b	129	GLY
32	z	66	LYS
32	z	67	LYS
32	z	82	ILE
32	z	243	PHE
2	C	48	ASN
6	Q	10	ALA
6	Q	85	VAL
10	e	140	ASP
13	G	54	PRO
14	I	232	PRO
15	J	105	SER
17	g	163	ASN
20	k	82	ALA
22	o	605	HIS
24	F	12	ALA
31	n	180	ALA
31	n	181	GLY
32	z	244	SER
2	C	47	GLY
3	E	195	GLY
3	E	238	LYS
5	P	27	THR
8	c	133	LYS
10	e	47	ASP
17	g	175	GLN
21	m	61	PHE
22	o	420	GLN
24	F	71	PRO
26	O	194	TYR
31	n	153	LEU
32	z	218	PRO

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Mol	Chain	Res	Type
3	E	151	SER
10	e	131	ASN
11	j	137	HIS
17	g	48	SER
20	k	161	SER
20	k	304	GLU
22	o	66	ASP
22	o	69	ALA
22	o	447	ASN
28	U	83	PRO
4	L	76	ALA
10	e	322	GLU
12	p	113	LEU
12	p	229	GLY
25	K	186	HIS
11	j	27	ARG
14	I	287	GLY
19	i	99	GLY
22	o	453	PRO
20	k	64	VAL
20	k	93	VAL
17	g	254	VAL
8	c	145	GLY
11	j	196	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	106/142 (75%)	106 (100%)	0	100	100
3	E	258/346 (75%)	256 (99%)	2 (1%)	81	92
4	L	94/118 (80%)	94 (100%)	0	100	100
5	P	95/113 (84%)	95 (100%)	0	100	100
6	Q	95/115 (83%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	a	255/307 (83%)	255 (100%)	0	100	100
8	c	152/155 (98%)	152 (100%)	0	100	100
9	d	147/168 (88%)	146 (99%)	1 (1%)	84	93
10	e	321/362 (89%)	315 (98%)	6 (2%)	57	80
11	j	190/193 (98%)	188 (99%)	2 (1%)	73	88
12	p	166/226 (74%)	165 (99%)	1 (1%)	86	94
13	G	183/208 (88%)	178 (97%)	5 (3%)	44	72
14	I	267/333 (80%)	265 (99%)	2 (1%)	84	93
15	J	118/182 (65%)	117 (99%)	1 (1%)	81	92
16	N	91/113 (80%)	90 (99%)	1 (1%)	73	88
17	g	312/312 (100%)	306 (98%)	6 (2%)	57	80
18	h	94/341 (28%)	94 (100%)	0	100	100
19	i	88/94 (94%)	87 (99%)	1 (1%)	73	88
20	k	252/292 (86%)	252 (100%)	0	100	100
21	m	102/102 (100%)	102 (100%)	0	100	100
22	o	277/369 (75%)	276 (100%)	1 (0%)	91	96
23	B	186/230 (81%)	184 (99%)	2 (1%)	73	88
24	F	109/109 (100%)	109 (100%)	0	100	100
25	K	102/151 (68%)	100 (98%)	2 (2%)	55	79
26	O	159/226 (70%)	158 (99%)	1 (1%)	86	94
27	R	89/126 (71%)	89 (100%)	0	100	100
28	U	77/78 (99%)	75 (97%)	2 (3%)	46	73
29	b	115/163 (71%)	115 (100%)	0	100	100
30	f	85/160 (53%)	85 (100%)	0	100	100
31	n	66/173 (38%)	65 (98%)	1 (2%)	65	84
32	z	168/219 (77%)	167 (99%)	1 (1%)	86	94
All	All	4819/6226 (77%)	4781 (99%)	38 (1%)	82	92

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	177	GLU
3	E	407	ASP

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Mol	Chain	Res	Type
9	d	169	THR
10	e	123	ASP
10	e	209	LEU
10	e	241	ARG
10	e	244	TYR
10	e	269	SER
10	e	277	ARG
11	j	4	ARG
11	j	166	TYR
12	p	235	MET
13	G	64	TYR
13	G	180	ARG
13	G	197	ARG
13	G	205	LEU
13	G	234	ARG
14	I	251	GLN
14	I	253	LYS
15	J	132	VAL
16	N	58	ARG
17	g	86	PHE
17	g	98	LEU
17	g	319	ARG
17	g	333	PHE
17	g	367	HIS
17	g	384	ASN
19	i	66	ARG
22	o	61	LYS
23	B	87	ARG
23	B	115	GLN
25	K	151	ARG
25	K	153	VAL
26	O	170	ARG
28	U	1	MET
28	U	52	ARG
31	n	161	ARG
32	z	217	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
10	e	245	HIS
17	g	363	ASN

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Mol	Chain	Res	Type
18	h	294	GLN
23	B	115	GLN
23	B	119	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	952/955 (99%)	227 (23%)	7 (0%)

All (227) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	A	10	G
1	A	16	A
1	A	33	U
1	A	40	A
1	A	41	C
1	A	53	A
1	A	59	U
1	A	64	C
1	A	79	C
1	A	80	U
1	A	82	U
1	A	91	A
1	A	92	A
1	A	97	A
1	A	101	G
1	A	103	A
1	A	107	G
1	A	112	C
1	A	114	A
1	A	117	A
1	A	123	C
1	A	124	C
1	A	125	U
1	A	137	C
1	A	143	G
1	A	148	A
1	A	159	C
1	A	160	G

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Mol	Chain	Res	Type
1	A	165	A
1	A	179	A
1	A	181	U
1	A	183	A
1	A	185	G
1	A	186	C
1	A	188	A
1	A	189	U
1	A	190	A
1	A	207	A
1	A	211	A
1	A	212	U
1	A	218	U
1	A	219	U
1	A	221	G
1	A	230	A
1	A	231	A
1	A	238	G
1	A	239	C
1	A	240	C
1	A	248	G
1	A	253	C
1	A	254	A
1	A	268	A
1	A	278	A
1	A	282	C
1	A	288	A
1	A	289	A
1	A	304	C
1	A	305	C
1	A	306	A
1	A	308	A
1	A	310	C
1	A	311	A
1	A	312	A
1	A	313	A
1	A	321	A
1	A	325	U
1	A	329	A
1	A	333	A
1	A	334	G
1	A	353	A

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Mol	Chain	Res	Type
1	A	355	A
1	A	360	A
1	A	361	A
1	A	362	A
1	A	363	U
1	A	364	A
1	A	365	A
1	A	369	A
1	A	370	C
1	A	386	A
1	A	388	A
1	A	389	G
1	A	390	C
1	A	394	C
1	A	411	C
1	A	415	A
1	A	416	C
1	A	427	U
1	A	428	A
1	A	443	G
1	A	451	C
1	A	452	A
1	A	455	G
1	A	458	A
1	A	465	U
1	A	466	A
1	A	472	A
1	A	478	U
1	A	479	C
1	A	483	A
1	A	497	A
1	A	498	A
1	A	499	C
1	A	500	A
1	A	513	A
1	A	524	G
1	A	525	G
1	A	529	U
1	A	533	U
1	A	534	A
1	A	535	U
1	A	536	C

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Mol	Chain	Res	Type
1	A	550	C
1	A	557	A
1	A	561	U
1	A	566	A
1	A	569	C
1	A	571	C
1	A	572	C
1	A	574	A
1	A	578	A
1	A	584	C
1	A	587	A
1	A	588	U
1	A	589	U
1	A	592	U
1	A	593	G
1	A	599	A
1	A	600	C
1	A	601	A
1	A	604	C
1	A	611	C
1	A	614	C
1	A	615	C
1	A	619	U
1	A	620	U
1	A	630	C
1	A	632	A
1	A	634	A
1	A	635	A
1	A	639	A
1	A	640	A
1	A	641	A
1	A	642	A
1	A	644	A
1	A	645	A
1	A	657	U
1	A	658	A
1	A	659	U
1	A	660	G
1	A	661	A
1	A	676	A
1	A	677	G
1	A	680	C

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Mol	Chain	Res	Type
1	A	681	A
1	A	682	A
1	A	684	G
1	A	685	U
1	A	686	G
1	A	693	A
1	A	703	A
1	A	706	A
1	A	712	G
1	A	714	U
1	A	719	U
1	A	723	U
1	A	725	C
1	A	726	A
1	A	727	C
1	A	729	A
1	A	730	A
1	A	741	C
1	A	746	A
1	A	757	A
1	A	759	A
1	A	760	C
1	A	769	A
1	A	784	A
1	A	785	G
1	A	788	A
1	A	796	A
1	A	801	G
1	A	808	G
1	A	809	U
1	A	815	U
1	A	819	C
1	A	821	A
1	A	832	A
1	A	833	C
1	A	835	C
1	A	836	A
1	A	839	G
1	A	856	A
1	A	857	A
1	A	860	G
1	A	866	G

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Mol	Chain	Res	Type
1	A	868	G
1	A	869	C
1	A	870	A
1	A	871	U
1	A	873	U
1	A	874	A
1	A	878	C
1	A	879	U
1	A	881	U
1	A	886	A
1	A	887	C
1	A	892	U
1	A	894	G
1	A	895	C
1	A	896	U
1	A	900	U
1	A	905	G
1	A	910	C
1	A	911	A
1	A	912	A
1	A	913	G
1	A	918	A
1	A	921	A
1	A	923	G
1	A	927	A
1	A	936	G
1	A	948	G
1	A	949	G
1	A	954	A
1	A	955	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	184	A
1	A	188	A
1	A	363	U
1	A	556	U
1	A	808	G
1	A	818	G

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	o	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	383:TYR	C	386:UNK	N	27.14
1	o	143:GLU	C	145:UNK	N	22.62
1	o	399:UNK	C	417:MET	N	21.79
1	o	173:UNK	C	220:UNK	N	13.77
1	o	300:UNK	C	311:UNK	N	13.39
1	o	285:UNK	C	290:UNK	N	12.01
1	o	362:UNK	C	371:SER	N	11.43
1	o	232:UNK	C	237:UNK	N	9.83
1	o	326:UNK	C	331:UNK	N	9.04
1	o	345:UNK	C	353:UNK	N	8.23
1	o	250:UNK	C	255:UNK	N	7.87
1	o	156:UNK	C	161:UNK	N	7.19
1	o	269:UNK	C	272:UNK	N	4.31

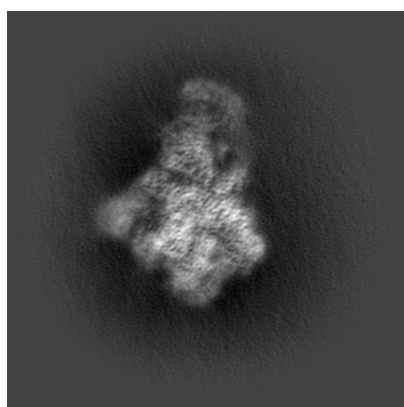
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9362. These allow visual inspection of the internal detail of the map and identification of artifacts.

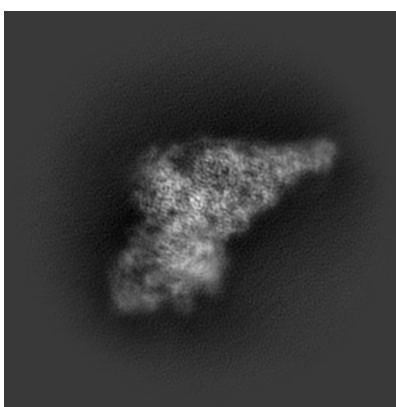
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

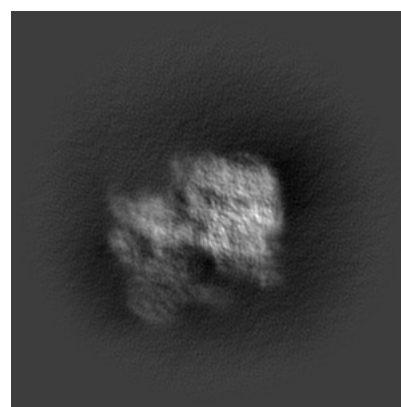
6.1.1 Primary map



X



Y

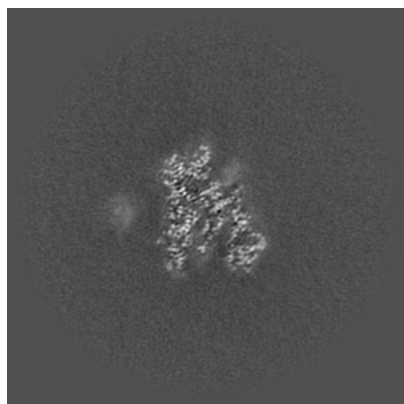


Z

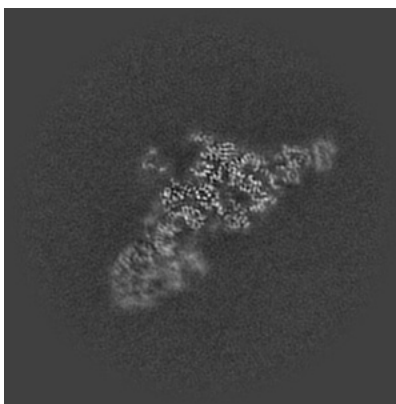
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

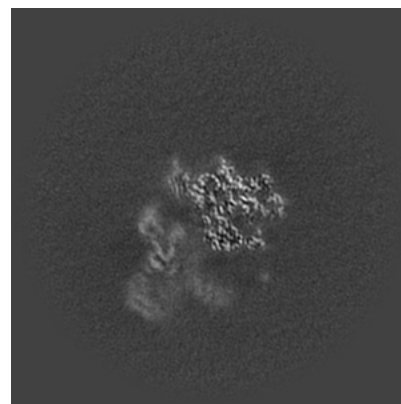
6.2.1 Primary map



X Index: 200



Y Index: 200

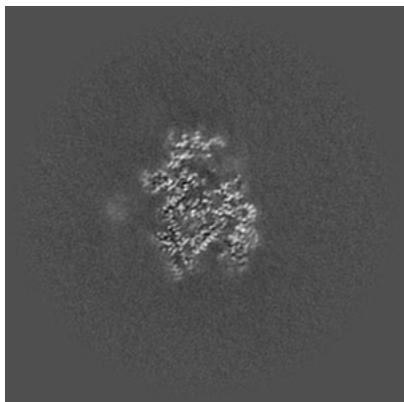


Z Index: 200

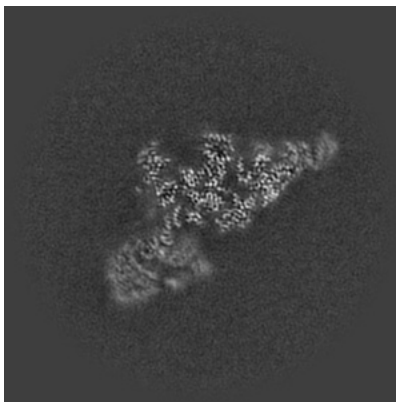
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

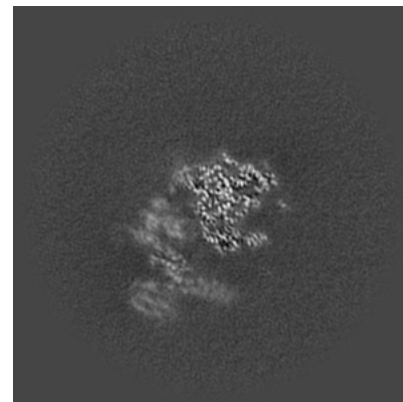
6.3.1 Primary map



X Index: 213



Y Index: 193

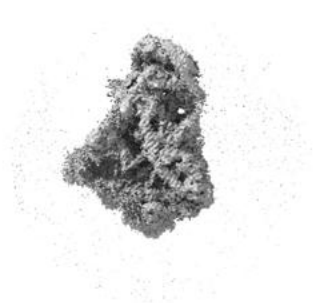


Z Index: 193

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

6.4 Orthogonal surface views [i](#)

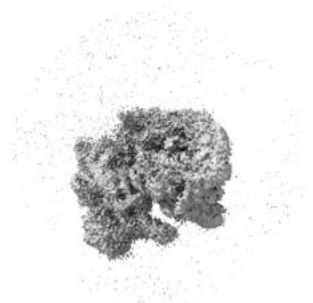
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

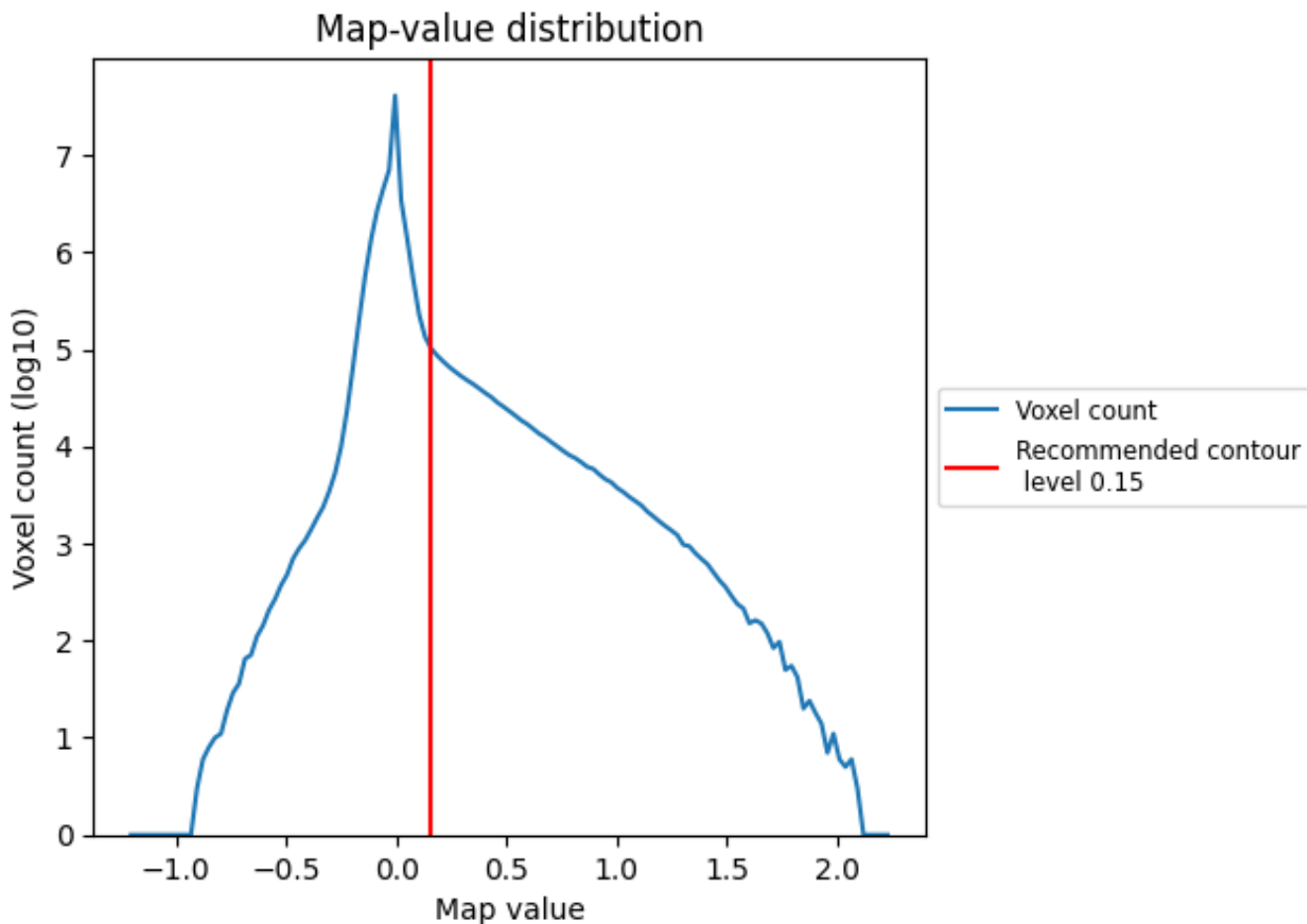
6.5 Mask visualisation

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

7 Map analysis [i](#)

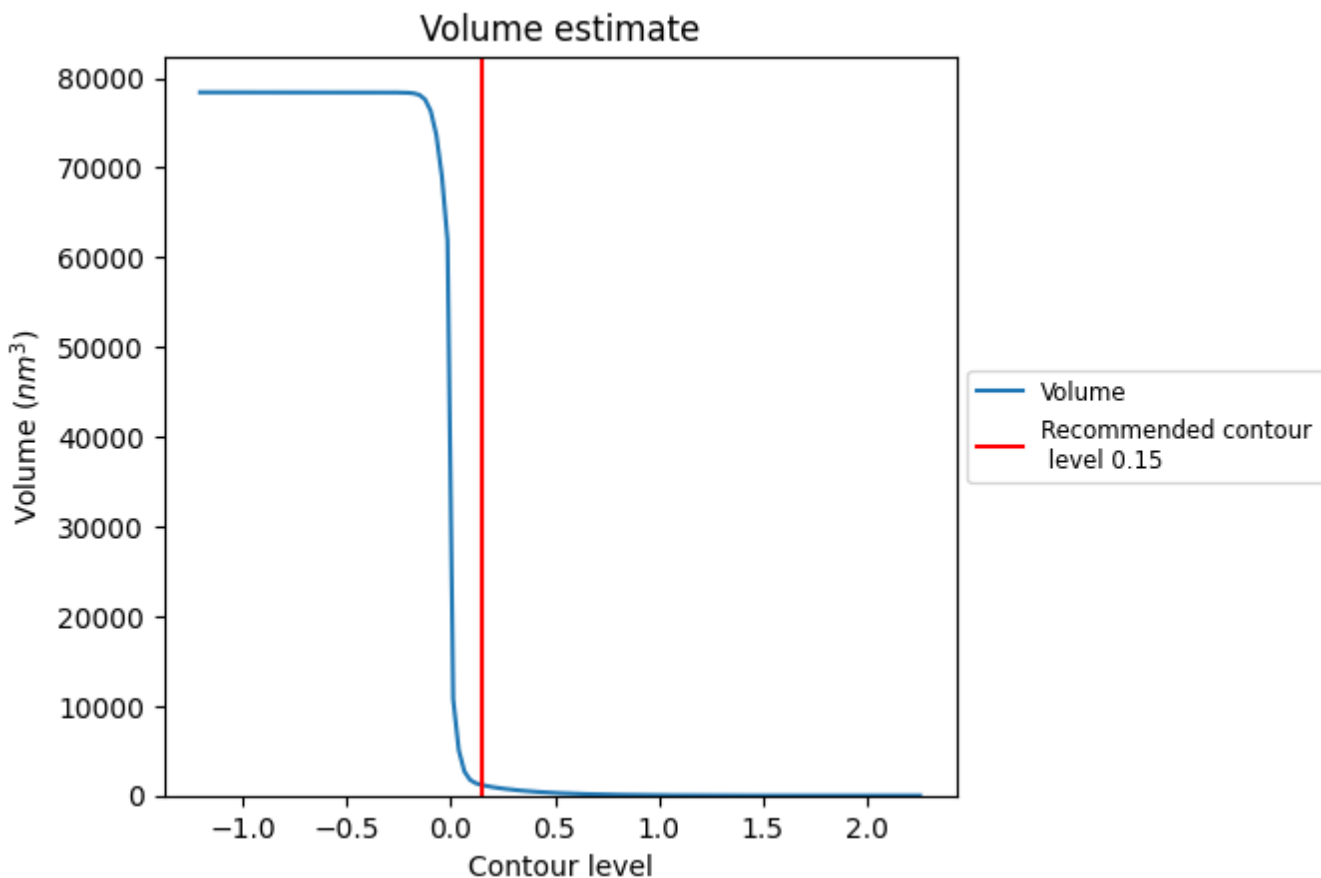
This section contains the results of statistical analysis of the map.

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.

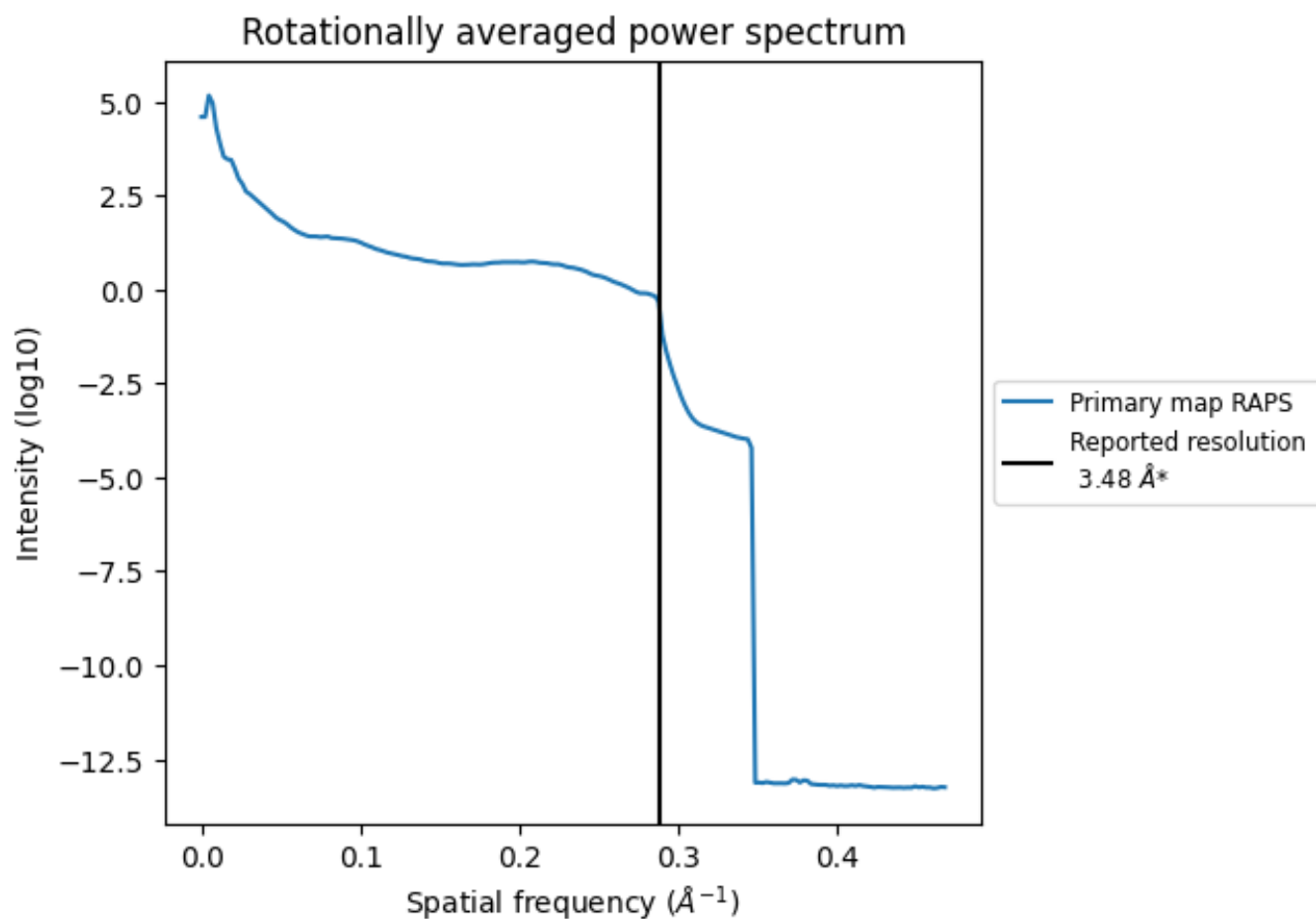
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1173 nm³; this corresponds to an approximate mass of 1059 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 0.287\AA^{-1}

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

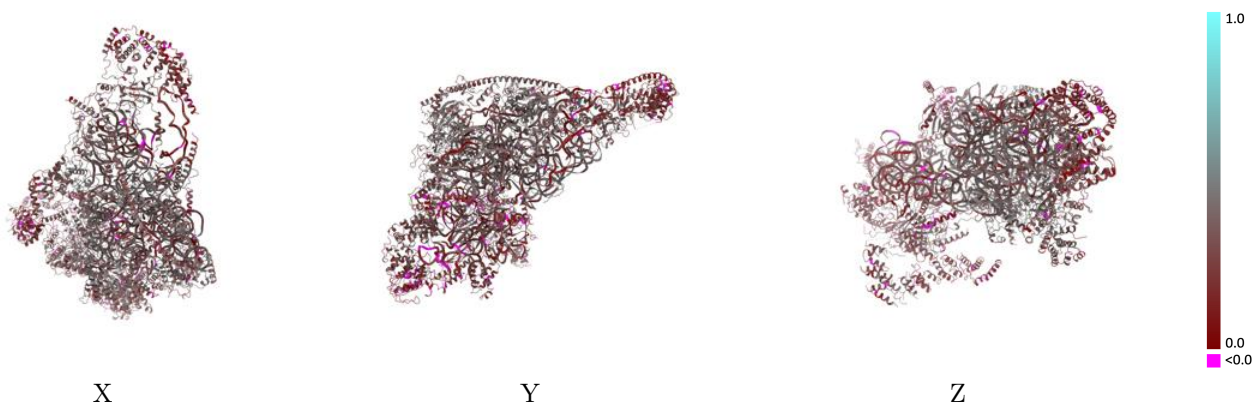
This section contains information regarding the fit between EMDB map EMD-9362 and PDB model 6NF8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



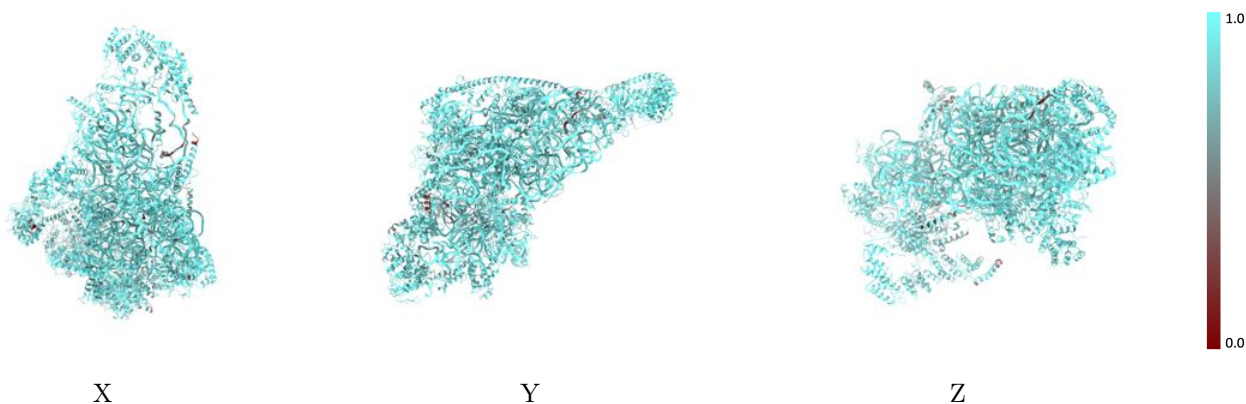
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



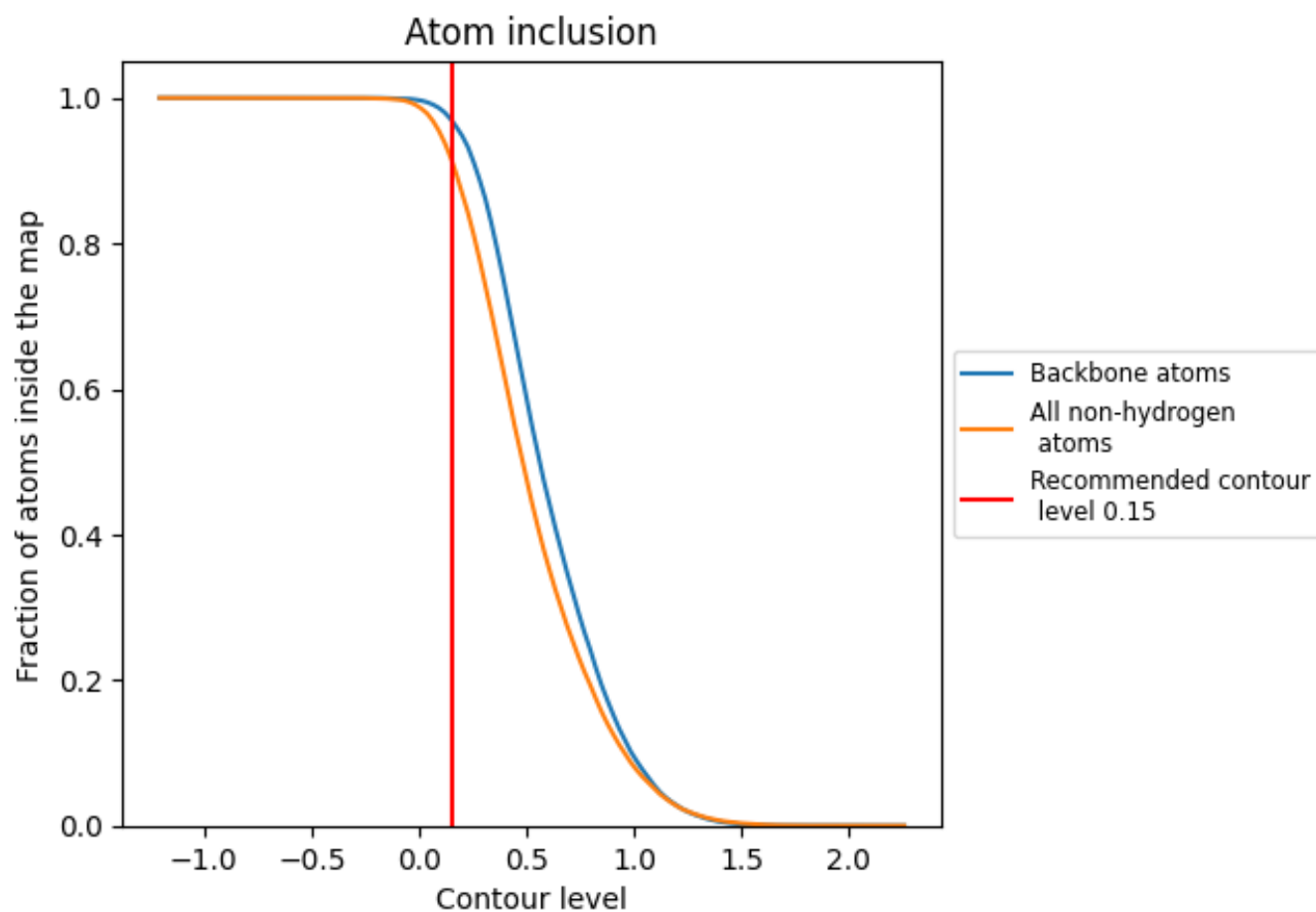
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.3120
A	 0.9465	 0.3060
B	 0.9400	 0.4110
C	 0.8525	 0.2970
E	 0.8928	 0.3410
F	 0.9201	 0.3940
G	 0.9145	 0.3420
I	 0.8893	 0.3320
J	 0.8869	 0.3240
K	 0.9357	 0.3800
L	 0.9446	 0.4140
N	 0.9350	 0.2760
O	 0.8946	 0.3720
P	 0.9414	 0.3930
Q	 0.9095	 0.4090
R	 0.9273	 0.4030
U	 0.9330	 0.3790
a	 0.9376	 0.3570
b	 0.9032	 0.3760
c	 0.9203	 0.4060
d	 0.9240	 0.3590
e	 0.9376	 0.2290
f	 0.9091	 0.4000
g	 0.9204	 0.2380
h	 0.9071	 0.2690
i	 0.8924	 0.2010
j	 0.9173	 0.3190
k	 0.8253	 0.2010
m	 0.8253	 0.2960
n	 0.8931	 0.3410
o	 0.8966	 0.2240
p	 0.9481	 0.3850
z	 0.7262	 0.1750

