WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Jun 7, 2025 – 02:10 pm BST

PDB ID	:	9HCC / pdb_00009hcc
EMDB ID	:	EMD-52044
Title	:	Mouse mitoribosome large subunit assembly intermediate (without uL16m) bound to MRM3-dimer, DDX28 and the MALSU-L0R8F8-mt-ACP complex, State A1 (SAMC knock-out)
Authors	:	Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenberg, A.
Deposited on	:	2024-11-08
Resolution	:	5.67 Å(reported)

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

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

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

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

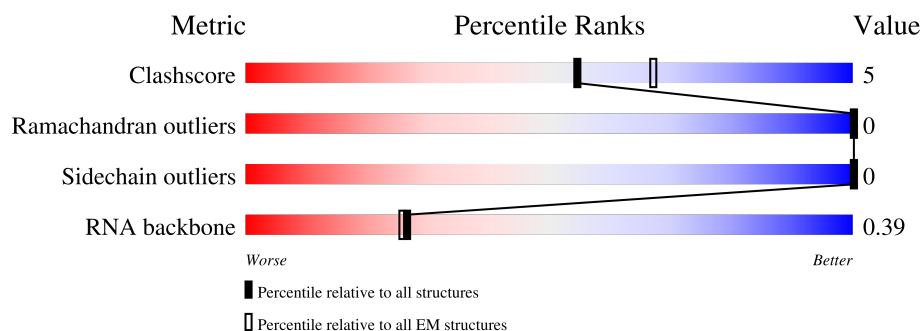|		
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 5.67 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0
RNA backbone		0.39

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1584	11% / 41% 23% 7% 29%
2	B	68	21% / 43% 38% 9% 10%
3	D	246	50% / 60% 10% 30%
4	E	348	6% / 70% 6% 24%
5	F	294	8% / 63% 10% 27%
6	H	268	15% / 27% 9% 65%
7	I	262	43% / 50% 8% 41%

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Mol	Chain	Length	Quality of chain
8	J	192	70% / 64% 10% 26%
9	K	178	6% / 88% 8% •
10	L	145	50% / 72% 8% 21%
11	M	295	7% / 72% 13% 16%
12	O	176	• / 73% 12% 15%
13	P	180	10% / 64% 14% 22%
14	Q	292	7% / 66% 9% 26%
15	R	149	6% / 83% 5% 12%
16	S	209	5% / 69% 7% 24%
17	T	206	7% / 72% 8% 19%
18	U	146	23% / 77% 9% 14%
19	V	216	59% / 78% 13% 8%
20	X	294	28% / 73% 10% 18%
21	Y	252	19% / 65% 5% 30%
22	Z	160	6% / 68% • 28%
23	0	187	• / 49% 9% 42%
24	5	423	51% / 85% 6% 9%
25	6	380	29% / 62% 17% 22%
26	7	336	7% / 79% 7% 13%
27	8	206	23% / 26% • 71%
28	9	135	23% / 66% 5% 29%
29	a	142	15% / 65% 7% 27%
30	b	159	• / 84% 9% 7%
31	c	308	5% / 81% 9% 9%
32	d	306	21% / 55% 12% 33%

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Mol	Chain	Length	Quality of chain
33	e	283	59% / 53% / 10% / 37%
34	f	211	38% / 35% / 7% / 58%
35	g	166	5% / 70% / 9% / 20%
36	h	159	8% / 61% / 8% / 31%
37	i	128	12% / 62% / 10% / 27%
38	j	121	6% / 66% / · / 30%
39	k	118	36% / 56% / 12% / 32%
40	l	135	44% / 47% / 9% / 44%
41	o	102	5% / 73% / · / 24%
42	p	206	11% / 53% / 11% / 36%
43	q	222	· / 39% / 5% / 56%
44	r	196	8% / 71% / 9% / 20%
45	s	442	16% / 74% / 12% / 15%
46	u	228	29% / 47% / 8% / 45%
47	v	70	77% / 90% / 9% / ·
48	w	156	49% / 46% / 5% / 49%
49	x	418	35% / 56% / 14% / 29%
49	y	418	31% / 52% / 18% / 30%
50	z	540	36% / 79% / 6% / 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	FES	r	301	-	-	X	-

2 Entry composition ⓘ

There are 52 unique types of molecules in this entry. The entry contains 174926 atoms, of which 81656 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 16S rRNA (1584-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1129	Total 36145	C 10796	H 12126	N 4363	O 7731	P 1129	0	0

- Molecule 2 is a RNA chain called tRNA-Phe (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	61	Total 1960	C 585	H 657	N 240	O 417	P 61	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	172	Total 2708	C 835	H 1373	N 253	O 240	S 7	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	264	Total 4219	C 1367	H 2097	N 361	O 388	S 6	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	214	Total 3483	C 1113	H 1755	N 305	O 304	S 6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	95	Total 1593	C 492	H 814	N 150	O 137		0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	154	Total	C	H	N	O	S	0	0
			2575	810	1330	222	207	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	142	Total	C	H	N	O	S	0	0
			2220	690	1145	191	191	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	171	Total	C	H	N	O	S	0	0
			2794	894	1398	253	243	6		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1837	560	944	174	155	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	249	Total	C	H	N	O	S	0	0
			4090	1285	2080	365	355	5		

- Molecule 12 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	149	Total	C	H	N	O	S	0	0
			2476	774	1254	230	213	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	P	141	Total	C	H	N	O	S	0	0
			2302	725	1148	221	203	5		

- Molecule 14 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Q	217	Total 3612	C 1150	H 1822	N 309	O 322	S 9	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	R	131	Total 2214	C 685	H 1137	N 214	O 175	S 3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	S	159	Total 2673	C 840	H 1372	N 233	O 226	S 2	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	T	166	Total 2771	C 871	H 1402	N 256	O 234	S 8	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	U	125	Total 2072	C 664	H 1038	N 193	O 174	S 3	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	198	Total 3250	C 1026	H 1622	N 302	O 294	S 6	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein bL28m,Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	X	242	Total 4072	C 1304	H 2051	N 358	O 355	S 4	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Y	176	Total 3076	C 973	H 1553	N 290	O 255	S 5	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Z	115	Total 1913	C 598	H 979	N 171	O 162	S 3	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	0	108	Total 1789	C 546	H 908	N 174	O 155	S 6	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	5	387	Total 6355	C 2045	H 3187	N 554	O 560	S 9	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	6	297	Total 4954	C 1630	H 2420	N 462	O 437	S 5	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	7	292	Total 4757	C 1517	H 2378	N 409	O 438	S 15	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	8	59	Total 977	C 306	H 484	N 87	O 98	S 2	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	9	96	Total	C	H	N	O	S	0	0
			1550	510	772	123	144	1		

- Molecule 29 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	a	103	Total	C	H	N	O	S	0	0
			1703	542	843	156	159	3		

- Molecule 30 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	b	148	Total	C	H	N	O	S	0	0
			2376	731	1195	234	214	2		

- Molecule 31 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	c	279	Total	C	H	N	O	S	0	0
			4502	1440	2256	389	409	8		

- Molecule 32 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	d	204	Total	C	H	N	O	S	0	0
			3358	1085	1670	299	293	11		

- Molecule 33 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	e	177	Total	C	H	N	O	S	0	0
			2911	922	1474	258	252	5		

- Molecule 34 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	f	89	Total	C	H	N	O	S	0	0
			1418	452	704	120	138	4		

- Molecule 35 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	g	132	Total 2184	C 709	H 1094	N 187	O 192	S 2	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	h	110	Total 1740	C 552	H 868	N 156	O 160	S 4	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	i	93	Total 1611	C 517	H 816	N 153	O 123	S 2	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	j	85	Total 1376	C 426	H 692	N 135	O 121	S 2	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	k	80	Total 1268	C 393	H 639	N 114	O 117	S 5	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	l	76	Total 1266	C 403	H 631	N 114	O 116	S 2	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	o	78	Total 1263	C 402	H 623	N 118	O 116	S 4	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	p	132	Total 2201	C 682	H 1112	N 205	O 198	S 4	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	q	97	Total 1584	C 501	H 785	N 155	O 142	S 1	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	r	156	Total 2586	C 806	H 1319	N 241	O 209	S 11	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	s	377	Total 6102	C 1938	H 3057	N 555	O 540	S 12	0	0

- Molecule 46 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	u	125	Total 2041	C 659	H 1012	N 170	O 191	S 9	0	0

- Molecule 47 is a protein called Predicted gene, 55359.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	v	69	Total 1189	C 374	H 603	N 112	O 99	S 1	0	0

- Molecule 48 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	w	79	Total 1277	C 410	H 640	N 95	O 127	S 5	0	0

- Molecule 49 is a protein called rRNA methyltransferase 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	x	295	Total	C	H	N	O	S	0	0
			4661	1478	2356	399	420	8		
49	y	293	Total	C	H	N	O	S	0	0
			4631	1469	2340	397	417	8		

- Molecule 50 is a protein called Probable ATP-dependent RNA helicase DDX28.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	z	458	Total	C	H	N	O	S	0	0
			7236	2259	3681	643	644	9		

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	0	1	Total	Zn	0
			1	1	

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).
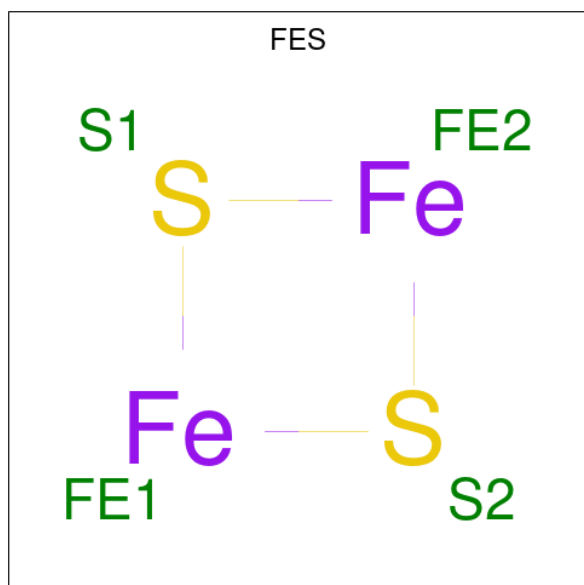
Mol	Chain	Residues	Atoms			AltConf
52	r	1	Total	Fe	S	0
			4	2	2	

3   Residue-property plots ⓘ

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: 16S rRNA (1584-MER)

- Molecule 2: tRNA-Phe (68-MER)
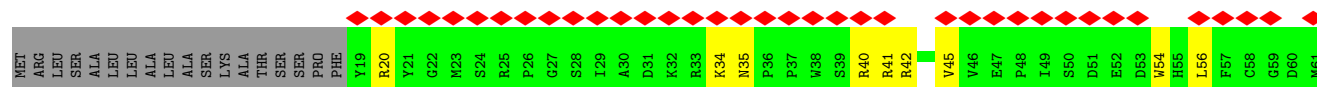
Chain B:

21%
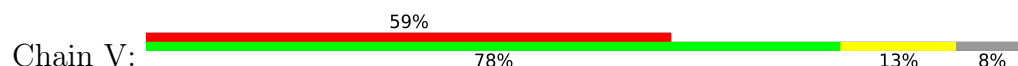
43%   38%   9%   10%
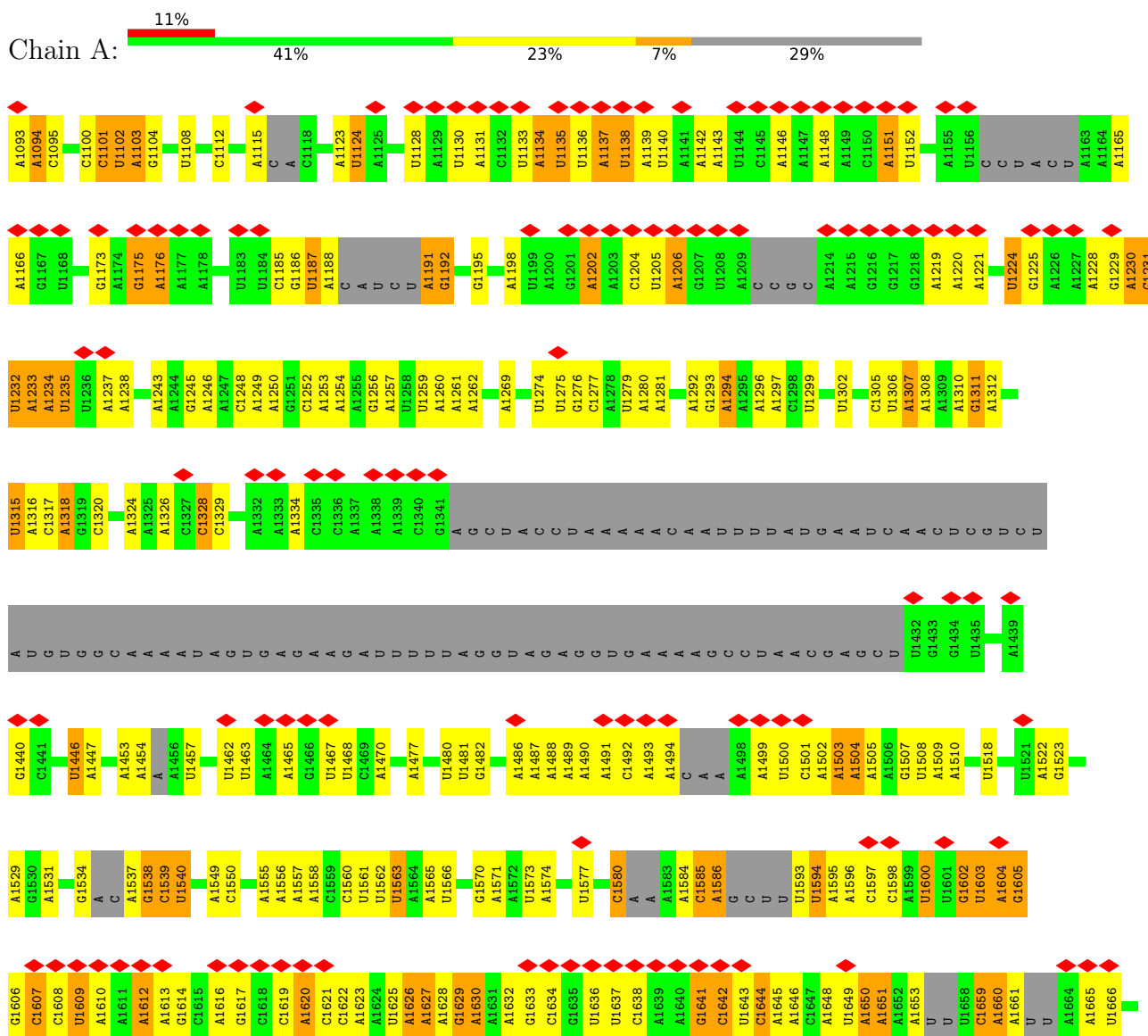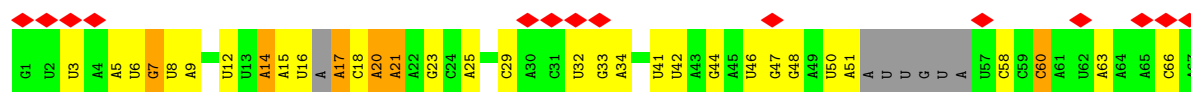
• Molecule 3: Large ribosomal subunit protein uL2m
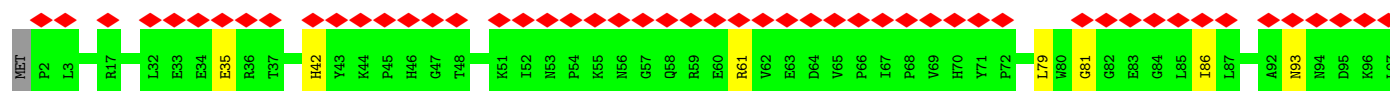
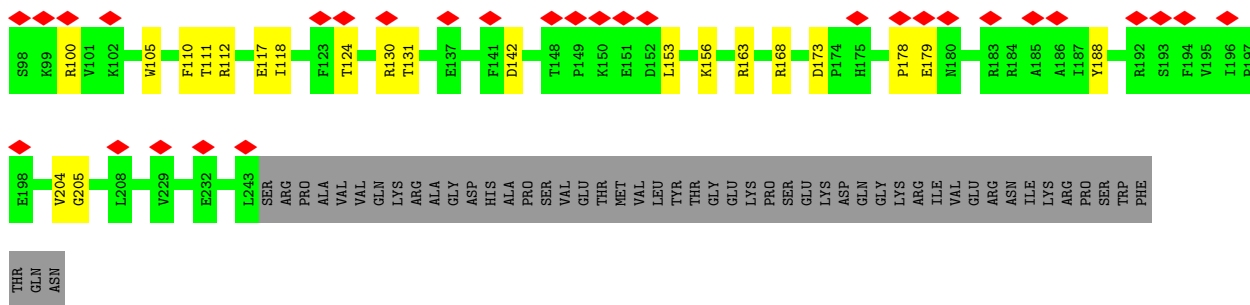Chain D:
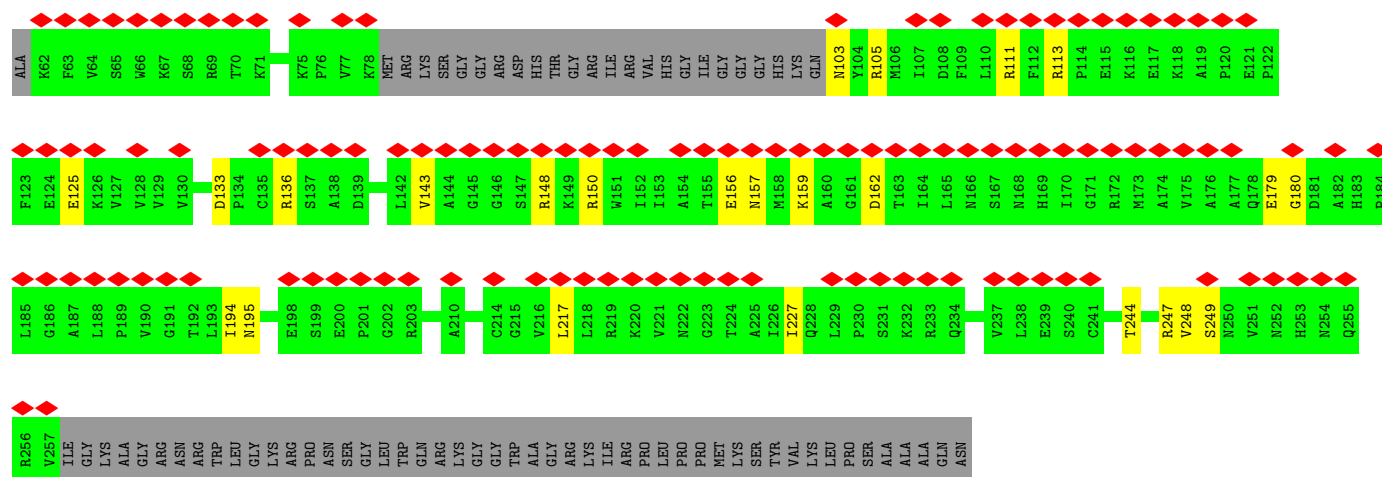
• Molecule 4: Large ribosomal subunit protein uL3m

Chain E:
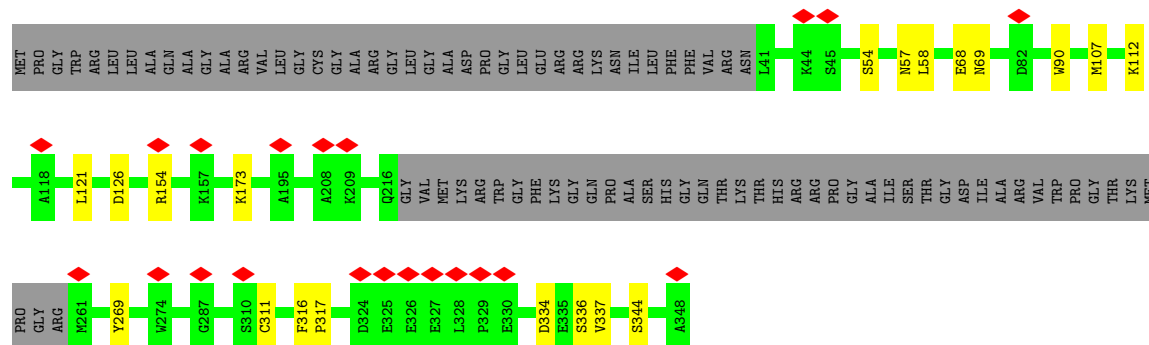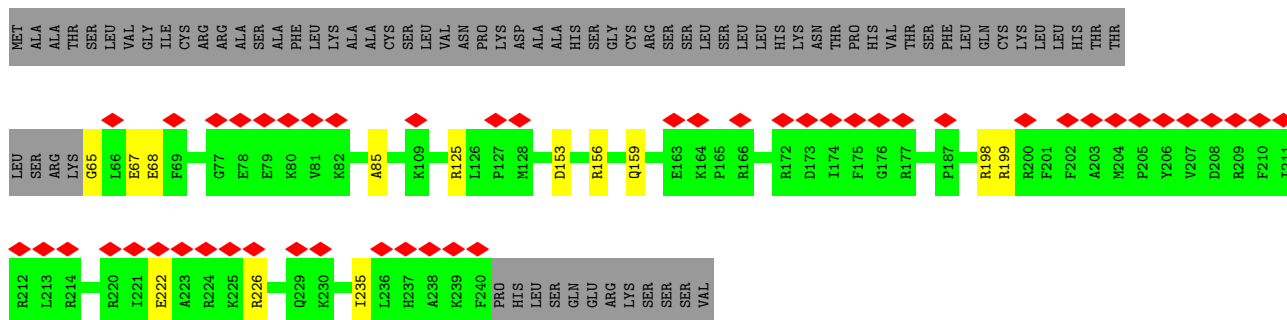

• Molecule 5: Large ribosomal subunit protein uL4m

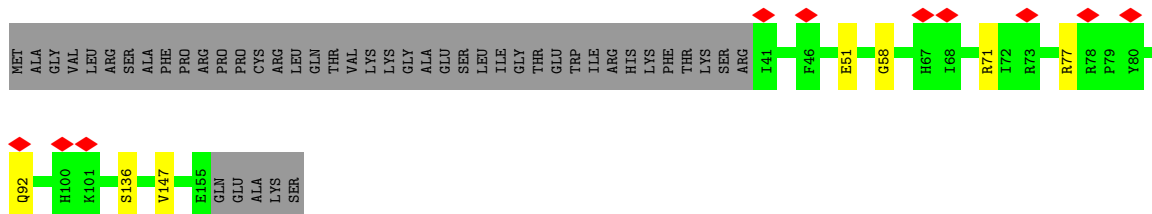Chain F:
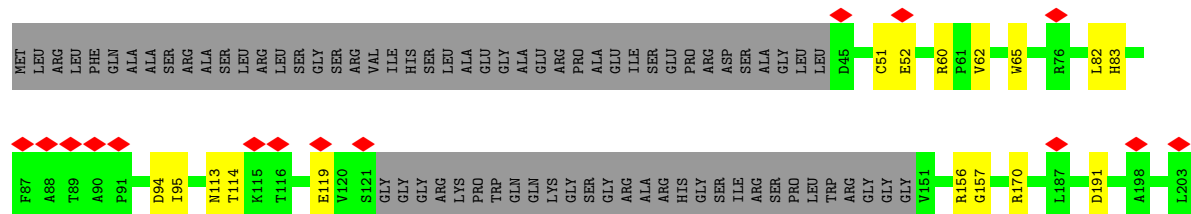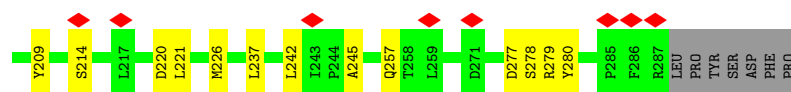
• Molecule 6: Large ribosomal subunit protein bL9m

Chain H:
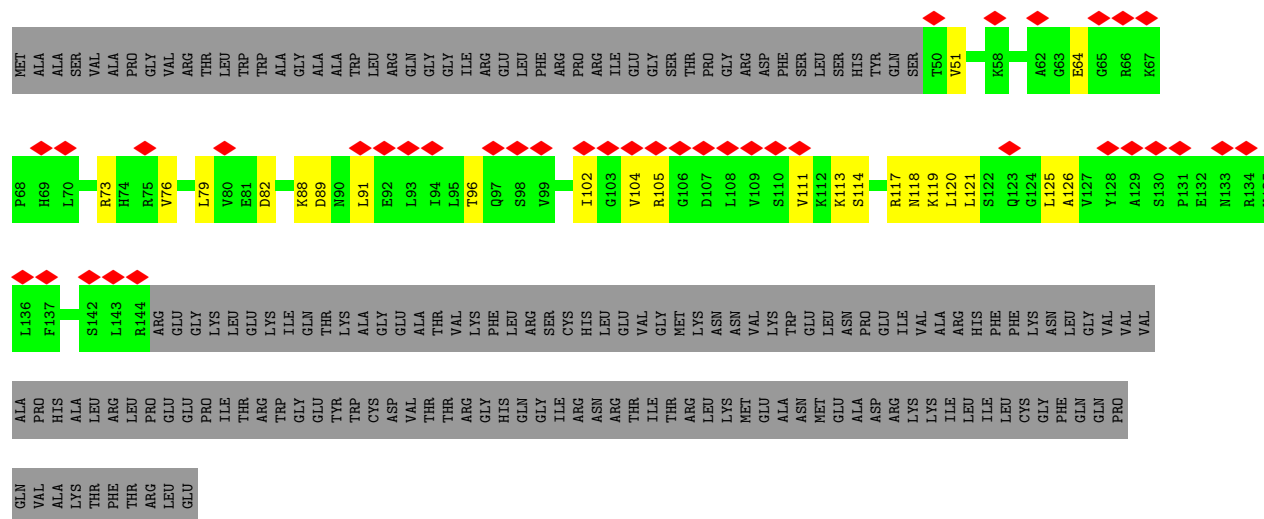
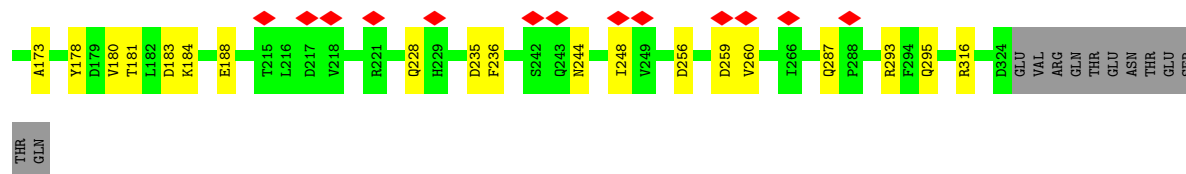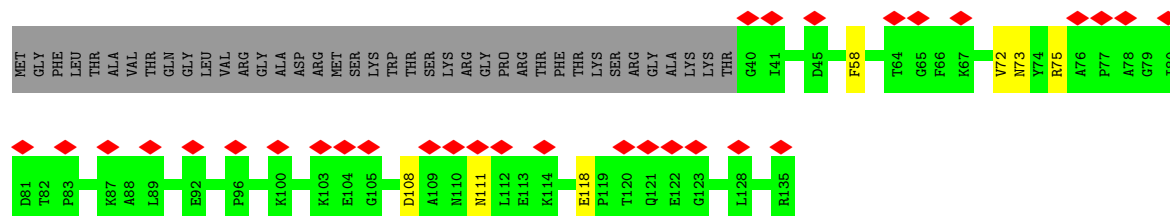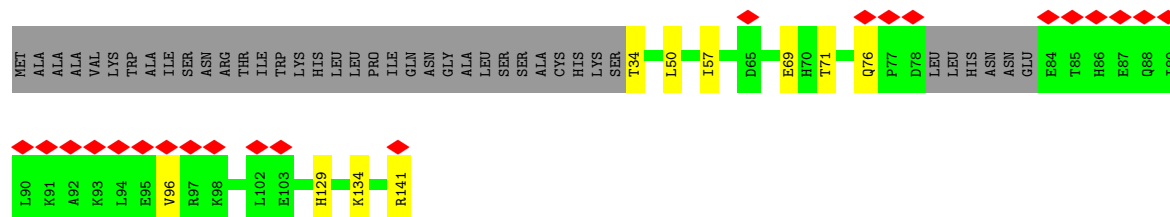• Molecule 7: Large ribosomal subunit protein uL10m
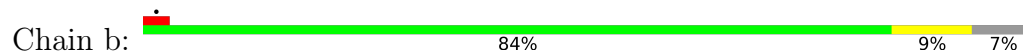
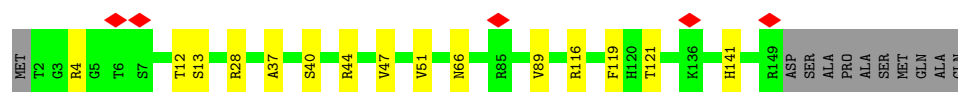Chain I:
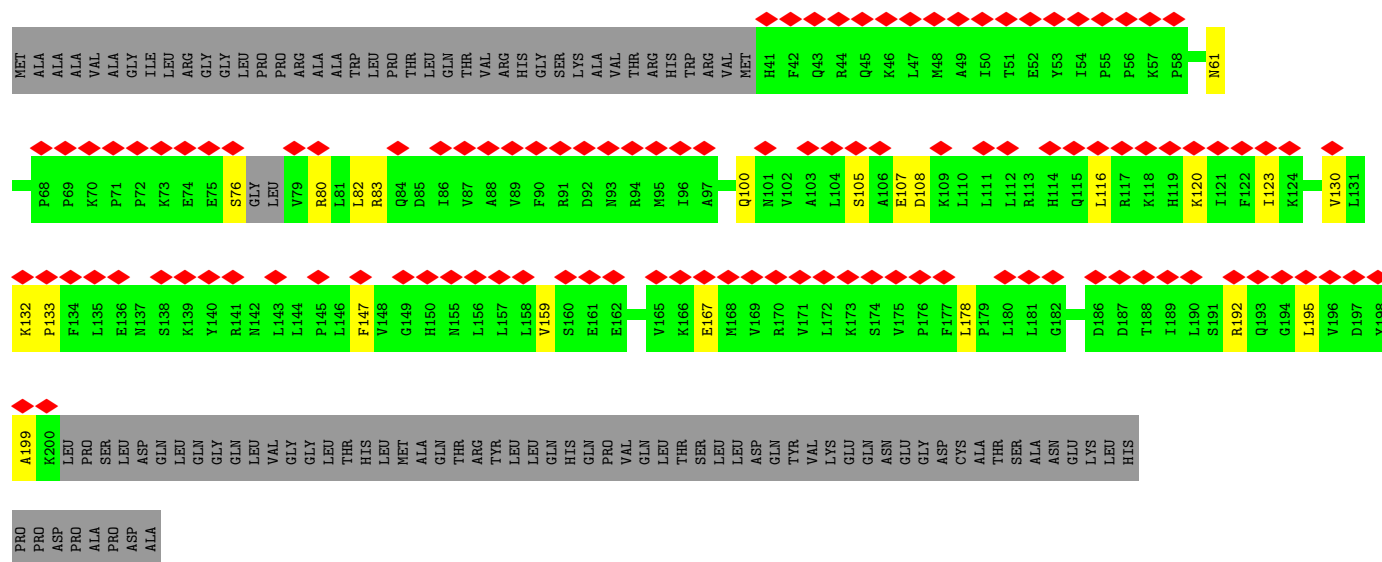
• Molecule 8: Large ribosomal subunit protein uL11m

Chain J:

MET SER LYS LEU SER ARG ALA THR ARG THR LEU LYS LYS PRO GLU ALA GLY G18 V19 I20 R21 S22 I23 V24 R25 A26 C27 Q28 A29 I30 P31 G32 P33 P34 L35 G36 P37 I38 L39 G40 Q41 R42 G43 V44 S45 I46 N47 Q48 F49 C50 K51 E52 F53 N54 E55 K56 T57 K58 D59 I60

K61 E62 G63 I64 P65 L66 P67 T68 K69 I70 F71 I72 K73 P74 D75 R76 T77 F78 E79 L80 K81 I82 G83 Q84 P85 T86 V87 S88 Y89 F90 L91 K92 A93 A94 A95 G96 I97 E98 K99 G100 A101 R102 H103 T104 K106 E107 V108 A109 G110 L111 V112 S113 L114 K115 H116 V117 Y118 E119 I120

A121 C122 V123 K124 A125 K126 D127 D128 A129 F130 A131 M132 Q133 D134 V135 P136 L137 S138 S139 V140 V141 R142 S143 I144 I145 G146 S147 A148 R149 G152 I153 R154 V155 V156 K157 D158 L159 SER ALA GLU GLU LEU GLU ALA PHE GLN LYS GLU ARG ALA VAL PHE LEU ALA ALA GLN LYS GLU ALA

ASP LEU ALA ALA GLN ALA GLU ALA GLU LYS LYS

- Molecule 9: Large ribosomal subunit protein uL13m

Chain K:

6%

88% 8%

MET S2 A7 P8 F14 L21 Q26 L50 V58 G69 Y77 Y83 P84 F87 R88 Q89 A92 A93 K98 G110 K114 N140 Q147 D156 E157 T171 P172 PRO ASP ASP PHE ARG MET
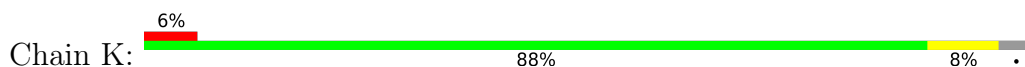
- Molecule 10: Large ribosomal subunit protein uL14m

Chain L:

50%

72% 8% 21%

MET ALA ALA LEU THR GLY LEU TRP GLY SER PHE ALA HIS VAL SER ARG ALA PHE SER GLN ARG CYS PHE SER THR SER GLY SER LEU SER A31 V32 Q33 T36 R37 V38 R39 V40 V41 D42 N43 S44 A45 S48 R53 P54 P55 R56 C57 I58 H59 V60 Y61 N62 K63 S64 G65

V66 G67 K68 V69 G70 D71 Q72 I73 L74 L75 A76 K81 K82 K83 I86 V87 G88 G93 S94 R95 F100 D101 S102 N103 L107 I108 E109 D110 N111 G112 N113 P114 I119 K120 I121 P122 I123 P124 T125 R128 R129 R130 E131 G132 E133 Y134 S135 K136 V137 L138 A139 I140 A141

Q142 N143 F144 V145

- Molecule 11: Large ribosomal subunit protein uL15m

Chain M:

7%

72% 13% 16%

MET ALA GLY THR ALA ARG GLY CYS G9 V21 S22 L23 A24 K34 R38 P39 R40 D41 R42 R43 R46 K47 CYS GLY ARG GLY HIS LYS GLY GLU ARG GLN GLY THR ARG PRO ARG LEU GLY PHE GLU GLY GLY GLN THR PRO PHE TYR ILE ARG ILE PRO LYS TYR GLY

PHE ASN GLU GLY H86 S87 F88 Q91 Y92 Q93 P94 L95 S96 L100 R108 G123 I128 L131 K132 R133 L139 V140 E141 D145 Q148 N152 A158 S159 E160 C187 R195 R202 E207 K217 L222 R232 A236 G240 E250

R253 M254 L255 S256 A257 R258 R262 Q263 I264 F265 N275 K280 I281 L282 K283 P284 T285 D286 E287 S295

• Molecule 12: Large ribosomal subunit protein bL17m

Chain O:

73%　　12%　　15%

• Molecule 13: Large ribosomal subunit protein uL18m

Chain P:

10%　　64%　　14%　　22%

• Molecule 14: Large ribosomal subunit protein bL19m

Chain Q:

7%　　66%　　9%　　26%

• Molecule 15: Large ribosomal subunit protein bL20m

Chain R:

6%　　83%　　5%　　12%

• Molecule 16: Large ribosomal subunit protein bL21m

Chain S:

5%　　69%　　7%　　24%

L117 D125 I126 R133 L134 E135 K136 I165 T168 E169 I174 N175 M176 K177 F178 K182 N183 F184 R185 K186 Q194 R198 I199 I204 L208 LEU

• Molecule 17: Large ribosomal subunit protein uL22m

Chain T:

MET ALA ALA ALA LEU LEU ARG GLU LEU GLY ALA LEU ARG VAL PRO ASN LEU ARG ILE TRP ALA THR GLN THR LEU ARG VAL LEU PRO PRO SER CYS ILE HIS THR SER ALA SER LEU ASP I41 W45 E46 N49 E60 R63 Y68 A85 E101 D104 R124

D125 N133 S139 R143 R151 Y152 H153 G154 R155 G156 R157 F158 G159 I160 M161 E174 P180 E181 V182 P183 K184 R200 T201 I202 L206
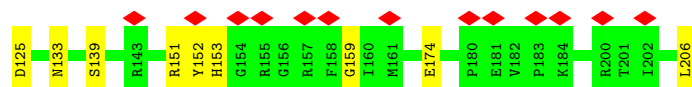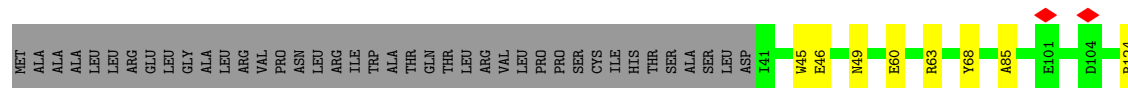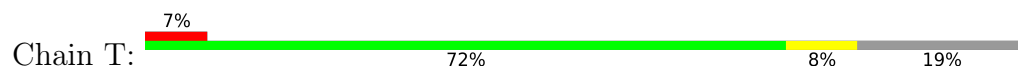
• Molecule 18: Large ribosomal subunit protein uL23m

Chain U:

MET A2 L6 Y7 P8 L9 V19 T22 N23 F24 V29 R30 P31 G32 T33 A34 Q35 D38 T39 M46 E47 R54 Q59 I60 Y61 V65 V68 G75 R79 R80 D81 H82 K83 N84 V85 R86 V97 Q98 L99 Q103 T104 F105 T106 F107 F111

P112 GLU LYS ASP PRO ARG SER PRO GLU PRO LEU GLU GLU GLU LEU PRO GLN GLN ARG GLN SER S133 P138 G139 G145 L146
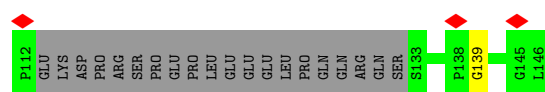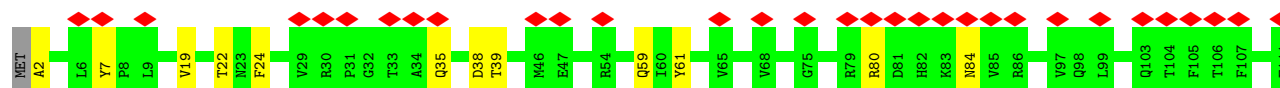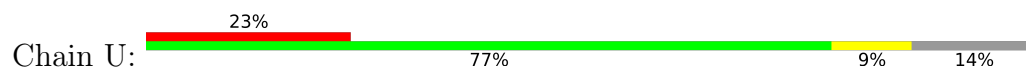
• Molecule 19: Large ribosomal subunit protein uL24m

Chain V:

MET ARG LEU SER ALA LEU LEU ALA LEU SER LYS ALA THR SER SER PRO PHE Y19 R20 Y21 G22 M23 S24 R25 P26 G27 S28 I29 A30 D31 K32 R33 K34 N35 P36 P37 W38 S39 R40 R41 R42 V45 V46 E47 P48 I49 S50 D51 E52 D53 W54 H55 L56 F57 C58 G59 D60 M61

V62 E63 I64 L65 E66 G67 K68 D69 A70 G71 K72 Q73 C74 K75 V76 V77 Q78 V79 V80 R81 Q82 R83 N84 W85 V86 V87 L88 E89 G90 L91 N92 T93 H94 Y95 R96 T101 K102 D103 H104 R105 A110 S111 E112 A113 P114 L115 H118 Q119 V120 K121 L122 V123 D124 P125 V126 D127 R128

K129 P130 T131 E132 I133 Q134 W135 R136 F137 T138 E139 A140 G141 E142 R143 V144 R145 V146 S147 T148 R149 S150 G151 R152 I153 I154 P155 K156 P157 E158 F159 P160 R161 A162 D163 G164 E168 T169 W170 K175 D176 T177 A182 L183 E195 M199 E200 A201 M202 G203 E206 T207 W215

Y216

• Molecule 20: Large ribosomal subunit protein bL28m,Large ribosomal subunit protein bL32m

Chain X:

MET P2 L3 R17 L32 E33 E34 E35 R36 T37 H42 Y43 K44 P45 H46 G47 T48 K51 I52 N53 P54 K55 N56 G57 Q58 R59 E60 R61 V62 E63 D64 V65 P66 I67 P68 V69 H70 Y71 P72 L79 W80 G81 G82 E83 G84 L85 I86 L87 A92 N93 N94 D95 K96 L97

• Molecule 21: Large ribosomal subunit protein uL29m

Chain Y:

• Molecule 22: Large ribosomal subunit protein uL30m

Chain Z:

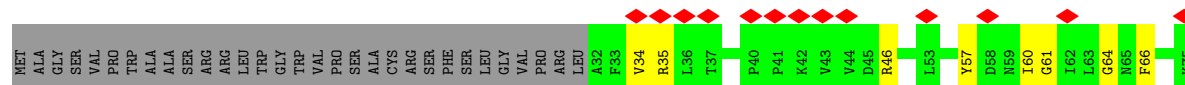• Molecule 23: Large ribosomal subunit protein bL32m
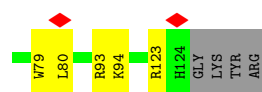
Chain 0:
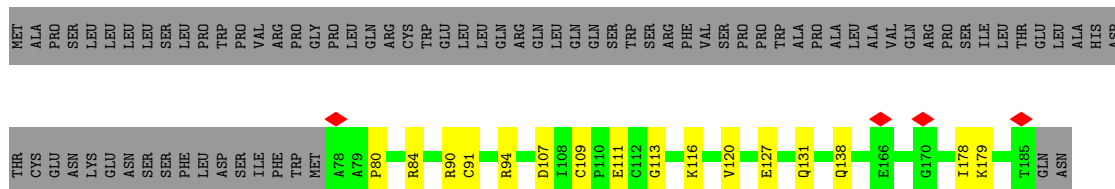
• Molecule 24: Large ribosomal subunit protein mL37

Chain 5:

• Molecule 25: Large ribosomal subunit protein mL38

Chain 6:

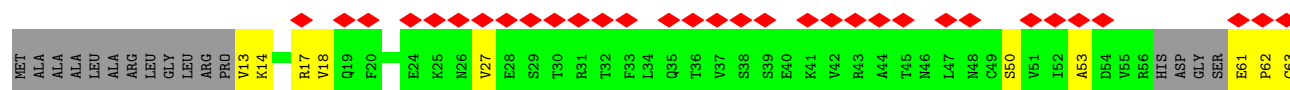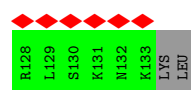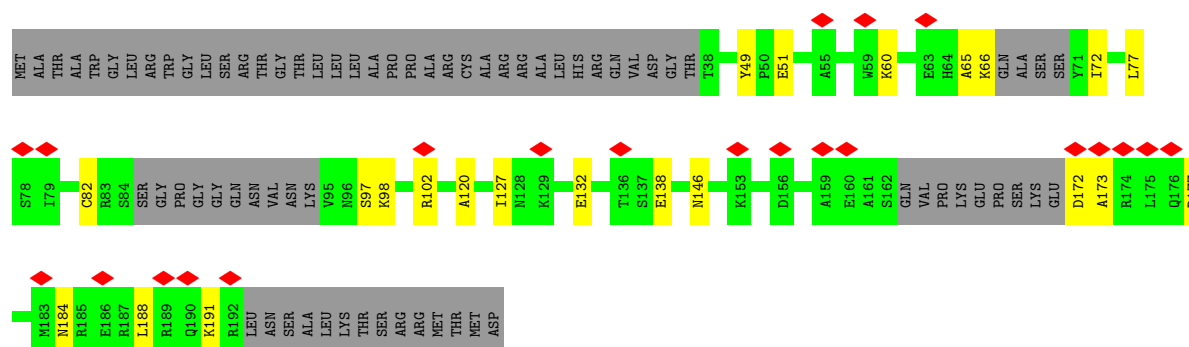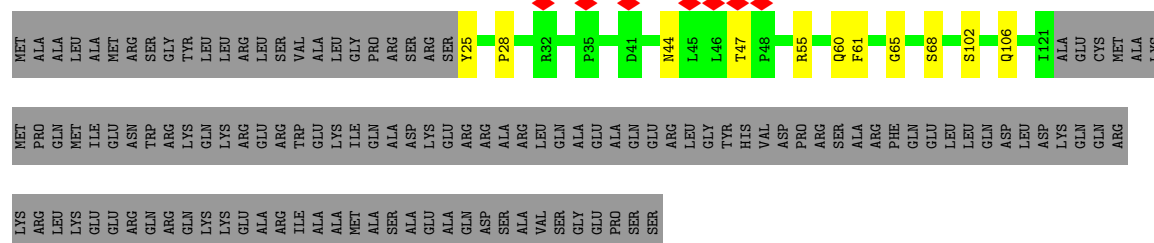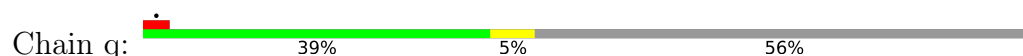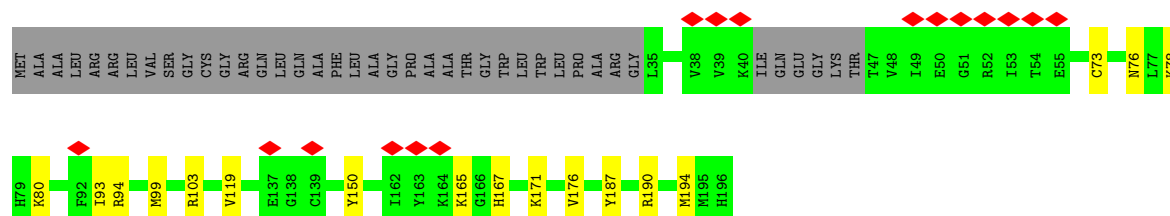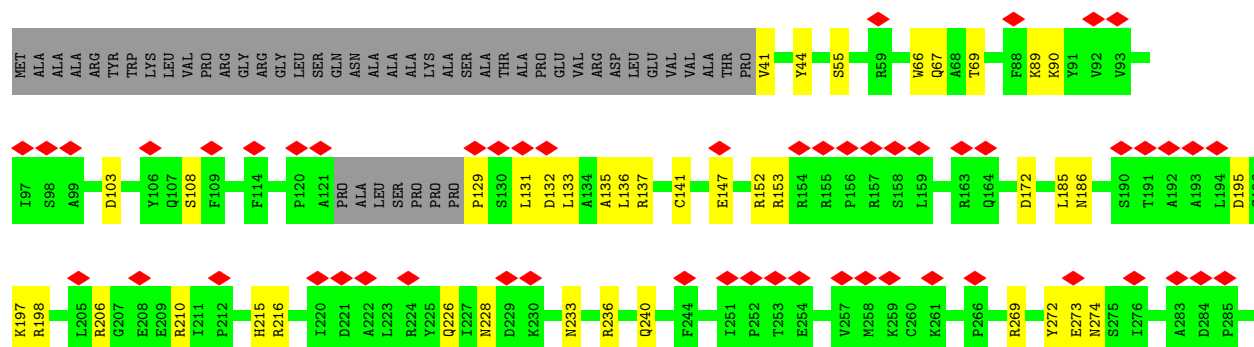• Molecule 26: Large ribosomal subunit protein mL39

Chain 7:

A173 Y178 D179 V180 T181 L182 D183 K184 E188 T215 L216 D217 V218 R221 Q228 H229 D235 F236 S242 Q243 N244 I248 V249 D256 D259 V260 I266 Q287 P288 R293 F294 Q295 R316 D324 GLU VAL ARG GLN THR GLU ASN THR GLU SER
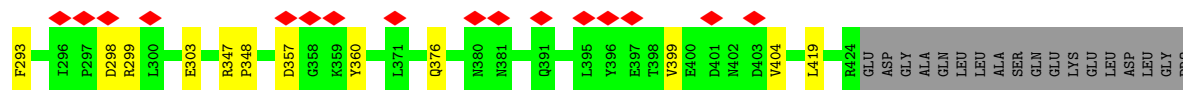
THR GLN

• Molecule 27: Large ribosomal subunit protein mL40

Chain 8:

23%

26%   •   71%

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

ASP GLN ALA ALA LYS ASP ARG LEU LYS LYS ARG ILE LYS LEU LYS LYS ALA SER GLN GLU LEU ILE PRO ILE GLU ASP PHE ILE THR PRO VAL ARG PHE LEU ASP LYS SER ARG ARG GLN GLN GLU E105 H106 S107 P108 E109 E110 S111 E112 R113 R114 A115 L116 L117 L118 K119 R120

W121 A122 L123 M131 D134 R137 S138 M139 L140 E141 A142 Q143 Q144 E145 A146 L147 E148 E149 L150 K151 L152 E153 S154 A155 E156 L157 Y158 A159 E160 A161 I162 K163 ARG ASP THR SER LEU PHE PRO PHE GLU LYS GLY PRO HIS TYR THR PRO PRO ILE SER ASN TYR GLN ALA PRO

GLU GLY ARG TYR ASN ASP ILE THR LYS VAL TYR THR GLN VAL GLU PHE LYS ARG
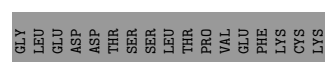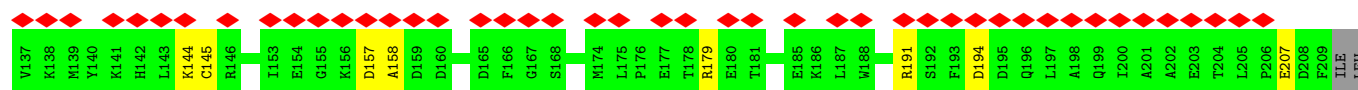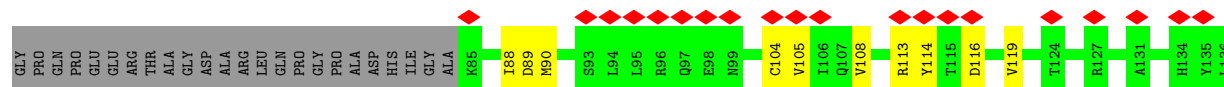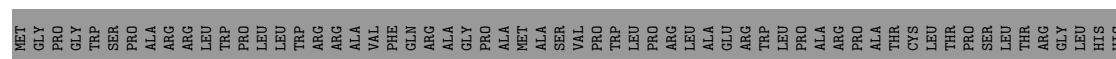
• Molecule 28: Large ribosomal subunit protein mL41

Chain 9:

23%

66%   5%   29%

MET GLY PHE LEU THR ALA VAL THR GLN GLY LEU VAL ARG GLY ALA ASP ARG MET SER LYS TRP THR SER LYS ARG GLY PRO ARG THR PHE THR LYS SER ARG GLY ALA LYS LYS THR G40 I41 D45 F58 T64 G65 F66 K67 V72 N73 Y74 R75 A76 P77 A78 G79 I80

D81 T82 P83 K87 A88 L89 E92 P96 K100 K103 E104 G105 D108 A109 N110 N111 L112 E113 K114 E118 P119 T120 Q121 E122 G123 L128 R135

• Molecule 29: Large ribosomal subunit protein mL42

Chain a:

15%

65%   7%   27%

MET ALA ALA ALA VAL LYS TRP ALA ILE SER ASN ARG THR ILE TRP LYS HIS LEU LEU PRO ILE GLN ASN GLY ALA LEU SER SER ALA CYS HIS LYS SER T34 L50 I57 D65 E69 H70 T71 Q76 P77 D78 LEU LEU HIS ASN ASN GLU E84 T85 H86 E87 Q88 I89

L90 K91 A92 K93 L94 E95 V96 R97 K98 L102 E103 H129 K134 R141

• Molecule 30: Large ribosomal subunit protein mL43

Chain b:

84%   9%   7%

MET T2 G3 R4 G5 T6 S7 T12 S13 R28 A37 S40 R44 V47 V51 N66 R85 V89 R116 F119 H120 T121 K136 H141 R149 ASP SER ALA PRO ALA SER MET GLN ALA GLN

• Molecule 31: Large ribosomal subunit protein mL44

Chain c: 5% 81% 9% 9%

PRO PRO VAL ARG GLY V31 K32 K33 G34 F35 R52 C53 P54 P55 P56 P57 V58 R59 R60 P64 E71 R78 L79 Q80 D86 L87 T90 S107 LEU GLY ILE GLU LYS GLU ALA ALA LEU LEU ASN L119 E144 F145 S155 C167 R171 S181 A182 E183

I199 E209 R210 W232 R256 T264 L269 I281 P285 E294 R298 R312 P313 W314 D315 Y316 S317 K320 GLU SER PRO LYS ARG ALA GLU GLN THR SER VAL ALA SER

• Molecule 32: Large ribosomal subunit protein mL45

Chain d: 21% 55% 12% 33%

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

ARG LYS ALA GLY LEU VAL ILE PRO GLN GLU ARG LEU GLU ARG PRO ILE H77 L78 A79 I84 F85 D86 P87 Y88 V89 E92 A95 R96 M97 SER SER LEU SER LYS GLU GLY L105 T106 Q107 R111 L112 R113 K114 N115 A116 A117 L120 A121 I122 R123 K124 I125 R126 E127 F128

D129 A130 N131 F132 K133 T134 K135 D136 F137 P138 E139 K140 I146 C151 S155 D156 H157 D158 R159 L160 H161 F169 P170 D171 L176 K177 Y178 K179 F185 V186 E187 S188 L189 V195 H196 V197 R198 C199 SER GLY LEU VAL ASN GLN SER N207 V212 T213 V214 H217

D226 R230 L231 M232 D237 V238 D241 V242 L243 E244 Y245 H251 N254 P255 Y256 I265 V266 P267 A268 W269 A270 P271 P272 K273 M281 Q286 L287 W290 E291 E292 Y293 E294 GLU THR GLN GLY GLU ALA GLN LYS PRO GLN LEU ALA

• Molecule 33: Large ribosomal subunit protein mL46

Chain e: 59% 53% 10% 37%

MET ALA ALA PRO VAL GLY ARG THR LEU LEU GLY LEU ALA ARG GLY TRP ARG GLN LEU ASP ARG PHE TRP ALA GLY SER SER ARG GLY LEU LEU SER LEU GLU ALA ALA SER SER SER ARG SER PRO W43 R44 L45 S46 G47 A48 L49 C50 L51 Q52 R53 P54 P55 L56 I57 T58 K59 A60

L61 T62 P63 L64 Q65 E66 E67 M68 A69 G70 L71 L72 Q73 Q74 I75 E76 V77 E78 R79 S80 L81 Y82 SER ASP HIS GLU LEU ARG ALA LEU ASP GLU ALA GLN ARG LEU ALA LYS LYS LYS ALA ASP LEU TYR ASP GLU GLN GLN GLN GLY ILE THR LEU ALA GLN ASP LEU GLU ASP

MET TRP GLU GLN ALA PHE LEU GLN PHE R130 P131 G132 A133 R134 E135 T136 E137 A138 D139 K140 K141 N142 D143 R144 T145 S146 L147 H148 R149 K150 L151 D152 R153 N154 L155 V156 L157 L158 V159 R160 E161 K162 L163 G164 D165 Q166 D167 V168 W169 M170 L171 P172 Q173 V174 E175 W176 Q177 P178 G179 E180

T181 L182 R183 G184 T185 A186 E187 R188 I189 L190 A191 T192 L193 S194 E195 N196 N197 M198 E199 A200 K201 F202 L203 G204 N205 A206 H210 Y211 K212 F213 K214 F215 PRO LYS ALA ILE GLN THR GLU LEU SER ASP L225 G226 V227 K228 V229 F230 F231 F232 K233 A234 L235 L236 L237 T238 G239 D240 F241 V242

Q243 A244 G245 K246 K247 S248 R249 H250 V251 W252 A253 S254 K255 E256 E257 L258 G259 D260 Y261 L262 Q263 P264 K265 Y266 A267 A268 R271 R272 F273 L274 L275 ASP SER ASP GLY LEU SER CYS LEU

• Molecule 34: Large ribosomal subunit protein mL48

Chain f:
38%
35% 7% 58%

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

LEU VAL LYS VAL GLN GLU PRO LYS LYS LYS ALA LYS VAL GLU LEU ARG ALA ILE ASN VAL GLY THR D84 Y85 E86 Y87 G88 V89 L90 N91 I92 H93 L94 T95 A96 Y97 D98 M99 S100 L101 A102 E103 S104 Y105 A106 Q107 Y108 V109 H110 R111 L112 C113 N114 R115 L116 S117 I118 K119 V120

E121 E122 S123 Y124 A125 M126 P127 T128 K129 T130 M131 GLU VAL MET ARG LEU PRO ASP GLN GLY ASN LYS MET VAL LEU ASP SER VAL L149 T150 T151 H152 E153 R154 V155 V156 Q157 I158 S159 G160 L161 S162 A163 T164 F165 A166 E167 I168 F169 L170 E171 V172 L173 Q174 S175 N176 L177 P178 E179 G180

V181 R182 L183 S184 V185 R186 E187 H188 T189 GLU GLU ASP PHE LYS GLY ARG PHE LYS ALA ARG PRO GLU LEU GLU GLU LEU LEU ALA LYS LEU ASN

• Molecule 35: Large ribosomal subunit protein mL49

Chain g:
5%
70% 9% 20%

MET ALA ALA ALA VAL LEU ARG ALA ALA LEU GLN ASP TRP ARG SER CYS LEU GLY ARG SER TYR GLY ARG ARG LYS LEU SER GLN THR GLN GLY PRO PRO ASP N35 F38 V39 E40 S41 V42 D43 E44 E49 R50 L51 L52 K64 F85 E99 R105 Q106 M107 R111

E114 S129 P130 G151 D154 F166

• Molecule 36: Large ribosomal subunit protein mL50

Chain h:
8%
61% 8% 31%

MET ALA ALA LEU ILE VAL SER ARG LEU ALA ARG ARG GLY LEU TRP LEU TRP LYS LEU PRO LEU ALA THR ARG ARG GLU LEU TRP SER SER ARG ALA LYS GLU LYS GLU PRO VAL VAL ALA GLU THR VAL GLU GLU VAL LYS LYS GLU PRO V50 L51 V52 C53 P54 R57 S58 L71

L79 D89 D107 A112 N115 C122 R123 V124 R125 D126 V127 L128 D129 F130 Q136 S156 W157 S158 Y159

• Molecule 37: Large ribosomal subunit protein mL51

Chain i:
12%
62% 10% 27%

MET ALA GLY SER VAL PRO TRP ALA ALA SER ARG ARG LEU TRP GLY TRP VAL PRO SER ALA CYS ARG SER PHE SER LEU GLY LEU VAL PRO ARG LEU A32 F33 V34 R35 L36 T37 P40 P41 K42 V43 V44 D45 R46 L53 Y57 D58 N59 I60 G61 I62 L63 G64 N65 F66 K75

W79 L80 R93 K94 R123 H124 GLY LYS TYR ARG

• Molecule 38: Large ribosomal subunit protein mL52

Chain j:

6%
66%　　　　　　　　　　・　　　　30%

MET ALA ALA LEU GLY THR TRP LEU SER SER VAL ARG ARG LEU HIS CYS SER VAL VAL ALA ARG A22 L45 S49 M59 I87 E100 R101 K102 K103 E104 H105 D106 LEU LYS PRO LYS GLY THR LEU LEU ARG SER PRO LEU PRO ASN GLN

• Molecule 39: Large ribosomal subunit protein mL53

Chain k:

36%
56%　　　　12%　　　　32%

MET ALA ALA ALA LEU ALA ARG ARG LEU GLY LEU ARG PRO V13 K14 R17 V18 Q19 F20 E24 K25 N26 V27 E28 S29 T30 R31 T32 F33 L34 Q35 T36 V37 S38 S39 E40 K41 V42 R43 A44 T45 N46 L47 N48 C49 S50 V51 I52 A53 D54 V55 R56 HIS ASP GLY SER E61 P62 C63

V64 D65 V66 D70 R73 A79 H80 L81 A89 S92 H93 I94 R95 D96 ARG ASN ALA ALA ALA SER ALA PRO GLY ALA ASP LYS VAL ALA PRO GLY THR SER THR ARG ARG

• Molecule 40: Large ribosomal subunit protein mL54

Chain l:

44%
47%　　　　9%　　　　44%

MET ALA ALA ALA HIS LEU LEU ARG ALA ALA SER ARG VAL THR ALA ARG TRP HIS PRO ARG ALA LEU PRO VAL LEU ARG ARG PRO GLY GLY PHE SER ILE ARG GLU TYR ALA LYS LYS PRO VAL GLY LYS GLY LYS GLY LYS GLY VAL ALA ALA GLU ALA LEU LYS ASP PRO GLU V58 C59 T60

D61 P62 T63 Q64 L65 T66 T67 H68 A69 M70 G71 V72 N73 I74 Y75 K76 E77 G78 Q79 D80 V81 A82 L83 K84 A85 D86 S87 E88 Y89 P90 T91 W92 L93 F94 Q95 V96 N97 L98 G99 P100 P101 K102 K103 L104 E105 E106 L107 E108 P109 R112 E113 Y114 L117 W124 R125 H126 N127

R128 L129 S130 K131 N132 K133 LYS LEU

• Molecule 41: Large ribosomal subunit protein mL63

Chain o:

5%
73%　　　　　　・　　　　24%

MET PHE LEU THR ALA VAL LEU LEU ARG GLY ILE PRO GLY ARG GLN TRP ILE GLY LYS HIS ARG ARG PRO R25 Y47 Y53 R66 T79 S80 R86 S102

• Molecule 42: Large ribosomal subunit protein mL62

Chain p:

11%
53%　　　　11%　　　　36%

• Molecule 43: Large ribosomal subunit protein mL64

Chain q:

• Molecule 44: Large ribosomal subunit protein mL66

Chain r:

• Molecule 45: Large ribosomal subunit protein mL65

Chain s:

F293 I296 P297 D298 R299 L300 E303 R347 P348 D357 G358 K359 Y360 L371 Q376 N380 N381 Q391 L395 Y396 E397 T398 V399 E400 D401 N402 D403 V404 L419 R424 GLU ASP GLY ALA GLN LEU LEU ALA SER GLN GLU LYS GLU ASP LEU GLY PRO

• Molecule 46: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:

29%

47%   8%   45%

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

GLY PRO GLN PRO GLU GLU ARG THR ALA GLY ASP ALA ARG ARG LEU GLN PRO GLY PRO ALA ASP HIS ILE GLY ALA K85 I88 D89 M90 S93 L94 L95 R96 Q97 E98 N99 C104 V105 I106 Q107 V108 R113 Y114 T115 D116 V119 T124 R127 A131 H134 Y135 L136

V137 K138 M139 Y140 K141 H142 L143 K144 C145 R146 I153 E154 G155 K156 D157 A158 D159 D160 D165 F166 G167 S168 M174 L175 P176 E177 T178 R179 E180 T181 E185 K186 L187 W188 R191 S192 F193 D194 D195 Q196 L197 A198 Q199 I200 A201 A202 E203 T204 L205 P206 E207 D208 F209 ILE LEU

GLY LEU GLU ASP THR SER LEU THR PRO VAL GLU PHE LYS CYS LYS

• Molecule 47: Predicted gene, 55359

Chain v:

77%

90%   9% •

MET A2 P3 W4 E7 A8 V9 L10 C11 L12 Y13 R14 A15 L16 L17 R18 Q19 G20 R21 E22 L23 R24 Y25 T26 D27 R28 F32 A33 S34 I35 R36 R37 E38 F39 R40 K41 N42 Q43 K44 L45 E46 N47 L48 E49 A50 R51 E52 K53 Q54 L55 E56 K57 G58 L59 V60 F61 L62 H63

S64 K65 L66 G67 G68 L69 I70
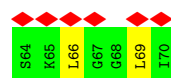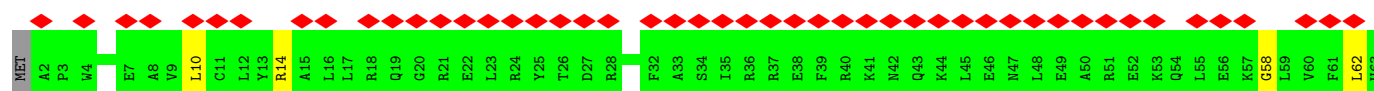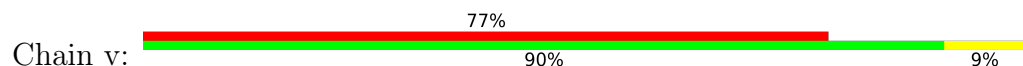
• Molecule 48: Acyl carrier protein, mitochondrial

Chain w:

49%

46%   5%   49%

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

VAL THR HIS LEU CYS ARG GLN TYR SER ASP ALA PRO PRO L74 T75 L76 D77 G78 I79 K80 D81 R82 V83 L84 Y85 V86 L87 K88 L89 Y90 D91 K92 I93 D94 P95 E96 K97 L98 S99 V100 N101 S102 H103 F104 M105 K106 D107 L108 G109 L110 D111 S112 L113 D114 Q115 V116 E117 I118 I119 M120

A121 M122 E123 D124 E125 F126 G127 F128 E129 I130 P131 D132 I133 D134 A135 E136 K137 L138 M139 C140 P141 Q142 E143 I144 V145 D146 Y147 I148 A149 D150 K151 L152 ASP VAL TYR GLU

• Molecule 49: rRNA methyltransferase 3, mitochondrial

Chain x:

35%

56%   14%   29%

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

• Molecule 49: rRNA methyltransferase 3, mitochondrial

Chain y:

31%

52% 18% 30%

• Molecule 50: Probable ATP-dependent RNA helicase DDX28

Chain z:

36%

79% 6% 15%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	457.2936, 457.2936, 457.2936	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84684, 0.84684, 0.84684	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.07	0/26881	0.18	0/41775
2	B	0.07	0/1459	0.17	0/2266
3	D	0.08	0/1357	0.23	0/1831
4	E	0.07	0/2186	0.20	0/2972
5	F	0.07	0/1772	0.20	0/2415
6	H	0.08	0/793	0.23	0/1066
7	I	0.09	0/1273	0.24	0/1722
8	J	0.09	0/1093	0.25	0/1472
9	K	0.06	0/1436	0.19	0/1948
10	L	0.07	0/908	0.21	0/1224
11	M	0.08	0/2054	0.24	0/2776
12	O	0.06	0/1246	0.19	0/1679
13	P	0.07	0/1181	0.21	0/1600
14	Q	0.08	0/1832	0.21	0/2471
15	R	0.06	0/1096	0.17	0/1469
16	S	0.08	0/1328	0.22	0/1798
17	T	0.07	0/1402	0.19	0/1885
18	U	0.07	0/1062	0.21	0/1441
19	V	0.07	0/1669	0.20	0/2259
20	X	0.07	0/2075	0.20	0/2806
21	Y	0.06	0/1561	0.17	0/2093
22	Z	0.07	0/959	0.21	0/1298
23	0	0.07	0/896	0.20	0/1200
24	5	0.07	0/3256	0.21	0/4432
25	6	0.09	0/2622	0.23	0/3560
26	7	0.07	0/2436	0.21	0/3300
27	8	0.06	0/499	0.17	0/666
28	9	0.09	0/800	0.22	0/1082
29	a	0.07	0/884	0.20	0/1197
30	b	0.07	0/1203	0.21	0/1625
31	c	0.07	0/2297	0.20	0/3106
32	d	0.07	0/1736	0.20	0/2353

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.07	0/1465	0.22	0/1971
34	f	0.09	0/726	0.22	0/983
35	g	0.08	0/1126	0.22	0/1533
36	h	0.09	0/894	0.24	0/1216
37	i	0.07	0/818	0.21	0/1099
38	j	0.06	0/698	0.18	0/937
39	k	0.07	0/636	0.20	0/857
40	l	0.07	0/651	0.19	0/882
41	o	0.06	0/655	0.17	0/880
42	p	0.07	0/1104	0.22	0/1476
43	q	0.07	0/825	0.19	0/1126
44	r	0.08	0/1301	0.21	0/1756
45	s	0.07	0/3118	0.20	0/4232
46	u	0.07	0/1053	0.20	0/1425
47	v	0.08	0/596	0.23	0/795
48	w	0.11	0/646	0.27	0/869
49	x	0.08	0/2357	0.24	0/3198
49	y	0.09	0/2342	0.25	0/3174
50	z	0.07	0/3623	0.20	0/4918
All	All	0.07	0/97886	0.20	0/138114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24019	12126	12156	204	0
2	B	1303	657	658	14	0
3	D	1335	1373	1373	14	0
4	E	2122	2097	2097	14	0
5	F	1728	1755	1754	20	0
6	H	779	814	814	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1245	1330	1330	17	0
8	J	1075	1145	1145	15	0
9	K	1396	1398	1398	9	0
10	L	893	944	944	10	0
11	M	2010	2080	2080	29	0
12	O	1222	1254	1254	14	0
13	P	1154	1148	1148	21	0
14	Q	1790	1822	1822	18	0
15	R	1077	1137	1137	6	0
16	S	1301	1372	1372	11	0
17	T	1369	1402	1402	12	0
18	U	1034	1038	1038	9	0
19	V	1628	1622	1622	23	0
20	X	2021	2051	2051	20	0
21	Y	1523	1553	1553	13	0
22	Z	934	979	979	5	0
23	0	881	908	908	13	0
24	5	3168	3187	3187	18	0
25	6	2534	2420	2418	45	0
26	7	2379	2378	2378	15	0
27	8	493	484	484	7	0
28	9	778	772	772	6	0
29	a	860	843	843	9	0
30	b	1181	1195	1195	13	0
31	c	2246	2256	2256	20	0
32	d	1688	1670	1670	24	0
33	e	1437	1474	1474	21	0
34	f	714	704	704	11	0
35	g	1090	1094	1094	12	0
36	h	872	868	867	10	0
37	i	795	816	816	11	0
38	j	684	692	692	5	0
39	k	629	639	639	8	0
40	l	635	631	631	10	0
41	o	640	623	623	4	0
42	p	1089	1112	1112	16	0
43	q	799	785	785	9	0
44	r	1267	1319	1319	15	0
45	s	3045	3057	3057	34	0
46	u	1029	1012	1012	12	0
47	v	586	603	603	5	0
48	w	637	640	640	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	x	2305	2356	2356	50	0
49	y	2291	2340	2340	59	0
50	z	3555	3681	3681	22	0
51	0	1	0	0	0	0
52	r	4	0	0	2	0
All	All	93270	81656	81683	823	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 5.

All (823) 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:2168:U:O2'	50:z:99:HIS:O	1.83	0.95
1:A:1093:A:O2'	1:A:1094:A:OP1	1.92	0.87
34:f:99:MET:SD	34:f:154:ARG:NH2	2.48	0.86
5:F:209:TYR:O	36:h:57:ARG:NH1	2.08	0.86
1:A:1477:A:OP1	35:g:105:ARG:NH2	2.09	0.86
1:A:1597:C:N4	1:A:1644:C:OP1	2.10	0.85
1:A:2466:U:O2'	1:A:2467:A:OP1	1.94	0.84
1:A:1307:A:N6	1:A:1318:A:O4'	2.11	0.83
1:A:2168:U:OP2	50:z:73:ARG:NH1	2.12	0.83
1:A:2181:A:O2'	1:A:2241:A:N6	2.13	0.82
1:A:2268:A:N6	1:A:2276:U:O4	2.12	0.82
6:H:51:VAL:HG13	20:X:86:ILE:HD12	1.62	0.82
1:A:2562:C:OP2	1:A:2563:A:O2'	1.97	0.81
1:A:1758:A:O2'	45:s:210:ARG:NH2	2.13	0.80
1:A:2092:G:N2	1:A:2096:C:O2'	2.14	0.80
18:U:59:GLN:NE2	28:9:58:PHE:O	2.14	0.80
31:c:80:GLN:O	31:c:210:ARG:NH2	2.14	0.80
1:A:1806:A:O2'	1:A:1809:C:N4	2.15	0.80
1:A:2507:U:O2'	1:A:2508:C:OP1	2.00	0.80
2:B:14:A:N1	2:B:21:A:O2'	2.14	0.79
1:A:1310:A:OP2	5:F:279:ARG:NE	2.16	0.79
45:s:240:GLN:NE2	45:s:348:PRO:O	2.16	0.79
45:s:89:LYS:O	45:s:269:ARG:NH2	2.16	0.79
1:A:1187:U:O4	43:q:60:GLN:NE2	2.16	0.78
49:x:228:ARG:NH1	49:x:257:MET:SD	2.56	0.78
4:E:107:MET:HE3	4:E:121:LEU:HD11	1.65	0.78
49:x:398:PHE:CE2	49:y:391:MET:HE3	2.18	0.78
24:5:280:GLN:OE1	45:s:152:ARG:NE	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:A:N6	1:A:2245:U:OP1	2.17	0.77
1:A:2247:C:O3'	1:A:2364:G:OP2	2.02	0.77
11:M:202:ARG:O	11:M:262:ARG:NH2	2.17	0.77
3:D:195:ASN:OD1	3:D:244:THR:OG1	2.01	0.77
17:T:133:ASN:ND2	17:T:174:GLU:OE2	2.18	0.76
10:L:119:ILE:O	10:L:142:GLN:NE2	2.19	0.76
6:H:96:THR:N	6:H:125:LEU:O	2.19	0.76
46:u:88:ILE:HD11	46:u:105:VAL:HG11	1.67	0.76
1:A:1315:U:O2'	1:A:1320:C:OP1	2.03	0.75
44:r:94:ARG:NH1	44:r:99:MET:O	2.19	0.75
2:B:29:C:OP2	34:f:111:ARG:NH1	2.18	0.75
50:z:73:ARG:NH2	50:z:93:ALA:O	2.18	0.75
25:6:220:ASN:OD1	25:6:234:HIS:NE2	2.20	0.75
2:B:12:U:O2'	2:B:14:A:OP1	2.05	0.75
11:M:207:GLU:OE2	43:q:106:GLN:NE2	2.20	0.75
1:A:1507:G:OP2	41:o:66:ARG:NH2	2.18	0.74
1:A:1641:G:OP1	8:J:42:ARG:NH2	2.20	0.74
4:E:112:LYS:NZ	4:E:337:VAL:O	2.19	0.74
1:A:2275:A:O2'	1:A:2276:U:OP1	2.03	0.74
1:A:1191:A:O2'	1:A:1192:G:OP1	2.06	0.74
25:6:161:LEU:HD22	25:6:219:ILE:HD13	1.69	0.74
1:A:1822:A:OP1	24:5:112:ARG:NH1	2.20	0.74
18:U:2:ALA:O	18:U:7:TYR:OH	2.05	0.74
3:D:156:GLU:N	3:D:247:ARG:O	2.21	0.73
11:M:232:ARG:NH2	42:p:60:LYS:O	2.21	0.73
1:A:1246:A:OP2	23:0:94:ARG:NH1	2.20	0.73
1:A:1262:A:OP1	30:b:4:ARG:NH2	2.22	0.73
1:A:1713:U:OP2	37:i:46:ARG:NH1	2.21	0.73
1:A:2659:C:O2'	1:A:2660:U:OP1	2.07	0.73
8:J:23:ILE:HD11	8:J:86:THR:CG2	2.19	0.73
1:A:1234:A:O2'	1:A:1235:U:OP1	2.05	0.73
1:A:2437:G:O3'	49:y:148:ARG:NH2	2.22	0.73
11:M:108:ARG:NH2	11:M:123:GLY:O	2.20	0.73
47:v:14:ARG:NH2	48:w:124:ASP:OD1	2.21	0.72
1:A:1305:C:OP2	35:g:111:ARG:NH2	2.22	0.72
1:A:2469:U:O4	49:x:102:ARG:NH2	2.22	0.72
13:P:112:ILE:HD13	13:P:131:VAL:HG21	1.71	0.72
1:A:1869:C:N4	17:T:153:HIS:O	2.22	0.72
49:x:155:LEU:HD11	49:x:185:ILE:HD11	1.71	0.72
1:A:1560:C:OP2	22:Z:77:ARG:NH1	2.22	0.72
11:M:250:GLU:O	11:M:253:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:U:OP2	30:b:116:ARG:NH1	2.23	0.72
1:A:1580:C:OP2	44:r:190:ARG:NH1	2.22	0.72
1:A:2598:A:OP1	14:Q:271:ARG:NH2	2.22	0.71
10:L:142:GLN:O	46:u:191:ARG:NH2	2.23	0.71
25:6:198:ALA:O	25:6:254:TYR:OH	2.08	0.71
20:X:35:GLU:N	20:X:35:GLU:OE1	2.24	0.70
49:x:283:ARG:NH1	49:x:285:TYR:OH	2.24	0.70
1:A:2487:A:O2'	49:x:218:ARG:O	2.07	0.70
20:X:156:LYS:NZ	20:X:205:GLY:O	2.25	0.70
14:Q:126:ALA:HB1	14:Q:129:LYS:HD3	1.74	0.70
49:x:135:LEU:HD11	49:x:144:PHE:CZ	2.27	0.70
1:A:2436:U:O2'	49:y:147:SER:O	2.08	0.70
49:y:203:PRO:O	49:y:207:THR:N	2.25	0.70
49:x:135:LEU:HD12	49:x:156:PRO:HG2	1.73	0.69
49:x:381:VAL:N	49:y:262:GLN:OE1	2.25	0.69
46:u:89:ASP:OD1	46:u:90:MET:N	2.25	0.69
1:A:2302:U:O2'	1:A:2303:A:OP1	2.11	0.69
1:A:2436:U:O4'	49:y:96:LYS:NZ	2.25	0.69
1:A:1894:C:O2'	12:O:17:ARG:NH2	2.25	0.69
4:E:57:ASN:OD1	12:O:147:ASN:ND2	2.25	0.69
13:P:51:ARG:O	25:6:159:ARG:NH2	2.25	0.69
1:A:1907:G:H4'	10:L:36:THR:HG22	1.72	0.69
13:P:173:ARG:O	42:p:177:ARG:NH2	2.25	0.69
1:A:1137:A:O2'	1:A:1138:U:OP1	2.10	0.69
1:A:1204:C:O2	1:A:1206:A:O2'	2.09	0.68
1:A:2648:A:OP1	9:K:98:LYS:NZ	2.27	0.68
1:A:1101:C:O2'	1:A:1102:U:OP2	2.10	0.68
1:A:1124:U:O2'	1:A:1133:U:O4	2.11	0.68
19:V:45:VAL:CG2	21:Y:235:ILE:HG22	2.23	0.68
1:A:1108:U:OP1	37:i:94:LYS:NZ	2.26	0.68
11:M:152:ASN:ND2	11:M:255:LEU:O	2.27	0.68
26:7:228:GLN:OE1	26:7:228:GLN:N	2.26	0.68
49:y:335:LEU:HD12	49:y:369:GLU:HB2	1.76	0.67
49:y:399:GLU:OE2	49:y:402:ARG:NH1	2.28	0.67
1:A:1095:C:OP1	17:T:45:TRP:N	2.27	0.67
49:y:148:ARG:NH1	49:y:151:TYR:OH	2.28	0.67
49:y:128:ARG:NH1	49:y:154:GLU:OE1	2.27	0.67
1:A:1103:A:O2'	19:V:40:ARG:NH2	2.28	0.67
1:A:1953:A:O2'	1:A:1954:C:OP1	2.13	0.67
49:x:135:LEU:HD12	49:x:156:PRO:CG	2.25	0.67
1:A:1847:U:OP1	24:5:223:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:127:GLU:OE2	23:O:131:GLN:NE2	2.28	0.66
1:A:1756:C:OP1	23:O:138:GLN:NE2	2.27	0.66
1:A:1762:C:OP2	45:s:55:SER:OG	2.13	0.66
8:J:84:GLN:N	8:J:127:ASP:OD2	2.29	0.66
23:O:116:LYS:NZ	23:O:120:VAL:O	2.28	0.66
49:y:247:ALA:O	49:y:260:HIS:NE2	2.28	0.66
16:S:168:THR:O	16:S:194:GLN:N	2.28	0.65
45:s:66:TRP:O	45:s:69:THR:OG1	2.10	0.65
49:x:405:ARG:NH2	49:y:339:SER:OG	2.29	0.65
1:A:1829:C:OP1	24:5:173:ARG:NH2	2.29	0.65
40:l:107:LEU:HD11	40:l:117:LEU:HD12	1.78	0.65
1:A:1446:U:OP1	11:M:42:ARG:NH1	2.28	0.65
1:A:2448:U:O4'	1:A:2471:A:N6	2.30	0.65
30:b:40:SER:OG	30:b:44:ARG:NH1	2.29	0.65
33:e:154:ASN:C	33:e:155:LEU:HD12	2.22	0.65
42:p:51:GLU:OE1	42:p:51:GLU:N	2.30	0.65
1:A:2466:U:HO2'	1:A:2467:A:P	2.20	0.65
17:T:46:GLU:OE1	17:T:46:GLU:N	2.29	0.65
1:A:1292:A:O2'	1:A:1328:C:O2	2.12	0.65
4:E:344:SER:OG	14:Q:169:PRO:O	2.08	0.65
13:P:88:HIS:O	13:P:119:THR:OG1	2.05	0.65
6:H:64:GLU:O	20:X:61:ARG:NH1	2.29	0.64
19:V:132:GLU:OE1	19:V:148:THR:OG1	2.09	0.64
49:x:338:GLN:O	49:x:377:LEU:N	2.29	0.64
49:y:213:ILE:N	49:y:351:VAL:O	2.30	0.64
19:V:101:THR:OG1	19:V:103:ASP:OD1	2.14	0.64
33:e:263:GLN:N	33:e:263:GLN:OE1	2.30	0.64
23:O:107:ASP:N	23:O:116:LYS:O	2.29	0.64
25:6:304:TYR:O	25:6:308:GLN:N	2.31	0.64
14:Q:161:GLU:OE1	14:Q:191:ARG:NH2	2.30	0.64
20:X:81:GLY:N	20:X:131:THR:OG1	2.30	0.64
11:M:283:LYS:NZ	35:g:41:SER:OG	2.20	0.64
45:s:90:LYS:NZ	45:s:272:TYR:O	2.31	0.64
32:d:157:HIS:O	32:d:161:HIS:ND1	2.30	0.64
23:O:131:GLN:OE1	32:d:290:TRP:NE1	2.31	0.64
11:M:91:GLN:O	11:M:93:GLN:NE2	2.29	0.64
3:D:157:ASN:ND2	3:D:179:GLU:OE1	2.31	0.64
1:A:1889:A:O2'	1:A:1891:A:OP1	2.14	0.63
1:A:1198:A:N1	19:V:40:ARG:NH1	2.45	0.63
50:z:227:GLY:O	50:z:231:GLY:N	2.30	0.63
31:c:167:CYS:SG	31:c:171:ARG:NH1	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:G:N2	2:B:60:C:N3	2.46	0.63
1:A:2119:A:OP1	15:R:34:ARG:NH2	2.32	0.63
33:e:150:LYS:HB2	33:e:155:LEU:HD11	1.80	0.63
5:F:60:ARG:NH1	36:h:122:CYS:SG	2.71	0.63
49:y:253:LEU:O	49:y:257:MET:N	2.32	0.63
1:A:1600:U:O2	7:I:107:GLU:N	2.32	0.63
49:x:145:PHE:HE1	49:x:166:ILE:HD12	1.63	0.63
8:J:23:ILE:HD11	8:J:86:THR:HG21	1.81	0.62
3:D:103:ASN:O	3:D:105:ARG:NH1	2.31	0.62
14:Q:129:LYS:NZ	46:u:114:TYR:O	2.32	0.62
49:x:279:PRO:O	49:x:282:THR:OG1	2.10	0.62
8:J:90:PHE:CE2	8:J:120:ILE:HG21	2.34	0.62
45:s:137:ARG:NH1	45:s:141:CYS:SG	2.72	0.62
7:I:61:ASN:OD1	44:r:78:LYS:NZ	2.33	0.62
1:A:1800:U:O2'	21:Y:125:ARG:NH2	2.33	0.62
1:A:2192:C:OP2	6:H:88:LYS:NZ	2.26	0.62
49:x:229:SER:O	49:y:391:MET:HE2	1.99	0.62
12:O:64:LYS:NZ	12:O:100:GLN:O	2.33	0.62
20:X:163:ARG:NH1	20:X:204:VAL:O	2.33	0.62
49:x:222:ASN:O	49:x:226:ILE:N	2.30	0.62
49:x:386:SER:O	49:y:129:ARG:NH2	2.33	0.62
50:z:97:TRP:NE1	50:z:105:ASP:OD2	2.33	0.62
7:I:116:LEU:HD12	7:I:123:ILE:HG13	1.81	0.61
5:F:94:ASP:OD1	5:F:95:ILE:N	2.33	0.61
25:6:152:ALA:HB2	25:6:316:LEU:HD13	1.81	0.61
1:A:1202:A:N6	1:A:1205:U:OP2	2.33	0.61
1:A:1728:A:OP2	11:M:40:ARG:NE	2.25	0.61
32:d:189:LEU:HD12	32:d:217:HIS:CD2	2.35	0.61
27:8:150:LEU:HD22	33:e:230:PHE:CZ	2.36	0.61
49:y:88:GLU:N	49:y:88:GLU:OE1	2.34	0.61
5:F:237:LEU:O	43:q:25:TYR:N	2.34	0.61
1:A:2667:G:N7	12:O:11:HIS:NE2	2.48	0.61
3:D:194:ILE:HD11	3:D:227:ILE:HD12	1.83	0.61
1:A:2116:U:O2'	23:0:80:PRO:O	2.18	0.60
1:A:2342:U:O2'	1:A:2343:A:OP1	2.18	0.60
32:d:126:ARG:O	32:d:130:ALA:N	2.33	0.60
11:M:131:LEU:O	11:M:133:ARG:NH1	2.34	0.60
33:e:194:SER:O	33:e:246:LYS:NZ	2.31	0.60
1:A:1725:U:O2'	11:M:38:ARG:NH2	2.34	0.60
36:h:136:GLN:N	36:h:136:GLN:OE1	2.34	0.60
1:A:2593:C:O4'	10:L:95:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1606:G:N2	8:J:103:HIS:O	2.34	0.60
34:f:187:GLU:OE1	34:f:187:GLU:N	2.35	0.60
49:x:388:ASN:O	49:y:228:ARG:NH1	2.35	0.60
4:E:68:GLU:OE1	4:E:154:ARG:NH2	2.34	0.59
8:J:120:ILE:HG22	40:l:71:GLY:O	2.01	0.59
11:M:141:GLU:N	11:M:141:GLU:OE1	2.35	0.59
16:S:168:THR:HG22	16:S:169:GLU:H	1.66	0.59
4:E:126:ASP:O	4:E:173:LYS:NZ	2.33	0.59
25:6:204:VAL:HG11	25:6:216:LEU:HD11	1.83	0.59
46:u:104:CYS:SG	46:u:179:ARG:NH2	2.74	0.59
49:x:145:PHE:CE1	49:x:166:ILE:HD12	2.36	0.59
49:x:225:THR:O	49:x:229:SER:N	2.29	0.59
7:I:167:GLU:N	7:I:167:GLU:OE1	2.34	0.59
13:P:169:GLY:O	42:p:184:ASN:ND2	2.35	0.59
33:e:264:PRO:O	33:e:268:ALA:N	2.33	0.59
49:x:288:ASP:OD2	49:x:375:ARG:NH1	2.35	0.59
7:I:195:LEU:O	7:I:199:ALA:N	2.33	0.59
14:Q:251:GLU:OE1	14:Q:251:GLU:N	2.33	0.59
25:6:60:ARG:NH2	25:6:64:GLU:OE1	2.36	0.59
49:y:222:ASN:O	49:y:226:ILE:N	2.31	0.59
5:F:214:SER:N	5:F:257:GLN:OE1	2.36	0.59
13:P:122:VAL:HG22	13:P:157:SER:HB3	1.85	0.59
17:T:49:ASN:ND2	17:T:68:TYR:O	2.34	0.59
20:X:117:GLU:N	20:X:142:ASP:OD2	2.36	0.58
42:p:97:SER:O	42:p:146:ASN:ND2	2.36	0.58
5:F:277:ASP:O	5:F:278:SER:OG	2.14	0.58
6:H:79:LEU:HD11	6:H:82:ASP:HB2	1.85	0.58
1:A:1744:G:N2	1:A:2113:A:OP2	2.37	0.58
1:A:1626:A:O2'	1:A:1627:A:O5'	2.19	0.58
49:x:155:LEU:HD11	49:x:185:ILE:CD1	2.34	0.58
49:y:150:GLU:OE1	49:y:150:GLU:N	2.34	0.58
1:A:2122:U:O4'	1:A:2134:G:N2	2.37	0.58
8:J:60:ILE:HG21	8:J:66:LEU:HD11	1.86	0.58
31:c:78:ARG:O	31:c:80:GLN:NE2	2.36	0.58
1:A:1603:U:HO2'	1:A:1605:G:P	2.27	0.58
31:c:315:ASP:OD1	31:c:317:SER:N	2.37	0.58
26:7:162:SER:OG	26:7:181:THR:OG1	2.22	0.58
49:y:117:ARG:O	49:y:121:GLY:N	2.36	0.58
27:8:139:MET:HE1	33:e:275:LEU:HD23	1.86	0.57
49:x:95:ASP:O	49:x:167:LYS:N	2.35	0.57
25:6:227:GLU:OE1	25:6:230:ALA:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:u:207:GLU:N	46:u:207:GLU:OE1	2.37	0.57
19:V:65:LEU:N	19:V:119:GLN:O	2.36	0.57
20:X:81:GLY:O	20:X:130:ARG:NE	2.35	0.57
25:6:157:LEU:HD11	25:6:318:PHE:CD1	2.40	0.57
36:h:89:ASP:O	36:h:123:ARG:NH1	2.37	0.57
1:A:1123:A:OP2	21:Y:199:ARG:NH1	2.37	0.57
19:V:54:TRP:NE1	19:V:56:LEU:O	2.32	0.57
31:c:155:SER:HG	31:c:232:TRP:CD1	2.23	0.57
31:c:155:SER:HG	31:c:232:TRP:CG	2.23	0.57
43:q:60:GLN:O	43:q:68:SER:OG	2.22	0.57
1:A:1206:A:N7	1:A:1221:A:N6	2.53	0.57
11:M:263:GLN:NE2	11:M:265:PHE:O	2.37	0.57
48:w:81:ASP:OD1	48:w:82:ARG:N	2.38	0.57
4:E:69:ASN:OD1	4:E:154:ARG:NH1	2.36	0.57
8:J:87:VAL:HG11	8:J:144:ILE:HG22	1.87	0.57
6:H:121:LEU:HD23	6:H:126:ALA:O	2.05	0.56
1:A:1224:U:O4	19:V:34:LYS:NZ	2.37	0.56
1:A:1246:A:O2'	23:0:91:CYS:SG	2.63	0.56
1:A:1629:G:HO2'	40:l:124:TRP:CD1	2.23	0.56
1:A:1730:C:O2'	15:R:40:ARG:NE	2.38	0.56
26:7:183:ASP:OD1	26:7:184:LYS:N	2.36	0.56
45:s:172:ASP:OD2	45:s:197:LYS:NZ	2.38	0.56
1:A:1191:A:HO2'	1:A:1192:G:P	2.28	0.56
3:D:111:ARG:O	3:D:150:ARG:NH2	2.38	0.56
19:V:20:ARG:N	19:V:35:ASN:OD1	2.38	0.56
34:f:114:ASN:OD1	34:f:115:ARG:N	2.38	0.56
49:x:332:LEU:HD23	49:x:332:LEU:H	1.69	0.56
1:A:1230:A:OP2	19:V:94:HIS:NE2	2.38	0.56
1:A:1571:A:OP2	15:R:65:ARG:NH1	2.38	0.56
19:V:199:MET:O	19:V:203:GLY:N	2.38	0.56
6:H:51:VAL:HG21	20:X:105:TRP:CG	2.41	0.56
6:H:117:ARG:O	6:H:117:ARG:NH1	2.37	0.56
44:r:176:VAL:N	44:r:194:MET:O	2.35	0.56
18:U:139:GLY:O	32:d:179:LYS:NZ	2.39	0.56
30:b:66:ASN:OD1	36:h:156:SER:OG	2.19	0.56
40:l:59:CYS:HB2	40:l:70:MET:HE2	1.86	0.56
32:d:106:THR:OG1	32:d:107:GLN:N	2.38	0.56
48:w:120:MET:HE2	48:w:120:MET:N	2.21	0.55
49:x:135:LEU:HD11	49:x:144:PHE:CE2	2.41	0.55
50:z:239:GLY:N	50:z:262:THR:OG1	2.38	0.55
1:A:2485:C:O2'	1:A:2486:A:OP2	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:302:ASP:OD1	25:6:303:PHE:N	2.39	0.55
32:d:244:GLU:N	32:d:244:GLU:OE1	2.39	0.55
49:x:215:ASP:OD2	49:x:361:SER:N	2.38	0.55
4:E:90:TRP:CD1	4:E:311:CYS:HG	2.25	0.55
19:V:177:THR:O	28:9:73:ASN:ND2	2.40	0.55
25:6:75:ARG:O	25:6:79:VAL:N	2.39	0.55
1:A:1293:G:N1	11:M:46:ARG:O	2.39	0.55
49:x:399:GLU:OE2	49:x:403:GLN:NE2	2.40	0.55
1:A:2617:A:O2'	1:A:2618:A:OP2	2.18	0.55
21:Y:67:GLU:OE1	21:Y:67:GLU:N	2.38	0.55
26:7:244:ASN:ND2	26:7:248:ILE:O	2.39	0.55
12:O:67:ASP:OD2	45:s:44:TYR:OH	2.18	0.55
2:B:25:A:OP2	13:P:87:GLN:NE2	2.37	0.55
29:a:76:GLN:N	29:a:76:GLN:OE1	2.40	0.55
49:x:402:ARG:NH2	49:y:395:ILE:O	2.39	0.55
24:5:139:LEU:O	24:5:145:ASN:ND2	2.39	0.54
25:6:187:VAL:HG13	25:6:319:PHE:HB3	1.90	0.54
30:b:89:VAL:HG12	30:b:89:VAL:O	2.07	0.54
32:d:111:ARG:NH2	32:d:195:VAL:HG22	2.22	0.54
1:A:1790:A:N6	17:T:152:TYR:O	2.36	0.54
1:A:2395:U:O4	1:A:2396:A:N6	2.39	0.54
36:h:71:LEU:HD22	36:h:128:LEU:HD13	1.89	0.54
1:A:2481:U:O4	49:x:386:SER:OG	2.24	0.54
5:F:119:GLU:OE2	5:F:156:ARG:NH2	2.40	0.54
19:V:215:TRP:O	24:5:64:LYS:NZ	2.40	0.54
13:P:42:GLU:OE2	25:6:338:ARG:NH1	2.41	0.54
24:5:207:CYS:HB2	24:5:229:ILE:HD12	1.90	0.54
49:y:340:TYR:CE1	49:y:395:ILE:HD11	2.41	0.54
1:A:1137:A:HO2'	1:A:1138:U:P	2.30	0.54
42:p:82:CYS:O	42:p:98:LYS:N	2.40	0.54
1:A:1311:G:N7	5:F:170:ARG:NH2	2.55	0.54
1:A:2625:A:O2'	44:r:99:MET:O	2.25	0.54
38:j:87:ILE:HD11	41:o:53:TYR:HE2	1.73	0.54
27:8:150:LEU:HD23	27:8:158:TYR:CZ	2.43	0.54
31:c:60:ARG:NH1	31:c:64:PRO:O	2.41	0.54
1:A:1609:U:N3	1:A:1612:A:OP2	2.39	0.54
1:A:2194:A:OP2	6:H:118:ASN:ND2	2.41	0.54
49:y:235:CYS:SG	49:y:397:LEU:HD22	2.48	0.54
45:s:147:GLU:OE1	45:s:153:ARG:NH2	2.39	0.53
49:y:351:VAL:CG1	49:y:396:LEU:HD13	2.38	0.53
50:z:505:HIS:HB2	50:z:506:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:56:GLU:OE1	24:5:56:GLU:N	2.41	0.53
39:k:17:ARG:NH1	39:k:63:CYS:O	2.42	0.53
1:A:2302:U:HO2'	1:A:2303:A:P	2.31	0.53
1:A:2568:G:N2	1:A:2571:A:OP2	2.42	0.53
1:A:1324:A:O2'	11:M:34:LYS:N	2.39	0.53
19:V:45:VAL:HG23	21:Y:235:ILE:HG22	1.89	0.53
45:s:108:SER:O	45:s:206:ARG:NE	2.42	0.53
49:y:95:ASP:N	49:y:165:LEU:O	2.33	0.53
16:S:136:LYS:NZ	38:j:45:LEU:O	2.35	0.53
16:S:168:THR:HG22	16:S:169:GLU:N	2.24	0.53
45:s:132:ASP:O	45:s:135:ALA:N	2.41	0.53
37:i:61:GLY:O	37:i:66:PHE:N	2.41	0.53
49:y:128:ARG:NH2	49:y:183:GLN:OE1	2.42	0.53
11:M:145:ASP:O	11:M:148:GLN:NE2	2.42	0.53
14:Q:153:ASN:OD1	14:Q:154:THR:N	2.41	0.53
16:S:66:GLN:OE1	16:S:66:GLN:N	2.41	0.53
4:E:90:TRP:NE1	4:E:311:CYS:SG	2.81	0.53
35:g:99:GLU:O	35:g:107:MET:N	2.42	0.53
50:z:93:ALA:O	50:z:97:TRP:NE1	2.42	0.53
1:A:1675:U:O2	44:r:187:TYR:N	2.42	0.52
33:e:233:LYS:NZ	33:e:273:PHE:O	2.42	0.52
49:x:150:GLU:N	49:x:150:GLU:OE1	2.41	0.52
11:M:275:ASN:N	11:M:280:LYS:O	2.38	0.52
1:A:1604:A:O2'	1:A:1605:G:OP1	2.26	0.52
3:D:195:ASN:O	3:D:244:THR:OG1	2.27	0.52
1:A:2625:A:O2'	44:r:94:ARG:NH1	2.42	0.52
30:b:28:ARG:NH2	31:c:71:GLU:OE2	2.43	0.52
37:i:79:TRP:O	37:i:93:ARG:NE	2.39	0.52
25:6:191:ASN:O	25:6:320:GLN:N	2.34	0.52
32:d:137:PHE:CD2	32:d:212:VAL:HG11	2.45	0.52
43:q:61:PHE:O	43:q:65:GLY:N	2.37	0.52
14:Q:131:SER:OG	46:u:113:ARG:NH1	2.43	0.52
22:Z:71:ARG:NH2	22:Z:92:GLN:O	2.42	0.52
1:A:1296:A:O4'	1:A:1326:A:N6	2.43	0.51
1:A:1593:U:O2'	1:A:1594:U:O5'	2.28	0.51
1:A:1789:G:O2'	1:A:1791:U:OP2	2.28	0.51
38:j:59:MET:SD	38:j:59:MET:N	2.83	0.51
5:F:114:THR:O	5:F:156:ARG:NH1	2.38	0.51
25:6:152:ALA:CB	25:6:316:LEU:HD13	2.40	0.51
45:s:233:ASN:O	45:s:293:PHE:N	2.36	0.51
2:B:42:U:O4	13:P:120:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:282:LEU:HD22	35:g:38:PHE:HD2	1.75	0.51
42:p:120:ALA:HA	42:p:127:ILE:HD11	1.92	0.51
49:y:327:THR:HG22	49:y:327:THR:O	2.10	0.51
8:J:23:ILE:HD11	8:J:86:THR:HG22	1.92	0.51
1:A:1650:A:O2'	1:A:1651:A:O4'	2.24	0.51
25:6:49:GLU:OE1	25:6:49:GLU:N	2.44	0.51
26:7:259:ASP:OD1	26:7:260:VAL:N	2.43	0.51
1:A:1453:A:O2'	1:A:1699:A:N6	2.44	0.51
1:A:1620:A:H61	1:A:1630:A:C2'	2.24	0.51
1:A:1953:A:HO2'	1:A:1954:C:P	2.33	0.51
3:D:133:ASP:OD2	3:D:136:ARG:NH1	2.44	0.51
13:P:138:GLU:OE1	25:6:136:ARG:NH2	2.44	0.51
28:9:108:ASP:OD1	28:9:111:ASN:ND2	2.43	0.51
45:s:195:ASP:OD1	45:s:198:ARG:NH2	2.44	0.51
50:z:78:GLN:NE2	50:z:82:LEU:O	2.44	0.51
36:h:125:ARG:NH1	36:h:126:ASP:OD2	2.44	0.51
47:v:10:LEU:HD23	48:w:120:MET:HE3	1.93	0.51
49:y:237:LYS:NZ	49:y:239:LEU:HD21	2.25	0.51
49:x:289:ASN:ND2	49:x:385:ASP:O	2.44	0.50
1:A:2186:A:N6	1:A:2236:G:O6	2.44	0.50
26:7:77:VAL:HG23	26:7:77:VAL:O	2.12	0.50
33:e:158:LEU:N	33:e:251:VAL:O	2.43	0.50
26:7:147:LEU:HD22	26:7:178:TYR:HB3	1.93	0.50
26:7:293:ARG:O	26:7:295:GLN:NE2	2.42	0.50
45:s:240:GLN:OE1	45:s:347:ARG:NH1	2.45	0.50
1:A:1953:A:O2'	1:A:1954:C:P	2.69	0.50
21:Y:222:GLU:OE2	21:Y:226:ARG:NE	2.44	0.50
26:7:173:ALA:O	26:7:316:ARG:NH1	2.45	0.50
1:A:1626:A:O3'	40:l:112:ARG:NH2	2.44	0.50
19:V:93:THR:HG21	19:V:110:ALA:HB1	1.92	0.50
25:6:242:SER:OG	25:6:243:ASN:N	2.45	0.50
1:A:1777:U:O2	1:A:1803:G:N2	2.35	0.50
33:e:137:GLU:N	33:e:137:GLU:OE1	2.44	0.50
40:l:107:LEU:HD13	40:l:114:TYR:HA	1.94	0.50
6:H:76:VAL:HG12	20:X:100:ARG:HD2	1.94	0.50
25:6:179:VAL:HG21	25:6:185:ILE:HD12	1.92	0.50
1:A:1563:U:OP1	1:A:1685:U:O2'	2.28	0.50
49:x:152:VAL:HA	49:x:155:LEU:HD12	1.94	0.50
20:X:118:ILE:O	20:X:168:ARG:NH1	2.44	0.49
25:6:240:ILE:HD12	25:6:245:VAL:HA	1.94	0.49
1:A:2437:G:O2'	49:y:148:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:206:LEU:HD12	30:b:119:PHE:CE1	2.48	0.49
49:y:239:LEU:HD23	49:y:266:VAL:HB	1.94	0.49
1:A:1243:A:OP2	23:0:90:ARG:NH2	2.41	0.49
1:A:1629:G:N2	40:l:127:ASN:OD1	2.45	0.49
5:F:220:ASP:O	5:F:245:ALA:N	2.44	0.49
24:5:206:ASN:OD1	45:s:153:ARG:NH1	2.45	0.49
1:A:1503:A:O2'	1:A:1504:A:P	2.70	0.49
12:O:36:LEU:O	12:O:40:GLU:N	2.40	0.49
19:V:105:ARG:NH2	32:d:171:ASP:OD1	2.43	0.49
1:A:1185:C:OP1	11:M:195:ARG:NE	2.44	0.49
10:L:58:ILE:HG22	10:L:58:ILE:O	2.13	0.49
16:S:116:ASP:OD1	16:S:117:LEU:N	2.45	0.49
1:A:1742:G:O2'	1:A:2115:A:N6	2.44	0.49
3:D:159:LYS:N	3:D:162:ASP:OD2	2.44	0.49
13:P:121:ASN:OD1	13:P:122:VAL:N	2.46	0.49
31:c:59:ARG:NH1	31:c:181:SER:O	2.41	0.49
50:z:186:LEU:HD12	50:z:282:PHE:CE2	2.48	0.49
1:A:1606:G:H2'	1:A:1607:C:H5'	1.93	0.49
32:d:251:HIS:ND1	32:d:254:ASN:OD1	2.45	0.49
45:s:399:VAL:HG22	45:s:404:VAL:HG12	1.95	0.49
1:A:1538:G:H2'	1:A:1539:C:O4'	2.12	0.49
1:A:1742:G:OP1	23:0:84:ARG:NH2	2.46	0.49
24:5:225:THR:O	24:5:226:SER:OG	2.25	0.49
46:u:105:VAL:HG13	46:u:119:VAL:HG22	1.95	0.49
7:I:76:SER:O	7:I:80:ARG:N	2.42	0.49
25:6:161:LEU:HD13	25:6:271:LEU:HD11	1.95	0.49
11:M:287:GLU:N	11:M:287:GLU:OE1	2.43	0.48
29:a:34:THR:HG22	29:a:34:THR:O	2.13	0.48
42:p:65:ALA:O	42:p:66:LYS:C	2.55	0.48
50:z:428:GLN:OE1	50:z:430:GLN:N	2.39	0.48
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.95	0.48
5:F:113:ASN:OD1	5:F:157:GLY:N	2.46	0.48
25:6:62:GLU:OE2	25:6:66:ARG:NH2	2.46	0.48
25:6:70:TRP:O	25:6:72:ARG:NH2	2.46	0.48
1:A:1234:A:HO2'	1:A:1235:U:P	2.36	0.48
1:A:2613:A:O4'	1:A:2648:A:N6	2.47	0.48
49:y:208:LEU:HD12	49:y:404:LEU:HD12	1.95	0.48
1:A:1885:G:OP1	45:s:216:ARG:NE	2.36	0.48
9:K:21:LEU:N	9:K:58:VAL:O	2.42	0.48
36:h:124:VAL:O	36:h:127:VAL:N	2.47	0.48
49:y:191:LYS:HZ2	49:y:248:TRP:CD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:268:ASP:OD1	14:Q:268:ASP:O	2.31	0.48
25:6:181:GLU:N	25:6:181:GLU:OE1	2.46	0.48
25:6:184:LEU:HD23	25:6:184:LEU:H	1.77	0.48
10:L:140:ILE:HG22	10:L:140:ILE:O	2.12	0.48
44:r:73:CYS:N	52:r:301:FES:S2	2.87	0.48
24:5:251:HIS:O	24:5:371:LYS:NZ	2.45	0.48
44:r:76:ASN:O	44:r:80:LYS:NZ	2.42	0.48
49:x:101:ASP:OD1	49:x:102:ARG:N	2.46	0.48
26:7:188:GLU:OE1	26:7:188:GLU:N	2.46	0.47
1:A:2489:G:OP2	49:x:114:ARG:NH2	2.41	0.47
5:F:62:VAL:O	5:F:82:LEU:N	2.36	0.47
34:f:89:VAL:HG23	34:f:89:VAL:O	2.13	0.47
45:s:226:GLN:NE2	45:s:228:ASN:OD1	2.41	0.47
49:y:114:ARG:NE	49:y:118:GLU:OE2	2.47	0.47
5:F:65:TRP:N	36:h:115:ASN:OD1	2.44	0.47
14:Q:77:SER:OG	14:Q:79:GLU:OE1	2.28	0.47
17:T:151:ARG:O	17:T:159:GLY:N	2.46	0.47
1:A:1137:A:O2'	1:A:1138:U:P	2.73	0.47
1:A:2628:A:O4'	44:r:103:ARG:NH2	2.40	0.47
11:M:96:SER:O	11:M:100:LEU:N	2.45	0.47
26:7:235:ASP:OD1	26:7:236:PHE:N	2.47	0.47
44:r:73:CYS:CA	52:r:301:FES:S2	3.02	0.47
49:x:328:ARG:O	49:x:332:LEU:HD21	2.14	0.47
49:y:288:ASP:OD2	49:y:375:ARG:NH1	2.47	0.47
1:A:1220:A:N6	1:A:1221:A:N1	2.62	0.47
11:M:222:LEU:O	42:p:49:TYR:OH	2.32	0.47
20:X:178:PRO:O	20:X:179:GLU:HG2	2.15	0.47
34:f:112:LEU:HD13	34:f:115:ARG:NH2	2.29	0.47
46:u:157:ASP:OD1	46:u:158:ALA:N	2.48	0.47
49:y:351:VAL:HG13	49:y:396:LEU:HD13	1.97	0.47
35:g:42:VAL:HG12	35:g:42:VAL:O	2.14	0.47
36:h:125:ARG:NH1	36:h:126:ASP:CG	2.72	0.47
49:x:213:ILE:HD11	49:x:278:LEU:HD11	1.95	0.47
49:y:378:ILE:HD13	49:y:395:ILE:HG21	1.95	0.47
1:A:1225:G:N1	1:A:1228:A:OP2	2.47	0.47
1:A:1671:U:OP1	44:r:165:LYS:NZ	2.43	0.47
50:z:481:TYR:O	50:z:485:ALA:N	2.43	0.47
1:A:1232:U:H1'	1:A:1233:A:OP2	2.15	0.47
1:A:1602:G:N2	8:J:143:SER:OG	2.44	0.47
13:P:41:ASN:OD1	25:6:293:LEU:N	2.42	0.47
31:c:209:GLU:OE1	31:c:209:GLU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:202:THR:OG1	49:x:203:PRO:HD3	2.15	0.47
4:E:90:TRP:NE1	4:E:311:CYS:HG	2.13	0.47
35:g:85:PHE:N	35:g:114:GLU:O	2.40	0.47
37:i:57:TYR:OH	43:q:28:PRO:O	2.28	0.47
37:i:60:ILE:O	37:i:64:GLY:N	2.47	0.47
1:A:1146:A:O4'	37:i:123:ARG:NH1	2.47	0.47
16:S:96:TYR:O	31:c:312:ARG:NH2	2.43	0.47
24:5:385:HIS:O	24:5:404:VAL:N	2.45	0.47
44:r:93:ILE:HD11	44:r:119:VAL:HG21	1.96	0.47
50:z:207:LEU:O	50:z:284:VAL:N	2.45	0.47
18:U:80:ARG:NH1	18:U:84:ASN:O	2.48	0.46
19:V:206:GLU:OE1	19:V:207:THR:N	2.48	0.46
25:6:247:GLU:OE1	25:6:247:GLU:N	2.47	0.46
45:s:357:ASP:OD1	45:s:360:TYR:N	2.46	0.46
49:x:135:LEU:HD12	49:x:156:PRO:HG3	1.97	0.46
15:R:85:ALA:O	15:R:89:ASN:ND2	2.48	0.46
25:6:60:ARG:O	25:6:60:ARG:NH1	2.49	0.46
27:8:139:MET:HE1	33:e:275:LEU:CD2	2.45	0.46
29:a:71:THR:O	31:c:256:ARG:NH2	2.48	0.46
39:k:80:HIS:C	39:k:81:LEU:HD22	2.40	0.46
45:s:298:ASP:OD1	45:s:299:ARG:N	2.49	0.46
1:A:1769:C:OP1	45:s:215:HIS:NE2	2.46	0.46
2:B:20:A:HO2'	2:B:21:A:P	2.37	0.46
11:M:236:ALA:O	11:M:240:GLY:N	2.47	0.46
21:Y:159:GLN:OE1	28:9:118:GLU:N	2.48	0.46
1:A:1175:G:O2'	1:A:1176:A:OP2	2.31	0.46
2:B:15:A:H4'	2:B:17:A:H62	1.81	0.46
9:K:26:GLN:NE2	9:K:147:GLN:OE1	2.48	0.46
32:d:137:PHE:CE2	32:d:212:VAL:HG11	2.51	0.46
17:T:60:GLU:OE2	17:T:63:ARG:NH2	2.48	0.46
6:H:102:ILE:O	6:H:102:ILE:HG22	2.16	0.46
13:P:61:VAL:HG12	13:P:61:VAL:O	2.16	0.46
19:V:45:VAL:HG22	21:Y:235:ILE:HG22	1.96	0.46
26:7:42:ASN:ND2	26:7:256:ASP:OD1	2.48	0.46
32:d:111:ARG:O	32:d:115:ASN:N	2.48	0.46
49:y:212:LEU:HD13	49:y:397:LEU:HD21	1.97	0.46
1:A:1642:C:H2'	1:A:1643:U:O4'	2.15	0.46
16:S:103:VAL:HG11	16:S:134:LEU:HD13	1.96	0.46
29:a:69:GLU:O	30:b:141:HIS:N	2.40	0.46
49:x:398:PHE:CD1	49:y:395:ILE:HD12	2.51	0.46
1:A:1486:A:O2'	1:A:1503:A:N1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:140:GLY:HA2	42:p:188:LEU:HD11	1.97	0.46
14:Q:123:ASP:HB2	14:Q:126:ALA:HB3	1.97	0.46
20:X:110:PHE:HB3	20:X:112:ARG:CZ	2.45	0.46
35:g:44:GLU:OE1	35:g:44:GLU:N	2.49	0.46
47:v:10:LEU:HD22	48:w:132:ASP:HB2	1.98	0.46
1:A:2109:A:N3	12:O:116:GLN:NE2	2.64	0.46
24:5:114:LEU:N	24:5:264:ASP:OD2	2.45	0.46
32:d:226:ASP:OD1	32:d:232:MET:HE2	2.16	0.46
37:i:34:VAL:HG12	37:i:35:ARG:N	2.31	0.46
1:A:1134:A:H1'	1:A:1135:U:H5'	1.98	0.45
1:A:1135:U:OP2	21:Y:198:ARG:NH1	2.49	0.45
4:E:54:SER:O	4:E:58:LEU:N	2.40	0.45
25:6:363:LEU:O	25:6:367:ASP:N	2.46	0.45
47:v:58:GLY:O	47:v:62:LEU:N	2.46	0.45
1:A:1185:C:OP2	43:q:55:ARG:NH2	2.50	0.45
1:A:1233:A:H2'	1:A:1234:A:O4'	2.16	0.45
1:A:1248:C:OP1	29:a:129:HIS:NE2	2.48	0.45
3:D:111:ARG:NH2	3:D:180:GLY:O	2.42	0.45
13:P:130:ARG:HG3	13:P:164:ALA:HB1	1.98	0.45
14:Q:165:GLU:O	14:Q:171:ILE:HD12	2.16	0.45
21:Y:65:GLY:N	21:Y:68:GLU:OE2	2.50	0.45
27:8:117:LEU:HD13	33:e:64:LEU:HD13	1.97	0.45
27:8:150:LEU:HD22	33:e:230:PHE:CE2	2.51	0.45
45:s:186:ASN:ND2	45:s:419:LEU:O	2.41	0.45
1:A:1659:C:O2'	1:A:1660:A:OP2	2.32	0.45
1:A:2486:A:H2'	1:A:2487:A:O4'	2.17	0.45
14:Q:245:PHE:O	14:Q:249:LEU:N	2.48	0.45
31:c:87:LEU:O	31:c:90:THR:OG1	2.25	0.45
32:d:151:CYS:O	32:d:155:SER:N	2.49	0.45
45:s:303:GLU:OE1	45:s:303:GLU:N	2.47	0.45
49:y:194:PRO:HB3	49:y:264:PRO:HA	1.98	0.45
50:z:335:GLU:N	50:z:335:GLU:OE1	2.48	0.45
1:A:1260:A:OP1	29:a:134:LYS:NZ	2.46	0.45
16:S:133:ARG:N	38:j:49:SER:O	2.41	0.45
18:U:38:ASP:OD1	18:U:39:THR:N	2.50	0.45
9:K:140:ASN:OD1	31:c:264:THR:OG1	2.23	0.45
1:A:1302:U:OP1	41:o:86:ARG:NH2	2.48	0.45
3:D:125:GLU:HB3	3:D:143:VAL:HG22	1.98	0.45
4:E:334:ASP:OD2	4:E:336:SER:OG	2.31	0.45
8:J:56:LYS:HZ1	8:J:80:LEU:HB3	1.81	0.45
10:L:38:VAL:HG22	10:L:39:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:188:TYR:OH	42:p:191:LYS:N	2.49	0.45
1:A:1561:U:O2'	1:A:1574:A:N3	2.41	0.45
1:A:2676:A:H4'	1:A:2676:A:OP2	2.17	0.45
6:H:104:VAL:HG22	6:H:105:ARG:N	2.32	0.45
7:I:116:LEU:O	7:I:120:LYS:N	2.50	0.45
7:I:192:ARG:NH2	39:k:53:ALA:O	2.43	0.45
1:A:1234:A:O2'	1:A:1235:U:P	2.74	0.45
1:A:1644:C:H2'	1:A:1645:A:O4'	2.17	0.45
1:A:2361:C:N3	1:A:2362:A:N6	2.64	0.45
25:6:171:VAL:HG21	25:6:214:TRP:CH2	2.52	0.45
49:y:217:LEU:N	49:y:244:CYS:SG	2.86	0.45
6:H:120:LEU:O	6:H:125:LEU:N	2.48	0.45
32:d:186:VAL:HG12	32:d:187:GLU:N	2.32	0.45
39:k:18:VAL:HG13	39:k:64:VAL:HG22	1.98	0.45
40:l:74:ILE:HG22	40:l:74:ILE:O	2.16	0.45
49:x:217:LEU:C	49:x:245:VAL:HG23	2.41	0.45
26:7:151:ILE:HD13	26:7:180:VAL:HG21	1.98	0.45
32:d:196:HIS:N	32:d:213:THR:OG1	2.50	0.45
48:w:112:SER:O	48:w:116:VAL:HG23	2.17	0.45
49:x:282:THR:O	49:x:284:VAL:HG23	2.17	0.45
1:A:1660:A:N3	1:A:1660:A:H2'	2.32	0.44
1:A:2168:U:O2	1:A:2168:U:H2'	2.17	0.44
1:A:2467:A:OP2	49:x:103:ARG:NE	2.50	0.44
1:A:2507:U:HO2'	1:A:2508:C:P	2.34	0.44
5:F:52:GLU:OE1	5:F:52:GLU:N	2.47	0.44
12:O:86:ILE:HB	12:O:87:PRO:HD3	1.99	0.44
42:p:102:ARG:NE	42:p:132:GLU:OE2	2.49	0.44
2:B:20:A:O2'	2:B:21:A:P	2.75	0.44
31:c:294:GLU:OE2	31:c:298:ARG:NE	2.50	0.44
32:d:121:ALA:O	32:d:125:ILE:HD12	2.17	0.44
1:A:1906:A:N3	10:L:33:GLN:NE2	2.59	0.44
18:U:61:TYR:O	21:Y:65:GLY:N	2.50	0.44
30:b:37:ALA:O	30:b:44:ARG:NH1	2.42	0.44
49:y:335:LEU:HD11	49:y:368:ALA:HB3	1.98	0.44
1:A:1677:A:OP1	15:R:82:LYS:NZ	2.44	0.44
2:B:20:A:O2'	2:B:21:A:OP1	2.35	0.44
16:S:165:ILE:HD11	16:S:198:ARG:HB3	2.00	0.44
25:6:157:LEU:HD11	25:6:318:PHE:CG	2.52	0.44
31:c:86:ASP:N	31:c:86:ASP:OD1	2.48	0.44
33:e:158:LEU:HD11	33:e:262:LEU:HD11	1.99	0.44
1:A:1101:C:O4'	19:V:42:ARG:NH2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:185:ILE:O	24:5:189:LYS:N	2.45	0.44
1:A:1573:U:OP2	38:j:22:ALA:N	2.51	0.44
8:J:103:HIS:O	8:J:104:THR:OG1	2.32	0.44
24:5:174:GLU:N	24:5:298:ASN:OD1	2.44	0.44
26:7:67:VAL:O	26:7:67:VAL:HG22	2.18	0.44
49:x:352:VAL:HG11	49:x:364:SER:HB2	2.00	0.44
49:y:203:PRO:O	49:y:206:HIS:N	2.50	0.44
1:A:1311:G:N2	37:i:66:PHE:O	2.51	0.44
1:A:2487:A:H5'	49:x:220:PRO:HG3	1.99	0.44
2:B:34:A:OP1	34:f:107:GLN:NE2	2.51	0.44
3:D:113:ARG:O	3:D:148:ARG:NH2	2.49	0.44
17:T:85:ALA:O	17:T:139:SER:OG	2.35	0.44
32:d:226:ASP:N	32:d:230:ARG:O	2.40	0.44
1:A:1537:A:O2'	1:A:1538:G:O4'	2.34	0.44
5:F:226:MET:SD	5:F:242:LEU:HD21	2.57	0.44
8:J:33:PRO:N	8:J:34:PRO:HD2	2.33	0.44
9:K:171:THR:HG23	9:K:171:THR:O	2.18	0.44
11:M:38:ARG:CG	11:M:39:PRO:HD2	2.48	0.44
26:7:287:GLN:N	26:7:287:GLN:OE1	2.51	0.44
17:T:124:ARG:NH1	17:T:125:ASP:OD1	2.51	0.43
33:e:168:VAL:HG12	33:e:169:TRP:N	2.33	0.43
49:y:237:LYS:HZ3	49:y:239:LEU:HD21	1.82	0.43
1:A:1224:U:OP1	19:V:41:ARG:NE	2.42	0.43
1:A:1585:C:O2'	1:A:1586:A:O5'	2.36	0.43
1:A:2129:G:O2'	1:A:2132:G:O6	2.31	0.43
2:B:20:A:C2'	2:B:21:A:O5'	2.66	0.43
6:H:88:LYS:HG2	6:H:114:SER:H	1.83	0.43
7:I:159:VAL:HG23	7:I:159:VAL:O	2.18	0.43
19:V:122:LEU:HD21	19:V:154:ILE:HG21	1.99	0.43
22:Z:51:GLU:OE1	22:Z:51:GLU:N	2.50	0.43
31:c:314:TRP:HD1	31:c:316:TYR:CE1	2.36	0.43
32:d:245:TYR:O	32:d:265:ILE:N	2.45	0.43
45:s:273:GLU:OE1	45:s:273:GLU:N	2.47	0.43
1:A:1603:U:O2'	1:A:1605:G:O5'	2.30	0.43
7:I:83:ARG:NH2	7:I:130:VAL:O	2.46	0.43
30:b:12:THR:HG22	30:b:13:SER:N	2.32	0.43
39:k:13:VAL:O	39:k:13:VAL:HG13	2.18	0.43
1:A:2302:U:O2'	1:A:2303:A:P	2.74	0.43
5:F:51:CYS:SG	5:F:83:HIS:N	2.91	0.43
14:Q:151:LEU:H	14:Q:151:LEU:HD23	1.82	0.43
25:6:219:ILE:HG23	25:6:231:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:141:ARG:NH2	30:b:121:THR:OG1	2.43	0.43
33:e:73:GLN:NE2	34:f:98:ASP:OD1	2.50	0.43
5:F:220:ASP:OD1	5:F:221:LEU:N	2.50	0.43
7:I:132:LYS:NZ	7:I:147:PHE:O	2.50	0.43
21:Y:153:ASP:OD1	21:Y:156:ARG:NH1	2.46	0.43
25:6:175:VAL:HG22	25:6:204:VAL:HG13	2.00	0.43
49:y:201:GLU:O	49:y:204:LEU:N	2.51	0.43
19:V:103:ASP:OD1	19:V:104:HIS:N	2.51	0.43
39:k:27:VAL:HG21	39:k:79:ALA:HA	2.00	0.43
7:I:83:ARG:NH1	7:I:130:VAL:HG12	2.33	0.43
8:J:119:GLU:OE2	40:l:83:LEU:HD21	2.18	0.43
9:K:110:GLY:O	9:K:114:LYS:NZ	2.49	0.43
22:Z:136:SER:OG	22:Z:147:VAL:O	2.35	0.43
34:f:160:GLY:O	34:f:161:LEU:HD22	2.19	0.43
49:y:222:ASN:ND2	49:y:356:GLU:OE2	2.51	0.43
1:A:1894:C:H1'	1:A:1895:A:OP2	2.18	0.43
1:A:2342:U:O2'	1:A:2343:A:P	2.76	0.43
49:x:217:LEU:O	49:x:245:VAL:HG23	2.18	0.43
49:y:392:ALA:O	49:y:396:LEU:HD12	2.18	0.43
1:A:1805:U:O4	18:U:35:GLN:NE2	2.52	0.43
1:A:2187:C:N4	1:A:2188:U:O4	2.51	0.43
5:F:191:ASP:OD1	5:F:191:ASP:N	2.51	0.43
6:H:118:ASN:OD1	6:H:119:LYS:N	2.51	0.43
16:S:112:VAL:HG13	16:S:199:ILE:HG13	2.01	0.43
25:6:179:VAL:HG21	25:6:185:ILE:CD1	2.48	0.43
25:6:351:HIS:ND1	42:p:138:GLU:OE1	2.52	0.43
35:g:106:GLN:O	35:g:151:GLY:N	2.40	0.43
6:H:73:ARG:O	6:H:76:VAL:HG22	2.19	0.43
7:I:100:GLN:O	7:I:178:LEU:HD12	2.18	0.43
12:O:88:LYS:O	12:O:92:VAL:N	2.51	0.43
25:6:177:TYR:N	25:6:185:ILE:O	2.52	0.43
31:c:183:GLU:OE1	31:c:183:GLU:N	2.51	0.43
34:f:184:SER:OG	34:f:186:ARG:NE	2.52	0.43
35:g:154:ASP:OD1	35:g:154:ASP:N	2.50	0.43
49:x:391:MET:HG3	49:y:225:THR:HG22	2.01	0.43
50:z:505:HIS:O	50:z:507:TRP:N	2.52	0.43
11:M:207:GLU:OE1	43:q:102:SER:OG	2.37	0.42
29:a:50:LEU:HD23	29:a:57:ILE:HG12	2.01	0.42
49:y:202:THR:HB	49:y:203:PRO:HD3	1.99	0.42
1:A:1101:C:OP1	37:i:35:ARG:NH2	2.52	0.42
1:A:1231:C:H3'	1:A:1232:U:C5'	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2182:U:OP2	1:A:2240:G:N1	2.51	0.42
1:A:2637:A:H3'	1:A:2638:U:H5"	2.01	0.42
30:b:47:VAL:O	30:b:51:VAL:HG12	2.18	0.42
45:s:131:LEU:HD13	45:s:136:LEU:CD1	2.49	0.42
46:u:108:VAL:N	46:u:116:ASP:O	2.51	0.42
1:A:1094:A:HO2'	1:A:1095:C:H6	1.66	0.42
1:A:1684:C:H1'	1:A:1685:U:P	2.59	0.42
24:5:207:CYS:CB	24:5:229:ILE:HD12	2.49	0.42
45:s:103:ASP:OD1	45:s:103:ASP:N	2.52	0.42
50:z:338:ASN:O	50:z:342:SER:N	2.51	0.42
1:A:2285:U:N3	1:A:2332:U:OP1	2.52	0.42
3:D:248:VAL:HG12	3:D:249:SER:N	2.34	0.42
15:R:104:ASP:CG	17:T:206:LEU:HD22	2.44	0.42
18:U:22:THR:HG22	18:U:24:PHE:H	1.83	0.42
49:y:380:VAL:HG23	49:y:380:VAL:O	2.19	0.42
1:A:1256:G:O6	30:b:4:ARG:NH1	2.53	0.42
2:B:23:G:OP2	13:P:89:HIS:ND1	2.53	0.42
13:P:117:TYR:OH	25:6:120:GLU:HG2	2.19	0.42
18:U:19:VAL:O	18:U:19:VAL:HG13	2.18	0.42
20:X:124:THR:O	20:X:124:THR:HG23	2.20	0.42
25:6:125:LEU:O	25:6:126:ARG:HG2	2.19	0.42
49:y:125:LEU:HD12	49:y:189:PHE:CE1	2.55	0.42
7:I:105:SER:OG	7:I:108:ASP:OD2	2.37	0.42
12:O:94:ALA:HB3	12:O:95:PRO:HD3	2.00	0.42
14:Q:237:ASN:OD1	14:Q:238:PHE:N	2.52	0.42
23:0:111:GLU:OE1	23:0:111:GLU:N	2.46	0.42
32:d:189:LEU:HD12	32:d:217:HIS:NE2	2.35	0.42
32:d:197:VAL:HG12	32:d:212:VAL:HG13	2.01	0.42
1:A:1558:A:H2'	1:A:1558:A:N3	2.34	0.42
7:I:132:LYS:HB2	7:I:133:PRO:HD3	2.01	0.42
10:L:55:PRO:HB2	10:L:75:LEU:HD11	2.02	0.42
14:Q:246:ASP:OD1	14:Q:247:LEU:N	2.52	0.42
32:d:169:PHE:N	32:d:170:PRO:HD2	2.35	0.42
33:e:181:THR:HG23	33:e:184:GLY:H	1.85	0.42
34:f:95:THR:O	34:f:95:THR:HG23	2.20	0.42
1:A:2450:C:O2'	1:A:2493:A:N3	2.46	0.42
12:O:84:ASP:N	12:O:84:ASP:OD1	2.53	0.42
14:Q:225:LYS:HB2	14:Q:226:PRO:CD	2.50	0.42
33:e:159:VAL:HA	33:e:250:HIS:HA	2.00	0.42
1:A:1539:C:H2'	1:A:1540:U:H5'	2.02	0.42
25:6:334:LEU:HD23	25:6:334:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:p:72:ILE:HG21	42:p:77:LEU:HD11	2.01	0.42
44:r:167:HIS:O	44:r:171:LYS:N	2.52	0.42
45:s:67:GLN:NE2	45:s:376:GLN:OE1	2.49	0.42
1:A:1888:A:N7	1:A:1889:A:N6	2.65	0.42
1:A:2485:C:O2	1:A:2485:C:O4'	2.37	0.42
11:M:38:ARG:HG2	11:M:39:PRO:HD2	2.02	0.42
13:P:133:ALA:O	13:P:137:LEU:N	2.41	0.42
45:s:131:LEU:HD11	45:s:133:LEU:HD23	2.02	0.42
1:A:2235:A:OP1	20:X:93:ASN:ND2	2.54	0.41
20:X:79:LEU:CD1	20:X:153:LEU:HD11	2.50	0.41
31:c:31:VAL:O	31:c:31:VAL:HG13	2.20	0.41
33:e:171:LEU:HG	33:e:172:PRO:HD2	2.01	0.41
42:p:82:CYS:N	42:p:98:LYS:O	2.48	0.41
46:u:194:ASP:OD1	46:u:194:ASP:N	2.52	0.41
48:w:132:ASP:HA	48:w:135:ALA:HB3	2.02	0.41
1:A:1629:G:H3'	1:A:1629:G:OP1	2.20	0.41
1:A:2436:U:H2'	1:A:2437:G:O4'	2.20	0.41
23:O:178:ILE:HG22	23:O:179:LYS:N	2.36	0.41
29:a:96:VAL:O	29:a:96:VAL:HG13	2.19	0.41
46:u:144:LYS:O	46:u:145:CYS:SG	2.74	0.41
50:z:159:ILE:N	50:z:160:PRO:HD2	2.35	0.41
1:A:1142:A:H2'	1:A:1143:A:O4'	2.19	0.41
1:A:2651:U:O2'	4:E:269:TYR:OH	2.36	0.41
13:P:98:ASN:ND2	13:P:100:GLN:OE1	2.53	0.41
37:i:80:LEU:HD12	37:i:80:LEU:O	2.20	0.41
39:k:14:LYS:O	39:k:50:SER:N	2.52	0.41
49:y:128:ARG:HE	49:y:183:GLN:HE22	1.68	0.41
1:A:2617:A:O2'	1:A:2618:A:P	2.78	0.41
12:O:77:ASP:OD1	12:O:83:LYS:NZ	2.45	0.41
45:s:195:ASP:OD2	45:s:236:ARG:NE	2.44	0.41
49:x:287:ALA:O	49:x:317:HIS:NE2	2.42	0.41
49:y:252:VAL:HG12	49:y:260:HIS:CE1	2.56	0.41
1:A:2366:U:O2'	1:A:2368:C:OP1	2.26	0.41
6:H:88:LYS:HG2	6:H:114:SER:HB2	2.03	0.41
33:e:51:LEU:HD23	33:e:252:TRP:CH2	2.55	0.41
39:k:61:GLU:N	39:k:62:PRO:CD	2.84	0.41
40:l:105:GLU:OE1	40:l:105:GLU:N	2.45	0.41
1:A:2168:U:C2'	50:z:99:HIS:O	2.67	0.41
2:B:41:U:OP2	13:P:122:VAL:HG23	2.20	0.41
6:H:91:LEU:N	6:H:111:VAL:O	2.45	0.41
12:O:144:THR:OG1	12:O:147:ASN:OD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:170:TRP:O	28:9:75:ARG:NE	2.53	0.41
24:5:33:TRP:O	24:5:39:ARG:NH2	2.54	0.41
45:s:41:VAL:HG22	45:s:41:VAL:O	2.20	0.41
45:s:90:LYS:NZ	45:s:274:ASN:OD1	2.48	0.41
50:z:457:ALA:HB1	50:z:461:LEU:HD13	2.01	0.41
12:O:41:ARG:NE	12:O:125:GLU:OE1	2.53	0.41
49:x:398:PHE:CG	49:y:395:ILE:HB	2.56	0.41
1:A:1165:A:OP2	1:A:1166:A:O2'	2.34	0.41
1:A:1306:U:O2'	1:A:1318:A:N1	2.51	0.41
6:H:51:VAL:O	20:X:42:HIS:ND1	2.52	0.41
6:H:89:ASP:O	6:H:113:LYS:N	2.52	0.41
9:K:156:ASP:OD1	9:K:157:GLU:N	2.54	0.41
35:g:129:SER:OG	35:g:130:PRO:HD3	2.21	0.41
47:v:66:LEU:HG	47:v:69:LEU:HD12	2.03	0.41
7:I:82:LEU:HB3	7:I:130:VAL:HG11	2.02	0.41
11:M:21:VAL:HG12	11:M:22:SER:N	2.36	0.41
14:Q:225:LYS:HB2	14:Q:226:PRO:HD2	2.02	0.41
20:X:111:THR:HG23	20:X:111:THR:O	2.20	0.41
23:0:109:CYS:O	23:0:113:GLY:N	2.51	0.41
25:6:237:LEU:HD13	25:6:240:ILE:HD11	2.02	0.41
43:q:44:ASN:O	43:q:47:THR:HG22	2.21	0.41
49:x:256:GLY:C	49:x:257:MET:HG3	2.46	0.41
49:y:173:ILE:HG22	49:y:182:PRO:HB3	2.03	0.41
50:z:186:LEU:C	50:z:186:LEU:HD23	2.45	0.41
1:A:1294:A:N6	1:A:1329:C:OP1	2.54	0.41
1:A:2168:U:C5	50:z:97:TRP:CG	3.08	0.41
11:M:282:LEU:HD22	35:g:38:PHE:CD2	2.56	0.41
49:y:226:ILE:HD11	49:y:389:SER:CB	2.51	0.41
22:Z:58:GLY:O	41:o:47:TYR:OH	2.38	0.40
25:6:283:GLU:OE1	25:6:283:GLU:N	2.50	0.40
33:e:171:LEU:O	33:e:172:PRO:C	2.62	0.40
49:y:141:PRO:HA	49:y:189:PHE:HA	2.03	0.40
49:y:141:PRO:HB2	49:y:163:VAL:CG1	2.50	0.40
5:F:279:ARG:O	5:F:280:TYR:C	2.64	0.40
7:I:130:VAL:O	7:I:130:VAL:HG12	2.20	0.40
21:Y:85:ALA:N	28:9:72:VAL:O	2.54	0.40
25:6:371:ASP:N	25:6:371:ASP:OD1	2.53	0.40
31:c:144:GLU:HB2	31:c:314:TRP:HZ3	1.85	0.40
45:s:129:PRO:HB2	45:s:185:LEU:HD23	2.03	0.40
49:x:128:ARG:NH1	49:x:129:ARG:HB2	2.35	0.40
1:A:1503:A:O2'	1:A:1504:A:OP2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1603:U:O2'	1:A:1605:G:P	2.79	0.40
1:A:1609:U:C6	1:A:1609:U:OP2	2.74	0.40
3:D:217:LEU:HA	3:D:227:ILE:HD13	2.04	0.40
9:K:7:ALA:HB3	9:K:8:PRO:HD3	2.02	0.40
20:X:111:THR:C	20:X:112:ARG:HD2	2.47	0.40
20:X:173:ASP:O	20:X:188:TYR:OH	2.37	0.40
24:5:167:THR:O	24:5:167:THR:HG22	2.21	0.40
25:6:290:CYS:SG	25:6:296:ARG:NE	2.91	0.40
9:K:69:GLY:N	44:r:150:TYR:O	2.42	0.40
10:L:33:GLN:H	10:L:36:THR:HG21	1.87	0.40
27:8:114:ARG:O	27:8:118:LEU:HD13	2.21	0.40
42:p:172:ASP:OD1	42:p:173:ALA:N	2.54	0.40
13:P:156:ASP:OD1	13:P:156:ASP:N	2.55	0.40
32:d:160:LEU:HD22	32:d:169:PHE:CD2	2.56	0.40
49:y:386:SER:O	49:y:387:LEU:C	2.64	0.40
50:z:61:LEU:H	50:z:61:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	168/246 (68%)	164 (98%)	4 (2%)	0	100	100
4	E	260/348 (75%)	253 (97%)	7 (3%)	0	100	100
5	F	210/294 (71%)	205 (98%)	5 (2%)	0	100	100
6	H	93/268 (35%)	89 (96%)	4 (4%)	0	100	100
7	I	150/262 (57%)	142 (95%)	8 (5%)	0	100	100
8	J	140/192 (73%)	136 (97%)	4 (3%)	0	100	100
9	K	169/178 (95%)	168 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
11	M	245/295 (83%)	239 (98%)	6 (2%)	0	100	100
12	O	147/176 (84%)	144 (98%)	3 (2%)	0	100	100
13	P	139/180 (77%)	138 (99%)	1 (1%)	0	100	100
14	Q	215/292 (74%)	211 (98%)	4 (2%)	0	100	100
15	R	129/149 (87%)	129 (100%)	0	0	100	100
16	S	157/209 (75%)	152 (97%)	5 (3%)	0	100	100
17	T	164/206 (80%)	164 (100%)	0	0	100	100
18	U	121/146 (83%)	121 (100%)	0	0	100	100
19	V	196/216 (91%)	196 (100%)	0	0	100	100
20	X	240/294 (82%)	238 (99%)	2 (1%)	0	100	100
21	Y	174/252 (69%)	174 (100%)	0	0	100	100
22	Z	113/160 (71%)	112 (99%)	1 (1%)	0	100	100
23	0	106/187 (57%)	106 (100%)	0	0	100	100
24	5	383/423 (90%)	379 (99%)	4 (1%)	0	100	100
25	6	289/380 (76%)	278 (96%)	11 (4%)	0	100	100
26	7	290/336 (86%)	286 (99%)	4 (1%)	0	100	100
27	8	57/206 (28%)	56 (98%)	1 (2%)	0	100	100
28	9	94/135 (70%)	93 (99%)	1 (1%)	0	100	100
29	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
30	b	146/159 (92%)	141 (97%)	5 (3%)	0	100	100
31	c	275/308 (89%)	275 (100%)	0	0	100	100
32	d	198/306 (65%)	195 (98%)	3 (2%)	0	100	100
33	e	171/283 (60%)	160 (94%)	11 (6%)	0	100	100
34	f	85/211 (40%)	81 (95%)	4 (5%)	0	100	100
35	g	130/166 (78%)	129 (99%)	1 (1%)	0	100	100
36	h	108/159 (68%)	106 (98%)	2 (2%)	0	100	100
37	i	91/128 (71%)	91 (100%)	0	0	100	100
38	j	83/121 (69%)	82 (99%)	1 (1%)	0	100	100
39	k	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
40	l	74/135 (55%)	72 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	o	76/102 (74%)	76 (100%)	0	0	100	100
42	p	124/206 (60%)	122 (98%)	2 (2%)	0	100	100
43	q	95/222 (43%)	95 (100%)	0	0	100	100
44	r	152/196 (78%)	146 (96%)	6 (4%)	0	100	100
45	s	373/442 (84%)	365 (98%)	8 (2%)	0	100	100
46	u	123/228 (54%)	121 (98%)	2 (2%)	0	100	100
47	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
48	w	77/156 (49%)	75 (97%)	2 (3%)	0	100	100
49	x	291/418 (70%)	285 (98%)	6 (2%)	0	100	100
49	y	287/418 (69%)	282 (98%)	5 (2%)	0	100	100
50	z	452/540 (84%)	441 (98%)	11 (2%)	0	100	100
All	All	8215/11409 (72%)	8055 (98%)	160 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	143/197 (73%)	143 (100%)	0	100	100
4	E	237/298 (80%)	237 (100%)	0	100	100
5	F	190/250 (76%)	190 (100%)	0	100	100
6	H	86/231 (37%)	86 (100%)	0	100	100
7	I	143/230 (62%)	143 (100%)	0	100	100
8	J	116/152 (76%)	116 (100%)	0	100	100
9	K	151/158 (96%)	151 (100%)	0	100	100
10	L	99/122 (81%)	99 (100%)	0	100	100
11	M	219/252 (87%)	219 (100%)	0	100	100
12	O	129/152 (85%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	P	123/157 (78%)	123 (100%)	0	100	100
14	Q	197/258 (76%)	197 (100%)	0	100	100
15	R	110/128 (86%)	110 (100%)	0	100	100
16	S	145/180 (81%)	145 (100%)	0	100	100
17	T	147/180 (82%)	147 (100%)	0	100	100
18	U	112/133 (84%)	112 (100%)	0	100	100
19	V	176/190 (93%)	176 (100%)	0	100	100
20	X	219/265 (83%)	219 (100%)	0	100	100
21	Y	162/228 (71%)	162 (100%)	0	100	100
22	Z	108/146 (74%)	108 (100%)	0	100	100
23	0	97/170 (57%)	97 (100%)	0	100	100
24	5	349/372 (94%)	349 (100%)	0	100	100
25	6	264/335 (79%)	264 (100%)	0	100	100
26	7	269/301 (89%)	269 (100%)	0	100	100
27	8	51/182 (28%)	51 (100%)	0	100	100
28	9	83/114 (73%)	83 (100%)	0	100	100
29	a	97/129 (75%)	97 (100%)	0	100	100
30	b	130/138 (94%)	130 (100%)	0	100	100
31	c	243/266 (91%)	243 (100%)	0	100	100
32	d	182/272 (67%)	182 (100%)	0	100	100
33	e	152/238 (64%)	152 (100%)	0	100	100
34	f	80/185 (43%)	80 (100%)	0	100	100
35	g	122/148 (82%)	122 (100%)	0	100	100
36	h	100/143 (70%)	100 (100%)	0	100	100
37	i	84/111 (76%)	84 (100%)	0	100	100
38	j	68/99 (69%)	68 (100%)	0	100	100
39	k	72/95 (76%)	72 (100%)	0	100	100
40	l	70/112 (62%)	70 (100%)	0	100	100
41	o	65/85 (76%)	65 (100%)	0	100	100
42	p	118/177 (67%)	118 (100%)	0	100	100
43	q	84/187 (45%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	r	141/168 (84%)	141 (100%)	0	100	100
45	s	329/378 (87%)	329 (100%)	0	100	100
46	u	115/197 (58%)	115 (100%)	0	100	100
47	v	60/61 (98%)	60 (100%)	0	100	100
48	w	73/135 (54%)	73 (100%)	0	100	100
49	x	251/358 (70%)	251 (100%)	0	100	100
49	y	249/358 (70%)	249 (100%)	0	100	100
50	z	394/464 (85%)	394 (100%)	0	100	100
All	All	7404/9885 (75%)	7404 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	88	HIS
4	E	138	HIS
4	E	176	HIS
4	E	281	ASN
4	E	294	ASN
6	H	74	HIS
8	J	133	GLN
13	P	55	ASN
15	R	79	HIS
16	S	144	ASN
17	T	153	HIS
18	U	35	GLN
22	Z	95	HIS
24	5	88	HIS
25	6	361	GLN
26	7	204	HIS
28	9	50	GLN
29	a	88	GLN
29	a	110	GLN
30	b	123	ASN
31	c	128	GLN
32	d	107	GLN
32	d	115	ASN
35	g	102	HIS

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Mol	Chain	Res	Type
37	i	59	ASN
38	j	94	GLN
38	j	95	GLN
40	l	126	HIS
42	p	123	HIS
42	p	146	ASN
45	s	107	GLN
45	s	173	GLN
49	x	403	GLN
49	y	120	GLN
49	y	206	HIS
49	y	317	HIS
50	z	367	GLN
50	z	388	GLN
50	z	424	HIS
50	z	430	GLN

5.3.3　RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1100/1584 (69%)	357 (32%)	27 (2%)
2	B	59/68 (86%)	24 (40%)	1 (1%)
All	All	1159/1652 (70%)	381 (32%)	28 (2%)

All (381) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	A
1	A	1100	C
1	A	1101	C
1	A	1102	U
1	A	1103	A
1	A	1104	G
1	A	1112	C
1	A	1115	A
1	A	1124	U
1	A	1128	U
1	A	1130	U
1	A	1131	A
1	A	1134	A
1	A	1135	U

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Mol	Chain	Res	Type
1	A	1136	U
1	A	1138	U
1	A	1139	A
1	A	1140	U
1	A	1148	A
1	A	1151	A
1	A	1152	U
1	A	1173	G
1	A	1175	G
1	A	1176	A
1	A	1186	G
1	A	1188	A
1	A	1192	G
1	A	1195	G
1	A	1202	A
1	A	1206	A
1	A	1219	A
1	A	1224	U
1	A	1229	G
1	A	1230	A
1	A	1231	C
1	A	1232	U
1	A	1233	A
1	A	1234	A
1	A	1235	U
1	A	1237	A
1	A	1238	A
1	A	1245	G
1	A	1249	A
1	A	1250	A
1	A	1252	C
1	A	1253	A
1	A	1254	A
1	A	1257	A
1	A	1261	A
1	A	1269	A
1	A	1274	U
1	A	1275	U
1	A	1276	G
1	A	1277	C
1	A	1279	U
1	A	1280	A

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Mol	Chain	Res	Type
1	A	1281	A
1	A	1294	A
1	A	1297	A
1	A	1299	U
1	A	1307	A
1	A	1308	A
1	A	1311	G
1	A	1312	A
1	A	1315	U
1	A	1316	A
1	A	1317	C
1	A	1318	A
1	A	1328	C
1	A	1334	A
1	A	1440	G
1	A	1446	U
1	A	1447	A
1	A	1454	A
1	A	1457	U
1	A	1462	U
1	A	1463	U
1	A	1465	A
1	A	1467	U
1	A	1468	U
1	A	1470	A
1	A	1480	U
1	A	1481	U
1	A	1482	G
1	A	1487	A
1	A	1488	A
1	A	1489	A
1	A	1490	A
1	A	1491	A
1	A	1492	C
1	A	1493	A
1	A	1494	A
1	A	1499	A
1	A	1500	U
1	A	1501	C
1	A	1502	A
1	A	1503	A
1	A	1504	A

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Mol	Chain	Res	Type
1	A	1505	A
1	A	1508	U
1	A	1509	A
1	A	1510	A
1	A	1518	U
1	A	1522	A
1	A	1523	G
1	A	1529	A
1	A	1531	A
1	A	1534	G
1	A	1538	G
1	A	1539	C
1	A	1540	U
1	A	1549	A
1	A	1550	C
1	A	1555	A
1	A	1556	A
1	A	1557	A
1	A	1562	U
1	A	1563	U
1	A	1565	A
1	A	1566	U
1	A	1570	G
1	A	1577	U
1	A	1580	C
1	A	1584	A
1	A	1585	C
1	A	1586	A
1	A	1594	U
1	A	1595	A
1	A	1596	A
1	A	1598	C
1	A	1600	U
1	A	1602	G
1	A	1603	U
1	A	1604	A
1	A	1605	G
1	A	1607	C
1	A	1608	C
1	A	1609	U
1	A	1610	A
1	A	1612	A

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Mol	Chain	Res	Type
1	A	1613	A
1	A	1614	G
1	A	1616	A
1	A	1617	G
1	A	1619	C
1	A	1620	A
1	A	1621	C
1	A	1622	C
1	A	1623	A
1	A	1625	U
1	A	1626	A
1	A	1627	A
1	A	1628	A
1	A	1629	G
1	A	1630	A
1	A	1632	A
1	A	1633	G
1	A	1634	C
1	A	1636	U
1	A	1637	U
1	A	1638	C
1	A	1641	G
1	A	1642	C
1	A	1644	C
1	A	1646	A
1	A	1648	A
1	A	1649	U
1	A	1650	A
1	A	1651	A
1	A	1653	A
1	A	1659	C
1	A	1660	A
1	A	1661	A
1	A	1665	A
1	A	1666	U
1	A	1670	A
1	A	1672	A
1	A	1674	U
1	A	1676	U
1	A	1679	A
1	A	1683	A
1	A	1684	C

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Mol	Chain	Res	Type
1	A	1685	U
1	A	1691	A
1	A	1694	U
1	A	1698	A
1	A	1699	A
1	A	1718	U
1	A	1719	U
1	A	1728	A
1	A	1731	A
1	A	1734	G
1	A	1749	A
1	A	1750	A
1	A	1756	C
1	A	1757	C
1	A	1758	A
1	A	1759	A
1	A	1767	G
1	A	1768	G
1	A	1770	A
1	A	1785	C
1	A	1786	U
1	A	1794	C
1	A	1802	A
1	A	1805	U
1	A	1806	A
1	A	1807	A
1	A	1808	U
1	A	1824	A
1	A	1827	C
1	A	1832	U
1	A	1833	A
1	A	1838	U
1	A	1845	C
1	A	1847	U
1	A	1852	C
1	A	1870	A
1	A	1872	C
1	A	1879	C
1	A	1881	U
1	A	1883	A
1	A	1888	A
1	A	1889	A

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Mol	Chain	Res	Type
1	A	1890	G
1	A	1895	A
1	A	1905	A
1	A	1923	G
1	A	1924	A
1	A	1925	A
1	A	1953	A
1	A	1954	C
1	A	2091	U
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2123	U
1	A	2128	U
1	A	2131	A
1	A	2132	G
1	A	2143	A
1	A	2146	A
1	A	2155	C
1	A	2156	G
1	A	2158	G
1	A	2159	A
1	A	2160	A
1	A	2161	G
1	A	2162	A
1	A	2168	U
1	A	2169	G
1	A	2170	G
1	A	2177	A
1	A	2180	U
1	A	2182	U
1	A	2183	A
1	A	2186	A
1	A	2187	C
1	A	2193	U
1	A	2195	U
1	A	2197	U
1	A	2236	G
1	A	2239	U
1	A	2241	A
1	A	2247	C
1	A	2275	A

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Mol	Chain	Res	Type
1	A	2276	U
1	A	2277	C
1	A	2278	C
1	A	2284	A
1	A	2285	U
1	A	2286	G
1	A	2287	A
1	A	2292	A
1	A	2293	A
1	A	2295	C
1	A	2297	A
1	A	2303	A
1	A	2333	U
1	A	2334	G
1	A	2339	A
1	A	2340	G
1	A	2342	U
1	A	2343	A
1	A	2351	A
1	A	2358	G
1	A	2360	C
1	A	2361	C
1	A	2362	A
1	A	2363	A
1	A	2367	A
1	A	2369	C
1	A	2373	G
1	A	2391	U
1	A	2394	U
1	A	2396	A
1	A	2397	A
1	A	2398	G
1	A	2408	C
1	A	2410	A
1	A	2412	A
1	A	2438	G
1	A	2447	A
1	A	2458	G
1	A	2462	A
1	A	2467	A
1	A	2468	U
1	A	2475	U

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Mol	Chain	Res	Type
1	A	2480	U
1	A	2481	U
1	A	2482	G
1	A	2486	A
1	A	2493	A
1	A	2495	A
1	A	2496	G
1	A	2497	U
1	A	2498	C
1	A	2501	A
1	A	2502	C
1	A	2505	G
1	A	2506	A
1	A	2507	U
1	A	2508	C
1	A	2509	U
1	A	2562	C
1	A	2564	G
1	A	2565	U
1	A	2575	C
1	A	2582	A
1	A	2598	A
1	A	2600	A
1	A	2601	U
1	A	2605	C
1	A	2614	C
1	A	2615	U
1	A	2617	A
1	A	2618	A
1	A	2619	U
1	A	2621	U
1	A	2625	A
1	A	2628	A
1	A	2629	A
1	A	2631	A
1	A	2635	A
1	A	2636	A
1	A	2638	U
1	A	2640	A
1	A	2647	U
1	A	2648	A
1	A	2650	G

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Mol	Chain	Res	Type
1	A	2655	C
1	A	2656	C
1	A	2659	C
1	A	2660	U
1	A	2665	U
1	A	2666	A
1	A	2676	A
2	B	3	U
2	B	5	A
2	B	6	U
2	B	7	G
2	B	8	U
2	B	9	A
2	B	14	A
2	B	16	U
2	B	17	A
2	B	18	C
2	B	20	A
2	B	21	A
2	B	32	U
2	B	33	G
2	B	44	G
2	B	46	U
2	B	47	G
2	B	48	G
2	B	50	U
2	B	51	A
2	B	58	C
2	B	60	C
2	B	63	A
2	B	66	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1134	A
1	A	1137	A
1	A	1187	U
1	A	1191	A
1	A	1232	U
1	A	1234	A
1	A	1489	A

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Mol	Chain	Res	Type
1	A	1502	A
1	A	1538	G
1	A	1584	A
1	A	1612	A
1	A	1628	A
1	A	1637	U
1	A	1684	C
1	A	1894	C
1	A	1953	A
1	A	2182	U
1	A	2275	A
1	A	2302	U
1	A	2342	U
1	A	2466	U
1	A	2480	U
1	A	2485	C
1	A	2507	U
1	A	2564	G
1	A	2659	C
1	A	2675	U
2	B	20	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
52	FES	r	301	44,7	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	FES	r	301	44,7	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	r	301	FES	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

6   Map visualisation   ⓘ

This section contains visualisations of the EMDB entry EMD-52044. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1   Orthogonal projections   ⓘ
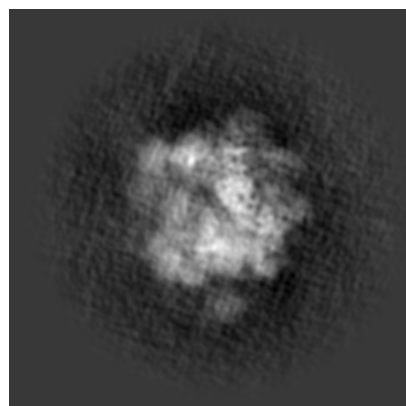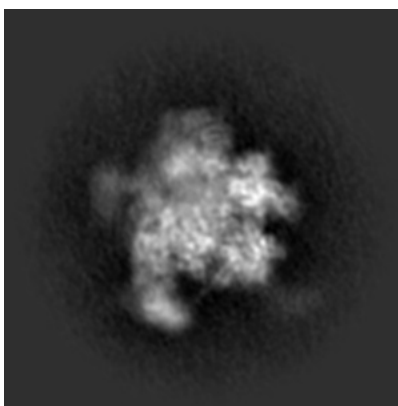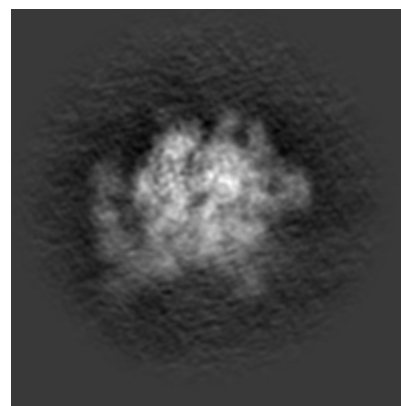
6.1.1   Primary map

| X | Y | Z |

6.1.2   Raw map

| X | Y | Z |
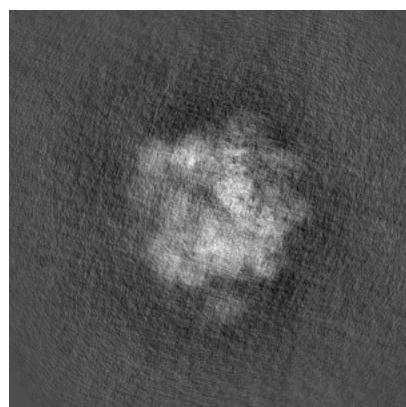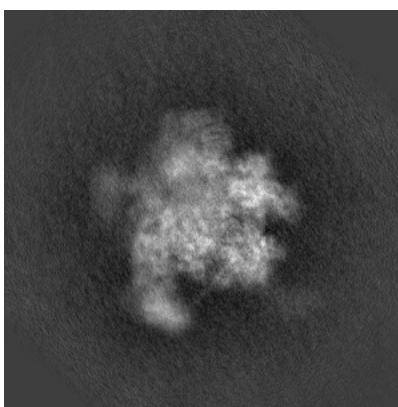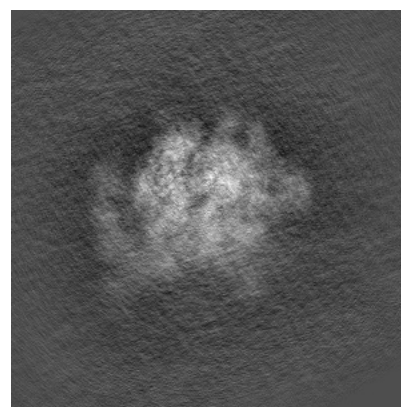
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
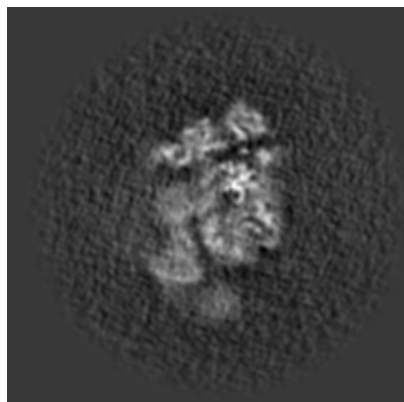
6.2.1 Primary map
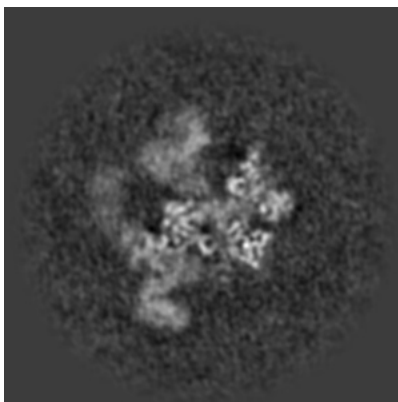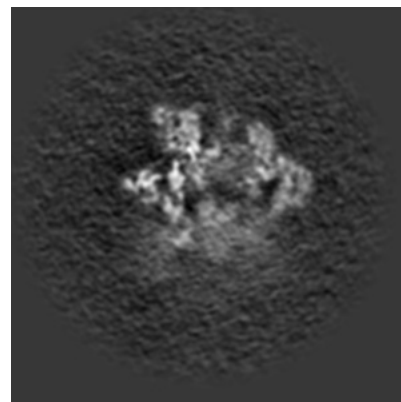
| X Index: 270 | Y Index: 270 | Z Index: 270 |

6.2.2 Raw map
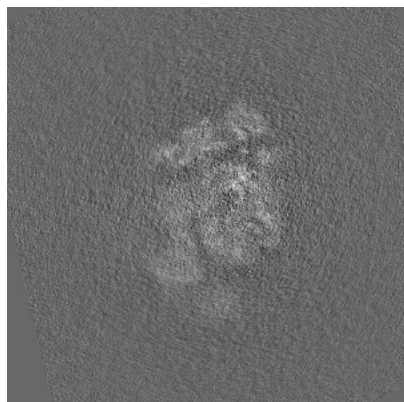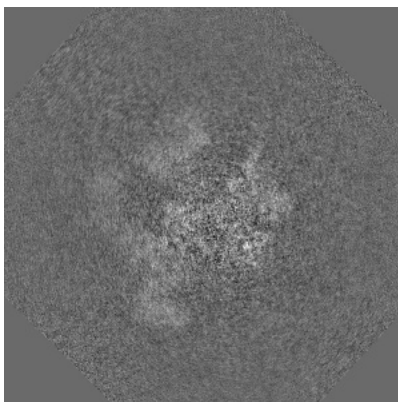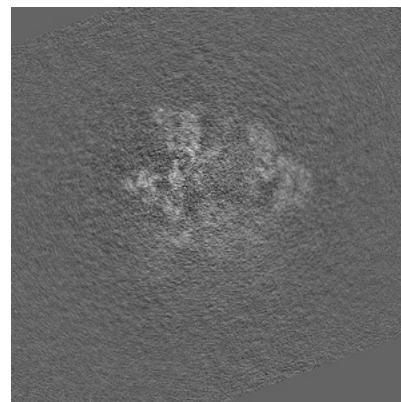
| X Index: 270 | Y Index: 270 | Z Index: 270 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
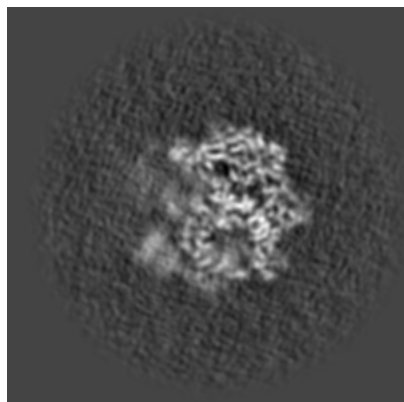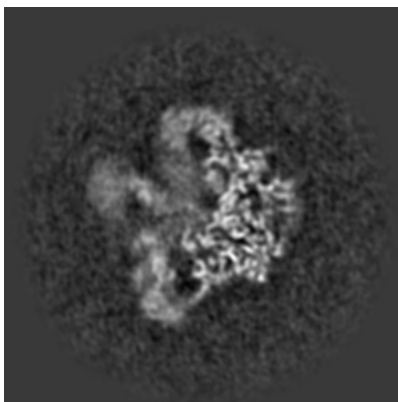
| X Index: 222 | Y Index: 298 | Z Index: 340 |
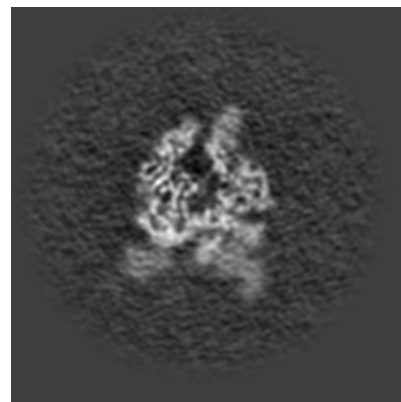
6.3.2 Raw map
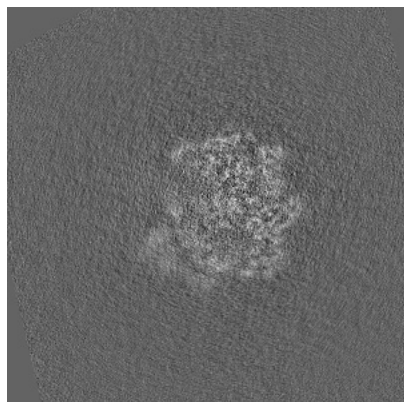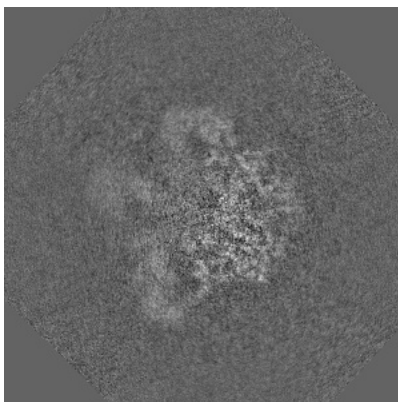
| X Index: 229 | Y Index: 299 | Z Index: 296 |
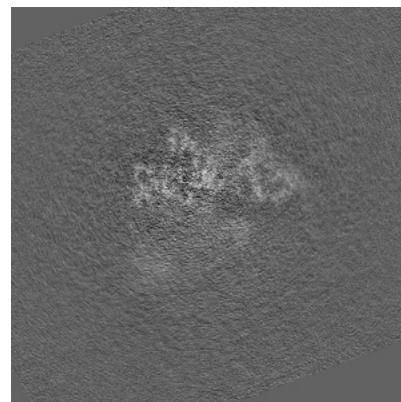
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
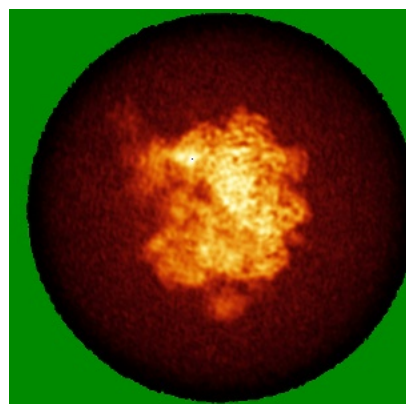
X
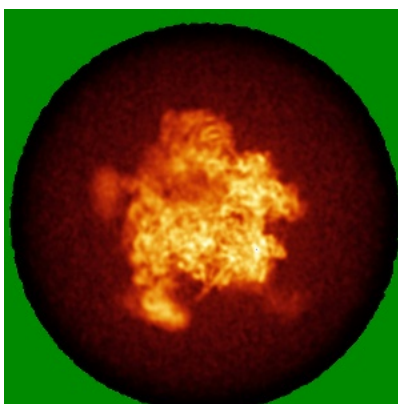
Y
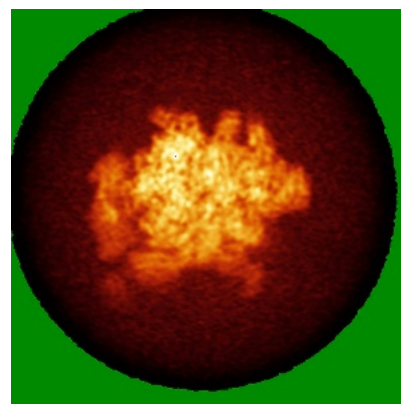
Z

6.4.2 Raw map

X

Y

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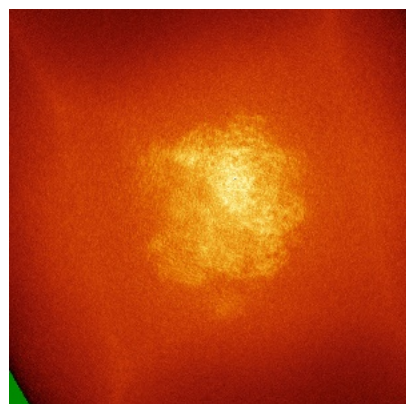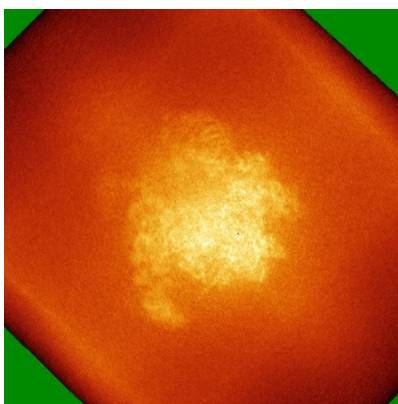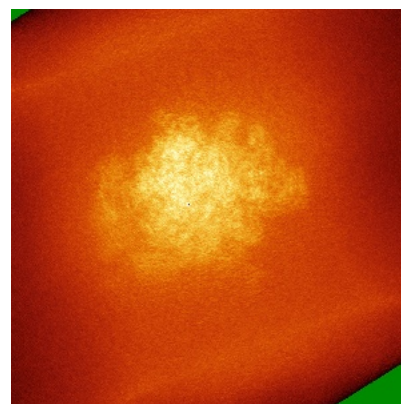
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
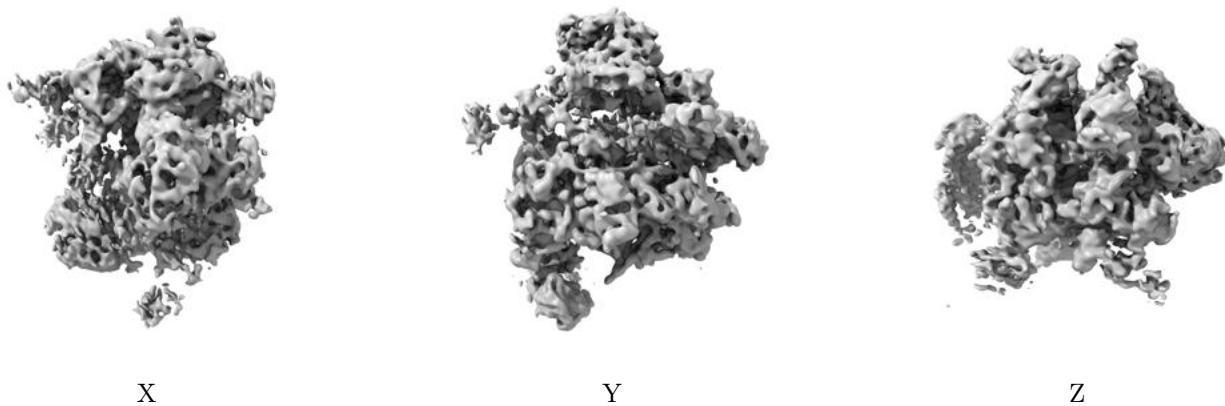
The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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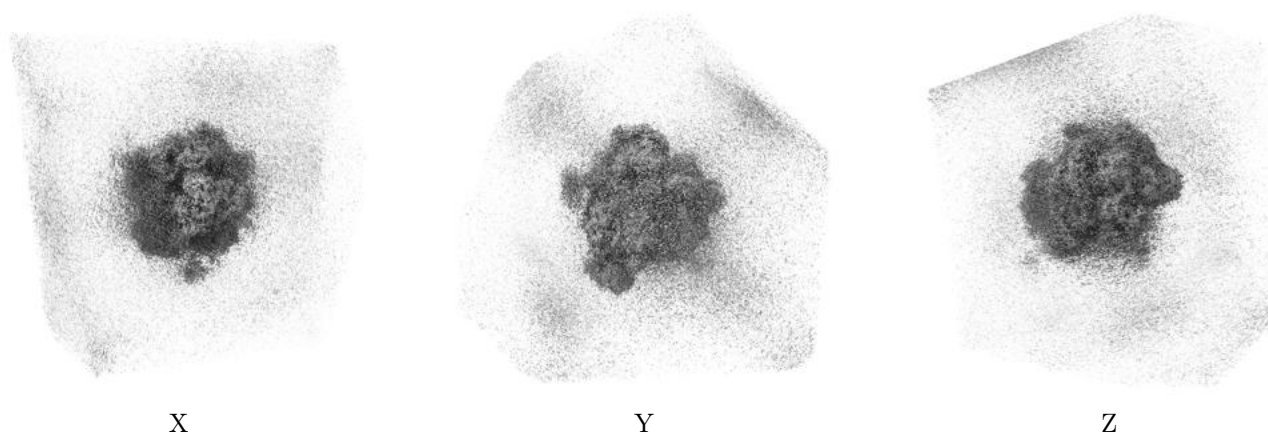
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7　Map analysis ⓘ

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

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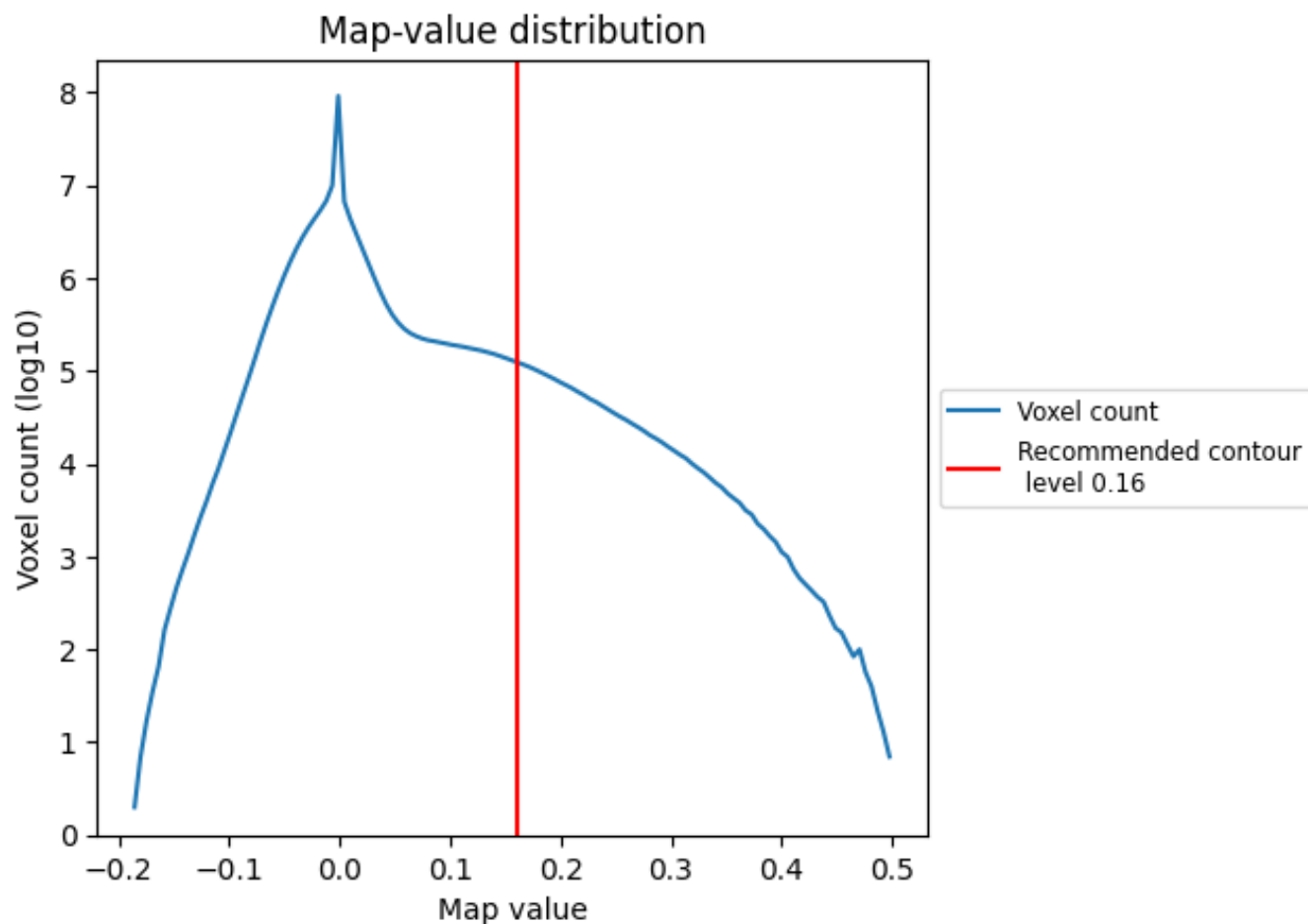
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
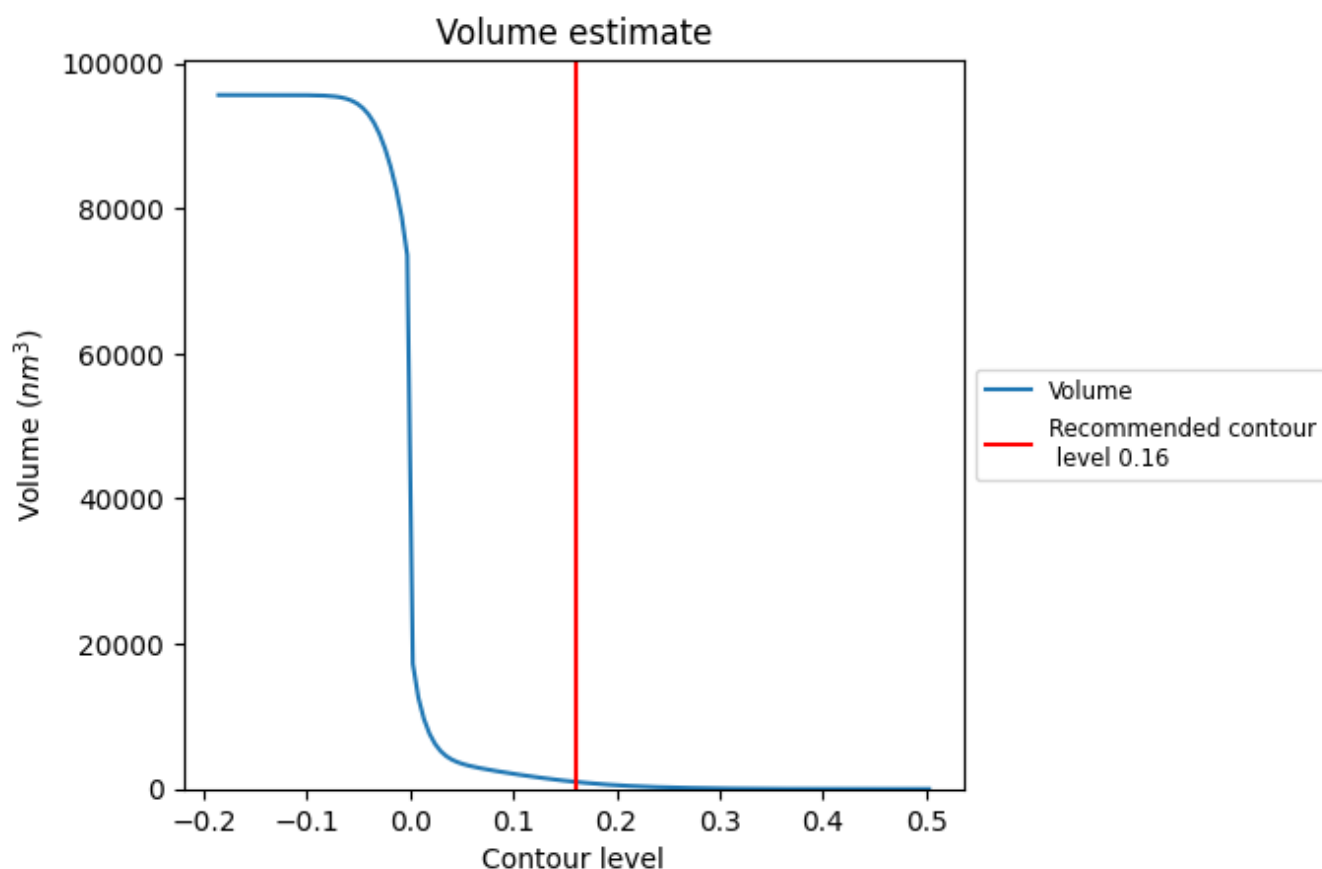
The volume at the recommended contour level is 982 nm^3; this corresponds to an approximate mass of 887 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ
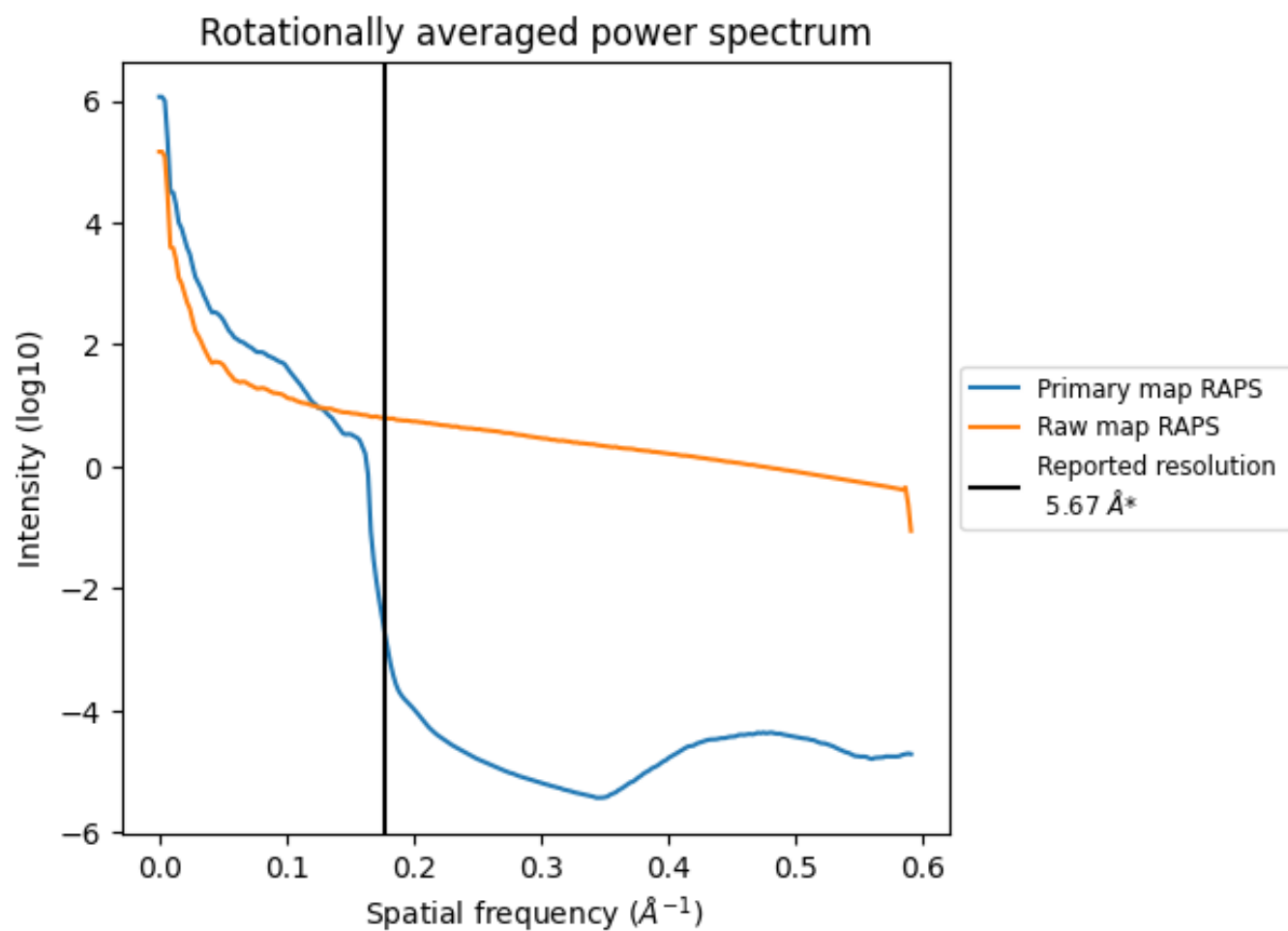
*Reported resolution corresponds to spatial frequency of 0.176 Å^{-1}

8　Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1　FSC ⓘ
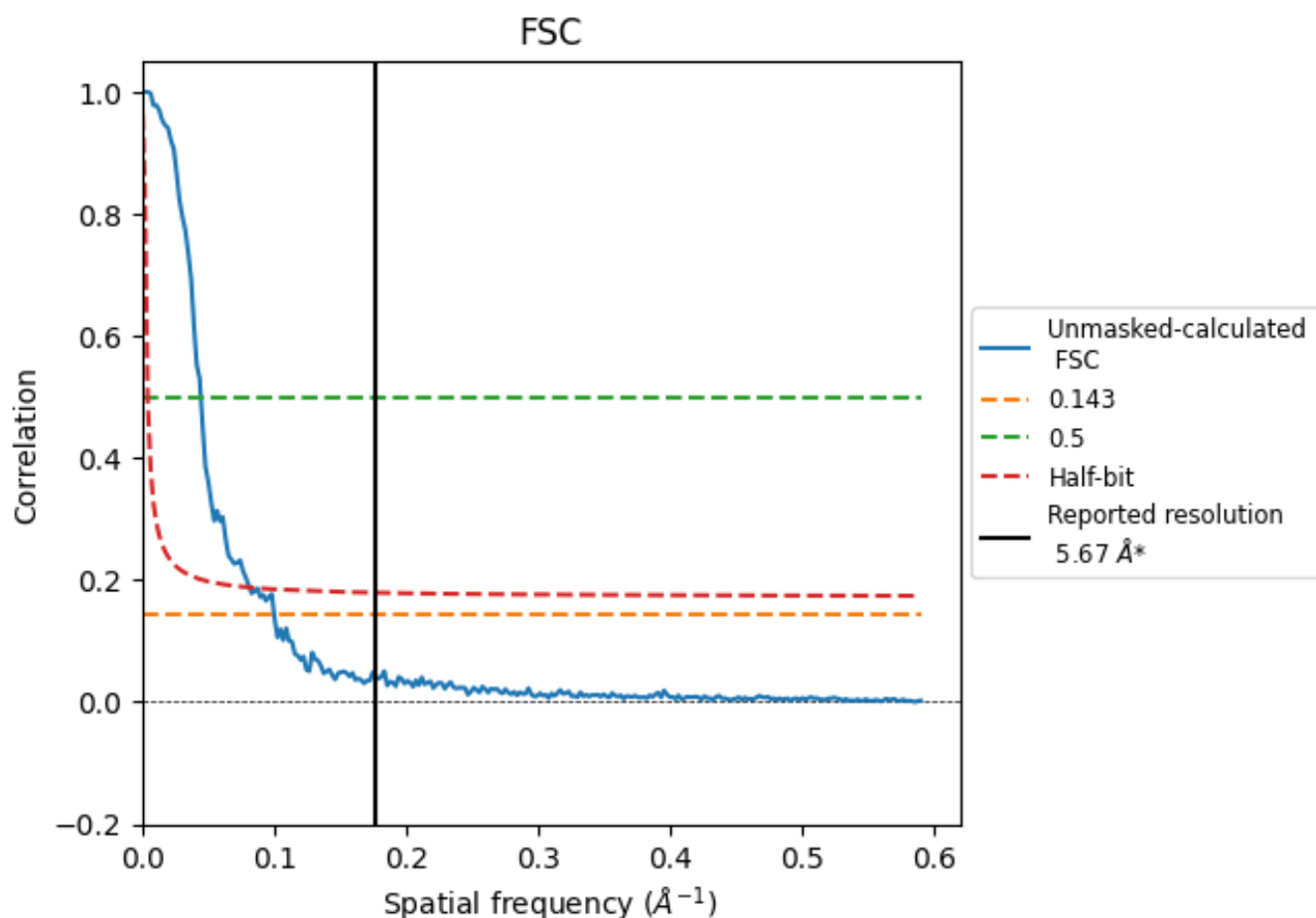
*Reported resolution corresponds to spatial frequency of 0.176 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.67	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.98	22.42	12.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.98 differs from the reported value 5.67 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-52044 and PDB model 9HCC. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay ⓘ
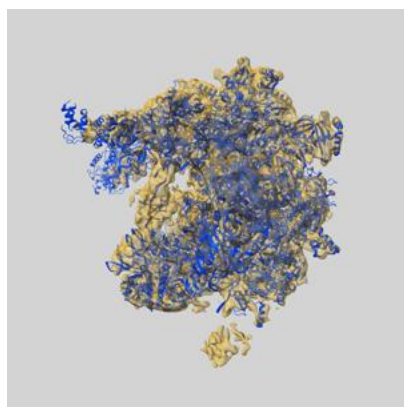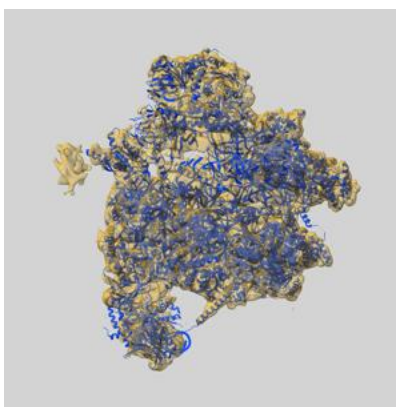
| X | Y | Z |
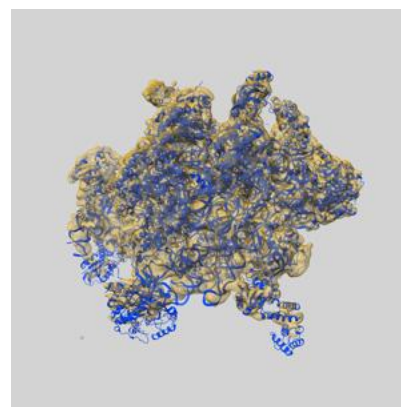
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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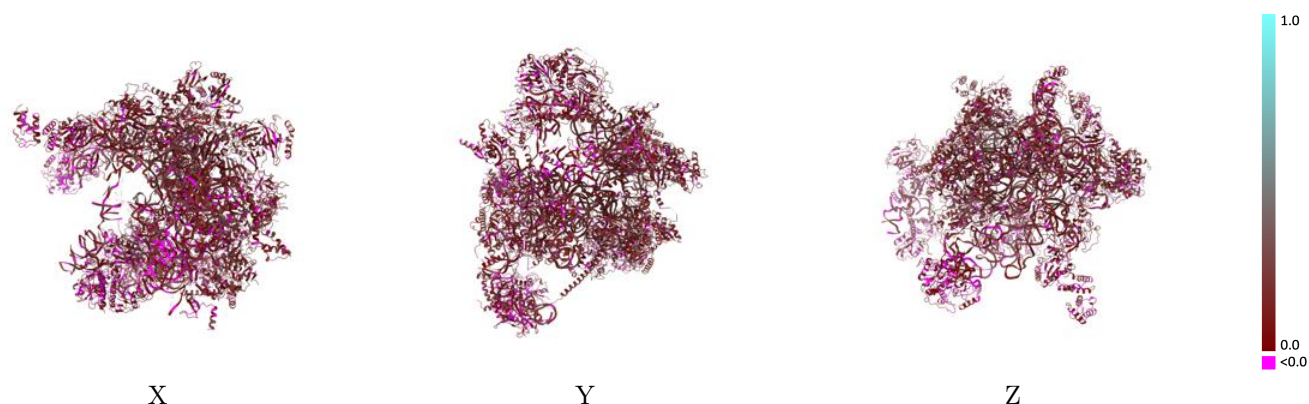
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
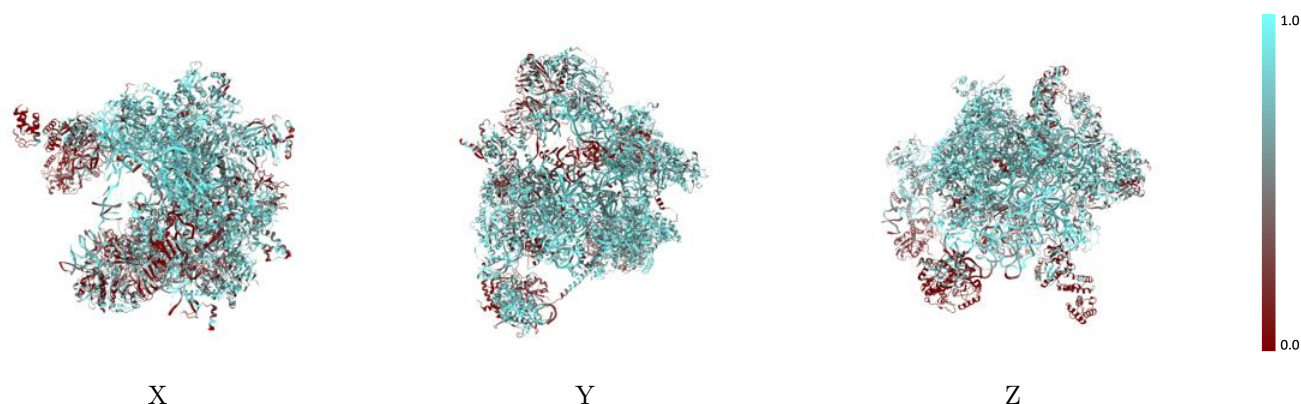
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion ⓘ
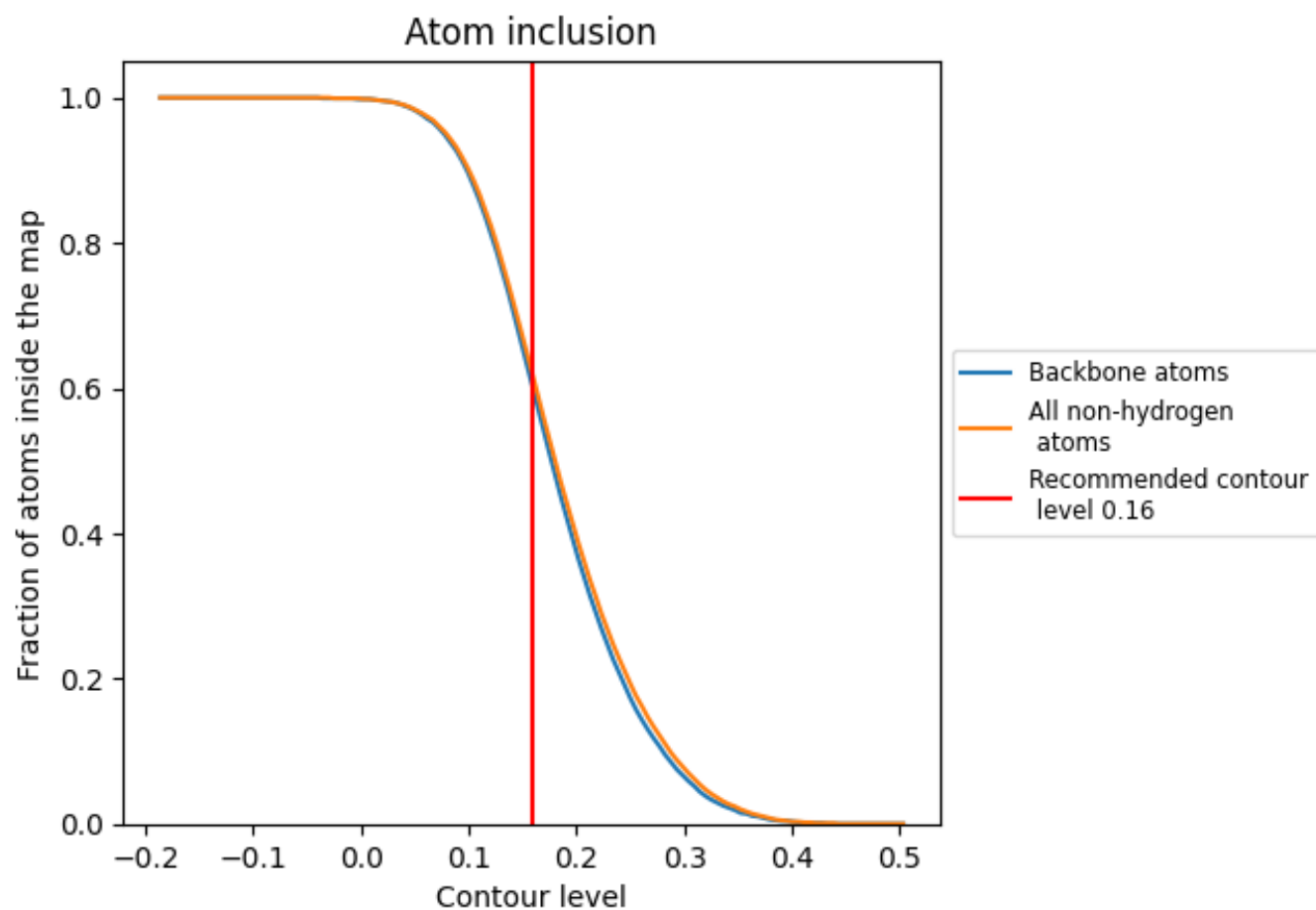
At the recommended contour level, 60% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.1460
0	0.7730	0.1800
5	0.3780	0.1160
6	0.5750	0.0880
7	0.7260	0.1710
8	0.1770	0.1090
9	0.5780	0.1330
A	0.7570	0.1640
B	0.6740	0.1230
D	0.2500	0.0740
E	0.7660	0.1590
F	0.7240	0.1510
H	0.5590	0.1060
I	0.2300	0.1160
J	0.0470	0.0410
K	0.7450	0.1800
L	0.3200	0.1180
M	0.7090	0.1750
O	0.7510	0.1570
P	0.7430	0.1090
Q	0.7490	0.1720
R	0.6850	0.1680
S	0.7250	0.1900
T	0.7200	0.1690
U	0.5850	0.1190
V	0.3010	0.1330
X	0.5350	0.1460
Y	0.5990	0.1130
Z	0.6840	0.1920
a	0.6210	0.1840
b	0.7340	0.1830
c	0.7270	0.1700
d	0.5810	0.1580
e	0.0440	0.0740
f	0.1020	0.0360

1.0

0.0
<0.0

Continued on next page...

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Chain	Atom inclusion	Q-score
g	0.8250	0.1900
h	0.6960	0.1930
i	0.6380	0.1510
j	0.7050	0.2010
k	0.3500	0.1210
l	0.1970	0.0570
o	0.7430	0.1700
p	0.6460	0.1490
q	0.7420	0.2080
r	0.7340	0.1730
s	0.6670	0.1570
u	0.4210	0.1190
v	0.2220	0.1080
w	0.0440	0.0920
x	0.4320	0.0830
y	0.5060	0.1080
z	0.4680	0.1380