



## Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 02:37 am 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

The following versions of software and data (see [references ⓘ](#)) 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) : 2.44

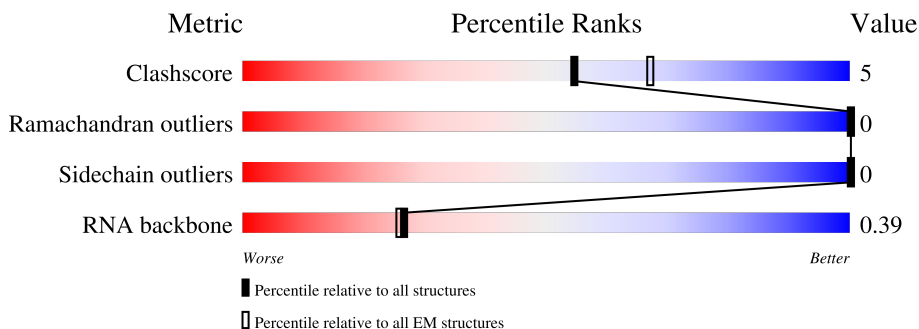
# 1 Overall quality at a glance

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

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

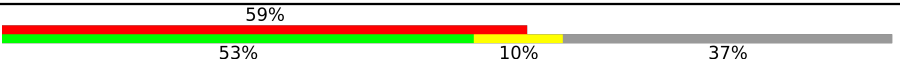

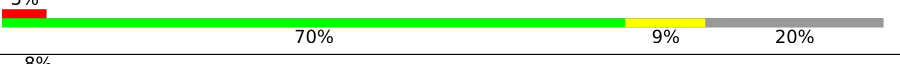
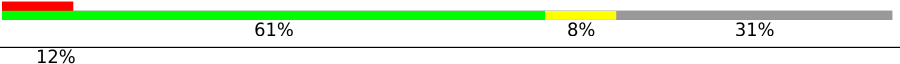
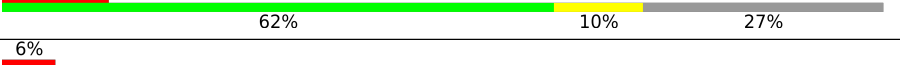
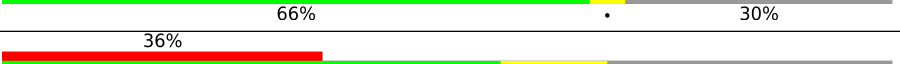

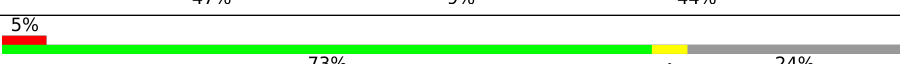
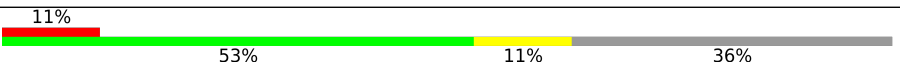

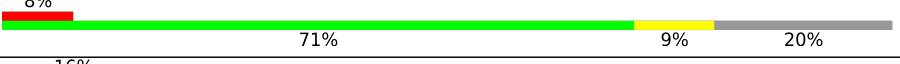

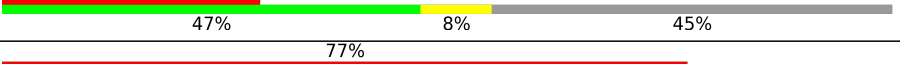
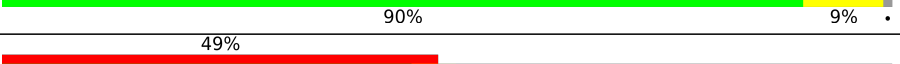
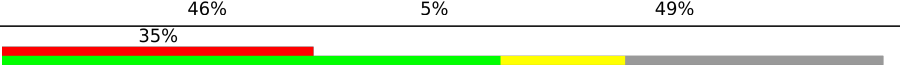

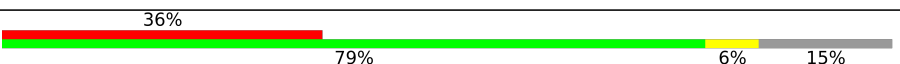

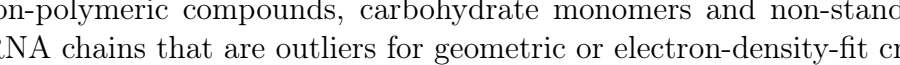
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	192	
9	K	178	
10	L	145	
11	M	295	
12	O	176	
13	P	180	
14	Q	292	
15	R	149	
16	S	209	
17	T	206	
18	U	146	
19	V	216	
20	X	294	
21	Y	252	
22	Z	160	
23	0	187	
24	5	423	
25	6	380	
26	7	336	
27	8	206	
28	9	135	
29	a	142	
30	b	159	
31	c	308	
32	d	306	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	e	283	
34	f	211	
35	g	166	
36	h	159	
37	i	128	
38	j	121	
39	k	118	
40	l	135	
41	o	102	
42	p	206	
43	q	222	
44	r	196	
45	s	442	
46	u	228	
47	v	70	
48	w	156	
49	x	418	
49	y	418	
50	z	540	

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 [i](#)

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	C	H	N	O	P	0	0
			36145	10796	12126	4363	7731	1129		

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

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

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

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

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

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

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

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

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

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

- 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	C	H	N	O	S	0	0
			3612	1150	1822	309	322	9		

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

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

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

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

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

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

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

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

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

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

- 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	C	H	N	O	S	0	0
			4072	1304	2051	358	355	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	C	H	N	O	S	0	0
			2184	709	1094	187	192	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

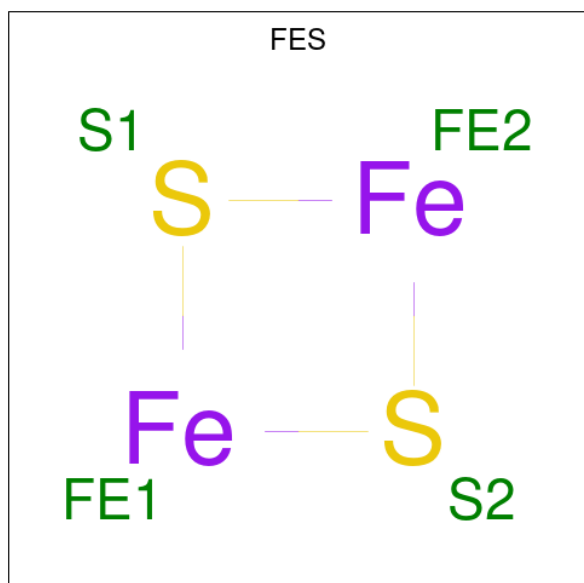
- Molecule 50 is a protein called Probable ATP-dependent RNA helicase DDX28.

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).

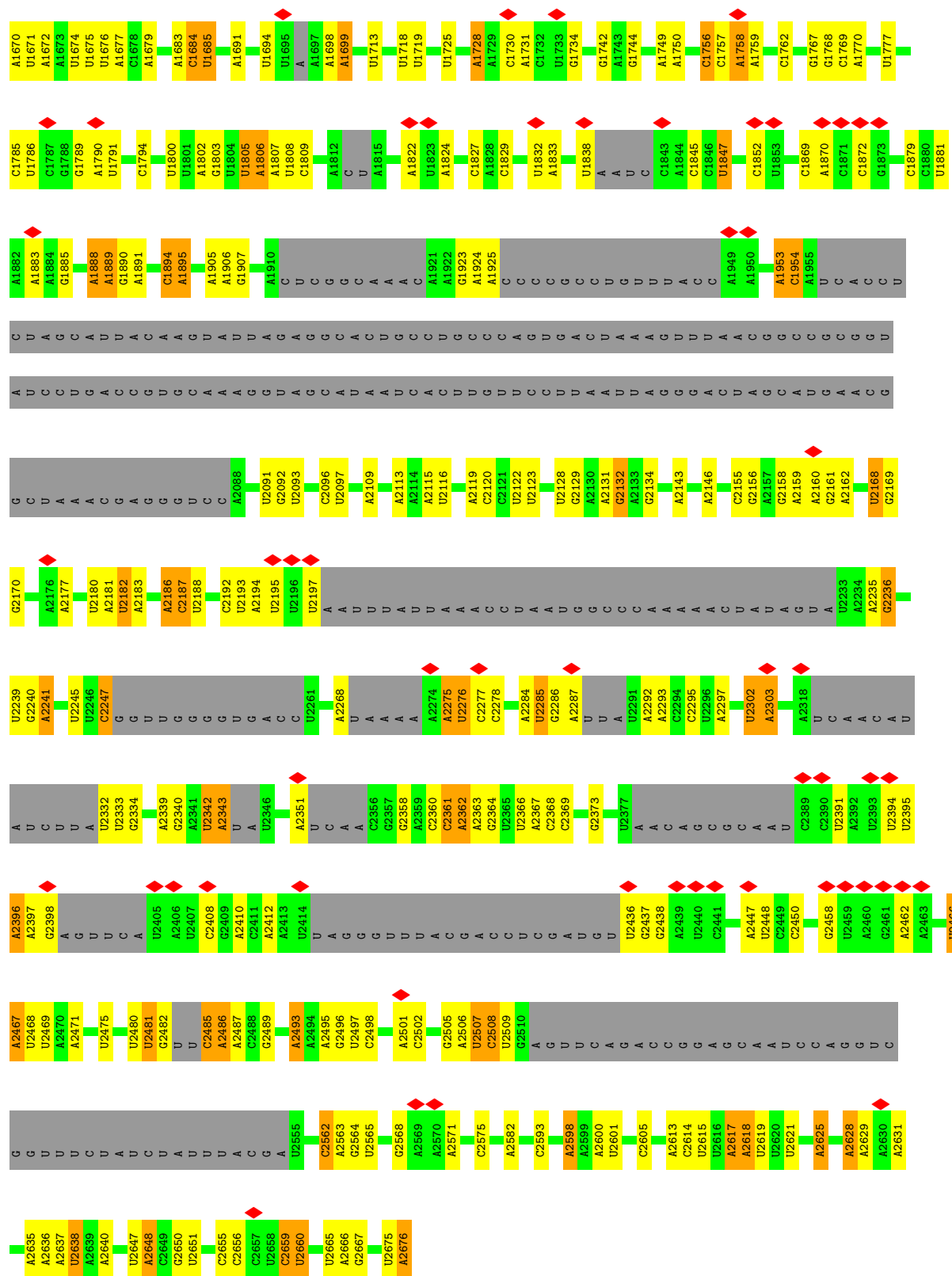
Mol	Chain	Residues	Atoms		AltConf
51	0	1	Total	Zn	0
			1	1	

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

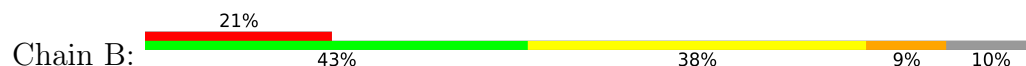


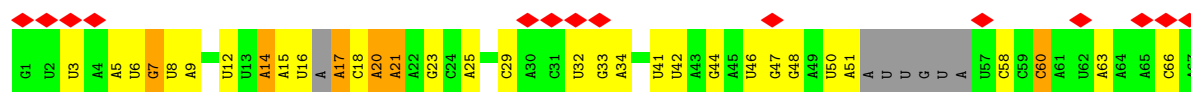
Mol	Chain	Residues	Atoms			AltConf
52	r	1	Total	Fe	S	0
			4	2	2	



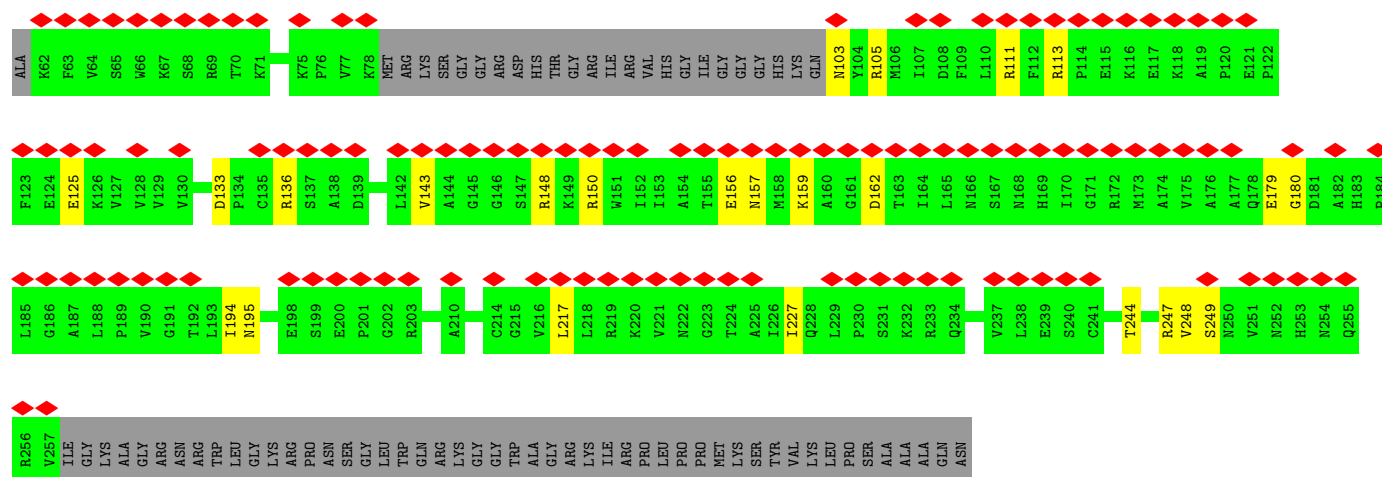


• Molecule 2: tRNA-Phe (68-MER)

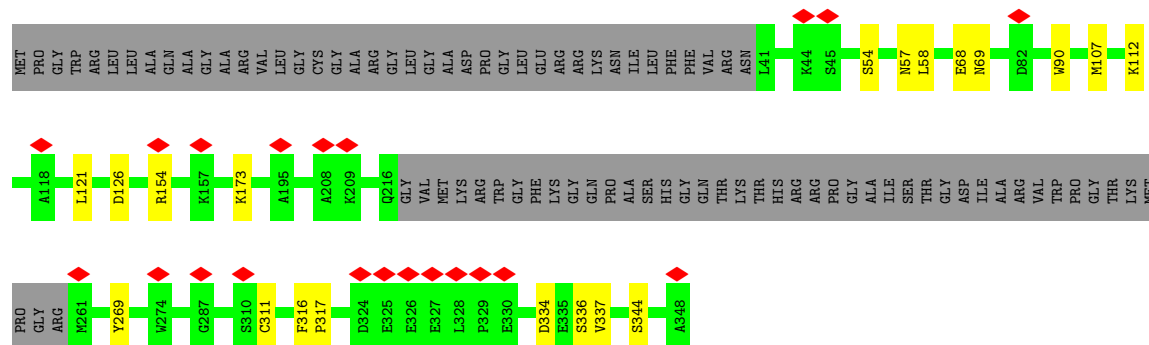




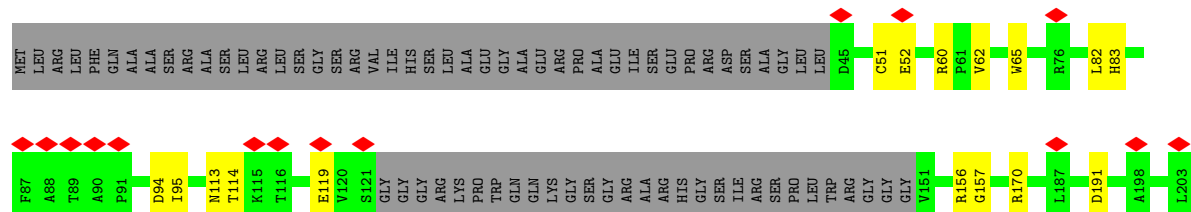
• Molecule 3: Large ribosomal subunit protein uL2m

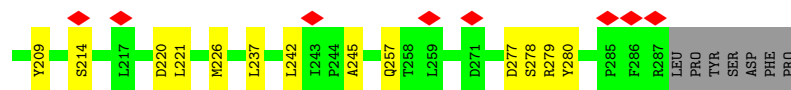


• Molecule 4: Large ribosomal subunit protein uL3m

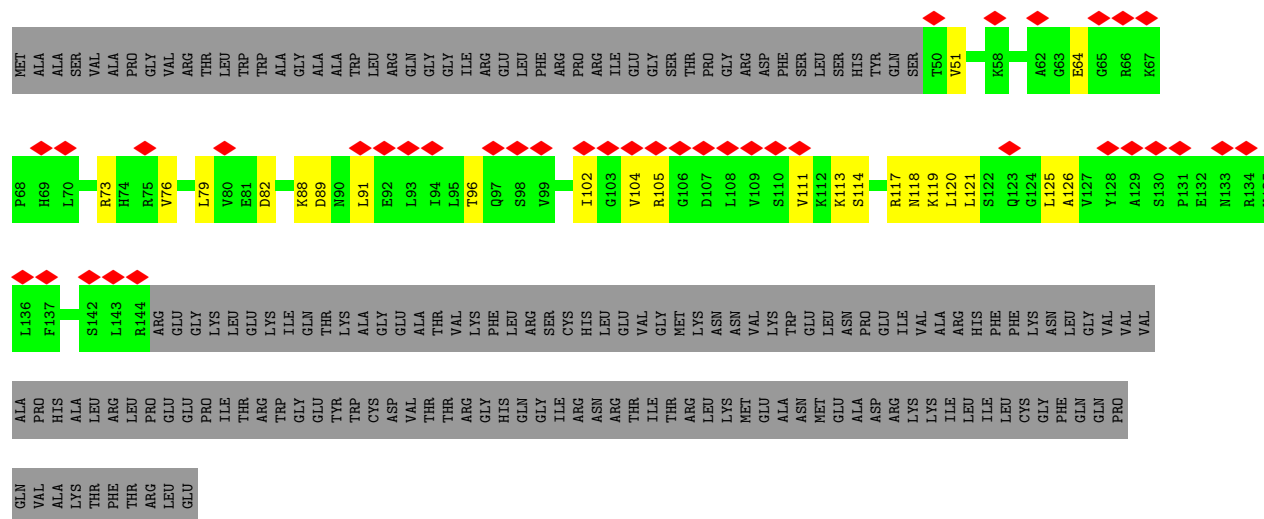


• Molecule 5: Large ribosomal subunit protein uL4m

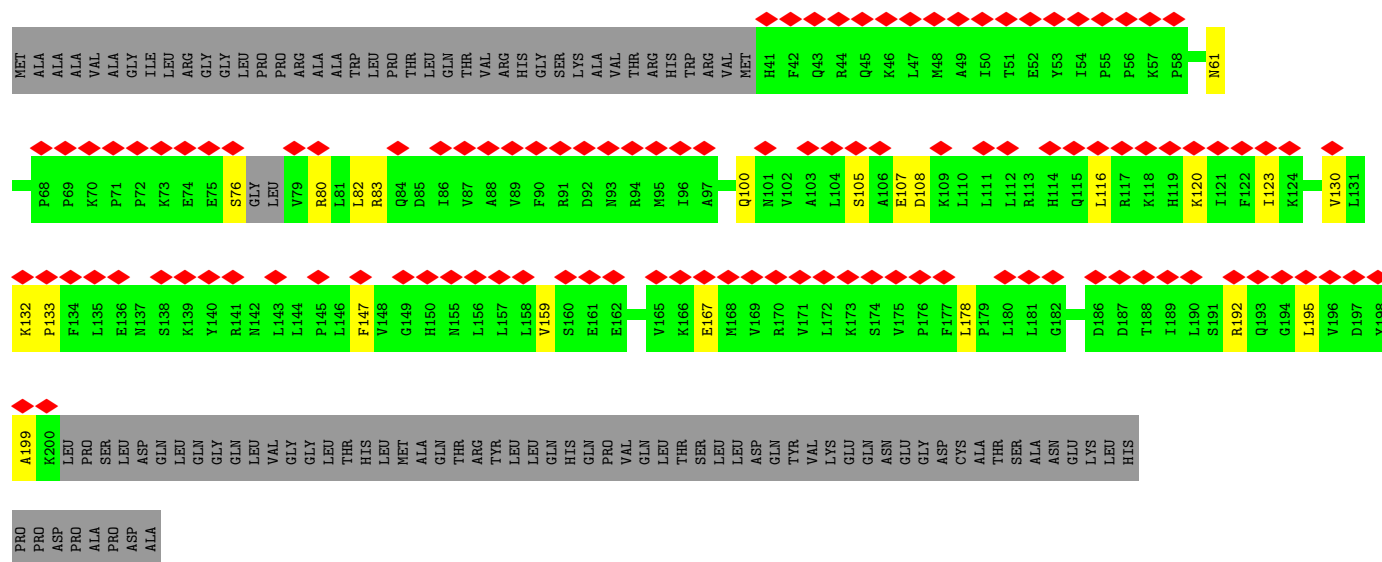




• Molecule 6: Large ribosomal subunit protein bL9m



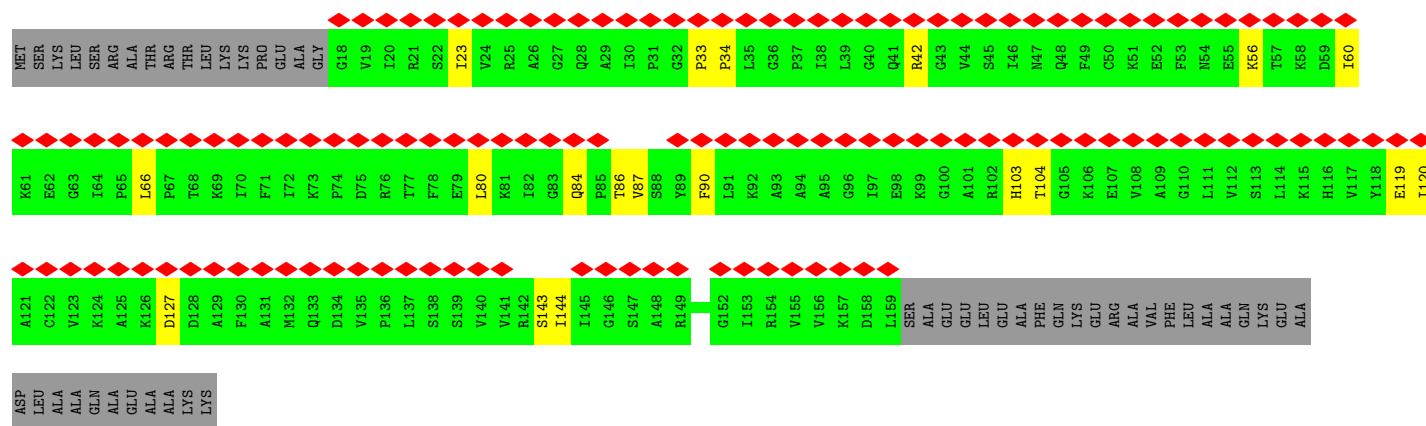
• Molecule 7: Large ribosomal subunit protein uL10m



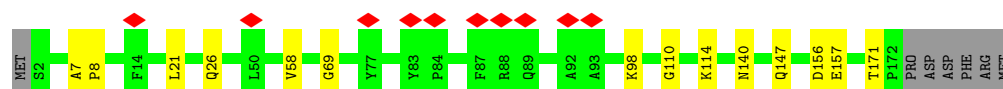
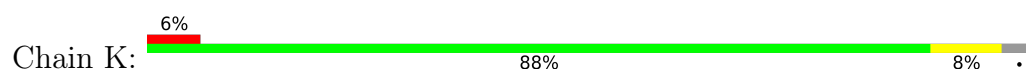
• Molecule 8: Large ribosomal subunit protein uL11m



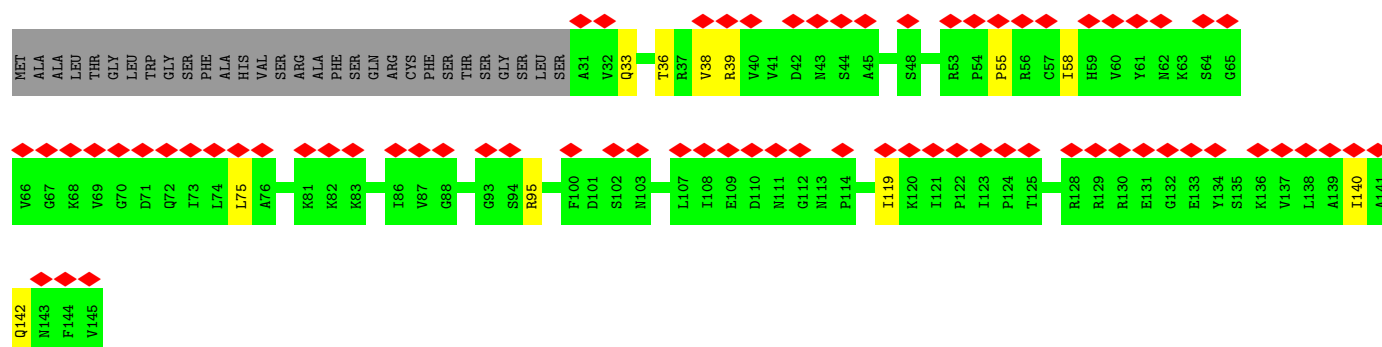




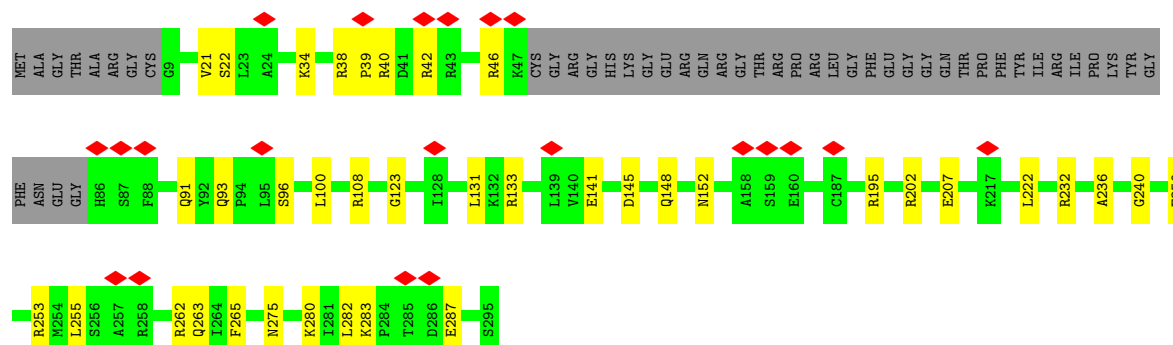
- Molecule 9: Large ribosomal subunit protein uL13m



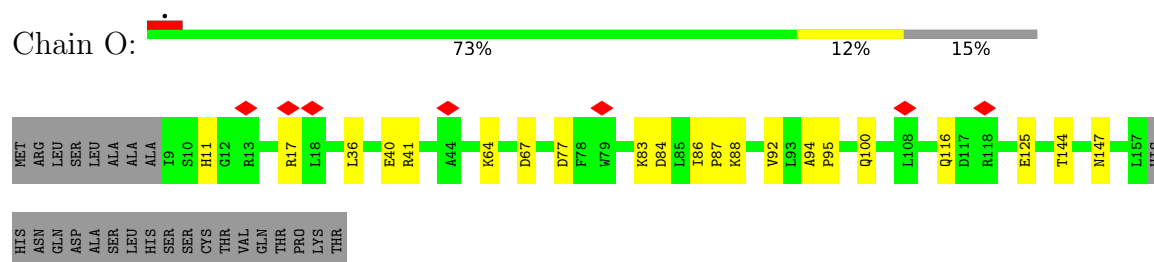
- Molecule 10: Large ribosomal subunit protein uL14m



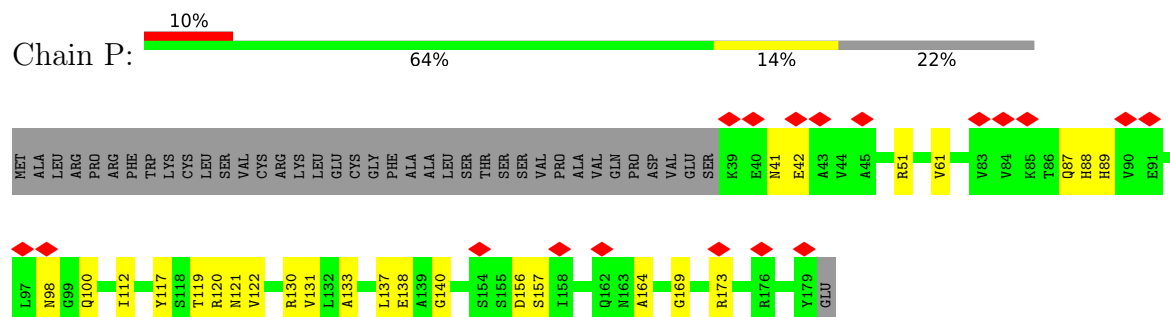
- Molecule 11: Large ribosomal subunit protein uL15m



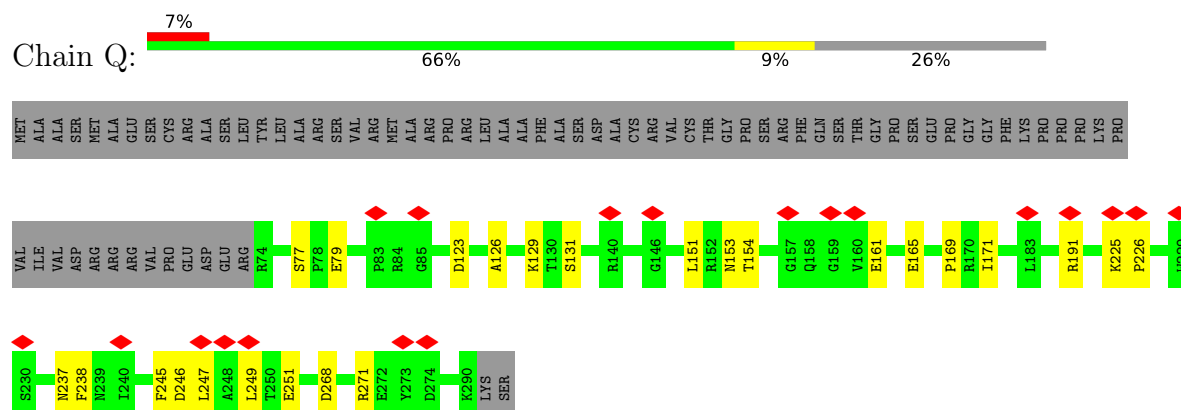
- Molecule 12: Large ribosomal subunit protein bL17m



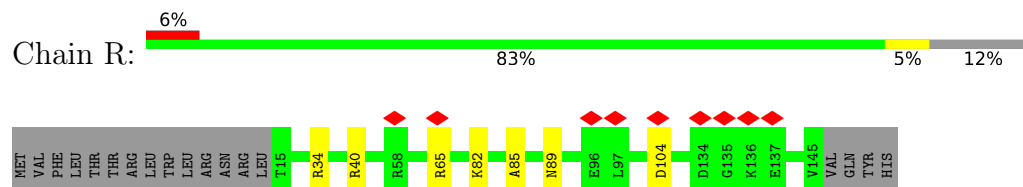
- Molecule 13: Large ribosomal subunit protein uL18m



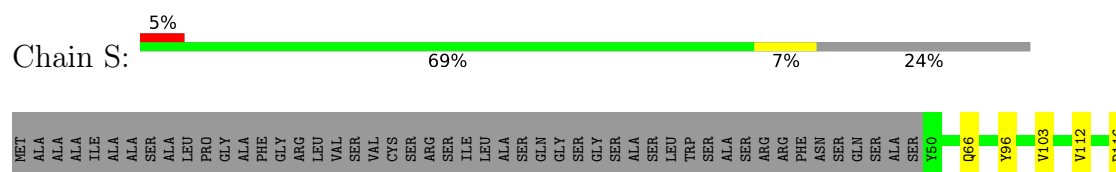
- Molecule 14: Large ribosomal subunit protein bL19m

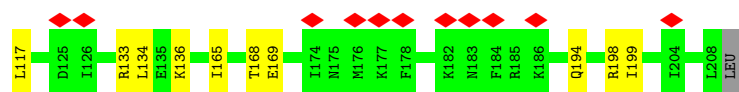


- Molecule 15: Large ribosomal subunit protein bL20m

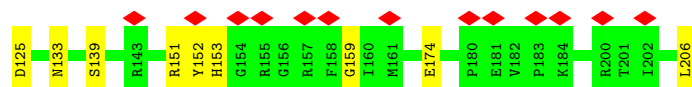
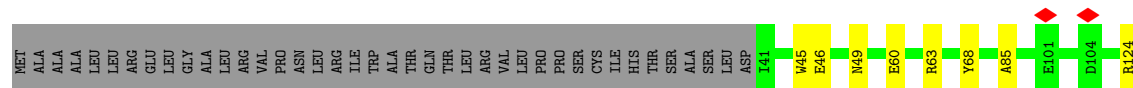


- Molecule 16: Large ribosomal subunit protein bL21m

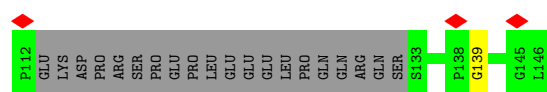
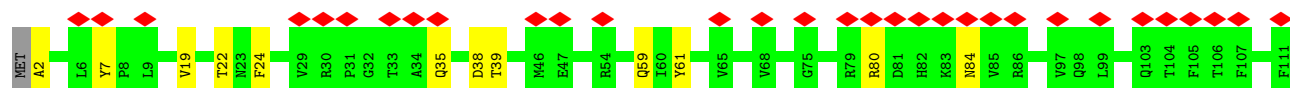
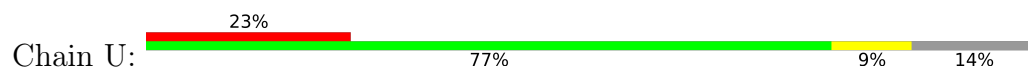




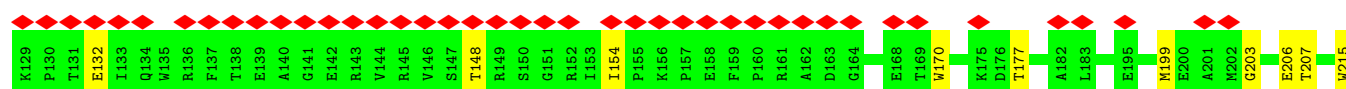
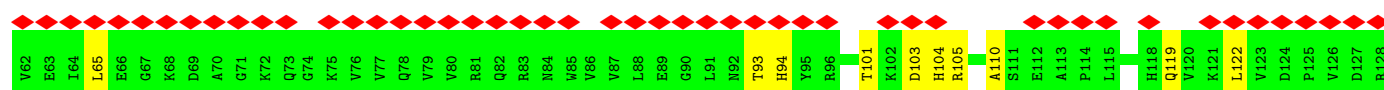
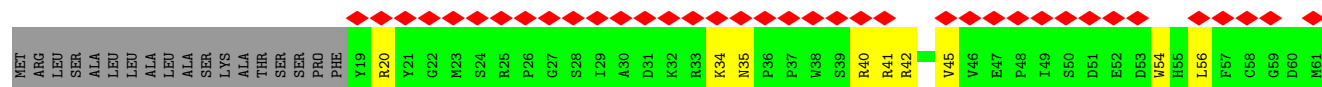
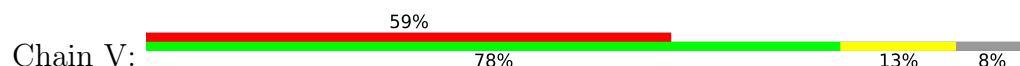
- Molecule 17: Large ribosomal subunit protein uL22m



- Molecule 18: Large ribosomal subunit protein uL23m

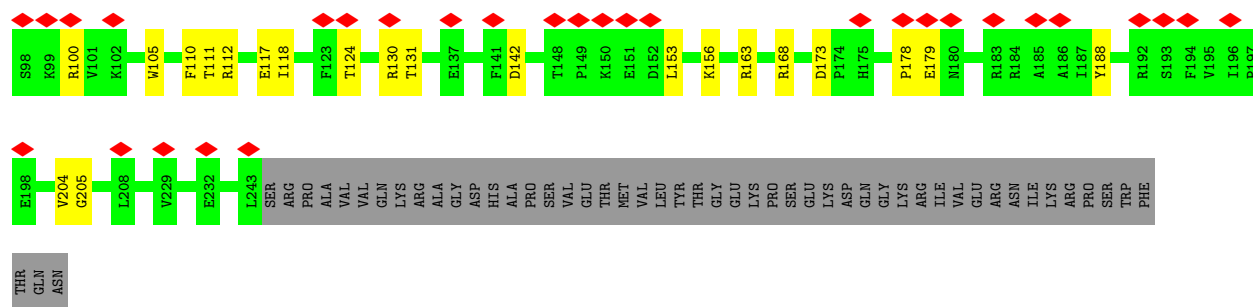


- Molecule 19: Large ribosomal subunit protein uL24m

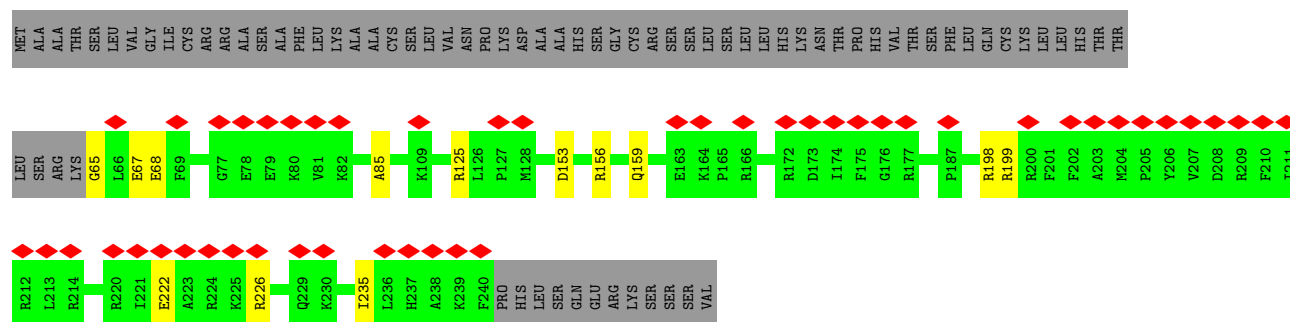


- Molecule 20: Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m

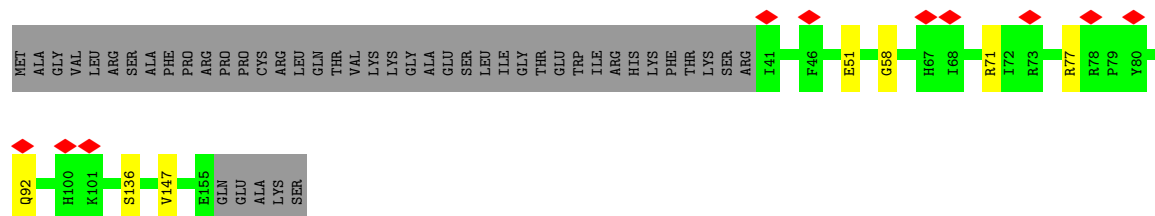




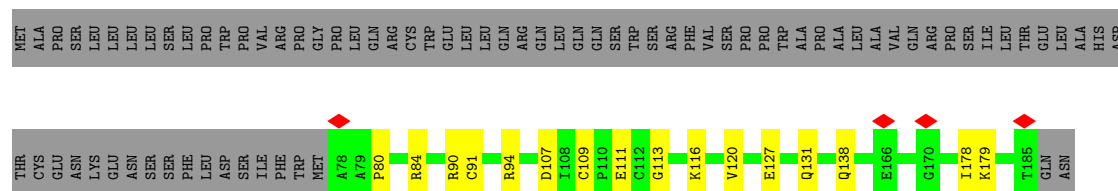
- Molecule 21: Large ribosomal subunit protein uL29m



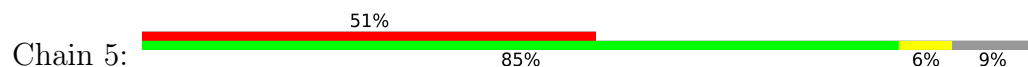
- Molecule 22: Large ribosomal subunit protein uL30m



- Molecule 23: Large ribosomal subunit protein bL32m

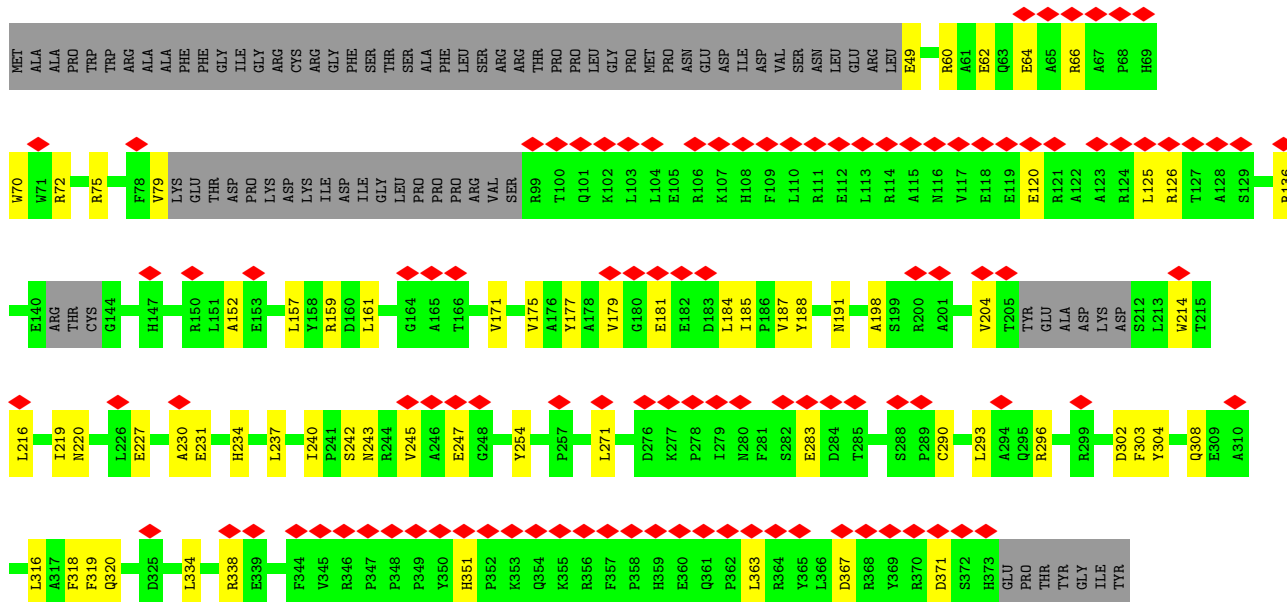


- Molecule 24: Large ribosomal subunit protein mL37

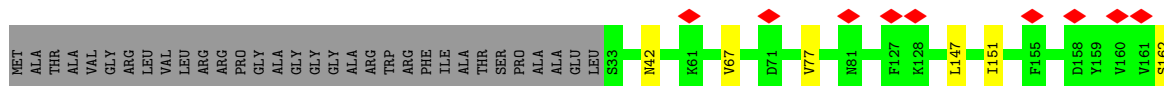
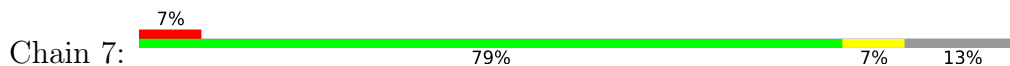


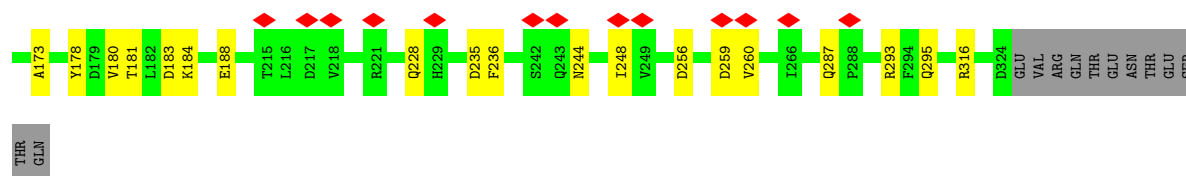


• Molecule 25: Large ribosomal subunit protein mL38

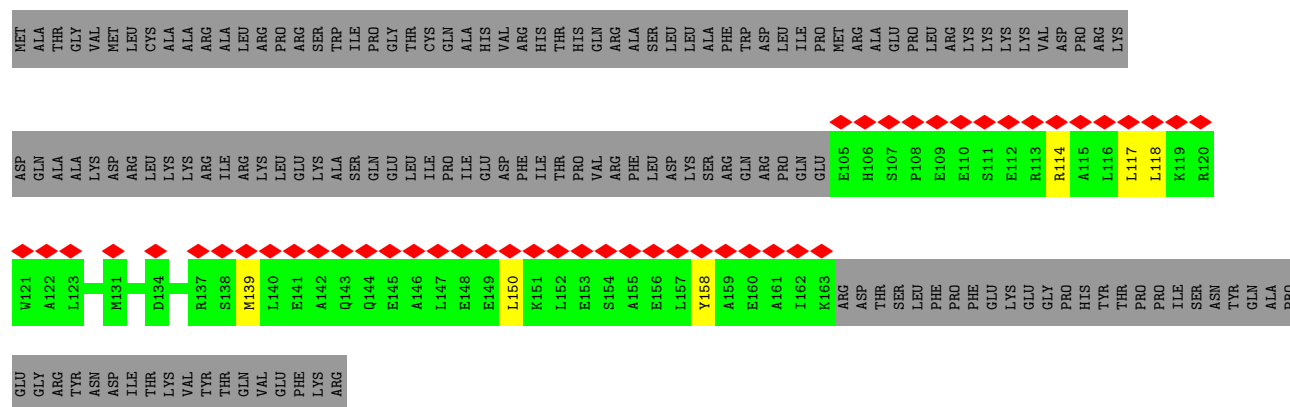


• Molecule 26: Large ribosomal subunit protein mL39

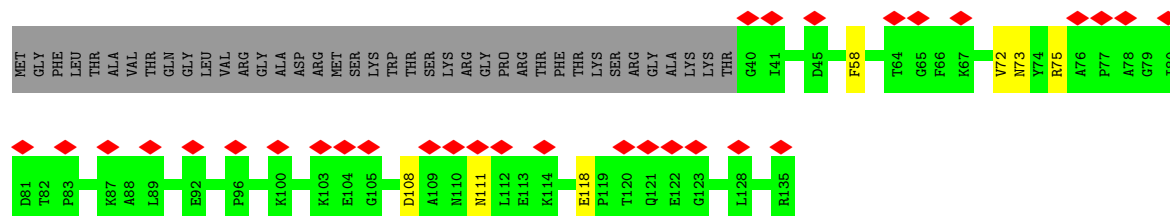




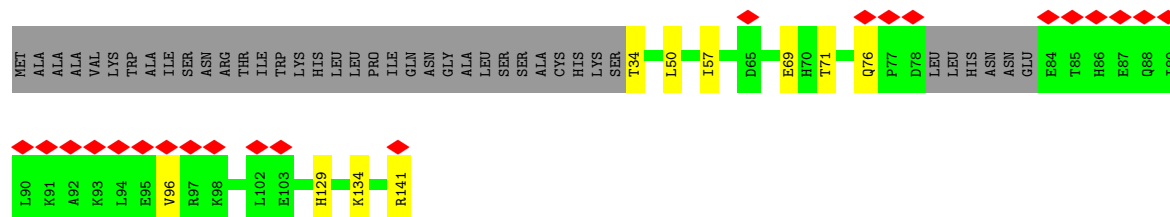
- Molecule 27: Large ribosomal subunit protein mL40



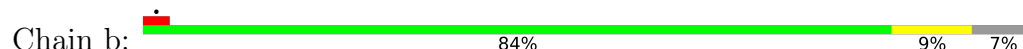
- Molecule 28: Large ribosomal subunit protein mL41



- Molecule 29: Large ribosomal subunit protein mL42

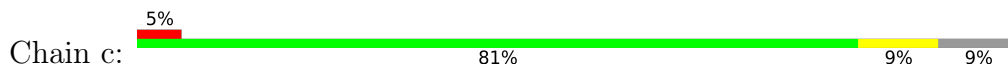


- Molecule 30: Large ribosomal subunit protein mL43

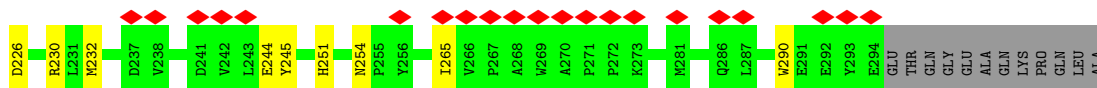
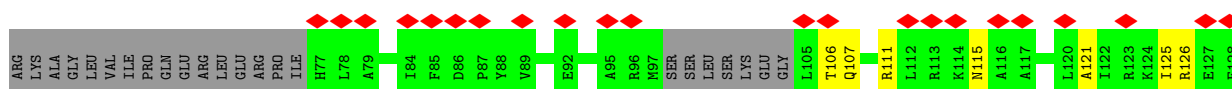
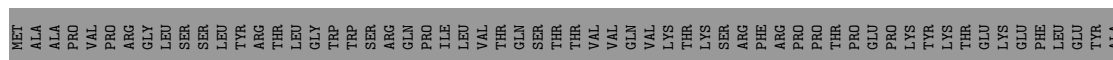




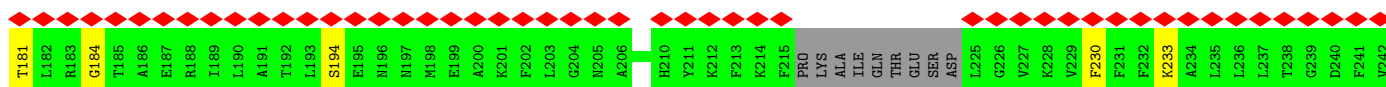
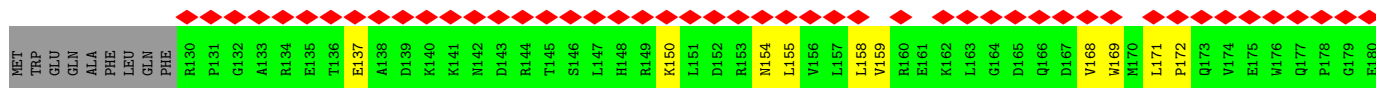
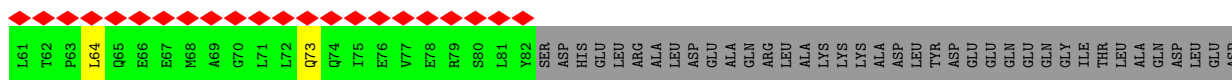
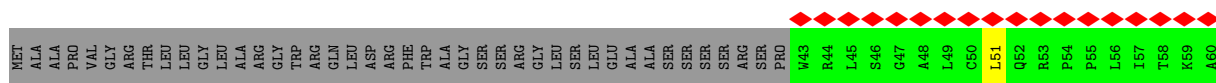
- Molecule 31: Large ribosomal subunit protein mL44

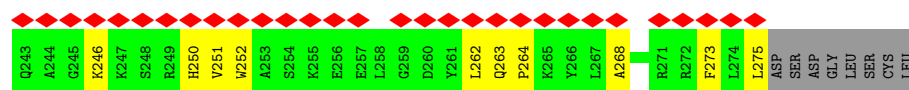


- Molecule 32: Large ribosomal subunit protein mL45

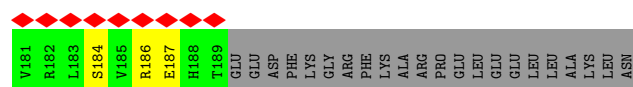
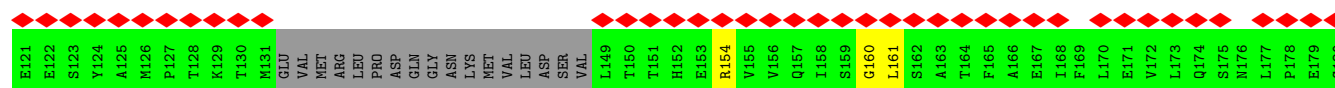
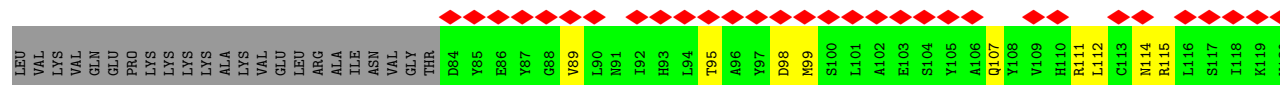
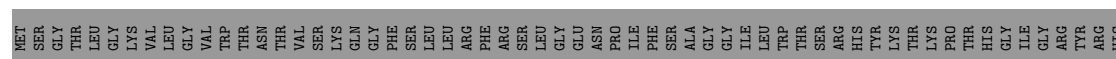
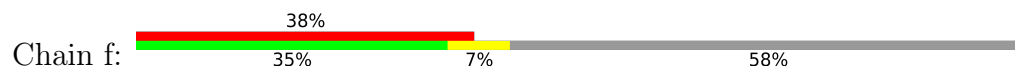


- Molecule 33: Large ribosomal subunit protein mL46

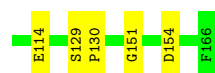
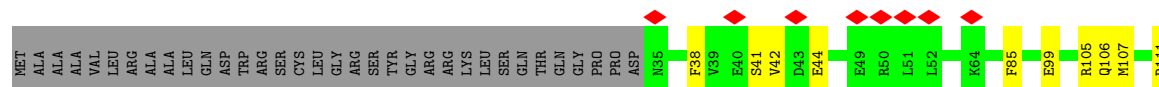




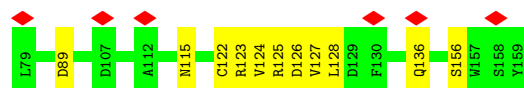
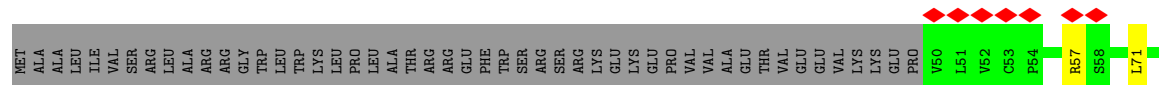
• Molecule 34: Large ribosomal subunit protein mL48



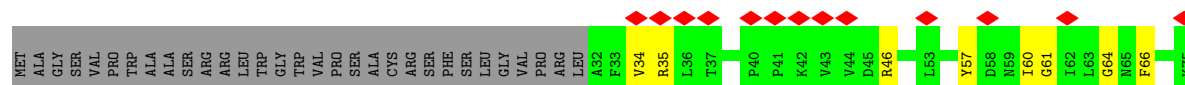
• Molecule 35: Large ribosomal subunit protein mL49



• Molecule 36: Large ribosomal subunit protein mL50



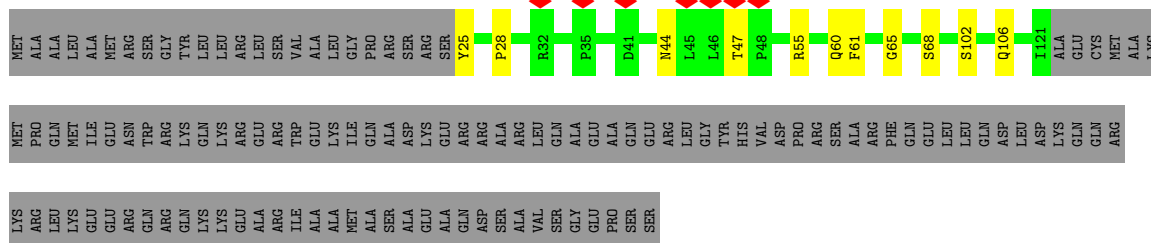
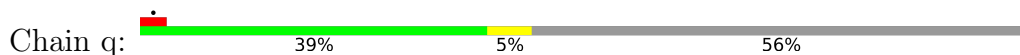
• Molecule 37: Large ribosomal subunit protein mL51



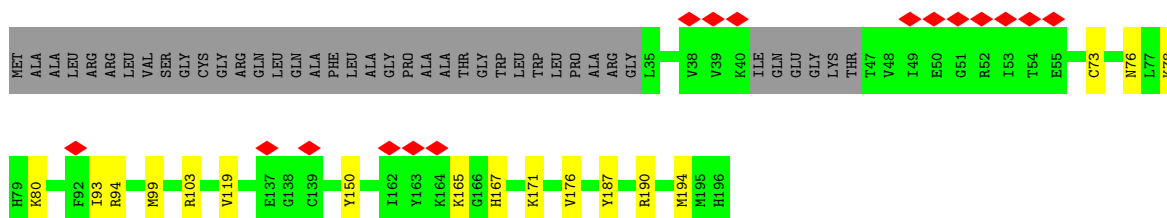




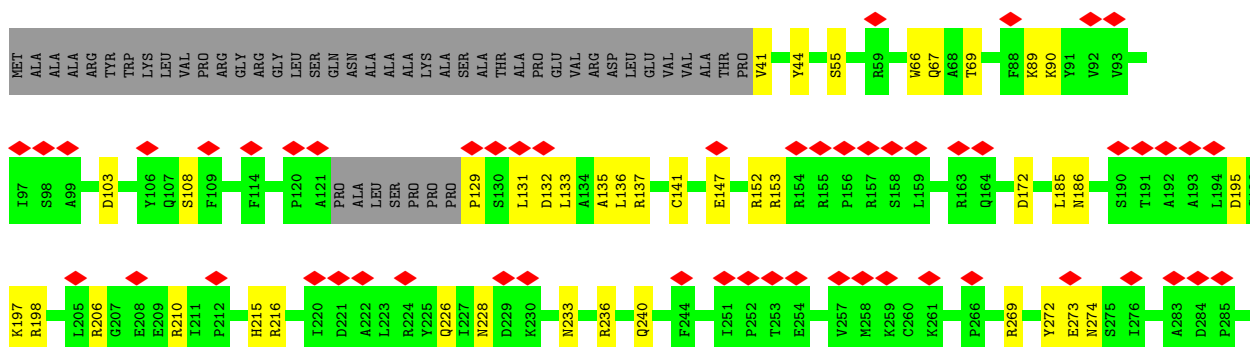
- Molecule 43: Large ribosomal subunit protein mL64

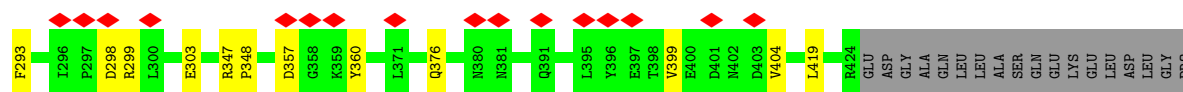


- Molecule 44: Large ribosomal subunit protein mL66

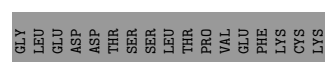
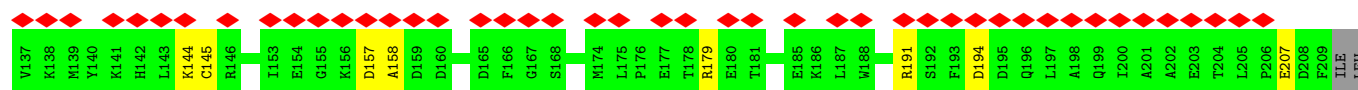
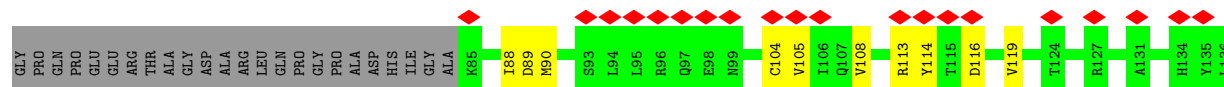
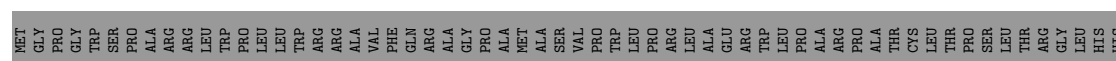


- Molecule 45: Large ribosomal subunit protein mL65

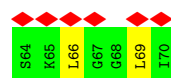
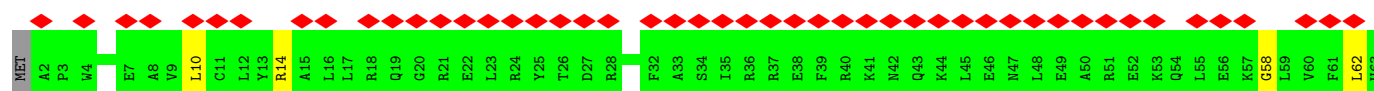
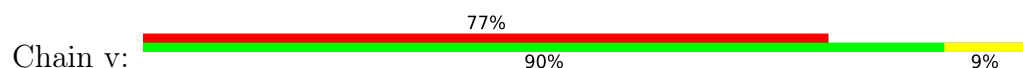




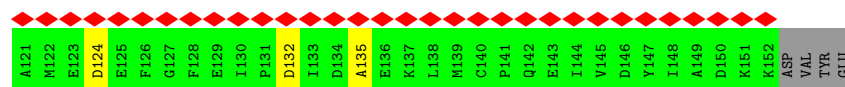
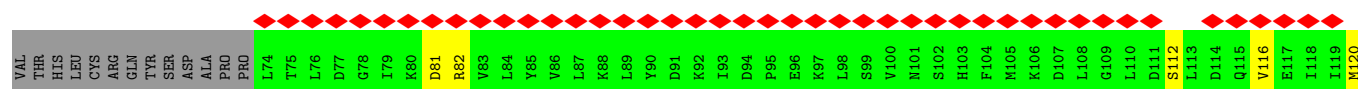
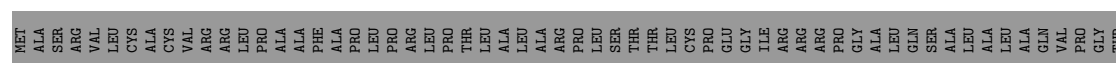
- Molecule 46: Mitochondrial assembly of ribosomal large subunit protein 1



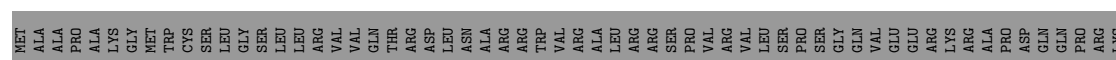
- Molecule 47: Predicted gene, 55359

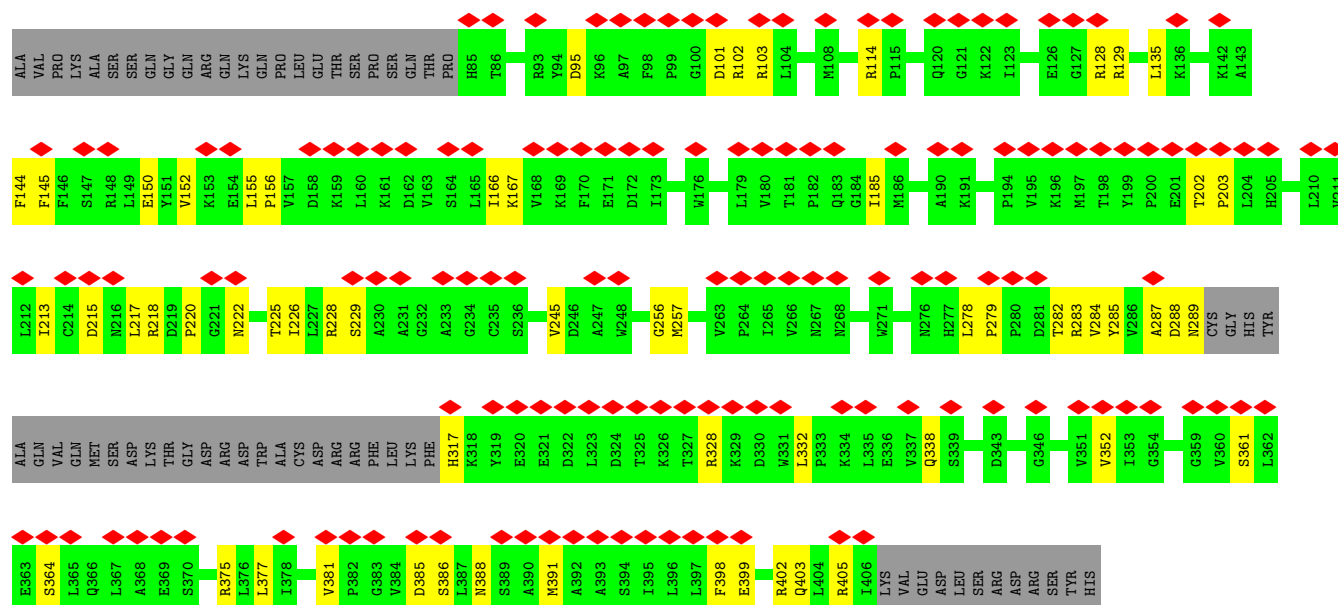


- Molecule 48: Acyl carrier protein, mitochondrial

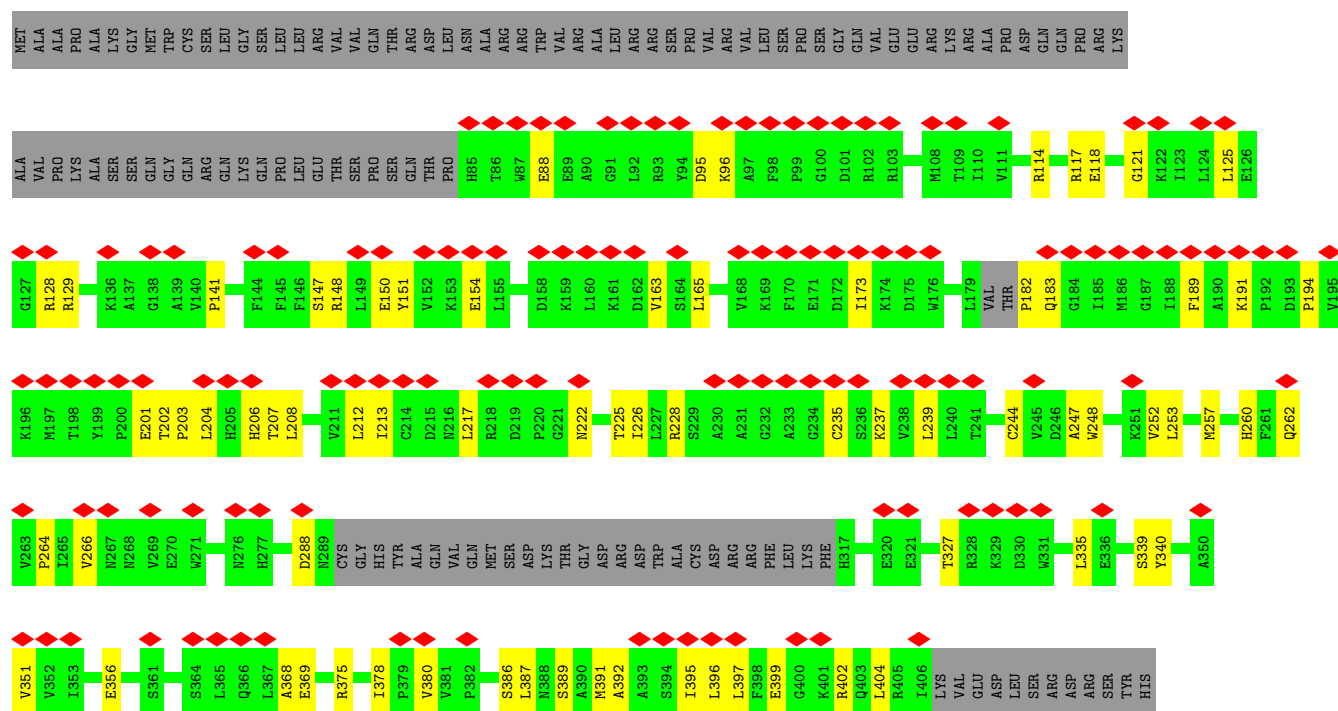


- Molecule 49: rRNA methyltransferase 3, mitochondrial

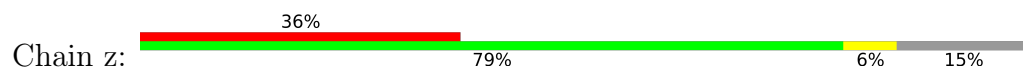


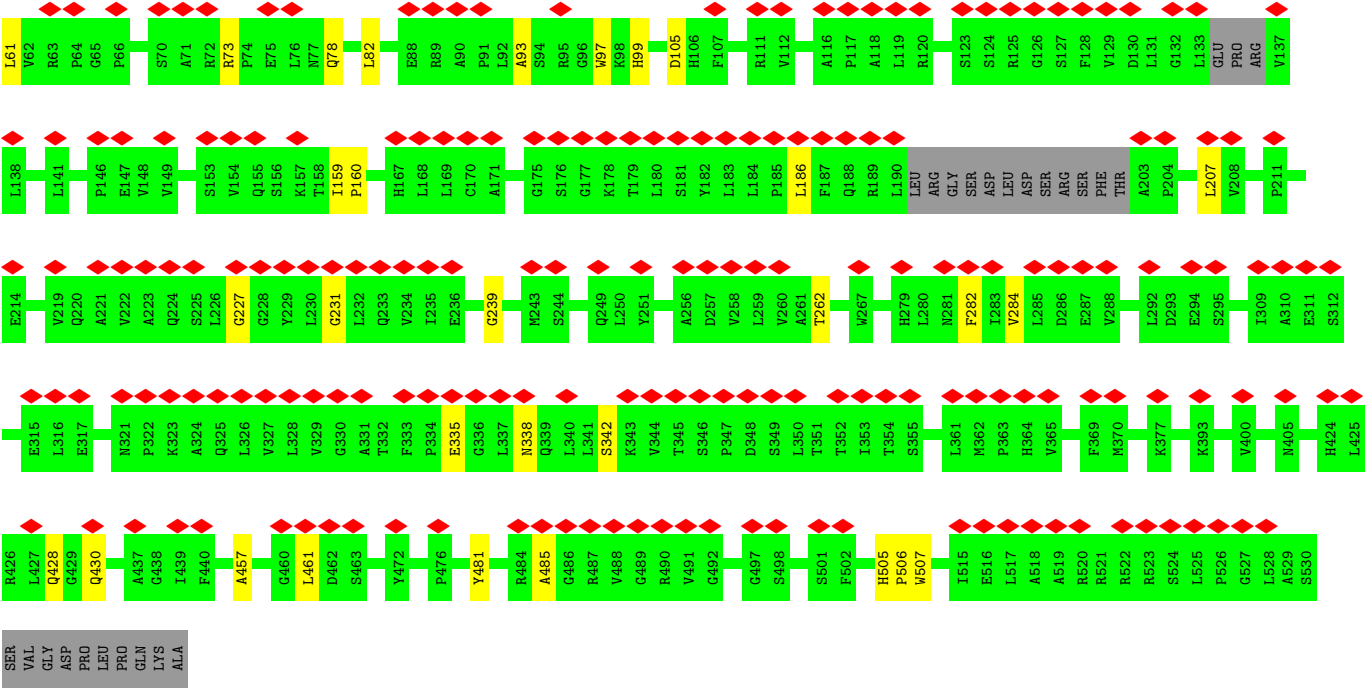


• Molecule 49: rRNA methyltransferase 3, mitochondrial



• Molecule 50: Probable ATP-dependent RNA helicase DDX28





## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:127:GLU:OE2	23:0:131:GLN:NE2	2.28	0.66
1:A:1756:C:OP1	23:0:138: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
23:0:116:LYS:NZ	23:0:120: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
23:0:107:ASP:N	23:0:116: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
23:0:131: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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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
23:0:178:ILE:HG22	23:0:179: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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	7,44	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	7,44	-	-	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

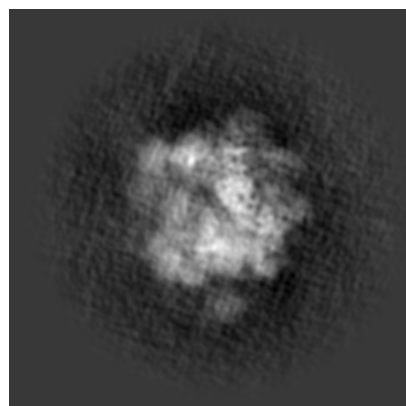
## 6 Map visualisation [i](#)

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

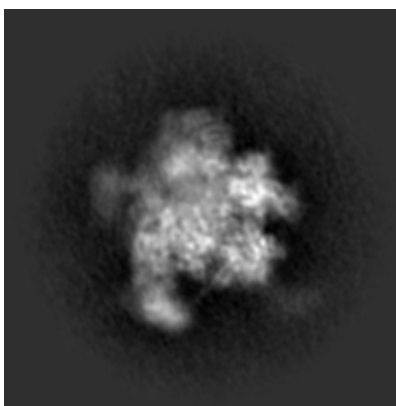
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

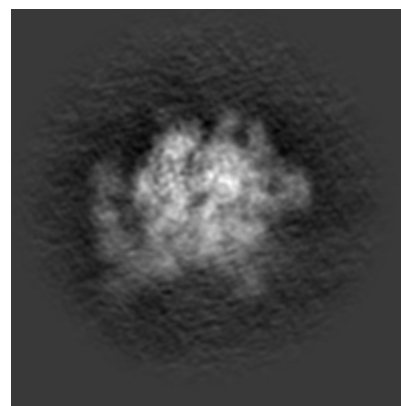
#### 6.1.1 Primary map



X

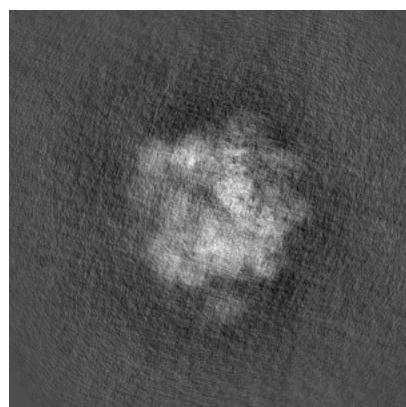


Y

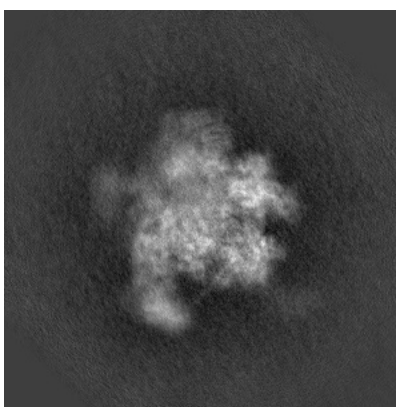


Z

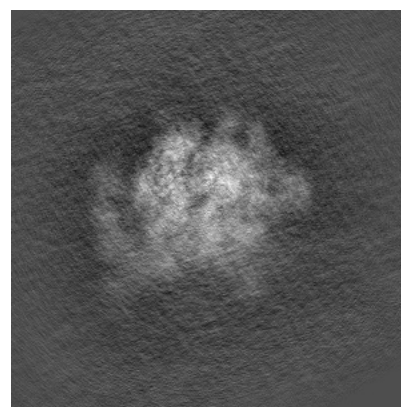
#### 6.1.2 Raw map



X



Y

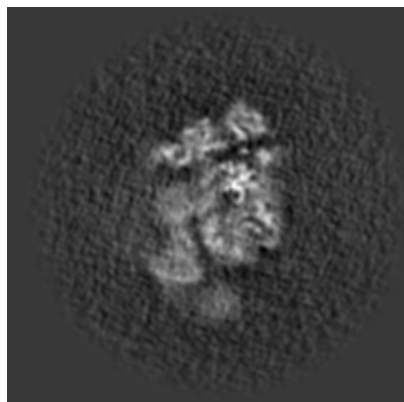


Z

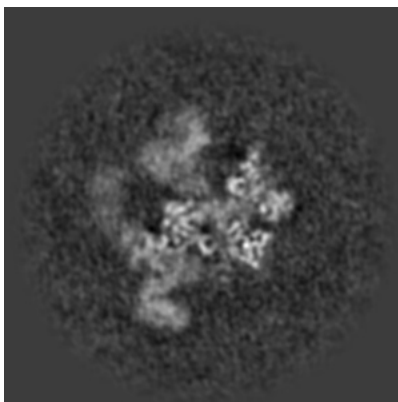
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

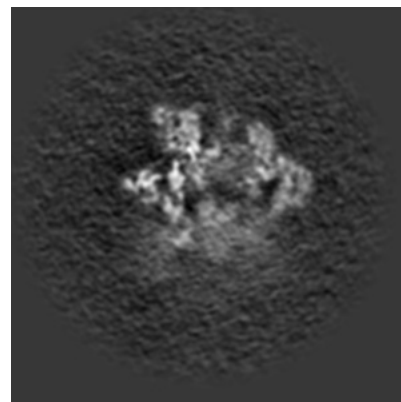
### 6.2.1 Primary map



X Index: 270

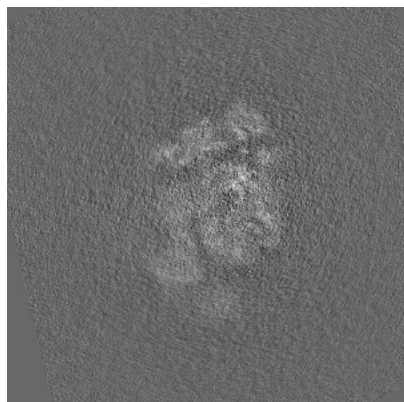


Y Index: 270

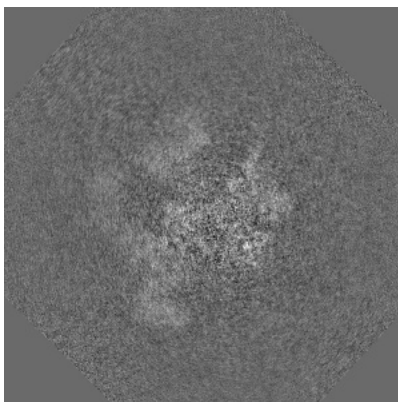


Z Index: 270

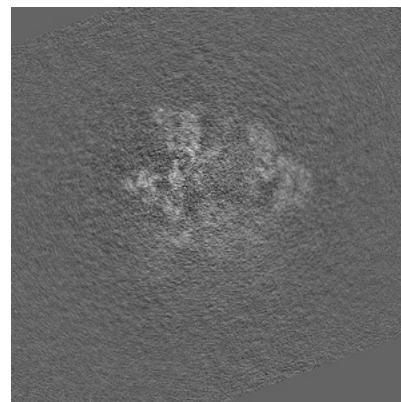
### 6.2.2 Raw map



X Index: 270



Y Index: 270



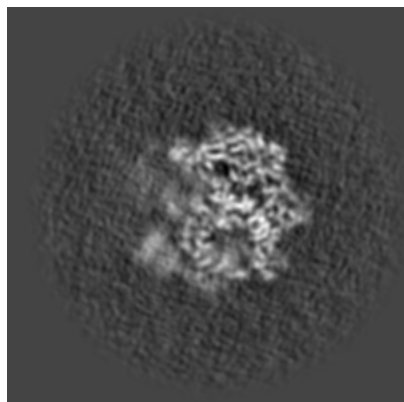
Z Index: 270

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

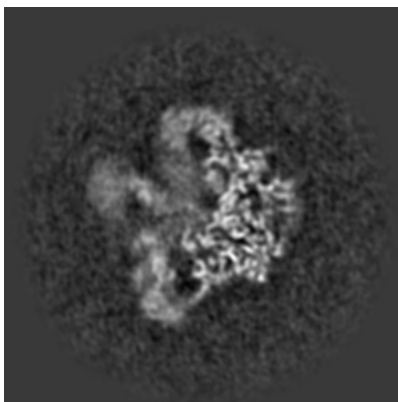


## 6.3 Largest variance slices [i](#)

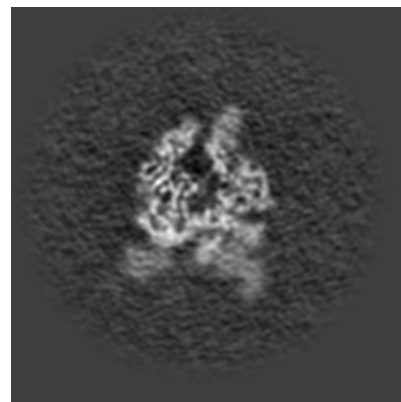
### 6.3.1 Primary map



X Index: 222

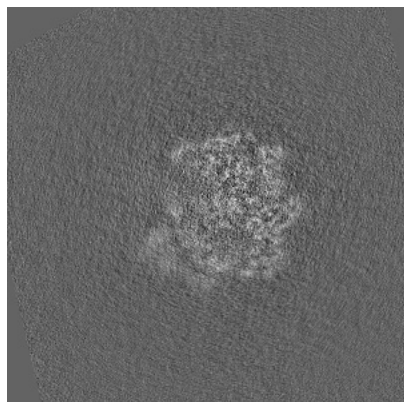


Y Index: 298

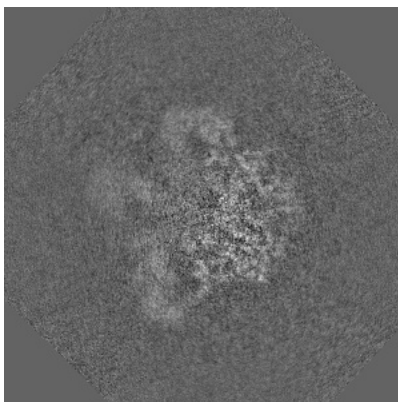


Z Index: 340

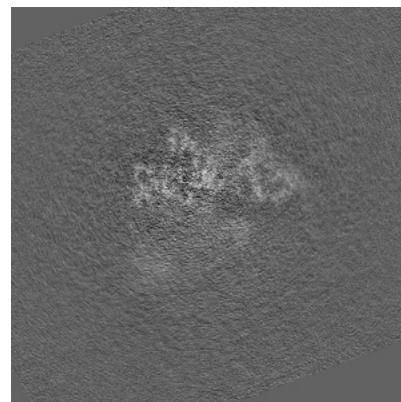
### 6.3.2 Raw map



X Index: 229



Y Index: 299

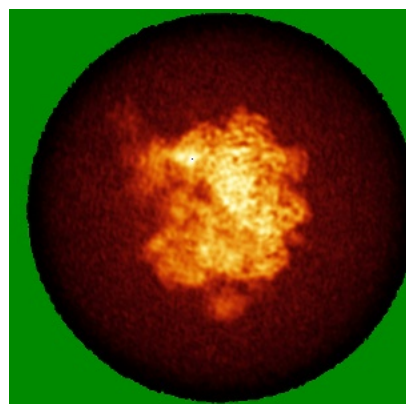


Z Index: 296

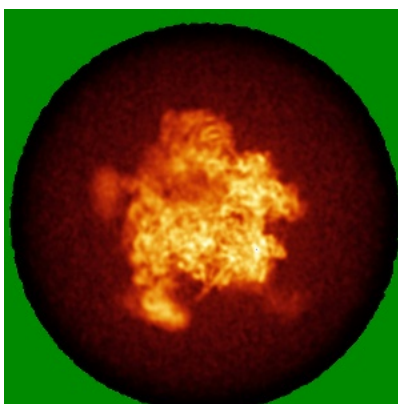
The images above show the largest variance slices of the map in three orthogonal directions.

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

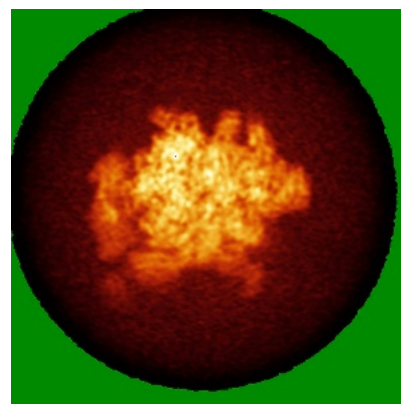
### 6.4.1 Primary map



X

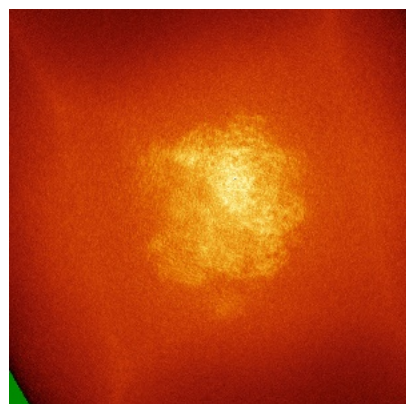


Y

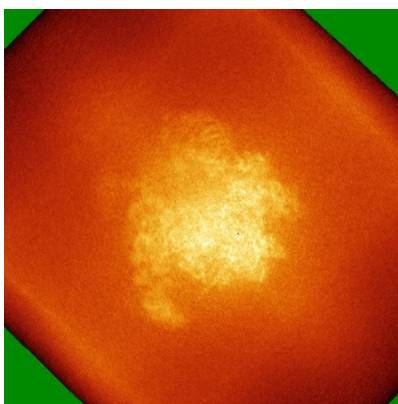


Z

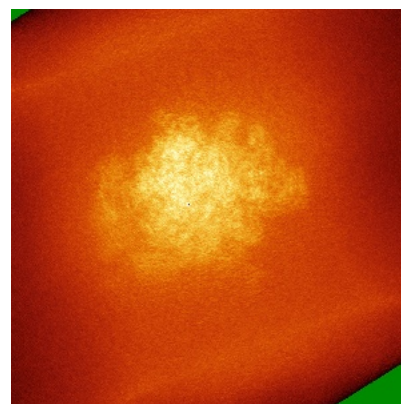
### 6.4.2 Raw map



X



Y

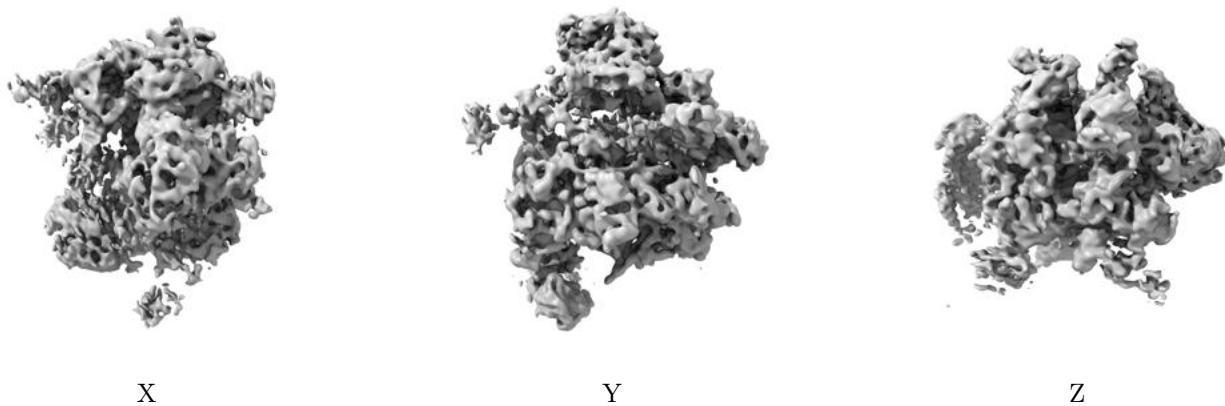


Z

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.

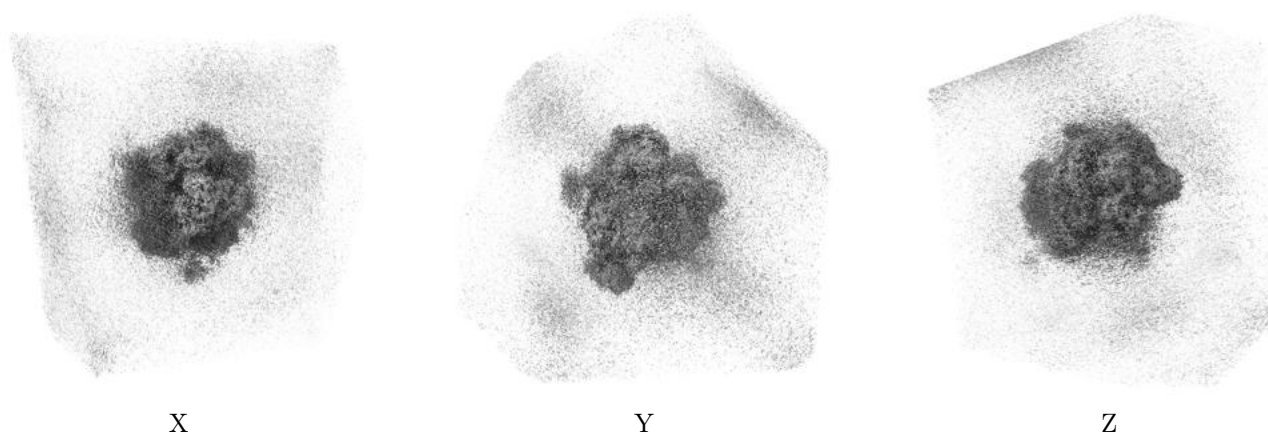
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



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

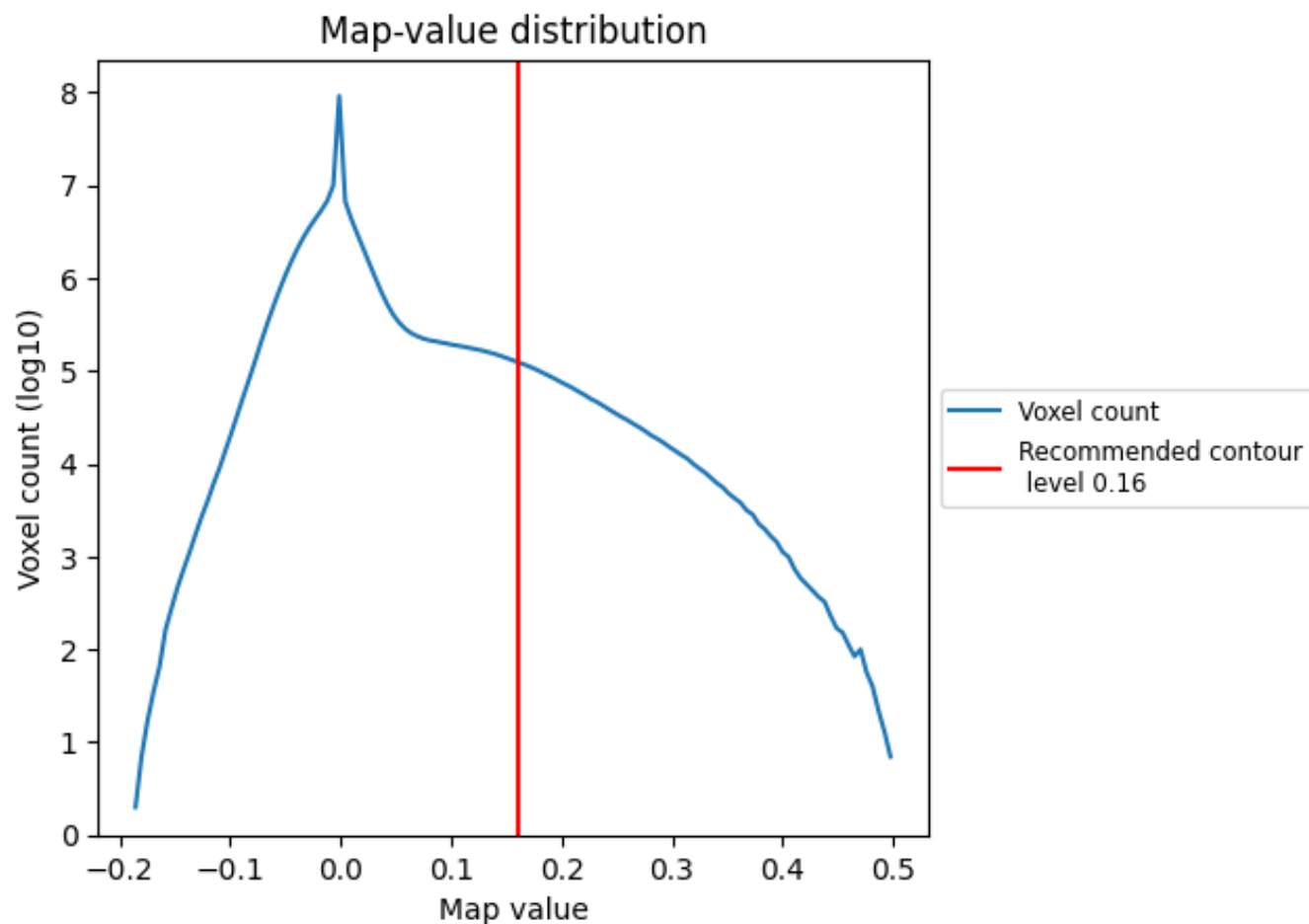
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

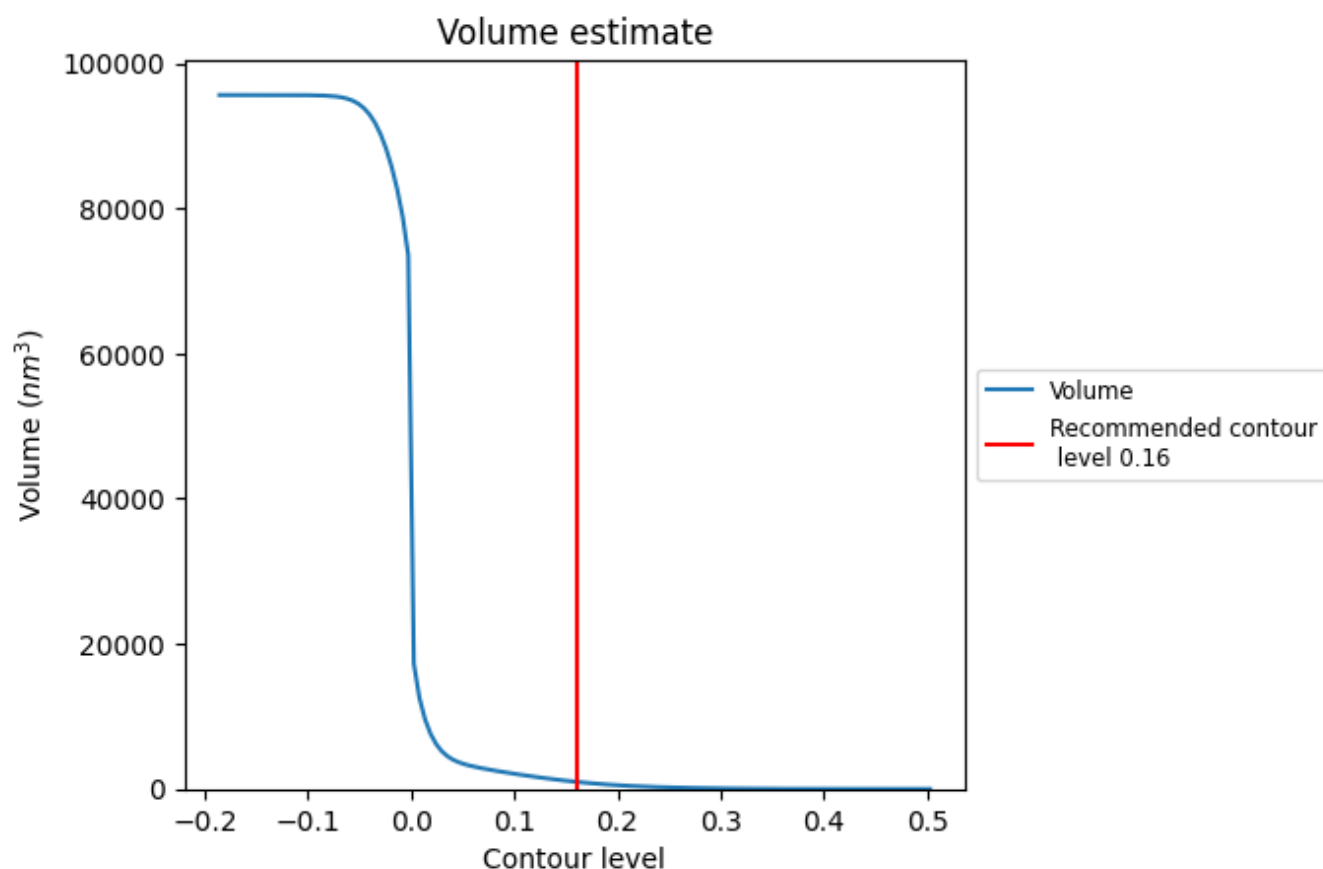
This section contains the results of statistical analysis of the map.

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



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

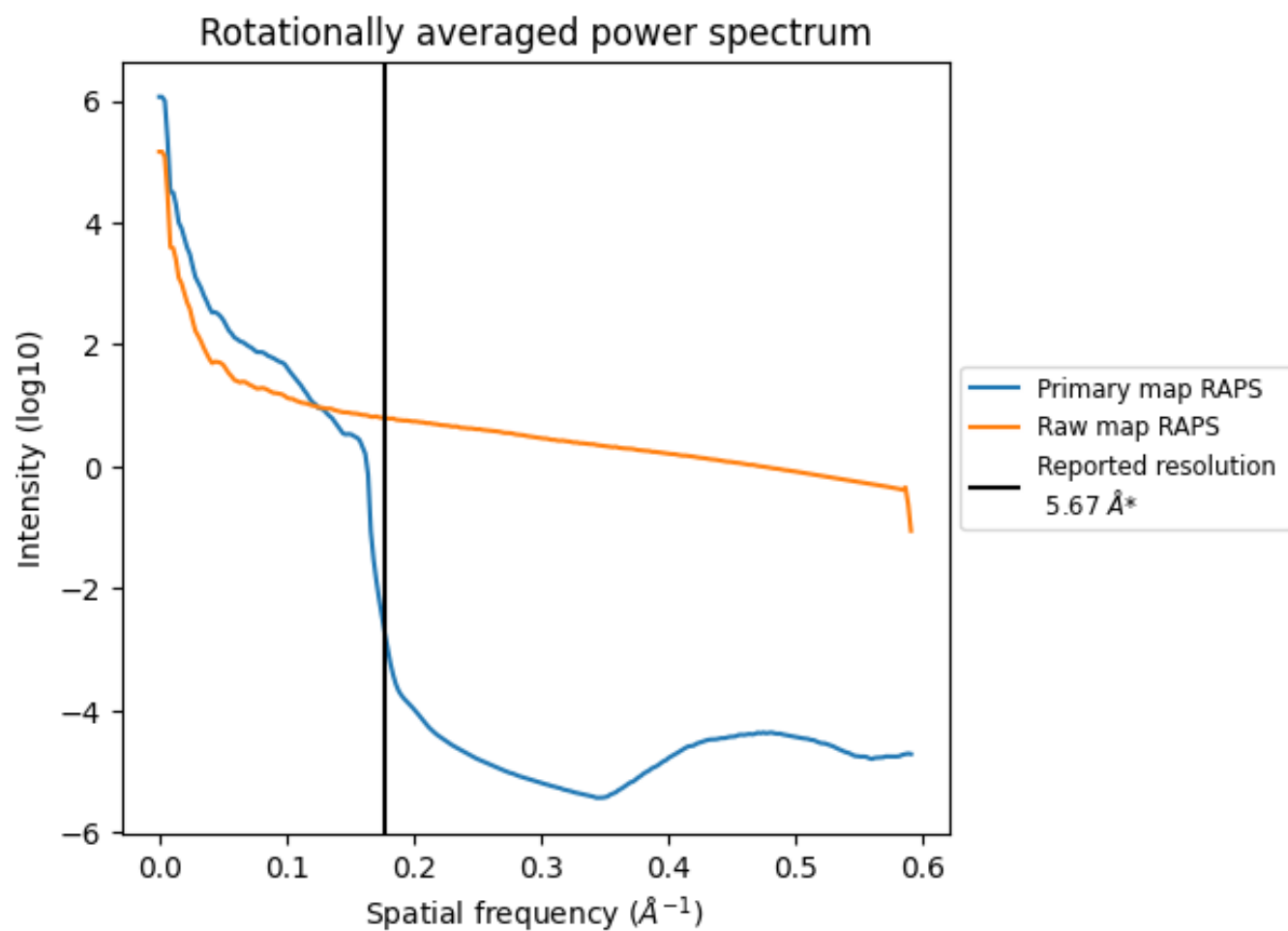
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm<sup>3</sup>; 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 ⓘ

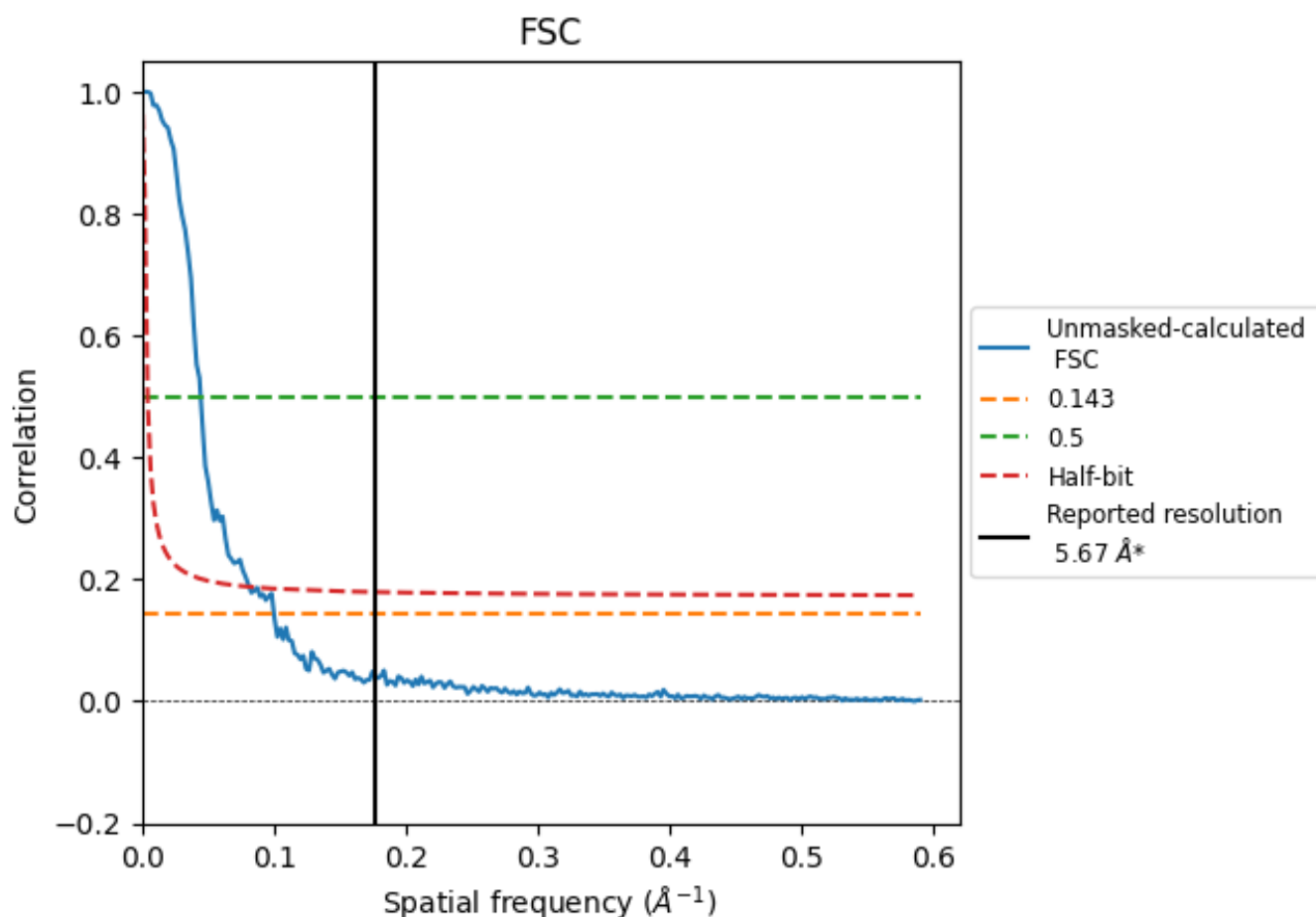


\*Reported resolution corresponds to spatial frequency of 0.176 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.176  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

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

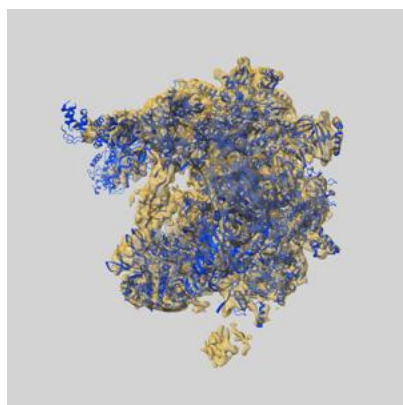
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.98 differs from the reported value 5.67 by more than 10 %



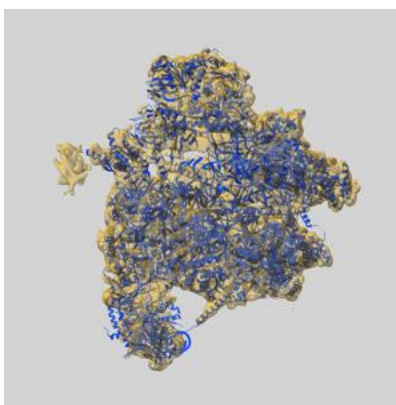
## 9 Map-model fit [i](#)

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.

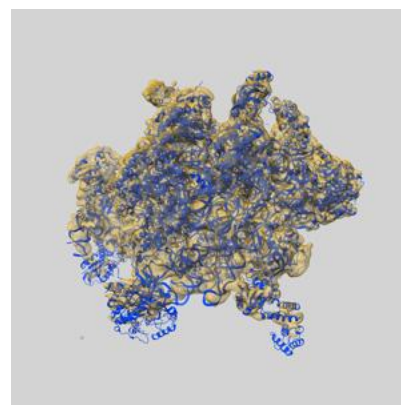
### 9.1 Map-model overlay [i](#)



X



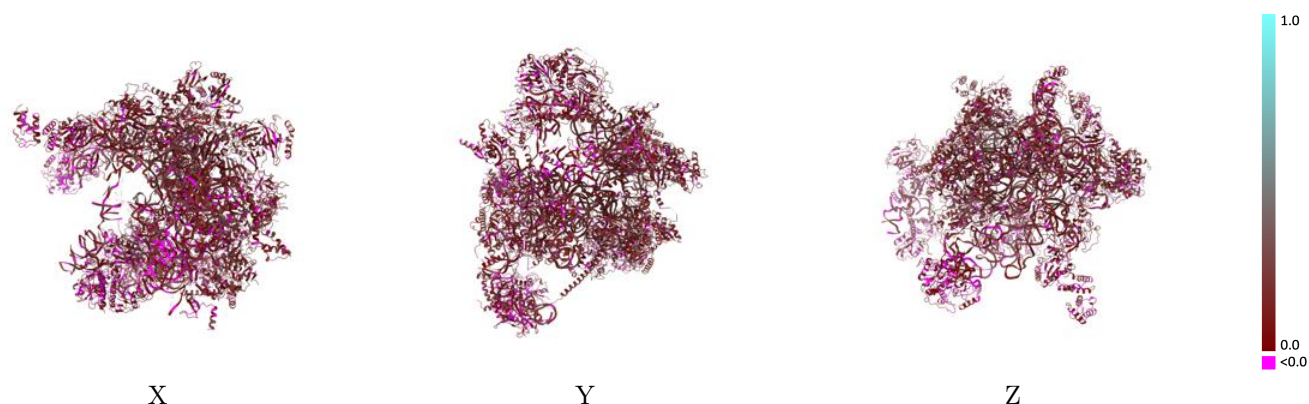
Y



Z

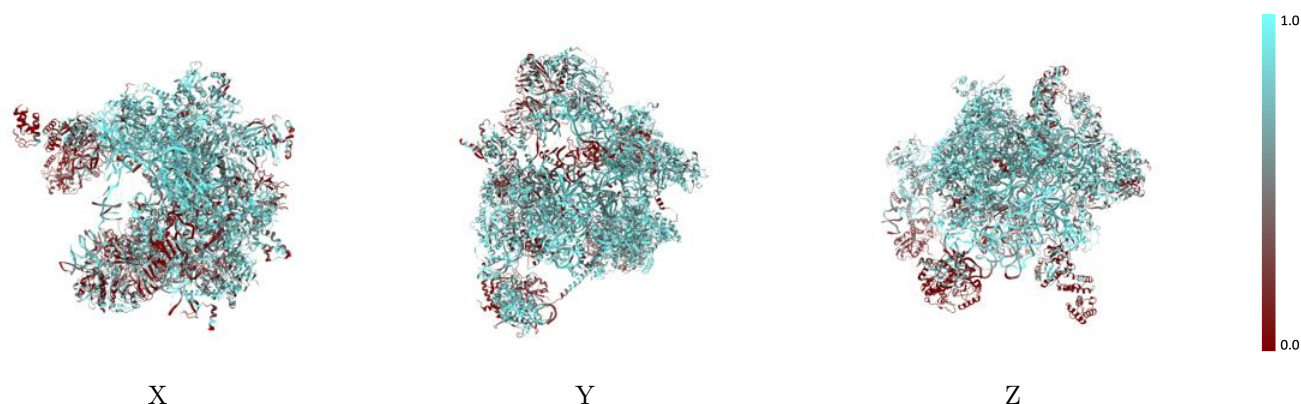
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



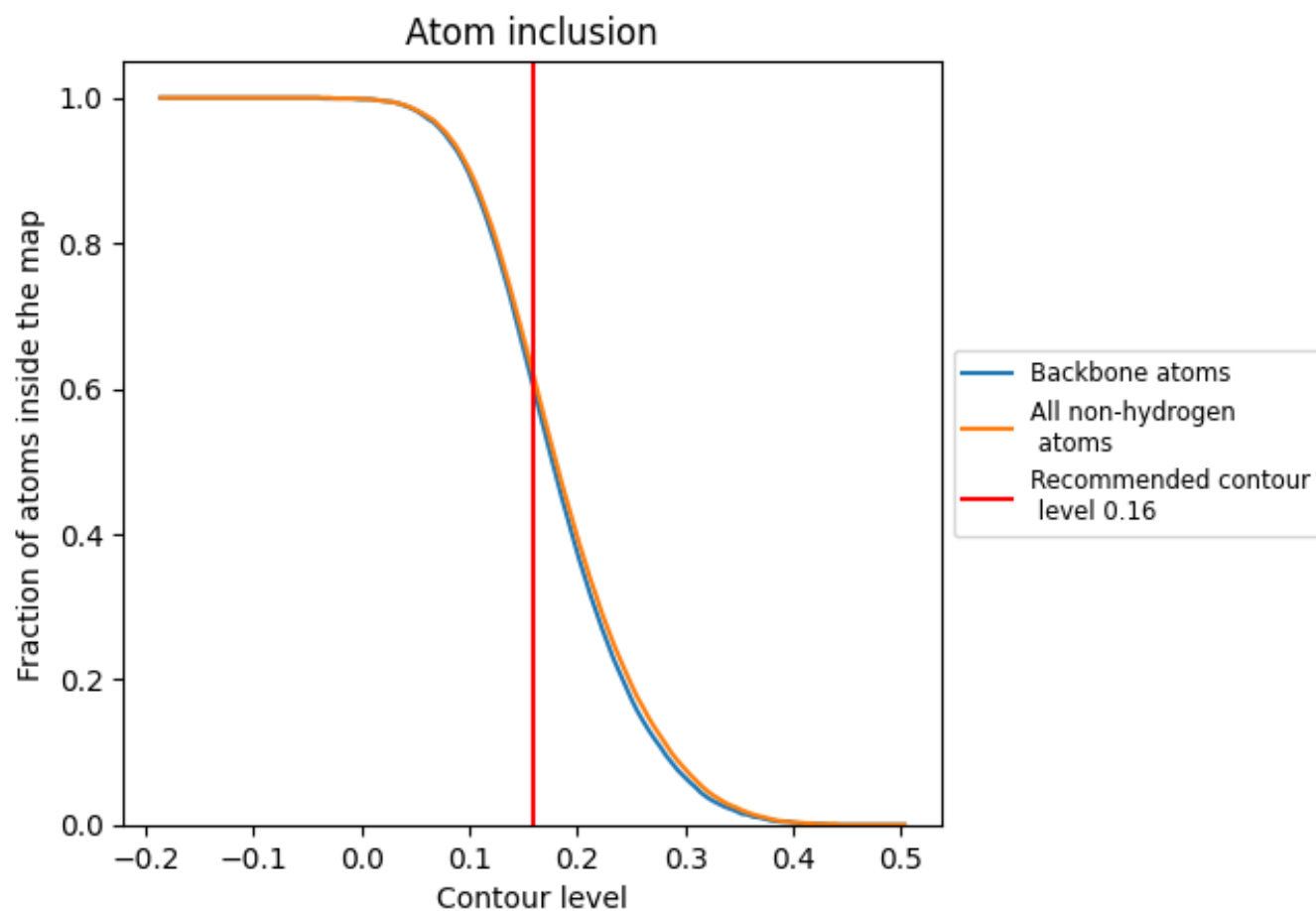
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



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



*Continued on next page...*

*Continued from previous page...*

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