



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 9HCE / pdb_00009hce
EMDB ID : EMD-52046
Title : Mouse mitoribosome large subunit assembly intermediate (without uL16m)
bound to MRM3 dimer and the MALSU-L0R8F8-mt-ACP complex, State A3
(SAMC knock out)
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.
Deposited on : 2024-11-08
Resolution : 7.31 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

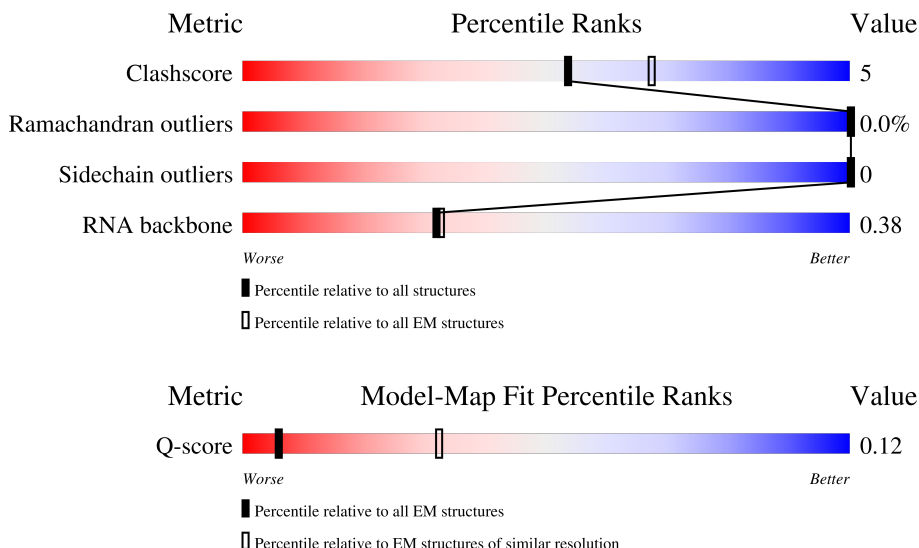
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.31 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	395 (6.81 - 7.80)

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

Mol	Chain	Length	Quality of chain
1	A	1584	19% 40% 21% 7% 31%
2	B	68	76% 49% 28% 13% 10%
3	D	246	41% 56% 14% 30%

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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	294	
6	H	268	
7	I	262	
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	198	
20	X	294	
21	Y	252	
22	Z	160	
23	0	187	
24	1	65	
25	5	423	
26	6	380	
27	7	336	
28	8	206	

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Mol	Chain	Length	Quality of chain
29	g	135	
30	a	142	
31	b	159	
32	c	308	
33	d	306	
34	e	283	
35	f	211	
36	g	166	
37	h	159	
38	i	128	
39	j	121	
40	k	118	
41	l	135	
42	o	102	
43	p	206	
44	q	222	
45	r	196	
46	s	442	
47	u	228	
48	v	70	
49	w	156	
50	x	418	
50	y	418	

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 158544 atoms, of which 72833 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	1086	Total	C	H	N	O	P	0	0
			34758	10383	11663	4192	7434	1086		

- 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	128	Total	C	H	N	O	S	0	0
			2129	667	1099	185	173	5		

- 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	144	Total	C	H	N	O	S	0	0
			2398	751	1215	220	207	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
			2674	840	1373	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 bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	1	56	Total	C	H	N	O		0	0
			967	296	508	86	77			

- Molecule 25 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	5	387	Total	C	H	N	O	S	0	0
			6355	2045	3187	554	560	9		

- Molecule 26 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	6	313	Total	C	H	N	O	S	0	0
			5218	1718	2545	484	465	6		

- Molecule 27 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	7	292	Total	C	H	N	O	S	0	0
			4757	1517	2378	409	438	15		

- Molecule 28 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	8	50	Total	C	H	N	O	S	0	0
			836	260	413	77	84	2		

- Molecule 29 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	9	96	Total	C	H	N	O	S	0	0
			1550	510	772	123	144	1		

- Molecule 30 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	84	Total	C	H	N	O	S	0	0
			1368	442	667	126	130	3		

- Molecule 31 is a protein called Large ribosomal subunit protein mL43.

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

- Molecule 32 is a protein called Large ribosomal subunit protein mL44.

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

- Molecule 33 is a protein called Large ribosomal subunit protein mL45.

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

- Molecule 34 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	118	Total	C	H	N	O	S	0	0
			1962	638	991	169	159	5		

- Molecule 35 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	83	Total	C	H	N	O	S	0	0
			1320	423	653	113	128	3		

- Molecule 36 is a protein called Large ribosomal subunit protein mL49.

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

- Molecule 37 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	110	Total	C	H	N	O	S	0	0
			1739	552	867	156	160	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL51.

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

- Molecule 39 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	j	84	Total	C	H	N	O	S	0	0
			1366	423	687	134	120	2		

- Molecule 40 is a protein called Large ribosomal subunit protein mL53.

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

- Molecule 41 is a protein called Large ribosomal subunit protein mL54.

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

- Molecule 42 is a protein called Large ribosomal subunit protein mL63.

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

- Molecule 43 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	103	Total	C	H	N	O		0	0
			853	332	301	106	114			

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

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

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	156	Total	C	H	N	O	S	0	0
			2585	806	1318	241	209	11		

- Molecule 46 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	s	377	Total	C	H	N	O	S	0	0
			6103	1938	3058	555	540	12		

- Molecule 47 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 48 is a protein called Predicted gene, 55359.

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

- Molecule 49 is a protein called Acyl carrier protein, mitochondrial.

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

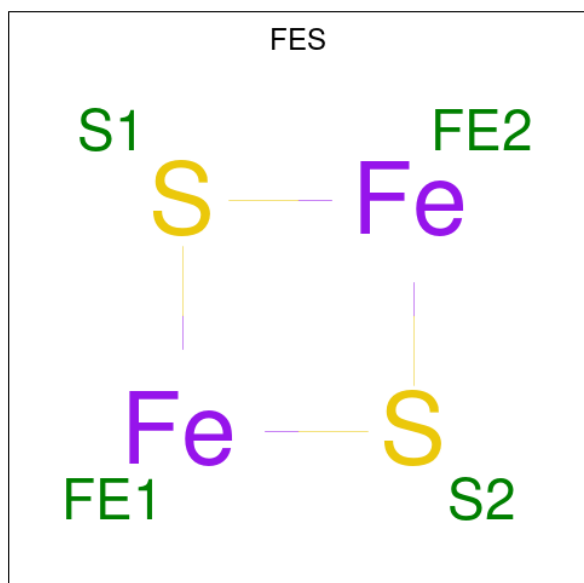
- Molecule 50 is a protein called rRNA methyltransferase 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	237	Total	C	H	N	O		
			1798	715	602	241	240		
50	y	247	Total	C	H	N	O		
			1909	756	649	252	252		
								0	0

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

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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

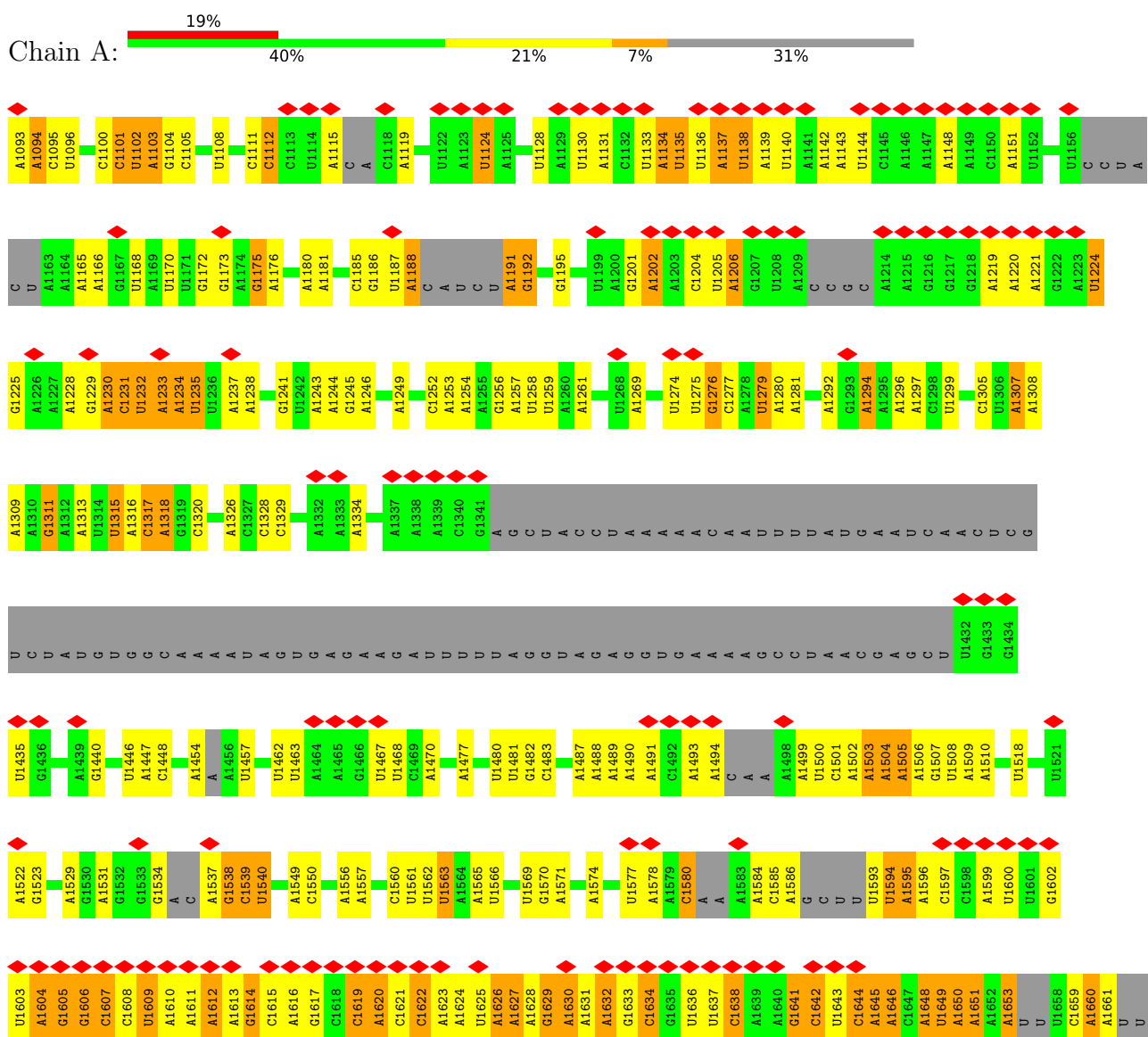


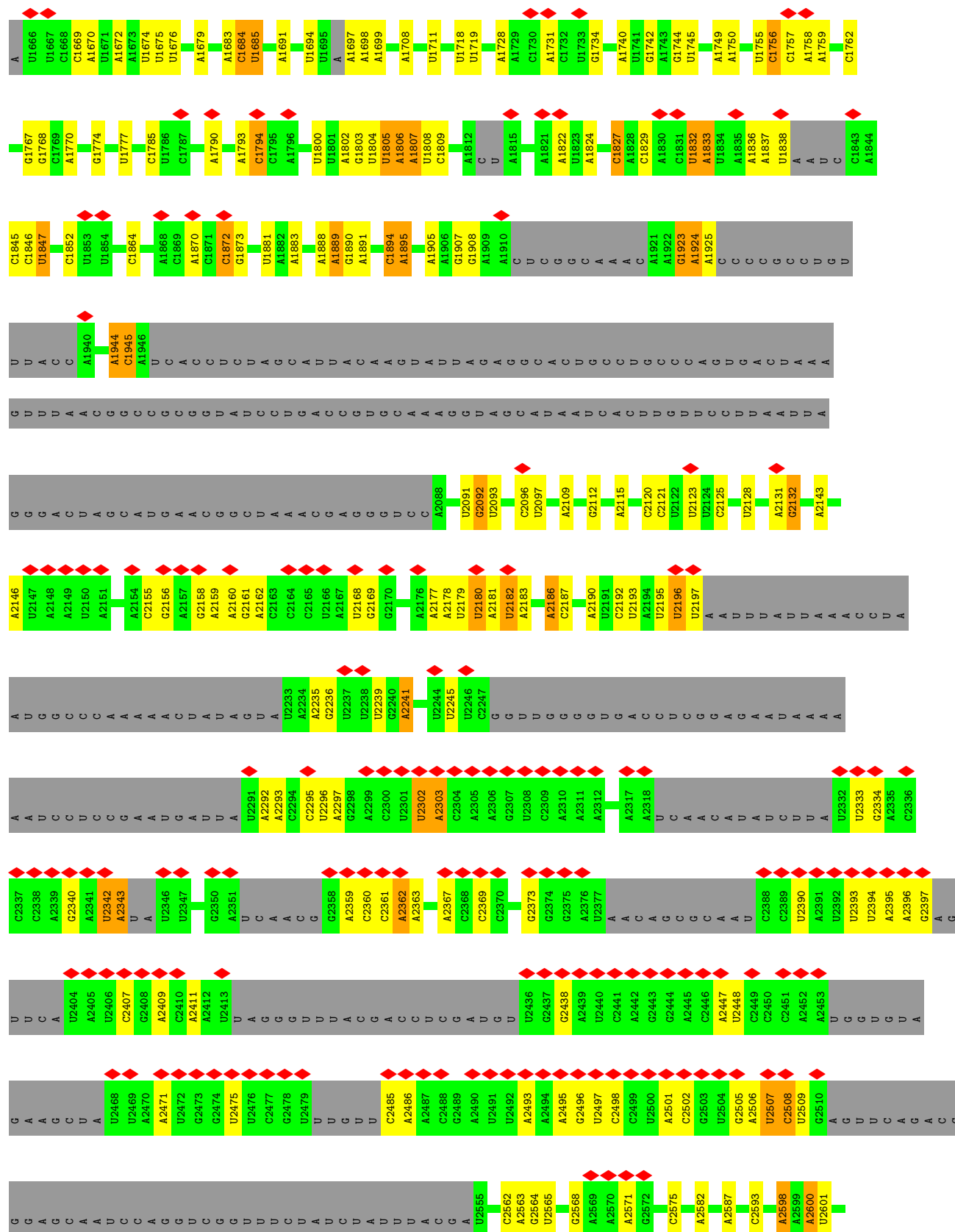
Mol	Chain	Residues	Atoms			AltConf
52	r	1	Total	Fe	S	
			4	2	2	
						0

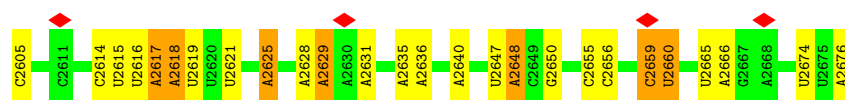
3 Residue-property plots

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

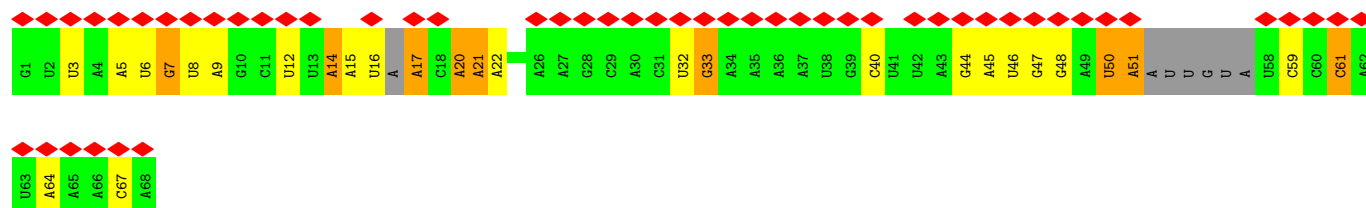
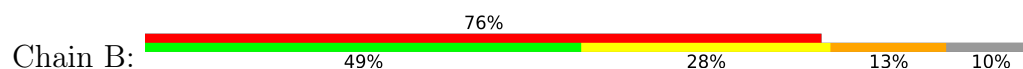
• Molecule 1: 16S rRNA (1584-MER)



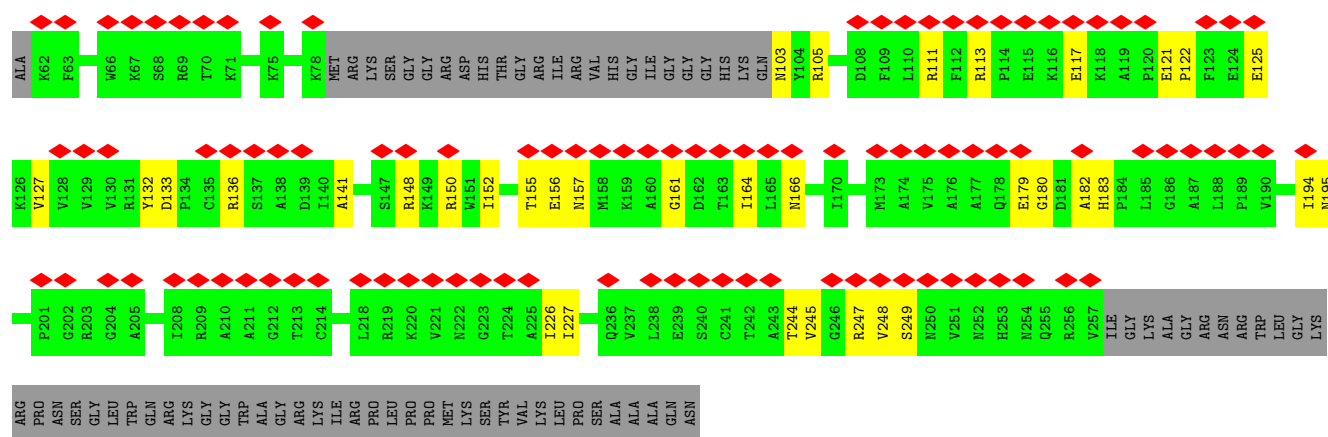
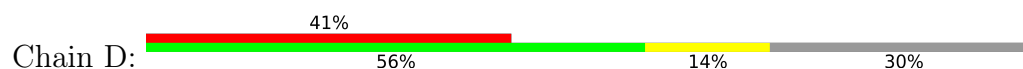




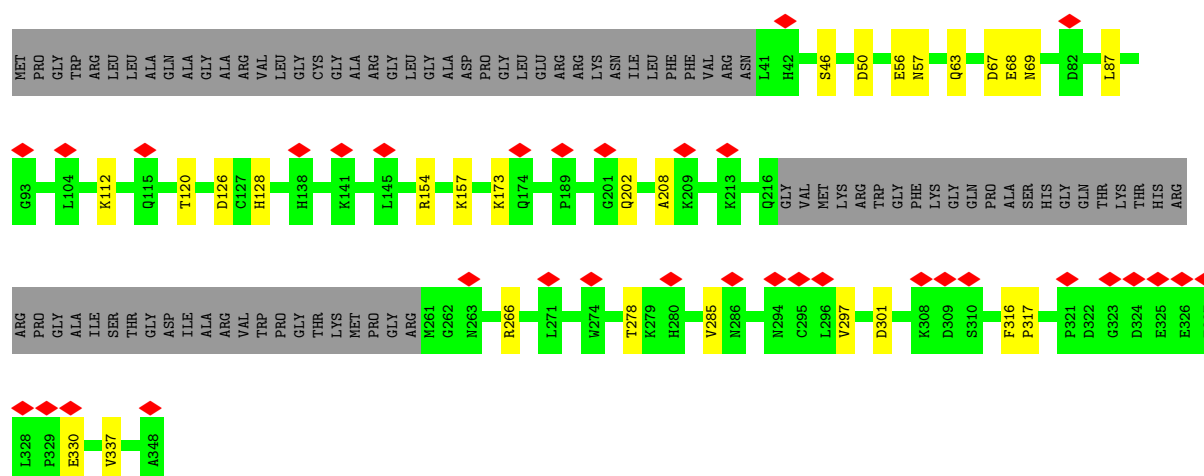
• Molecule 2: tRNA-Phe (68-MER)



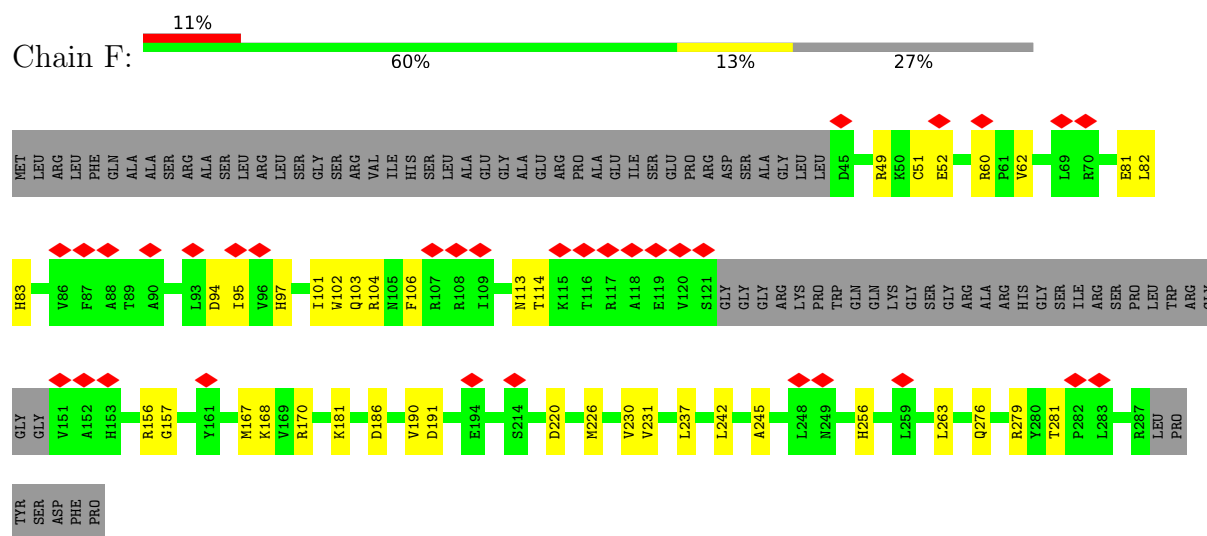
• Molecule 3: Large ribosomal subunit protein uL2m



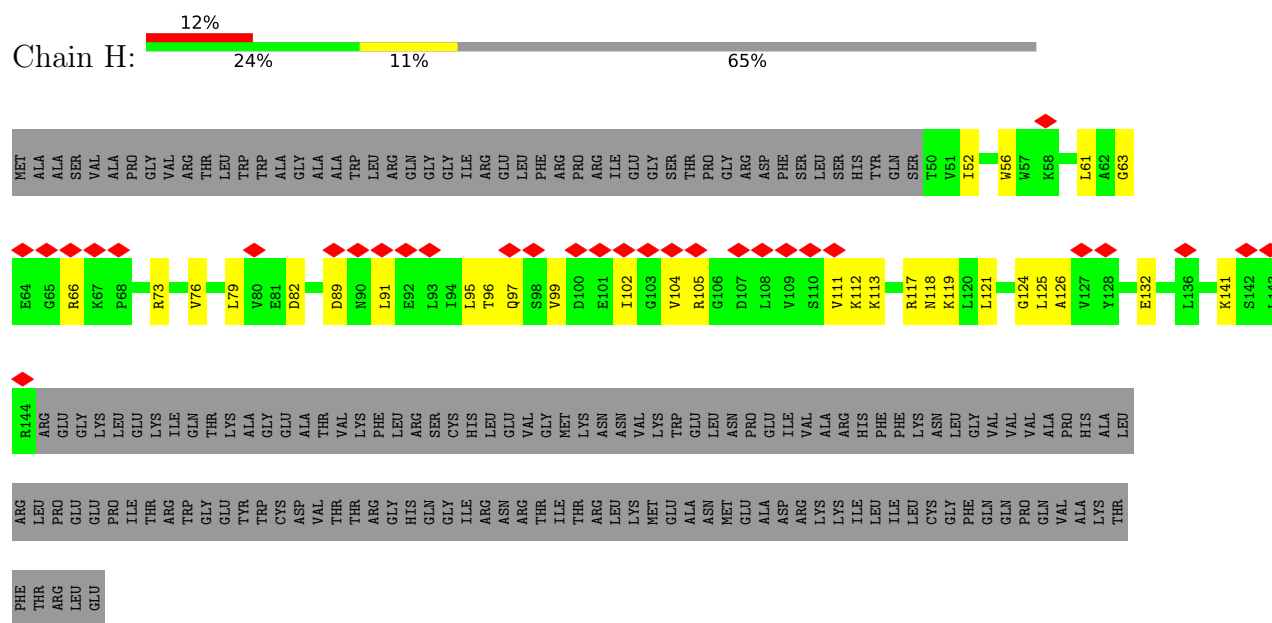
• Molecule 4: Large ribosomal subunit protein uL3m



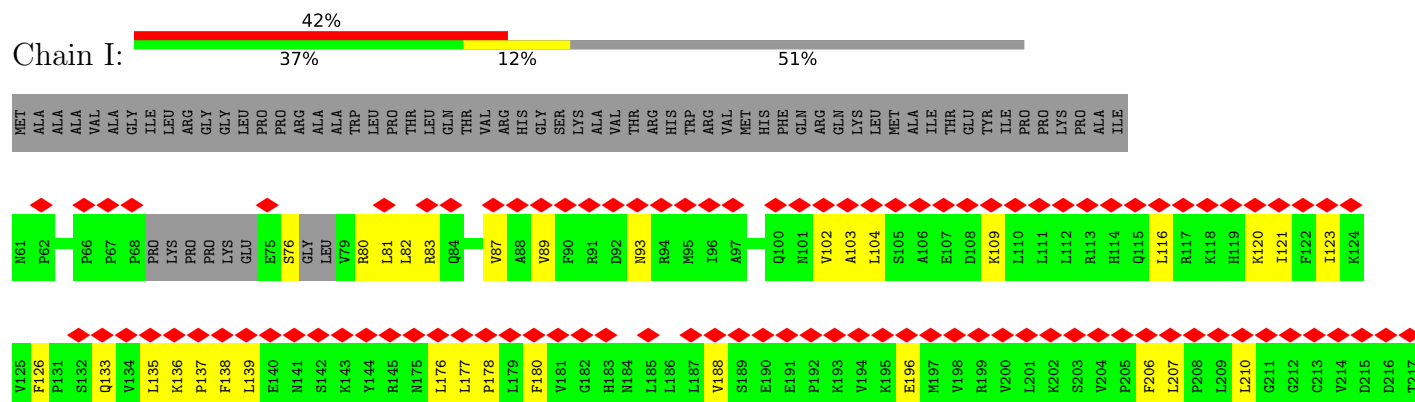
- Molecule 5: Large ribosomal subunit protein uL4m

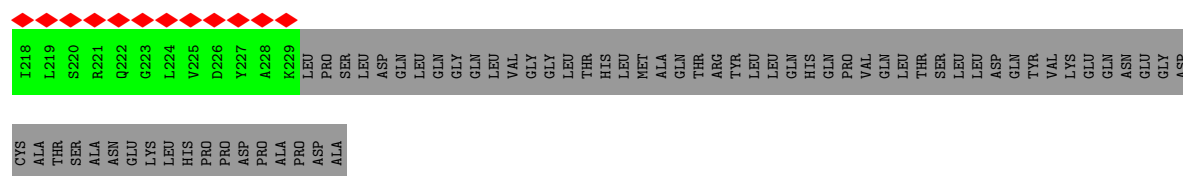


- Molecule 6: Large ribosomal subunit protein bL9m

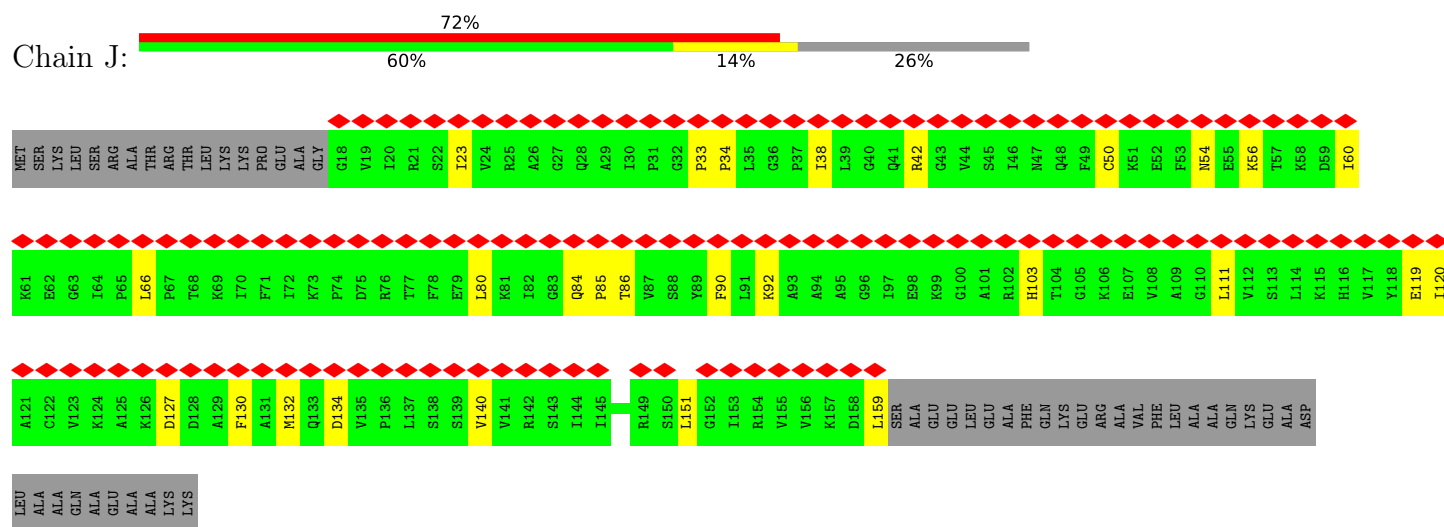


- Molecule 7: Large ribosomal subunit protein uL10m

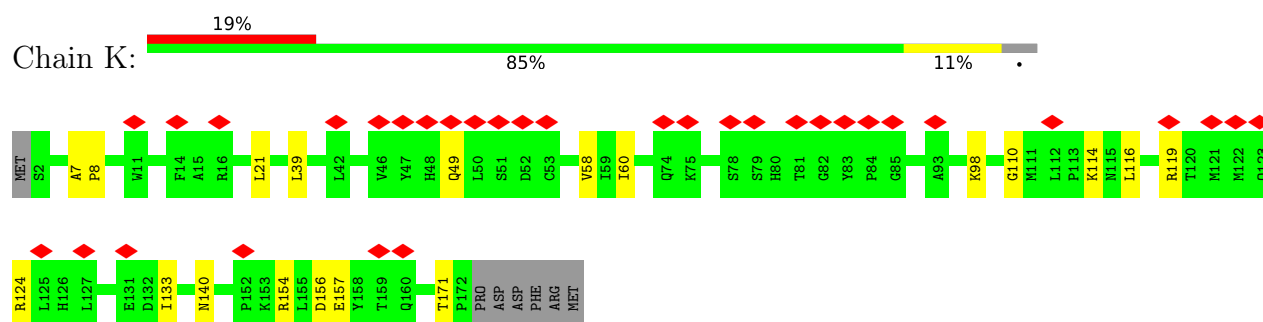




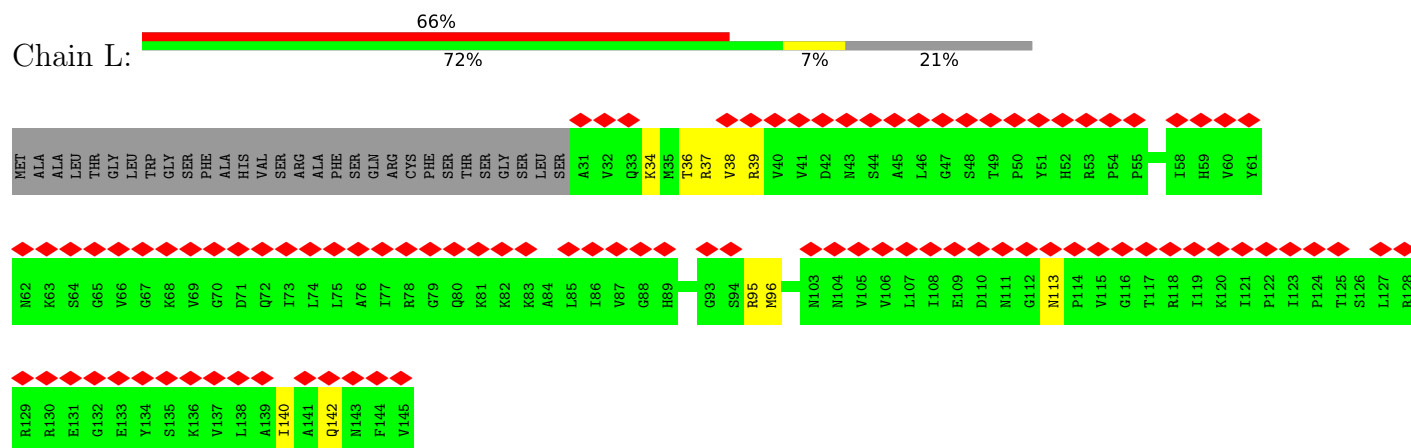
- Molecule 8: Large ribosomal subunit protein uL11m



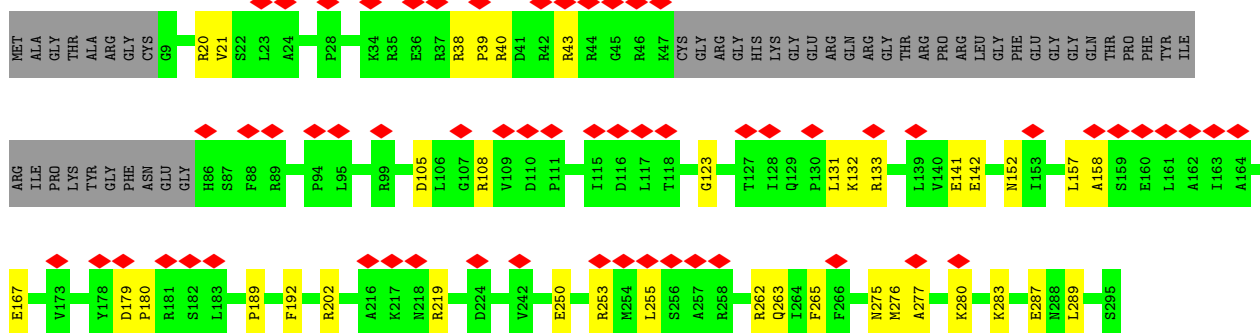
- Molecule 9: Large ribosomal subunit protein uL13m



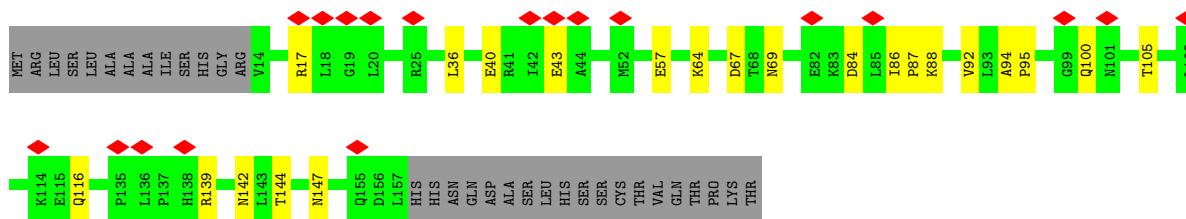
- Molecule 10: Large ribosomal subunit protein uL14m



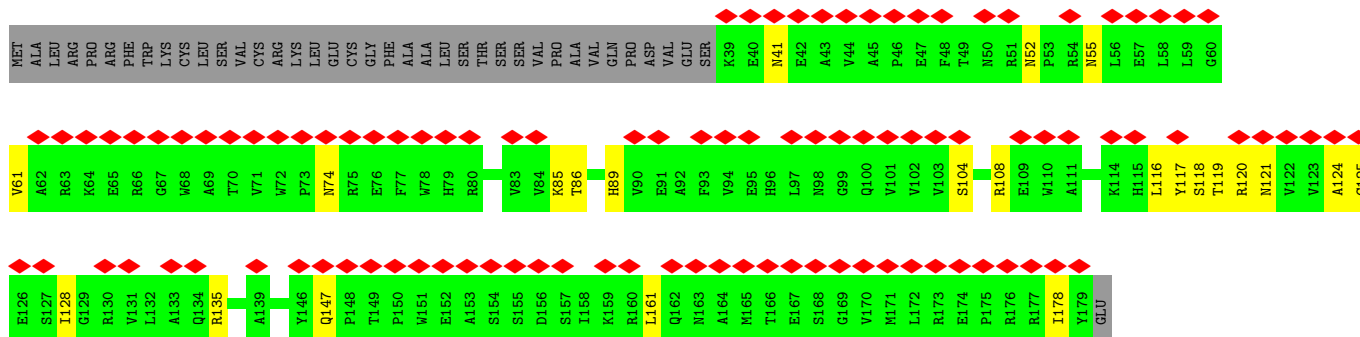
- Molecule 11: Large ribosomal subunit protein uL15m



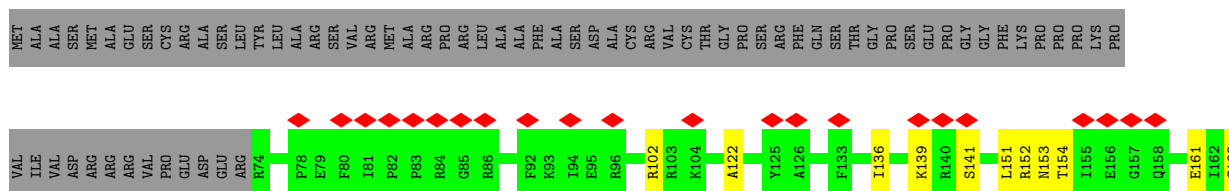
- Molecule 12: Large ribosomal subunit protein bL17m

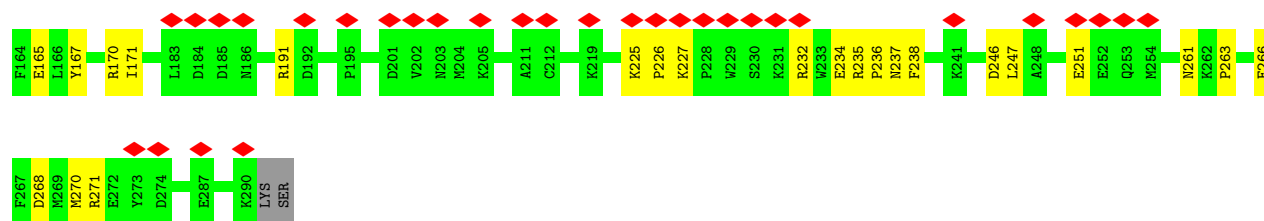


- Molecule 13: Large ribosomal subunit protein uL18m

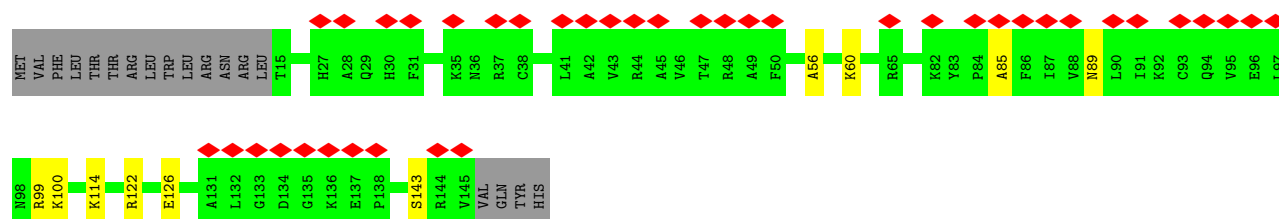
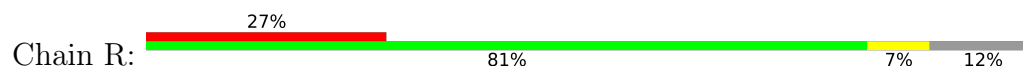


- Molecule 14: Large ribosomal subunit protein bL19m

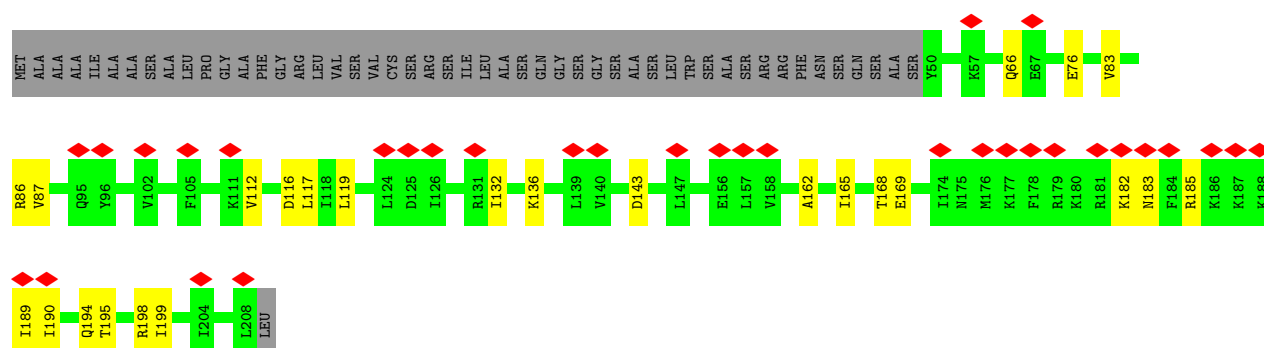




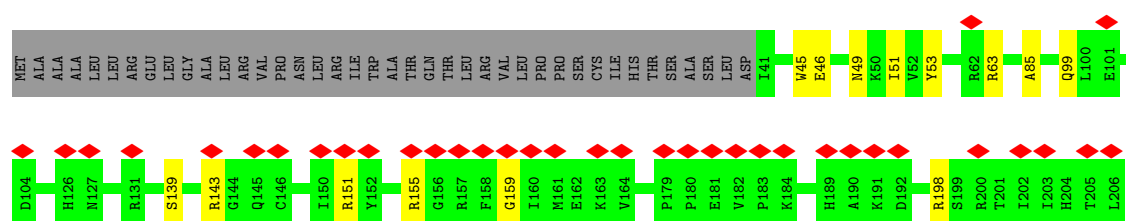
- Molecule 15: Large ribosomal subunit protein bL20m



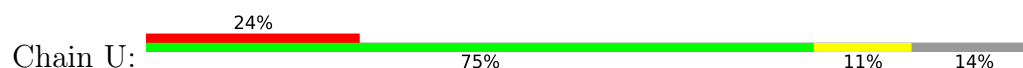
- Molecule 16: Large ribosomal subunit protein bL21m

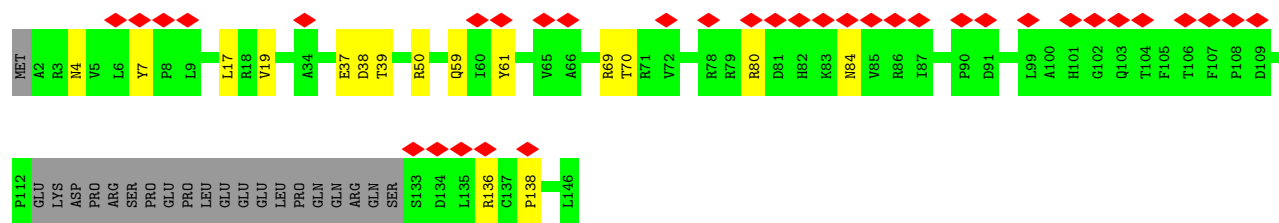


- Molecule 17: Large ribosomal subunit protein uL22m

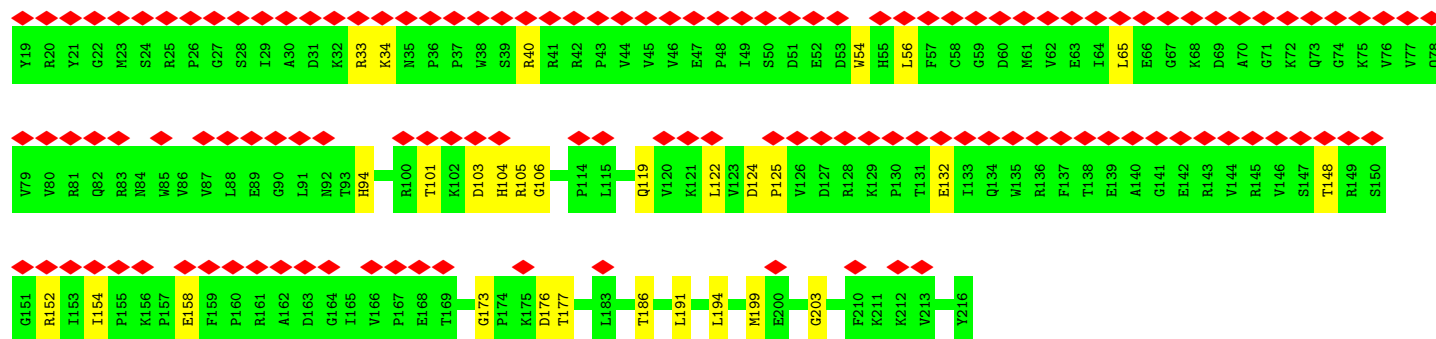
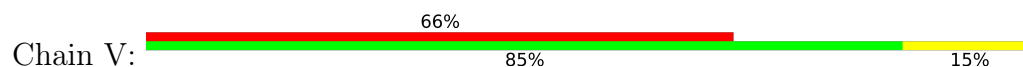


- Molecule 18: Large ribosomal subunit protein uL23m

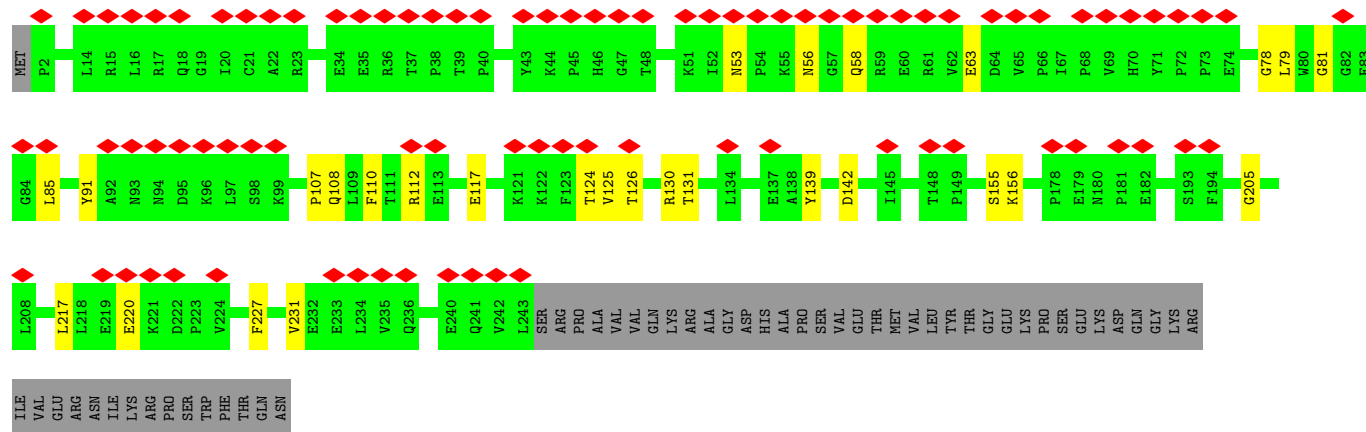
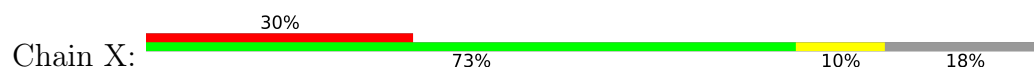




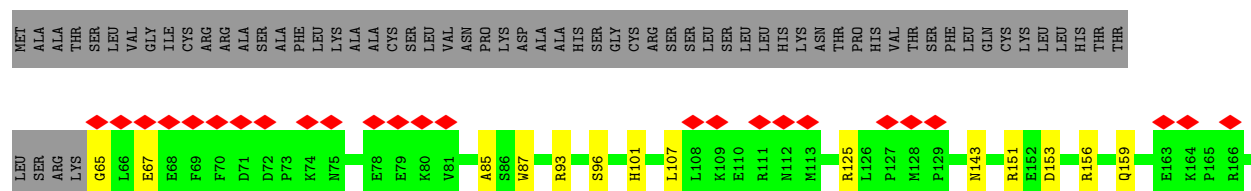
- Molecule 19: Large ribosomal subunit protein uL24m

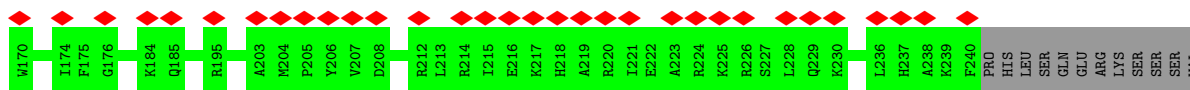


- Molecule 20: Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m

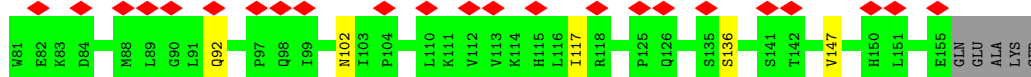
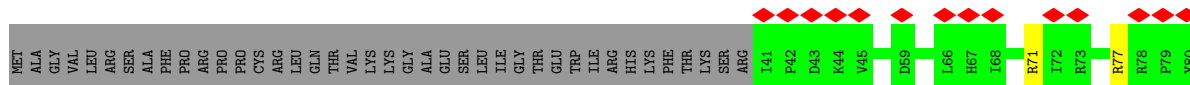


- Molecule 21: Large ribosomal subunit protein uL29m

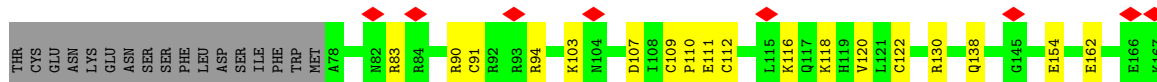
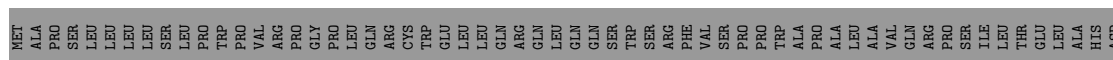




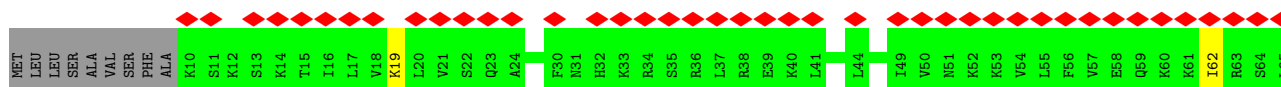
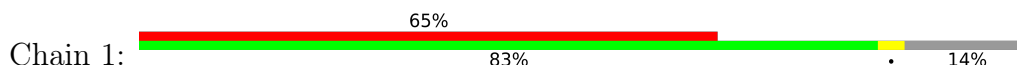
- Molecule 22: Large ribosomal subunit protein uL30m



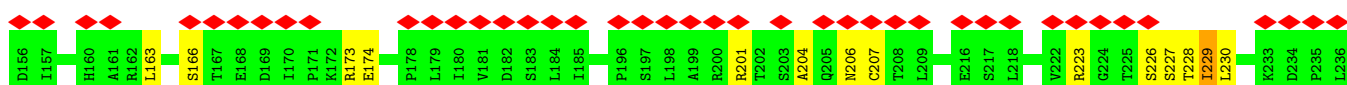
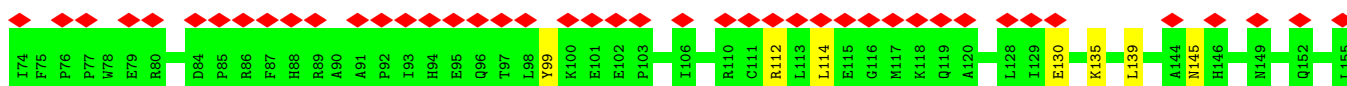
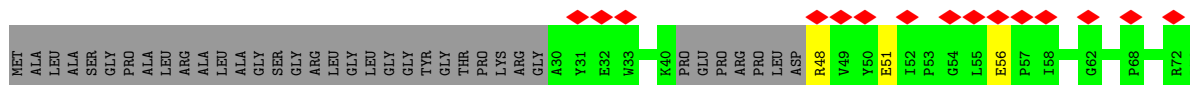
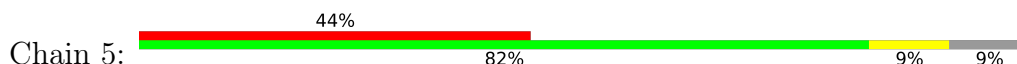
- Molecule 23: Large ribosomal subunit protein bL32m

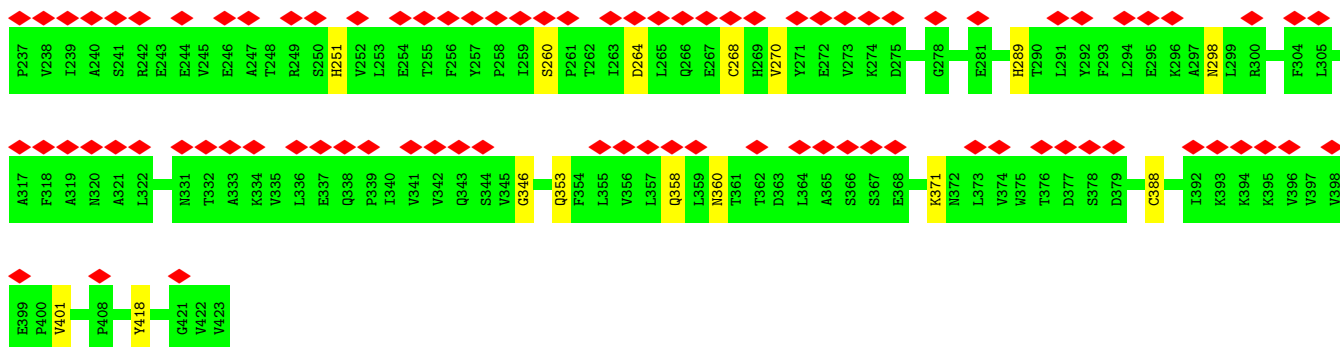


- Molecule 24: Large ribosomal subunit protein bL33m

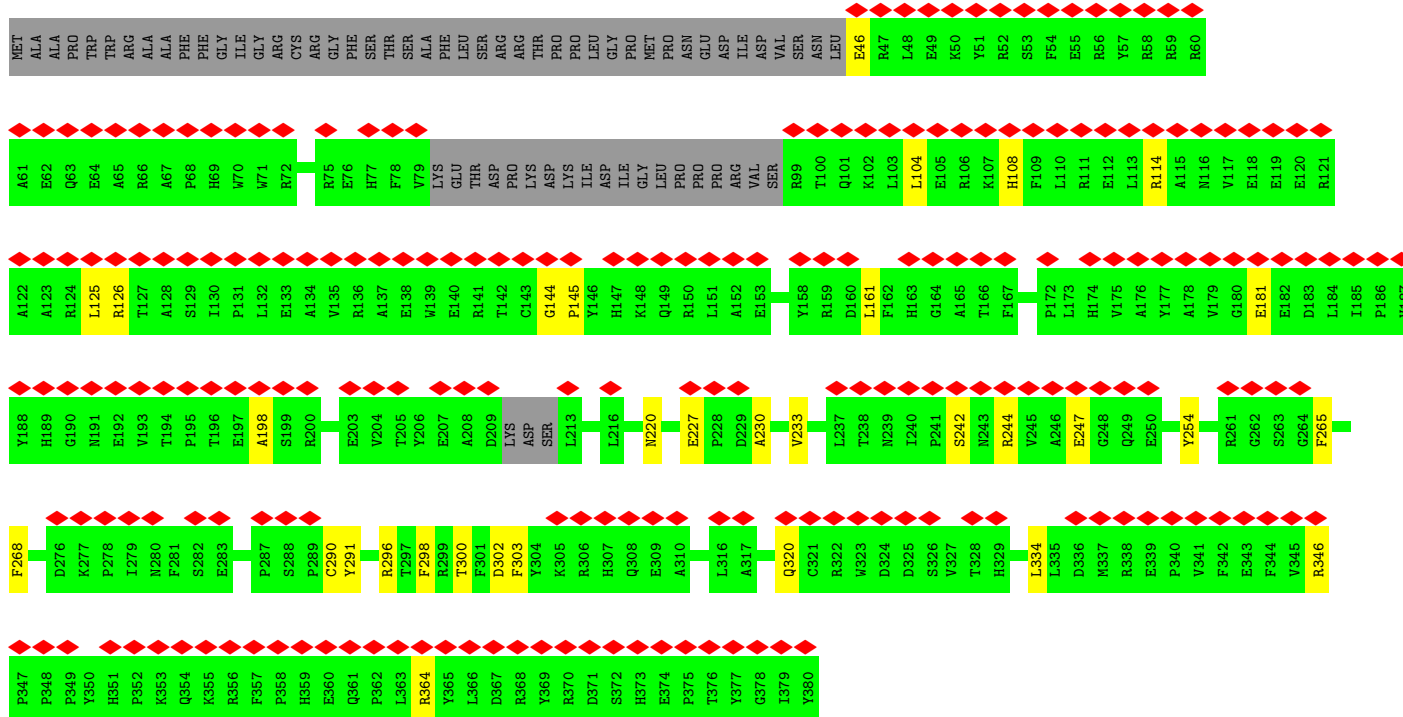
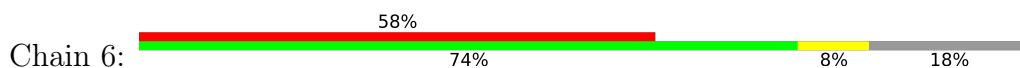


- Molecule 25: Large ribosomal subunit protein mL37

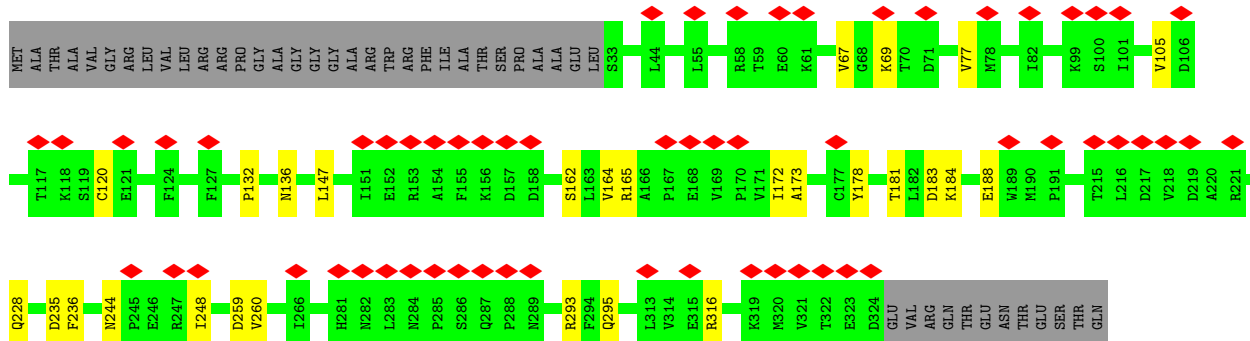
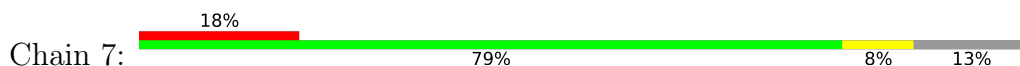


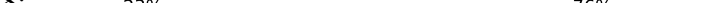


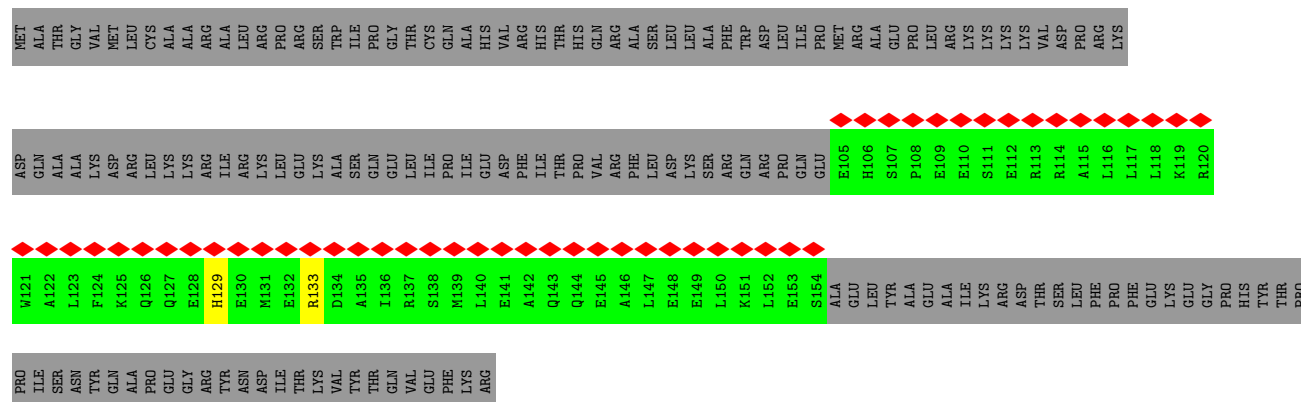
• Molecule 26: Large ribosomal subunit protein mL38

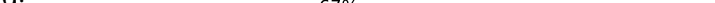


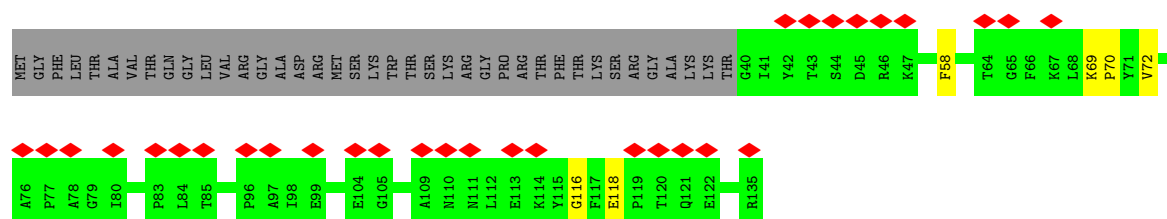
• Molecule 27: Large ribosomal subunit protein mL39

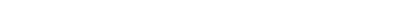


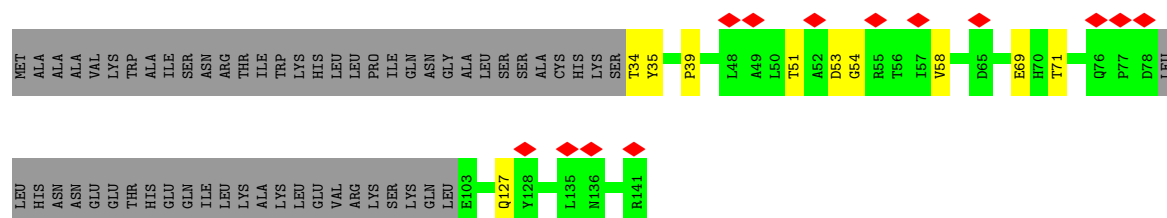
- Chain 8:  24% 23% 76%



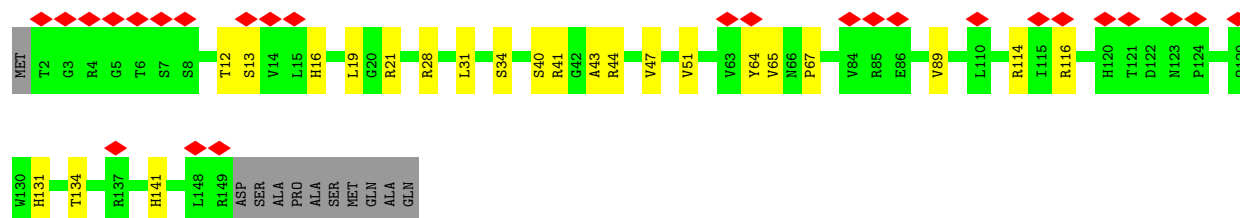
- Chain 9:  23% 67% 29%



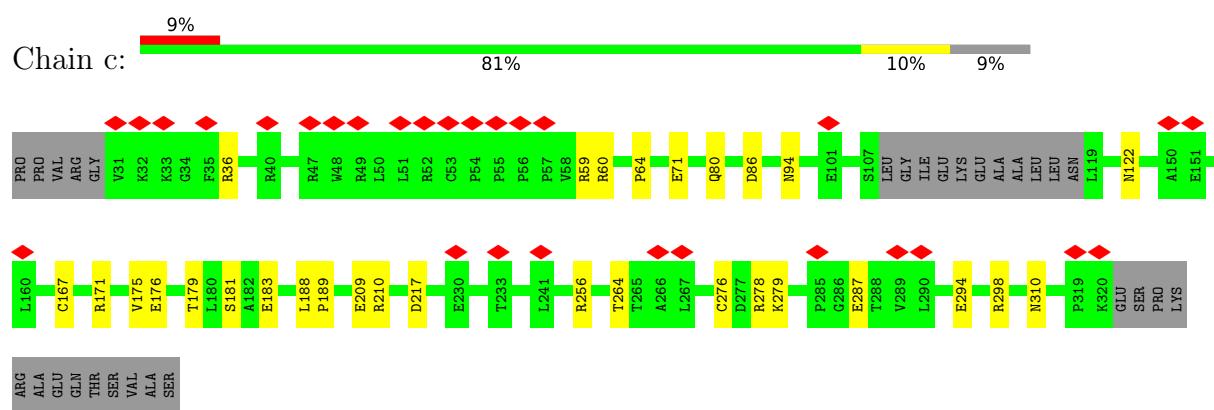
- Chain a: 



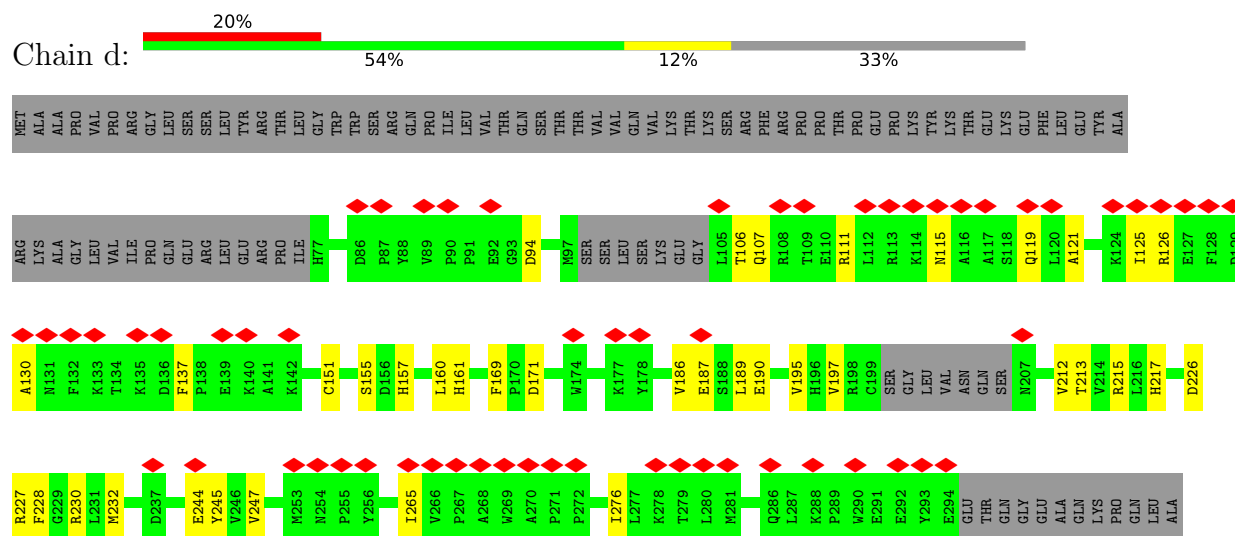
- Chain b: 16% 79% 14% 7%



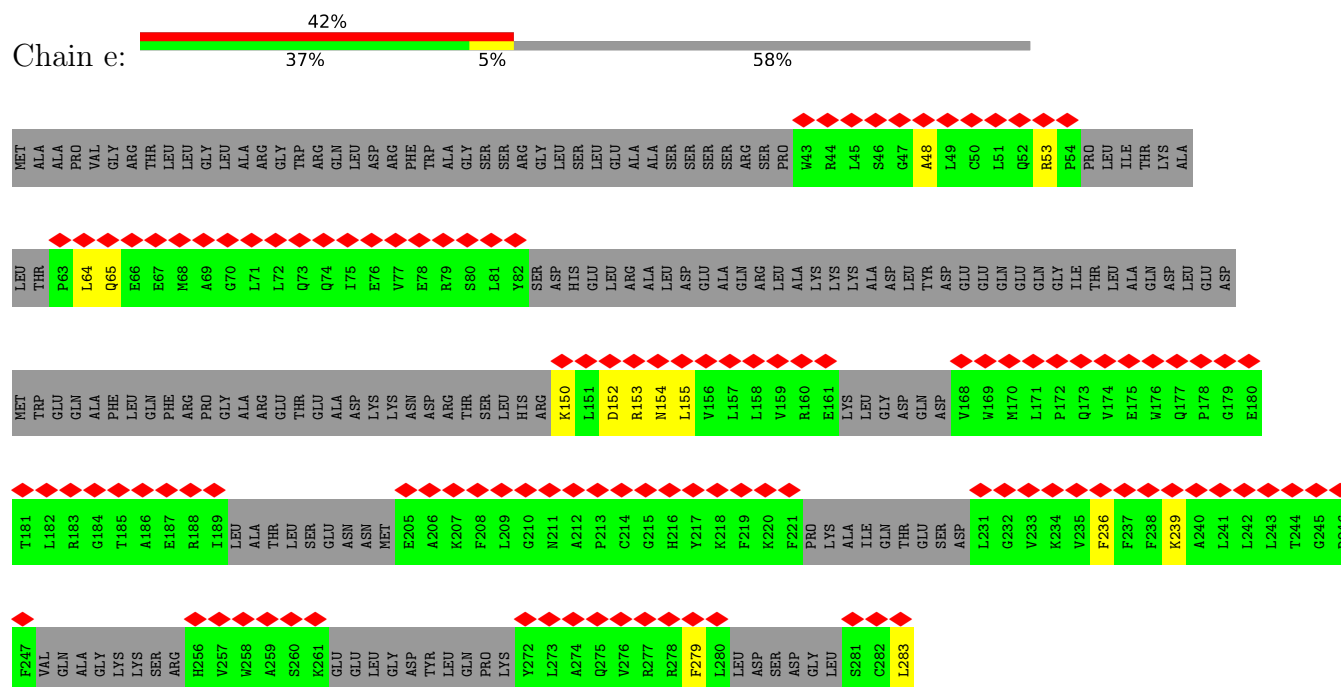
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

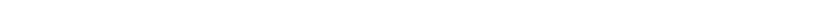


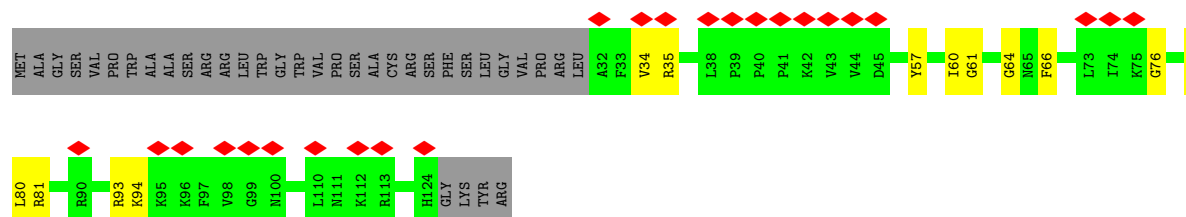
- Molecule 33: Large ribosomal subunit protein mL45



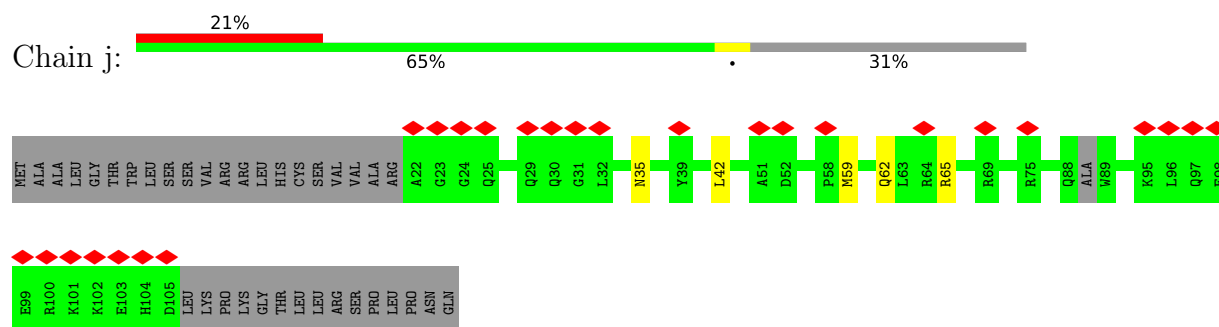
- Molecule 34: Large ribosomal subunit protein mL46



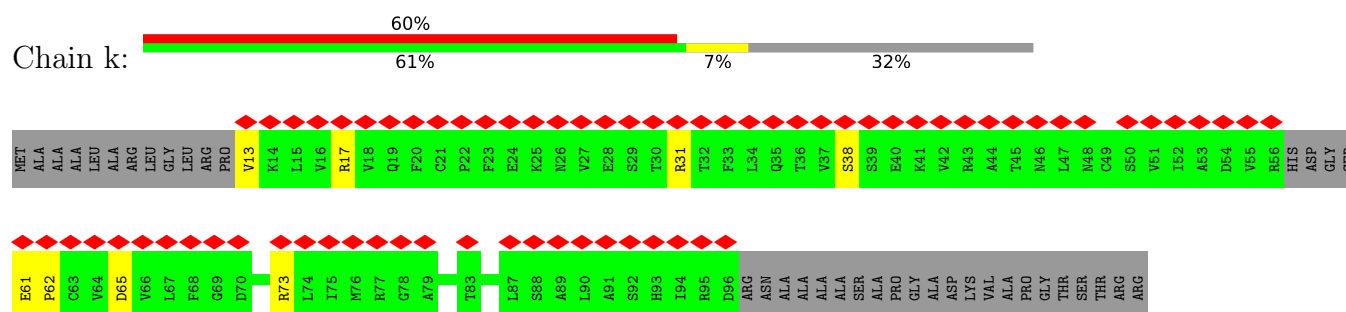
- Chain f: 



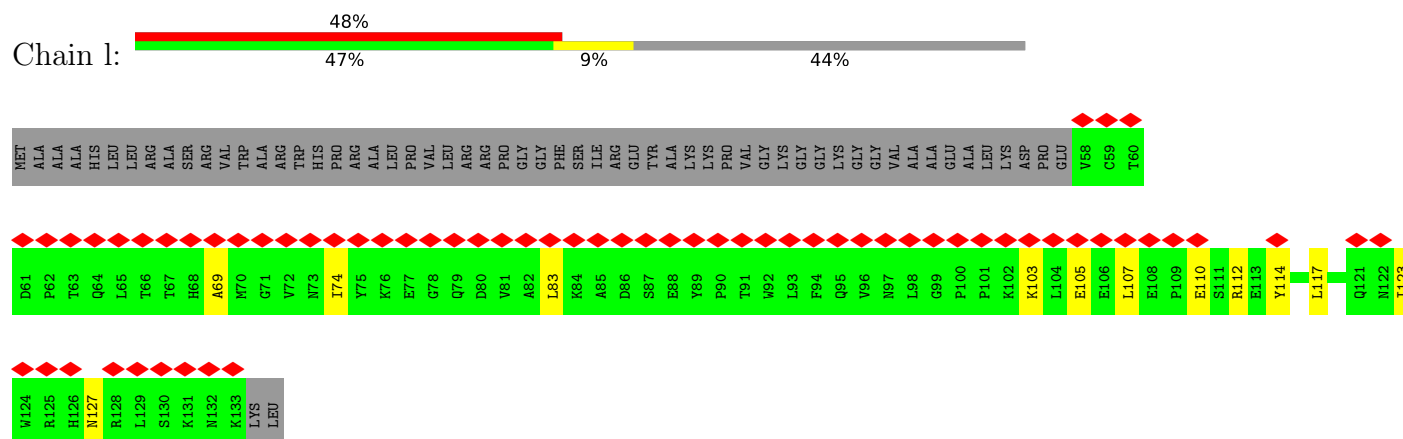
- Molecule 39: Large ribosomal subunit protein mL52



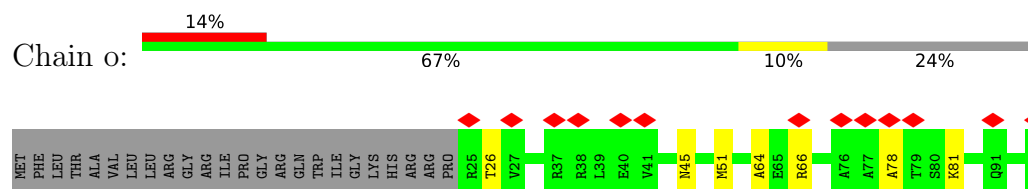
- Molecule 40: Large ribosomal subunit protein mL53



- Molecule 41: Large ribosomal subunit protein mL54

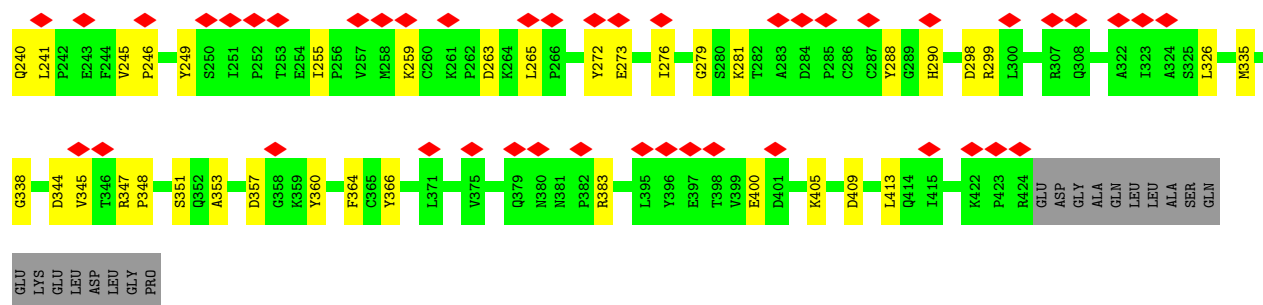


- Molecule 42: Large ribosomal subunit protein mL63

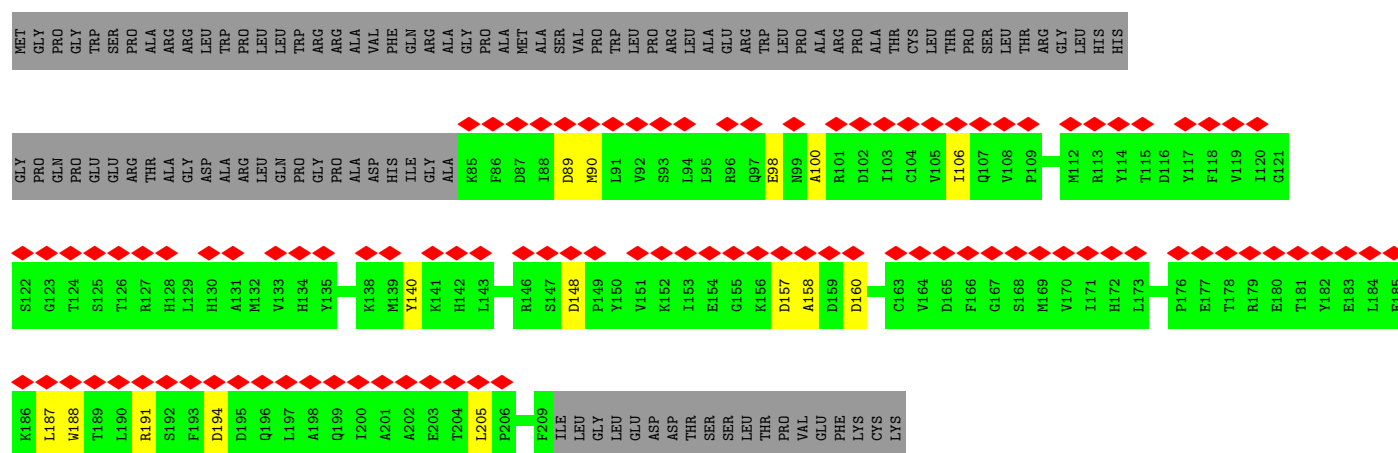


- Molecule 43: Large ribosomal subunit protein mL62

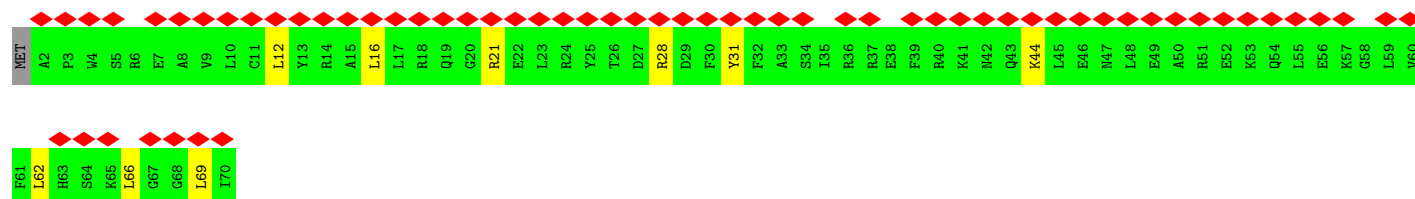
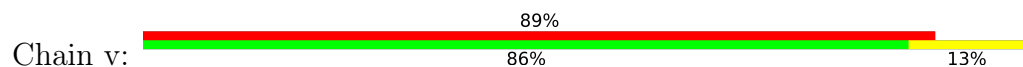




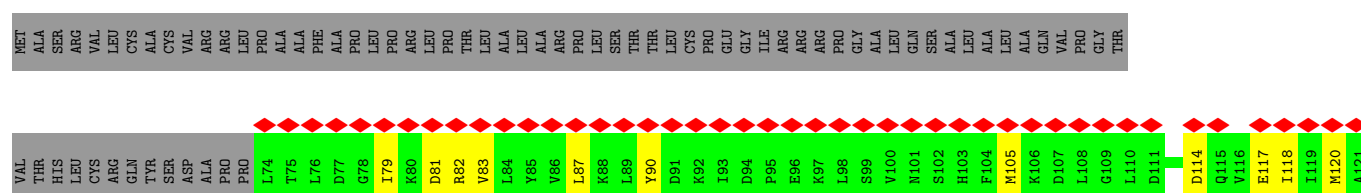
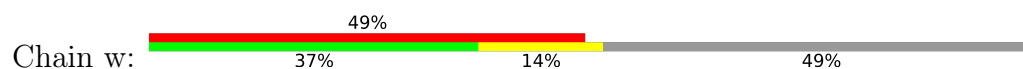
- Molecule 47: Mitochondrial assembly of ribosomal large subunit protein 1

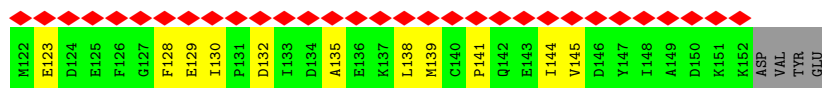


- Molecule 48: Predicted gene, 55359

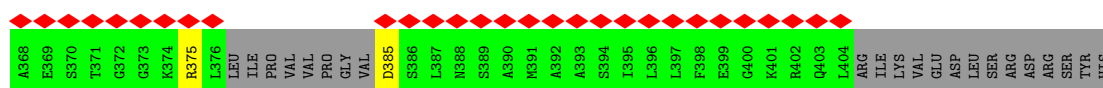
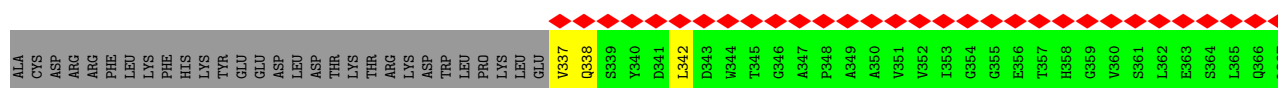
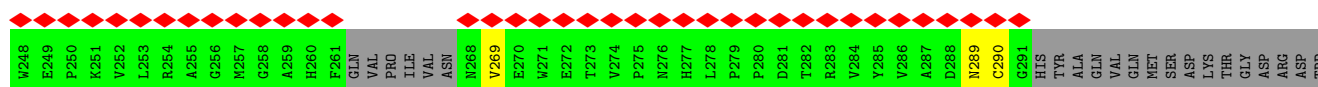
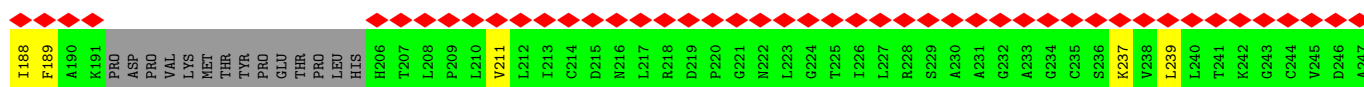
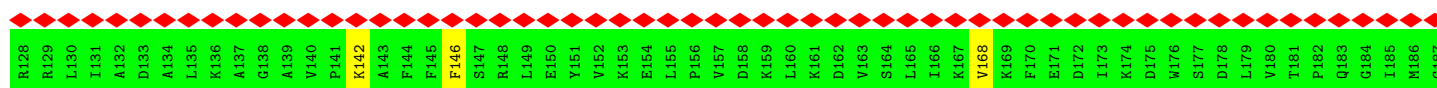
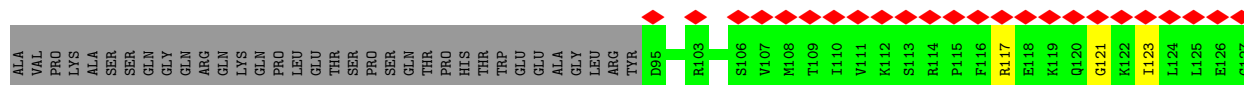


- Molecule 49: Acyl carrier protein, mitochondrial

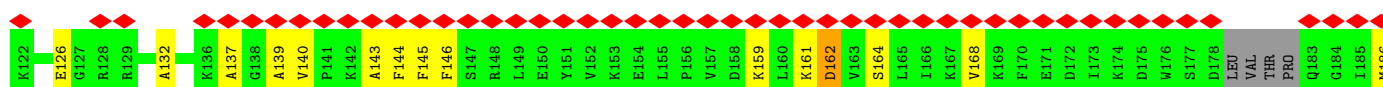
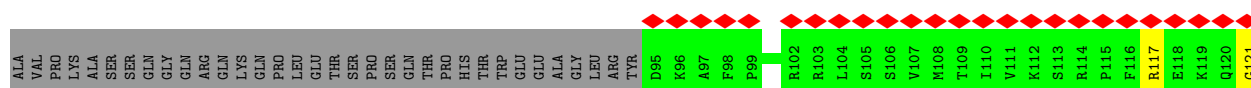




• Molecule 50: rRNA methyltransferase 3, mitochondrial



• Molecule 50: rRNA methyltransferase 3, mitochondrial



L367	L368	E369	S370	G372	G373	K374	L376	L377	L378	P379	V380	V381	P382	V384	S386	L387	N388	S389	A390	M391	A392	A393	S394	L396	L397	F398	E399	G400	K401	K402	Q403	L404	ARG	ILE	LYS	VAL	GLU	ASP	LEU	SER	ARG	ASP	ARG	THR	TYR	HIS													
ALA	CYS	ASP	ARG	ARG	PHE	LEU	PHE	HIS	LYS	TYR	GLU	GLU	ASP	LEU	ASP	THR	THR	ARG	LYS	ASP	TRP	LEU	LEU	LEU	GLU	V337	Q338	S339	V340	D341	L342	D343	V344	T345	G346	A347	P348	A349	A350	V351	V352	L353	G354	G355	E356	T357	H358	G359	V360	S361	L362	E363	S364	L365	Q366				
A247	W248	E249	P250	K251	V252	L253	R254	A255	G256	M257	G258	A259	H260	F261	Q262	V263	P264	L265	V266	M267	N268	V269	E270	W271	T272	T273	V274	P275	N276	H277	L278	P279	P280	D281	T282	R283	V284	V285	V286	A287	D288	N289	C290	G291	HIS	TYR	ALA	GLN	VAL	GLN	MET	SER	ASP	LYS	THR	GLY	ASP	ARG	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5173	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	0.443	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	457.2925, 457.2925, 457.2925	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.846838, 0.846838, 0.846838	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	0/25846	0.19	0/40163
2	B	0.06	0/1458	0.16	0/2262
3	D	0.08	0/1357	0.23	0/1831
4	E	0.07	0/2186	0.21	0/2972
5	F	0.07	0/1772	0.22	0/2415
6	H	0.09	0/793	0.27	0/1066
7	I	0.11	0/1048	0.27	0/1414
8	J	0.09	0/1093	0.25	0/1472
9	K	0.06	0/1436	0.20	0/1948
10	L	0.08	0/908	0.23	0/1224
11	M	0.09	0/2054	0.25	0/2776
12	O	0.07	0/1206	0.20	0/1626
13	P	0.07	0/1181	0.25	0/1600
14	Q	0.08	0/1832	0.22	0/2471
15	R	0.06	0/1096	0.18	0/1469
16	S	0.08	0/1328	0.23	0/1798
17	T	0.07	0/1402	0.20	0/1885
18	U	0.07	0/1062	0.22	0/1441
19	V	0.07	0/1669	0.21	0/2259
20	X	0.08	0/2075	0.22	0/2806
21	Y	0.07	0/1561	0.18	0/2093
22	Z	0.07	0/959	0.22	0/1298
23	0	0.08	0/896	0.22	0/1200
24	1	0.08	0/465	0.21	0/616
25	5	0.07	0/3256	0.22	0/4432
26	6	0.08	0/2766	0.20	0/3758
27	7	0.07	0/2436	0.21	0/3300
28	8	0.06	0/428	0.18	0/570
29	9	0.08	0/800	0.22	0/1082
30	a	0.07	0/724	0.21	0/985
31	b	0.07	0/1203	0.22	0/1625
32	c	0.07	0/2297	0.19	0/3106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.08	0/1736	0.22	0/2353
34	e	0.07	0/989	0.21	0/1323
35	f	0.07	0/679	0.19	0/920
36	g	0.09	0/1126	0.24	0/1533
37	h	0.07	0/894	0.21	0/1216
38	i	0.06	0/818	0.20	0/1099
39	j	0.07	0/693	0.20	0/930
40	k	0.07	0/636	0.20	0/857
41	l	0.07	0/651	0.22	0/882
42	o	0.06	0/655	0.18	0/880
43	p	0.05	0/550	0.18	0/758
44	q	0.07	0/825	0.20	0/1126
45	r	0.08	0/1301	0.23	0/1756
46	s	0.10	0/3118	0.25	0/4232
47	u	0.07	0/1053	0.21	0/1425
48	v	0.08	0/596	0.22	0/795
49	w	0.12	0/646	0.33	0/869
50	x	0.07	0/1194	0.22	0/1650
50	y	0.09	0/1260	0.28	0/1743
All	All	0.08	0/90013	0.21	0/127310

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	23095	11663	11692	197	0
2	B	1303	657	659	10	0
3	D	1335	1373	1373	23	0
4	E	2122	2097	2097	19	0
5	F	1728	1755	1754	27	0
6	H	779	814	814	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1030	1099	1099	27	0
8	J	1075	1145	1145	22	0
9	K	1396	1398	1398	12	0
10	L	893	944	944	11	0
11	M	2010	2080	2080	26	0
12	O	1183	1215	1215	17	0
13	P	1154	1148	1148	17	0
14	Q	1790	1822	1822	22	0
15	R	1077	1137	1137	9	0
16	S	1301	1373	1372	18	0
17	T	1369	1402	1402	12	0
18	U	1034	1038	1038	12	0
19	V	1628	1622	1622	21	0
20	X	2021	2051	2051	20	0
21	Y	1523	1553	1553	11	0
22	Z	934	979	979	5	0
23	0	881	908	908	18	0
24	1	459	508	508	1	0
25	5	3168	3187	3187	28	0
26	6	2673	2545	2545	23	0
27	7	2379	2378	2378	19	0
28	8	423	413	413	1	0
29	9	778	772	772	6	0
30	a	701	667	667	10	0
31	b	1181	1195	1195	18	0
32	c	2246	2256	2256	21	0
33	d	1688	1670	1670	30	0
34	e	971	991	991	8	0
35	f	667	653	653	9	0
36	g	1090	1094	1094	15	0
37	h	872	867	867	5	0
38	i	795	816	816	10	0
39	j	679	687	687	4	0
40	k	629	639	639	6	0
41	l	635	631	631	11	0
42	o	640	623	623	9	0
43	p	552	301	301	0	0
44	q	799	785	785	8	0
45	r	1267	1318	1318	14	0
46	s	3045	3058	3057	47	0
47	u	1029	1012	1012	11	0
48	v	586	603	603	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	w	637	640	640	16	0
50	x	1196	602	602	12	0
50	y	1260	649	649	26	0
51	0	1	0	0	0	0
52	r	4	0	0	2	0
All	All	85711	72833	72861	795	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 (795) 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)
6:H:105:ARG:O	6:H:141:LYS:NZ	2.05	0.90
45:r:73:CYS:N	52:r:301:FES:S2	2.44	0.90
1:A:1305:C:OP2	36:g:111:ARG:NH2	2.06	0.88
1:A:2507:U:O2'	1:A:2508:C:OP1	1.95	0.84
1:A:1907:G:H4'	10:L:36:THR:HG22	1.58	0.84
19:V:105:ARG:NH1	19:V:106:GLY:O	2.11	0.83
1:A:1093:A:O2'	1:A:1094:A:OP1	1.99	0.81
9:K:39:LEU:O	9:K:124:ARG:NH2	2.13	0.81
1:A:1259:U:OP2	31:b:116:ARG:NH1	2.15	0.79
3:D:195:ASN:OD1	3:D:244:THR:OG1	1.99	0.79
23:0:110:PRO:O	27:7:69:LYS:NZ	2.15	0.79
31:b:41:ARG:NH2	42:o:99:LYS:O	2.15	0.79
1:A:1774:G:N2	1:A:1864:C:O2'	2.16	0.78
11:M:108:ARG:NH2	11:M:123:GLY:O	2.16	0.78
1:A:1627:A:OP1	41:l:112:ARG:NH2	2.16	0.78
1:A:1837:A:OP2	3:D:105:ARG:NH2	2.17	0.78
13:P:117:TYR:O	26:6:114:ARG:NH2	2.16	0.78
46:s:240:GLN:NE2	46:s:348:PRO:O	2.18	0.78
18:U:59:GLN:NE2	29:9:58:PHE:O	2.17	0.77
25:5:166:SER:O	46:s:281:LYS:NZ	2.13	0.77
1:A:2598:A:OP1	14:Q:271:ARG:NH2	2.17	0.77
1:A:1315:U:O2'	1:A:1320:C:OP1	2.03	0.77
1:A:1307:A:N6	1:A:1318:A:O4'	2.17	0.77
1:A:2192:C:OP1	20:X:108:GLN:NE2	2.16	0.77
32:c:80:GLN:O	32:c:210:ARG:NH2	2.18	0.77
25:5:163:LEU:O	46:s:281:LYS:NZ	2.18	0.76
3:D:156:GLU:N	3:D:247:ARG:O	2.19	0.76
1:A:1641:G:OP1	8:J:42:ARG:NH2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:A:HO2'	23:0:91:CYS:HG	1.33	0.75
1:A:1822:A:OP1	25:5:112:ARG:NH1	2.19	0.75
1:A:1191:A:O2'	1:A:1192:G:OP1	2.05	0.75
1:A:1560:C:OP2	22:Z:77:ARG:NH1	2.20	0.75
30:a:71:THR:O	32:c:256:ARG:NH2	2.20	0.75
12:O:64:LYS:NZ	12:O:100:GLN:O	2.21	0.74
1:A:1103:A:O2'	19:V:40:ARG:NH2	2.20	0.74
1:A:1230:A:OP2	19:V:94:HIS:NE2	2.20	0.74
1:A:2181:A:O2'	1:A:2241:A:N6	2.20	0.74
1:A:2562:C:OP2	1:A:2563:A:O2'	2.04	0.73
1:A:1894:C:O2	12:O:17:ARG:NH2	2.21	0.73
11:M:250:GLU:O	11:M:253:ARG:NH1	2.20	0.73
7:I:116:LEU:HD12	7:I:123:ILE:HG13	1.69	0.73
1:A:1649:U:HO2'	1:A:1650:A:P	2.11	0.73
1:A:1829:C:OP1	25:5:173:ARG:NH2	2.20	0.73
13:P:121:ASN:OD1	13:P:124:ALA:N	2.21	0.73
12:O:69:ASN:O	46:s:43:ARG:NH2	2.21	0.72
6:H:79:LEU:HD11	6:H:82:ASP:HB2	1.72	0.72
41:l:107:LEU:HD11	41:l:117:LEU:HD12	1.72	0.72
11:M:202:ARG:O	11:M:262:ARG:NH2	2.22	0.72
3:D:133:ASP:OD2	3:D:136:ARG:NH1	2.21	0.72
15:R:114:LYS:NZ	30:a:39:PRO:O	2.21	0.72
1:A:1648:A:OP1	7:I:133:GLN:NE2	2.23	0.72
49:w:90:TYR:OH	49:w:117:GLU:OE2	2.06	0.72
33:d:111:ARG:O	33:d:115:ASN:N	2.23	0.72
5:F:114:THR:O	5:F:156:ARG:NH1	2.22	0.72
1:A:1185:C:OP2	44:q:55:ARG:NH2	2.23	0.72
12:O:43:GLU:OE1	23:0:130:ARG:NH1	2.22	0.72
46:s:90:LYS:NZ	46:s:272:TYR:O	2.23	0.72
30:a:69:GLU:OE2	32:c:278:ARG:NH2	2.22	0.72
46:s:79:LYS:NZ	46:s:338:GLY:O	2.23	0.72
5:F:237:LEU:O	44:q:25:TYR:N	2.23	0.71
1:A:1728:A:OP2	11:M:40:ARG:NE	2.23	0.71
1:A:1889:A:O2'	1:A:1891:A:OP1	2.07	0.71
13:P:74:ASN:O	13:P:147:GLN:NE2	2.24	0.71
1:A:1234:A:O2'	1:A:1235:U:OP1	2.07	0.71
46:s:49:ALA:O	46:s:61:ARG:NH1	2.24	0.71
1:A:2616:U:OP1	45:r:144:LYS:NZ	2.24	0.71
1:A:1624:A:O2'	8:J:134:ASP:OD1	2.09	0.71
25:5:226:SER:O	25:5:227:SER:OG	2.09	0.71
1:A:1119:A:O2'	18:U:4:ASN:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:162:SER:OG	27:7:181:THR:OG1	2.09	0.70
1:A:1606:G:N2	8:J:103:HIS:O	2.25	0.70
3:D:111:ARG:O	3:D:150:ARG:NH2	2.25	0.70
16:S:136:LYS:NZ	39:j:42:LEU:O	2.17	0.70
1:A:1944:A:O2'	1:A:1945:C:OP1	2.08	0.69
17:T:46:GLU:OE1	17:T:46:GLU:N	2.26	0.69
1:A:1847:U:OP1	25:5:223:ARG:NH1	2.25	0.69
31:b:41:ARG:NH1	42:o:96:ASN:O	2.26	0.69
6:H:117:ARG:O	6:H:117:ARG:NH1	2.24	0.69
18:U:37:GLU:OE1	46:s:259:LYS:NZ	2.25	0.69
1:A:1246:A:OP2	23:0:94:ARG:NH1	2.26	0.68
1:A:1315:U:OP2	11:M:132:LYS:NZ	2.23	0.68
1:A:2659:C:O2'	1:A:2660:U:OP1	2.12	0.68
8:J:60:ILE:HG21	8:J:66:LEU:HD11	1.74	0.68
15:R:122:ARG:NH1	30:a:35:TYR:O	2.26	0.68
27:7:228:GLN:OE1	27:7:228:GLN:N	2.26	0.68
50:y:139:ALA:HB2	50:y:263:VAL:HG23	1.74	0.68
16:S:143:ASP:OD2	32:c:310:ASN:ND2	2.27	0.68
16:S:119:LEU:HD12	16:S:195:THR:O	1.94	0.68
16:S:168:THR:O	16:S:194:GLN:N	2.27	0.68
1:A:2092:G:N2	1:A:2096:C:O2'	2.26	0.68
10:L:142:GLN:O	47:u:191:ARG:NH2	2.26	0.68
1:A:1101:C:O2'	1:A:1102:U:OP2	2.11	0.67
1:A:1580:C:OP2	45:r:190:ARG:NH1	2.27	0.67
1:A:1507:G:OP2	42:o:66:ARG:NH2	2.27	0.67
1:A:1872:C:N3	17:T:155:ARG:NH2	2.42	0.67
3:D:194:ILE:HD11	3:D:227:ILE:HD12	1.75	0.67
4:E:112:LYS:NZ	4:E:337:VAL:O	2.26	0.67
1:A:1137:A:O2'	1:A:1138:U:OP1	2.11	0.67
1:A:1626:A:O2'	1:A:1627:A:O5'	2.12	0.67
32:c:167:CYS:SG	32:c:171:ARG:NH1	2.67	0.67
1:A:2302:U:O2'	1:A:2303:A:OP1	2.13	0.67
1:A:1571:A:OP1	15:R:99:ARG:NH1	2.28	0.67
8:J:23:ILE:HD11	8:J:86:THR:CG2	2.23	0.67
47:u:205:LEU:HD12	47:u:205:LEU:O	1.95	0.66
11:M:289:LEU:HD21	44:q:76:TRP:HB3	1.77	0.66
20:X:156:LYS:NZ	20:X:205:GLY:O	2.28	0.66
45:r:94:ARG:HH11	45:r:100:LEU:HD23	1.60	0.66
35:f:114:ASN:OD1	35:f:115:ARG:N	2.29	0.66
46:s:66:TRP:O	46:s:69:THR:OG1	2.12	0.66
3:D:125:GLU:OE1	3:D:166:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2600:A:N6	14:Q:270:MET:O	2.28	0.66
26:6:198:ALA:O	26:6:254:TYR:OH	2.13	0.66
25:5:130:GLU:N	25:5:130:GLU:OE1	2.30	0.65
47:u:89:ASP:OD1	47:u:90:MET:N	2.29	0.65
17:T:51:ILE:O	33:d:227:ARG:NH2	2.30	0.65
20:X:117:GLU:N	20:X:142:ASP:OD2	2.30	0.65
19:V:105:ARG:NH2	33:d:171:ASP:OD1	2.28	0.65
26:6:161:LEU:O	26:6:300:THR:OG1	2.15	0.65
34:e:239:LYS:NZ	34:e:279:PHE:O	2.29	0.65
1:A:1571:A:O2'	39:j:35:ASN:OD1	2.10	0.64
25:5:251:HIS:O	25:5:371:LYS:NZ	2.30	0.64
21:Y:85:ALA:N	29:9:72:VAL:O	2.30	0.64
19:V:54:TRP:NE1	19:V:56:LEU:O	2.30	0.64
1:A:1101:C:OP1	38:i:35:ARG:NH2	2.31	0.64
1:A:1477:A:OP1	36:g:105:ARG:NH2	2.31	0.64
26:6:233:VAL:O	26:6:296:ARG:NH1	2.30	0.64
46:s:67:GLN:O	46:s:71:HIS:ND1	2.30	0.64
46:s:273:GLU:N	46:s:273:GLU:OE1	2.31	0.64
26:6:46:GLU:N	26:6:46:GLU:OE1	2.31	0.64
1:A:1105:C:O2	1:A:1201:G:O2'	2.16	0.64
1:A:2507:U:HO2'	1:A:2508:C:P	2.19	0.64
1:A:1202:A:N6	1:A:1205:U:OP2	2.29	0.63
6:H:73:ARG:O	6:H:76:VAL:HG22	1.98	0.63
5:F:94:ASP:OD1	5:F:95:ILE:N	2.32	0.63
7:I:102:VAL:HG12	7:I:207:LEU:HD12	1.81	0.63
1:A:1649:U:O2'	1:A:1650:A:O5'	2.11	0.63
25:5:230:LEU:O	25:5:289:HIS:N	2.29	0.63
1:A:1847:U:O2'	25:5:268:CYS:SG	2.55	0.62
6:H:89:ASP:O	6:H:113:LYS:N	2.31	0.62
50:y:145:PHE:N	50:y:186:MET:O	2.28	0.62
20:X:81:GLY:N	20:X:131:THR:OG1	2.33	0.62
31:b:89:VAL:HG12	31:b:89:VAL:O	1.98	0.62
7:I:196:GLU:N	7:I:196:GLU:OE1	2.32	0.62
1:A:1762:C:OP2	46:s:55:SER:OG	2.14	0.62
33:d:126:ARG:O	33:d:130:ALA:N	2.32	0.62
3:D:117:GLU:OE1	25:5:260:SER:N	2.33	0.61
50:x:117:ARG:O	50:x:121:GLY:N	2.33	0.61
5:F:49:ARG:NH1	5:F:81:GLU:O	2.34	0.61
14:Q:102:ARG:NH1	14:Q:167:TYR:O	2.33	0.61
20:X:56:ASN:OD1	20:X:58:GLN:N	2.34	0.61
31:b:40:SER:OG	31:b:44:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:23:ILE:HD11	8:J:86:THR:HG21	1.81	0.61
19:V:132:GLU:OE1	19:V:148:THR:OG1	2.17	0.61
1:A:1224:U:O4	19:V:34:LYS:NZ	2.33	0.60
25:5:56:GLU:OE1	25:5:56:GLU:N	2.33	0.60
33:d:213:THR:HG22	33:d:247:VAL:HG22	1.82	0.60
23:0:116:LYS:NZ	23:0:120:VAL:O	2.28	0.60
46:s:241:LEU:HD11	46:s:290:HIS:HA	1.83	0.60
1:A:1711:U:O2	5:F:104:ARG:NH2	2.34	0.60
11:M:131:LEU:O	11:M:133:ARG:NH1	2.35	0.60
17:T:49:ASN:O	33:d:227:ARG:NH2	2.34	0.60
6:H:121:LEU:HD23	6:H:126:ALA:O	2.01	0.60
49:w:128:PHE:O	49:w:130:ILE:HD12	2.02	0.60
37:h:136:GLN:N	37:h:136:GLN:OE1	2.33	0.60
41:l:107:LEU:HD13	41:l:114:TYR:HA	1.84	0.60
50:x:211:VAL:HG22	50:x:237:LYS:CB	2.32	0.60
39:j:62:GLN:OE1	39:j:65:ARG:NH1	2.35	0.59
1:A:1204:C:O2	1:A:1206:A:O2'	2.18	0.59
32:c:60:ARG:NH1	32:c:64:PRO:O	2.35	0.59
33:d:189:LEU:HD12	33:d:217:HIS:CD2	2.37	0.59
31:b:34:SER:O	31:b:44:ARG:NH1	2.35	0.59
33:d:157:HIS:O	33:d:161:HIS:ND1	2.35	0.59
23:0:154:GLU:O	23:0:172:ARG:N	2.35	0.59
46:s:237:ILE:N	46:s:288:TYR:O	2.36	0.59
46:s:108:SER:O	46:s:206:ARG:NH1	2.36	0.59
11:M:141:GLU:N	11:M:141:GLU:OE1	2.36	0.58
20:X:227:PHE:O	20:X:231:VAL:HG23	2.03	0.58
1:A:1311:G:N7	5:F:170:ARG:NH2	2.51	0.58
1:A:1561:U:O2'	1:A:1574:A:N3	2.31	0.58
24:1:19:LYS:HG3	24:1:62:ILE:HD11	1.85	0.58
50:x:289:ASN:N	50:x:385:ASP:O	2.34	0.58
7:I:102:VAL:HG11	7:I:206:PHE:HE1	1.68	0.58
4:E:69:ASN:OD1	4:E:154:ARG:NH1	2.36	0.58
1:A:1777:U:O2	1:A:1803:G:N2	2.35	0.58
30:a:51:THR:OG1	30:a:53:ASP:OD1	2.20	0.58
4:E:87:LEU:HD12	4:E:317:PRO:CG	2.33	0.57
22:Z:71:ARG:NH2	22:Z:92:GLN:O	2.37	0.57
6:H:102:ILE:O	6:H:102:ILE:HG22	2.04	0.57
11:M:275:ASN:N	11:M:280:LYS:O	2.35	0.57
6:H:104:VAL:HG13	6:H:141:LYS:NZ	2.18	0.57
21:Y:159:GLN:OE1	29:9:118:GLU:N	2.38	0.57
6:H:63:GLY:N	20:X:63:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:173:ALA:O	27:7:316:ARG:NH1	2.37	0.57
26:6:227:GLU:OE1	26:6:230:ALA:N	2.36	0.57
7:I:81:LEU:HD13	41:l:110:GLU:O	2.05	0.57
21:Y:107:LEU:HD23	29:9:70:PRO:HA	1.86	0.57
4:E:50:ASP:O	12:O:139:ARG:NH1	2.37	0.57
49:w:128:PHE:O	49:w:129:GLU:HG2	2.03	0.57
2:B:12:U:O2'	2:B:14:A:OP1	2.23	0.56
1:A:1538:G:H2'	1:A:1539:C:O4'	2.05	0.56
4:E:57:ASN:OD1	12:O:147:ASN:ND2	2.38	0.56
33:d:111:ARG:NH2	33:d:195:VAL:HG22	2.20	0.56
7:I:102:VAL:HG23	40:k:38:SER:O	2.06	0.56
27:7:244:ASN:ND2	27:7:248:ILE:O	2.36	0.56
35:f:94:LEU:N	35:f:154:ARG:O	2.38	0.56
38:i:79:TRP:O	38:i:93:ARG:NE	2.35	0.56
7:I:82:LEU:O	7:I:82:LEU:HD23	2.06	0.56
11:M:152:ASN:ND2	11:M:255:LEU:O	2.38	0.56
26:6:302:ASP:OD1	26:6:303:PHE:N	2.38	0.56
1:A:1597:C:N4	1:A:1644:C:OP1	2.37	0.56
6:H:117:ARG:HE	20:X:112:ARG:HG2	1.70	0.56
31:b:21:ARG:NH2	32:c:217:ASP:OD2	2.37	0.56
5:F:190:VAL:O	5:F:263:LEU:N	2.39	0.56
1:A:1258:U:OP2	31:b:114:ARG:NH2	2.38	0.56
46:s:357:ASP:OD1	46:s:360:TYR:N	2.36	0.56
47:u:140:TYR:OH	47:u:148:ASP:OD2	2.23	0.56
1:A:1578:A:O2'	42:o:26:THR:HG23	2.06	0.56
1:A:2361:C:OP2	1:A:2362:A:N6	2.39	0.56
10:L:34:LYS:O	10:L:36:THR:HG23	2.06	0.56
25:5:114:LEU:N	25:5:264:ASP:OD2	2.37	0.55
1:A:1846:C:OP2	46:s:154:ARG:NH2	2.38	0.55
8:J:56:LYS:HZ1	8:J:80:LEU:HB3	1.72	0.55
38:i:61:GLY:O	38:i:66:PHE:N	2.37	0.55
1:A:1225:G:N1	1:A:1228:A:OP2	2.40	0.55
1:A:1793:A:OP2	1:A:1794:C:N4	2.39	0.55
3:D:103:ASN:O	3:D:105:ARG:NH1	2.37	0.55
20:X:79:LEU:HD23	20:X:125:VAL:HG11	1.87	0.55
50:x:342:LEU:HD11	50:x:375:ARG:C	2.31	0.55
1:A:1095:C:OP1	17:T:45:TRP:N	2.38	0.55
14:Q:237:ASN:OD1	14:Q:238:PHE:N	2.40	0.55
1:A:1675:U:O2	45:r:187:TYR:N	2.36	0.55
3:D:155:THR:HG21	3:D:180:GLY:HA2	1.89	0.55
16:S:168:THR:HG22	16:S:169:GLU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:199:MET:O	19:V:203:GLY:N	2.40	0.55
1:A:2394:U:O4	1:A:2395:A:N6	2.40	0.55
1:A:2617:A:O2'	1:A:2618:A:OP2	2.20	0.55
16:S:116:ASP:OD1	16:S:117:LEU:N	2.40	0.55
27:7:183:ASP:OD1	27:7:184:LYS:N	2.38	0.54
33:d:121:ALA:O	33:d:125:ILE:HD12	2.05	0.54
49:w:141:PRO:O	49:w:145:VAL:HG23	2.07	0.54
19:V:101:THR:OG1	19:V:103:ASP:OD1	2.19	0.54
1:A:1629:G:N2	41:l:127:ASN:OD1	2.38	0.54
1:A:1708:A:OP1	32:c:36:ARG:NH2	2.41	0.54
31:b:28:ARG:NH2	32:c:71:GLU:OE2	2.40	0.54
16:S:66:GLN:OE1	16:S:66:GLN:N	2.40	0.54
13:P:55:ASN:OD1	26:6:265:PHE:N	2.39	0.54
11:M:179:ASP:OD1	11:M:180:PRO:HD2	2.08	0.54
1:A:1742:G:O2'	1:A:2115:A:N6	2.40	0.53
5:F:62:VAL:O	5:F:82:LEU:N	2.35	0.53
25:5:48:ARG:NH2	25:5:51:GLU:OE1	2.42	0.53
1:A:1653:A:O2'	45:r:113:ARG:NH2	2.41	0.53
1:A:1805:U:O2	18:U:69:ARG:NH1	2.40	0.53
2:B:22:A:OP2	2:B:45:A:N6	2.41	0.53
1:A:1309:A:C8	5:F:281:THR:HG21	2.43	0.53
1:A:1448:C:OP2	11:M:43:ARG:NH1	2.41	0.53
3:D:141:ALA:N	3:D:152:ILE:O	2.40	0.53
11:M:283:LYS:NZ	36:g:41:SER:OG	2.27	0.53
26:6:233:VAL:HG23	26:6:298:PHE:CE1	2.43	0.53
27:7:147:LEU:HD22	27:7:178:TYR:HB3	1.90	0.53
3:D:157:ASN:ND2	3:D:179:GLU:OE1	2.41	0.53
26:6:242:SER:OG	26:6:244:ARG:NH1	2.41	0.53
50:x:142:LYS:N	50:x:188:ILE:O	2.39	0.53
1:A:1124:U:O2'	1:A:1133:U:O4	2.25	0.53
4:E:126:ASP:O	4:E:173:LYS:NZ	2.35	0.53
1:A:1276:G:N2	1:A:1697:A:O2'	2.41	0.53
2:B:20:A:HO2'	2:B:21:A:P	2.31	0.53
22:Z:117:ILE:O	42:o:45:ASN:ND2	2.42	0.53
1:A:1234:A:HO2'	1:A:1235:U:P	2.32	0.53
1:A:2302:U:HO2'	1:A:2303:A:P	2.31	0.53
33:d:244:GLU:N	33:d:244:GLU:OE1	2.42	0.53
50:y:144:PHE:N	50:y:164:SER:O	2.41	0.52
11:M:263:GLN:NE2	11:M:265:PHE:O	2.42	0.52
30:a:69:GLU:O	31:b:141:HIS:N	2.39	0.52
8:J:119:GLU:OE2	41:l:83:LEU:HD21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:180:ARG:NH1	23:0:185:THR:O	2.42	0.52
18:U:50:ARG:NH2	18:U:70:THR:OG1	2.43	0.52
36:g:99:GLU:O	36:g:107:MET:N	2.41	0.52
48:v:31:TYR:CE2	48:v:66:LEU:HD21	2.44	0.52
1:A:1096:U:O2'	17:T:143:ARG:NH1	2.43	0.52
1:A:1506:A:OP1	42:o:64:ALA:N	2.42	0.52
45:r:73:CYS:CA	52:r:301:FES:S2	2.93	0.52
5:F:97:HIS:NE2	5:F:101:ILE:HD11	2.24	0.52
1:A:1241:G:O2'	1:A:1740:A:O5'	2.27	0.52
1:A:1649:U:H4'	1:A:1650:A:OP1	2.10	0.52
2:B:50:U:O4	2:B:51:A:N6	2.41	0.52
6:H:104:VAL:HG13	6:H:141:LYS:HZ2	1.75	0.52
27:7:293:ARG:O	27:7:295:GLN:NE2	2.43	0.52
35:f:112:LEU:O	35:f:116:LEU:HD23	2.10	0.52
49:w:132:ASP:HA	49:w:135:ALA:HB3	1.92	0.52
1:A:1220:A:N6	1:A:1221:A:N1	2.57	0.51
1:A:1539:C:H2'	1:A:1540:U:H5'	1.91	0.51
2:B:40:C:OP2	13:P:120:ARG:NH2	2.43	0.51
8:J:111:LEU:HD22	8:J:159:LEU:HD13	1.92	0.51
45:r:94:ARG:NH1	45:r:100:LEU:HD23	2.25	0.51
1:A:1137:A:HO2'	1:A:1138:U:P	2.33	0.51
6:H:91:LEU:N	6:H:111:VAL:O	2.41	0.51
26:6:247:GLU:OE1	26:6:247:GLU:N	2.43	0.51
34:e:152:ASP:OD2	34:e:153:ARG:NH2	2.44	0.51
34:e:283:LEU:HD23	35:f:168:ILE:HD11	1.91	0.51
5:F:60:ARG:NH2	37:h:119:HIS:O	2.43	0.51
25:5:139:LEU:O	25:5:145:ASN:ND2	2.43	0.51
46:s:91:TYR:OH	46:s:263:ASP:OD2	2.24	0.51
1:A:1807:A:O2'	46:s:299:ARG:NH1	2.44	0.51
14:Q:227:LYS:NZ	14:Q:234:GLU:OE2	2.38	0.51
10:L:96:MET:N	14:Q:163:CYS:O	2.42	0.51
27:7:259:ASP:OD1	27:7:260:VAL:N	2.44	0.51
50:x:337:VAL:HG12	50:x:338:GLN:N	2.26	0.51
1:A:1944:A:HO2'	1:A:1945:C:P	2.33	0.51
5:F:167:MET:SD	5:F:279:ARG:NH2	2.83	0.50
21:Y:87:TRP:O	21:Y:143:ASN:ND2	2.41	0.50
27:7:235:ASP:OD1	27:7:236:PHE:N	2.44	0.50
1:A:1134:A:H1'	1:A:1135:U:H5'	1.93	0.50
36:g:44:GLU:OE1	36:g:44:GLU:N	2.45	0.50
38:i:57:TYR:OH	44:q:28:PRO:O	2.29	0.50
5:F:113:ASN:OD1	5:F:157:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:104:LEU:O	7:I:109:LYS:NZ	2.44	0.50
13:P:116:LEU:HD21	13:P:118:SER:O	2.11	0.50
16:S:83:VAL:HG22	16:S:86:ARG:HH21	1.75	0.50
50:x:342:LEU:HD11	50:x:375:ARG:O	2.11	0.50
50:y:338:GLN:O	50:y:341:ASP:N	2.45	0.50
3:D:195:ASN:O	3:D:244:THR:OG1	2.28	0.50
20:X:85:LEU:HD23	20:X:107:PRO:HD2	1.94	0.50
26:6:181:GLU:N	26:6:181:GLU:OE1	2.45	0.50
47:u:157:ASP:OD1	47:u:158:ALA:N	2.45	0.50
1:A:1233:A:H2'	1:A:1234:A:O4'	2.12	0.50
1:A:1561:U:O3'	1:A:1574:A:O2'	2.29	0.50
25:5:207:CYS:HB2	25:5:229:ILE:HD12	1.94	0.50
1:A:1744:G:O2'	1:A:2112:G:O6	2.23	0.50
7:I:82:LEU:HD11	7:I:126:PHE:HB3	1.94	0.50
9:K:110:GLY:O	9:K:114:LYS:NZ	2.45	0.50
11:M:105:ASP:OD2	36:g:70:SER:N	2.43	0.50
32:c:59:ARG:NH1	32:c:181:SER:O	2.40	0.50
33:d:226:ASP:N	33:d:230:ARG:O	2.41	0.50
46:s:202:PHE:HD1	46:s:276:ILE:HG23	1.77	0.50
30:a:34:THR:HG22	30:a:34:THR:O	2.12	0.49
49:w:123:GLU:O	49:w:128:PHE:N	2.39	0.49
15:R:85:ALA:O	15:R:89:ASN:ND2	2.43	0.49
33:d:106:THR:OG1	33:d:107:GLN:N	2.42	0.49
37:h:79:LEU:O	37:h:81:SER:N	2.45	0.49
1:A:2593:C:O4'	10:L:95:ARG:NH1	2.46	0.49
6:H:121:LEU:HG	6:H:126:ALA:HB3	1.94	0.49
8:J:56:LYS:O	8:J:60:ILE:HG22	2.13	0.49
14:Q:161:GLU:OE1	14:Q:191:ARG:NH2	2.41	0.49
14:Q:268:ASP:OD1	14:Q:268:ASP:O	2.30	0.49
22:Z:102:ASN:ND2	42:o:51:MET:O	2.40	0.49
12:O:57:GLU:OE2	12:O:105:THR:N	2.38	0.49
2:B:33:G:O2'	35:f:103:GLU:OE2	2.28	0.49
7:I:136:LYS:HB2	7:I:137:PRO:HD3	1.93	0.49
21:Y:153:ASP:OD1	21:Y:156:ARG:NH1	2.41	0.49
1:A:1503:A:O2'	1:A:1504:A:P	2.71	0.49
14:Q:153:ASN:OD1	14:Q:154:THR:N	2.44	0.49
17:T:53:TYR:N	33:d:227:ARG:O	2.44	0.49
23:0:107:ASP:N	23:0:116:LYS:O	2.36	0.49
33:d:94:ASP:OD2	33:d:215:ARG:NE	2.46	0.49
38:i:60:ILE:O	38:i:64:GLY:N	2.45	0.49
50:y:342:LEU:HB2	50:y:345:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:188:VAL:HG23	7:I:188:VAL:O	2.13	0.49
36:g:68:THR:O	36:g:71:GLY:N	2.46	0.49
46:s:344:ASP:OD1	46:s:345:VAL:N	2.46	0.49
1:A:1191:A:HO2'	1:A:1192:G:P	2.35	0.49
7:I:136:LYS:NZ	7:I:180:PHE:O	2.38	0.49
22:Z:136:SER:OG	22:Z:147:VAL:O	2.30	0.49
1:A:1669:C:OP1	45:r:164:LYS:NZ	2.25	0.49
7:I:102:VAL:HG11	7:I:206:PHE:CE1	2.47	0.49
37:h:89:ASP:O	37:h:123:ARG:NH1	2.46	0.49
49:w:123:GLU:HG2	49:w:130:ILE:HD13	1.94	0.49
4:E:56:GLU:OE1	12:O:142:ASN:ND2	2.41	0.49
8:J:130:PHE:HB2	8:J:132:MET:HG2	1.95	0.49
42:o:78:ALA:O	42:o:81:LYS:NZ	2.20	0.49
11:M:38:ARG:CG	11:M:39:PRO:HD2	2.43	0.48
25:5:228:THR:O	25:5:229:ILE:C	2.56	0.48
46:s:51:MET:SD	46:s:65:ARG:NH1	2.86	0.48
1:A:2625:A:O2'	45:r:99:MET:O	2.20	0.48
10:L:38:VAL:HG22	10:L:39:ARG:N	2.29	0.48
13:P:41:ASN:ND2	26:6:291:TYR:O	2.46	0.48
50:y:146:PHE:O	50:y:168:VAL:N	2.45	0.48
1:A:1279:U:O2'	1:A:2132:G:N1	2.39	0.48
1:A:1305:C:O2'	5:F:168:LYS:NZ	2.45	0.48
1:A:1827:C:O2	25:5:388:CYS:N	2.46	0.48
6:H:96:THR:OG1	6:H:124:GLY:O	2.31	0.48
6:H:118:ASN:OD1	6:H:119:LYS:N	2.47	0.48
8:J:132:MET:HE1	8:J:140:VAL:HG22	1.96	0.48
13:P:61:VAL:HG12	13:P:61:VAL:O	2.12	0.48
34:e:154:ASN:C	34:e:155:LEU:HD12	2.39	0.48
1:A:1740:A:O2'	23:0:83:ARG:NH2	2.39	0.48
1:A:1800:U:O2	21:Y:125:ARG:NH2	2.47	0.48
1:A:1944:A:O2'	1:A:1945:C:P	2.71	0.48
5:F:231:VAL:HG13	44:q:26:ARG:HD3	1.95	0.48
49:w:81:ASP:OD1	49:w:82:ARG:N	2.46	0.48
1:A:1744:G:O2'	1:A:1745:U:OP2	2.32	0.48
6:H:96:THR:N	6:H:125:LEU:O	2.46	0.48
13:P:178:ILE:O	26:6:346:ARG:NH2	2.44	0.48
26:6:104:LEU:O	26:6:108:HIS:ND1	2.46	0.48
4:E:68:GLU:OE1	4:E:154:ARG:NH2	2.47	0.48
19:V:65:LEU:N	19:V:119:GLN:O	2.39	0.48
34:e:150:LYS:HB2	34:e:155:LEU:HD11	1.94	0.48
1:A:1231:C:H3'	1:A:1232:U:C5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:U:H1'	1:A:1233:A:OP2	2.14	0.48
2:B:20:A:O2'	2:B:21:A:OP1	2.23	0.48
1:A:1206:A:N7	1:A:1221:A:N6	2.60	0.48
11:M:276:MET:SD	11:M:277:ALA:N	2.86	0.48
25:5:201:ARG:NH1	25:5:418:TYR:O	2.46	0.48
3:D:248:VAL:HG12	3:D:249:SER:N	2.29	0.47
33:d:226:ASP:OD1	33:d:232:MET:HE2	2.14	0.47
1:A:1305:C:P	36:g:111:ARG:NH2	2.87	0.47
9:K:21:LEU:N	9:K:58:VAL:O	2.44	0.47
16:S:87:VAL:HG21	30:a:58:VAL:CG1	2.45	0.47
46:s:195:ASP:OD1	46:s:198:ARG:NH2	2.46	0.47
1:A:2568:G:N2	1:A:2571:A:OP2	2.47	0.47
6:H:99:VAL:HB	6:H:125:LEU:HD13	1.96	0.47
7:I:89:VAL:O	7:I:93:ASN:ND2	2.45	0.47
46:s:298:ASP:OD1	46:s:299:ARG:N	2.47	0.47
48:v:12:LEU:O	48:v:16:LEU:HD23	2.14	0.47
1:A:1137:A:O2'	1:A:1138:U:P	2.73	0.47
2:B:7:G:N2	2:B:61:C:N3	2.62	0.47
15:R:122:ARG:NH2	16:S:76:GLU:OE2	2.47	0.47
1:A:1180:A:O3'	6:H:66:ARG:NH1	2.48	0.47
10:L:113:ASN:ND2	47:u:160:ASP:OD1	2.45	0.47
14:Q:251:GLU:OE1	14:Q:251:GLU:N	2.41	0.47
18:U:80:ARG:NH1	18:U:84:ASN:O	2.48	0.47
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.97	0.47
27:7:172:ILE:O	27:7:316:ARG:NH2	2.47	0.47
31:b:47:VAL:O	31:b:51:VAL:HG12	2.13	0.47
33:d:197:VAL:HG12	33:d:212:VAL:HG13	1.96	0.47
1:A:2186:A:N6	1:A:2236:G:O6	2.47	0.47
12:O:94:ALA:HB3	12:O:95:PRO:HD3	1.96	0.47
32:c:94:ASN:OD1	32:c:122:ASN:ND2	2.47	0.47
36:g:68:THR:HG22	36:g:69:PRO:HD2	1.97	0.47
36:g:154:ASP:OD1	36:g:154:ASP:N	2.47	0.47
47:u:98:GLU:OE2	47:u:100:ALA:HB2	2.15	0.47
50:y:338:GLN:O	50:y:342:LEU:HG	2.15	0.47
1:A:1180:A:O2'	6:H:61:LEU:O	2.29	0.47
1:A:1620:A:H61	1:A:1630:A:C2'	2.28	0.47
5:F:226:MET:SD	5:F:242:LEU:HD21	2.55	0.47
6:H:97:GLN:HB2	6:H:125:LEU:HA	1.97	0.47
8:J:60:ILE:HG21	8:J:66:LEU:CD1	2.42	0.47
12:O:36:LEU:O	12:O:40:GLU:N	2.43	0.47
3:D:127:VAL:O	3:D:161:GLY:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:95:LEU:HA	6:H:126:ALA:HA	1.97	0.47
50:y:287:ALA:HB2	50:y:376:LEU:CB	2.45	0.47
1:A:1908:G:N1	1:A:2092:G:OP2	2.44	0.46
10:L:38:VAL:HG22	10:L:39:ARG:H	1.80	0.46
25:5:174:GLU:N	25:5:298:ASN:OD1	2.40	0.46
25:5:204:ALA:N	25:5:228:THR:O	2.49	0.46
26:6:290:CYS:SG	26:6:296:ARG:NE	2.84	0.46
49:w:83:VAL:O	49:w:87:LEU:HD23	2.15	0.46
6:H:52:ILE:O	6:H:79:LEU:HD12	2.14	0.46
27:7:105:VAL:HG13	27:7:120:CYS:SG	2.55	0.46
44:q:61:PHE:O	44:q:65:GLY:N	2.42	0.46
46:s:400:GLU:OE1	46:s:405:LYS:NZ	2.43	0.46
1:A:2196:U:O4	6:H:102:ILE:HD11	2.15	0.46
16:S:183:ASN:OD1	16:S:185:ARG:NH2	2.48	0.46
33:d:151:CYS:O	33:d:155:SER:N	2.48	0.46
46:s:95:PRO:HG3	46:s:227:ILE:HG23	1.98	0.46
48:v:21:ARG:O	48:v:28:ARG:NH2	2.48	0.46
1:A:1181:A:N3	20:X:53:ASN:ND2	2.64	0.46
1:A:1609:U:N3	1:A:1612:A:OP2	2.46	0.46
1:A:2296:U:OP2	26:6:364:ARG:NE	2.39	0.46
5:F:51:CYS:SG	5:F:83:HIS:N	2.88	0.46
19:V:103:ASP:OD1	19:V:104:HIS:N	2.49	0.46
21:Y:67:GLU:OE1	21:Y:67:GLU:N	2.42	0.46
45:r:50:GLU:OE2	45:r:52:ARG:NH2	2.48	0.46
1:A:1660:A:N3	1:A:1660:A:H2'	2.30	0.46
1:A:1908:G:P	10:L:37:ARG:NH1	2.88	0.46
4:E:202:GLN:NE2	4:E:301:ASP:OD1	2.48	0.46
1:A:1134:A:H2'	1:A:1134:A:N3	2.31	0.46
1:A:1648:A:H2'	1:A:1649:U:C1'	2.45	0.46
6:H:56:TRP:HB2	6:H:76:VAL:HG23	1.98	0.46
8:J:84:GLN:HG3	8:J:85:PRO:HD2	1.98	0.46
18:U:38:ASP:OD1	18:U:39:THR:N	2.49	0.46
19:V:173:GLY:N	19:V:176:ASP:OD2	2.48	0.46
33:d:190:GLU:OE2	33:d:215:ARG:NH2	2.48	0.46
46:s:195:ASP:OD2	46:s:236:ARG:NE	2.44	0.46
16:S:165:ILE:HD11	16:S:198:ARG:HB3	1.98	0.46
16:S:168:THR:HG22	16:S:169:GLU:H	1.79	0.46
17:T:151:ARG:O	17:T:159:GLY:N	2.43	0.46
20:X:81:GLY:O	20:X:130:ARG:NE	2.47	0.46
33:d:137:PHE:CD2	33:d:212:VAL:HG11	2.51	0.46
33:d:245:TYR:O	33:d:265:ILE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:116:LEU:O	7:I:120:LYS:N	2.49	0.46
47:u:187:LEU:C	47:u:187:LEU:HD23	2.41	0.46
1:A:1243:A:OP2	23:0:90:ARG:NH2	2.42	0.46
18:U:61:TYR:O	21:Y:65:GLY:N	2.49	0.46
2:B:15:A:O2'	2:B:17:A:N7	2.49	0.45
4:E:87:LEU:HD12	4:E:317:PRO:HG2	1.97	0.45
10:L:140:ILE:HG22	10:L:140:ILE:O	2.16	0.45
14:Q:151:LEU:H	14:Q:151:LEU:HD23	1.82	0.45
20:X:124:THR:HG23	20:X:124:THR:O	2.16	0.45
26:6:233:VAL:HG23	26:6:298:PHE:CD1	2.51	0.45
39:j:59:MET:SD	39:j:59:MET:N	2.89	0.45
47:u:194:ASP:OD1	47:u:194:ASP:N	2.48	0.45
1:A:1614:G:H2'	1:A:1615:C:O4'	2.16	0.45
12:O:144:THR:OG1	12:O:147:ASN:OD1	2.34	0.45
13:P:85:LYS:O	13:P:86:THR:C	2.59	0.45
23:0:162:GLU:OE1	23:0:180:ARG:NH2	2.49	0.45
32:c:175:VAL:O	32:c:179:THR:N	2.50	0.45
33:d:186:VAL:HG12	33:d:187:GLU:N	2.31	0.45
1:A:1172:G:N2	1:A:1175:G:O2'	2.50	0.45
1:A:1234:A:O2'	1:A:1235:U:P	2.73	0.45
1:A:1756:C:OP1	23:0:138:GLN:NE2	2.49	0.45
46:s:241:LEU:HD12	46:s:351:SER:HA	1.98	0.45
49:w:79:ILE:HG22	49:w:145:VAL:HG22	1.99	0.45
1:A:1538:G:O2'	1:A:1539:C:OP1	2.34	0.45
28:8:129:HIS:O	28:8:133:ARG:N	2.41	0.45
3:D:111:ARG:NH2	3:D:180:GLY:O	2.44	0.45
41:l:69:ALA:HB2	41:l:83:LEU:HD23	1.99	0.45
46:s:132:ASP:O	46:s:135:ALA:N	2.49	0.45
47:u:106:ILE:CD1	48:v:69:LEU:HD23	2.46	0.45
4:E:63:GLN:NE2	4:E:67:ASP:OD2	2.49	0.45
7:I:76:SER:O	7:I:80:ARG:N	2.49	0.45
7:I:83:ARG:O	7:I:87:VAL:HG23	2.17	0.45
12:O:67:ASP:O	46:s:43:ARG:NH2	2.47	0.45
3:D:182:ALA:O	3:D:183:HIS:ND1	2.49	0.45
5:F:97:HIS:CE1	5:F:101:ILE:HD11	2.51	0.45
5:F:220:ASP:O	5:F:245:ALA:N	2.50	0.45
8:J:33:PRO:N	8:J:34:PRO:HD2	2.32	0.45
20:X:125:VAL:HG12	20:X:126:THR:N	2.32	0.45
25:5:226:SER:O	25:5:227:SER:CB	2.65	0.45
1:A:2302:U:O2'	1:A:2303:A:P	2.73	0.45
8:J:34:PRO:O	8:J:38:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:67:VAL:O	27:7:67:VAL:HG22	2.17	0.45
35:f:114:ASN:OD1	35:f:114:ASN:C	2.60	0.45
1:A:1188:A:N3	44:q:34:ARG:NH1	2.64	0.45
6:H:104:VAL:HG22	6:H:105:ARG:N	2.31	0.45
30:a:53:ASP:OD1	30:a:54:GLY:N	2.50	0.45
36:g:85:PHE:N	36:g:114:GLU:O	2.44	0.45
50:x:337:VAL:HG12	50:x:338:GLN:H	1.82	0.45
14:Q:139:LYS:NZ	14:Q:141:SER:OG	2.35	0.45
33:d:115:ASN:O	33:d:119:GLN:N	2.32	0.45
13:P:52:ASN:ND2	26:6:320:GLN:OE1	2.50	0.44
19:V:122:LEU:HD21	19:V:154:ILE:HG21	1.99	0.44
25:5:346:GLY:O	25:5:353:GLN:N	2.40	0.44
50:x:123:ILE:O	50:x:189:PHE:N	2.46	0.44
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.99	0.44
27:7:164:VAL:HG13	27:7:165:ARG:N	2.32	0.44
27:7:188:GLU:OE1	27:7:188:GLU:N	2.48	0.44
31:b:65:VAL:HG12	31:b:67:PRO:HD3	1.99	0.44
1:A:1806:A:O2'	1:A:1809:C:N4	2.50	0.44
7:I:89:VAL:CG2	7:I:188:VAL:HG21	2.46	0.44
12:O:84:ASP:N	12:O:84:ASP:OD1	2.51	0.44
19:V:124:ASP:OD2	19:V:152:ARG:NH1	2.49	0.44
36:g:77:ASP:OD1	36:g:78:PRO:HA	2.17	0.44
50:y:190:ALA:HB3	50:y:262:GLN:HG3	1.99	0.44
1:A:2179:U:H2'	1:A:2180:U:O4'	2.18	0.44
13:P:104:SER:O	13:P:135:ARG:NH1	2.50	0.44
19:V:186:THR:OG1	21:Y:96:SER:N	2.50	0.44
31:b:131:HIS:O	31:b:134:THR:OG1	2.28	0.44
49:w:87:LEU:CD1	49:w:118:ILE:HG23	2.47	0.44
50:y:283:ARG:CB	50:y:344:TRP:HA	2.47	0.44
7:I:102:VAL:O	7:I:102:VAL:HG13	2.18	0.44
18:U:19:VAL:O	18:U:19:VAL:HG13	2.16	0.44
31:b:12:THR:HG22	31:b:13:SER:N	2.31	0.44
41:l:105:GLU:OE1	41:l:105:GLU:N	2.46	0.44
46:s:76:VAL:HG13	46:s:335:MET:O	2.18	0.44
1:A:1629:G:O6	1:A:1632:A:N6	2.51	0.44
11:M:189:PRO:HA	11:M:192:PHE:CE1	2.53	0.44
12:O:86:ILE:HB	12:O:87:PRO:HD3	1.98	0.44
14:Q:139:LYS:HZ3	14:Q:141:SER:CB	2.30	0.44
15:R:126:GLU:OE1	15:R:143:SER:N	2.51	0.44
20:X:110:PHE:HB3	20:X:112:ARG:NE	2.32	0.44
27:7:77:VAL:HG23	27:7:77:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:U:OP1	38:i:94:LYS:NZ	2.45	0.44
1:A:1246:A:OP1	30:a:127:GLN:NE2	2.51	0.44
40:k:73:ARG:NH1	45:r:48:VAL:HG23	2.32	0.44
49:w:105:MET:HG2	49:w:139:MET:HE1	1.98	0.44
1:A:2342:U:O2'	1:A:2343:A:P	2.76	0.44
1:A:2629:A:N3	1:A:2629:A:H2'	2.33	0.44
7:I:135:LEU:O	7:I:138:PHE:HB3	2.18	0.44
45:r:93:ILE:HD11	45:r:119:VAL:HG21	1.99	0.44
50:y:259:ALA:O	50:y:263:VAL:HB	2.18	0.44
1:A:1256:G:O3'	15:R:60:LYS:NZ	2.48	0.44
1:A:1894:C:H1'	1:A:1895:A:OP2	2.17	0.44
16:S:112:VAL:HG13	16:S:199:ILE:HG13	1.99	0.44
33:d:125:ILE:HD12	33:d:125:ILE:H	1.83	0.44
50:y:161:LYS:O	50:y:162:ASP:CB	2.66	0.44
9:K:156:ASP:OD1	9:K:157:GLU:N	2.51	0.43
32:c:86:ASP:N	32:c:86:ASP:OD1	2.49	0.43
1:A:1593:U:O2'	1:A:1594:U:O5'	2.36	0.43
11:M:38:ARG:HG2	11:M:39:PRO:HD2	2.00	0.43
35:f:158:ILE:HD13	35:f:169:PHE:CE2	2.53	0.43
50:x:146:PHE:O	50:x:168:VAL:N	2.44	0.43
11:M:287:GLU:OE1	11:M:287:GLU:N	2.47	0.43
17:T:85:ALA:O	17:T:139:SER:OG	2.36	0.43
20:X:217:LEU:O	20:X:220:GLU:HG2	2.18	0.43
32:c:209:GLU:OE1	32:c:209:GLU:N	2.46	0.43
46:s:111:LYS:HA	46:s:255:ILE:HG21	2.00	0.43
46:s:147:GLU:OE1	46:s:153:ARG:NH2	2.50	0.43
1:A:1093:A:HO2'	1:A:1094:A:P	2.37	0.43
20:X:78:GLY:O	20:X:155:SER:OG	2.31	0.43
20:X:110:PHE:HB3	20:X:112:ARG:CZ	2.48	0.43
1:A:2092:G:N2	1:A:2096:C:HO2'	2.16	0.43
1:A:2587:A:H4'	4:E:266:ARG:HE	1.83	0.43
33:d:195:VAL:HG21	33:d:215:ARG:HB2	2.00	0.43
50:y:137:ALA:O	50:y:263:VAL:HG13	2.18	0.43
50:y:291:GLY:N	50:y:376:LEU:O	2.52	0.43
1:A:1296:A:O4'	1:A:1326:A:N6	2.47	0.43
1:A:2245:U:O2'	1:A:2362:A:N7	2.47	0.43
21:Y:93:ARG:O	21:Y:151:ARG:NH2	2.51	0.43
25:5:99:TYR:HA	25:5:270:VAL:HG22	1.99	0.43
50:y:263:VAL:HG12	50:y:265:ILE:H	1.84	0.43
16:S:169:GLU:N	16:S:169:GLU:OE1	2.52	0.43
25:5:401:VAL:HG23	25:5:401:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:31:LEU:N	31:b:64:TYR:O	2.45	0.43
50:x:290:CYS:O	50:y:232:GLY:N	2.49	0.43
1:A:1165:A:OP2	1:A:1166:A:O2'	2.23	0.43
8:J:84:GLN:N	8:J:127:ASP:OD2	2.50	0.43
17:T:63:ARG:NH1	33:d:228:PHE:O	2.50	0.43
36:g:42:VAL:HG12	36:g:42:VAL:O	2.19	0.43
46:s:245:VAL:HG22	46:s:246:PRO:HD2	2.01	0.43
9:K:140:ASN:CG	32:c:264:THR:HG1	2.20	0.43
14:Q:236:PRO:CG	14:Q:261:ASN:HA	2.49	0.43
32:c:294:GLU:OE2	32:c:298:ARG:NE	2.52	0.43
46:s:245:VAL:HG21	46:s:249:TYR:CD2	2.54	0.43
46:s:345:VAL:O	46:s:383:ARG:NH1	2.42	0.43
49:w:120:MET:HE2	49:w:120:MET:N	2.34	0.43
50:y:140:VAL:N	50:y:262:GLN:OE1	2.51	0.43
1:A:1604:A:O2'	1:A:1605:G:OP1	2.36	0.43
2:B:14:A:N1	2:B:21:A:O2'	2.47	0.43
3:D:180:GLY:N	3:D:245:VAL:O	2.52	0.43
50:y:342:LEU:HD21	50:y:376:LEU:HA	2.01	0.43
10:L:36:THR:O	10:L:37:ARG:C	2.62	0.42
46:s:326:LEU:HD13	46:s:366:TYR:HB2	2.01	0.42
48:v:44:LYS:NZ	49:w:114:ASP:OD1	2.52	0.42
1:A:1244:A:OP2	23:0:94:ARG:NH2	2.46	0.42
1:A:1684:C:H1'	1:A:1685:U:P	2.59	0.42
1:A:2109:A:N3	12:O:116:GLN:NE2	2.67	0.42
4:E:208:ALA:HB2	4:E:297:VAL:HG12	2.02	0.42
6:H:117:ARG:HD2	6:H:121:LEU:CD1	2.49	0.42
14:Q:225:LYS:HB2	14:Q:226:PRO:CD	2.49	0.42
35:f:92:ILE:HG23	35:f:184:SER:O	2.20	0.42
50:y:190:ALA:O	50:y:261:PHE:N	2.51	0.42
1:A:1622:C:OP1	41:l:103:LYS:NZ	2.36	0.42
1:A:1642:C:H2'	1:A:1643:U:O4'	2.19	0.42
1:A:1836:A:H2'	3:D:132:TYR:HB3	2.01	0.42
9:K:171:THR:HG23	9:K:171:THR:O	2.20	0.42
38:i:76:GLY:O	38:i:81:ARG:NE	2.52	0.42
49:w:138:LEU:CD1	49:w:144:ILE:HD13	2.49	0.42
50:x:239:LEU:HA	50:x:269:VAL:HG21	2.01	0.42
50:y:338:GLN:O	50:y:339:SER:C	2.62	0.42
1:A:1638:C:N3	8:J:38:ILE:HD11	2.34	0.42
6:H:111:VAL:HG12	6:H:112:LYS:N	2.35	0.42
8:J:23:ILE:HD11	8:J:86:THR:HG22	2.01	0.42
13:P:85:LYS:O	13:P:89:HIS:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:198:ARG:NH2	32:c:287:GLU:OE2	2.44	0.42
26:6:144:GLY:N	26:6:145:PRO:CD	2.82	0.42
33:d:111:ARG:HH22	33:d:195:VAL:HG22	1.84	0.42
7:I:116:LEU:HB3	7:I:121:ILE:HB	2.00	0.42
15:R:56:ALA:O	15:R:60:LYS:N	2.52	0.42
16:S:132:ILE:N	16:S:162:ALA:O	2.37	0.42
16:S:182:LYS:O	16:S:183:ASN:HB3	2.20	0.42
40:k:61:GLU:N	40:k:62:PRO:CD	2.83	0.42
46:s:103:ASP:OD1	46:s:103:ASP:N	2.52	0.42
1:A:1111:C:H2'	1:A:1112:C:H4'	2.01	0.42
1:A:1649:U:C2	1:A:1650:A:C2	3.07	0.42
4:E:46:SER:O	23:0:118:LYS:NZ	2.47	0.42
5:F:103:GLN:HA	5:F:106:PHE:CE1	2.55	0.42
9:K:154:ARG:NH1	9:K:156:ASP:OD1	2.52	0.42
13:P:119:THR:O	13:P:120:ARG:C	2.62	0.42
50:y:143:ALA:O	50:y:188:ILE:N	2.53	0.42
3:D:226:ILE:O	3:D:227:ILE:HD13	2.20	0.42
6:H:117:ARG:HD2	6:H:121:LEU:HD13	2.01	0.42
18:U:136:ARG:NH1	27:7:77:VAL:HG11	2.34	0.42
38:i:34:VAL:HG12	38:i:35:ARG:N	2.35	0.42
38:i:80:LEU:HD12	38:i:80:LEU:O	2.20	0.42
46:s:353:ALA:O	46:s:364:PHE:N	2.39	0.42
5:F:102:TRP:O	5:F:106:PHE:HD1	2.03	0.42
5:F:230:VAL:HG12	5:F:242:LEU:HD12	2.01	0.42
16:S:189:ILE:HG22	16:S:190:ILE:N	2.35	0.42
17:T:99:GLN:O	23:0:103:LYS:NZ	2.53	0.42
23:0:109:CYS:SG	23:0:122:CYS:HB2	2.59	0.42
46:s:240:GLN:OE1	46:s:347:ARG:NH1	2.53	0.42
1:A:1594:U:H1'	1:A:1595:A:C8	2.55	0.42
3:D:121:GLU:HB3	3:D:122:PRO:HD2	2.02	0.42
7:I:210:LEU:HD11	40:k:31:ARG:HE	1.84	0.42
23:0:109:CYS:HB3	23:0:112:CYS:SG	2.60	0.42
47:u:106:ILE:HG21	47:u:188:TRP:HB3	2.01	0.42
50:y:126:GLU:H	50:y:254:ARG:HA	1.85	0.42
1:A:1580:C:N4	45:r:195:MET:O	2.48	0.42
1:A:1832:U:H2'	1:A:1833:A:O4'	2.19	0.42
1:A:2342:U:O2'	1:A:2343:A:OP1	2.33	0.42
1:A:2342:U:H4'	1:A:2343:A:OP1	2.19	0.42
3:D:113:ARG:O	3:D:148:ARG:NH2	2.50	0.42
5:F:191:ASP:N	5:F:191:ASP:OD1	2.52	0.42
13:P:125:CYS:HA	13:P:128:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:246:ASP:OD1	14:Q:247:LEU:N	2.52	0.42
40:k:13:VAL:O	40:k:13:VAL:HG13	2.20	0.42
5:F:52:GLU:OE1	5:F:52:GLU:N	2.49	0.41
14:Q:232:ARG:CD	14:Q:235:ARG:HG3	2.50	0.41
34:e:48:ALA:N	34:e:236:PHE:O	2.53	0.41
50:y:117:ARG:O	50:y:121:GLY:N	2.53	0.41
1:A:1649:U:HO2'	1:A:1650:A:C5'	2.23	0.41
1:A:1908:G:N2	1:A:2092:G:OP2	2.47	0.41
1:A:2182:U:N3	1:A:2235:A:OP1	2.53	0.41
4:E:128:HIS:HB2	4:E:173:LYS:HZ1	1.84	0.41
6:H:76:VAL:HG21	20:X:91:TYR:CZ	2.54	0.41
27:7:132:PRO:O	27:7:136:ASN:N	2.44	0.41
31:b:131:HIS:CE1	31:b:134:THR:HG23	2.55	0.41
41:l:74:ILE:HG22	41:l:74:ILE:O	2.19	0.41
46:s:41:VAL:HG22	46:s:41:VAL:O	2.20	0.41
7:I:102:VAL:O	7:I:103:ALA:C	2.62	0.41
31:b:43:ALA:HB2	31:b:89:VAL:HG11	2.01	0.41
32:c:171:ARG:NE	32:c:176:GLU:OE1	2.53	0.41
44:q:44:ASN:O	44:q:47:THR:HG22	2.21	0.41
1:A:1294:A:N6	1:A:1329:C:OP1	2.53	0.41
11:M:21:VAL:HG22	42:o:95:LEU:HD22	2.03	0.41
32:c:183:GLU:OE1	32:c:183:GLU:N	2.53	0.41
1:A:1311:G:N2	38:i:66:PHE:O	2.53	0.41
1:A:1569:U:O2'	15:R:100:LYS:NZ	2.54	0.41
11:M:157:LEU:HD23	11:M:158:ALA:N	2.35	0.41
14:Q:165:GLU:O	14:Q:171:ILE:HD12	2.20	0.41
14:Q:263:PRO:O	14:Q:266:GLU:HG2	2.21	0.41
25:5:358:GLN:NE2	25:5:360:ASN:OD1	2.54	0.41
31:b:16:HIS:HB3	31:b:19:LEU:HD12	2.02	0.41
40:k:17:ARG:O	40:k:65:ASP:N	2.46	0.41
1:A:1669:C:N4	1:A:2125:C:O2	2.49	0.41
7:I:116:LEU:CD1	7:I:123:ILE:HG13	2.43	0.41
12:O:67:ASP:O	46:s:43:ARG:NH1	2.52	0.41
32:c:276:CYS:N	32:c:279:LYS:O	2.49	0.41
1:A:1317:C:N4	11:M:142:GLU:OE2	2.54	0.41
1:A:1606:G:H2'	1:A:1607:C:H5'	2.03	0.41
3:D:164:ILE:HD11	3:D:180:GLY:C	2.46	0.41
4:E:278:THR:N	4:E:330:GLU:O	2.46	0.41
6:H:117:ARG:HD2	6:H:121:LEU:HB2	2.03	0.41
7:I:139:LEU:HD11	7:I:176:LEU:HB2	2.03	0.41
8:J:50:CYS:O	8:J:54:ASN:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:136:ILE:N	14:Q:152:ARG:O	2.52	0.41
19:V:124:ASP:OD1	19:V:125:PRO:HD2	2.20	0.41
19:V:194:LEU:HD21	21:Y:101:HIS:HB2	2.02	0.41
33:d:137:PHE:CE2	33:d:212:VAL:HG11	2.56	0.41
48:v:62:LEU:C	48:v:62:LEU:HD23	2.46	0.41
50:y:342:LEU:HD11	50:y:376:LEU:HA	2.03	0.41
1:A:1504:A:H3'	1:A:1505:A:H5''	2.02	0.41
1:A:2617:A:O2'	1:A:2618:A:P	2.79	0.41
1:A:2674:U:OP1	4:E:157:LYS:NZ	2.54	0.41
5:F:276:GLN:O	36:g:90:ARG:NH1	2.54	0.41
14:Q:225:LYS:HB2	14:Q:226:PRO:HD2	2.02	0.41
19:V:191:LEU:HD13	29:9:116:GLY:HA3	2.02	0.41
23:0:111:GLU:OE1	23:0:111:GLU:N	2.47	0.41
25:5:206:ASN:N	25:5:227:SER:O	2.49	0.41
34:e:64:LEU:HD12	34:e:65:GLN:N	2.36	0.41
36:g:129:SER:OG	36:g:130:PRO:HD3	2.21	0.41
1:A:2448:U:O4'	1:A:2471:A:N6	2.54	0.41
1:A:2648:A:OP1	9:K:98:LYS:NZ	2.54	0.41
11:M:189:PRO:HA	11:M:192:PHE:HE1	1.86	0.41
12:O:88:LYS:O	12:O:92:VAL:N	2.50	0.41
13:P:161:LEU:HD23	13:P:161:LEU:C	2.46	0.41
19:V:177:THR:CG2	29:9:69:LYS:H	2.34	0.41
33:d:160:LEU:HD22	33:d:169:PHE:CD2	2.56	0.41
1:A:1142:A:H2'	1:A:1143:A:O4'	2.20	0.41
1:A:1595:A:H1'	1:A:1651:A:C2	2.57	0.41
1:A:1611:A:H2'	1:A:1612:A:O4'	2.21	0.41
9:K:60:ILE:HG21	9:K:133:ILE:HD11	2.03	0.41
9:K:116:LEU:O	9:K:119:ARG:NH1	2.53	0.41
18:U:7:TYR:CD2	18:U:17:LEU:HD21	2.56	0.41
26:6:125:LEU:O	26:6:126:ARG:HG2	2.21	0.41
34:e:53:ARG:HD3	34:e:155:LEU:HD13	2.03	0.41
1:A:1144:U:O2'	1:A:1435:U:O4	2.39	0.40
1:A:1644:C:H2'	1:A:1645:A:O4'	2.20	0.40
1:A:1653:A:OP2	1:A:1653:A:C8	2.74	0.40
4:E:120:THR:HG22	4:E:285:VAL:O	2.21	0.40
5:F:181:LYS:NZ	5:F:256:HIS:O	2.54	0.40
5:F:186:ASP:OD1	11:M:20:ARG:NH1	2.54	0.40
7:I:177:LEU:N	7:I:178:PRO:HD2	2.35	0.40
26:6:334:LEU:HD23	26:6:334:LEU:H	1.86	0.40
46:s:107:GLN:O	46:s:111:LYS:N	2.54	0.40
46:s:409:ASP:O	46:s:413:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1563:U:OP1	1:A:1685:U:O2'	2.40	0.40
1:A:1629:G:O4'	41:l:123:ILE:HG21	2.20	0.40
8:J:90:PHE:CE2	8:J:120:ILE:HG21	2.56	0.40
11:M:167:GLU:OE2	11:M:219:ARG:NH1	2.54	0.40
13:P:108:ARG:O	13:P:108:ARG:NH1	2.40	0.40
18:U:138:PRO:HD2	33:d:276:ILE:HD13	2.03	0.40
26:6:220:ASN:HA	26:6:268:PHE:CD1	2.57	0.40
27:7:147:LEU:C	27:7:147:LEU:HD23	2.46	0.40
32:c:188:LEU:N	32:c:189:PRO:HD2	2.36	0.40
1:A:1228:A:O2'	19:V:33:ARG:NH2	2.53	0.40
1:A:1645:A:H2'	1:A:1646:A:H5''	2.03	0.40
6:H:132:GLU:OE1	20:X:139:TYR:HD1	2.03	0.40
19:V:158:GLU:N	19:V:158:GLU:OE1	2.54	0.40
35:f:160:GLY:C	35:f:161:LEU:HD22	2.45	0.40
37:h:132:ASN:OD1	37:h:132:ASN:C	2.65	0.40
46:s:99:ALA:HB1	46:s:265:LEU:HD11	2.04	0.40
46:s:202:PHE:CD1	46:s:276:ILE:HG23	2.54	0.40
1:A:1634:C:N4	1:A:1641:G:H22	2.19	0.40
14:Q:122:ALA:N	14:Q:170:ARG:O	2.41	0.40
25:5:135:LYS:O	25:5:139:LEU:HD23	2.22	0.40
50:y:132:ALA:HB2	50:y:159:LYS:O	2.22	0.40
1:A:1537:A:O2'	1:A:1538:G:O4'	2.36	0.40
1:A:1605:G:N1	1:A:1619:C:N3	2.60	0.40
1:A:1923:G:H2'	1:A:1924:A:H5''	2.04	0.40
8:J:92:LYS:HE2	8:J:151:LEU:HD22	2.03	0.40
9:K:49:GLN:OE1	9:K:49:GLN:N	2.46	0.40
46:s:198:ARG:NH1	46:s:279:GLY:O	2.46	0.40
49:w:141:PRO:HA	49:w:144:ILE:HG22	2.04	0.40
50:y:349:ALA:HB2	50:y:400:GLY:HA3	2.02	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%)	165 (98%)	3 (2%)	0	100	100
4	E	260/348 (75%)	252 (97%)	8 (3%)	0	100	100
5	F	210/294 (71%)	210 (100%)	0	0	100	100
6	H	93/268 (35%)	88 (95%)	5 (5%)	0	100	100
7	I	122/262 (47%)	117 (96%)	5 (4%)	0	100	100
8	J	140/192 (73%)	137 (98%)	3 (2%)	0	100	100
9	K	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
10	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
11	M	245/295 (83%)	239 (98%)	6 (2%)	0	100	100
12	O	142/176 (81%)	139 (98%)	3 (2%)	0	100	100
13	P	139/180 (77%)	132 (95%)	7 (5%)	0	100	100
14	Q	215/292 (74%)	212 (99%)	3 (1%)	0	100	100
15	R	129/149 (87%)	129 (100%)	0	0	100	100
16	S	157/209 (75%)	153 (98%)	4 (2%)	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	196/198 (99%)	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%)	113 (100%)	0	0	100	100
23	0	106/187 (57%)	106 (100%)	0	0	100	100
24	1	54/65 (83%)	54 (100%)	0	0	100	100
25	5	383/423 (90%)	375 (98%)	7 (2%)	1 (0%)	36	72
26	6	307/380 (81%)	299 (97%)	8 (3%)	0	100	100
27	7	290/336 (86%)	285 (98%)	5 (2%)	0	100	100
28	8	48/206 (23%)	48 (100%)	0	0	100	100
29	9	94/135 (70%)	94 (100%)	0	0	100	100
30	a	80/142 (56%)	78 (98%)	2 (2%)	0	100	100
31	b	146/159 (92%)	141 (97%)	5 (3%)	0	100	100
32	c	275/308 (89%)	275 (100%)	0	0	100	100
33	d	198/306 (65%)	196 (99%)	2 (1%)	0	100	100
34	e	102/283 (36%)	101 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	f	79/211 (37%)	75 (95%)	4 (5%)	0	100	100
36	g	130/166 (78%)	129 (99%)	1 (1%)	0	100	100
37	h	108/159 (68%)	104 (96%)	4 (4%)	0	100	100
38	i	91/128 (71%)	91 (100%)	0	0	100	100
39	j	82/121 (68%)	81 (99%)	1 (1%)	0	100	100
40	k	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
41	l	74/135 (55%)	72 (97%)	2 (3%)	0	100	100
42	o	76/102 (74%)	76 (100%)	0	0	100	100
43	p	97/206 (47%)	95 (98%)	2 (2%)	0	100	100
44	q	95/222 (43%)	95 (100%)	0	0	100	100
45	r	152/196 (78%)	144 (95%)	8 (5%)	0	100	100
46	s	373/442 (84%)	362 (97%)	11 (3%)	0	100	100
47	u	123/228 (54%)	119 (97%)	4 (3%)	0	100	100
48	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
49	w	77/156 (49%)	74 (96%)	3 (4%)	0	100	100
50	x	227/418 (54%)	218 (96%)	9 (4%)	0	100	100
50	y	239/418 (57%)	215 (90%)	23 (10%)	1 (0%)	30	67
All	All	7559/10916 (69%)	7398 (98%)	159 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	5	229	ILE
50	y	162	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	143/197 (73%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	119/230 (52%)	119 (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	125/152 (82%)	125 (100%)	0	100	100
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	176/176 (100%)	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	1	53/60 (88%)	53 (100%)	0	100	100
25	5	349/372 (94%)	349 (100%)	0	100	100
26	6	278/335 (83%)	278 (100%)	0	100	100
27	7	269/301 (89%)	269 (100%)	0	100	100
28	8	45/182 (25%)	45 (100%)	0	100	100
29	9	83/114 (73%)	83 (100%)	0	100	100
30	a	79/129 (61%)	79 (100%)	0	100	100
31	b	130/138 (94%)	130 (100%)	0	100	100
32	c	243/266 (91%)	243 (100%)	0	100	100
33	d	182/272 (67%)	182 (100%)	0	100	100
34	e	102/238 (43%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	74/185 (40%)	74 (100%)	0	100	100
36	g	122/148 (82%)	122 (100%)	0	100	100
37	h	100/143 (70%)	100 (100%)	0	100	100
38	i	84/111 (76%)	84 (100%)	0	100	100
39	j	68/99 (69%)	68 (100%)	0	100	100
40	k	72/95 (76%)	72 (100%)	0	100	100
41	l	70/112 (62%)	70 (100%)	0	100	100
42	o	65/85 (76%)	65 (100%)	0	100	100
43	p	12/177 (7%)	12 (100%)	0	100	100
44	q	84/187 (45%)	84 (100%)	0	100	100
45	r	141/168 (84%)	141 (100%)	0	100	100
46	s	329/378 (87%)	329 (100%)	0	100	100
47	u	115/197 (58%)	115 (100%)	0	100	100
48	v	60/61 (98%)	60 (100%)	0	100	100
49	w	73/135 (54%)	73 (100%)	0	100	100
50	x	10/358 (3%)	10 (100%)	0	100	100
50	y	14/358 (4%)	14 (100%)	0	100	100
All	All	6387/9467 (68%)	6387 (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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	117	HIS
4	E	174	GLN
4	E	281	ASN
4	E	294	ASN
5	F	98	GLN
5	F	105	ASN
5	F	249	ASN
6	H	123	GLN
7	I	184	ASN
9	K	40	GLN
9	K	70	ASN
14	Q	132	GLN

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Mol	Chain	Res	Type
15	R	27	HIS
17	T	56	GLN
17	T	73	GLN
18	U	98	GLN
20	X	94	ASN
22	Z	95	HIS
23	0	82	ASN
25	5	88	HIS
25	5	206	ASN
26	6	77	HIS
26	6	174	HIS
26	6	351	HIS
29	9	50	GLN
30	a	110	GLN
30	a	125	HIS
31	b	16	HIS
31	b	102	GLN
31	b	123	ASN
31	b	141	HIS
32	c	139	GLN
32	c	260	GLN
33	d	119	GLN
34	e	73	GLN
35	f	107	GLN
35	f	152	HIS
37	h	96	HIS
37	h	111	HIS
38	i	59	ASN
42	o	91	GLN
42	o	94	HIS
45	r	131	HIS
46	s	94	HIS
46	s	333	GLN
47	u	134	HIS
48	v	54	GLN
50	y	277	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1058/1584 (66%)	338 (31%)	25 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	59/68 (86%)	23 (38%)	1 (1%)
All	All	1117/1652 (67%)	361 (32%)	26 (2%)

All (361) 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
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	1168	U
1	A	1170	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

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Mol	Chain	Res	Type
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	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
1	A	1281	A
1	A	1292	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	1313	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

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Mol	Chain	Res	Type
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	1483	C
1	A	1487	A
1	A	1488	A
1	A	1489	A
1	A	1490	A
1	A	1491	A
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
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	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

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Mol	Chain	Res	Type
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	1599	A
1	A	1600	U
1	A	1602	G
1	A	1603	U
1	A	1604	A
1	A	1605	G
1	A	1606	G
1	A	1607	C
1	A	1608	C
1	A	1609	U
1	A	1610	A
1	A	1612	A
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	1631	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

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Mol	Chain	Res	Type
1	A	1641	G
1	A	1642	C
1	A	1644	C
1	A	1645	A
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	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
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	1731	A
1	A	1734	G
1	A	1749	A
1	A	1750	A
1	A	1755	U
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	1790	A
1	A	1794	C

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Mol	Chain	Res	Type
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	1873	G
1	A	1881	U
1	A	1883	A
1	A	1888	A
1	A	1889	A
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	1944	A
1	A	1945	C
1	A	2091	U
1	A	2092	G
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2121	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

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Mol	Chain	Res	Type
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	2177	A
1	A	2178	A
1	A	2180	U
1	A	2182	U
1	A	2183	A
1	A	2186	A
1	A	2187	C
1	A	2190	A
1	A	2193	U
1	A	2195	U
1	A	2196	U
1	A	2197	U
1	A	2239	U
1	A	2241	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	2340	G
1	A	2342	U
1	A	2343	A
1	A	2359	A
1	A	2360	C
1	A	2362	A
1	A	2363	A
1	A	2367	A
1	A	2369	C
1	A	2373	G
1	A	2390	U
1	A	2393	U
1	A	2396	A
1	A	2397	G

Continued on next page...

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Mol	Chain	Res	Type
1	A	2407	C
1	A	2409	A
1	A	2411	A
1	A	2438	G
1	A	2447	A
1	A	2475	U
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	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	2640	A
1	A	2647	U
1	A	2648	A

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Mol	Chain	Res	Type
1	A	2650	G
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	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	59	C
2	B	61	C
2	B	64	A
2	B	67	C

All (26) 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...

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Mol	Chain	Res	Type
1	A	1502	A
1	A	1538	G
1	A	1584	A
1	A	1612	A
1	A	1628	A
1	A	1637	U
1	A	1649	U
1	A	1684	C
1	A	1804	U
1	A	1894	C
1	A	1944	A
1	A	2182	U
1	A	2302	U
1	A	2342	U
1	A	2485	C
1	A	2507	U
1	A	2564	G
1	A	2659	C
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	45,7	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	FES	r	301	45,7	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

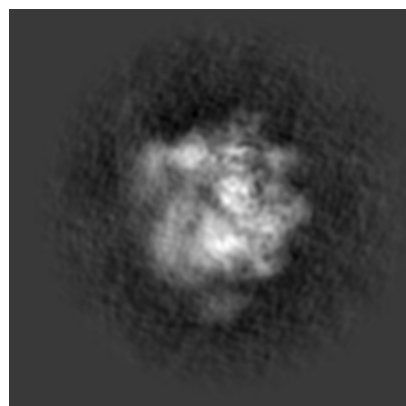
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52046. These allow visual inspection of the internal detail of the map and identification of artifacts.

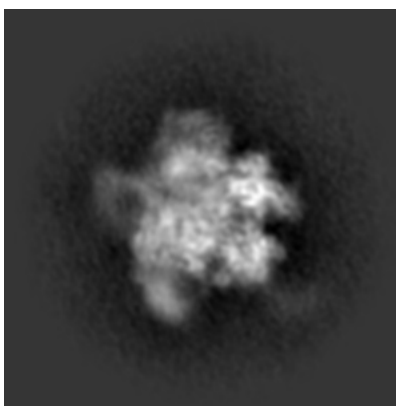
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

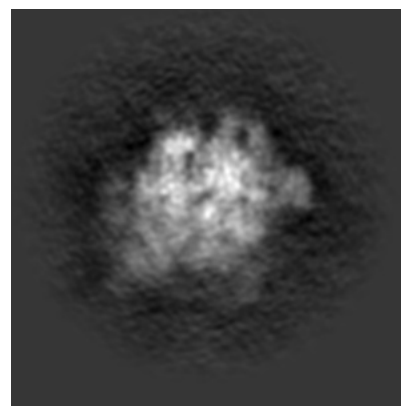
6.1.1 Primary map



X

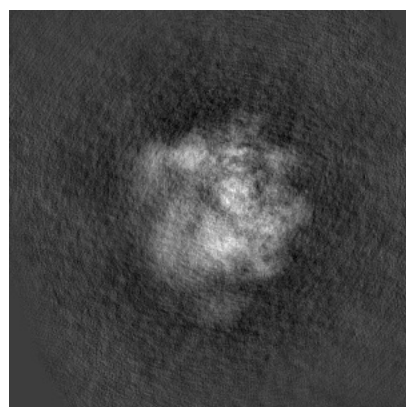


Y

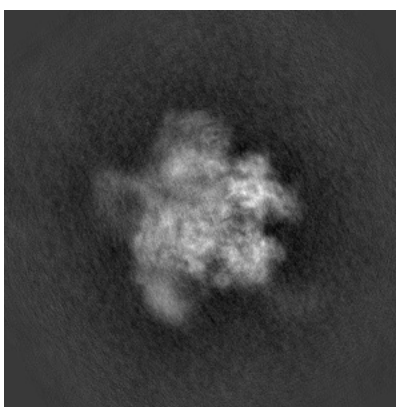


Z

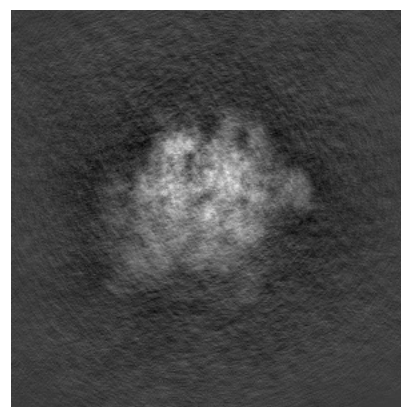
6.1.2 Raw map



X



Y

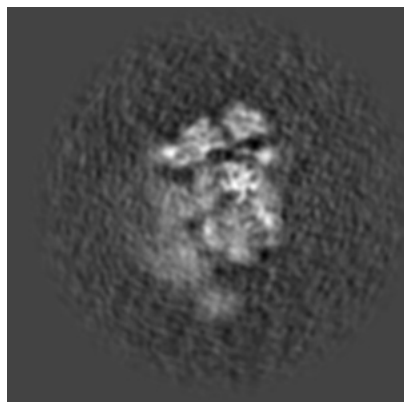


Z

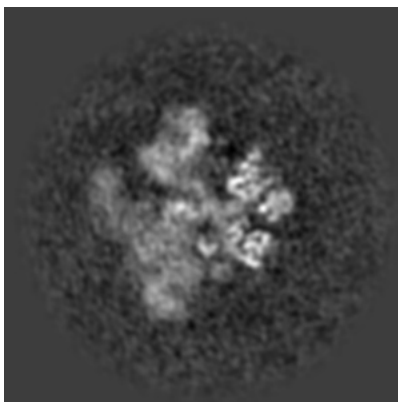
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

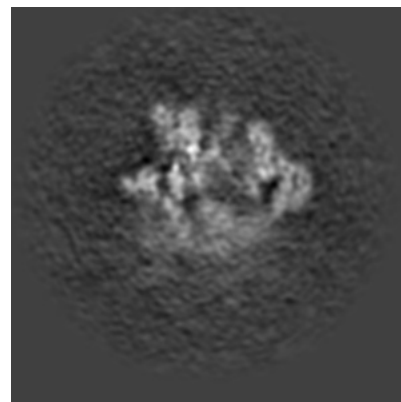
6.2.1 Primary map



X Index: 270

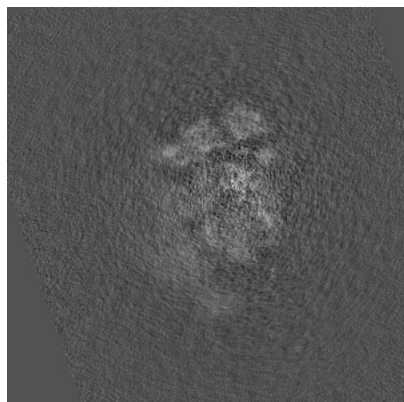


Y Index: 270

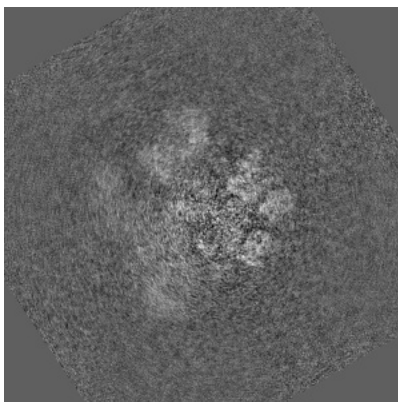


Z Index: 270

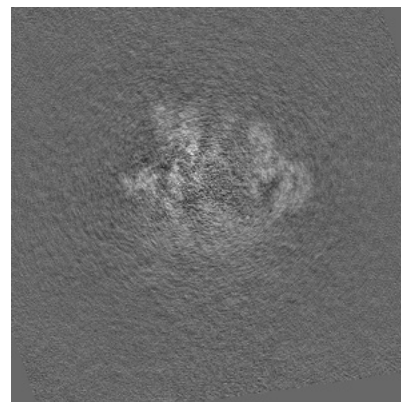
6.2.2 Raw map



X Index: 270



Y Index: 270

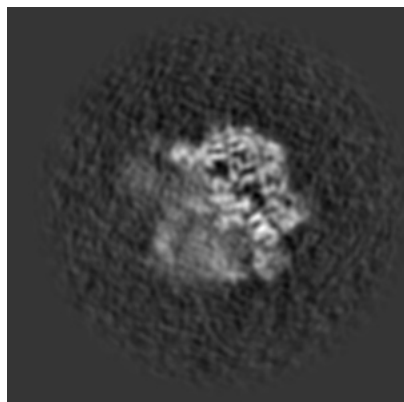


Z Index: 270

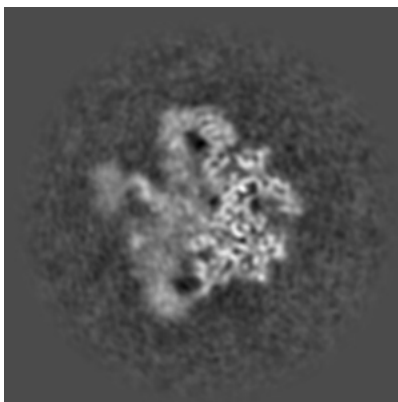
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

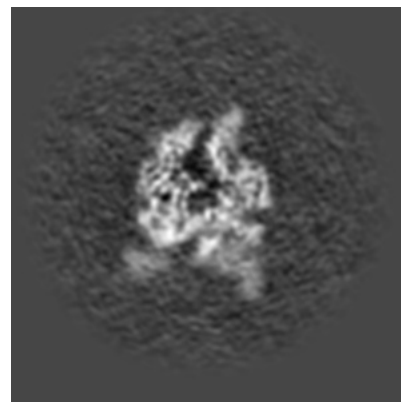
6.3.1 Primary map



X Index: 220

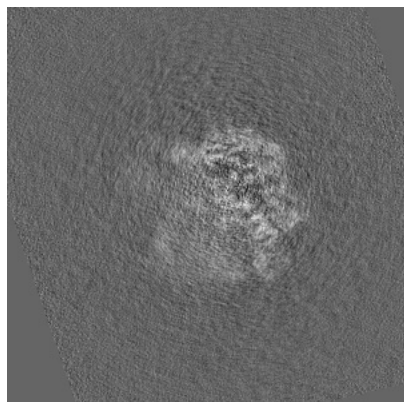


Y Index: 302

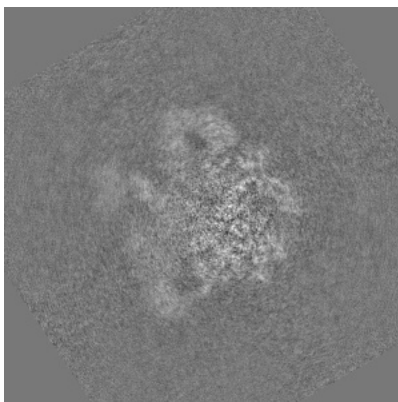


Z Index: 340

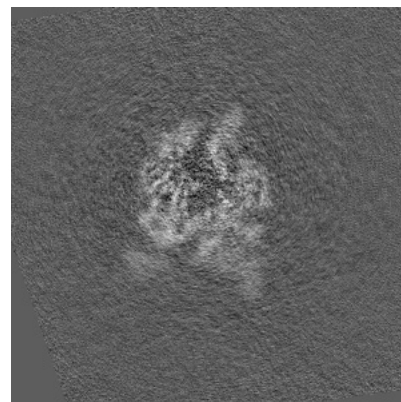
6.3.2 Raw map



X Index: 221



Y Index: 303

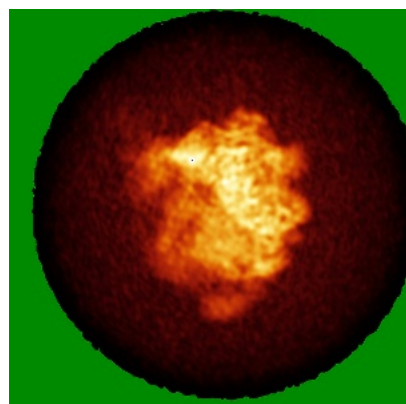


Z Index: 339

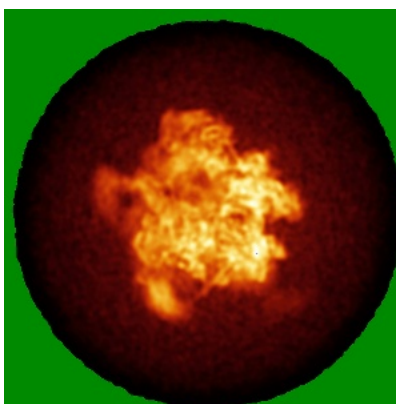
The images above show the largest variance slices of the map in three orthogonal directions.

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

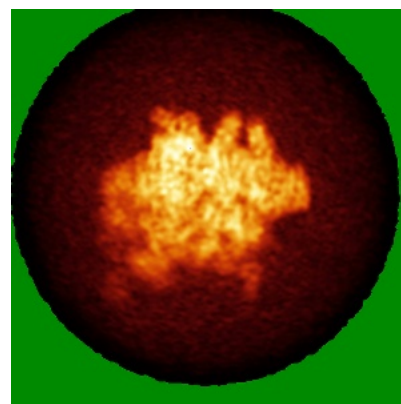
6.4.1 Primary map



X

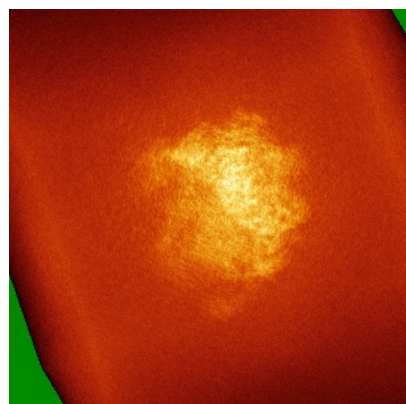


Y

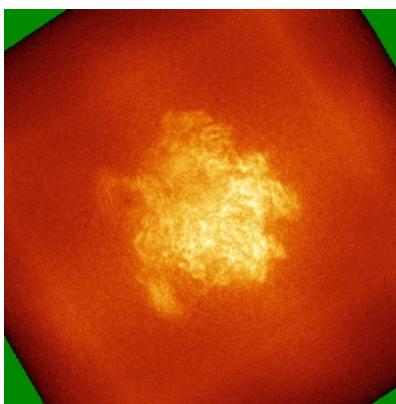


Z

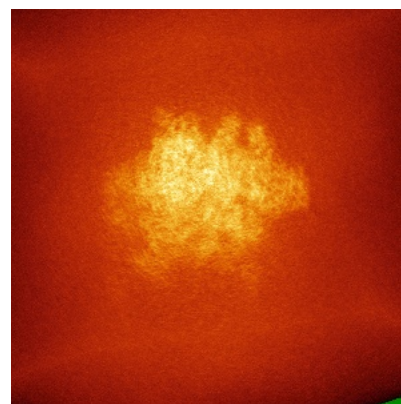
6.4.2 Raw map



X



Y

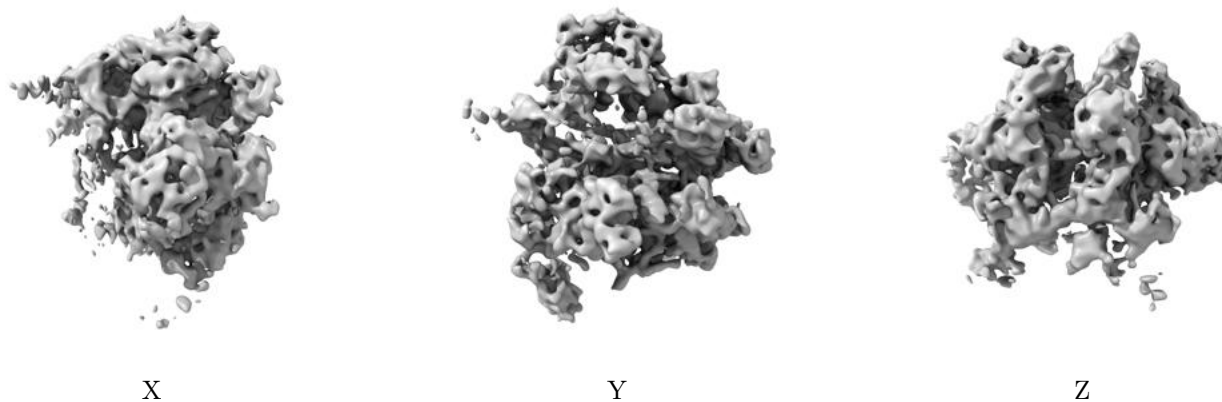


Z

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

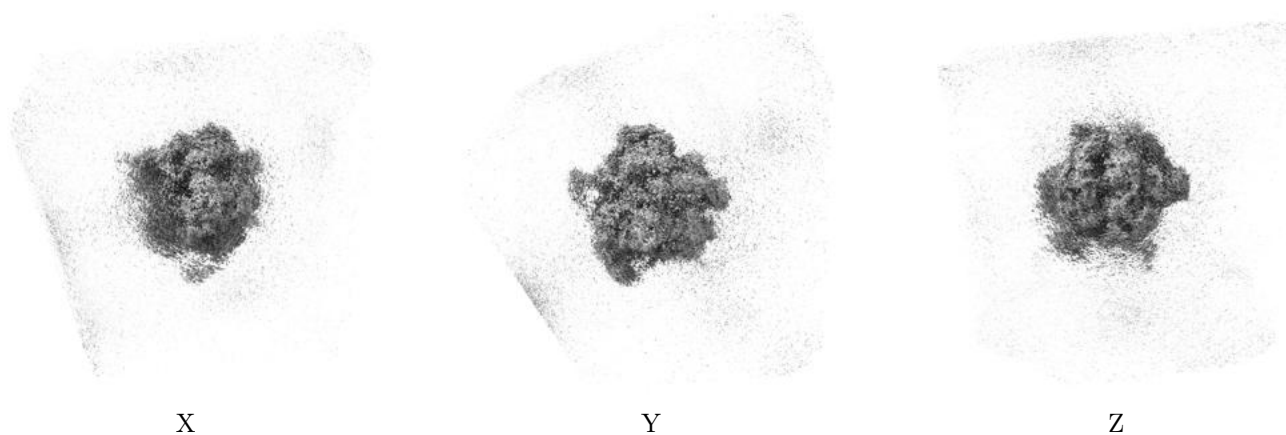
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

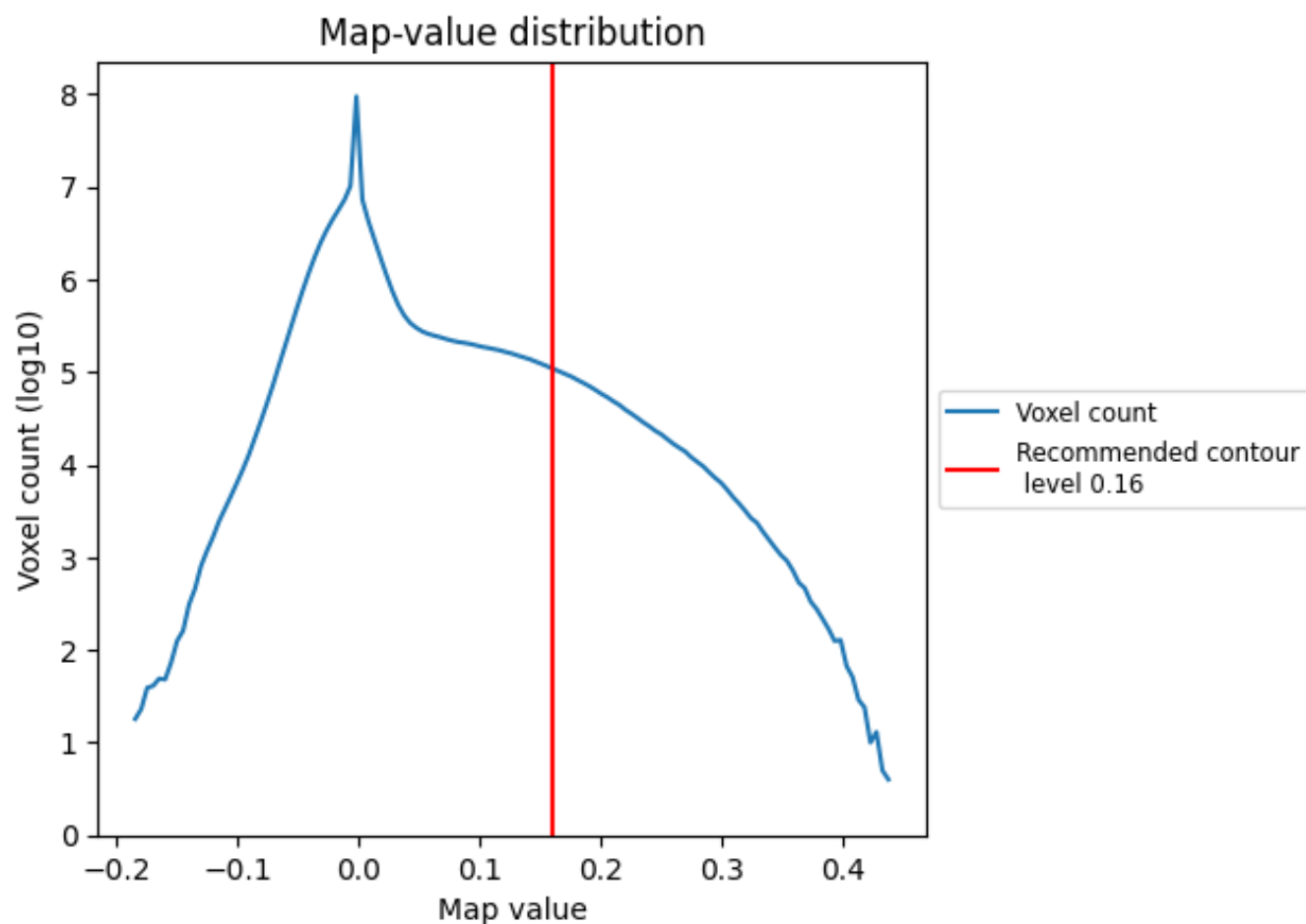
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

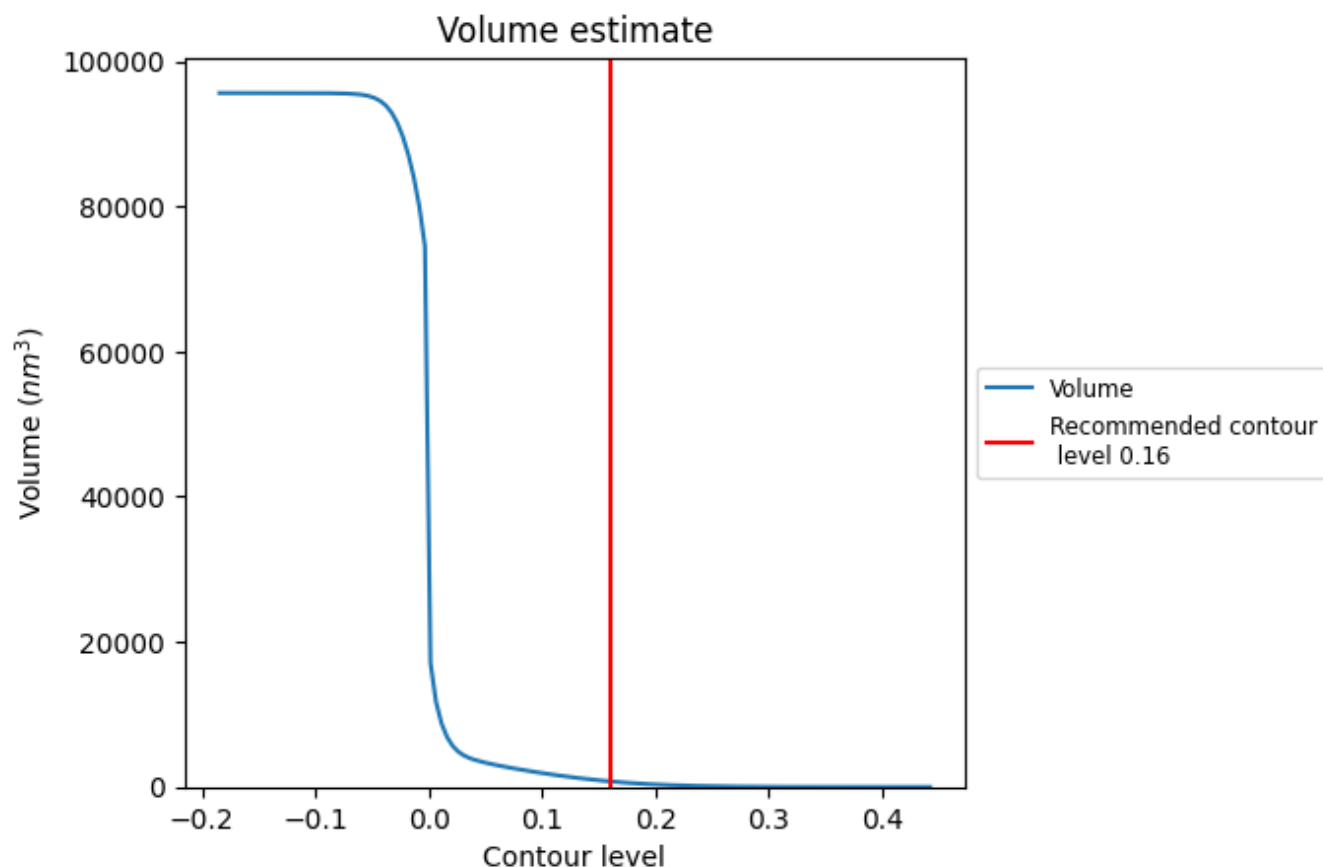
This section contains the results of statistical analysis of the map.

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.

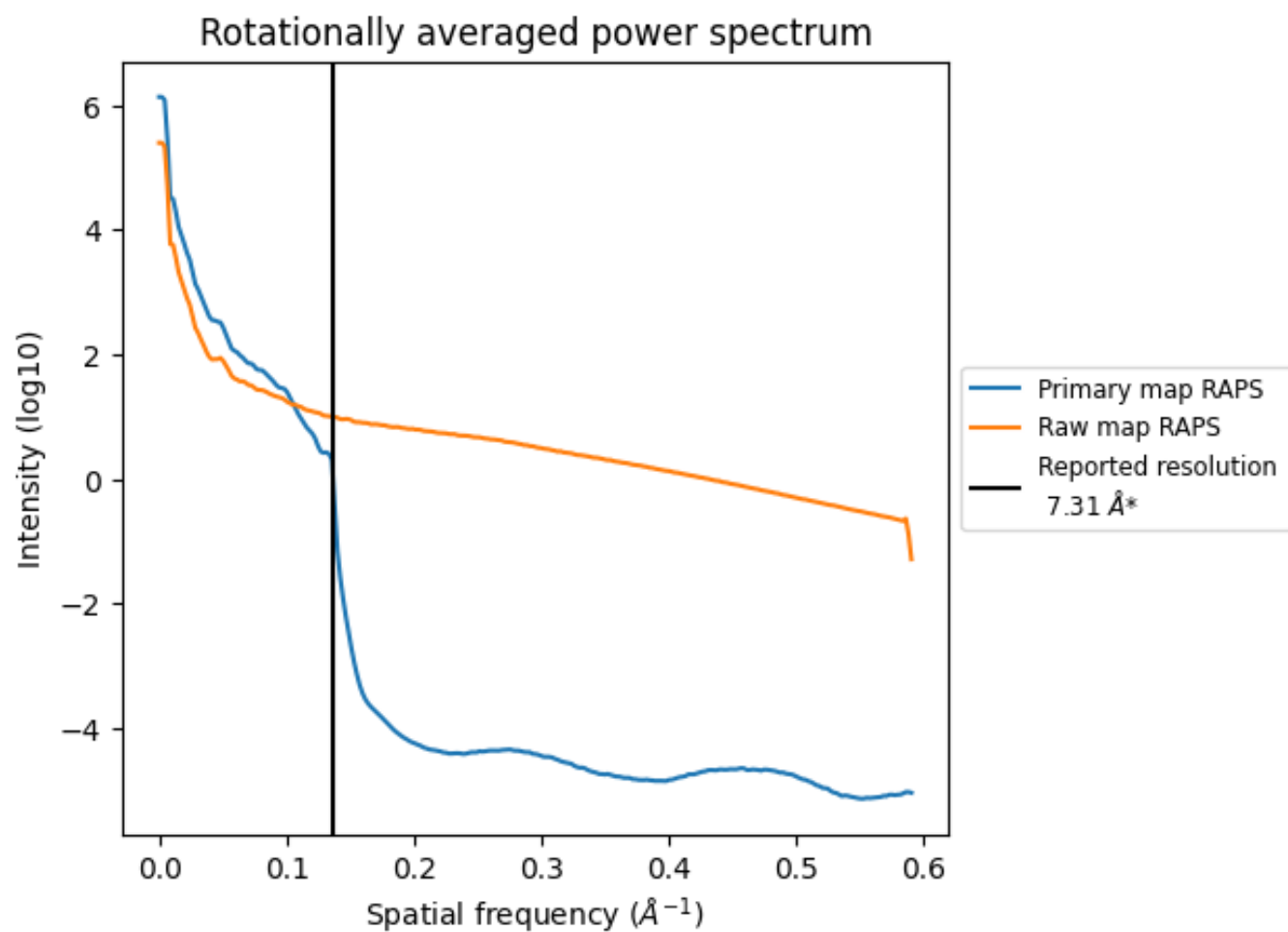
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm³; this corresponds to an approximate mass of 697 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 ⓘ

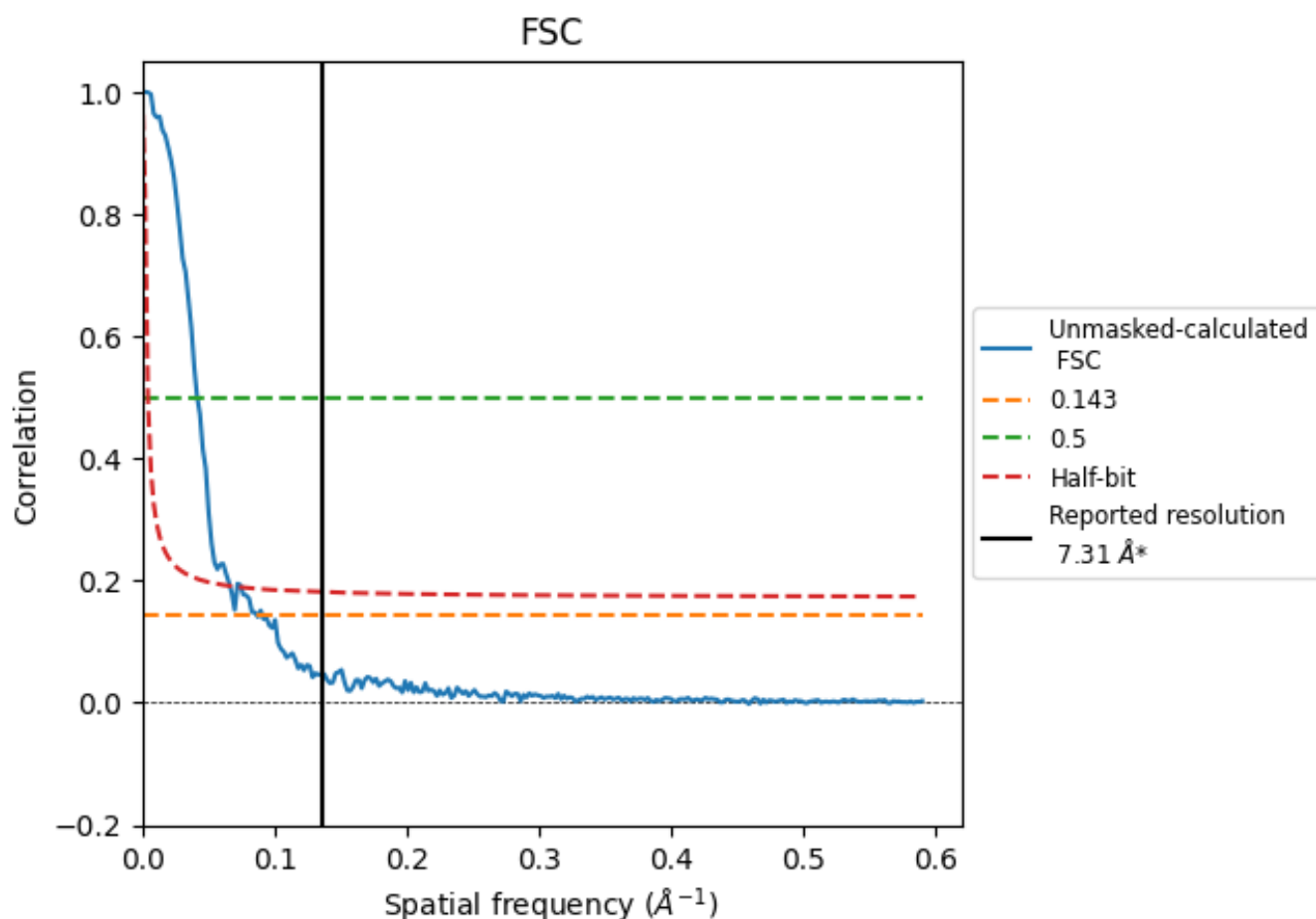


*Reported resolution corresponds to spatial frequency of 0.137 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

8.2 Resolution estimates [i](#)

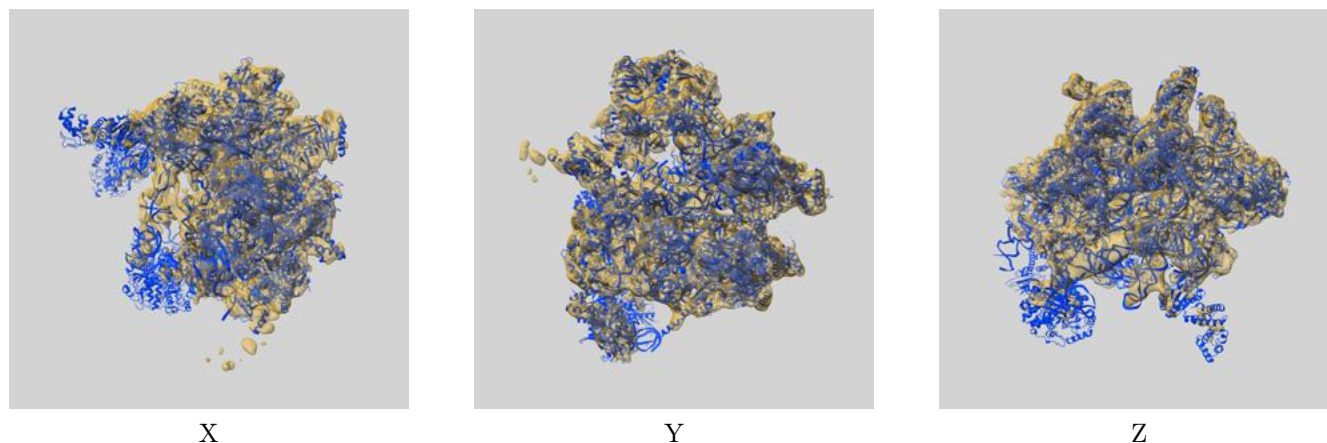
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.53	23.98	15.08

*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 11.53 differs from the reported value 7.31 by more than 10 %

9 Map-model fit [i](#)

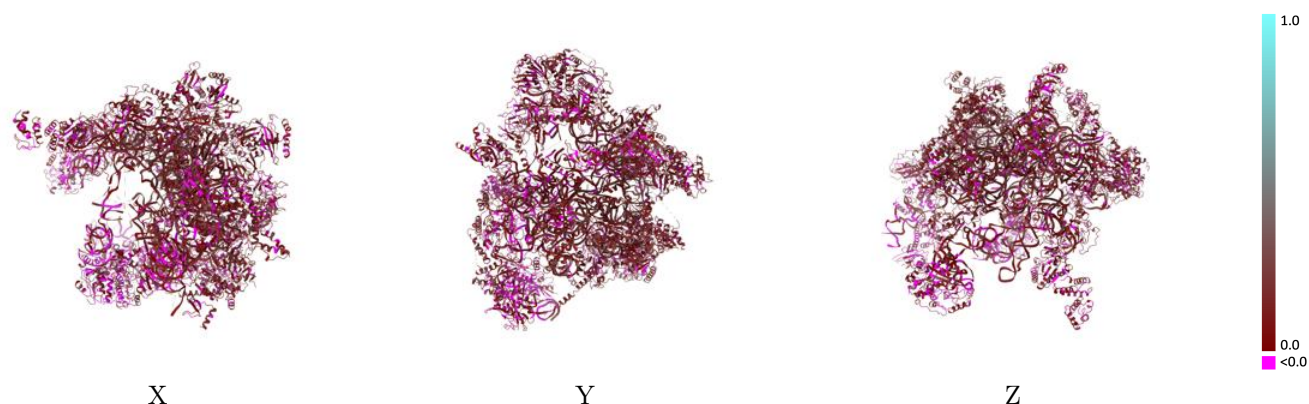
This section contains information regarding the fit between EMDB map EMD-52046 and PDB model 9HCE. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.16 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](#)

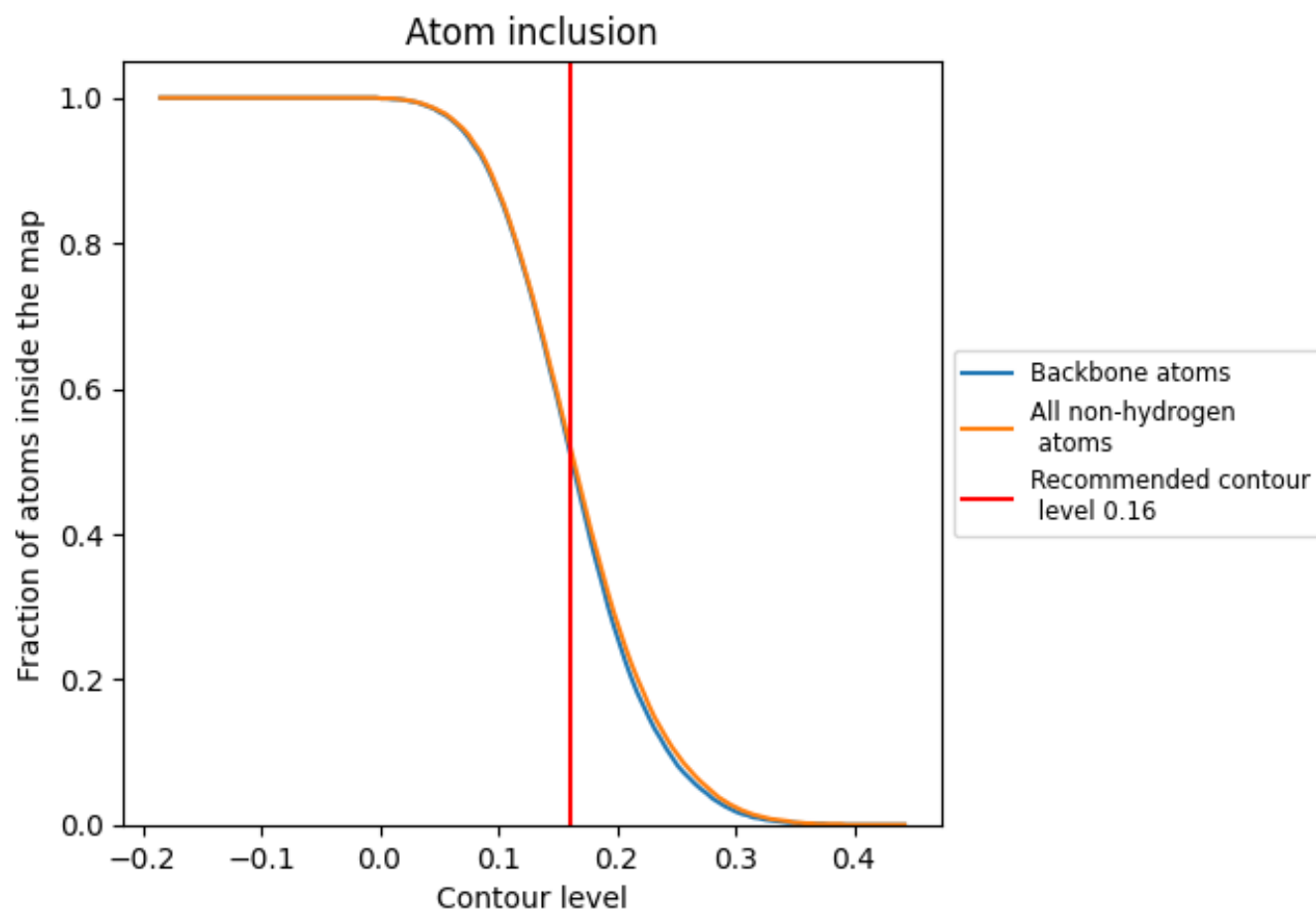


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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	 0.5250	 0.1200
0	 0.7510	 0.1570
1	 0.2180	 0.0440
5	 0.4490	 0.1060
6	 0.2790	 0.0440
7	 0.6510	 0.1410
8	 0.0000	 0.0190
9	 0.5980	 0.1080
A	 0.6330	 0.1350
B	 0.1580	 0.0500
D	 0.3530	 0.0620
E	 0.7370	 0.1360
F	 0.7160	 0.1240
H	 0.6150	 0.0860
I	 0.1210	 0.0820
J	 0.0210	 0.0340
K	 0.6650	 0.1410
L	 0.1570	 0.0780
M	 0.6090	 0.1270
O	 0.7190	 0.1270
P	 0.2540	 0.0350
Q	 0.6390	 0.1450
R	 0.5510	 0.1450
S	 0.6230	 0.1610
T	 0.6300	 0.1370
U	 0.6240	 0.1240
V	 0.3230	 0.1020
X	 0.5400	 0.1280
Y	 0.5820	 0.1140
Z	 0.5140	 0.1520
a	 0.6740	 0.1620
b	 0.6580	 0.1520
c	 0.7440	 0.1570
d	 0.6140	 0.1190
e	 0.0000	 0.0390



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Chain	Atom inclusion	Q-score
f	 0.0000	 0.0340
g	 0.7740	 0.1630
h	 0.6160	 0.1710
i	 0.5970	 0.1360
j	 0.5430	 0.1700
k	 0.0960	 0.0980
l	 0.1500	 0.0660
o	 0.6930	 0.1610
p	 0.4770	 0.1710
q	 0.6530	 0.1850
r	 0.7360	 0.1470
s	 0.5800	 0.1360
u	 0.1730	 0.0900
v	 0.1070	 0.1000
w	 0.0360	 0.0720
x	 0.0490	 0.0710
y	 0.0870	 0.1010