



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 12:23 PM UTC

PDB ID : 7A5F / pdb_00007a5f
EMDB ID : EMD-11641
Title : Structure of the stalled human mitoribosome with P- and E-site mt-tRNAs
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 4.40 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:

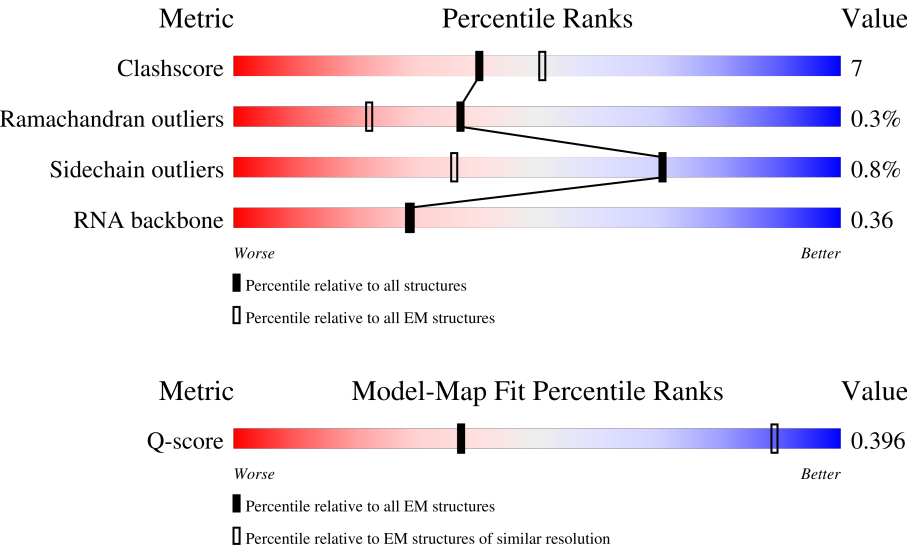
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.40 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	3132 (3.91 - 4.90)

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	Y2	29	93% 97%
2	A3	1559	6% 55% 35% 6%
3	B3	69	12% 51% 28% 19%

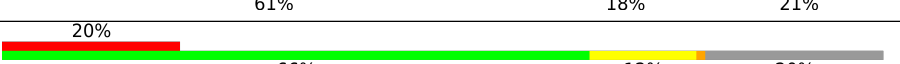
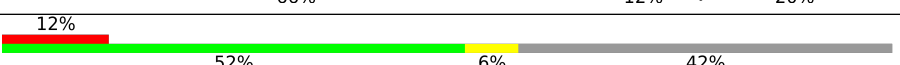
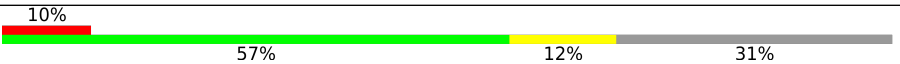
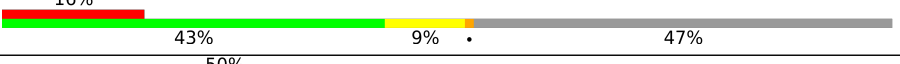
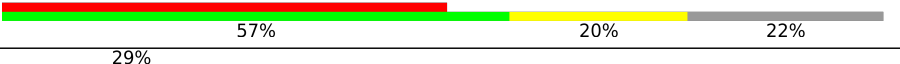
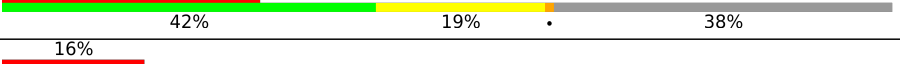
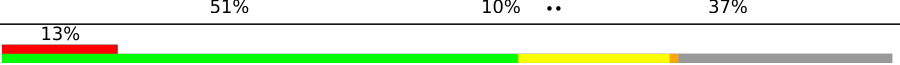
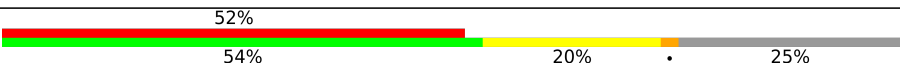
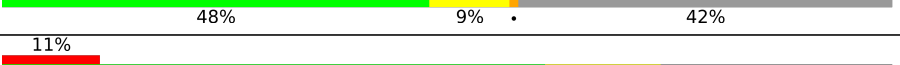
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Mol	Chain	Length	Quality of chain
4	D3	305	
5	E3	348	
6	F3	311	
7	D	267	
7	H3	267	
8	I3	261	
9	J3	192	
10	K3	178	
11	L3	145	
12	M3	296	
13	N3	251	
14	O3	175	
15	P3	180	
16	Q3	292	
17	R3	149	
18	S3	205	
19	T3	206	
20	U3	153	
21	V3	216	
22	W3	148	
23	X3	256	
24	Y3	250	
25	Z3	161	
26	O3	188	
27	I3	65	

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Mol	Chain	Length	Quality of chain
28	23	92	
29	33	188	
30	43	103	
31	53	423	
32	63	380	
33	73	338	
34	93	137	
35	a3	142	
36	b3	215	
37	c3	332	
38	d3	306	
39	e3	279	
40	f3	212	
41	g3	166	
42	h3	158	
43	i3	128	
44	j3	123	
45	k3	112	
46	l3	138	
47	m3	128	
48	o3	102	
49	p3	206	
50	q3	222	
51	r3	196	
52	s3	467	

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Mol	Chain	Length	Quality of chain
52	t3	467	
53	A5	28	
54	B6	296	
55	C6	167	
56	D6	430	
57	E6	125	
58	F6	242	
59	G6	396	
60	H6	201	
61	I6	194	
62	J6	138	
63	K6	128	
64	L6	257	
65	M6	137	
66	N6	130	
67	O6	258	
68	P6	142	
69	Q6	87	
70	R6	360	
71	S6	190	
72	T6	173	
73	U6	205	
74	V6	414	
75	W6	187	
76	X6	398	

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Mol	Chain	Length	Quality of chain
77	Y6	395	
78	Z6	106	
79	a6	218	
80	b6	323	
81	c6	118	
82	d6	199	
83	e6	689	
84	A6	954	
85	24	73	
85	C	73	
86	i4	10	
87	A	206	
88	n	229	

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
94	CL	n	307	-	-	X	-

2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 165767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Y2	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A3	1503	Total	C	N	O	P	0	0
			31913	14319	5761	10330	1503		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679

- Molecule 3 is a RNA chain called mt-tRNA Val.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B3	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 4 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D3	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 5 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E3	300	Total	C	N	O	S	0	0
			2365	1523	410	422	10		

- Molecule 6 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F3	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 7 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H3	95	Total	C	N	O		0	0
			784	498	152	134			
7	D	80	Total	C	N	O	S	0	0
			648	421	111	112	4		

- Molecule 8 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I3	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 9 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J3	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 10 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K3	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 11 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L3	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 12 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M3	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 13 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N3	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 14 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O3	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 15 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P3	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 16 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q3	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 17 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R3	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 18 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S3	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 19 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T3	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 20 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U3	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 21 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V3	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 22 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W3	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 23 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X3	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X3	148	ALA	THR	conflict	UNP Q13084
X3	149	SER	PRO	conflict	UNP Q13084
X3	150	GLY	LYS	conflict	UNP Q13084

- Molecule 24 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y3	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 25 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z3	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 26 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	03	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 27 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 28 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	23	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 29 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	33	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 30 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	43	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 31 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	53	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 32 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	63	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 33 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	73	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	93	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a3	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b3	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c3	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d3	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e3	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f3	131	Total	C	N	O	S	0	0
			1039	663	169	203	4		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g3	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h3	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i3	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j3	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k3	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l3	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m3	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o3	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p3	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q3	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r3	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s3	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		
52	t3	28	Total	C	N	O		0	0
			140	84	28	28			

- Molecule 53 is a protein called Oxa1L.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	A5	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 54 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 55 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	C6	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 56 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	D6	322	Total	C	N	O	S	0	0
			2557	1611	476	457	13		

- Molecule 57 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	E6	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 58 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	F6	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 59 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G6	305	Total	C	N	O	S	0	0
			2516	1599	448	455	14		

- Molecule 60 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	H6	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 61 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	I6	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 62 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	J6	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 63 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	K6	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 64 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	L6	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 65 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	M6	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 66 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	N6	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 67 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	O6	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 68 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	P6	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 69 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Q6	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q6	50	ARG	CYS	conflict	UNP P82921

- Molecule 70 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	R6	242	Total	C	N	O	S	0	0
			2008	1285	343	372	8		

- Molecule 71 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	S6	126	Total	C	N	O	S	0	0
			1042	673	183	185	1		

- Molecule 72 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	T6	162	Total	C	N	O	S	0	0
			1330	850	231	238	11		

- Molecule 73 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	U6	173	Total	C	N	O	S	0	0
			1461	900	294	263	4		

- Molecule 74 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	V6	328	Total	C	N	O	S	0	0
			2702	1737	452	502	11		

- Molecule 75 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	W6	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 76 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	X6	316	Total	C	N	O	S	0	0
			2531	1625	440	455	11		

- Molecule 77 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Y6	108	Total	C	N	O	S	0	0
			914	593	150	169	2		

- Molecule 78 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Z6	87	Total	C	N	O	S	0	0
			740	473	133	130	4		

- Molecule 79 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	a6	201	Total	C	N	O	S	0	0
			1684	1065	322	292	5		

- Molecule 80 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	b6	256	Total	C	N	O	S	0	0
			2076	1321	350	395	10		

- Molecule 81 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	c6	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 82 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	d6	69	Total	C	N	O	S	0	0
			610	393	130	86	1		

- Molecule 83 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	e6	414	Total	C	N	O	S	0	0
			2838	1805	490	529	14		

- Molecule 84 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A6	928	Total	C	N	O	P	0	0
			19716	8840	3560	6388	928		

- Molecule 85 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
85	C	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 86 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	i4	10	Total	C	N	O	P	0	0
			219	99	47	63	10		

- Molecule 87 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	A	162	Total	C	N	O	S	0	0
			1375	876	247	249	3		

- Molecule 88 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	n	228	Total	C	N	O	S	4	0
			1766	1121	321	321	3		

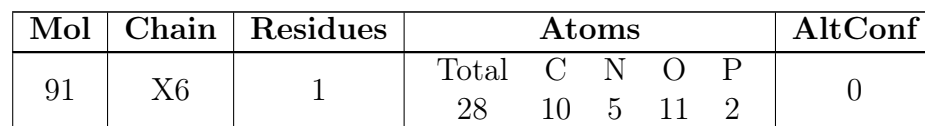
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	A3	97	Total	Mg	0
			97	97	
89	D3	1	Total	Mg	0
			1	1	
89	g3	1	Total	Mg	0
			1	1	
89	A6	28	Total	Mg	0
			28	28	
89	n	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	03	1	Total	Zn	0
			1	1	
90	43	1	Total	Zn	0
			1	1	
90	r3	1	Total	Zn	0
			1	1	
90	B6	1	Total	Zn	0
			1	1	
90	O6	1	Total	Zn	0
			1	1	
90	P6	1	Total	Zn	0
			1	1	
90	T6	1	Total	Zn	0
			1	1	

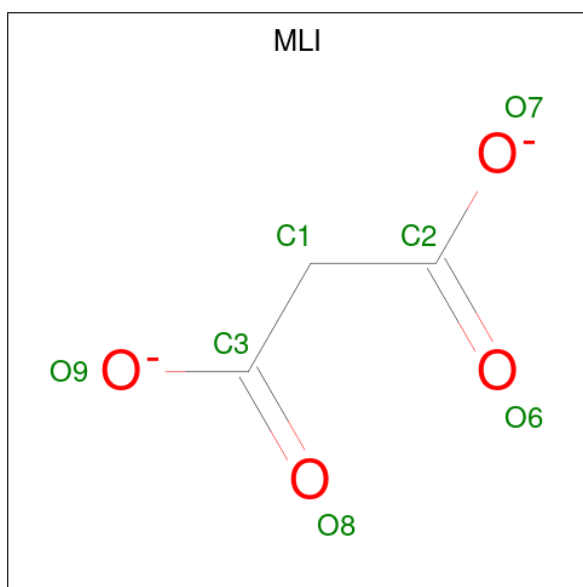
- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



-
- Diagram illustrating the Lewis structure of the sulfate ion (SO_4^{2-}). The central sulfur atom (S) is bonded to four oxygen atoms. Two oxygen atoms are double-bonded to sulfur (top and bottom), and two are single-bonded (left and right). Each single-bonded oxygen has a negative charge (O^-). The sulfur atom has a formal charge of +6. The overall charge of the ion is -2.

Mol	Chain	Residues	Atoms			AltConf
92	n	1	Total	O	S	0
			5	4	1	

- Molecule 93 is MALONATE ION (CCD ID: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



Mol	Chain	Residues	Atoms			AltConf
93	n	1	Total	C	O	0
			7	3	4	
93	n	1	Total	C	O	0
			7	3	4	
93	n	1	Total	C	O	0
			7	3	4	

- Molecule 94 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
94	n	2	Total	Cl	0
			2	2	

- Molecule 95 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
95	n	2	Total	Na	0
			2	2	
95	D	2	Total	Na	0
			2	2	

- Molecule 96 is water.

Mol	Chain	Residues	Atoms		AltConf
96	A3	4	Total	O	0
			4	4	

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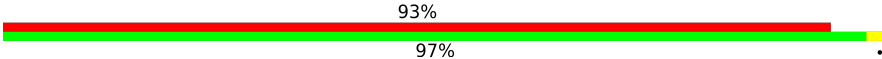
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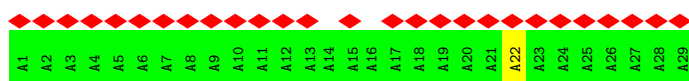
Mol	Chain	Residues	Atoms		AltConf
96	n	67	Total 67	O 67	0
96	D	8	Total 8	O 8	0

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.

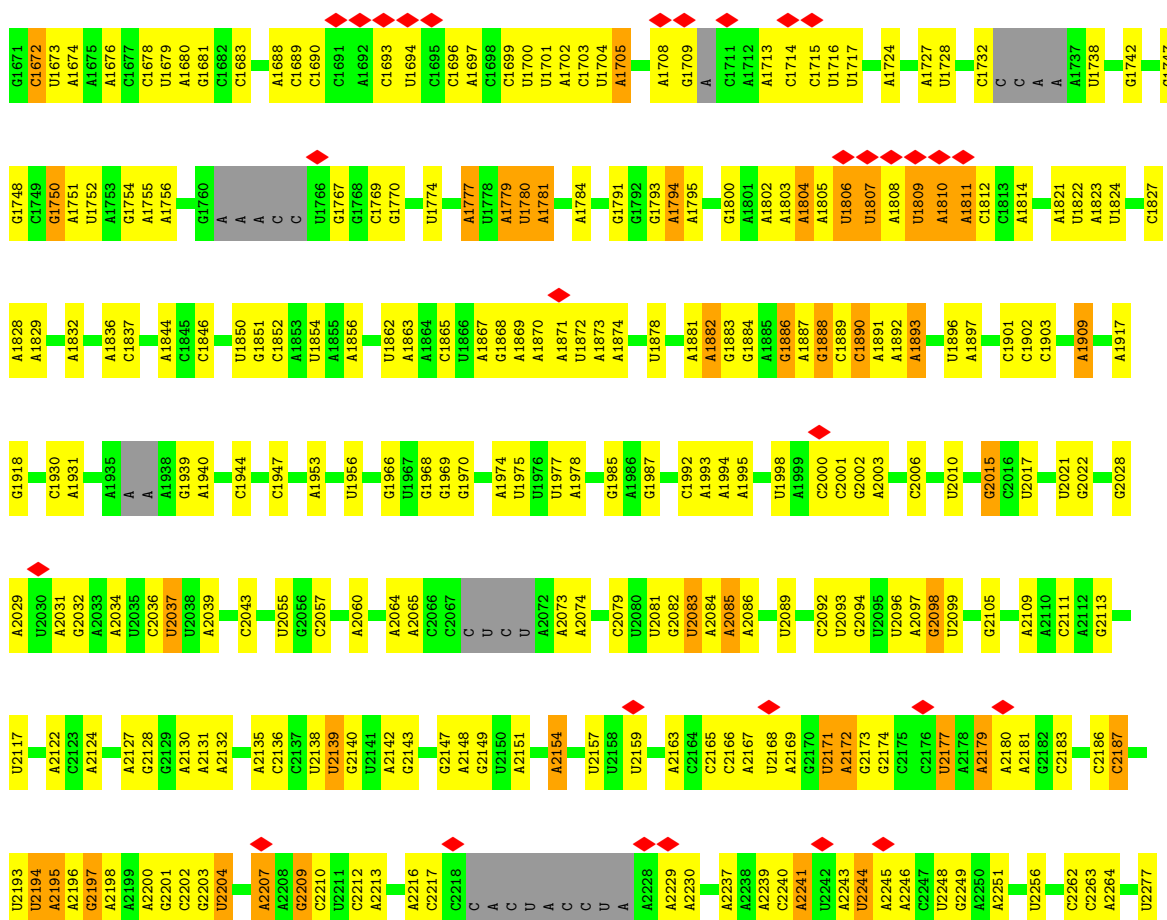
- Molecule 1: nascent chain

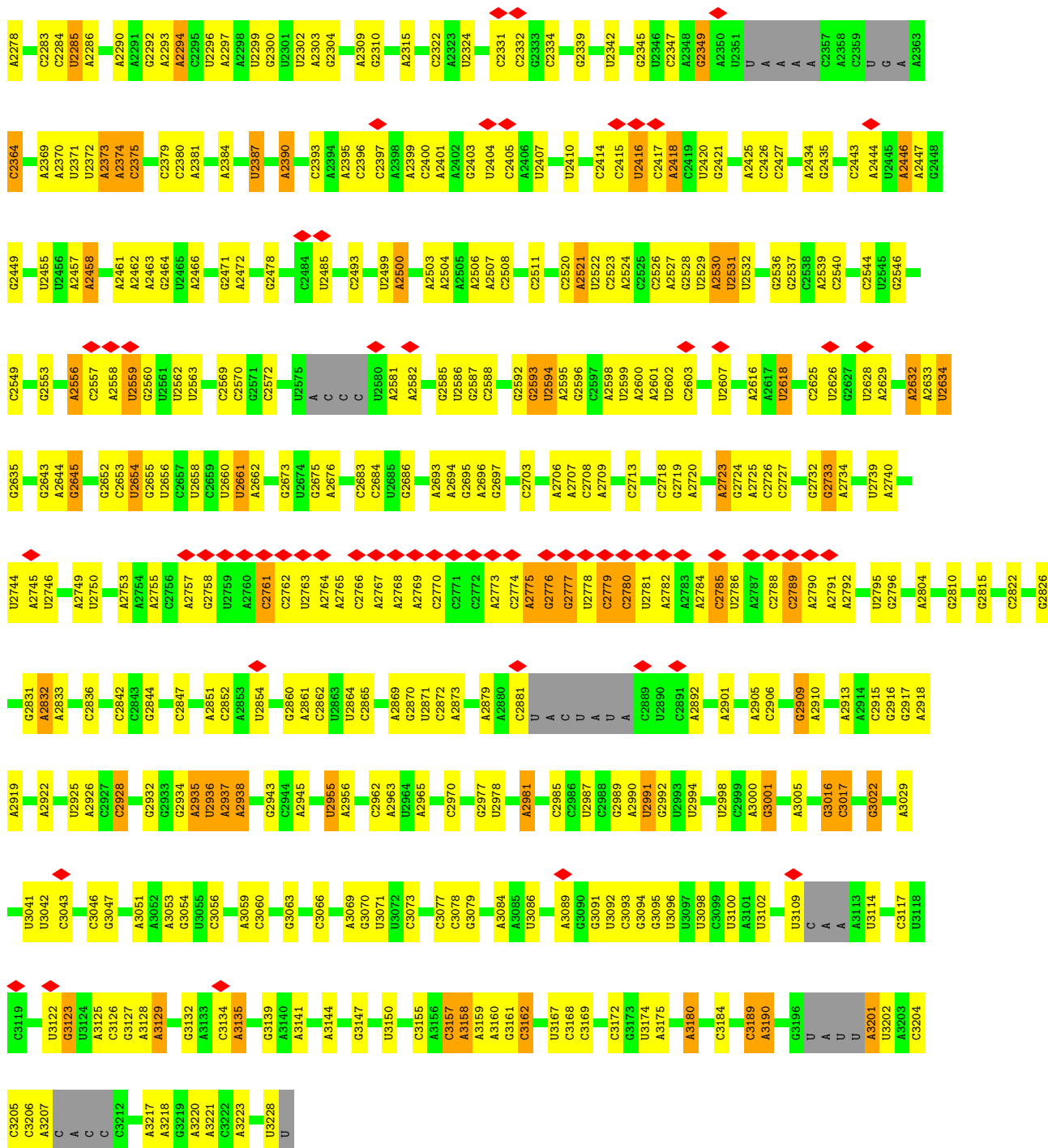
Chain Y2: 



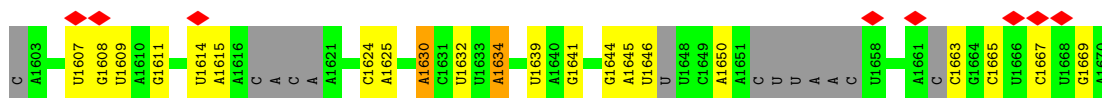
- Molecule 2: 16S rRNA

Chain A3: 

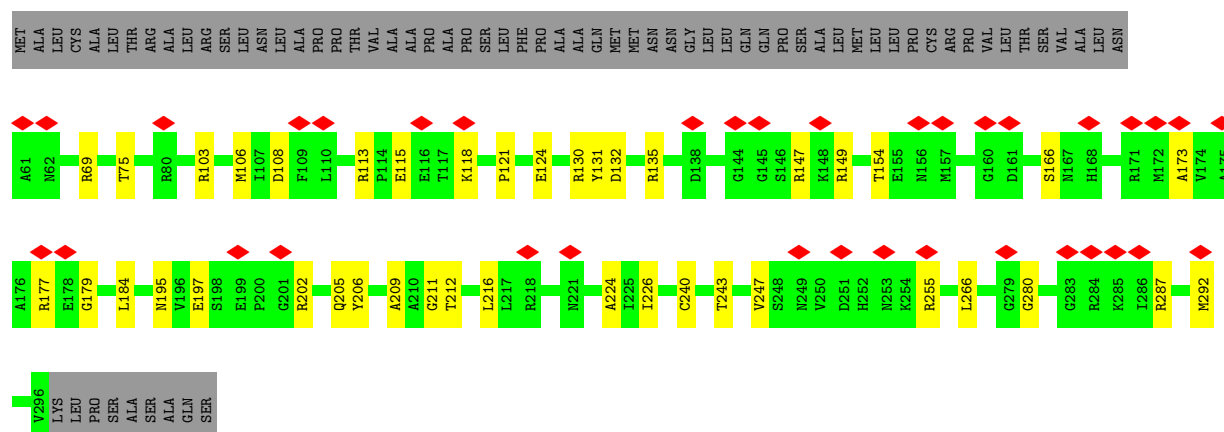




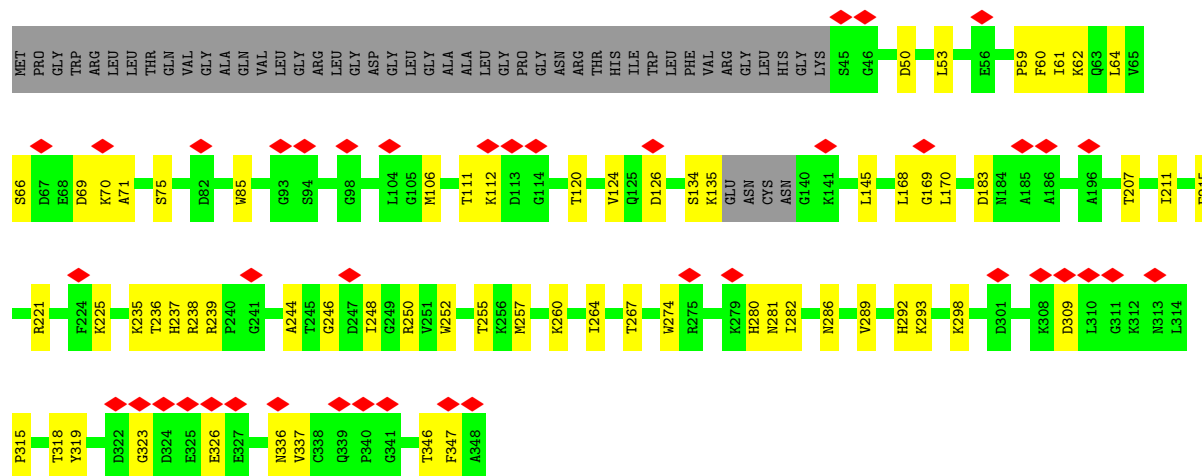
• Molecule 3: mt-tRNA Val



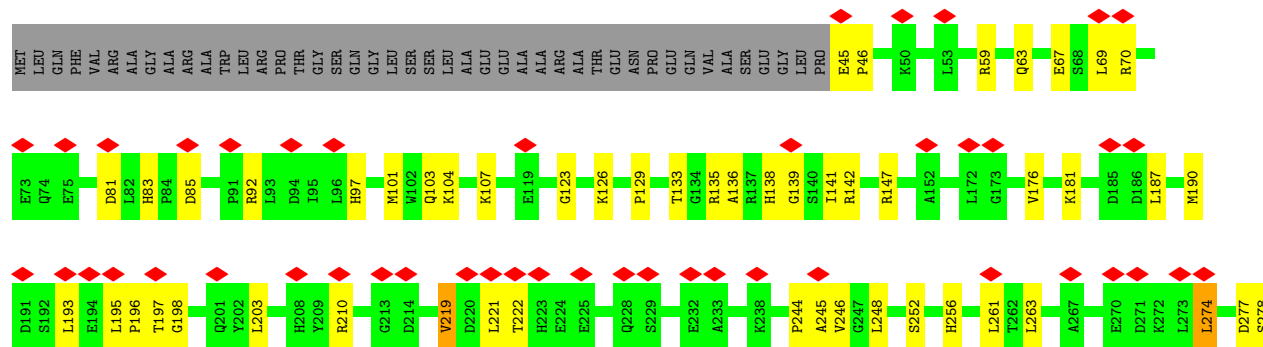
• Molecule 4: 39S ribosomal protein L2, mitochondrial

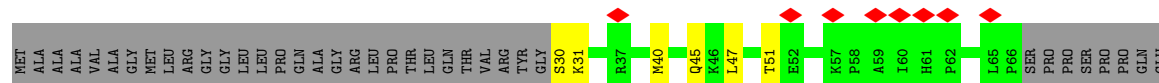


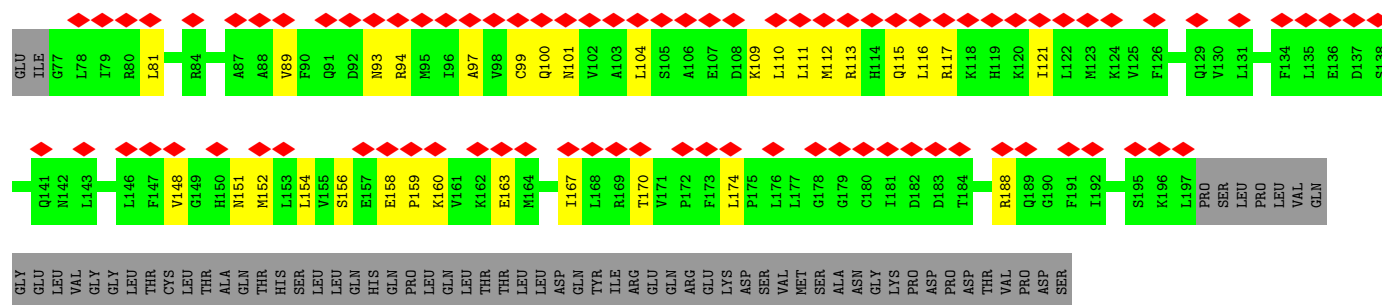
- Molecule 5: 39S ribosomal protein L3, mitochondrial



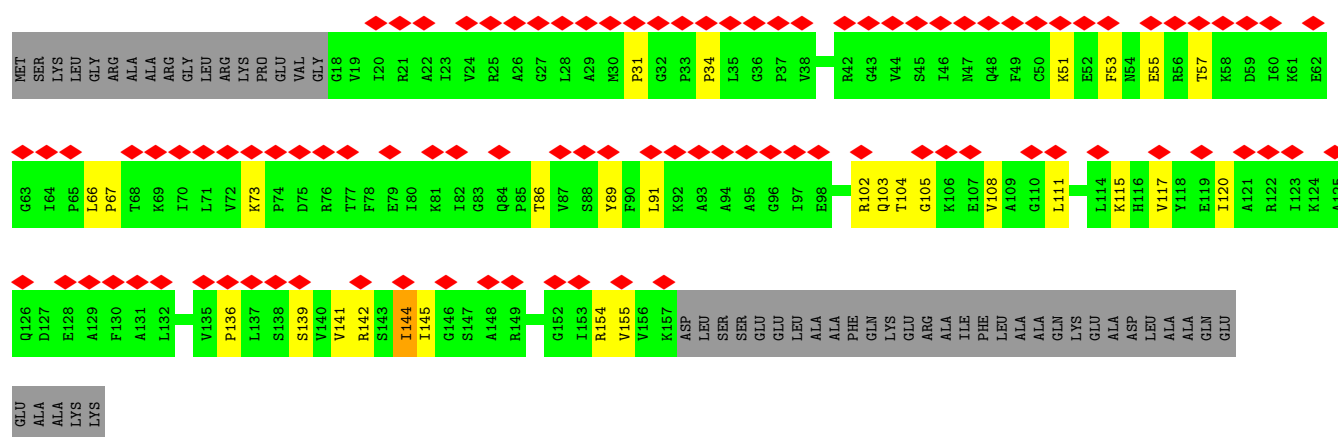
- Molecule 6: 39S ribosomal protein L4, mitochondrial



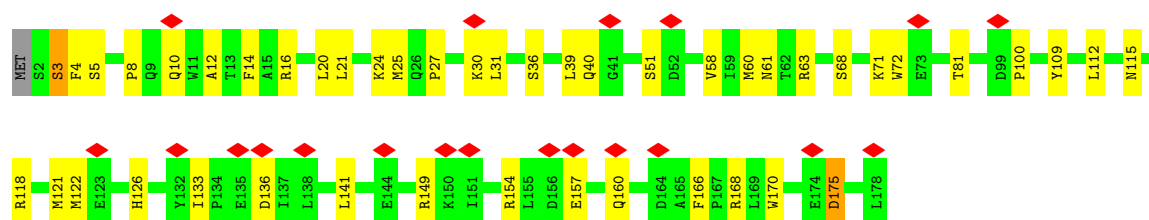
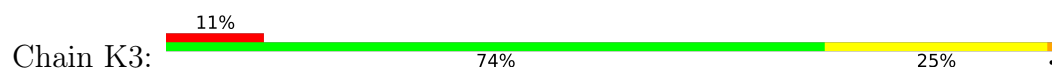




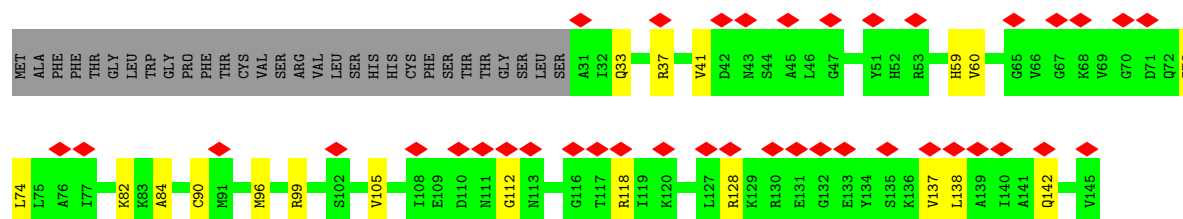
• Molecule 9: 39S ribosomal protein L11, mitochondrial



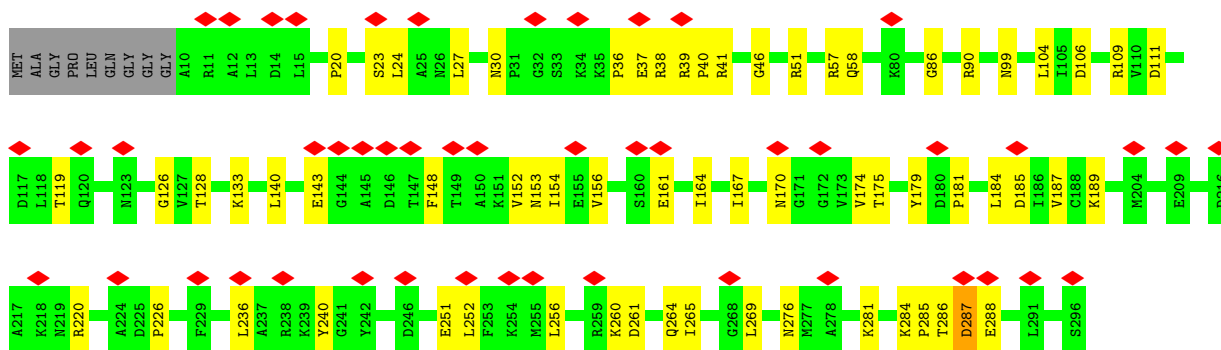
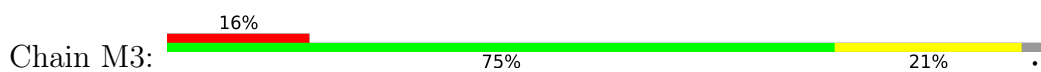
• Molecule 10: 39S ribosomal protein L13, mitochondrial



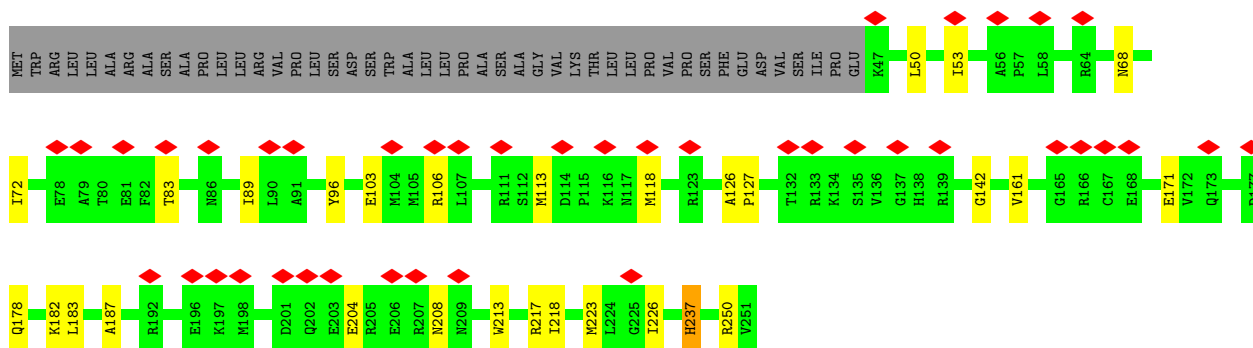
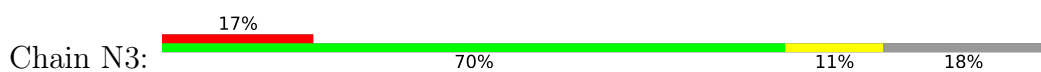
• Molecule 11: 39S ribosomal protein L14, mitochondrial



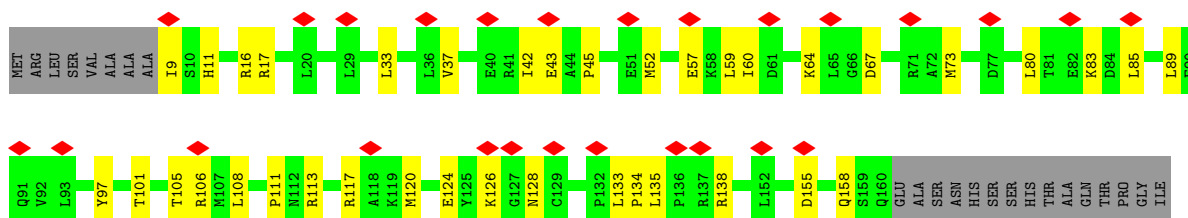
• Molecule 12: 39S ribosomal protein L15, mitochondrial



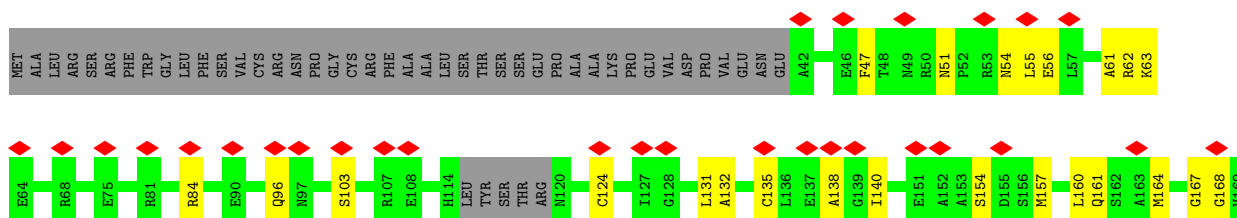
- Molecule 13: 39S ribosomal protein L16, mitochondrial



- Molecule 14: 39S ribosomal protein L17, mitochondrial

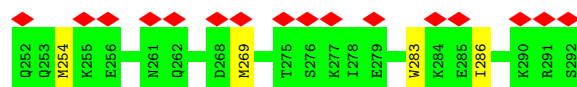
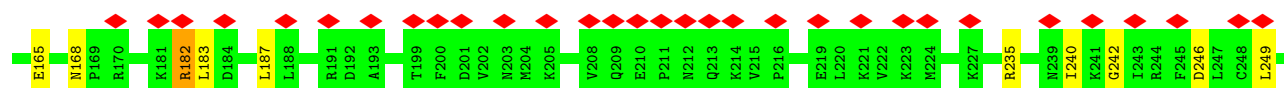
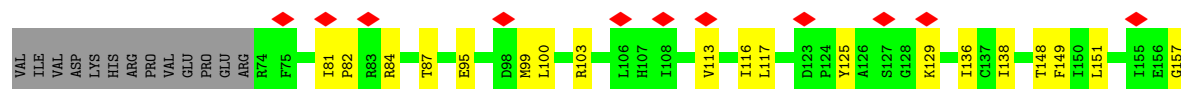
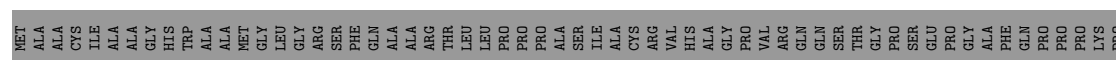


- Molecule 15: 39S ribosomal protein L18, mitochondrial

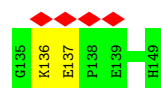
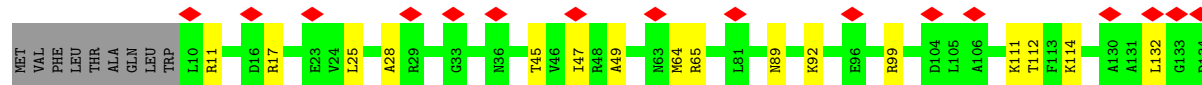
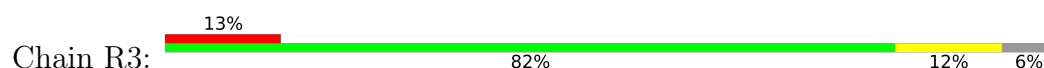




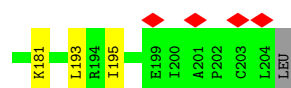
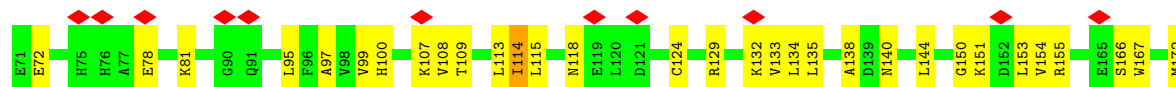
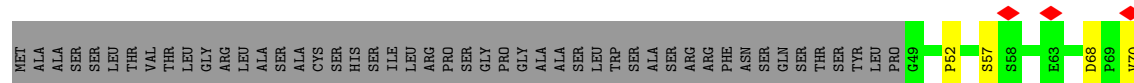
- Molecule 16: 39S ribosomal protein L19, mitochondrial



- Molecule 17: 39S ribosomal protein L20, mitochondrial

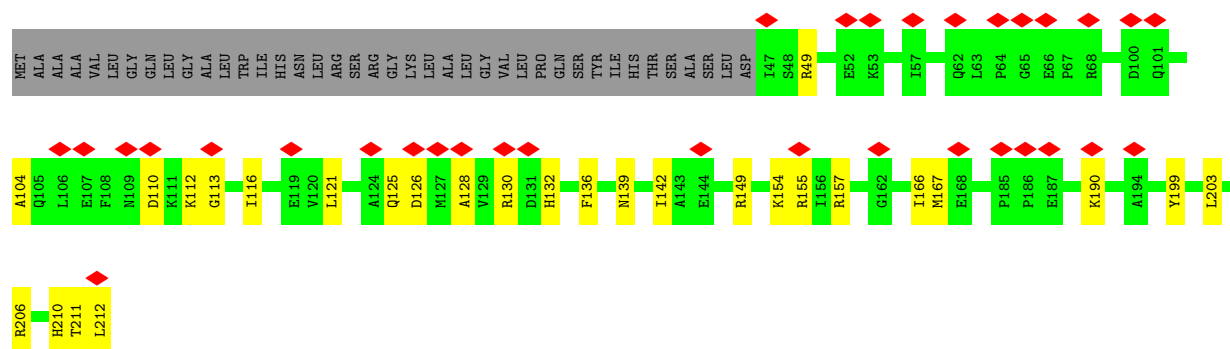


- Molecule 18: 39S ribosomal protein L21, mitochondrial

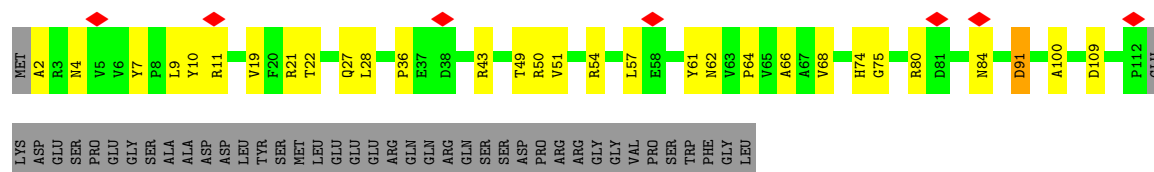


- Molecule 19: 39S ribosomal protein L22, mitochondrial

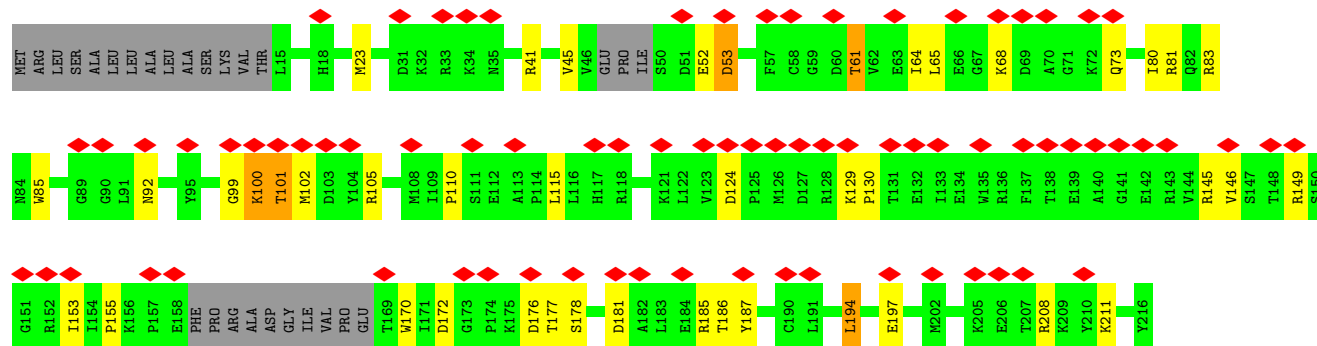




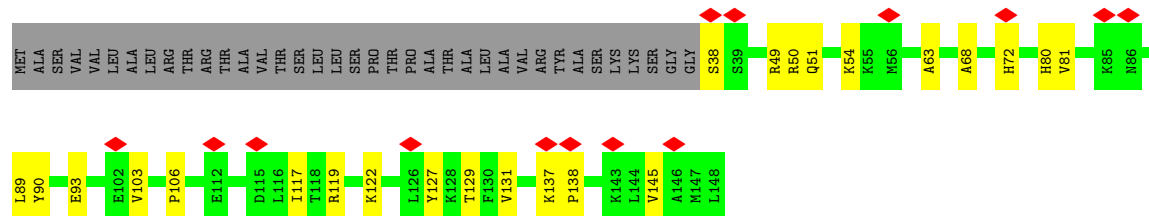
- Molecule 20: 39S ribosomal protein L23, mitochondrial



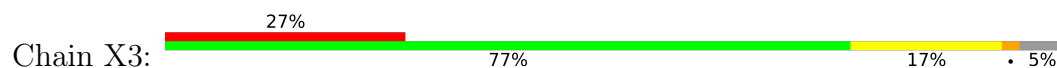
- Molecule 21: 39S ribosomal protein L24, mitochondrial

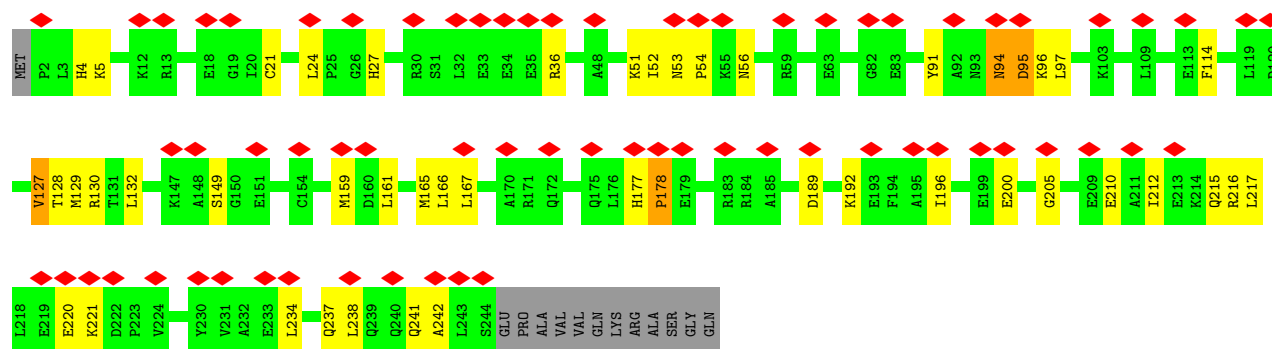


- Molecule 22: 39S ribosomal protein L27, mitochondrial

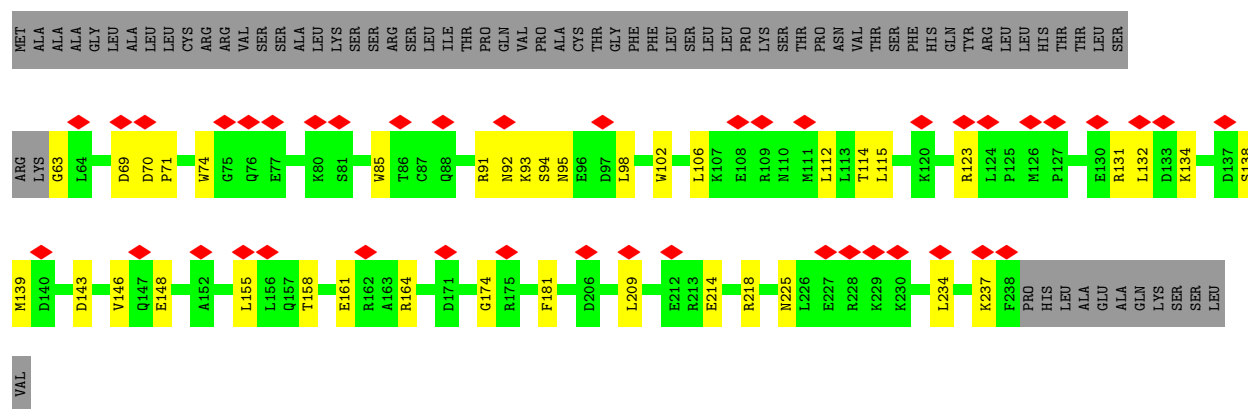


- Molecule 23: 39S ribosomal protein L28, mitochondrial

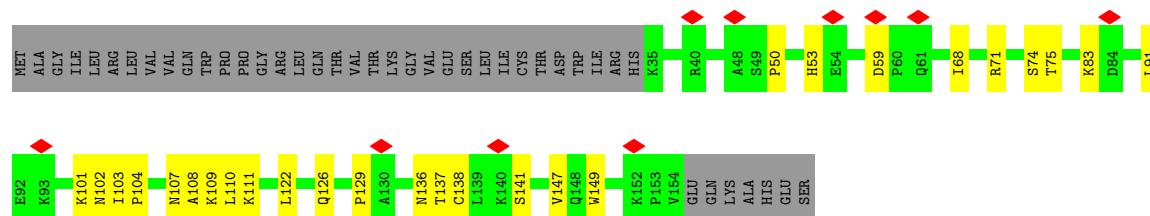




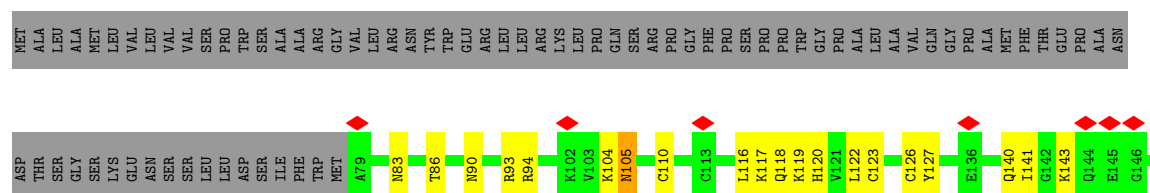
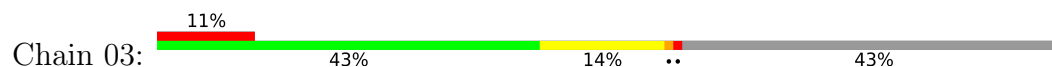
• Molecule 24: 39S ribosomal protein L47, mitochondrial

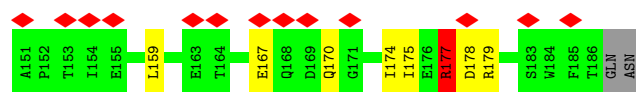


• Molecule 25: 39S ribosomal protein L30, mitochondrial

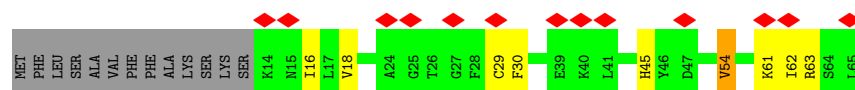


• Molecule 26: 39S ribosomal protein L32, mitochondrial

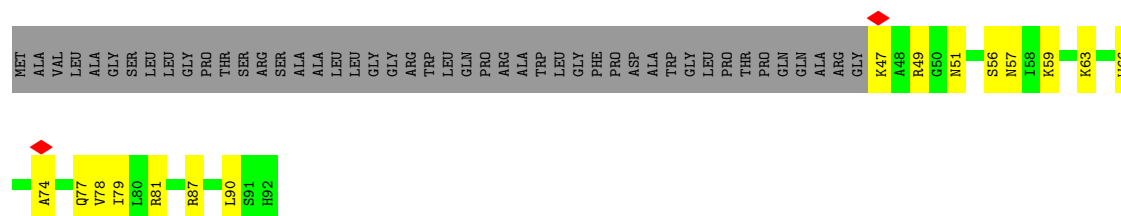
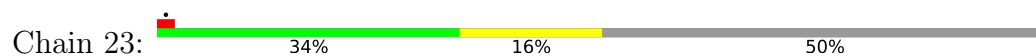




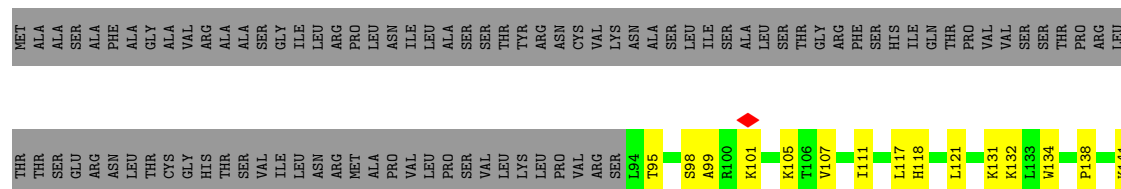
- Molecule 27: 39S ribosomal protein L33, mitochondrial



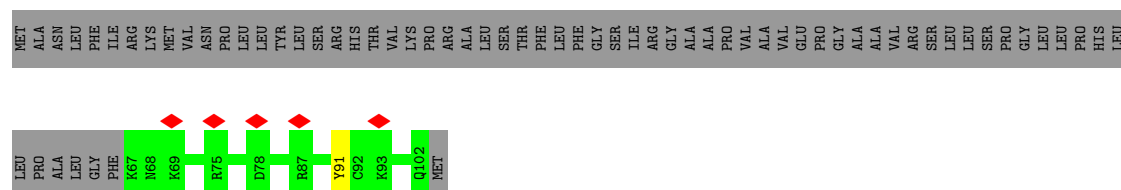
- Molecule 28: 39S ribosomal protein L34, mitochondrial



- Molecule 29: 39S ribosomal protein L35, mitochondrial

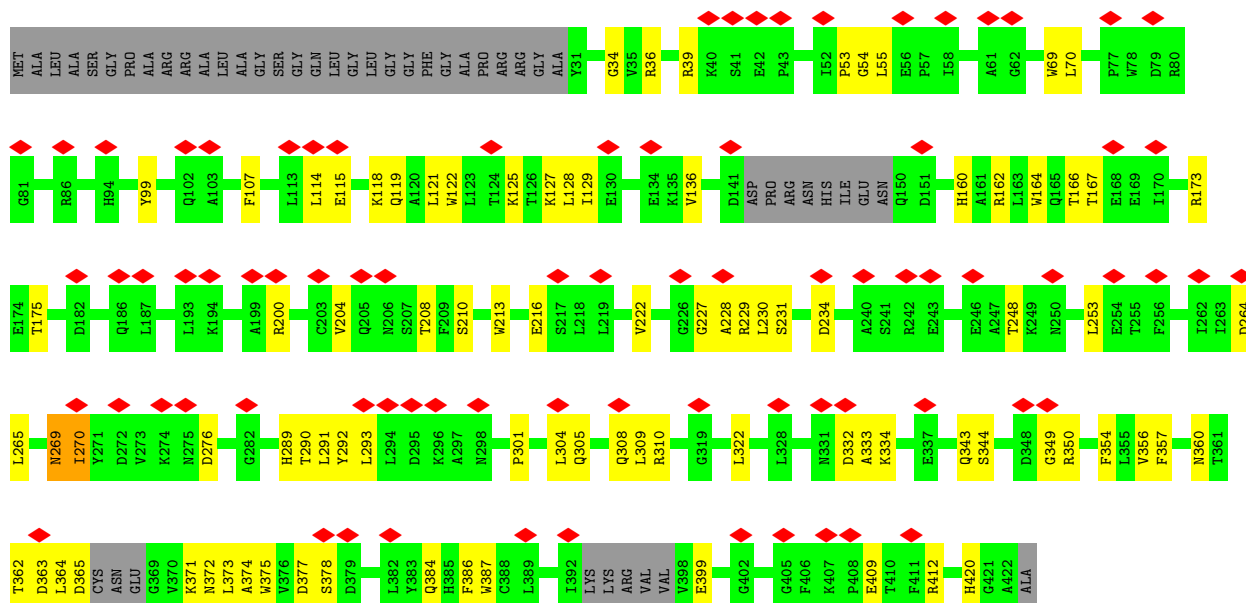


- Molecule 30: 39S ribosomal protein L36, mitochondrial

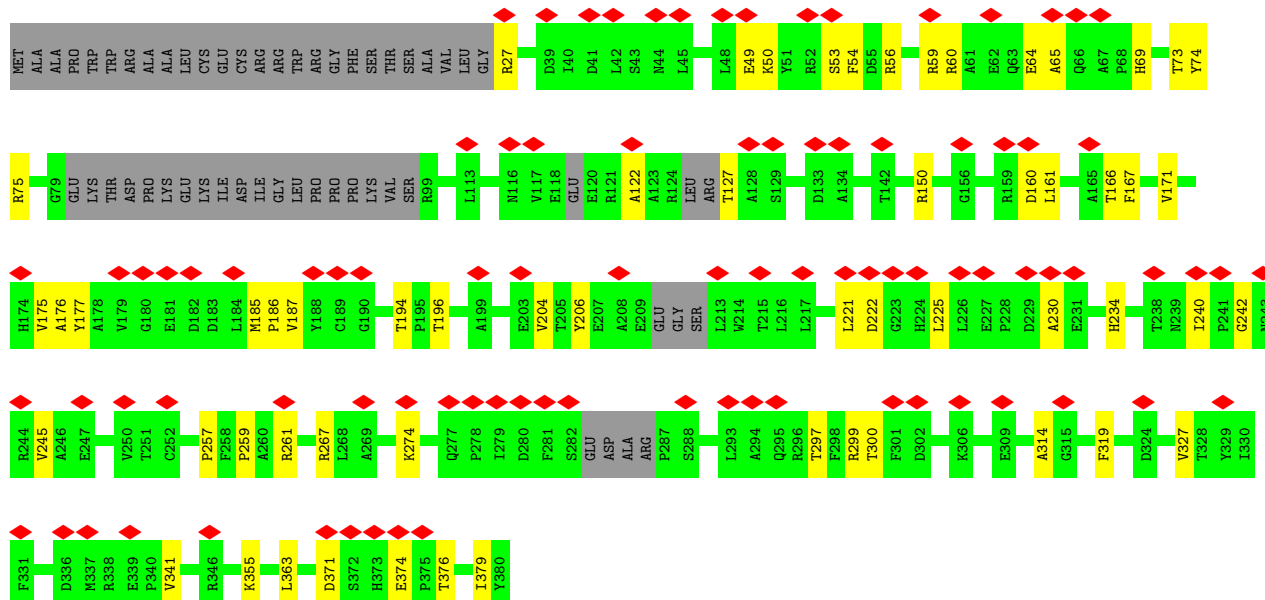
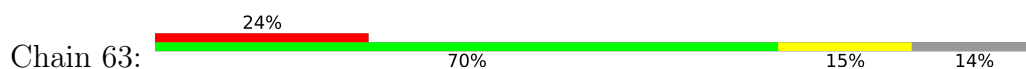


- Molecule 31: 39S ribosomal protein L37, mitochondrial

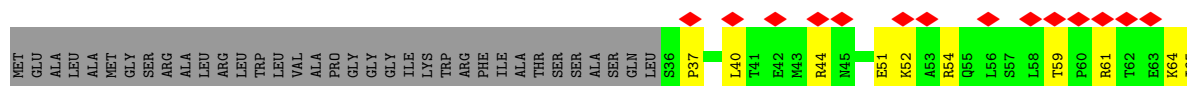


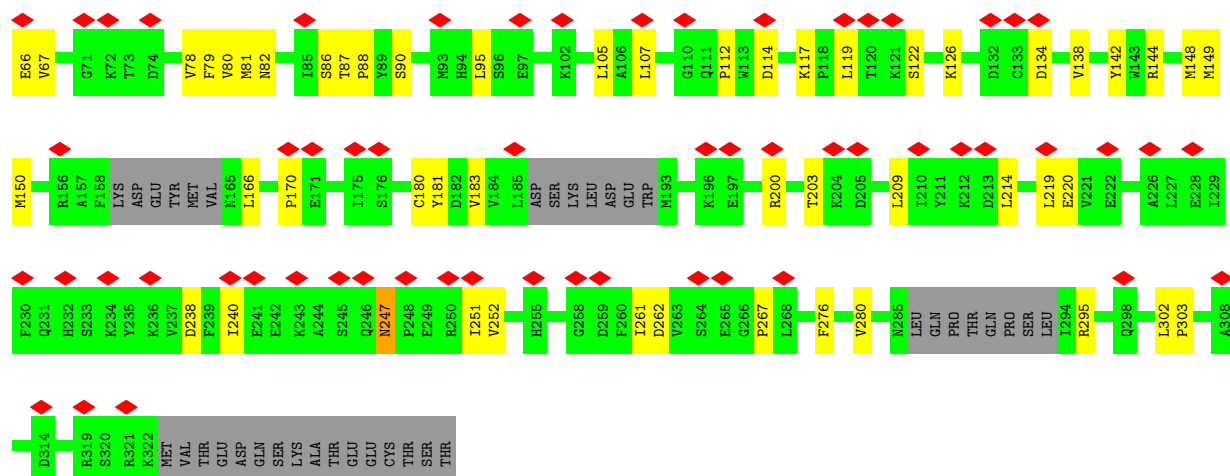


• Molecule 32: 39S ribosomal protein L38, mitochondrial

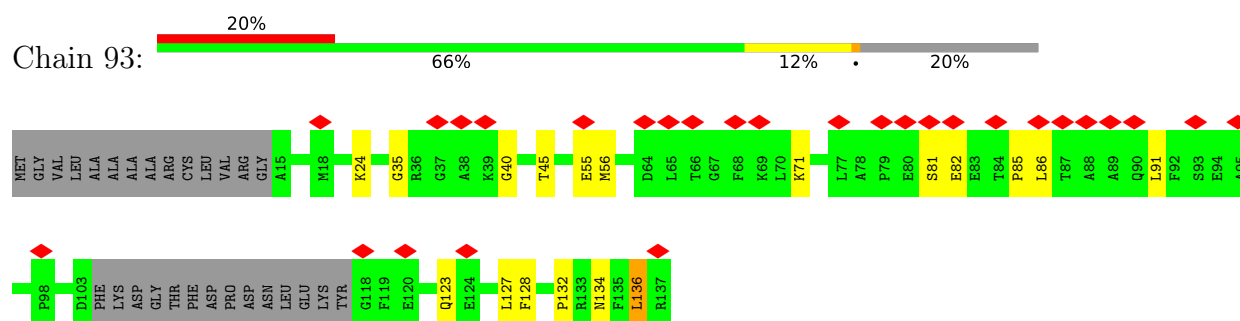


• Molecule 33: 39S ribosomal protein L39, mitochondrial

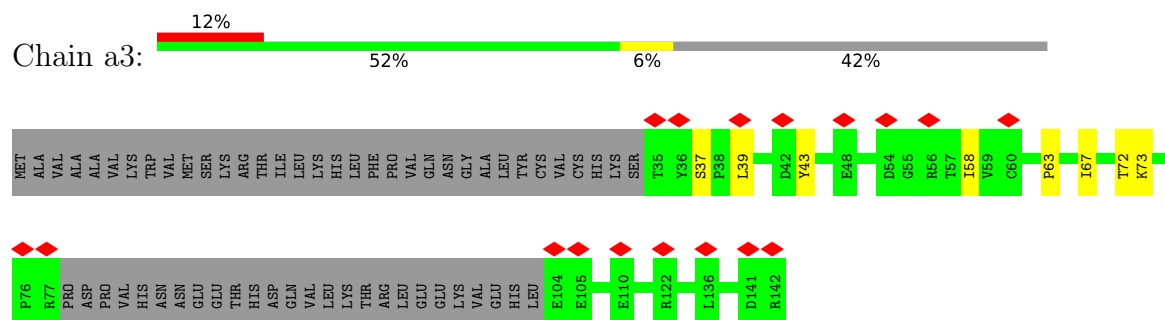




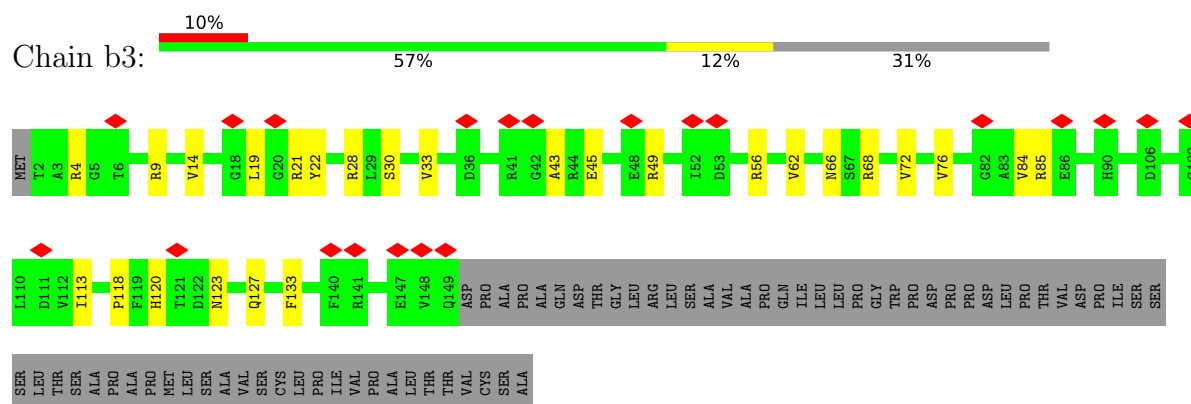
- Molecule 34: 39S ribosomal protein L41, mitochondrial



- Molecule 35: 39S ribosomal protein L42, mitochondrial

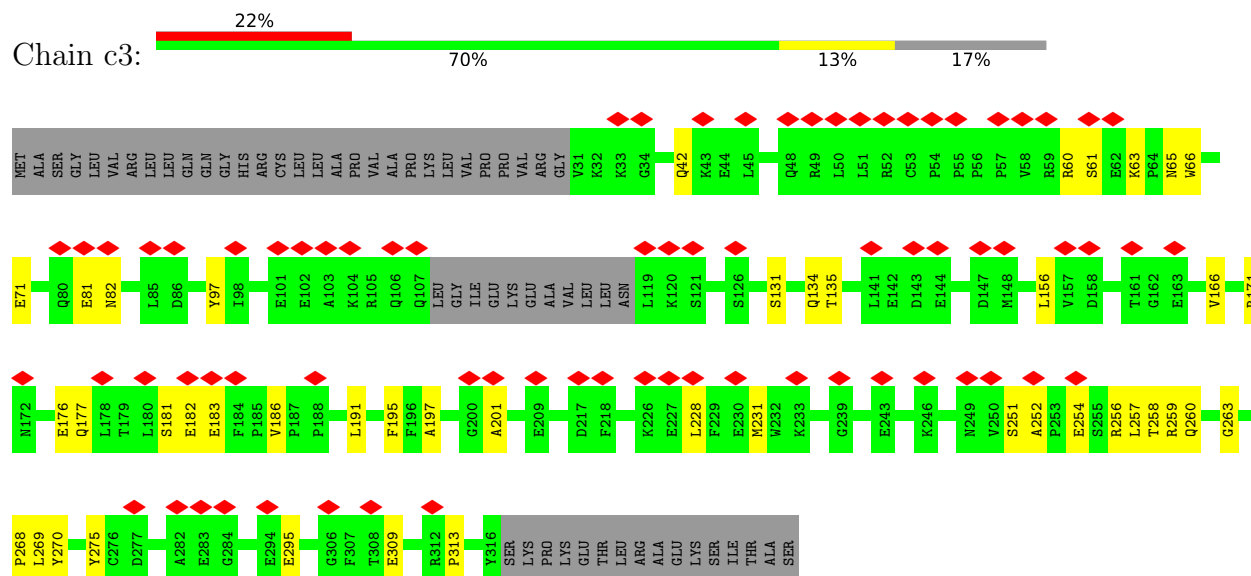


- Molecule 36: 39S ribosomal protein L43, mitochondrial



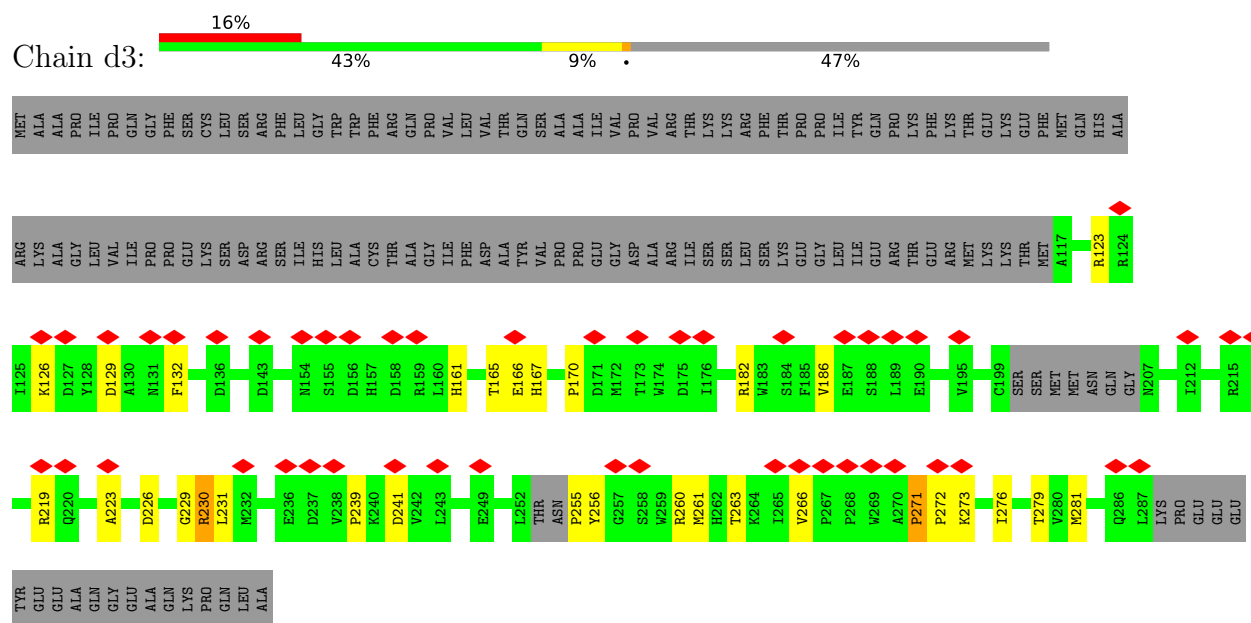
- Molecule 37: 39S ribosomal protein L44, mitochondrial

Chain c3:



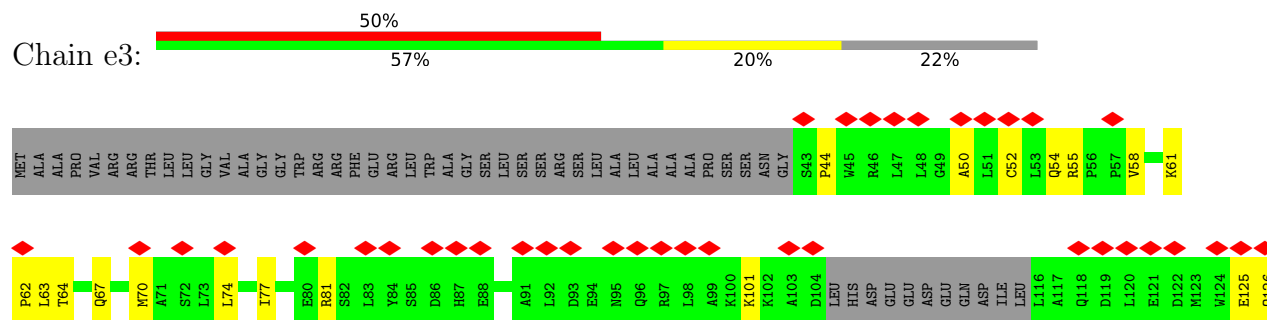
- Molecule 38: 39S ribosomal protein L45, mitochondrial

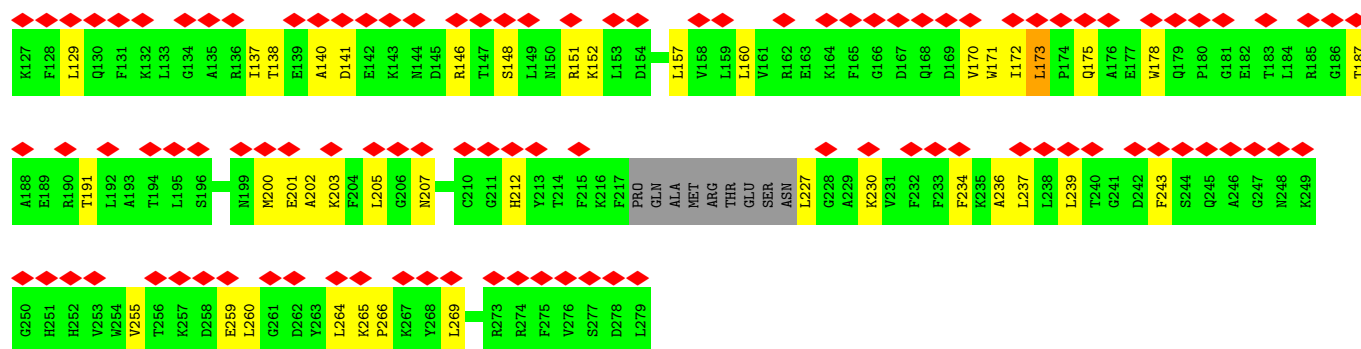
Chain d3:



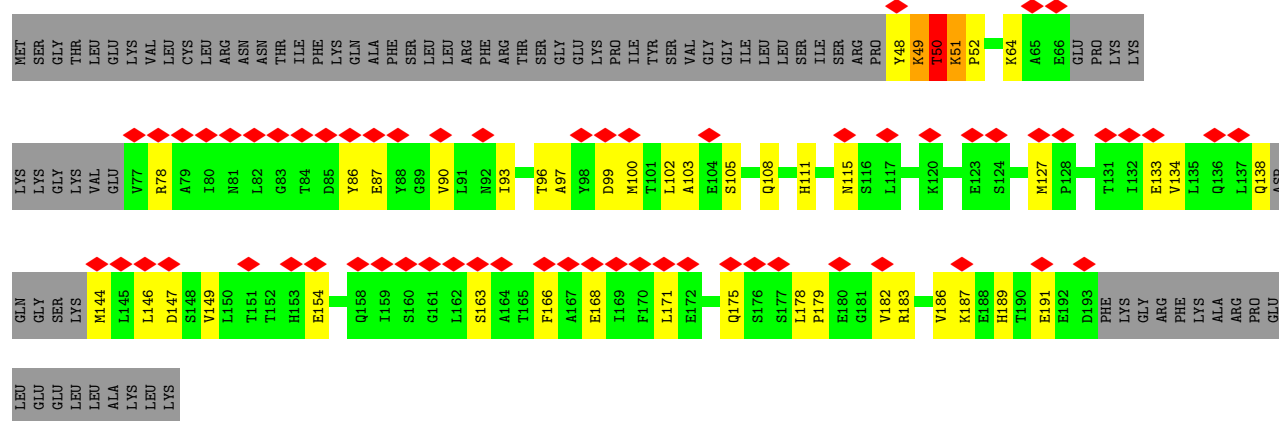
- Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e3:

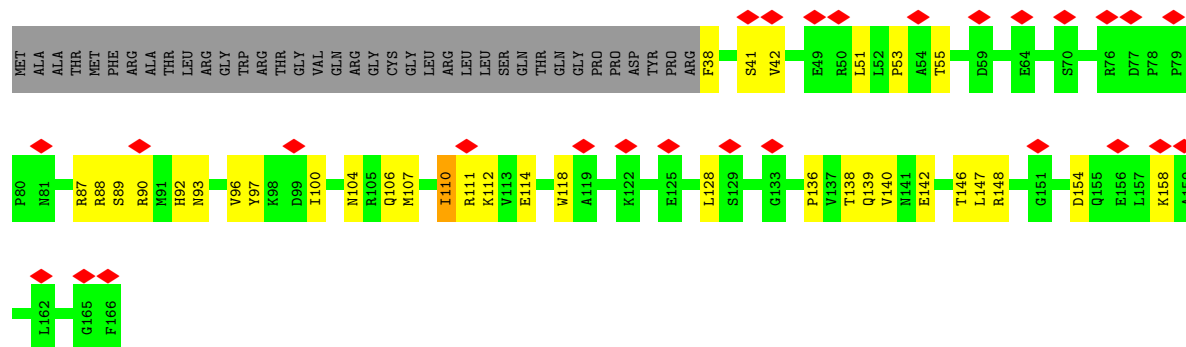




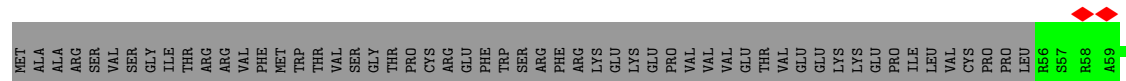
• Molecule 40: 39S ribosomal protein L48, mitochondrial

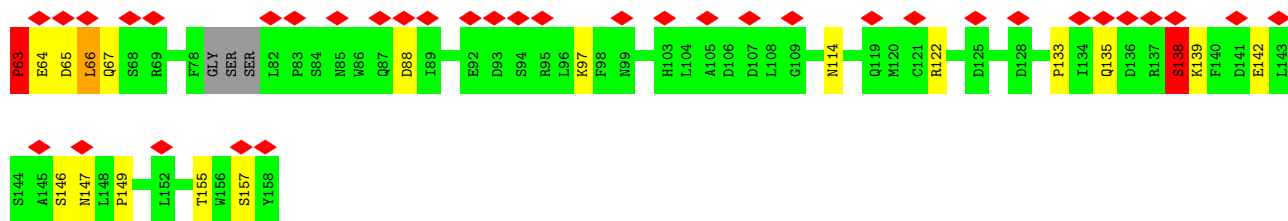


• Molecule 41: 39S ribosomal protein L49, mitochondrial

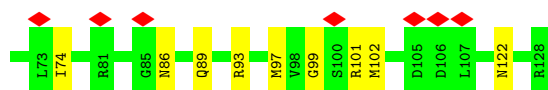
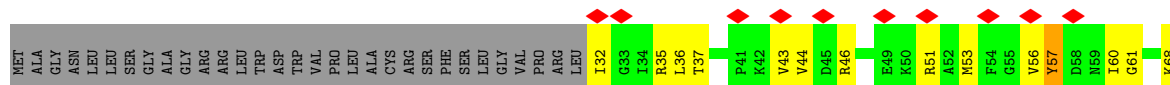


• Molecule 42: 39S ribosomal protein L50, mitochondrial

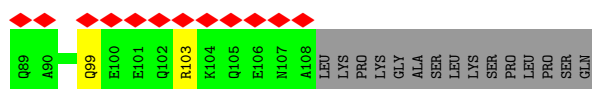
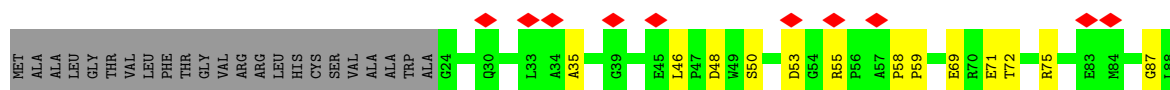




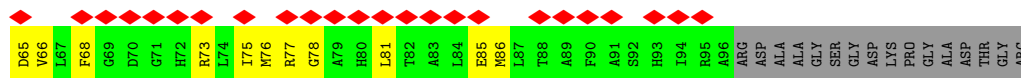
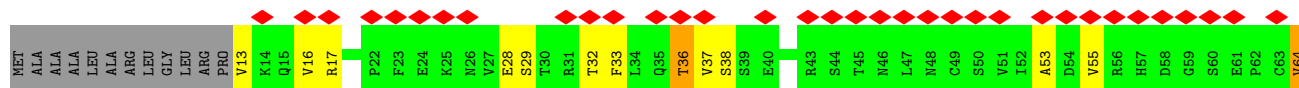
- Molecule 43: 39S ribosomal protein L51, mitochondrial



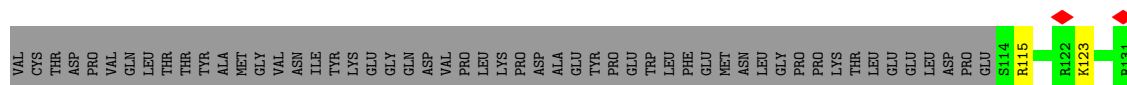
- Molecule 44: 39S ribosomal protein L52, mitochondrial



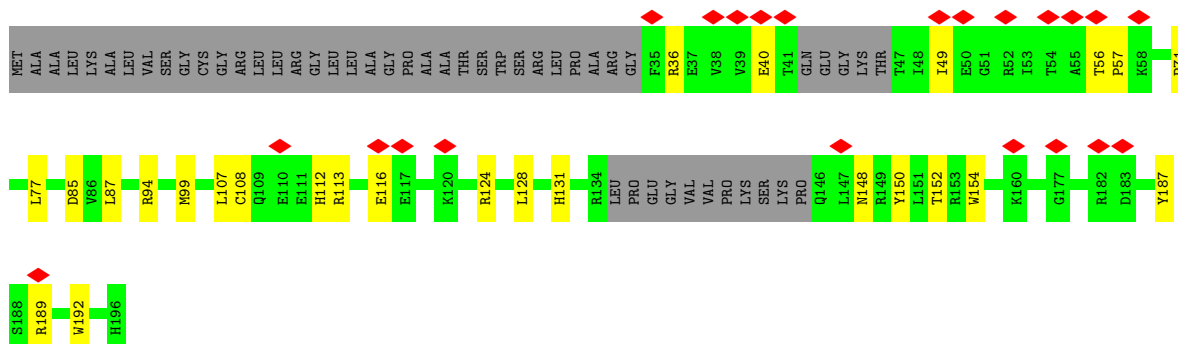
- Molecule 45: 39S ribosomal protein L53, mitochondrial



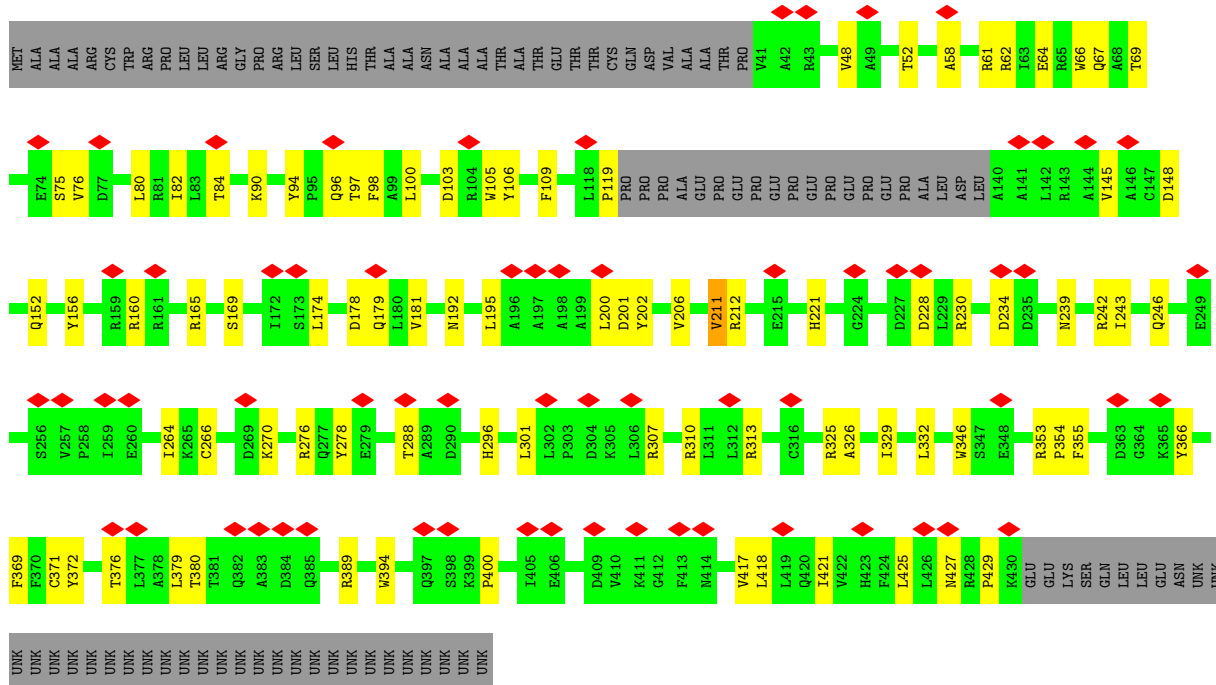
- Molecule 46: 39S ribosomal protein L54, mitochondrial



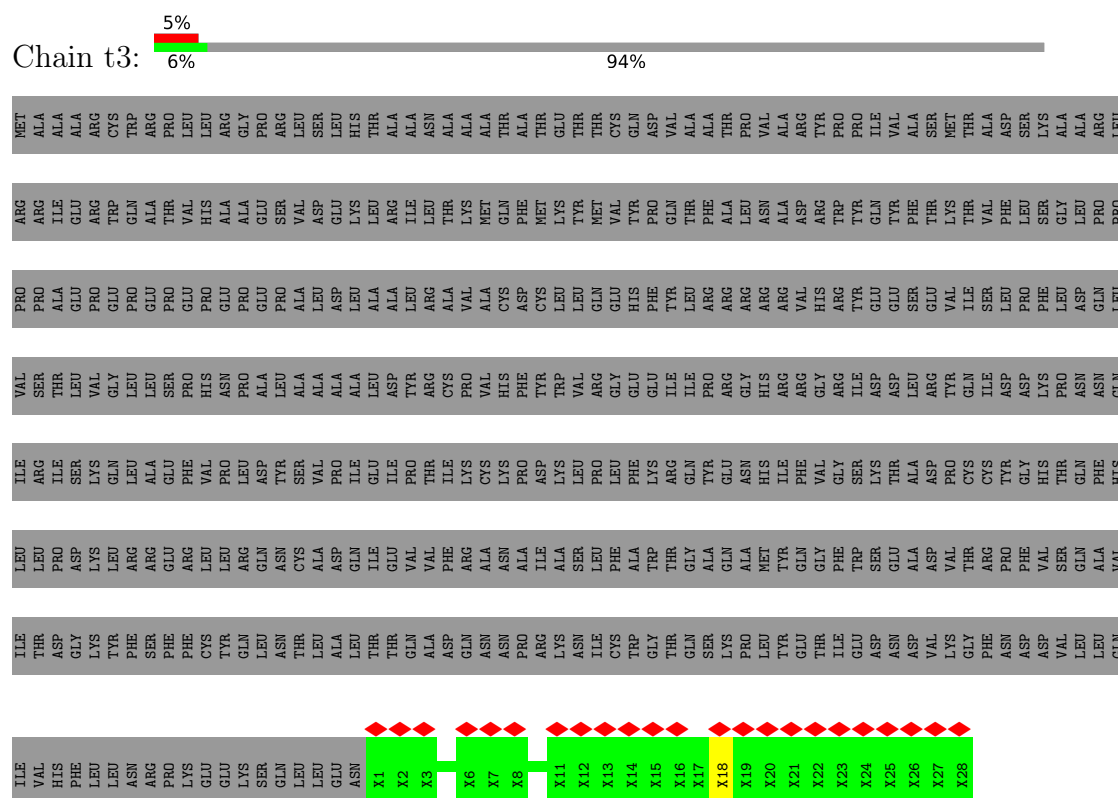
- Molecule 51: 39S ribosomal protein S18a, mitochondrial



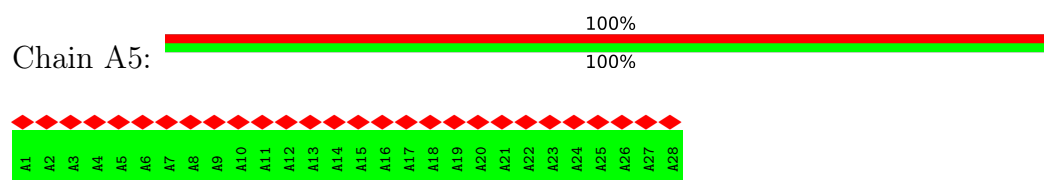
- Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65



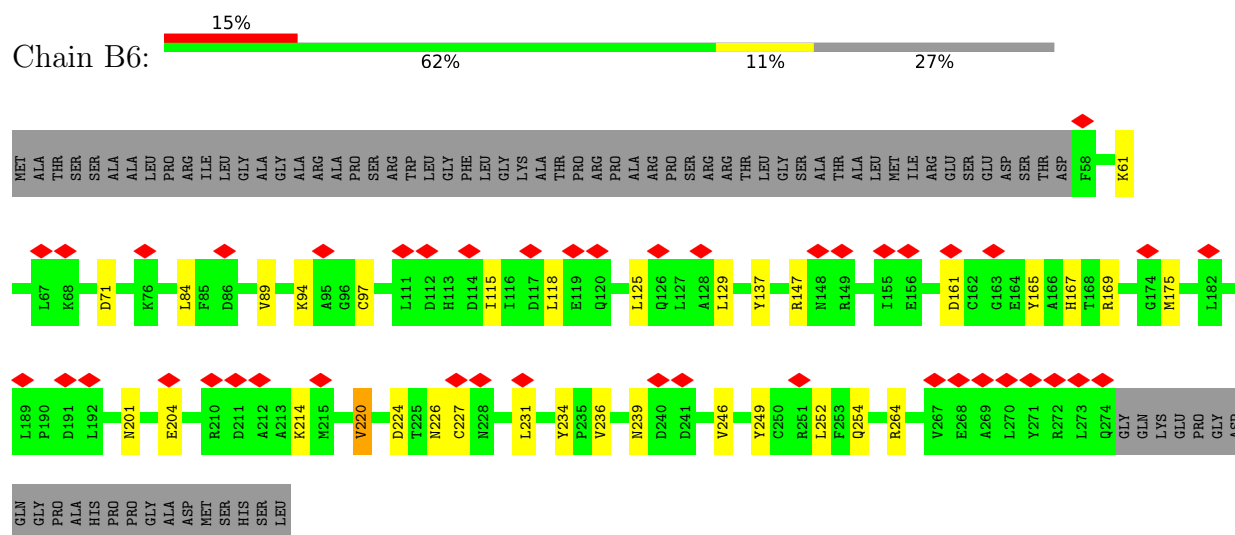
- Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65



- Molecule 53: Oxa1L

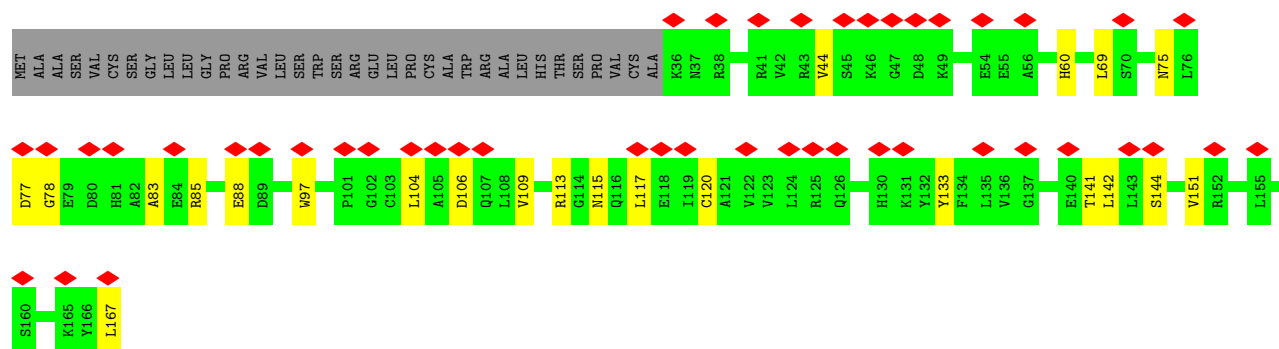


- Molecule 54: 28S ribosomal protein S2, mitochondrial

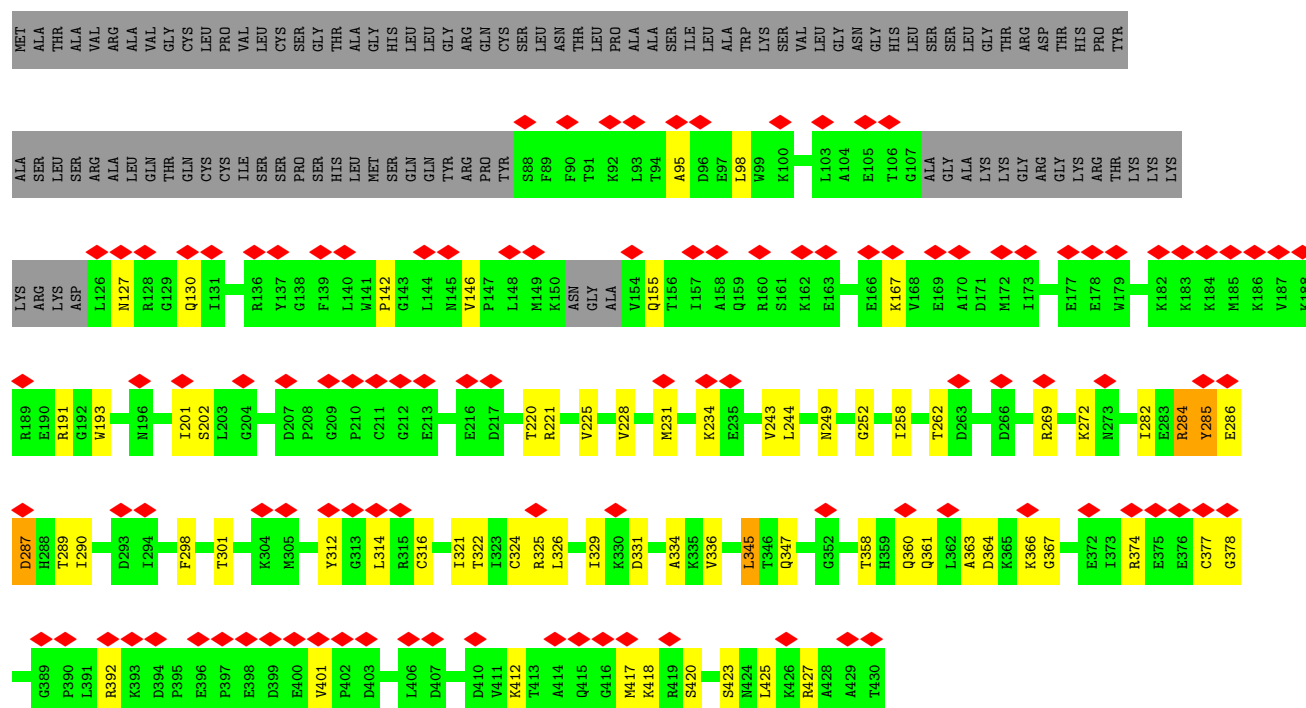


- Molecule 55: 28S ribosomal protein S24, mitochondrial

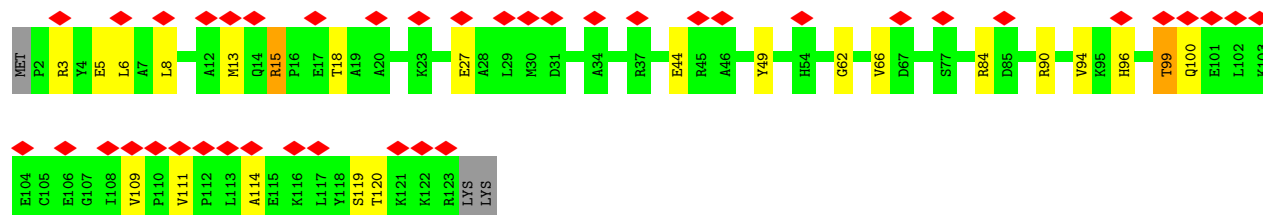
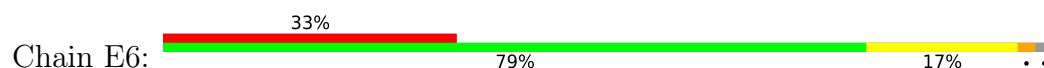




- Molecule 56: 28S ribosomal protein S5, mitochondrial

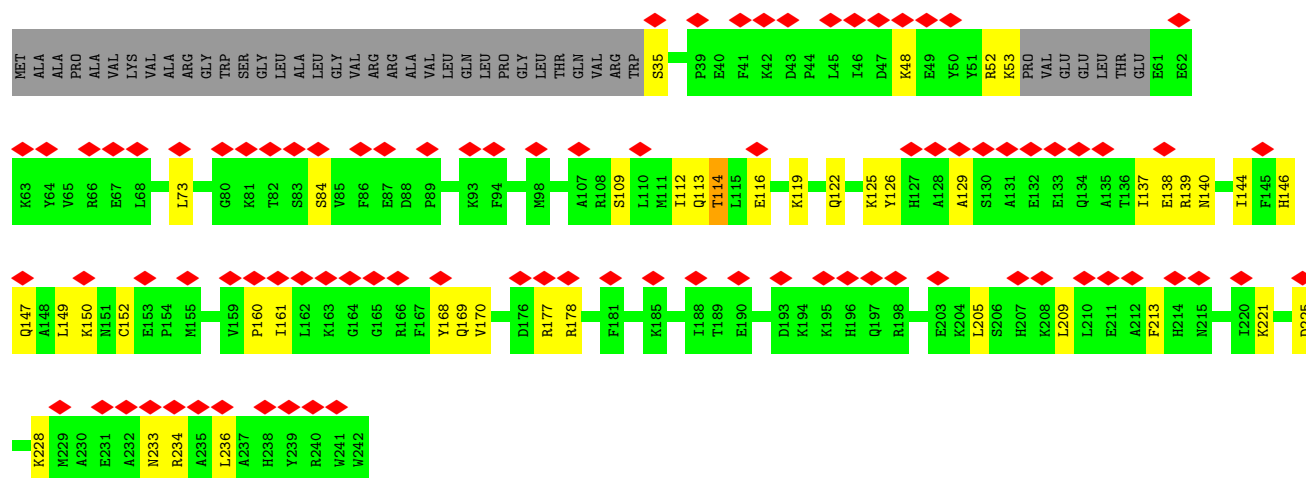


- Molecule 57: 28S ribosomal protein S6, mitochondrial

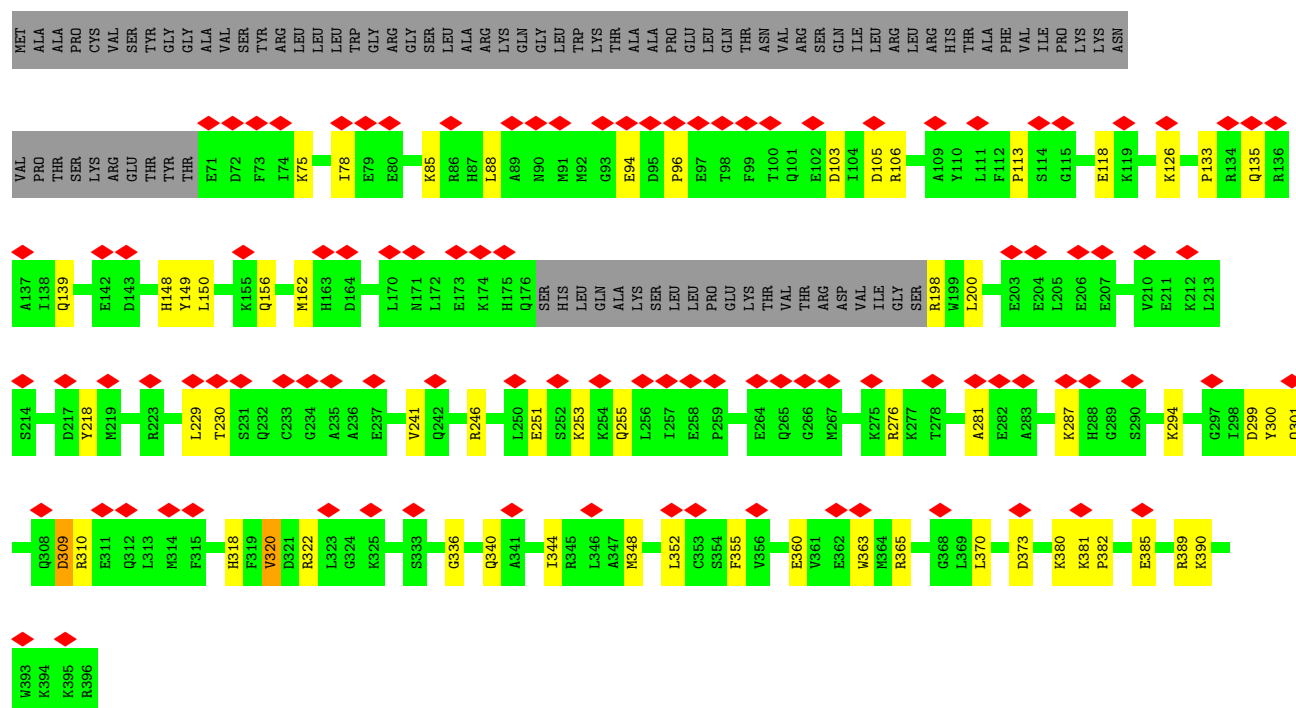


- Molecule 58: 28S ribosomal protein S7, mitochondrial

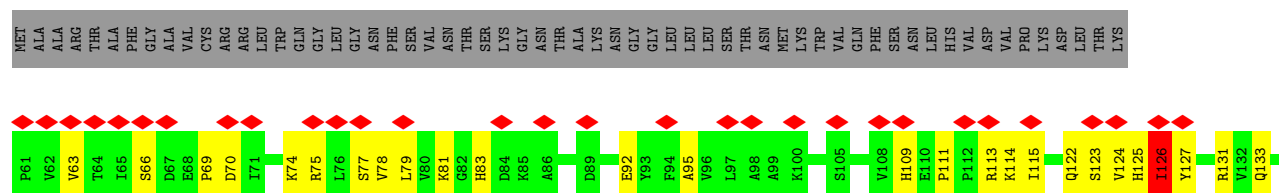




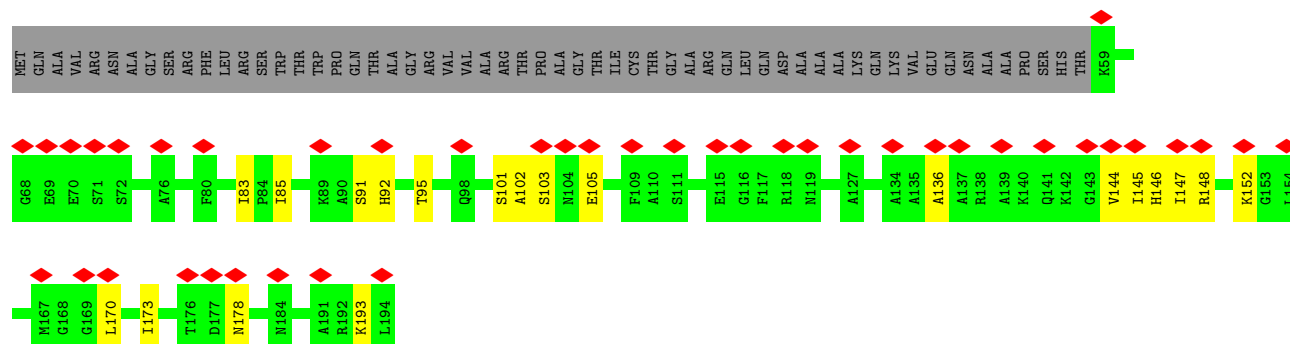
- Molecule 59: 28S ribosomal protein S9, mitochondrial



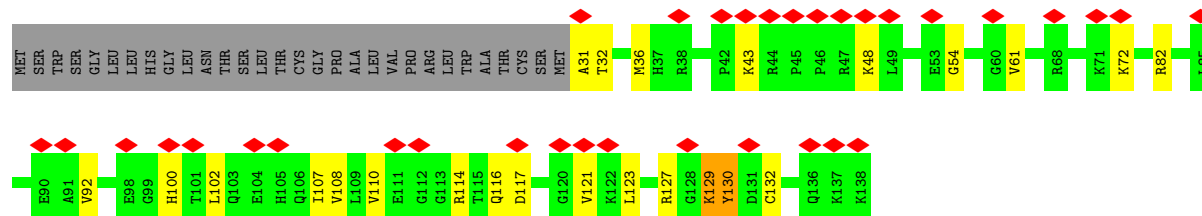
- Molecule 60: 28S ribosomal protein S10, mitochondrial



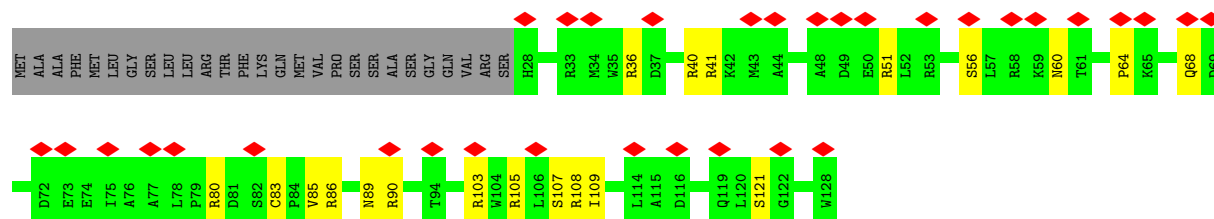
- Molecule 61: 28S ribosomal protein S11, mitochondrial



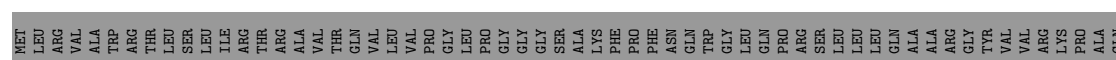
- Molecule 62: 28S ribosomal protein S12, mitochondrial

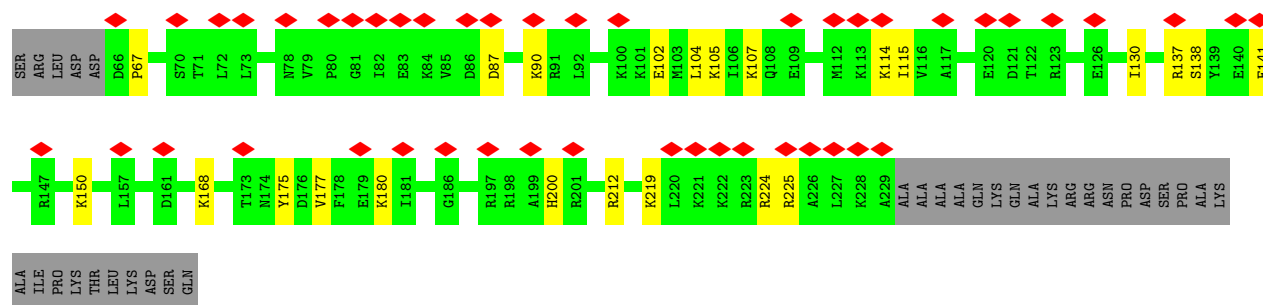


- Molecule 63: 28S ribosomal protein S14, mitochondrial

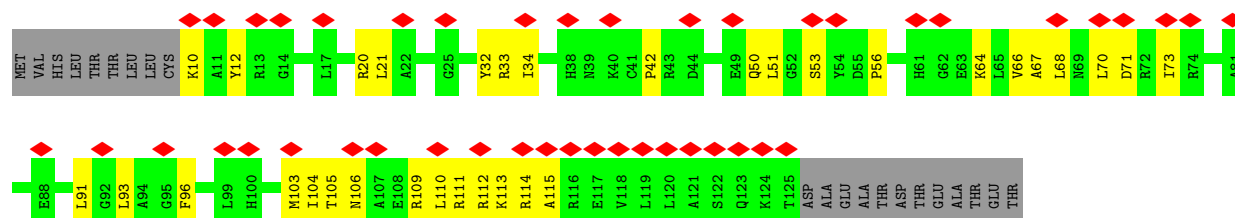


- Molecule 64: 28S ribosomal protein S15, mitochondrial

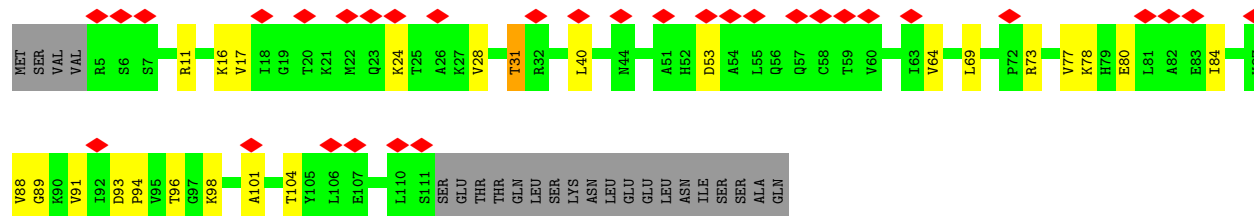




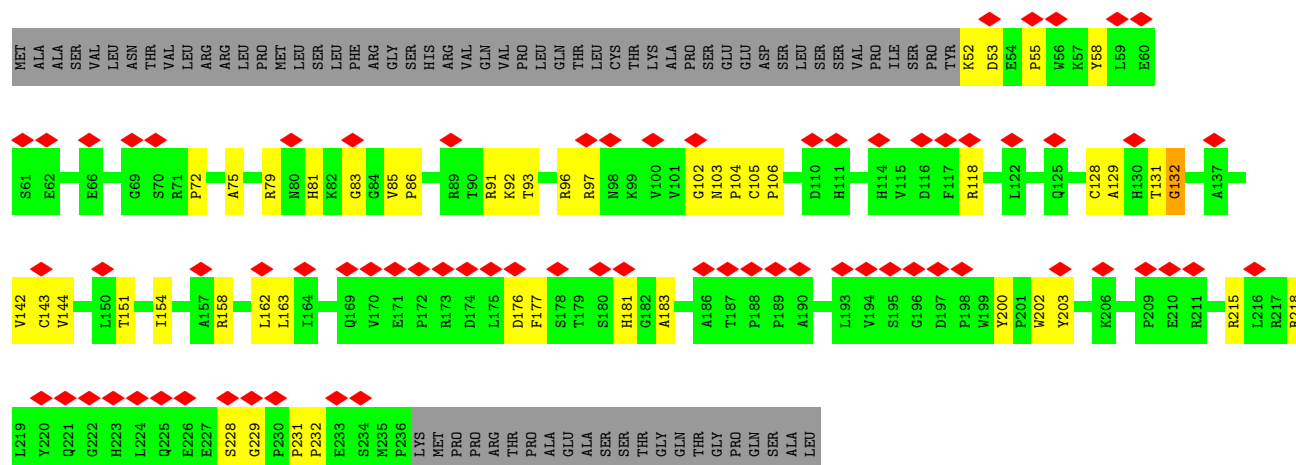
- Molecule 65: 28S ribosomal protein S16, mitochondrial



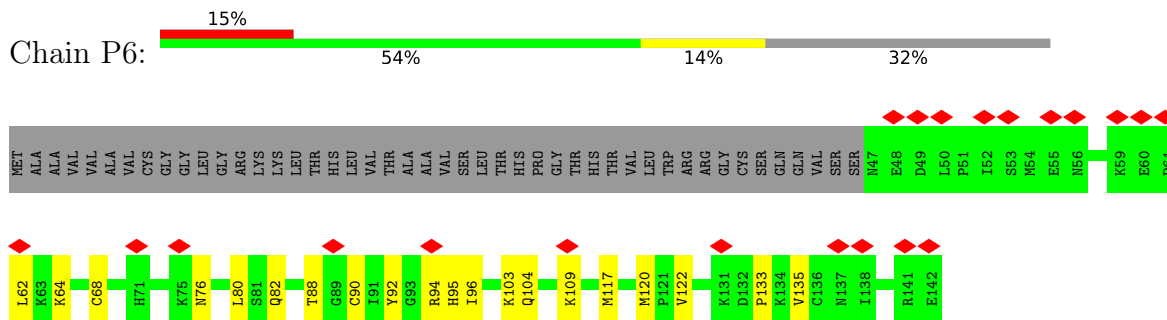
- Molecule 66: 28S ribosomal protein S17, mitochondrial



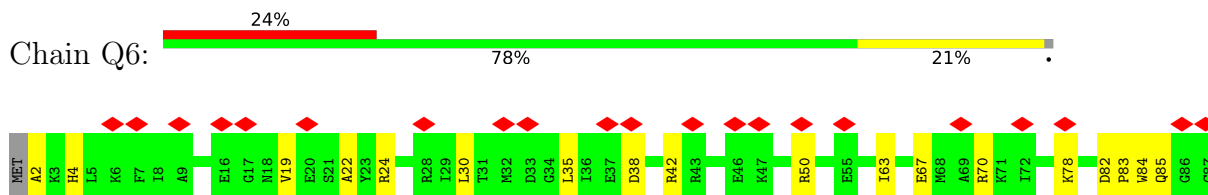
- Molecule 67: 28S ribosomal protein S18b, mitochondrial



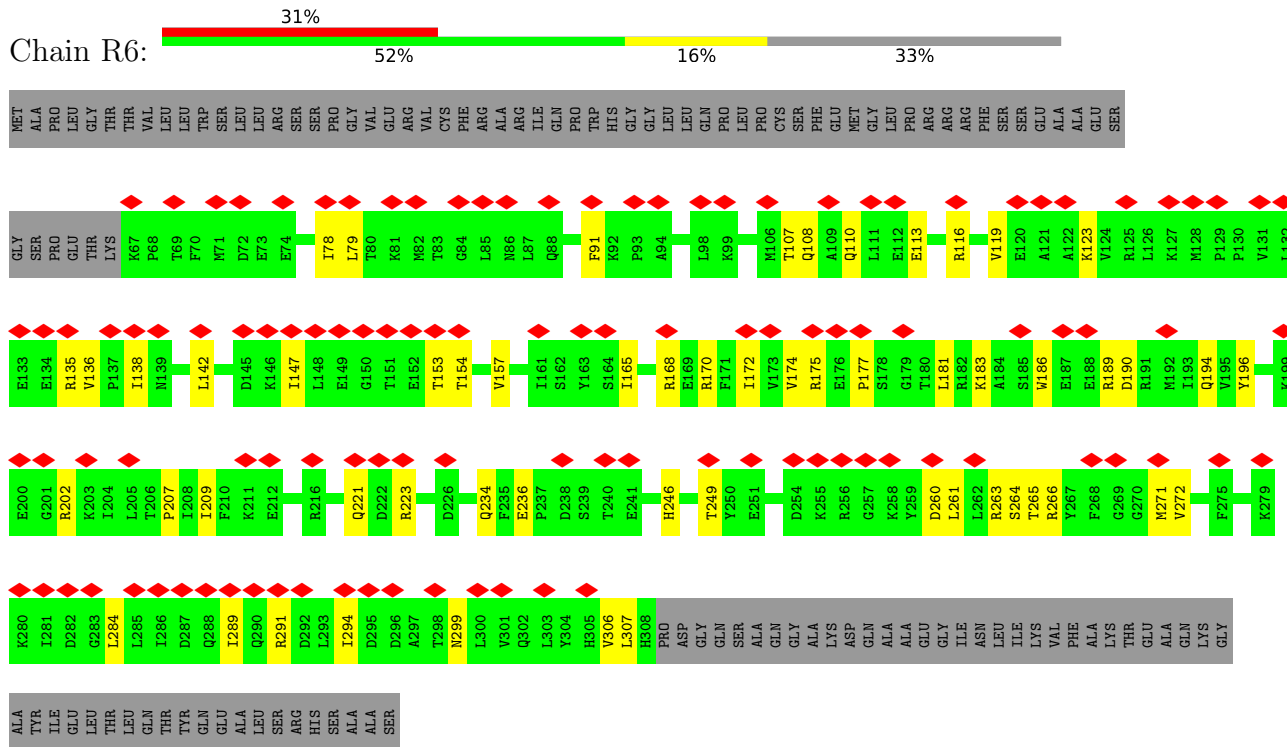
- Chain P6:



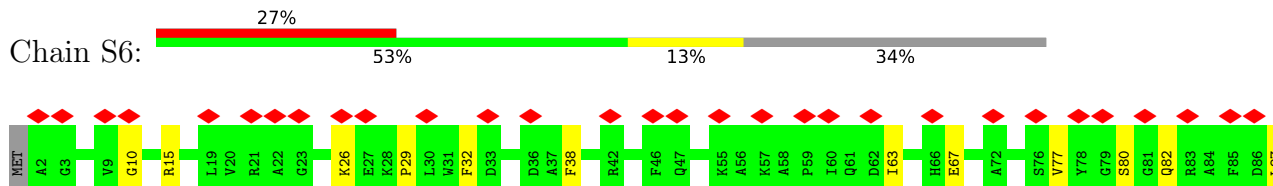
- Chain Q6:

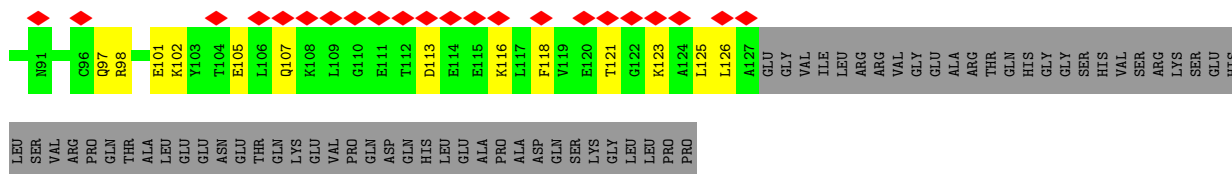


- Chain R6:

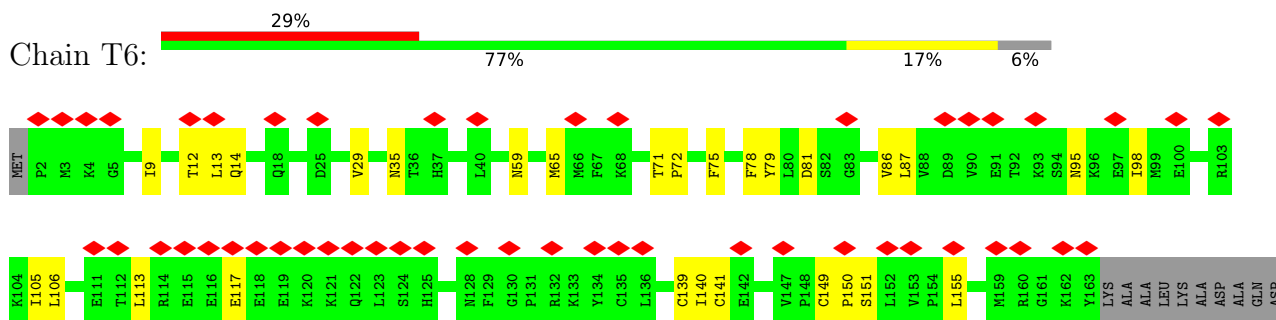


- Chain S6:

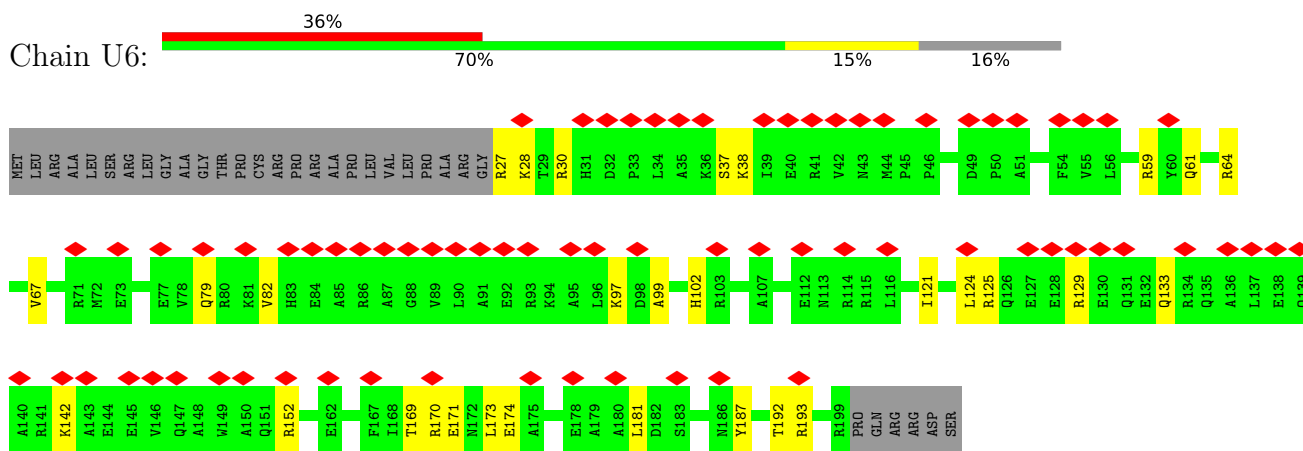




- Molecule 72: 28S ribosomal protein S25, mitochondrial

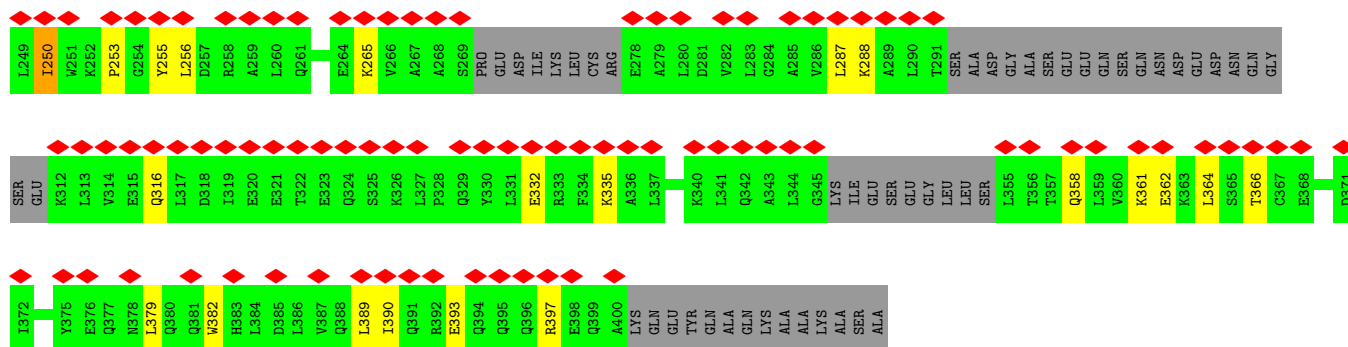


- Molecule 73: 28S ribosomal protein S26, mitochondrial

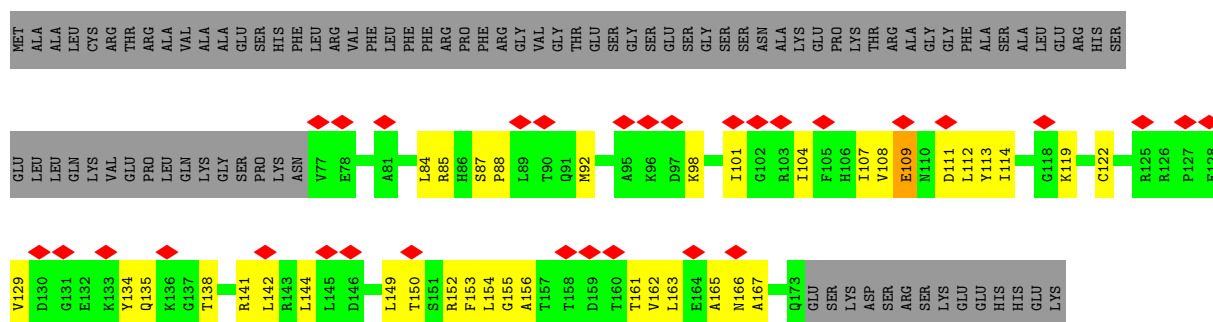
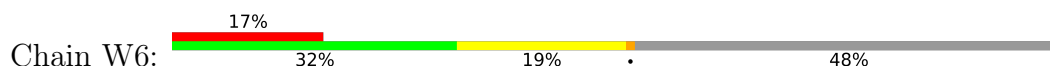


- Molecule 74: 28S ribosomal protein S27, mitochondrial

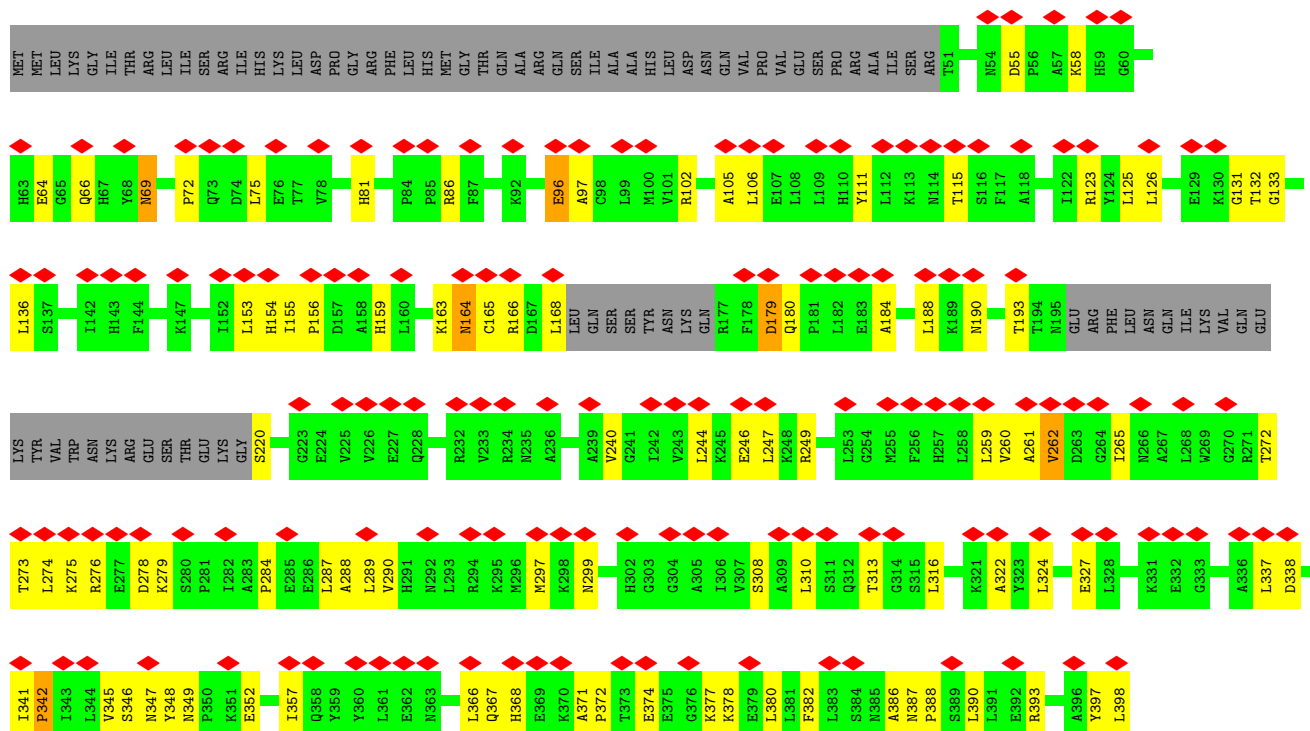
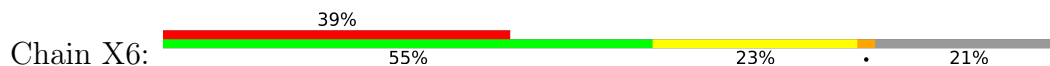


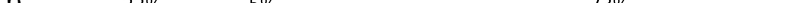


- Molecule 75: 28S ribosomal protein S28, mitochondrial



- Molecule 76: 28S ribosomal protein S29, mitochondrial



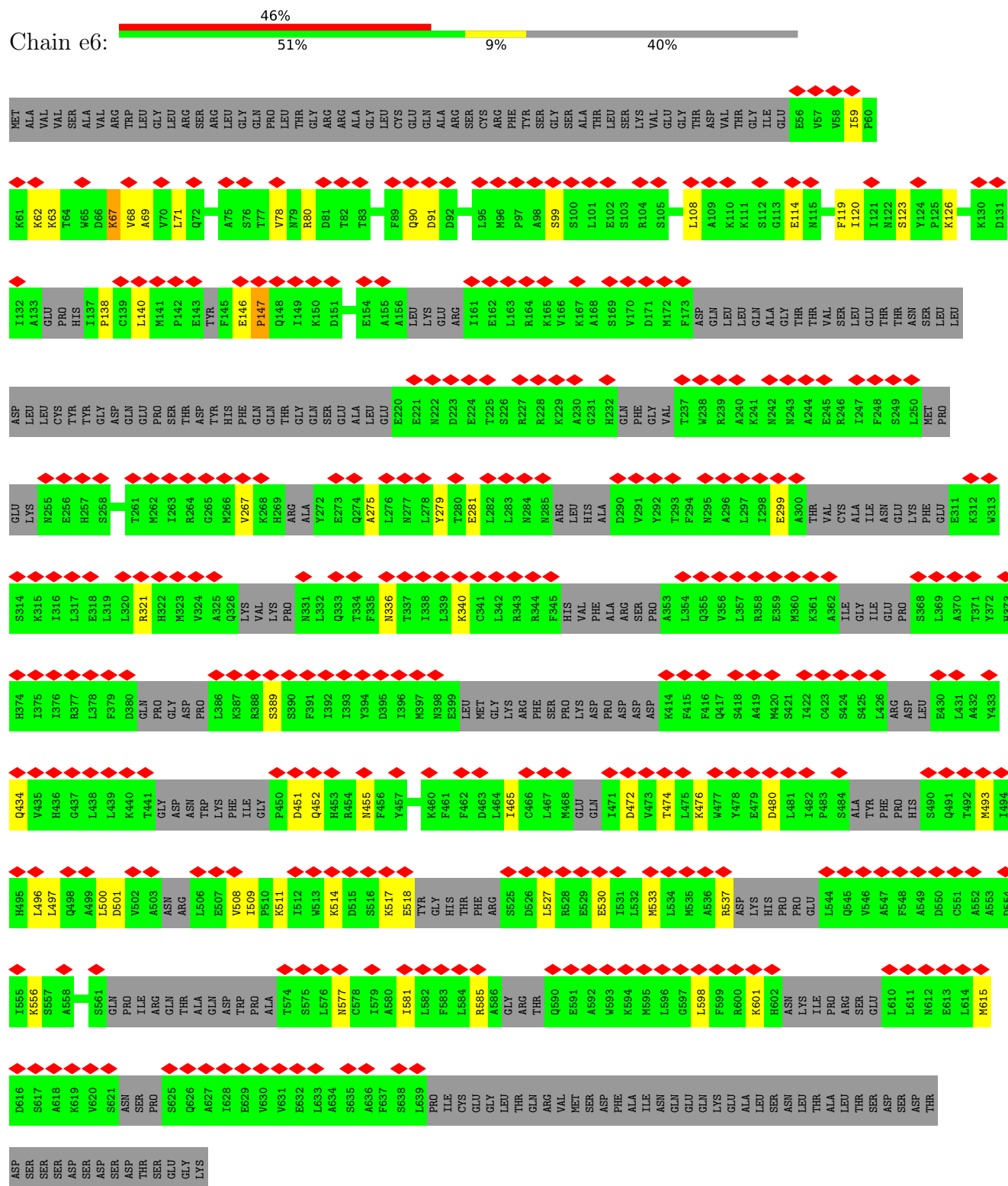
- Chain Y6: 



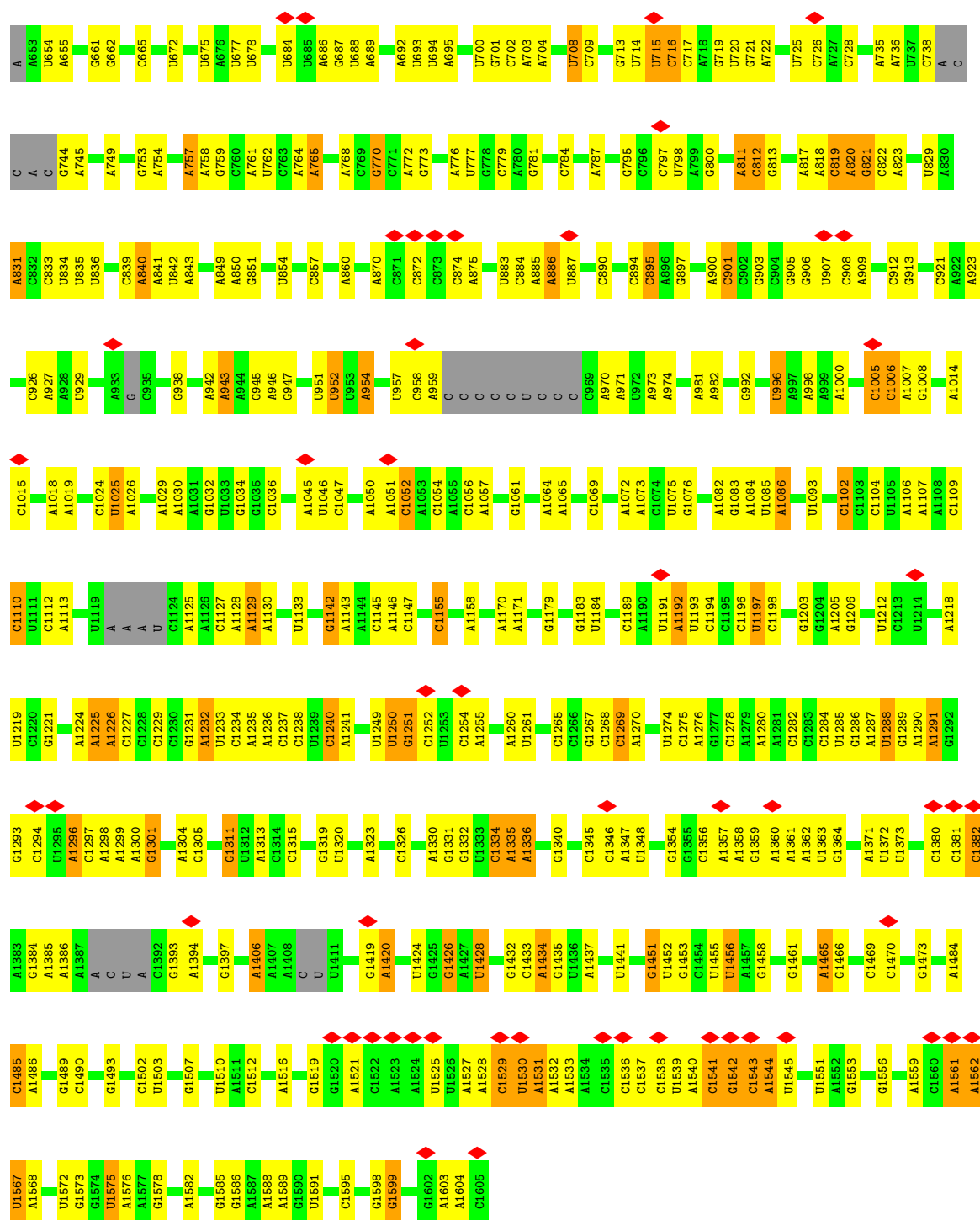
LYS

- Molecule 83: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain e6:

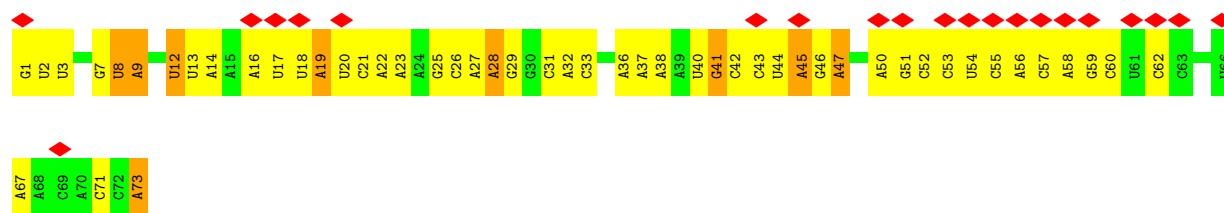


- Molecule 84: 12S rRNA



• Molecule 85: mt-tRNA

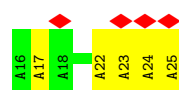
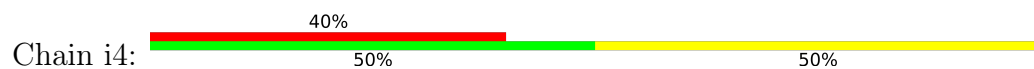




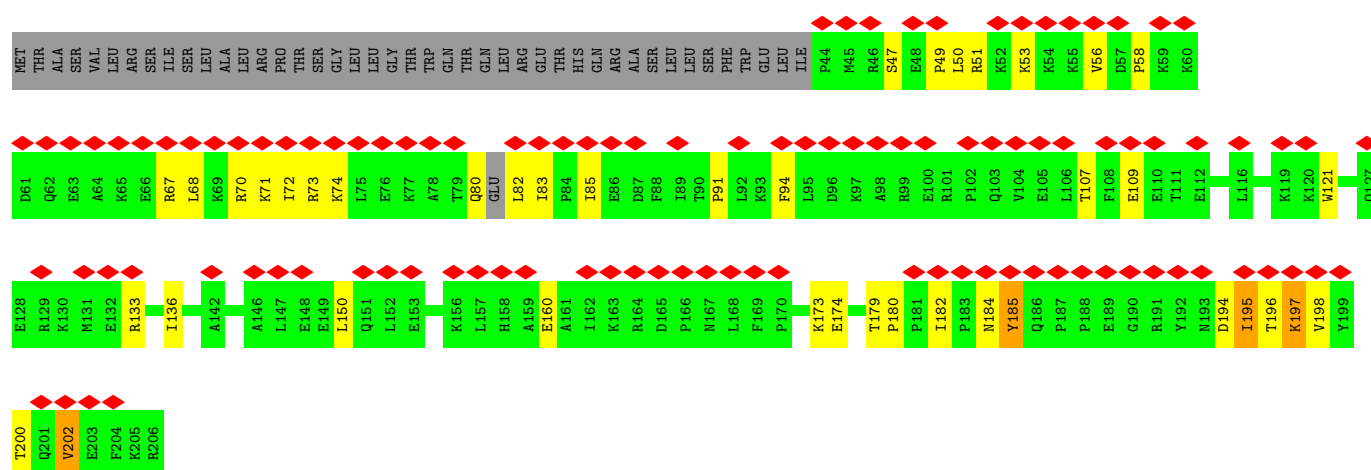
• Molecule 85: mt-tRNA



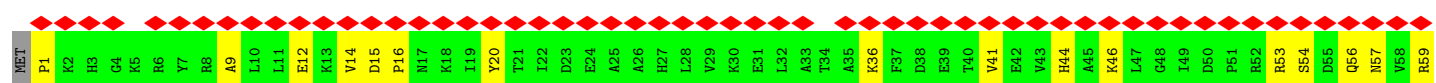
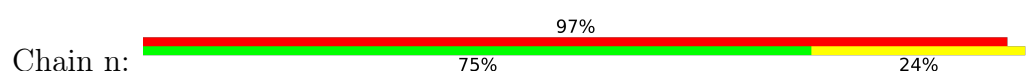
• Molecule 86: mRNA



• Molecule 87: 39S ribosomal protein L40, mitochondrial



• Molecule 88: 50S ribosomal protein L1



F180	P181	P182	E183	K184	L185	A186	D187	N188	I189	R190	A191	F192	I193	R194	A195	L196	E197	A198	H199	K200	P201	E202	G203	A204	K205	G206	T207	F208	L209	R210	S211	V212	Y213	V214	T215	T216	T217	M218	G219	P220	S221	V222	R223	I224	N225	P226	H227	S228											
M120	G121	A122	V123	G124	S125	K126	L127	G128	R129	I130	L131	G132	P133	R134	G135	L136	L137	P138	N139	P140	K141	A142	G143	T144	V145	G146	F147	N148	I149	G150	E151	I152	I153	R154	E155	I156	K157	A158	G159	R160	I161	E162	F163	R164	N165	D166	K167	T168	G169	A170	I171	H172	A173	P174	V175	G176	K177	A178	S179
G60	T61	V62	S63	L64	P65	H66	G67	L68	G69	K70	Q71	V72	R73	V74	L75	A76	I77	A78	K79	G80	E81	K82	I83	K84	E85	A86	E87	E88	A89	G90	A91	D92	Y93	V94	G95	G96	E97	E98	I99	I100	Q101	K102	I103	L104	D105	G106	W107	M108	D109	F110	D111	A112	V113	V114	A115	T116	P117	D118	V119

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MLI, ZN, CL, GDP, SO4, MG

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	Y2	0.38	0/144	0.94	0/200
2	A3	0.36	0/35697	0.45	4/55544 (0.0%)
3	B3	0.26	0/1328	0.39	0/2056
4	D3	0.36	0/1879	0.67	0/2527
5	E3	0.37	0/2433	0.69	2/3299 (0.1%)
6	F3	0.37	0/2071	0.72	0/2817
7	D	0.30	0/665	0.72	0/905
7	H3	0.33	0/798	0.66	0/1073
8	I3	0.30	0/1308	0.63	0/1761
9	J3	0.30	0/1077	0.73	0/1452
10	K3	0.36	0/1495	0.66	0/2029
11	L3	0.35	0/904	0.67	2/1218 (0.2%)
12	M3	0.35	0/2359	0.73	2/3185 (0.1%)
13	N3	0.33	0/1697	0.67	2/2281 (0.1%)
14	O3	0.37	0/1269	0.67	0/1708
15	P3	0.36	0/1103	0.67	0/1491
16	Q3	0.33	0/1863	0.64	1/2509 (0.0%)
17	R3	0.38	0/1174	0.69	1/1572 (0.1%)
18	S3	0.39	0/1276	0.67	0/1729
19	T3	0.36	0/1402	0.63	0/1886
20	U3	0.38	0/946	0.65	0/1283
21	V3	0.32	0/1590	0.71	2/2151 (0.1%)
22	W3	0.39	0/893	0.64	0/1204
23	X3	0.32	0/2081	0.71	2/2812 (0.1%)
24	Y3	0.35	0/1552	0.60	0/2079
25	Z3	0.37	0/1003	0.63	0/1354
26	O3	0.34	0/895	0.71	2/1201 (0.2%)
27	13	0.33	0/438	0.78	0/583
28	23	0.37	0/382	0.53	0/507
29	33	0.37	0/852	0.58	0/1136
30	43	0.36	0/329	0.60	0/435
31	53	0.34	0/3154	0.69	2/4295 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	63	0.33	0/2722	0.68	0/3709
33	73	0.32	0/2207	0.63	0/2978
34	93	0.33	0/896	0.69	0/1205
35	a3	0.33	0/709	0.66	0/963
36	b3	0.36	0/1202	0.66	0/1626
37	c3	0.31	0/2264	0.61	0/3059
38	d3	0.32	0/1385	0.76	4/1877 (0.2%)
39	e3	0.29	0/1797	0.68	0/2422
40	f3	0.34	0/1055	0.91	1/1427 (0.1%)
41	g3	0.37	0/1102	0.61	0/1503
42	h3	0.32	0/847	0.87	5/1150 (0.4%)
43	i3	0.37	0/849	0.65	0/1135
44	j3	0.32	0/698	0.61	0/940
45	k3	0.28	0/665	0.73	0/897
46	l3	0.24	0/226	0.61	0/299
47	m3	0.33	0/379	0.84	2/510 (0.4%)
48	o3	0.40	0/818	0.63	0/1097
49	p3	0.27	0/1071	0.59	0/1433
50	q3	0.29	0/1107	0.65	0/1498
51	r3	0.36	0/1238	0.65	0/1676
52	s3	0.37	1/3114 (0.0%)	0.66	0/4225
53	A5	0.26	0/139	0.93	0/193
54	B6	0.35	0/1811	0.63	1/2451 (0.0%)
55	C6	0.33	0/1112	0.58	0/1505
56	D6	0.32	0/2607	0.70	2/3498 (0.1%)
57	E6	0.31	0/989	0.69	0/1335
58	F6	0.30	0/1708	0.64	0/2291
59	G6	0.32	0/2570	0.67	2/3443 (0.1%)
60	H6	0.37	0/1019	0.80	3/1379 (0.2%)
61	I6	0.30	0/1031	0.63	0/1390
62	J6	0.32	0/854	0.61	0/1148
63	K6	0.34	0/879	0.62	0/1182
64	L6	0.31	0/1406	0.63	0/1878
65	M6	0.34	0/941	0.68	0/1265
66	N6	0.33	0/864	0.70	0/1169
67	O6	0.32	0/1580	0.72	4/2150 (0.2%)
68	P6	0.34	0/791	0.65	1/1062 (0.1%)
69	Q6	0.34	0/752	0.70	0/1001
70	R6	0.35	1/2050 (0.0%)	0.74	0/2770
71	S6	0.31	0/1069	0.63	0/1441
72	T6	0.31	0/1361	0.68	0/1829
73	U6	0.27	0/1482	0.63	0/1987
74	V6	0.26	0/2758	0.66	2/3724 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	W6	0.32	0/778	0.76	2/1048 (0.2%)
76	X6	0.32	0/2596	0.77	8/3519 (0.2%)
77	Y6	0.30	0/943	0.62	0/1274
78	Z6	0.28	0/757	0.64	2/1011 (0.2%)
79	a6	0.32	0/1727	0.69	0/2338
80	b6	0.30	0/2121	0.72	0/2873
81	c6	0.33	0/939	0.71	0/1256
82	d6	0.33	0/621	0.62	0/820
83	e6	0.34	2/2859 (0.1%)	0.80	4/3864 (0.1%)
84	A6	0.32	0/22053	0.43	0/34324
85	24	0.23	0/1731	0.41	0/2693
85	C	0.23	0/1731	0.41	0/2693
86	i4	0.27	0/247	0.42	0/383
87	A	0.36	1/1403 (0.1%)	0.89	3/1880 (0.2%)
88	n	0.30	0/1812	0.68	2/2443 (0.1%)
All	All	0.34	5/174499 (0.0%)	0.60	70/248421 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y2	0	1
4	D3	0	1
5	E3	0	6
6	F3	0	1
7	H3	0	1
9	J3	0	1
10	K3	0	2
12	M3	0	4
16	Q3	0	1
17	R3	0	1
21	V3	0	2
22	W3	0	1
23	X3	0	3
25	Z3	0	1
26	03	0	1
27	13	0	1
31	53	0	1
34	93	0	2
38	d3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	e3	0	1
40	f3	0	4
41	g3	0	1
42	h3	0	2
43	i3	0	1
45	k3	0	1
48	o3	0	1
50	q3	0	1
56	D6	0	3
62	J6	0	2
63	K6	0	1
67	O6	0	1
70	R6	0	3
71	S6	0	1
74	V6	0	3
75	W6	0	1
76	X6	0	2
77	Y6	0	1
81	c6	0	1
83	e6	0	1
87	A	0	4
All	All	0	69

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	e6	91	ASP	C-N	-6.55	1.23	1.33
87	A	83	ILE	C-N	6.07	1.40	1.33
70	R6	91	PHE	C-N	-5.75	1.21	1.33
52	s3	427	ASN	C-N	-5.69	1.21	1.33
83	e6	509	ILE	CA-CB	5.64	1.61	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	A	202	VAL	N-CA-C	-8.87	105.29	113.71
47	m3	51	LEU	CA-C-N	8.47	133.56	120.68
47	m3	51	LEU	C-N-CA	8.47	133.56	120.68
42	h3	63	PRO	CA-C-N	7.64	135.45	121.70
42	h3	63	PRO	C-N-CA	7.64	135.45	121.70
40	f3	50	THR	N-CA-C	-7.48	101.41	111.96
83	e6	147	PRO	N-CA-CB	7.34	110.96	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	h3	64	GLU	CA-C-N	6.95	134.81	121.54
42	h3	64	GLU	C-N-CA	6.95	134.81	121.54
13	N3	237	HIS	CA-C-N	6.85	134.63	121.54
13	N3	237	HIS	C-N-CA	6.85	134.63	121.54
83	e6	321	ARG	N-CA-C	-6.80	105.26	113.97
76	X6	96	GLU	CA-C-N	6.66	134.26	121.54
76	X6	96	GLU	C-N-CA	6.66	134.26	121.54
78	Z6	90	GLY	CA-C-N	6.55	133.49	121.70
78	Z6	90	GLY	C-N-CA	6.55	133.49	121.70
59	G6	320	VAL	CA-C-N	6.46	133.88	121.54
59	G6	320	VAL	C-N-CA	6.46	133.88	121.54
5	E3	323	GLY	CA-C-N	6.43	133.27	121.70
5	E3	323	GLY	C-N-CA	6.43	133.27	121.70
88	n	115	ALA	CA-C-N	6.40	137.84	122.36
88	n	115	ALA	C-N-CA	6.40	137.84	122.36
68	P6	135	VAL	N-CA-C	-6.39	107.01	113.47
38	d3	129	ASP	CA-C-N	6.35	133.13	121.70
38	d3	129	ASP	C-N-CA	6.35	133.13	121.70
42	h3	64	GLU	CA-CB-CG	6.19	126.49	114.10
60	H6	179	GLN	N-CA-C	6.12	118.67	111.02
74	V6	195	ASP	CA-C-N	6.10	133.19	121.54
74	V6	195	ASP	C-N-CA	6.10	133.19	121.54
16	Q3	157	GLY	N-CA-C	5.99	119.99	113.58
12	M3	46	GLY	CA-C-N	5.98	132.96	121.54
12	M3	46	GLY	C-N-CA	5.98	132.96	121.54
54	B6	204	GLU	N-CA-C	-5.94	101.91	110.40
60	H6	126	ILE	CA-C-N	5.91	131.05	122.36
60	H6	126	ILE	C-N-CA	5.91	131.05	122.36
76	X6	341	ILE	CB-CA-C	5.91	116.13	110.16
11	L3	112	GLY	CA-C-N	5.76	132.07	121.70
11	L3	112	GLY	C-N-CA	5.76	132.07	121.70
67	O6	102	GLY	CA-C-N	-5.75	113.62	121.61
67	O6	102	GLY	C-N-CA	-5.75	113.62	121.61
87	A	180	PRO	CA-C-N	5.69	140.66	127.00
87	A	180	PRO	C-N-CA	5.69	140.66	127.00
83	e6	267	VAL	N-CA-C	-5.68	106.77	112.17
76	X6	342	PRO	CA-C-N	5.67	127.64	121.97
76	X6	342	PRO	C-N-CA	5.67	127.64	121.97
21	V3	99	GLY	CA-C-N	5.50	132.04	121.54
21	V3	99	GLY	C-N-CA	5.50	132.04	121.54
38	d3	230	ARG	CA-C-N	5.49	132.02	121.54
38	d3	230	ARG	C-N-CA	5.49	132.02	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	53	216	GLU	CA-C-N	5.45	131.51	121.70
31	53	216	GLU	C-N-CA	5.45	131.51	121.70
2	A3	2789	C	C2'-C3'-O3'	5.42	117.64	109.50
83	e6	281	GLU	N-CA-C	-5.38	107.36	114.31
2	A3	1806	U	P-O3'-C3'	5.37	128.25	120.20
26	03	177	ARG	CA-C-N	5.35	131.75	121.54
26	03	177	ARG	C-N-CA	5.35	131.75	121.54
2	A3	3201	A	P-O3'-C3'	5.34	128.21	120.20
23	X3	178	PRO	CA-C-N	5.29	131.65	121.54
23	X3	178	PRO	C-N-CA	5.29	131.65	121.54
76	X6	179	ASP	CA-C-N	5.25	129.88	122.74
76	X6	179	ASP	C-N-CA	5.25	129.88	122.74
17	R3	136	LYS	N-CA-C	5.16	116.95	110.91
76	X6	164	ASN	N-CA-C	5.11	117.96	110.30
75	W6	129	VAL	CA-C-N	5.07	129.61	122.46
75	W6	129	VAL	C-N-CA	5.07	129.61	122.46
67	O6	53	ASP	CA-C-N	5.06	134.14	121.80
67	O6	53	ASP	C-N-CA	5.06	134.14	121.80
56	D6	298	PHE	CA-C-N	5.04	131.18	121.54
56	D6	298	PHE	C-N-CA	5.04	131.18	121.54
2	A3	1807	U	P-O3'-C3'	5.04	127.76	120.20

There are no chirality outliers.

All (69) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	03	177	ARG	Peptide
27	13	62	ILE	Peptide
31	53	269	ASN	Peptide
34	93	132	PRO	Peptide
34	93	45	THR	Peptide
87	A	184	ASN	Peptide
87	A	185	TYR	Peptide
87	A	196	THR	Peptide
87	A	197	LYS	Peptide
4	D3	206	TYR	Peptide
56	D6	284	ARG	Peptide
56	D6	285	TYR	Peptide
56	D6	286	GLU	Peptide
5	E3	126	ASP	Peptide
5	E3	169	GLY	Peptide
5	E3	244	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	E3	315	PRO	Peptide
5	E3	326	GLU	Peptide
5	E3	85	TRP	Peptide
6	F3	129	PRO	Peptide
7	H3	63	PRO	Peptide
9	J3	144	ILE	Peptide
62	J6	129	LYS	Peptide
62	J6	130	TYR	Peptide
10	K3	3	SER	Peptide
10	K3	5	SER	Peptide
63	K6	64	PRO	Peptide
12	M3	109	ARG	Peptide
12	M3	20	PRO	Peptide
12	M3	264	GLN	Peptide
12	M3	287	ASP	Peptide
67	O6	55	PRO	Peptide
16	Q3	182	ARG	Peptide
17	R3	137	GLU	Peptide
70	R6	154	THR	Peptide
70	R6	265	THR	Peptide
70	R6	291	ARG	Peptide
71	S6	107	GLN	Peptide
21	V3	100	LYS	Peptide
21	V3	170	TRP	Peptide
74	V6	155	GLU	Peptide
74	V6	196	PHE	Peptide
74	V6	41	GLU	Peptide
22	W3	72	HIS	Peptide
75	W6	107	ILE	Peptide
23	X3	51	LYS	Peptide
23	X3	94	ASN	Peptide
23	X3	95	ASP	Peptide
76	X6	66	GLN	Peptide
76	X6	96	GLU	Peptide
1	Y2	22	ALA	Peptide
77	Y6	339	GLU	Peptide
25	Z3	141	SER	Peptide
81	c6	60	GLU	Peptide
38	d3	230	ARG	Peptide
38	d3	271	PRO	Peptide
39	e3	173	LEU	Peptide
83	e6	67	LYS	Peptide

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Mol	Chain	Res	Type	Group
40	f3	189	HIS	Peptide
40	f3	49	LYS	Peptide
40	f3	50	THR	Peptide
40	f3	87	GLU	Peptide
41	g3	110	ILE	Peptide
42	h3	138	SER	Peptide
42	h3	63	PRO	Peptide
43	i3	57	TYR	Peptide
45	k3	36	THR	Peptide
48	o3	82	PHE	Peptide
50	q3	78	SER	Peptide

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	Y2	145	0	147	0	0
2	A3	31913	0	16213	233	0
3	B3	1191	0	607	4	0
4	D3	1842	0	1896	27	0
5	E3	2365	0	2378	39	0
6	F3	2013	0	2044	41	0
7	D	648	0	657	9	0
7	H3	784	0	832	12	0
8	I3	1283	0	1370	25	0
9	J3	1061	0	1141	19	0
10	K3	1451	0	1448	30	0
11	L3	889	0	941	11	0
12	M3	2305	0	2378	41	0
13	N3	1654	0	1681	20	0
14	O3	1245	0	1283	29	0
15	P3	1080	0	1081	18	0
16	Q3	1822	0	1859	20	0
17	R3	1153	0	1214	14	0
18	S3	1251	0	1322	25	0
19	T3	1368	0	1410	23	0
20	U3	922	0	935	25	0
21	V3	1551	0	1558	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W3	871	0	898	17	0
23	X3	2027	0	2040	33	0
24	Y3	1517	0	1561	30	0
25	Z3	978	0	1030	18	0
26	O3	880	0	903	18	0
27	I3	433	0	475	5	0
28	23	376	0	406	11	0
29	33	831	0	883	21	0
30	43	322	0	343	1	0
31	53	3064	0	3059	54	0
32	63	2636	0	2450	39	0
33	73	2158	0	2173	38	0
34	93	873	0	878	14	0
35	a3	686	0	658	7	0
36	b3	1178	0	1180	21	0
37	c3	2217	0	2220	30	0
38	d3	1347	0	1343	20	0
39	e3	1762	0	1767	39	0
40	f3	1039	0	1044	26	0
41	g3	1067	0	1056	28	0
42	h3	827	0	806	12	0
43	i3	827	0	857	18	0
44	j3	684	0	673	9	0
45	k3	655	0	656	15	0
46	l3	221	0	227	4	0
47	m3	372	0	387	8	0
48	o3	797	0	804	17	0
49	p3	1058	0	1083	16	0
50	q3	1076	0	1049	14	0
51	r3	1203	0	1220	21	0
52	s3	3036	0	3022	53	0
52	t3	140	0	31	1	0
53	A5	140	0	142	0	0
54	B6	1768	0	1765	22	0
55	C6	1082	0	1088	19	0
56	D6	2557	0	2596	45	0
57	E6	972	0	1000	16	0
58	F6	1668	0	1716	29	0
59	G6	2516	0	2503	43	0
60	H6	999	0	1024	37	0
61	I6	1011	0	1052	13	0
62	J6	838	0	887	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	K6	861	0	885	19	0
64	L6	1382	0	1472	16	0
65	M6	920	0	951	26	0
66	N6	846	0	908	17	0
67	O6	1528	0	1488	34	0
68	P6	774	0	803	14	0
69	Q6	740	0	754	15	0
70	R6	2008	0	2031	36	0
71	S6	1042	0	1037	15	0
72	T6	1330	0	1342	20	0
73	U6	1461	0	1471	28	0
74	V6	2702	0	2690	43	0
75	W6	766	0	785	27	0
76	X6	2531	0	2520	65	0
77	Y6	914	0	859	12	0
78	Z6	740	0	747	10	0
79	a6	1684	0	1685	40	0
80	b6	2076	0	2097	37	0
81	c6	925	0	962	12	0
82	d6	610	0	682	9	0
83	e6	2838	0	2416	34	0
84	A6	19716	0	10015	172	0
85	24	1547	0	787	18	0
85	C	1547	0	788	16	0
86	i4	219	0	110	1	0
87	A	1375	0	1426	28	0
88	n	1766	0	1829	34	0
89	A3	97	0	0	0	0
89	A6	28	0	0	0	0
89	D3	1	0	0	0	0
89	g3	1	0	0	0	0
89	n	1	0	0	0	0
90	03	1	0	0	0	0
90	43	1	0	0	0	0
90	B6	1	0	0	0	0
90	O6	1	0	0	0	0
90	P6	1	0	0	0	0
90	T6	1	0	0	0	0
90	r3	1	0	0	0	0
91	X6	28	0	12	2	0
92	n	5	0	0	0	0
93	n	21	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	n	2	0	0	2	0
95	D	2	0	0	0	0
95	n	2	0	0	0	0
96	A3	4	0	0	0	0
96	D	8	0	0	1	0
96	n	67	0	0	3	0
All	All	165767	0	138908	1951	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 7.

All (1951) 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)
52:s3:264:ILE:HG22	52:s3:266:CYS:H	1.52	0.74
2:A3:2015:G:H22	2:A3:2037:U:H5"	1.54	0.72
80:b6:250:GLU:HA	80:b6:301:ASN:HD21	1.54	0.71
65:M6:21:LEU:HD12	65:M6:32:TYR:HB3	1.71	0.71
74:V6:175:VAL:HG12	74:V6:177:SER:H	1.58	0.69
2:A3:1683:C:H41	24:Y3:225:ASN:HD21	1.40	0.68
41:g3:128:LEU:HB2	41:g3:136:PRO:HG3	1.76	0.67
73:U6:61:GLN:NE2	79:a6:198:MET:SD	2.67	0.67
62:J6:129:LYS:HG2	62:J6:130:TYR:HB2	1.77	0.67
84:A6:728:C:H42	84:A6:754:A:H61	1.42	0.67
2:A3:1794:A:OP1	6:F3:142:ARG:NH2	2.26	0.67
76:X6:102:ARG:H	76:X6:105:ALA:HB3	1.60	0.67
8:I3:174:LEU:HD21	45:k3:55:VAL:HG13	1.75	0.67
2:A3:2082:G:N3	25:Z3:109:LYS:NZ	2.43	0.67
55:C6:75:ASN:HA	63:K6:103:ARG:HH12	1.58	0.67
59:G6:113:PRO:HG2	80:b6:109:PRO:HG2	1.77	0.67
87:A:47:SER:HA	87:A:50:LEU:HB2	1.77	0.67
39:e3:152:LYS:HB3	39:e3:157:LEU:HD21	1.77	0.67
73:U6:169:THR:HG23	73:U6:171:GLU:H	1.60	0.66
25:Z3:126:GLN:HE21	25:Z3:147:VAL:HG22	1.60	0.66
33:73:65:ILE:HB	33:73:122:SER:HB2	1.77	0.66
57:E6:96:HIS:HB3	57:E6:99:THR:HG23	1.76	0.66
59:G6:382:PRO:O	60:H6:131:ARG:NH1	2.28	0.66
24:Y3:91:ARG:HH11	34:93:85:PRO:HA	1.61	0.66
24:Y3:164:ARG:NH1	24:Y3:181:PHE:O	2.27	0.66
58:F6:234:ARG:HD2	81:c6:53:MET:HG2	1.78	0.66
2:A3:3117:C:H42	2:A3:3139:G:H1	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:F6:126:TYR:HB2	58:F6:137:ILE:HG21	1.79	0.65
80:b6:251:TYR:HB3	80:b6:297:VAL:HG12	1.78	0.65
31:53:248:THR:HG21	31:53:373:LEU:HD11	1.78	0.65
38:d3:182:ARG:HB2	38:d3:223:ALA:HB3	1.78	0.65
54:B6:169:ARG:HH12	59:G6:150:LEU:HD21	1.61	0.65
55:C6:97:TRP:HD1	55:C6:104:LEU:HD22	1.61	0.65
69:Q6:67:GLU:HG2	75:W6:154:LEU:HB2	1.77	0.65
84:A6:1142:G:H2'	84:A6:1143:A:H8	1.62	0.65
15:P3:55:LEU:HB2	15:P3:61:ALA:HB2	1.77	0.65
15:P3:84:ARG:NH1	15:P3:124:CYS:SG	2.70	0.65
82:d6:129:ASN:HD22	82:d6:131:LEU:HB2	1.62	0.65
52:s3:152:GLN:HA	52:s3:156:TYR:HB2	1.79	0.65
2:A3:2599:U:OP2	2:A3:2625:C:N4	2.29	0.65
2:A3:1881:A:OP2	41:g3:111:ARG:NH2	2.30	0.65
2:A3:2500:A:HO2'	28:23:47:LYS:N	1.95	0.65
38:d3:226:ASP:HB3	38:d3:229:GLY:H	1.62	0.65
2:A3:1777:A:N6	2:A3:1780:U:OP2	2.31	0.64
17:R3:47:ILE:HG23	18:S3:172:MET:HE1	1.80	0.64
2:A3:1688:A:H3'	23:X3:5:LYS:HE3	1.79	0.64
23:X3:238:LEU:HA	23:X3:241:GLN:HB2	1.80	0.64
64:L6:87:ASP:HA	64:L6:90:LYS:HE2	1.78	0.64
56:D6:234:LYS:NZ	84:A6:1326:C:N3	2.45	0.64
58:F6:178:ARG:NH1	84:A6:1197:U:O2'	2.31	0.64
8:I3:101:ASN:HD21	8:I3:104:LEU:HB2	1.63	0.64
60:H6:66:SER:HB2	83:e6:62:LYS:HB3	1.80	0.64
2:A3:1884:G:N7	6:F3:281:ARG:NH1	2.45	0.63
52:s3:376:THR:HG22	52:s3:389:ARG:HG3	1.80	0.63
83:e6:598:LEU:HA	83:e6:601:LYS:HD2	1.79	0.63
84:A6:1128:A:H2'	84:A6:1129:A:H2'	1.79	0.63
2:A3:2559:U:OP2	84:A6:1005:C:N4	2.32	0.63
4:D3:108:ASP:OD2	4:D3:149:ARG:NH1	2.32	0.63
24:Y3:131:ARG:HA	24:Y3:134:LYS:HD2	1.80	0.63
26:03:90:ASN:HB3	26:03:94:ARG:HH21	1.64	0.63
52:s3:332:LEU:HD13	52:s3:372:TYR:HB2	1.81	0.63
56:D6:202:SER:OG	56:D6:221:ARG:NH1	2.32	0.63
21:V3:177:THR:OG1	21:V3:178:SER:N	2.32	0.63
31:53:229:ARG:NH1	31:53:231:SER:OG	2.32	0.63
70:R6:78:ILE:HG23	70:R6:299:ASN:HB3	1.79	0.63
79:a6:15:ALA:O	79:a6:19:ARG:NH1	2.31	0.63
12:M3:30:ASN:OD1	48:o3:91:GLN:NE2	2.32	0.62
84:A6:773:G:N2	84:A6:776:A:OP2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:A:107:THR:HG22	87:A:109:GLU:H	1.64	0.62
4:D3:132:ASP:OD2	4:D3:135:ARG:NH1	2.32	0.62
20:U3:9:LEU:O	20:U3:11:ARG:NH2	2.32	0.62
55:C6:69:LEU:HD23	80:b6:107:LYS:HD3	1.81	0.62
12:M3:140:LEU:HB2	12:M3:156:VAL:HG11	1.82	0.62
6:F3:282:PRO:O	6:F3:290:TYR:OH	2.17	0.62
38:d3:261:MET:N	38:d3:261:MET:SD	2.72	0.62
84:A6:702:C:H2'	84:A6:703:A:H8	1.64	0.62
34:93:127:LEU:O	34:93:134:ASN:ND2	2.32	0.62
32:63:53:SER:HB3	32:63:56:ARG:HD2	1.81	0.62
66:N6:17:VAL:HG12	66:N6:28:VAL:HG22	1.82	0.62
3:B3:1639:U:H5''	15:P3:154:SER:HB2	1.81	0.62
8:I3:97:ALA:HB3	8:I3:154:LEU:HB2	1.82	0.62
59:G6:389:ARG:HB2	84:A6:1437:A:H5''	1.81	0.62
87:A:185:TYR:HB3	87:A:194:ASP:HB2	1.81	0.62
2:A3:2256:U:O2'	18:S3:118:ASN:ND2	2.33	0.62
21:V3:53:ASP:OD1	21:V3:53:ASP:N	2.33	0.62
63:K6:56:SER:O	63:K6:60:ASN:ND2	2.33	0.62
80:b6:172:VAL:HG22	80:b6:208:LYS:HB3	1.82	0.62
7:H3:94:LEU:HB3	7:H3:116:LYS:HE2	1.81	0.61
38:d3:165:THR:HG23	38:d3:167:HIS:H	1.65	0.61
77:Y6:348:ARG:HA	77:Y6:351:MET:HB2	1.82	0.61
28:23:74:ALA:HA	28:23:77:GLN:HE21	1.64	0.61
79:a6:43:ARG:HE	79:a6:50:LEU:HD21	1.64	0.61
64:L6:114:LYS:HG3	64:L6:115:ILE:HG13	1.82	0.61
2:A3:2096:U:O4	12:M3:57:ARG:NH1	2.33	0.61
23:X3:97:LEU:H	85:C:73:A:H3'	1.65	0.61
58:F6:35:SER:N	84:A6:1434:A:OP1	2.34	0.61
70:R6:202:ARG:HG3	70:R6:234:GLN:HA	1.81	0.61
39:e3:264:LEU:HD12	39:e3:269:LEU:HB3	1.82	0.61
43:i3:53:MET:HE2	50:q3:27:ALA:HB2	1.81	0.61
31:53:290:THR:HG22	31:53:343:GLN:HB2	1.81	0.61
79:a6:19:ARG:NH2	84:A6:812:C:OP1	2.33	0.61
84:A6:1203:G:N1	84:A6:1426:G:OP2	2.34	0.61
18:S3:107:LYS:HD2	19:T3:212:LEU:HD11	1.81	0.61
2:A3:2248:U:OP1	17:R3:99:ARG:NH2	2.33	0.61
2:A3:2970:C:N3	13:N3:182:LYS:NZ	2.49	0.61
23:X3:96:LYS:N	85:C:73:A:O3'	2.34	0.61
2:A3:2909:G:N7	29:33:131:LYS:NZ	2.49	0.60
23:X3:177:HIS:ND1	23:X3:178:PRO:O	2.32	0.60
2:A3:1800:G:N7	21:V3:41:ARG:NH2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M3:104:LEU:HD11	12:M3:126:GLY:HA3	1.83	0.60
19:T3:154:LYS:O	19:T3:155:ARG:NH1	2.34	0.60
58:F6:169:GLN:OE1	58:F6:233:ASN:ND2	2.34	0.60
74:V6:393:GLU:OE2	74:V6:397:ARG:NH2	2.34	0.60
88:n:103:ILE:HA	88:n:107:TRP:HB2	1.81	0.60
4:D3:195:ASN:HB2	4:D3:243:THR:HG22	1.83	0.60
21:V3:194:LEU:HA	21:V3:197:GLU:HB2	1.82	0.60
24:Y3:174:GLY:HA3	24:Y3:209:LEU:HD21	1.83	0.60
40:f3:163:SER:HB2	40:f3:166:PHE:HB3	1.82	0.60
2:A3:1930:C:H5''	2:A3:1931:A:H5'	1.83	0.60
25:Z3:108:ALA:HA	25:Z3:111:LYS:HD2	1.83	0.60
42:h3:133:PRO:HB2	42:h3:135:GLN:HE22	1.66	0.60
43:i3:35:ARG:NH1	43:i3:37:THR:O	2.35	0.60
74:V6:70:LEU:HD11	74:V6:389:LEU:HB3	1.83	0.60
17:R3:112:THR:OG1	36:b3:127:GLN:NE2	2.33	0.60
33:73:107:LEU:HD12	33:73:126:LYS:HD3	1.84	0.60
56:D6:225:VAL:HG12	56:D6:243:VAL:HG12	1.84	0.60
64:L6:102:GLU:HA	64:L6:105:LYS:HE2	1.82	0.60
76:X6:313:THR:OG1	91:X6:500:GDP:O2B	2.19	0.60
17:R3:114:LYS:NZ	35:a3:43:TYR:O	2.34	0.60
12:M3:39:ARG:HE	12:M3:41:ARG:HH11	1.47	0.60
55:C6:44:VAL:HG12	55:C6:167:LEU:HB3	1.84	0.60
56:D6:360:GLN:NE2	56:D6:364:ASP:OD2	2.34	0.60
61:I6:144:VAL:HG13	61:I6:170:LEU:HD11	1.84	0.60
45:k3:85:GLU:OE1	51:r3:36:ARG:NH2	2.35	0.60
2:A3:2073:A:OP2	32:63:27:ARG:N	2.34	0.60
77:Y6:338:LEU:O	77:Y6:377:ARG:NH2	2.34	0.60
2:A3:1747:G:N2	2:A3:1750:G:O2'	2.35	0.59
13:N3:218:ILE:HA	13:N3:223:MET:HG3	1.84	0.59
79:a6:97:LEU:HD21	79:a6:100:VAL:HG13	1.84	0.59
18:S3:114:ILE:HG23	18:S3:193:LEU:HB2	1.82	0.59
36:b3:30:SER:HB2	36:b3:76:VAL:HB	1.84	0.59
79:a6:63:ARG:HA	79:a6:137:HIS:HA	1.84	0.59
80:b6:140:ASP:HA	80:b6:143:CYS:HB3	1.83	0.59
6:F3:279:ARG:NH1	6:F3:280:TYR:O	2.36	0.59
21:V3:45:VAL:HG11	24:Y3:237:LYS:HD3	1.83	0.59
56:D6:366:LYS:O	56:D6:392:ARG:NH2	2.35	0.59
74:V6:230:LEU:HA	74:V6:233:LYS:HG2	1.84	0.59
2:A3:2395:A:O2'	31:53:384:GLN:NE2	2.36	0.59
2:A3:2529:U:O4	4:D3:205:GLN:NE2	2.35	0.59
2:A3:2556:A:OP1	4:D3:287:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F3:85:ASP:HB3	6:F3:274:LEU:HD11	1.84	0.59
61:I6:101:SER:HB3	61:I6:105:GLU:HB2	1.84	0.59
67:O6:181:HIS:HD2	67:O6:183:ALA:H	1.49	0.59
76:X6:272:THR:HG22	76:X6:274:LEU:H	1.67	0.59
10:K3:109:TYR:HD1	10:K3:122:MET:HG3	1.68	0.59
59:G6:255:GLN:HE21	59:G6:370:LEU:HD23	1.67	0.59
2:A3:2130:A:O2'	48:o3:25:ARG:NH1	2.36	0.59
3:B3:1630:A:OP1	47:m3:42:ARG:NH1	2.35	0.59
57:E6:90:ARG:HH22	68:P6:117:MET:HA	1.67	0.59
65:M6:20:ARG:NH1	65:M6:42:PRO:O	2.36	0.59
79:a6:73:LEU:HD22	79:a6:76:LEU:HD13	1.84	0.59
88:n:116:THR:HG22	88:n:118:ASP:H	1.67	0.59
2:A3:2294:A:OP2	12:M3:41:ARG:NH1	2.36	0.59
56:D6:269:ARG:NH2	84:A6:1282:C:OP1	2.34	0.59
41:g3:107:MET:HE1	41:g3:148:ARG:HH11	1.67	0.59
56:D6:193:TRP:HE1	56:D6:322:THR:HG21	1.67	0.59
87:A:50:LEU:HG	87:A:68:LEU:HD23	1.84	0.59
4:D3:130:ARG:NH1	4:D3:131:TYR:O	2.35	0.58
51:r3:40:GLU:HB3	51:r3:49:ILE:HG12	1.86	0.58
84:A6:704:A:N1	84:A6:713:G:O2'	2.35	0.58
2:A3:1889:C:OP1	12:M3:133:LYS:NZ	2.36	0.58
6:F3:92:ARG:HB2	6:F3:176:VAL:HG21	1.86	0.58
13:N3:103:GLU:OE1	13:N3:106:ARG:NH2	2.36	0.58
73:U6:64:ARG:NH2	84:A6:849:A:OP1	2.36	0.58
87:A:68:LEU:HA	87:A:71:LYS:HB2	1.85	0.58
63:K6:40:ARG:HD3	63:K6:86:ARG:HG3	1.84	0.58
79:a6:101:ARG:HH11	84:A6:1532:A:H5'	1.68	0.58
69:Q6:50:ARG:NH1	84:A6:1599:G:O6	2.37	0.58
87:A:133:ARG:HA	87:A:136:ILE:HD12	1.84	0.58
40:f3:78:ARG:NH2	40:f3:86:TYR:O	2.32	0.58
2:A3:1850:U:O2'	2:A3:2098:G:N2	2.36	0.58
8:I3:51:THR:OG1	13:N3:250:ARG:NH2	2.37	0.58
49:p3:75:ARG:HH12	49:p3:109:GLU:H	1.52	0.58
76:X6:387:ASN:HB3	76:X6:390:LEU:HB2	1.86	0.58
2:A3:2727:C:O2'	2:A3:2815:G:N2	2.37	0.58
24:Y3:94:SER:OG	24:Y3:95:ASN:N	2.37	0.58
65:M6:104:ILE:HG23	70:R6:147:ILE:HG21	1.86	0.58
82:d6:132:LYS:NZ	84:A6:943:A:OP1	2.34	0.58
2:A3:2416:U:OP1	52:s3:313:ARG:NH2	2.36	0.58
19:T3:157:ARG:HG3	19:T3:167:MET:HE3	1.85	0.58
52:s3:201:ASP:OD1	52:s3:242:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B6:94:LYS:HE3	75:W6:150:THR:HB	1.84	0.58
56:D6:284:ARG:NH2	56:D6:287:ASP:OD1	2.37	0.58
56:D6:363:ALA:O	56:D6:367:GLY:N	2.37	0.58
59:G6:336:GLY:O	59:G6:340:GLN:NE2	2.37	0.58
76:X6:166:ARG:NH1	84:A6:1386:A:OP1	2.37	0.58
80:b6:56:ARG:H	80:b6:59:LYS:HB2	1.68	0.58
2:A3:2466:A:OP1	16:Q3:235:ARG:NH2	2.37	0.57
5:E3:221:ARG:NH1	5:E3:257:MET:O	2.34	0.57
39:e3:160:LEU:HD13	39:e3:171:TRP:HE1	1.68	0.57
71:S6:29:PRO:HG2	71:S6:32:PHE:HB2	1.86	0.57
12:M3:236:LEU:HD22	12:M3:240:TYR:HE2	1.70	0.57
37:c3:260:GLN:HB2	37:c3:270:TYR:HD1	1.69	0.57
75:W6:149:LEU:HD22	75:W6:166:ASN:HB2	1.86	0.57
55:C6:113:ARG:HG2	60:H6:166:GLU:HB3	1.86	0.57
57:E6:27:GLU:OE2	73:U6:170:ARG:NH1	2.37	0.57
57:E6:119:SER:OG	57:E6:120:THR:N	2.37	0.57
74:V6:58:ASP:HA	74:V6:61:PHE:HB2	1.87	0.57
76:X6:346:SER:OG	76:X6:347:ASN:N	2.36	0.57
83:e6:389:SER:O	83:e6:434:GLN:NE2	2.37	0.57
2:A3:1769:C:N4	6:F3:104:LYS:O	2.37	0.57
6:F3:126:LYS:NZ	6:F3:138:HIS:O	2.37	0.57
10:K3:25:MET:HE3	10:K3:149:ARG:HH12	1.68	0.57
73:U6:27:ARG:HB2	84:A6:716:C:H42	1.69	0.57
78:Z6:41:PRO:HG2	78:Z6:44:LYS:HD3	1.87	0.57
2:A3:2425:A:OP1	52:s3:221:HIS:ND1	2.37	0.57
14:O3:134:PRO:HG3	26:03:126:CYS:HB3	1.85	0.57
71:S6:10:GLY:O	71:S6:15:ARG:NH1	2.37	0.57
76:X6:276:ARG:HG3	76:X6:278:ASP:H	1.67	0.57
2:A3:3158:A:O2'	14:O3:11:HIS:O	2.22	0.57
25:Z3:138:CYS:HG	25:Z3:149:TRP:CG	2.23	0.57
76:X6:349:ASN:ND2	76:X6:352:GLU:OE2	2.37	0.57
2:A3:2530:A:H4'	2:A3:2531:U:H5'	1.87	0.57
52:s3:195:LEU:HD21	52:s3:425:LEU:HG	1.86	0.57
85:C:25:G:N2	85:C:42:C:O2	2.38	0.57
2:A3:2595:A:O2'	82:d6:151:ARG:NH1	2.37	0.57
8:I3:47:LEU:HD13	13:N3:226:ILE:HG12	1.86	0.57
31:53:230:LEU:HB3	31:53:289:HIS:HB3	1.86	0.57
56:D6:130:GLN:O	78:Z6:72:ARG:NH2	2.38	0.57
60:H6:113:ARG:NH2	84:A6:1315:C:OP2	2.38	0.57
70:R6:194:GLN:NE2	70:R6:202:ARG:O	2.37	0.57
74:V6:202:ARG:NH2	74:V6:238:GLN:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:24:25:G:N2	85:24:42:C:O2	2.38	0.57
88:n:210:ARG:HD3	88:n:211:SER:HB2	1.85	0.57
13:N3:89:ILE:HD11	13:N3:187:ALA:HB1	1.86	0.57
16:Q3:246:ASP:OD1	16:Q3:246:ASP:N	2.38	0.57
20:U3:80:ARG:NH2	20:U3:84:ASN:O	2.37	0.57
43:i3:68:LYS:HZ3	50:q3:33:ARG:HE	1.53	0.57
43:i3:86:ASN:H	43:i3:89:GLN:HB2	1.69	0.57
73:U6:121:ILE:HA	73:U6:124:LEU:HB2	1.87	0.57
76:X6:179:ASP:HB2	76:X6:288:ALA:HB3	1.87	0.57
76:X6:397:TYR:HB2	76:X6:398:LEU:HD12	1.85	0.57
2:A3:2943:G:H5''	48:o3:13:PRO:HB3	1.85	0.56
49:p3:97:SER:O	49:p3:146:ASN:ND2	2.38	0.56
70:R6:172:ILE:HD13	70:R6:189:ARG:HG3	1.87	0.56
2:A3:2339:G:H5''	28:23:57:ASN:HD22	1.70	0.56
32:63:185:MET:HE3	32:63:186:PRO:HD2	1.87	0.56
61:I6:193:LYS:NZ	84:A6:1575:U:O2	2.38	0.56
70:R6:165:ILE:HB	70:R6:170:ARG:HE	1.69	0.56
80:b6:81:VAL:HG12	80:b6:83:LEU:H	1.70	0.56
84:A6:1072:A:N6	84:A6:1093:U:OP2	2.36	0.56
2:A3:2503:A:HO2'	2:A3:3094:G:HO2'	1.53	0.56
6:F3:252:SER:O	6:F3:256:HIS:ND1	2.38	0.56
52:s3:64:GLU:HA	52:s3:67:GLN:HB2	1.87	0.56
54:B6:137:TYR:O	54:B6:264:ARG:NH2	2.38	0.56
59:G6:94:GLU:HG3	59:G6:96:PRO:HD2	1.86	0.56
66:N6:94:PRO:HB3	72:T6:87:LEU:HD11	1.86	0.56
76:X6:287:LEU:HB2	76:X6:290:VAL:HG12	1.85	0.56
10:K3:21:LEU:HD21	10:K3:31:LEU:HD22	1.87	0.56
32:63:374:GLU:OE1	49:p3:141:ARG:NH2	2.37	0.56
36:b3:28:ARG:NH1	37:c3:177:GLN:OE1	2.38	0.56
40:f3:144:MET:N	40:f3:144:MET:SD	2.79	0.56
66:N6:16:LYS:NZ	84:A6:954:A:OP2	2.35	0.56
2:A3:1837:C:OP1	36:b3:4:ARG:NH2	2.38	0.56
31:53:99:TYR:HA	31:53:270:ILE:HG22	1.86	0.56
83:e6:80:ARG:NH2	83:e6:480:ASP:OD2	2.38	0.56
84:A6:840:A:H2'	84:A6:841:A:H8	1.70	0.56
60:H6:113:ARG:HE	60:H6:115:ILE:HD11	1.69	0.56
2:A3:1697:A:OP2	24:Y3:164:ARG:NH2	2.38	0.56
21:V3:110:PRO:HD3	38:d3:166:GLU:HG2	1.86	0.56
26:03:105:ASN:N	26:03:105:ASN:OD1	2.38	0.56
26:03:167:GLU:HA	26:03:170:GLN:HE21	1.70	0.56
31:53:34:GLY:O	31:53:39:ARG:NE	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s3:246:GLN:OE1	52:s3:353:ARG:NH1	2.39	0.56
58:F6:125:LYS:HA	58:F6:129:ALA:HB3	1.86	0.56
62:J6:61:VAL:HA	62:J6:107:ILE:HA	1.88	0.56
66:N6:101:ALA:HB3	66:N6:104:THR:HB	1.87	0.56
88:n:190:ARG:NH2	96:n:413:HOH:O	2.38	0.56
2:A3:2089:U:H1'	41:g3:104:ASN:HD21	1.71	0.56
2:A3:3017:C:OP2	2:A3:3022:G:N2	2.37	0.56
10:K3:36:SER:O	10:K3:40:GLN:NE2	2.39	0.56
11:L3:96:MET:SD	16:Q3:168:ASN:ND2	2.79	0.56
60:H6:177:LEU:HB3	60:H6:179:GLN:HG2	1.88	0.56
70:R6:153:THR:HA	70:R6:177:PRO:HB3	1.88	0.56
2:A3:1742:G:H5'	29:33:163:THR:HG21	1.88	0.56
6:F3:195:LEU:HD11	6:F3:203:LEU:HD12	1.88	0.56
17:R3:111:LYS:HE3	36:b3:127:GLN:HB3	1.87	0.56
59:G6:381:LYS:NZ	84:A6:1320:U:O2'	2.32	0.56
65:M6:56:PRO:O	65:M6:64:LYS:NZ	2.39	0.56
66:N6:53:ASP:N	66:N6:53:ASP:OD1	2.39	0.56
74:V6:200:GLU:HG3	74:V6:203:ASN:HD22	1.70	0.56
5:E3:248:ILE:HG22	5:E3:250:ARG:H	1.70	0.56
14:O3:37:VAL:HB	14:O3:85:LEU:HD13	1.88	0.56
84:A6:735:A:H3'	84:A6:736:A:H8	1.71	0.56
37:c3:251:SER:OG	37:c3:252:ALA:N	2.39	0.55
65:M6:112:ARG:NH2	67:O6:229:GLY:O	2.39	0.55
2:A3:2521:A:N6	4:D3:202:ARG:O	2.39	0.55
5:E3:293:LYS:HD3	16:Q3:87:THR:HG22	1.88	0.55
6:F3:103:GLN:O	6:F3:107:LYS:NZ	2.33	0.55
36:b3:30:SER:HB3	37:c3:65:ASN:HD22	1.71	0.55
54:B6:246:VAL:HA	54:B6:249:TYR:HB2	1.87	0.55
7:D:165:LYS:HG2	7:D:168:LYS:HD2	1.87	0.55
33:73:148:MET:HE3	33:73:262:ASP:HB3	1.88	0.55
80:b6:97:MET:HE3	80:b6:98:ALA:H	1.72	0.55
82:d6:136:ARG:NH1	84:A6:1147:C:O2	2.40	0.55
7:D:191:ARG:NH2	96:D:401:HOH:O	2.39	0.55
2:A3:2057:C:N4	2:A3:2081:U:O4	2.40	0.55
3:B3:1634:A:H4'	40:f3:108:GLN:HE22	1.71	0.55
4:D3:115:GLU:HB2	4:D3:118:LYS:HD2	1.88	0.55
18:S3:115:LEU:HB3	36:b3:118:PRO:HB2	1.89	0.55
20:U3:50:ARG:NH1	20:U3:68:VAL:O	2.39	0.55
23:X3:24:LEU:HA	23:X3:215:GLN:HE21	1.71	0.55
56:D6:285:TYR:OH	56:D6:374:ARG:NH2	2.39	0.55
72:T6:71:THR:HG21	72:T6:75:PHE:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:1673:U:O2'	19:T3:149:ARG:NH2	2.39	0.55
8:I3:89:VAL:O	8:I3:93:ASN:ND2	2.36	0.55
9:J3:111:LEU:HG	9:J3:154:ARG:HB3	1.87	0.55
37:c3:171:ARG:NH1	37:c3:176:GLU:OE1	2.40	0.55
49:p3:76:LEU:HD13	49:p3:103:PHE:HB3	1.88	0.55
57:E6:109:VAL:HA	68:P6:62:LEU:HD13	1.87	0.55
66:N6:69:LEU:HD11	66:N6:80:GLU:HG3	1.89	0.55
2:A3:2661:U:OP2	5:E3:238:ARG:NH2	2.39	0.55
16:Q3:148:THR:OG1	16:Q3:149:PHE:N	2.39	0.55
67:O6:106:PRO:HD2	67:O6:142:VAL:HA	1.89	0.55
68:P6:94:ARG:HE	68:P6:104:GLN:HG2	1.70	0.55
76:X6:133:GLY:HA3	91:X6:500:GDP:HN22	1.72	0.55
2:A3:2616:A:HO2'	2:A3:3046:C:HO2'	1.53	0.55
2:A3:2658:U:OP1	5:E3:225:LYS:NZ	2.39	0.55
33:73:105:LEU:HD23	33:73:138:VAL:HG23	1.88	0.55
58:F6:177:ARG:NH2	84:A6:1465:A:OP2	2.40	0.55
84:A6:1428:U:OP1	85:C:32:A:O2'	2.23	0.55
2:A3:1705:A:N6	34:93:40:GLY:O	2.38	0.55
2:A3:2987:U:O2'	2:A3:2991:U:OP1	2.23	0.55
14:O3:117:ARG:HD2	19:T3:110:ASP:HB2	1.89	0.55
20:U3:61:TYR:O	24:Y3:63:GLY:N	2.40	0.55
37:c3:258:THR:OG1	37:c3:259:ARG:N	2.39	0.55
75:W6:161:THR:HG22	75:W6:163:LEU:H	1.71	0.55
79:a6:53:ARG:NH1	84:A6:708:U:OP1	2.40	0.55
84:A6:764:A:N1	84:A6:784:C:O2'	2.39	0.55
2:A3:2395:A:H4'	31:53:350:ARG:HH22	1.72	0.55
20:U3:64:PRO:HB2	20:U3:100:ALA:HB3	1.89	0.55
29:33:183:ARG:NH1	32:63:355:LYS:O	2.39	0.55
39:e3:148:SER:HB2	39:e3:151:ARG:HB2	1.88	0.55
41:g3:140:VAL:HG22	48:o3:85:HIS:HD2	1.71	0.55
59:G6:148:HIS:HD2	59:G6:156:GLN:HB2	1.72	0.55
63:K6:80:ARG:NH2	84:A6:1354:G:OP1	2.39	0.55
65:M6:109:ARG:O	65:M6:113:LYS:N	2.36	0.55
2:A3:2122:A:O2'	2:A3:2136:C:OP2	2.25	0.55
2:A3:2472:A:OP1	11:L3:37:ARG:NH2	2.40	0.55
10:K3:27:PRO:HG2	10:K3:30:LYS:HB2	1.89	0.55
14:O3:80:LEU:O	14:O3:83:LYS:NZ	2.40	0.55
32:63:60:ARG:NH2	32:63:64:GLU:OE2	2.39	0.55
35:a3:72:THR:OG1	37:c3:256:ARG:NH1	2.38	0.55
39:e3:77:ILE:HG12	39:e3:81:ARG:HH12	1.71	0.55
51:r3:94:ARG:NH1	51:r3:99:MET:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:I6:152:LYS:NZ	61:I6:178:ASN:OD1	2.39	0.55
63:K6:83:CYS:HB3	63:K6:85:VAL:HG12	1.89	0.55
73:U6:27:ARG:HH22	84:A6:854:U:H1'	1.71	0.55
76:X6:125:LEU:HD21	76:X6:337:LEU:HD22	1.88	0.55
88:n:54:SER:O	88:n:57:ASN:ND2	2.37	0.55
2:A3:1802:A:OP1	21:V3:83:ARG:NH1	2.39	0.54
2:A3:2662:A:OP1	2:A3:3159:A:O2'	2.25	0.54
5:E3:252:TRP:O	5:E3:255:THR:OG1	2.25	0.54
74:V6:197:SER:OG	74:V6:199:GLU:N	2.40	0.54
84:A6:819:C:O2	84:A6:822:C:N4	2.39	0.54
2:A3:2149:G:OP2	17:R3:65:ARG:NH2	2.40	0.54
2:A3:2822:C:O2'	2:A3:2915:C:OP2	2.25	0.54
5:E3:168:LEU:HB3	5:E3:170:LEU:HD13	1.90	0.54
6:F3:293:PHE:HB2	41:g3:55:THR:HG21	1.89	0.54
8:I3:113:ARG:O	8:I3:117:ARG:NH1	2.41	0.54
42:h3:138:SER:OG	42:h3:139:LYS:N	2.40	0.54
79:a6:133:HIS:HB3	79:a6:136:TYR:HB2	1.89	0.54
32:63:194:THR:HG22	32:63:196:THR:H	1.71	0.54
52:s3:243:ILE:HG21	52:s3:429:PRO:HG3	1.89	0.54
70:R6:142:LEU:HD22	70:R6:183:LYS:HE2	1.88	0.54
73:U6:30:ARG:HB2	84:A6:714:U:H2'	1.89	0.54
76:X6:102:ARG:NH1	76:X6:346:SER:O	2.40	0.54
85:C:25:G:H1	85:C:41:G:H1	1.55	0.54
2:A3:1742:G:O2'	2:A3:1754:G:O6	2.24	0.54
65:M6:50:GLN:NE2	65:M6:51:LEU:O	2.36	0.54
74:V6:248:PRO:HB2	79:a6:143:PRO:HB3	1.90	0.54
82:d6:145:LYS:NZ	84:A6:1585:G:O6	2.35	0.54
2:A3:2167:A:N6	2:A3:2212:C:OP2	2.37	0.54
24:Y3:158:THR:OG1	34:93:123:GLN:NE2	2.40	0.54
31:53:162:ARG:HE	31:53:386:PHE:HB3	1.72	0.54
37:c3:97:TYR:HB2	37:c3:181:SER:HA	1.89	0.54
52:s3:75:SER:OG	52:s3:76:VAL:N	2.39	0.54
65:M6:70:LEU:HA	65:M6:73:ILE:HG22	1.89	0.54
67:O6:92:LYS:HA	67:O6:144:VAL:HG12	1.90	0.54
84:A6:1082:A:H5'	85:24:37:A:H5'	1.90	0.54
2:A3:2249:G:OP2	17:R3:65:ARG:NH1	2.40	0.54
2:A3:2673:G:H5''	19:T3:112:LYS:HB2	1.89	0.54
3:B3:1624:C:OP1	32:63:59:ARG:NH1	2.40	0.54
10:K3:20:LEU:HD22	10:K3:141:LEU:HD13	1.90	0.54
13:N3:142:GLY:O	22:W3:38:SER:N	2.40	0.54
31:53:227:GLY:HA3	31:53:293:LEU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d3:123:ARG:HA	38:d3:126:LYS:HB2	1.89	0.54
56:D6:331:ASP:N	56:D6:331:ASP:OD1	2.40	0.54
60:H6:78:VAL:HB	60:H6:143:LEU:HB3	1.90	0.54
68:P6:109:LYS:NZ	84:A6:1036:C:OP1	2.41	0.54
2:A3:1890:C:OP2	29:33:168:ARG:NH2	2.40	0.54
31:53:115:GLU:HB3	31:53:119:GLN:HB2	1.88	0.54
31:53:387:TRP:NE1	31:53:399:GLU:OE2	2.41	0.54
32:63:234:HIS:HE1	32:63:257:PRO:HA	1.72	0.54
39:e3:207:ASN:ND2	87:A:160:GLU:O	2.40	0.54
73:U6:79:GLN:HA	73:U6:82:VAL:HG12	1.90	0.54
88:n:74:VAL:HG11	88:n:153:ILE:HG23	1.90	0.54
59:G6:139:GLN:OE1	59:G6:156:GLN:NE2	2.41	0.54
60:H6:114:LYS:O	60:H6:138:THR:OG1	2.23	0.54
67:O6:52:LYS:HG3	67:O6:58:TYR:HB2	1.90	0.54
67:O6:162:LEU:HA	70:R6:221:GLN:HE22	1.73	0.54
73:U6:129:ARG:O	73:U6:133:GLN:NE2	2.40	0.54
29:33:147:PHE:HB2	32:63:363:LEU:HB2	1.90	0.54
63:K6:41:ARG:NH2	63:K6:89:ASN:OD1	2.40	0.54
67:O6:132:GLY:O	67:O6:158:ARG:NH2	2.41	0.54
71:S6:97:GLN:NE2	71:S6:101:GLU:OE2	2.41	0.54
79:a6:65:LEU:HA	79:a6:68:LEU:HB2	1.89	0.54
87:A:47:SER:HB2	87:A:51:ARG:HD2	1.90	0.54
2:A3:2196:A:O2'	2:A3:2213:A:N1	2.37	0.54
21:V3:80:ILE:HB	21:V3:85:TRP:HB2	1.88	0.54
39:e3:265:LYS:HG3	39:e3:266:PRO:HD3	1.90	0.54
56:D6:191:ARG:NH2	84:A6:886:A:OP1	2.40	0.54
67:O6:118:ARG:HA	67:O6:162:LEU:HD11	1.90	0.54
70:R6:79:LEU:HD23	70:R6:272:VAL:HG23	1.90	0.54
84:A6:958:C:N4	84:A6:1047:C:O2	2.41	0.54
88:n:155:GLU:HB2	88:n:160:ARG:HH11	1.72	0.54
2:A3:1673:U:OP1	19:T3:49:ARG:NH2	2.41	0.53
2:A3:1755:A:O2'	7:H3:63:PRO:O	2.25	0.53
18:S3:135:LEU:HD13	18:S3:144:LEU:HB3	1.91	0.53
40:f3:127:MET:HE2	40:f3:154:GLU:HG3	1.89	0.53
59:G6:105:ASP:OD2	59:G6:126:LYS:NZ	2.42	0.53
85:24:25:G:H1	85:24:41:G:H1	1.55	0.53
2:A3:2194:U:O4	8:I3:109:LYS:NZ	2.39	0.53
5:E3:280:HIS:HB2	5:E3:282:ILE:HD11	1.90	0.53
20:U3:2:ALA:N	20:U3:7:TYR:HH	2.06	0.53
26:O3:119:LYS:O	26:O3:120:HIS:ND1	2.41	0.53
88:n:20:TYR:O	88:n:225:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:n:61:THR:N	94:n:307:CL:CL	2.78	0.53
6:F3:67:GLU:OE1	6:F3:210:ARG:NH1	2.40	0.53
23:X3:212:ILE:O	23:X3:216:ARG:N	2.41	0.53
59:G6:229:LEU:HD21	59:G6:241:VAL:HG11	1.90	0.53
59:G6:299:ASP:OD2	59:G6:301:GLN:NE2	2.41	0.53
31:53:36:ARG:HA	31:53:39:ARG:HG3	1.90	0.53
39:e3:146:ARG:NH1	39:e3:259:GLU:OE2	2.39	0.53
70:R6:168:ARG:NH2	70:R6:236:GLU:OE2	2.42	0.53
84:A6:1064:A:H2'	84:A6:1065:A:H8	1.73	0.53
8:I3:116:LEU:HB3	8:I3:121:ILE:HG23	1.89	0.53
20:U3:57:LEU:O	20:U3:62:ASN:N	2.42	0.53
31:53:332:ASP:N	31:53:332:ASP:OD2	2.42	0.53
52:s3:212:ARG:HD3	52:s3:379:LEU:HD23	1.89	0.53
68:P6:76:ASN:ND2	73:U6:187:TYR:O	2.41	0.53
74:V6:105:ARG:O	74:V6:108:THR:OG1	2.21	0.53
83:e6:451:ASP:O	83:e6:455:ASN:ND2	2.41	0.53
83:e6:508:VAL:HA	83:e6:511:LYS:HD3	1.91	0.53
84:A6:1250:U:H4'	84:A6:1251:G:H5'	1.88	0.53
16:Q3:240:ILE:HG22	16:Q3:242:GLY:H	1.72	0.53
60:H6:78:VAL:HG22	60:H6:173:THR:HG22	1.89	0.53
65:M6:91:LEU:HB3	65:M6:96:PHE:HB3	1.89	0.53
68:P6:82:GLN:NE2	68:P6:133:PRO:O	2.42	0.53
6:F3:63:GLN:HE22	42:h3:97:LYS:HE3	1.74	0.53
6:F3:63:GLN:HG2	6:F3:81:ASP:HB3	1.91	0.53
9:J3:141:VAL:O	9:J3:145:ILE:N	2.42	0.53
31:53:166:THR:OG1	31:53:167:THR:N	2.41	0.53
70:R6:165:ILE:O	70:R6:170:ARG:NH2	2.42	0.53
2:A3:2003:A:OP2	2:A3:2734:A:O2'	2.27	0.53
32:63:261:ARG:HB3	32:63:341:VAL:HG12	1.91	0.53
60:H6:111:PRO:HD2	60:H6:140:TYR:HB2	1.90	0.53
67:O6:215:ARG:NE	79:a6:87:TRP:O	2.40	0.53
80:b6:176:LYS:HG3	80:b6:204:VAL:HB	1.91	0.53
81:c6:9:ARG:NH2	84:A6:1025:U:OP2	2.42	0.53
2:A3:2375:C:O2'	52:s3:276:ARG:NH2	2.39	0.53
2:A3:2618:U:O4	2:A3:3043:C:N4	2.39	0.53
2:A3:3180:A:O3'	51:r3:94:ARG:NH1	2.42	0.53
16:Q3:81:ILE:HD12	16:Q3:82:PRO:HD2	1.91	0.53
62:J6:114:ARG:NH2	84:A6:901:C:OP1	2.41	0.53
81:c6:29:LEU:O	81:c6:113:ASN:ND2	2.42	0.53
2:A3:1882:A:N6	2:A3:1893:A:O4'	2.41	0.53
2:A3:2204:U:O2'	2:A3:2207:A:N7	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:2310:G:OP2	26:03:93:ARG:NH2	2.38	0.53
2:A3:2777:G:H2'	7:D:177:LYS:HE2	1.91	0.53
2:A3:2852:C:O2'	27:13:45:HIS:ND1	2.41	0.53
4:D3:177:ARG:HG3	4:D3:179:GLY:H	1.72	0.53
13:N3:171:GLU:O	46:I3:135:ASN:ND2	2.42	0.53
65:M6:34:ILE:HG13	65:M6:51:LEU:HB2	1.91	0.53
19:T3:126:ASP:HB3	19:T3:130:ARG:HH11	1.75	0.52
20:U3:28:LEU:H	24:Y3:114:THR:HG22	1.74	0.52
20:U3:74:HIS:HB2	34:93:24:LYS:HE3	1.91	0.52
27:13:29:CYS:SG	27:13:30:PHE:N	2.82	0.52
54:B6:129:LEU:HD11	54:B6:252:LEU:HB3	1.90	0.52
74:V6:256:LEU:HD11	74:V6:288:LYS:HE2	1.91	0.52
9:J3:86:THR:HG23	9:J3:89:TYR:H	1.74	0.52
18:S3:100:HIS:HB2	18:S3:134:LEU:HD11	1.91	0.52
76:X6:387:ASN:HD22	76:X6:390:LEU:H	1.56	0.52
84:A6:700:U:H2'	84:A6:701:G:H8	1.73	0.52
26:03:177:ARG:HH22	26:03:179:ARG:HD3	1.73	0.52
61:I6:101:SER:OG	61:I6:102:ALA:N	2.43	0.52
70:R6:157:VAL:HG22	70:R6:174:VAL:HG13	1.91	0.52
81:c6:109:GLN:NE2	84:A6:1296:A:OP1	2.42	0.52
6:F3:221:LEU:HA	6:F3:245:ALA:H	1.74	0.52
36:b3:21:ARG:NH1	37:c3:81:GLU:OE2	2.42	0.52
56:D6:377:CYS:SG	56:D6:378:GLY:N	2.83	0.52
62:J6:102:LEU:HD21	62:J6:132:CYS:HB2	1.90	0.52
65:M6:20:ARG:HB3	84:A6:843:A:H5''	1.91	0.52
2:A3:2593:G:N2	2:A3:2632:A:OP2	2.34	0.52
2:A3:2703:C:OP2	10:K3:118:ARG:NH2	2.40	0.52
5:E3:292:HIS:ND1	5:E3:293:LYS:O	2.39	0.52
14:O3:67:ASP:N	14:O3:67:ASP:OD1	2.43	0.52
17:R3:45:THR:O	17:R3:49:ALA:N	2.40	0.52
39:e3:187:THR:O	39:e3:191:THR:OG1	2.23	0.52
58:F6:146:HIS:HB3	58:F6:150:LYS:HE3	1.92	0.52
68:P6:122:VAL:H	69:Q6:4:HIS:CE1	2.28	0.52
76:X6:69:ASN:OD1	76:X6:69:ASN:N	2.41	0.52
83:e6:472:ASP:OD2	83:e6:472:ASP:N	2.42	0.52
7:D:207:LYS:HD2	7:D:224:THR:HG23	1.91	0.52
39:e3:138:THR:HA	39:e3:141:ASP:HB2	1.91	0.52
66:N6:78:LYS:NZ	84:A6:753:G:O3'	2.39	0.52
70:R6:175:ARG:HE	70:R6:181:LEU:HD13	1.75	0.52
9:J3:31:PRO:HB2	9:J3:34:PRO:HD2	1.91	0.52
16:Q3:100:LEU:HA	16:Q3:103:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e3:55:ARG:HH12	39:e3:58:VAL:HG12	1.75	0.52
61:I6:83:ILE:HG21	61:I6:173:ILE:HD11	1.92	0.52
84:A6:1102:C:OP1	84:A6:1155:C:N4	2.43	0.52
2:A3:1822:U:O2	2:A3:2707:A:O2'	2.27	0.52
7:H3:65:ALA:HB3	7:H3:71:PRO:HA	1.92	0.52
22:W3:68:ALA:HB3	22:W3:89:LEU:HD12	1.92	0.52
23:X3:128:THR:OG1	23:X3:129:MET:N	2.40	0.52
37:c3:182:GLU:HG3	37:c3:183:GLU:HG2	1.91	0.52
54:B6:220:VAL:HG12	54:B6:234:TYR:HB2	1.92	0.52
59:G6:133:PRO:O	59:G6:135:GLN:NE2	2.42	0.52
62:J6:31:ALA:N	84:A6:938:G:O6	2.43	0.52
71:S6:102:LYS:HA	71:S6:105:GLU:HG3	1.91	0.52
71:S6:123:LYS:HD3	71:S6:126:LEU:HD21	1.92	0.52
80:b6:184:ASP:OD1	80:b6:184:ASP:N	2.42	0.52
4:D3:211:GLY:H	4:D3:247:VAL:HG23	1.74	0.52
6:F3:277:ASP:OD1	6:F3:277:ASP:N	2.37	0.52
22:W3:49:ARG:HB3	22:W3:51:GLN:HG3	1.91	0.52
54:B6:234:TYR:OH	71:S6:38:PHE:O	2.27	0.52
58:F6:147:GLN:HA	58:F6:150:LYS:HD2	1.90	0.52
64:L6:67:PRO:HD3	64:L6:107:LYS:HD3	1.92	0.52
83:e6:138:PRO:HB2	83:e6:140:LEU:HG	1.92	0.52
10:K3:16:ARG:NH2	19:T3:199:TYR:OH	2.42	0.52
54:B6:201:ASN:ND2	84:A6:1298:A:OP1	2.43	0.52
84:A6:1510:U:OP2	84:A6:1543:C:N4	2.43	0.52
2:A3:1747:G:H5''	23:X3:96:LYS:HE2	1.91	0.51
10:K3:154:ARG:NH2	10:K3:157:GLU:OE2	2.43	0.51
13:N3:213:TRP:HB3	13:N3:218:ILE:HD11	1.92	0.51
23:X3:4:HIS:O	43:i3:101:ARG:NH1	2.38	0.51
52:s3:96:GLN:NE2	52:s3:301:LEU:O	2.43	0.51
52:s3:246:GLN:NE2	52:s3:354:PRO:O	2.43	0.51
57:E6:13:MET:HG3	57:E6:18:THR:HG22	1.92	0.51
84:A6:757:A:H2'	84:A6:758:A:H8	1.74	0.51
84:A6:1075:U:H2'	84:A6:1076:G:H8	1.74	0.51
84:A6:1363:U:H2'	84:A6:1364:G:H8	1.75	0.51
85:C:26:C:O2	85:C:41:G:N2	2.44	0.51
2:A3:2373:A:OP1	20:U3:50:ARG:NH2	2.42	0.51
4:D3:216:LEU:HD11	4:D3:224:ALA:HB1	1.91	0.51
12:M3:36:PRO:O	12:M3:38:ARG:NH2	2.40	0.51
31:53:354:PHE:HB2	31:53:377:ASP:HB3	1.92	0.51
62:J6:82:ARG:HD2	62:J6:92:VAL:HG22	1.91	0.51
64:L6:200:HIS:NE2	84:A6:765:A:OP2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:M6:105:THR:O	65:M6:109:ARG:N	2.41	0.51
85:C:25:G:H22	85:C:41:G:H1	1.58	0.51
27:13:54:VAL:HG13	50:q3:128:MET:HE3	1.91	0.51
33:73:240:ILE:HG23	33:73:252:VAL:HG21	1.91	0.51
60:H6:147:HIS:O	80:b6:133:TRP:NE1	2.44	0.51
61:I6:91:SER:OG	61:I6:92:HIS:N	2.42	0.51
8:I3:167:ILE:O	8:I3:170:THR:OG1	2.26	0.51
32:63:166:THR:OG1	32:63:167:PHE:N	2.43	0.51
32:63:230:ALA:HA	32:63:299:ARG:HG2	1.91	0.51
36:b3:62:VAL:HG21	37:c3:71:GLU:HG3	1.93	0.51
39:e3:64:THR:HG23	39:e3:67:GLN:H	1.75	0.51
39:e3:205:LEU:HD21	39:e3:237:LEU:HD13	1.91	0.51
67:O6:177:PHE:HA	70:R6:168:ARG:HE	1.76	0.51
74:V6:219:VAL:O	74:V6:223:SER:OG	2.29	0.51
74:V6:358:GLN:HA	74:V6:361:LYS:HD2	1.92	0.51
75:W6:108:VAL:HG23	75:W6:113:TYR:HE1	1.76	0.51
2:A3:3205:C:OP2	5:E3:298:LYS:NZ	2.35	0.51
10:K3:112:LEU:HD13	10:K3:121:MET:HE3	1.92	0.51
11:L3:73:ILE:HG13	11:L3:84:ALA:HB3	1.93	0.51
31:53:208:THR:OG1	52:s3:160:ARG:NH2	2.42	0.51
45:k3:64:VAL:HG13	45:k3:76:MET:HB2	1.91	0.51
59:G6:373:ASP:OD1	59:G6:373:ASP:N	2.44	0.51
68:P6:88:THR:HG23	68:P6:90:CYS:H	1.74	0.51
81:c6:38:ARG:HD2	81:c6:39:GLU:HB2	1.91	0.51
4:D3:184:LEU:HD11	4:D3:226:ILE:HD11	1.92	0.51
25:Z3:68:ILE:HD11	25:Z3:122:LEU:HD13	1.92	0.51
32:63:206:TYR:OH	32:63:242:GLY:O	2.23	0.51
40:f3:134:VAL:HG21	40:f3:146:LEU:HG	1.91	0.51
52:s3:67:GLN:HG2	52:s3:346:TRP:HH2	1.76	0.51
54:B6:97:CYS:SG	54:B6:226:ASN:ND2	2.82	0.51
72:T6:78:PHE:HB2	72:T6:86:VAL:HB	1.91	0.51
76:X6:324:LEU:HD22	80:b6:304:GLU:HB3	1.92	0.51
76:X6:348:TYR:HB2	76:X6:386:ALA:HB1	1.92	0.51
85:24:25:G:H22	85:24:41:G:H1	1.57	0.51
2:A3:2860:G:O2'	22:W3:63:ALA:O	2.25	0.51
14:O3:113:ARG:HG3	14:O3:120:MET:HE2	1.92	0.51
22:W3:103:VAL:HG22	22:W3:127:TYR:HE1	1.76	0.51
41:g3:88:ARG:NH1	41:g3:92:HIS:O	2.41	0.51
47:m3:70:GLU:O	47:m3:72:ARG:N	2.38	0.51
52:s3:174:LEU:HD12	52:s3:301:LEU:HD21	1.92	0.51
56:D6:401:VAL:HB	72:T6:9:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:M6:106:ASN:HA	65:M6:109:ARG:HB2	1.92	0.51
72:T6:105:ILE:HG22	72:T6:106:LEU:HG	1.92	0.51
2:A3:1977:U:H2'	2:A3:1978:A:H8	1.75	0.51
2:A3:3157:C:O2'	16:Q3:84:ARG:O	2.24	0.51
51:r3:85:ASP:OD1	51:r3:85:ASP:N	2.37	0.51
52:s3:105:TRP:HA	52:s3:264:ILE:HD11	1.91	0.51
58:F6:109:SER:HA	58:F6:112:ILE:HD12	1.92	0.51
2:A3:2064:A:H62	40:f3:48:TYR:N	2.09	0.51
16:Q3:182:ARG:HB3	16:Q3:187:LEU:HD21	1.92	0.51
21:V3:68:LYS:O	21:V3:92:ASN:ND2	2.44	0.51
36:b3:56:ARG:NH2	42:h3:147:ASN:O	2.43	0.51
66:N6:93:ASP:OD1	72:T6:71:THR:OG1	2.27	0.51
76:X6:154:HIS:ND1	76:X6:261:ALA:O	2.35	0.51
80:b6:56:ARG:HD2	80:b6:80:ALA:HA	1.93	0.51
87:A:68:LEU:O	87:A:72:ILE:N	2.44	0.51
2:A3:1784:A:H62	2:A3:1793:G:H21	1.58	0.51
2:A3:2938:A:O2'	85:24:73:A:O2'	2.28	0.51
2:A3:3046:C:H2'	2:A3:3047:G:H8	1.76	0.51
12:M3:261:ASP:OD2	49:p3:41:SER:OG	2.23	0.51
14:O3:106:ARG:HD3	14:O3:126:LYS:HE2	1.93	0.51
33:73:37:PRO:HA	33:73:40:LEU:HD13	1.93	0.51
41:g3:138:THR:OG1	41:g3:139:GLN:N	2.43	0.51
41:g3:139:GLN:HE21	48:o3:85:HIS:HA	1.76	0.51
56:D6:127:ASN:HD21	78:Z6:72:ARG:HD3	1.76	0.51
63:K6:85:VAL:HG22	84:A6:1237:C:H42	1.74	0.51
74:V6:212:GLY:O	74:V6:224:GLN:NE2	2.44	0.51
76:X6:357:ILE:HD11	76:X6:377:LYS:HG2	1.93	0.51
81:c6:11:ALA:HB2	81:c6:19:PRO:HB3	1.93	0.51
84:A6:1267:G:H21	84:A6:1336:A:H62	1.58	0.51
2:A3:2310:G:O2'	2:A3:2675:G:O6	2.25	0.50
2:A3:2553:G:N2	4:D3:280:GLY:O	2.43	0.50
2:A3:2594:U:H2'	2:A3:2595:A:H8	1.77	0.50
15:P3:62:ARG:HD3	22:W3:80:HIS:HE1	1.74	0.50
37:c3:257:LEU:HD21	37:c3:260:GLN:HB3	1.93	0.50
52:s3:228:ASP:O	52:s3:230:ARG:NH1	2.44	0.50
58:F6:161:ILE:HD12	58:F6:170:VAL:HG21	1.92	0.50
65:M6:33:ARG:HA	65:M6:53:SER:HA	1.93	0.50
67:O6:203:TYR:O	73:U6:59:ARG:NH2	2.40	0.50
76:X6:55:ASP:OD1	76:X6:55:ASP:N	2.43	0.50
84:A6:686:A:H2'	84:A6:687:G:H8	1.75	0.50
85:24:26:C:O2	85:24:41:G:N2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:2278:A:OP1	43:i3:51:ARG:NH1	2.35	0.50
2:A3:2779:C:H1'	2:A3:2780:C:H5''	1.93	0.50
12:M3:111:ASP:OD2	12:M3:111:ASP:N	2.40	0.50
20:U3:109:ASP:OD1	20:U3:109:ASP:N	2.42	0.50
23:X3:189:ASP:HA	23:X3:192:LYS:HB3	1.92	0.50
25:Z3:59:ASP:OD1	25:Z3:59:ASP:N	2.42	0.50
33:73:114:ASP:HB2	33:73:117:LYS:HB2	1.93	0.50
44:j3:53:ASP:OD1	44:j3:55:ARG:NH1	2.44	0.50
52:s3:97:THR:OG1	52:s3:98:PHE:N	2.44	0.50
57:E6:44:GLU:HG2	57:E6:62:GLY:HA2	1.94	0.50
76:X6:164:ASN:ND2	84:A6:1384:G:N3	2.60	0.50
84:A6:770:G:H1	84:A6:779:C:H42	1.59	0.50
2:A3:2139:U:H5''	25:Z3:74:SER:HB3	1.93	0.50
2:A3:2572:C:O2'	85:24:12:U:OP1	2.24	0.50
8:I3:81:LEU:HD21	46:l3:115:ARG:HH21	1.75	0.50
18:S3:78:GLU:HA	18:S3:81:LYS:HG2	1.94	0.50
19:T3:104:ALA:HA	26:o3:116:LEU:HD21	1.93	0.50
22:W3:137:LYS:HD2	22:W3:138:PRO:HD2	1.93	0.50
74:V6:332:GLU:HA	74:V6:335:LYS:HG2	1.92	0.50
2:A3:2131:A:OP1	48:o3:23:ARG:NH2	2.44	0.50
21:V3:146:VAL:HG22	21:V3:153:ILE:HG22	1.92	0.50
50:q3:48:PRO:HG2	50:q3:51:GLN:HG3	1.94	0.50
60:H6:126:ILE:HG22	60:H6:127:TYR:H	1.76	0.50
69:Q6:30:LEU:HD22	69:Q6:35:LEU:HD22	1.93	0.50
72:T6:95:ASN:HA	72:T6:98:ILE:HD12	1.93	0.50
76:X6:262:VAL:O	76:X6:308:SER:OG	2.26	0.50
2:A3:2017:U:O2'	2:A3:2723:A:N1	2.41	0.50
5:E3:50:ASP:HA	5:E3:53:LEU:HD13	1.93	0.50
14:O3:155:ASP:OD1	14:O3:158:GLN:NE2	2.44	0.50
41:g3:118:TRP:NE1	41:g3:142:GLU:OE2	2.39	0.50
50:q3:78:SER:O	50:q3:78:SER:OG	2.28	0.50
60:H6:83:HIS:H	60:H6:168:VAL:HG12	1.76	0.50
85:24:53:C:H2'	85:24:54:U:H2'	1.94	0.50
10:K3:68:SER:OG	10:K3:71:LYS:NZ	2.37	0.50
12:M3:153:ASN:HB2	12:M3:256:LEU:HD22	1.94	0.50
17:R3:89:ASN:HD22	17:R3:92:LYS:HD2	1.76	0.50
18:S3:124:CYS:HG	36:b3:22:TYR:HH	1.59	0.50
33:73:149:MET:HG3	33:73:209:LEU:HD23	1.94	0.50
33:73:150:MET:HE2	33:73:280:VAL:HG22	1.93	0.50
56:D6:412:LYS:HB3	56:D6:418:LYS:HG2	1.94	0.50
62:J6:61:VAL:HG22	62:J6:107:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:O6:163:LEU:O	70:R6:223:ARG:NH1	2.45	0.50
79:a6:24:GLN:O	79:a6:27:ARG:NH2	2.44	0.50
4:D3:113:ARG:O	4:D3:147:ARG:NH1	2.30	0.50
10:K3:175:ASP:OD1	10:K3:175:ASP:N	2.34	0.50
12:M3:24:LEU:HD13	12:M3:27:LEU:HD21	1.93	0.50
12:M3:148:PHE:O	12:M3:170:ASN:ND2	2.42	0.50
12:M3:286:THR:OG1	41:g3:38:PHE:O	2.29	0.50
15:P3:103:SER:OG	32:63:150:ARG:NH1	2.45	0.50
19:T3:113:GLY:HA2	19:T3:116:ILE:HD12	1.94	0.50
24:Y3:69:ASP:N	24:Y3:69:ASP:OD1	2.36	0.50
26:03:123:CYS:HB3	26:03:126:CYS:HB2	1.93	0.50
57:E6:3:ARG:HB3	57:E6:96:HIS:HB2	1.93	0.50
59:G6:310:ARG:HH22	76:X6:390:LEU:HD22	1.77	0.50
70:R6:107:THR:OG1	70:R6:108:GLN:N	2.44	0.50
71:S6:80:SER:O	71:S6:82:GLN:NE2	2.45	0.50
85:C:53:C:H2'	85:C:54:U:H2'	1.94	0.50
2:A3:1865:C:OP2	17:R3:17:ARG:NH1	2.45	0.50
2:A3:2420:U:H2'	2:A3:2421:G:H8	1.77	0.50
2:A3:2446:A:N6	52:s3:82:ILE:O	2.44	0.50
8:I3:100:GLN:HA	8:I3:151:ASN:HA	1.93	0.50
23:X3:167:LEU:HD21	31:53:55:LEU:HB3	1.94	0.50
31:53:69:TRP:HD1	31:53:70:LEU:HG	1.75	0.50
31:53:213:TRP:HD1	31:53:364:LEU:HG	1.77	0.50
41:g3:89:SER:HG	41:g3:93:ASN:H	1.59	0.50
60:H6:63:VAL:HG11	83:e6:63:LYS:HE2	1.93	0.50
60:H6:133:GLN:NE2	84:A6:1456:U:OP1	2.44	0.50
70:R6:221:GLN:HB2	70:R6:223:ARG:HG3	1.94	0.50
73:U6:192:THR:OG1	73:U6:193:ARG:N	2.45	0.50
76:X6:164:ASN:HD22	84:A6:1384:G:H21	1.59	0.50
78:Z6:73:ASP:N	78:Z6:73:ASP:OD1	2.40	0.50
84:A6:1269:C:H2'	84:A6:1270:A:H8	1.77	0.50
2:A3:2537:G:O2'	2:A3:2634:U:OP2	2.30	0.50
9:J3:66:LEU:HD12	9:J3:67:PRO:HD2	1.94	0.50
11:L3:128:ARG:HB2	16:Q3:125:TYR:HB3	1.94	0.50
32:63:161:LEU:O	32:63:300:THR:OG1	2.29	0.50
69:Q6:67:GLU:OE2	69:Q6:70:ARG:NH1	2.38	0.50
73:U6:173:LEU:HG	73:U6:174:GLU:HG3	1.94	0.50
76:X6:153:LEU:HD22	76:X6:260:VAL:HG23	1.94	0.50
79:a6:136:TYR:CZ	84:A6:709:C:H2'	2.46	0.50
2:A3:2421:G:H5''	34:93:24:LYS:HG2	1.93	0.49
14:O3:85:LEU:O	14:O3:89:LEU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X3:114:PHE:HE2	23:X3:127:VAL:HG11	1.77	0.49
25:Z3:71:ARG:NH1	25:Z3:91:LEU:O	2.43	0.49
25:Z3:75:THR:HB	25:Z3:83:LYS:HG2	1.94	0.49
27:13:18:VAL:HG12	27:13:61:LYS:HB3	1.93	0.49
31:53:125:LYS:HE3	31:53:364:LEU:HD13	1.93	0.49
32:63:160:ASP:OD2	32:63:267:ARG:NH2	2.44	0.49
41:g3:154:ASP:OD1	41:g3:154:ASP:N	2.42	0.49
65:M6:110:LEU:O	65:M6:114:ARG:N	2.43	0.49
69:Q6:78:LYS:HE3	75:W6:162:VAL:HG12	1.94	0.49
74:V6:41:GLU:HA	74:V6:43:ARG:HG3	1.93	0.49
2:A3:2177:U:O2'	2:A3:2179:A:N6	2.45	0.49
49:p3:56:ASP:OD1	49:p3:56:ASP:N	2.39	0.49
49:p3:104:HIS:HA	49:p3:132:GLU:HA	1.94	0.49
74:V6:107:TRP:HB3	74:V6:382:TRP:CD2	2.47	0.49
76:X6:72:PRO:HA	76:X6:75:LEU:HD23	1.94	0.49
2:A3:3000:A:H2'	2:A3:3001:G:C8	2.47	0.49
10:K3:8:PRO:HG2	37:c3:295:GLU:HG3	1.94	0.49
32:63:122:ALA:O	32:63:127:THR:N	2.45	0.49
37:c3:263:GLY:H	37:c3:268:PRO:HB3	1.77	0.49
49:p3:96:ASN:N	49:p3:96:ASN:OD1	2.43	0.49
55:C6:75:ASN:ND2	63:K6:121:SER:O	2.40	0.49
58:F6:146:HIS:O	58:F6:150:LYS:N	2.41	0.49
66:N6:11:ARG:NH1	72:T6:81:ASP:OD2	2.45	0.49
67:O6:151:THR:HA	67:O6:154:ILE:HG22	1.93	0.49
77:Y6:321:PHE:HB2	80:b6:164:ARG:HH12	1.77	0.49
83:e6:472:ASP:O	83:e6:476:LYS:N	2.45	0.49
2:A3:3220:A:OP1	5:E3:260:LYS:NZ	2.45	0.49
9:J3:102:ARG:NH1	52:t3:18:UNK:O	2.46	0.49
14:O3:155:ASP:HA	14:O3:158:GLN:HG2	1.94	0.49
25:Z3:102:ASN:OD1	25:Z3:107:ASN:ND2	2.41	0.49
33:73:64:LYS:NZ	38:d3:276:ILE:O	2.45	0.49
34:93:86:LEU:HD21	34:93:91:LEU:HD13	1.95	0.49
51:r3:113:ARG:HA	51:r3:116:GLU:HG2	1.93	0.49
32:63:176:ALA:HA	32:63:186:PRO:HA	1.94	0.49
67:O6:202:TRP:CD1	67:O6:202:TRP:H	2.30	0.49
71:S6:87:LEU:HD23	75:W6:88:PRO:HB2	1.95	0.49
88:n:63[A]:SER:HA	88:n:160:ARG:HA	1.94	0.49
4:D3:124:GLU:OE1	4:D3:149:ARG:NE	2.43	0.49
12:M3:51:ARG:HB3	12:M3:58:GLN:HA	1.95	0.49
12:M3:185:ASP:OD1	12:M3:185:ASP:N	2.43	0.49
16:Q3:283:TRP:HA	16:Q3:286:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:H6:77:SER:HA	60:H6:144:GLU:HA	1.94	0.49
63:K6:86:ARG:O	84:A6:1238:C:O2'	2.29	0.49
73:U6:169:THR:OG1	73:U6:170:ARG:N	2.46	0.49
80:b6:70:TYR:OH	80:b6:76:PHE:O	2.31	0.49
84:A6:1024:C:H42	84:A6:1034:G:H1	1.61	0.49
84:A6:1225:A:H3'	84:A6:1226:A:H2'	1.94	0.49
88:n:63[B]:SER:HA	88:n:160:ARG:HA	1.93	0.49
2:A3:1888:G:OP1	12:M3:189:LYS:NZ	2.40	0.49
2:A3:2277:U:O2	6:F3:104:LYS:NZ	2.41	0.49
12:M3:23:SER:OG	12:M3:24:LEU:N	2.46	0.49
12:M3:175:THR:HA	12:M3:220:ARG:HB3	1.94	0.49
40:f3:100:MET:HG2	47:m3:45:ARG:HH12	1.78	0.49
49:p3:104:HIS:HD2	49:p3:106:ALA:H	1.61	0.49
52:s3:418:LEU:HA	52:s3:421:ILE:HD12	1.94	0.49
59:G6:299:ASP:N	59:G6:299:ASP:OD1	2.43	0.49
65:M6:42:PRO:HD3	84:A6:717:C:H5'	1.95	0.49
67:O6:79:ARG:HH22	67:O6:86:PRO:HB2	1.78	0.49
2:A3:1791:G:N7	28:23:87:ARG:NH2	2.61	0.49
13:N3:53:ILE:HD11	13:N3:127:PRO:HD3	1.95	0.49
56:D6:314:LEU:HD13	56:D6:321:ILE:HA	1.94	0.49
70:R6:271:MET:HE1	70:R6:284:LEU:HD13	1.95	0.49
73:U6:64:ARG:HA	73:U6:67:VAL:HG22	1.94	0.49
84:A6:811:A:O2'	84:A6:813:G:N7	2.46	0.49
2:A3:2585:G:O2'	85:24:23:A:O2'	2.28	0.49
2:A3:3063:G:O2'	2:A3:3066:C:OP2	2.29	0.49
5:E3:318:THR:OG1	5:E3:319:TYR:N	2.46	0.49
18:S3:97:ALA:N	18:S3:108:VAL:O	2.44	0.49
21:V3:129:LYS:HD3	21:V3:130:PRO:HD2	1.95	0.49
25:Z3:129:PRO:HG3	25:Z3:147:VAL:HG12	1.95	0.49
60:H6:123:SER:OG	60:H6:124:VAL:N	2.46	0.49
62:J6:110:VAL:HG11	62:J6:123:LEU:HD13	1.94	0.49
2:A3:3128:A:O2'	2:A3:3129:A:O4'	2.31	0.49
21:V3:145:ARG:NH1	21:V3:155:PRO:O	2.45	0.49
41:g3:146:THR:OG1	41:g3:147:LEU:N	2.44	0.49
67:O6:83:GLY:O	84:A6:672:U:O2'	2.30	0.49
70:R6:142:LEU:HB3	70:R6:181:LEU:HD23	1.95	0.49
84:A6:1260:A:N6	84:A6:1340:G:O6	2.46	0.49
2:A3:2418:A:H5'	20:U3:51:VAL:HG13	1.95	0.48
5:E3:106:MET:HG2	5:E3:120:THR:HG22	1.94	0.48
5:E3:124:VAL:HB	5:E3:281:ASN:HB3	1.95	0.48
36:b3:133:PHE:HB3	37:c3:259:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:f3:147:ASP:N	40:f3:147:ASP:OD1	2.45	0.48
59:G6:276:ARG:NH1	59:G6:373:ASP:OD2	2.38	0.48
74:V6:41:GLU:HG2	74:V6:43:ARG:HH21	1.78	0.48
9:J3:91:LEU:HD11	9:J3:120:ILE:HD13	1.94	0.48
16:Q3:165:GLU:HB2	16:Q3:168:ASN:HB2	1.96	0.48
21:V3:124:ASP:N	21:V3:129:LYS:O	2.46	0.48
54:B6:84:LEU:HD12	54:B6:89:VAL:HG11	1.94	0.48
71:S6:67:GLU:OE2	75:W6:85:ARG:NH2	2.46	0.48
79:a6:90:ASP:N	79:a6:90:ASP:OD1	2.44	0.48
6:F3:59:ARG:NH2	41:g3:114:GLU:OE1	2.46	0.48
10:K3:10:GLN:NE2	19:T3:203:LEU:O	2.45	0.48
20:U3:10:TYR:HD2	34:93:56:MET:HE2	1.78	0.48
21:V3:100:LYS:O	21:V3:102:MET:N	2.46	0.48
29:33:131:LYS:HG3	29:33:132:LYS:HG3	1.95	0.48
42:h3:88:ASP:OD1	42:h3:122:ARG:NH2	2.46	0.48
47:m3:56:LEU:HB2	47:m3:66:ILE:HD13	1.95	0.48
58:F6:122:GLN:HB3	58:F6:139:ARG:HG2	1.95	0.48
70:R6:135:ARG:NH1	70:R6:190:ASP:OD1	2.47	0.48
80:b6:186:ALA:HA	80:b6:189:LYS:HB3	1.94	0.48
80:b6:194:VAL:HG23	80:b6:197:ARG:HH11	1.78	0.48
84:A6:719:G:H1'	84:A6:821:G:H5'	1.94	0.48
88:n:168:THR:OG1	88:n:169:GLY:N	2.46	0.48
2:A3:1672:C:O2'	19:T3:149:ARG:O	2.25	0.48
2:A3:2197:G:H5'	46:l3:123:LYS:HG3	1.94	0.48
2:A3:2292:G:O2'	17:R3:11:ARG:O	2.26	0.48
5:E3:50:ASP:O	14:O3:138:ARG:NH2	2.39	0.48
11:L3:60:VAL:HA	11:L3:73:ILE:HG22	1.95	0.48
12:M3:119:THR:HG21	41:g3:51:LEU:HD22	1.96	0.48
20:U3:27:GLN:HG3	20:U3:43:ARG:HB2	1.95	0.48
39:e3:77:ILE:HG12	39:e3:81:ARG:HH22	1.78	0.48
67:O6:93:THR:OG1	67:O6:96:ARG:NE	2.41	0.48
76:X6:265:ILE:HG22	76:X6:310:LEU:HB3	1.96	0.48
77:Y6:315:ILE:HG21	80:b6:163:VAL:HG21	1.95	0.48
83:e6:336:ASN:O	83:e6:340:LYS:N	2.47	0.48
2:A3:1868:G:H2'	12:M3:40:PRO:HG3	1.95	0.48
2:A3:1892:A:N6	32:63:376:THR:O	2.46	0.48
2:A3:2083:U:O4	2:A3:2084:A:N6	2.46	0.48
2:A3:2241:A:H2'	51:r3:192:TRP:HE3	1.78	0.48
2:A3:3175:A:OP2	30:43:91:TYR:OH	2.29	0.48
8:I3:30:SER:OG	8:I3:31:LYS:N	2.46	0.48
8:I3:188:ARG:HD2	45:k3:55:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J3:145:ILE:HG13	9:J3:155:VAL:HG11	1.95	0.48
10:K3:51:SER:O	19:T3:206:ARG:NH1	2.47	0.48
13:N3:68:ASN:N	13:N3:68:ASN:OD1	2.45	0.48
45:k3:73:ARG:HG2	45:k3:75:ILE:HD11	1.95	0.48
49:p3:151:LEU:O	49:p3:155:ARG:NH1	2.47	0.48
2:A3:2909:G:OP1	29:33:134:TRP:NE1	2.43	0.48
14:O3:108:LEU:HD22	26:03:122:LEU:HD21	1.95	0.48
39:e3:50:ALA:HB2	39:e3:175:GLN:HG2	1.95	0.48
76:X6:164:ASN:N	76:X6:164:ASN:OD1	2.47	0.48
79:a6:17:ARG:O	79:a6:21:LEU:N	2.43	0.48
2:A3:2094:G:OP2	12:M3:57:ARG:NH2	2.47	0.48
2:A3:2138:U:O2'	2:A3:2151:A:N3	2.47	0.48
2:A3:2461:A:H4'	5:E3:235:LYS:HG2	1.94	0.48
6:F3:83:HIS:CE1	6:F3:274:LEU:HD21	2.49	0.48
22:W3:122:LYS:HB2	32:63:49:GLU:HB2	1.95	0.48
23:X3:234:LEU:HD13	23:X3:237:GLN:HG3	1.94	0.48
60:H6:70:ASP:OD1	60:H6:70:ASP:N	2.40	0.48
76:X6:265:ILE:HD11	76:X6:297:MET:HE1	1.96	0.48
84:A6:1561:A:H1'	84:A6:1562:A:H5'	1.96	0.48
2:A3:2294:A:N7	12:M3:39:ARG:NH2	2.61	0.48
2:A3:2457:A:N3	14:O3:17:ARG:NH2	2.62	0.48
6:F3:70:ARG:HA	6:F3:196:PRO:HD3	1.96	0.48
10:K3:115:ASN:OD1	10:K3:115:ASN:N	2.47	0.48
12:M3:285:PRO:HB3	50:q3:76:TRP:HE1	1.79	0.48
14:O3:60:ILE:HG21	14:O3:97:TYR:HD2	1.78	0.48
32:63:187:VAL:HG21	32:63:319:PHE:HD1	1.78	0.48
52:s3:181:VAL:HG13	52:s3:200:LEU:HD21	1.96	0.48
55:C6:85:ARG:NH1	80:b6:159:SER:O	2.47	0.48
76:X6:81:HIS:HB2	76:X6:156:PRO:HB3	1.95	0.48
84:A6:1083:G:O6	84:A6:1084:A:N6	2.47	0.48
87:A:67:ARG:O	87:A:71:LYS:N	2.47	0.48
87:A:70:ARG:HE	87:A:74:LYS:HG3	1.79	0.48
2:A3:2203:G:H1'	2:A3:2209:G:H1	1.78	0.48
2:A3:2761:C:O2'	2:A3:2785:C:N4	2.41	0.48
7:H3:120:ARG:HD3	23:X3:132:LEU:HD22	1.95	0.48
23:X3:161:LEU:HD22	23:X3:165:MET:HE3	1.96	0.48
39:e3:125:GLU:OE2	47:m3:73:ARG:NE	2.45	0.48
40:f3:51:LYS:HG3	40:f3:52:PRO:HD2	1.96	0.48
55:C6:106:ASP:OD1	55:C6:106:ASP:N	2.43	0.48
83:e6:493:MET:HA	83:e6:496:LEU:HG	1.96	0.48
84:A6:1073:A:O2'	84:A6:1591:U:O2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:n:15:ASP:OD1	88:n:223:ARG:NH1	2.47	0.48
8:I3:94:ARG:N	8:I3:156:SER:O	2.41	0.48
12:M3:106:ASP:OD1	12:M3:106:ASP:N	2.44	0.48
18:S3:57:SER:O	51:r3:187:TYR:OH	2.30	0.48
25:Z3:107:ASN:HA	25:Z3:110:LEU:HD12	1.95	0.48
41:g3:87:ARG:HB2	41:g3:112:LYS:HB3	1.96	0.48
54:B6:161:ASP:OD1	54:B6:254:GLN:NE2	2.47	0.48
63:K6:80:ARG:NH1	84:A6:1354:G:OP2	2.47	0.48
73:U6:28:LYS:HE2	84:A6:704:A:H3'	1.96	0.48
11:L3:118:ARG:NH1	11:L3:142:GLN:OE1	2.38	0.47
24:Y3:91:ARG:NH1	24:Y3:148:GLU:OE1	2.47	0.47
31:53:200:ARG:NH2	31:53:234:ASP:OD2	2.47	0.47
31:53:356:VAL:HG23	31:53:375:TRP:HB2	1.95	0.47
32:63:53:SER:OG	32:63:54:PHE:N	2.47	0.47
38:d3:241:ASP:N	38:d3:241:ASP:OD1	2.45	0.47
58:F6:149:LEU:HA	58:F6:152:CYS:HB3	1.95	0.47
60:H6:75:ARG:HA	60:H6:146:GLU:HA	1.95	0.47
76:X6:184:ALA:HB2	76:X6:289:LEU:HD11	1.95	0.47
79:a6:93:CYS:HB2	79:a6:121:LYS:H	1.79	0.47
84:A6:895:C:N4	84:A6:905:G:O2'	2.47	0.47
84:A6:1334:C:H4'	84:A6:1335:A:H3'	1.94	0.47
12:M3:181:PRO:HA	12:M3:184:LEU:HB2	1.96	0.47
33:73:247:ASN:OD1	33:73:247:ASN:N	2.44	0.47
74:V6:197:SER:HG	74:V6:200:GLU:H	1.55	0.47
75:W6:92:MET:O	75:W6:98:LYS:NZ	2.47	0.47
78:Z6:6:GLU:HA	78:Z6:9:PHE:HB3	1.95	0.47
79:a6:129:ARG:NH1	79:a6:204:PRO:O	2.47	0.47
84:A6:1532:A:H2'	84:A6:1533:A:C8	2.49	0.47
2:A3:1809:U:H2'	2:A3:1810:A:H4'	1.96	0.47
2:A3:2278:A:OP2	43:i3:46:ARG:NH2	2.41	0.47
2:A3:2395:A:OP1	31:53:173:ARG:NH2	2.44	0.47
2:A3:2928:C:OP2	2:A3:3073:C:O2'	2.32	0.47
15:P3:157:MET:O	15:P3:161:GLN:N	2.47	0.47
22:W3:106:PRO:HD2	22:W3:117:ILE:HD11	1.95	0.47
23:X3:36:ARG:NH2	23:X3:149:SER:OG	2.48	0.47
31:53:304:LEU:HD23	31:53:309:LEU:HD12	1.95	0.47
31:53:357:PHE:HD1	31:53:374:ALA:HB2	1.79	0.47
36:b3:45:GLU:OE1	36:b3:49:ARG:NH2	2.43	0.47
59:G6:380:LYS:NZ	59:G6:385:GLU:O	2.41	0.47
77:Y6:304:TRP:HB3	77:Y6:309:LYS:HB2	1.96	0.47
12:M3:287:ASP:OD2	41:g3:38:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P3:170:VAL:HG21	49:p3:180:ILE:HD13	1.94	0.47
31:53:360:ASN:N	31:53:372:ASN:OD1	2.43	0.47
33:73:59:THR:O	33:73:61:ARG:NH2	2.47	0.47
33:73:82:ASN:O	33:73:86:SER:OG	2.28	0.47
60:H6:83:HIS:ND1	60:H6:137:ARG:O	2.48	0.47
62:J6:116:GLN:NE2	84:A6:901:C:OP2	2.41	0.47
70:R6:175:ARG:HH11	70:R6:181:LEU:HB2	1.79	0.47
78:Z6:85:LEU:HA	78:Z6:88:LEU:HB2	1.96	0.47
84:A6:1293:G:O2'	84:A6:1301:G:OP2	2.28	0.47
88:n:41:VAL:HG11	88:n:185:LEU:HD11	1.94	0.47
88:n:127:LEU:HB3	88:n:131:LEU:HG	1.96	0.47
2:A3:1814:A:N3	2:A3:1862:U:O2'	2.43	0.47
2:A3:2154:A:OP2	48:o3:30:ARG:NH2	2.43	0.47
2:A3:2299:U:H3'	6:F3:136:ALA:HB2	1.97	0.47
2:A3:2347:C:O2	24:Y3:123:ARG:NH2	2.48	0.47
8:I3:110:LEU:HA	8:I3:113:ARG:HB2	1.96	0.47
33:73:238:ASP:OD1	33:73:238:ASP:N	2.46	0.47
39:e3:170:VAL:HB	39:e3:172:ILE:HG23	1.97	0.47
56:D6:231:MET:HE2	84:A6:1484:A:H1'	1.96	0.47
60:H6:162:ARG:HH22	83:e6:71:LEU:HD13	1.79	0.47
63:K6:90:ARG:NH2	84:A6:1240:C:OP2	2.33	0.47
69:Q6:83:PRO:HB2	69:Q6:84:TRP:CE2	2.49	0.47
71:S6:98:ARG:HD2	71:S6:125:LEU:HD21	1.96	0.47
84:A6:1057:A:N1	84:A6:1104:C:O2'	2.36	0.47
88:n:36:LYS:NZ	96:n:414:HOH:O	2.41	0.47
2:A3:2458:A:O2'	5:E3:215:PHE:O	2.28	0.47
2:A3:3134:C:H3'	2:A3:3135:A:C8	2.49	0.47
10:K3:63:ARG:HE	10:K3:100:PRO:HG3	1.79	0.47
10:K3:136:ASP:N	10:K3:136:ASP:OD1	2.47	0.47
35:a3:37:SER:OG	35:a3:39:LEU:O	2.32	0.47
36:b3:84:VAL:O	36:b3:85:ARG:NH1	2.48	0.47
55:C6:109:VAL:HB	55:C6:120:CYS:HB2	1.96	0.47
56:D6:358:THR:HG23	56:D6:361:GLN:H	1.80	0.47
58:F6:122:GLN:NE2	58:F6:138:GLU:O	2.47	0.47
63:K6:107:SER:OG	63:K6:108:ARG:N	2.46	0.47
70:R6:260:ASP:HA	70:R6:263:ARG:HH11	1.78	0.47
72:T6:149:CYS:SG	72:T6:151:SER:OG	2.72	0.47
75:W6:104:ILE:HD13	75:W6:114:ILE:HG12	1.96	0.47
84:A6:1541:C:O2	84:A6:1542:G:N1	2.48	0.47
2:A3:1891:A:OP1	29:33:118:HIS:NE2	2.38	0.47
2:A3:2073:A:H62	2:A3:2832:A:H2	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:3000:A:H2'	2:A3:3001:G:H8	1.80	0.47
12:M3:161:GLU:HA	12:M3:164:ILE:HD12	1.97	0.47
17:R3:64:MET:HE1	19:T3:210:HIS:HB3	1.97	0.47
31:53:115:GLU:HG3	31:53:118:LYS:HB3	1.97	0.47
31:53:310:ARG:NE	31:53:378:SER:OG	2.45	0.47
32:63:274:LYS:HE3	32:63:314:ALA:HB2	1.96	0.47
38:d3:126:LYS:NZ	38:d3:132:PHE:O	2.48	0.47
39:e3:160:LEU:HD12	39:e3:255:VAL:HG21	1.96	0.47
40:f3:178:LEU:HD12	40:f3:179:PRO:HD2	1.95	0.47
52:s3:90:LYS:NZ	52:s3:278:TYR:O	2.48	0.47
66:N6:40:LEU:HD21	72:T6:13:LEU:HD13	1.97	0.47
75:W6:142:LEU:HB3	75:W6:167:ALA:HB1	1.95	0.47
80:b6:244:THR:HB	80:b6:246:ALA:H	1.79	0.47
84:A6:996:U:O2'	84:A6:998:A:OP2	2.29	0.47
84:A6:1313:A:N6	84:A6:1319:G:O6	2.47	0.47
84:A6:1512:C:N4	84:A6:1545:U:O4	2.47	0.47
88:n:75:LEU:HD21	88:n:103:ILE:HD13	1.97	0.47
2:A3:2127:A:H4'	2:A3:2251:A:C6	2.50	0.47
8:I3:174:LEU:HB3	45:k3:53:ALA:HB3	1.97	0.47
22:W3:145:VAL:HG23	32:63:341:VAL:HG23	1.96	0.47
24:Y3:102:TRP:O	24:Y3:106:LEU:N	2.47	0.47
26:03:90:ASN:OD1	26:03:93:ARG:NH1	2.37	0.47
31:53:121:LEU:HD21	31:53:128:LEU:HB2	1.96	0.47
49:p3:113:GLU:OE1	49:p3:116:ARG:NH2	2.48	0.47
76:X6:368:HIS:HB3	76:X6:371:ALA:HB3	1.97	0.47
2:A3:2187:C:H4'	9:J3:103:GLN:HE21	1.79	0.47
4:D3:197:GLU:HB2	4:D3:240:CYS:HB2	1.97	0.47
12:M3:179:TYR:OH	12:M3:260:LYS:NZ	2.36	0.47
15:P3:56:GLU:HG2	15:P3:61:ALA:HB3	1.97	0.47
21:V3:185:ARG:NH2	21:V3:187:TYR:O	2.46	0.47
76:X6:374:GLU:HG3	76:X6:378:LYS:HE3	1.96	0.47
84:A6:1084:A:O2'	84:A6:1086:A:N7	2.43	0.47
9:J3:51:LYS:O	9:J3:55:GLU:N	2.47	0.47
15:P3:51:ASN:HB3	15:P3:54:ASN:HB2	1.97	0.47
29:33:174:ASP:OD2	29:33:174:ASP:N	2.45	0.47
57:E6:6:LEU:HB3	57:E6:66:VAL:HB	1.97	0.47
75:W6:104:ILE:HD12	75:W6:112:LEU:HD12	1.95	0.47
75:W6:155:GLY:HA3	81:c6:28:ILE:HG23	1.97	0.47
87:A:56:VAL:HG12	87:A:58:PRO:HD3	1.96	0.47
52:s3:202:TYR:HA	52:s3:239:ASN:HB3	1.97	0.46
61:I6:145:ILE:HG23	61:I6:146:HIS:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Q6:63:ILE:HG12	81:c6:4:PRO:HG2	1.97	0.46
75:W6:101:ILE:HG22	75:W6:141:ARG:HB3	1.97	0.46
79:a6:129:ARG:NH2	79:a6:203:TYR:OH	2.46	0.46
84:A6:1485:C:H41	86:i4:25:A:H2'	1.80	0.46
2:A3:2775:A:H5'	2:A3:2776:G:C8	2.51	0.46
15:P3:62:ARG:NH1	22:W3:93:GLU:OE2	2.44	0.46
21:V3:130:PRO:O	21:V3:149:ARG:NH2	2.45	0.46
25:Z3:136:ASN:OD1	25:Z3:136:ASN:N	2.48	0.46
33:73:66:GLU:O	33:73:122:SER:OG	2.31	0.46
39:e3:202:ALA:HB1	39:e3:236:ALA:HB1	1.96	0.46
44:j3:50:SER:OG	44:j3:55:ARG:O	2.34	0.46
54:B6:214:LYS:HE2	84:A6:1284:C:H5''	1.97	0.46
55:C6:117:LEU:HD21	55:C6:151:VAL:HG12	1.97	0.46
55:C6:144:SER:HB2	55:C6:151:VAL:HG22	1.96	0.46
56:D6:252:GLY:O	56:D6:282:ILE:N	2.48	0.46
79:a6:73:LEU:HD13	79:a6:76:LEU:HD22	1.95	0.46
80:b6:199:CYS:SG	80:b6:201:THR:OG1	2.69	0.46
83:e6:275:ALA:O	83:e6:279:TYR:N	2.49	0.46
18:S3:99:VAL:HG22	18:S3:133:VAL:HG12	1.96	0.46
20:U3:54:ARG:NH2	20:U3:66:ALA:O	2.47	0.46
29:33:179:LYS:H	29:33:179:LYS:HG2	1.53	0.46
60:H6:124:VAL:HA	63:K6:108:ARG:HH22	1.79	0.46
76:X6:58:LYS:HA	76:X6:58:LYS:HD2	1.63	0.46
79:a6:99:ARG:HE	84:A6:1530:U:H1'	1.80	0.46
5:E3:62:LYS:O	5:E3:66:SER:OG	2.25	0.46
10:K3:168:ARG:HE	10:K3:170:TRP:CD1	2.33	0.46
19:T3:136:PHE:HB2	19:T3:139:ASN:HB2	1.97	0.46
31:53:53:PRO:HA	31:53:54:GLY:HA2	1.63	0.46
33:73:276:PHE:H	33:73:303:PRO:HA	1.80	0.46
39:e3:52:CYS:HB2	39:e3:173:LEU:HD21	1.97	0.46
56:D6:289:THR:OG1	56:D6:290:ILE:N	2.43	0.46
59:G6:281:ALA:HB1	59:G6:344:ILE:HD13	1.97	0.46
69:Q6:19:VAL:HA	69:Q6:22:ALA:HB3	1.97	0.46
76:X6:168:LEU:HA	76:X6:180:GLN:HG2	1.97	0.46
83:e6:556:LYS:HE2	83:e6:556:LYS:HB3	1.77	0.46
84:A6:661:G:O4'	84:A6:1484:A:O2'	2.31	0.46
87:A:80:GLN:O	87:A:82:LEU:N	2.49	0.46
4:D3:292:MET:N	4:D3:292:MET:SD	2.89	0.46
6:F3:278:SER:H	41:g3:90:ARG:HD2	1.80	0.46
14:O3:57:GLU:OE2	14:O3:105:THR:OG1	2.32	0.46
20:U3:66:ALA:HB3	52:s3:100:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k3:17:ARG:HB2	45:k3:65:ASP:HB3	1.96	0.46
59:G6:365:ARG:HB2	59:G6:370:LEU:HD22	1.96	0.46
60:H6:131:ARG:NH1	84:A6:1455:U:OP1	2.47	0.46
66:N6:96:THR:O	66:N6:98:LYS:N	2.49	0.46
67:O6:105:CYS:HB3	67:O6:143:CYS:H	1.80	0.46
69:Q6:2:ALA:N	84:A6:981:A:OP2	2.48	0.46
75:W6:135:GLN:H	75:W6:138:THR:HG1	1.62	0.46
79:a6:43:ARG:NH2	84:A6:709:C:O2'	2.48	0.46
79:a6:144:LYS:HA	79:a6:147:GLU:HB3	1.97	0.46
2:A3:2643:G:O2'	2:A3:2645:G:OP2	2.28	0.46
9:J3:117:VAL:HA	9:J3:120:ILE:HG12	1.97	0.46
20:U3:75:GLY:H	20:U3:91:ASP:HB3	1.80	0.46
31:53:409:GLU:HA	31:53:412:ARG:HD2	1.98	0.46
32:63:222:ASP:OD2	32:63:267:ARG:NH1	2.48	0.46
39:e3:201:GLU:HG2	39:e3:239:LEU:HD22	1.97	0.46
40:f3:111:HIS:O	40:f3:115:ASN:ND2	2.49	0.46
45:k3:13:VAL:HB	45:k3:68:PHE:HD2	1.80	0.46
61:I6:136:ALA:HB1	61:I6:170:LEU:HD23	1.98	0.46
62:J6:117:ASP:OD1	62:J6:117:ASP:N	2.40	0.46
65:M6:71:ASP:OD1	65:M6:71:ASP:N	2.39	0.46
84:A6:849:A:H2'	84:A6:850:A:C8	2.51	0.46
88:n:56:GLN:NE2	88:n:203:GLY:O	2.47	0.46
2:A3:1800:G:O6	21:V3:41:ARG:NH1	2.42	0.46
2:A3:2187:C:O2'	9:J3:104:THR:O	2.31	0.46
2:A3:2420:U:H4'	34:93:35:GLY:HA2	1.98	0.46
29:33:98:SER:OG	29:33:99:ALA:N	2.48	0.46
58:F6:48:LYS:O	58:F6:52:ARG:NH1	2.49	0.46
60:H6:95:ALA:O	60:H6:156:TYR:OH	2.34	0.46
60:H6:122:GLN:HG2	84:A6:1269:C:H5'	1.97	0.46
63:K6:60:ASN:O	63:K6:68:GLN:NE2	2.48	0.46
72:T6:12:THR:HG23	72:T6:14:GLN:H	1.80	0.46
74:V6:109:ILE:HG21	74:V6:139:PRO:HB3	1.97	0.46
83:e6:501:ASP:OD1	83:e6:537:ARG:NH2	2.47	0.46
2:A3:1882:A:C4	32:63:379:ILE:HD13	2.50	0.46
7:H3:98:LEU:HB3	7:H3:108:ARG:HA	1.97	0.46
15:P3:135:CYS:HA	15:P3:138:ALA:HB3	1.98	0.46
21:V3:172:ASP:HB2	21:V3:176:ASP:HB2	1.97	0.46
31:53:114:LEU:N	31:53:264:ASP:OD2	2.48	0.46
43:i3:57:TYR:OH	50:q3:28:ARG:O	2.24	0.46
60:H6:124:VAL:HG12	63:K6:109:ILE:HD12	1.97	0.46
85:24:45:A:H5''	87:A:51:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:n:72:VAL:O	88:n:157:LYS:NZ	2.45	0.46
2:A3:1851:G:H2'	2:A3:2693:A:N7	2.31	0.46
5:E3:145:LEU:HD23	5:E3:145:LEU:HA	1.80	0.46
13:N3:113:MET:HG3	13:N3:118:MET:HE3	1.97	0.46
33:73:81:MET:SD	38:d3:279:THR:OG1	2.72	0.46
33:73:247:ASN:ND2	33:73:251:ILE:O	2.49	0.46
54:B6:147:ARG:NH1	84:A6:1298:A:OP1	2.49	0.46
59:G6:320:VAL:HG23	59:G6:322:ARG:H	1.81	0.46
71:S6:77:VAL:HG21	71:S6:118:PHE:HZ	1.81	0.46
73:U6:99:ALA:HA	73:U6:102:HIS:HB3	1.97	0.46
79:a6:99:ARG:HH21	79:a6:115:TRP:HE1	1.64	0.46
80:b6:86:ARG:HB3	80:b6:96:PRO:HB2	1.97	0.46
87:A:197:LYS:HD3	87:A:200:THR:HA	1.98	0.46
2:A3:2602:U:OP1	2:A3:3091:G:O2'	2.30	0.46
12:M3:154:ILE:HG23	12:M3:174:VAL:HG12	1.98	0.46
32:63:177:TYR:O	32:63:185:MET:N	2.39	0.46
33:73:95:LEU:HD23	38:d3:281:MET:HE2	1.99	0.46
37:c3:197:ALA:O	37:c3:201:ALA:N	2.39	0.46
38:d3:219:ARG:HA	38:d3:241:ASP:HA	1.98	0.46
39:e3:63:LEU:HD13	39:e3:67:GLN:HB3	1.97	0.46
57:E6:100:GLN:H	57:E6:100:GLN:HG3	1.57	0.46
58:F6:228:LYS:HB3	85:C:39:A:H5''	1.98	0.46
64:L6:224:ARG:HH11	64:L6:225:ARG:HD3	1.81	0.46
74:V6:95:PHE:O	74:V6:98:SER:OG	2.30	0.46
74:V6:362:GLU:O	74:V6:366:THR:OG1	2.26	0.46
2:A3:1804:A:O2'	21:V3:23:MET:SD	2.72	0.45
2:A3:2658:U:O2	11:L3:33:GLN:NE2	2.38	0.45
6:F3:290:TYR:HE1	41:g3:53:PRO:HG2	1.81	0.45
11:L3:90:CYS:SG	11:L3:99:ARG:NH1	2.90	0.45
14:O3:33:LEU:HD21	14:O3:59:LEU:HD22	1.98	0.45
52:s3:326:ALA:HA	52:s3:329:ILE:HG12	1.97	0.45
64:L6:137:ARG:NE	64:L6:141:GLU:OE1	2.48	0.45
76:X6:244:LEU:HA	76:X6:247:LEU:HG	1.98	0.45
82:d6:139:ASN:ND2	84:A6:1145:C:OP1	2.49	0.45
84:A6:1527:A:H2'	84:A6:1528:A:C8	2.52	0.45
2:A3:2598:A:N1	2:A3:2625:C:O2'	2.43	0.45
10:K3:72:TRP:NE1	51:r3:148:ASN:O	2.49	0.45
14:O3:80:LEU:HD13	14:O3:85:LEU:HB2	1.97	0.45
23:X3:27:HIS:CE1	23:X3:200:GLU:HG2	2.51	0.45
33:73:51:GLU:HG2	33:73:54:ARG:HE	1.81	0.45
39:e3:172:ILE:HD12	39:e3:175:GLN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:T6:35:ASN:ND2	72:T6:72:PRO:O	2.45	0.45
76:X6:123:ARG:HE	76:X6:338:ASP:H	1.64	0.45
79:a6:61:GLU:HG2	79:a6:62:SER:H	1.81	0.45
83:e6:465:ILE:HG22	83:e6:474:THR:HG23	1.97	0.45
2:A3:2955:U:H5'	13:N3:178:GLN:HE22	1.81	0.45
12:M3:226:PRO:HG3	49:p3:45:LEU:HD13	1.98	0.45
19:T3:128:ALA:HA	19:T3:132:HIS:HB2	1.99	0.45
20:U3:21:ARG:NH2	24:Y3:143:ASP:OD1	2.38	0.45
21:V3:64:ILE:HD12	21:V3:115:LEU:HD22	1.98	0.45
22:W3:119:ARG:O	32:63:50:LYS:NZ	2.39	0.45
40:f3:97:ALA:HB3	40:f3:103:ALA:HB2	1.98	0.45
43:i3:99:GLY:HA2	43:i3:102:MET:HE3	1.98	0.45
56:D6:220:THR:HG21	56:D6:272:LYS:HG2	1.99	0.45
56:D6:324:CYS:HB3	56:D6:329:ILE:HB	1.98	0.45
60:H6:109:HIS:CE1	60:H6:142:CYS:HG	2.34	0.45
67:O6:228:SER:OG	67:O6:229:GLY:N	2.49	0.45
73:U6:79:GLN:OE1	84:A6:744:G:O2'	2.31	0.45
80:b6:296:VAL:HG22	80:b6:312:TYR:HE1	1.80	0.45
2:A3:1752:U:H5'	29:33:95:THR:HG23	1.99	0.45
8:I3:112:MET:HA	8:I3:115:GLN:HB2	1.97	0.45
28:23:51:ASN:OD1	28:23:51:ASN:N	2.48	0.45
29:33:138:PRO:HA	29:33:141:LYS:HD3	1.98	0.45
42:h3:65:ASP:O	42:h3:67:GLN:N	2.44	0.45
50:q3:96:LEU:O	50:q3:100:GLN:N	2.42	0.45
52:s3:366:TYR:HA	52:s3:400:PRO:HA	1.98	0.45
74:V6:102:TRP:CG	74:V6:103:TYR:H	2.34	0.45
78:Z6:16:ALA:O	78:Z6:21:GLU:N	2.49	0.45
87:A:49:PRO:O	87:A:53:LYS:HG2	2.16	0.45
5:E3:69:ASP:OD2	5:E3:70:LYS:N	2.50	0.45
8:I3:111:LEU:O	8:I3:115:GLN:N	2.50	0.45
10:K3:12:ALA:HA	37:c3:269:LEU:HD11	1.98	0.45
31:53:200:ARG:H	31:53:200:ARG:HG2	1.60	0.45
31:53:333:ALA:HB1	31:53:363:ASP:HA	1.98	0.45
34:93:128:PHE:HA	34:93:134:ASN:HD22	1.82	0.45
52:s3:66:TRP:O	52:s3:69:THR:OG1	2.33	0.45
52:s3:80:LEU:O	52:s3:84:THR:OG1	2.31	0.45
52:s3:192:ASN:HB3	52:s3:195:LEU:HD13	1.98	0.45
64:L6:212:ARG:NH2	82:d6:187:GLU:O	2.49	0.45
65:M6:67:ALA:HB2	70:R6:196:TYR:CZ	2.52	0.45
69:Q6:24:ARG:HD3	69:Q6:24:ARG:HA	1.69	0.45
70:R6:246:HIS:O	70:R6:249:THR:OG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:U6:30:ARG:NH1	84:A6:715:U:O2	2.45	0.45
82:d6:138:MET:HE2	84:A6:1493:G:H4'	1.98	0.45
84:A6:926:C:H2'	84:A6:927:A:C8	2.51	0.45
88:n:142:ALA:HA	94:n:307:CL:CL	2.54	0.45
2:A3:1953:A:O2'	2:A3:2463:A:OP1	2.35	0.45
2:A3:2334:C:OP1	52:s3:221:HIS:NE2	2.49	0.45
2:A3:2585:G:HO2'	85:24:23:A:HO2'	1.59	0.45
6:F3:197:THR:OG1	6:F3:198:GLY:N	2.50	0.45
13:N3:53:ILE:HD11	13:N3:126:ALA:HA	1.98	0.45
20:U3:91:ASP:OD1	20:U3:91:ASP:N	2.34	0.45
33:73:170:PRO:HG2	33:73:180:CYS:HB2	1.99	0.45
36:b3:9:ARG:HG2	36:b3:113:ILE:HG13	1.99	0.45
38:d3:273:LYS:HD3	38:d3:273:LYS:HA	1.72	0.45
50:q3:39:TRP:HE3	50:q3:40:PRO:HD2	1.81	0.45
52:s3:211:VAL:HG23	52:s3:380:THR:HG22	1.98	0.45
56:D6:420:SER:HB2	56:D6:423:SER:HB3	1.98	0.45
58:F6:140:ASN:HA	76:X6:367:GLN:HG3	1.98	0.45
62:J6:54:GLY:O	84:A6:929:U:O2'	2.35	0.45
65:M6:106:ASN:OD1	65:M6:109:ARG:NH1	2.50	0.45
74:V6:69:SER:OG	74:V6:105:ARG:NH2	2.50	0.45
77:Y6:365:SER:OG	77:Y6:368:GLN:OE1	2.33	0.45
83:e6:577:ASN:OD1	83:e6:577:ASN:N	2.45	0.45
84:A6:973:A:H2'	84:A6:974:A:H8	1.81	0.45
2:A3:1886:G:H1	43:i3:61:GLY:HA3	1.82	0.45
6:F3:219:VAL:HG21	6:F3:248:LEU:HD12	1.99	0.45
7:H3:59:TRP:HE3	7:H3:60:TRP:H	1.63	0.45
32:63:234:HIS:CE1	32:63:257:PRO:HA	2.52	0.45
56:D6:228:VAL:HG21	84:A6:1290:A:H4'	1.99	0.45
61:I6:85:ILE:HD11	61:I6:148:ARG:HH11	1.82	0.45
77:Y6:306:LYS:HE2	77:Y6:306:LYS:HB3	1.78	0.45
78:Z6:91:LYS:HE3	78:Z6:91:LYS:HB2	1.86	0.45
79:a6:166:TYR:H	79:a6:171:ARG:NH2	2.15	0.45
79:a6:184:THR:OG1	79:a6:185:SER:N	2.50	0.45
84:A6:700:U:H2'	84:A6:701:G:C8	2.51	0.45
7:D:185:ASN:HB3	7:D:187:GLU:H	1.81	0.45
7:D:185:ASN:ND2	7:D:187:GLU:OE2	2.49	0.45
2:A3:2945:A:N6	2:A3:2977:G:O2'	2.49	0.45
4:D3:154:THR:HA	4:D3:247:VAL:HA	1.99	0.45
16:Q3:117:LEU:HD12	16:Q3:151:LEU:HD21	1.99	0.45
18:S3:144:LEU:HG	35:a3:58:ILE:HB	1.99	0.45
20:U3:36:PRO:HD3	52:s3:270:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X3:97:LEU:H	85:C:73:A:C3'	2.30	0.45
24:Y3:214:GLU:OE2	24:Y3:218:ARG:NH1	2.44	0.45
59:G6:198:ARG:N	59:G6:246:ARG:O	2.49	0.45
73:U6:37:SER:OG	73:U6:38:LYS:N	2.47	0.45
76:X6:246:GLU:HA	76:X6:249:ARG:HD3	1.99	0.45
84:A6:823:A:N3	84:A6:835:U:O2'	2.49	0.45
84:A6:1542:G:O2'	84:A6:1544:A:OP2	2.30	0.45
5:E3:346:THR:OG1	5:E3:347:PHE:N	2.50	0.45
18:S3:129:ARG:HE	18:S3:155:ARG:HG3	1.82	0.45
18:S3:140:ASN:HD22	35:a3:63:PRO:HA	1.80	0.45
20:U3:19:VAL:HG11	20:U3:22:THR:HG23	1.99	0.45
32:63:64:GLU:HB3	32:63:69:HIS:HE1	1.82	0.45
40:f3:99:ASP:HB3	40:f3:102:LEU:HB2	1.98	0.45
58:F6:113:GLN:HA	58:F6:116:GLU:HG2	1.99	0.45
60:H6:92:GLU:HA	60:H6:95:ALA:HB3	1.99	0.45
76:X6:132:THR:OG1	76:X6:345:VAL:O	2.32	0.45
76:X6:275:LYS:HD2	76:X6:279:LYS:HA	1.99	0.45
78:Z6:46:LYS:HG3	78:Z6:49:TYR:HE1	1.82	0.45
80:b6:83:LEU:HB3	80:b6:85:VAL:HG13	1.98	0.45
87:A:73:ARG:HD3	87:A:73:ARG:HA	1.73	0.45
2:A3:1738:U:H5'	43:i3:93:ARG:HH22	1.82	0.45
5:E3:236:THR:HG23	5:E3:239:ARG:HD3	1.99	0.45
8:I3:148:VAL:HG21	45:k3:28:GLU:HG2	1.99	0.45
12:M3:281:LYS:HD2	41:g3:41:SER:HB3	1.99	0.45
23:X3:166:LEU:HD13	23:X3:196:ILE:HG22	1.98	0.45
41:g3:100:ILE:HG22	41:g3:106:GLN:HA	1.99	0.45
84:A6:829:U:O2'	84:A6:831:A:N7	2.39	0.45
2:A3:2826:G:OP1	22:W3:49:ARG:NH2	2.36	0.44
2:A3:3125:A:H62	2:A3:3132:G:H21	1.64	0.44
6:F3:181:LYS:O	6:F3:187:LEU:N	2.49	0.44
9:J3:53:PHE:O	9:J3:57:THR:OG1	2.29	0.44
31:53:175:THR:O	31:53:175:THR:OG1	2.34	0.44
40:f3:64:LYS:HA	40:f3:64:LYS:HD2	1.67	0.44
52:s3:243:ILE:HD11	52:s3:296:HIS:CE1	2.52	0.44
63:K6:51:ARG:NH1	84:A6:1406:A:O5'	2.50	0.44
68:P6:64:LYS:HB3	68:P6:68:CYS:HB2	1.99	0.44
84:A6:757:A:H2'	84:A6:758:A:C8	2.52	0.44
87:A:195:ILE:HD13	87:A:202:VAL:HG21	2.00	0.44
2:A3:2503:A:O2'	2:A3:3094:G:O2'	2.26	0.44
4:D3:197:GLU:OE2	4:D3:202:ARG:N	2.50	0.44
40:f3:171:LEU:O	40:f3:175:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D6:417:MET:N	56:D6:417:MET:SD	2.90	0.44
64:L6:104:LEU:HD21	64:L6:138:SER:HB2	2.00	0.44
64:L6:175:TYR:HB2	66:N6:89:GLY:HA3	1.98	0.44
74:V6:76:ILE:HD11	74:V6:92:LEU:HD21	1.99	0.44
5:E3:207:THR:HB	5:E3:267:THR:HG23	1.98	0.44
20:U3:64:PRO:O	20:U3:100:ALA:N	2.49	0.44
32:63:175:VAL:HG22	32:63:204:VAL:HG12	1.99	0.44
36:b3:66:ASN:HA	42:h3:155:THR:HG23	1.99	0.44
40:f3:93:ILE:HG12	40:f3:186:VAL:HG12	2.00	0.44
54:B6:165:TYR:HD1	59:G6:149:TYR:HA	1.81	0.44
56:D6:312:TYR:HB3	56:D6:331:ASP:HB2	1.98	0.44
72:T6:113:LEU:O	72:T6:117:GLU:N	2.50	0.44
84:A6:695:A:N7	84:A6:720:U:O2'	2.49	0.44
84:A6:708:U:OP1	84:A6:849:A:N6	2.46	0.44
2:A3:2683:C:N4	26:03:83:ASN:OD1	2.38	0.44
14:O3:108:LEU:HD11	14:O3:135:LEU:HD13	1.99	0.44
23:X3:56:ASN:N	23:X3:56:ASN:OD1	2.50	0.44
44:j3:71:GLU:OE1	44:j3:75:ARG:NH2	2.51	0.44
50:q3:79:PRO:HA	50:q3:82:LEU:HB3	1.99	0.44
52:s3:58:ALA:O	52:s3:62:ARG:N	2.49	0.44
56:D6:347:GLN:HE22	84:A6:1288:U:H2'	1.82	0.44
60:H6:69:PRO:HB2	83:e6:59:ILE:HD11	2.00	0.44
63:K6:36:ARG:NH2	84:A6:1241:A:OP1	2.51	0.44
64:L6:150:LYS:HD3	84:A6:1056:C:H5'	2.00	0.44
67:O6:72:PRO:HG2	67:O6:75:ALA:HB2	2.00	0.44
77:Y6:303:GLN:HA	77:Y6:306:LYS:HE2	1.99	0.44
79:a6:171:ARG:NH1	79:a6:188:GLU:OE2	2.50	0.44
2:A3:2458:A:OP2	14:O3:9:ILE:N	2.50	0.44
8:I3:167:ILE:HA	8:I3:170:THR:HG23	2.00	0.44
13:N3:50:LEU:HD21	13:N3:161:VAL:HG21	1.99	0.44
39:e3:44:PRO:HG2	39:e3:227:LEU:HD12	1.99	0.44
56:D6:244:LEU:HD13	56:D6:258:ILE:HG22	1.99	0.44
59:G6:162:MET:HE3	59:G6:162:MET:HB3	1.93	0.44
70:R6:207:PRO:HG2	70:R6:209:ILE:HG22	1.98	0.44
70:R6:289:ILE:HD12	70:R6:294:ILE:HG22	2.00	0.44
72:T6:139:CYS:SG	72:T6:140:ILE:N	2.91	0.44
76:X6:165:CYS:SG	76:X6:166:ARG:N	2.91	0.44
84:A6:1029:A:H2'	84:A6:1030:A:C8	2.53	0.44
2:A3:2028:G:N1	2:A3:2264:A:OP2	2.34	0.44
2:A3:2303:A:H2'	2:A3:2304:G:H8	1.83	0.44
6:F3:190:MET:N	6:F3:261:LEU:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P3:47:PHE:HE1	32:63:225:LEU:H	1.65	0.44
22:W3:50:ARG:O	22:W3:54:LYS:NZ	2.41	0.44
31:53:305:GLN:O	31:53:308:GLN:N	2.50	0.44
36:b3:68:ARG:HA	42:h3:157:SER:HB2	2.00	0.44
39:e3:52:CYS:N	39:e3:234:PHE:O	2.38	0.44
39:e3:260:LEU:HB2	39:e3:264:LEU:HD23	2.00	0.44
56:D6:314:LEU:HD23	56:D6:314:LEU:HA	1.85	0.44
64:L6:177:VAL:HG23	64:L6:180:LYS:HD3	1.99	0.44
74:V6:84:GLU:HA	74:V6:87:HIS:HB2	1.99	0.44
74:V6:120:ASP:OD1	74:V6:120:ASP:N	2.48	0.44
78:Z6:42:LEU:HD13	78:Z6:45:LYS:HD3	2.00	0.44
79:a6:98:THR:HG22	79:a6:116:GLY:HA2	2.00	0.44
80:b6:102:ASN:OD1	80:b6:104:GLU:N	2.49	0.44
81:c6:44:THR:OG1	81:c6:45:CYS:N	2.50	0.44
81:c6:55:CYS:HA	81:c6:58:GLN:HG2	1.99	0.44
82:d6:166:GLN:HE21	82:d6:170:GLU:HG2	1.83	0.44
88:n:9:ALA:HA	88:n:12:GLU:HB2	1.99	0.44
23:X3:210:GLU:HA	31:53:70:LEU:HD21	1.99	0.44
38:d3:161:HIS:O	38:d3:260:ARG:NH1	2.46	0.44
41:g3:96:VAL:HG22	41:g3:110:ILE:HG12	2.00	0.44
51:r3:108:CYS:O	51:r3:112:HIS:N	2.48	0.44
70:R6:119:VAL:O	70:R6:123:LYS:N	2.50	0.44
80:b6:211:ARG:HD2	80:b6:221:TYR:CE2	2.53	0.44
84:A6:773:G:H21	84:A6:776:A:H2	1.65	0.44
84:A6:1110:C:O2'	84:A6:1112:C:OP2	2.34	0.44
2:A3:2148:A:H2'	2:A3:2149:G:C8	2.53	0.44
2:A3:2285:U:H2'	2:A3:2286:A:H8	1.82	0.44
2:A3:2302:U:H2'	2:A3:2303:A:C8	2.53	0.44
2:A3:2528:G:H5''	4:D3:135:ARG:HE	1.83	0.44
4:D3:209:ALA:O	4:D3:212:THR:OG1	2.36	0.44
11:L3:137:VAL:HG13	11:L3:138:LEU:HD12	2.00	0.44
15:P3:131:LEU:HD22	15:P3:164:MET:HE1	2.00	0.44
24:Y3:98:LEU:HD23	24:Y3:98:LEU:HA	1.86	0.44
25:Z3:53:HIS:ND1	48:o3:47:TYR:OH	2.40	0.44
33:73:112:PRO:HB2	33:73:267:PRO:HG2	2.00	0.44
33:73:200:ARG:O	33:73:203:THR:OG1	2.34	0.44
48:o3:15:ARG:HA	48:o3:15:ARG:HD2	1.80	0.44
54:B6:115:ILE:HD13	71:S6:63:ILE:HD12	1.98	0.44
56:D6:427:ARG:HE	67:O6:85:VAL:HG12	1.83	0.44
59:G6:139:GLN:H	59:G6:139:GLN:HG2	1.64	0.44
69:Q6:82:ASP:HB3	69:Q6:85:GLN:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:A:91:PRO:HD2	87:A:94:PHE:HD2	1.82	0.44
2:A3:1696:C:H1'	20:U3:4:ASN:HD22	1.83	0.44
2:A3:2471:G:O2'	2:A3:2654:U:O4	2.34	0.44
2:A3:2962:C:H42	2:A3:3016:G:H22	1.65	0.44
37:c3:186:VAL:HG21	37:c3:191:LEU:HD13	2.00	0.44
45:k3:29:SER:HA	45:k3:32:THR:HG22	2.00	0.44
55:C6:133:TYR:HE1	83:e6:90:GLN:HG3	1.83	0.44
58:F6:119:LYS:NZ	76:X6:398:LEU:O	2.50	0.44
59:G6:300:TYR:OH	76:X6:382:PHE:O	2.32	0.44
59:G6:309:ASP:N	59:G6:309:ASP:OD1	2.51	0.44
61:I6:144:VAL:HG22	61:I6:147:ILE:HD11	1.99	0.44
75:W6:101:ILE:HA	75:W6:141:ARG:HA	2.00	0.44
84:A6:1393:G:H22	84:A6:1420:A:H5''	1.83	0.44
87:A:70:ARG:O	87:A:74:LYS:N	2.44	0.44
5:E3:211:ILE:HG12	5:E3:292:HIS:HB3	2.00	0.43
6:F3:69:LEU:HB3	6:F3:195:LEU:HD23	1.99	0.43
8:I3:99:CYS:O	8:I3:152:MET:N	2.40	0.43
23:X3:217:LEU:HD12	23:X3:217:LEU:HA	1.88	0.43
35:a3:67:ILE:O	37:c3:275:TYR:OH	2.32	0.43
37:c3:82:ASN:OD1	37:c3:82:ASN:N	2.51	0.43
41:g3:139:GLN:NE2	41:g3:140:VAL:O	2.51	0.43
48:o3:54:MET:HB3	48:o3:58:GLN:HB2	2.00	0.43
56:D6:412:LYS:HD2	56:D6:418:LYS:HB3	2.00	0.43
59:G6:320:VAL:HG21	59:G6:352:LEU:HD21	1.99	0.43
70:R6:264:SER:O	70:R6:264:SER:OG	2.34	0.43
84:A6:1082:A:OP1	85:24:36:A:O2'	2.27	0.43
84:A6:1082:A:N6	84:A6:1567:U:OP1	2.51	0.43
2:A3:2795:U:H2'	2:A3:2796:G:H8	1.82	0.43
2:A3:3189:C:H1'	51:r3:154:TRP:HB3	2.00	0.43
4:D3:121:PRO:HB3	4:D3:166:SER:HA	1.99	0.43
6:F3:63:GLN:HA	6:F3:81:ASP:HA	2.00	0.43
16:Q3:249:LEU:HD13	16:Q3:254:MET:HG2	2.00	0.43
21:V3:186:THR:N	24:Y3:92:ASN:O	2.52	0.43
33:73:88:PRO:HD3	33:73:119:LEU:HG	1.99	0.43
39:e3:126:GLN:HA	39:e3:129:LEU:HG	2.00	0.43
62:J6:43:LYS:HG3	84:A6:759:G:H5''	2.00	0.43
68:P6:94:ARG:HH12	84:A6:1024:C:H4'	1.83	0.43
68:P6:103:LYS:HD3	68:P6:103:LYS:HA	1.76	0.43
85:C:19:A:N6	85:C:44:U:O2'	2.51	0.43
88:n:223:ARG:NH2	96:n:403:HOH:O	2.52	0.43
7:H3:87:LYS:HG3	7:H3:88:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K3:122:MET:HE3	10:K3:122:MET:HB3	1.75	0.43
21:V3:105:ARG:HG2	38:d3:170:PRO:HB2	2.00	0.43
22:W3:81:VAL:HG21	22:W3:131:VAL:HG23	2.00	0.43
35:a3:73:LYS:HE2	35:a3:73:LYS:HB3	1.69	0.43
36:b3:56:ARG:HG2	42:h3:149:PRO:HG3	2.00	0.43
39:e3:200:MET:HE3	39:e3:243:PHE:HB2	2.00	0.43
50:q3:78:SER:O	50:q3:80:GLU:N	2.51	0.43
50:q3:147:GLN:O	50:q3:151:GLU:N	2.49	0.43
52:s3:371:CYS:HB2	52:s3:394:TRP:HB2	2.00	0.43
56:D6:127:ASN:ND2	56:D6:130:GLN:OE1	2.51	0.43
59:G6:103:ASP:OD1	59:G6:106:ARG:NH1	2.52	0.43
62:J6:100:HIS:HA	62:J6:127:ARG:HH22	1.82	0.43
67:O6:200:TYR:HB3	67:O6:202:TRP:CE2	2.52	0.43
74:V6:102:TRP:HH2	84:A6:1529:C:H3'	1.83	0.43
80:b6:149:ILE:HA	80:b6:175:VAL:HG12	2.01	0.43
84:A6:688:U:H2'	84:A6:689:A:C8	2.53	0.43
2:A3:2399:A:N7	2:A3:2400:C:N4	2.67	0.43
2:A3:2873:A:H4'	22:W3:90:TYR:CZ	2.53	0.43
14:O3:73:MET:HE3	14:O3:73:MET:HB2	1.85	0.43
15:P3:168:GLY:O	49:p3:184:ASN:ND2	2.46	0.43
17:R3:25:LEU:HA	17:R3:28:ALA:HB3	2.00	0.43
26:O3:159:LEU:HD13	26:O3:174:ILE:HG23	2.01	0.43
40:f3:133:GLU:HA	40:f3:149:VAL:HA	2.01	0.43
43:i3:53:MET:HE3	43:i3:56:VAL:HG11	2.00	0.43
52:s3:109:PHE:HA	52:s3:212:ARG:HG2	2.00	0.43
60:H6:170:MET:SD	60:H6:171:GLU:N	2.91	0.43
67:O6:128:CYS:HG	67:O6:131:THR:HG1	1.63	0.43
75:W6:112:LEU:HD11	75:W6:134:TYR:HB3	2.00	0.43
77:Y6:328:PHE:HB2	80:b6:221:TYR:HB2	1.99	0.43
79:a6:178:ARG:NH1	79:a6:187:GLU:O	2.50	0.43
83:e6:493:MET:HB2	83:e6:527:LEU:HD23	1.99	0.43
87:A:182:ILE:HD12	87:A:182:ILE:HA	1.97	0.43
85:C:8:U:H5'	85:C:47:A:H5'	2.01	0.43
2:A3:1702:A:OP2	28:23:66:TRP:N	2.52	0.43
2:A3:1791:G:O2'	2:A3:2006:C:O2'	2.32	0.43
11:L3:59:HIS:HB3	11:L3:74:LEU:HB2	2.01	0.43
12:M3:276:ASN:HD21	50:q3:66:ALA:H	1.65	0.43
15:P3:157:MET:HA	15:P3:160:LEU:HB3	2.01	0.43
23:X3:159:MET:HB3	23:X3:205:GLY:HA3	2.00	0.43
37:c3:131:SER:HA	37:c3:134:GLN:HB2	2.00	0.43
52:s3:369:PHE:HZ	52:s3:417:VAL:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:C6:77:ASP:H	60:H6:138:THR:HG21	1.84	0.43
56:D6:142:PRO:HA	56:D6:146:VAL:HG21	2.01	0.43
56:D6:336:VAL:HG21	56:D6:345:LEU:HD12	2.01	0.43
58:F6:168:TYR:HB3	58:F6:236:LEU:HD23	2.01	0.43
59:G6:75:LYS:HA	59:G6:78:ILE:HD12	2.00	0.43
69:Q6:38:ASP:O	69:Q6:42:ARG:N	2.51	0.43
74:V6:142:PHE:HD1	74:V6:145:ASN:HD22	1.65	0.43
84:A6:1205:A:H2'	84:A6:1206:G:H8	1.82	0.43
85:24:19:A:N6	85:24:44:U:O2'	2.51	0.43
2:A3:1947:C:H42	2:A3:1969:G:H1	1.66	0.43
2:A3:2937:A:O2'	85:24:73:A:N1	2.43	0.43
2:A3:3190:A:O3'	51:r3:124:ARG:NH2	2.52	0.43
5:E3:183:ASP:OD1	5:E3:183:ASP:N	2.52	0.43
6:F3:107:LYS:HG2	43:i3:74:ILE:HG22	2.00	0.43
40:f3:175:GLN:HG3	87:A:173:LYS:HD2	2.00	0.43
56:D6:155:GLN:HE22	83:e6:108:LEU:HD13	1.84	0.43
56:D6:316:CYS:HB2	56:D6:334:ALA:HB3	2.01	0.43
64:L6:168:LYS:HE2	84:A6:952:U:H5'	2.01	0.43
70:R6:113:GLU:HA	70:R6:116:ARG:HB3	2.01	0.43
74:V6:182:SER:HA	74:V6:185:VAL:HG12	2.00	0.43
79:a6:113:LYS:HD2	79:a6:113:LYS:HA	1.90	0.43
79:a6:118:LEU:HD21	79:a6:120:PHE:HB2	2.01	0.43
83:e6:99:SER:OG	83:e6:518:GLU:O	2.32	0.43
84:A6:1435:G:O2'	84:A6:1461:G:O6	2.34	0.43
87:A:70:ARG:HG3	87:A:74:LYS:HE3	2.01	0.43
2:A3:2127:A:H2'	2:A3:2128:G:H8	1.84	0.43
2:A3:2796:G:H21	7:H3:88:HIS:HE1	1.67	0.43
21:V3:65:LEU:HD23	21:V3:65:LEU:HA	1.87	0.43
33:73:220:GLU:HB2	33:73:251:ILE:HD11	2.01	0.43
39:e3:77:ILE:HG23	39:e3:81:ARG:HH22	1.83	0.43
76:X6:131:GLY:HA3	76:X6:387:ASN:HD21	1.84	0.43
79:a6:99:ARG:NE	84:A6:1530:U:O3'	2.52	0.43
2:A3:1800:G:H22	2:A3:1803:A:H5'	1.83	0.43
2:A3:3122:U:H4'	2:A3:3123:G:H4'	2.01	0.43
6:F3:246:VAL:HG22	43:i3:60:ILE:HG13	2.00	0.43
10:K3:14:PHE:HB3	19:T3:206:ARG:HH21	1.83	0.43
31:53:357:PHE:HA	31:53:374:ALA:HA	2.00	0.43
33:73:138:VAL:O	33:73:142:TYR:N	2.52	0.43
33:73:219:LEU:HA	33:73:219:LEU:HD23	1.80	0.43
33:73:302:LEU:HD23	33:73:302:LEU:HA	1.88	0.43
37:c3:60:ARG:HA	37:c3:63:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:f3:138:GLN:NE2	87:A:194:ASP:O	2.52	0.43
47:m3:55:LEU:HD11	47:m3:63:THR:HB	2.00	0.43
48:o3:93:ASP:O	48:o3:96:ASN:ND2	2.52	0.43
54:B6:61:LYS:HE2	54:B6:61:LYS:HB2	1.91	0.43
56:D6:325:ARG:HG3	56:D6:326:LEU:HD12	2.00	0.43
59:G6:200:LEU:O	59:G6:218:TYR:OH	2.31	0.43
67:O6:176:ASP:OD1	67:O6:176:ASP:N	2.43	0.43
76:X6:126:LEU:HD23	76:X6:126:LEU:HA	1.85	0.43
80:b6:218:ASN:O	80:b6:222:ALA:N	2.52	0.43
84:A6:1489:G:O6	84:A6:1573:G:N2	2.52	0.43
88:n:201:PRO:HG2	88:n:204:ALA:HB2	2.00	0.43
2:A3:2549:C:H41	2:A3:2562:U:H2'	1.84	0.43
9:J3:154:ARG:NH1	9:J3:155:VAL:O	2.52	0.43
31:53:230:LEU:HD12	31:53:230:LEU:HA	1.78	0.43
32:63:161:LEU:HB2	32:63:221:LEU:HD21	2.00	0.43
37:c3:61:SER:HA	37:c3:66:TRP:CD1	2.53	0.43
55:C6:142:LEU:HD13	83:e6:120:ILE:HD11	2.01	0.43
57:E6:5:GLU:N	57:E6:94:VAL:O	2.51	0.43
58:F6:160:PRO:HG3	85:C:31:C:P	2.59	0.43
60:H6:111:PRO:HB2	60:H6:140:TYR:HD2	1.84	0.43
76:X6:322:ALA:HB1	76:X6:327:GLU:HG3	2.01	0.43
83:e6:615:MET:HE3	83:e6:615:MET:HB3	1.85	0.43
2:A3:1795:A:H5''	6:F3:147:ARG:HH22	1.84	0.43
2:A3:2293:A:N6	12:M3:37:GLU:OE1	2.52	0.43
12:M3:284:LYS:HE3	41:g3:42:VAL:HG11	2.00	0.43
14:O3:133:LEU:HB2	14:O3:135:LEU:HD22	2.01	0.43
29:33:98:SER:HB2	29:33:105:LYS:HE3	2.01	0.43
29:33:163:THR:HG23	29:33:165:PHE:H	1.83	0.43
31:53:127:LYS:HE2	31:53:129:ILE:HG12	1.99	0.43
33:73:87:THR:O	33:73:90:SER:OG	2.29	0.43
33:73:166:LEU:HD22	33:73:181:TYR:HE2	1.84	0.43
39:e3:70:MET:HG2	87:A:121:TRP:CE2	2.53	0.43
74:V6:265:LYS:HD2	74:V6:265:LYS:HA	1.75	0.43
75:W6:153:PHE:H	75:W6:156:ALA:HB3	1.83	0.43
79:a6:137:HIS:H	84:A6:709:C:H41	1.66	0.43
84:A6:1075:U:H2'	84:A6:1076:G:C8	2.53	0.43
2:A3:2462:A:OP1	5:E3:237:HIS:NE2	2.51	0.42
10:K3:166:PHE:HB2	51:r3:87:LEU:HD13	1.99	0.42
19:T3:110:ASP:OD1	19:T3:110:ASP:N	2.52	0.42
24:Y3:112:LEU:HA	24:Y3:115:LEU:HD12	2.00	0.42
59:G6:251:GLU:O	59:G6:253:LYS:NZ	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:S6:97:GLN:HE21	71:S6:101:GLU:HG2	1.84	0.42
74:V6:40:TRP:HE3	74:V6:379:LEU:HD22	1.84	0.42
76:X6:284:PRO:HA	76:X6:287:LEU:HD12	2.01	0.42
79:a6:63:ARG:H	79:a6:66:GLN:HE21	1.67	0.42
2:A3:1917:A:OP1	28:23:63:LYS:NZ	2.51	0.42
2:A3:2085:A:H2'	2:A3:2086:A:C8	2.53	0.42
5:E3:59:PRO:HA	5:E3:62:LYS:HB2	2.00	0.42
5:E3:309:ASP:OD1	5:E3:309:ASP:N	2.48	0.42
6:F3:126:LYS:HG2	6:F3:139:GLY:HA2	2.01	0.42
13:N3:183:LEU:HD23	13:N3:183:LEU:HA	1.81	0.42
16:Q3:95:GLU:O	16:Q3:99:MET:N	2.42	0.42
25:Z3:50:PRO:HA	25:Z3:53:HIS:CD2	2.53	0.42
45:k3:81:LEU:HB2	45:k3:86:MET:HE2	2.00	0.42
65:M6:110:LEU:HA	65:M6:113:LYS:HB2	2.01	0.42
71:S6:26:LYS:HD3	71:S6:26:LYS:HA	1.86	0.42
74:V6:202:ARG:HG2	74:V6:234:VAL:HG11	2.01	0.42
74:V6:231:LEU:HD22	74:V6:243:VAL:HG23	2.00	0.42
74:V6:233:LYS:HD3	74:V6:288:LYS:HE3	2.01	0.42
2:A3:1909:A:HO2'	2:A3:2733:G:HO2'	1.55	0.42
5:E3:70:LYS:HA	5:E3:70:LYS:HD3	1.70	0.42
5:E3:71:ALA:O	5:E3:75:SER:OG	2.31	0.42
6:F3:45:GLU:HA	6:F3:46:PRO:HD3	1.91	0.42
12:M3:86:GLY:H	12:M3:90:ARG:NH2	2.17	0.42
14:O3:42:ILE:HD11	14:O3:52:MET:HE1	2.00	0.42
29:33:107:VAL:HG21	29:33:161:MET:HE2	1.99	0.42
42:h3:142:GLU:O	42:h3:146:SER:OG	2.32	0.42
54:B6:239:ASN:OD1	75:W6:119:LYS:NZ	2.48	0.42
60:H6:81:LYS:HB2	60:H6:170:MET:HE3	2.00	0.42
65:M6:111:ARG:O	65:M6:115:ALA:N	2.52	0.42
76:X6:123:ARG:HH12	76:X6:299:ASN:H	1.67	0.42
88:n:59:ARG:H	88:n:199:HIS:CE1	2.37	0.42
19:T3:121:LEU:O	19:T3:125:GLN:N	2.36	0.42
25:Z3:101:LYS:HB3	25:Z3:103:ILE:HG23	2.00	0.42
29:33:117:LEU:HD12	29:33:121:LEU:HB2	2.01	0.42
31:53:334:LYS:H	31:53:362:THR:HG23	1.84	0.42
40:f3:105:SER:OG	47:m3:38:ALA:O	2.31	0.42
44:j3:46:LEU:HD23	44:j3:46:LEU:HA	1.82	0.42
52:s3:234:ASP:OD2	52:s3:278:TYR:OH	2.36	0.42
62:J6:129:LYS:N	62:J6:132:CYS:O	2.52	0.42
65:M6:111:ARG:HG2	67:O6:232:PRO:HD2	2.00	0.42
66:N6:73:ARG:HE	66:N6:73:ARG:HB2	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:R6:136:VAL:HG23	70:R6:138:ILE:HD11	2.01	0.42
84:A6:688:U:H2'	84:A6:689:A:H8	1.84	0.42
5:E3:111:THR:HA	5:E3:337:VAL:HA	2.01	0.42
10:K3:60:MET:HB3	10:K3:133:ILE:HD11	1.99	0.42
18:S3:151:LYS:HE2	18:S3:151:LYS:HB2	1.89	0.42
20:U3:11:ARG:HH11	21:V3:211:LYS:H	1.68	0.42
20:U3:19:VAL:HG22	34:93:136:LEU:HD22	2.00	0.42
31:53:228:ALA:N	31:53:292:TYR:O	2.53	0.42
51:r3:128:LEU:HD22	51:r3:131:HIS:HD2	1.85	0.42
56:D6:167:LYS:HA	56:D6:167:LYS:HD2	1.84	0.42
57:E6:6:LEU:HD23	57:E6:8:LEU:HB2	2.01	0.42
60:H6:126:ILE:HD11	84:A6:1221:G:H21	1.84	0.42
67:O6:231:PRO:HA	67:O6:232:PRO:HD3	1.91	0.42
74:V6:109:ILE:HG12	74:V6:137:ILE:HG22	2.02	0.42
80:b6:176:LYS:HE2	80:b6:176:LYS:HB2	1.92	0.42
84:A6:719:G:N3	84:A6:820:A:O2'	2.52	0.42
84:A6:1285:U:H3	84:A6:1291:A:H61	1.68	0.42
2:A3:2244:U:HO2'	51:r3:189:ARG:HE	1.66	0.42
2:A3:2387:U:H3'	4:D3:75:THR:HG22	2.02	0.42
12:M3:152:VAL:HG23	12:M3:167:ILE:HD11	2.02	0.42
18:S3:52:PRO:HG2	51:r3:77:LEU:HD11	2.00	0.42
18:S3:113:LEU:HB2	36:b3:120:HIS:HB3	2.00	0.42
18:S3:166:SER:OG	18:S3:167:TRP:N	2.51	0.42
21:V3:177:THR:HG22	34:93:71:LYS:H	1.85	0.42
24:Y3:71:PRO:HA	24:Y3:74:TRP:CD1	2.55	0.42
29:33:95:THR:HA	43:i3:122:ASN:HB3	2.01	0.42
29:33:131:LYS:HE2	29:33:131:LYS:HB2	1.84	0.42
33:73:144:ARG:NH1	33:73:267:PRO:O	2.49	0.42
37:c3:156:LEU:HD22	37:c3:231:MET:HE2	2.01	0.42
55:C6:77:ASP:HA	55:C6:78:GLY:HA2	1.64	0.42
56:D6:249:ASN:OD1	56:D6:249:ASN:N	2.52	0.42
59:G6:344:ILE:O	59:G6:348:MET:N	2.49	0.42
63:K6:80:ARG:HD3	63:K6:86:ARG:HH22	1.83	0.42
67:O6:97:ARG:NH2	84:A6:875:A:OP2	2.51	0.42
71:S6:113:ASP:HB3	71:S6:116:LYS:H	1.84	0.42
2:A3:3161:G:H1'	2:A3:3162:C:H2'	2.00	0.42
9:J3:136:PRO:O	9:J3:139:SER:OG	2.36	0.42
11:L3:82:LYS:HA	11:L3:82:LYS:HD3	1.75	0.42
14:O3:43:GLU:OE2	26:03:127:TYR:OH	2.25	0.42
19:T3:155:ARG:O	19:T3:167:MET:N	2.53	0.42
24:Y3:70:ASP:OD1	24:Y3:70:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y3:234:LEU:HD23	24:Y3:234:LEU:HA	1.91	0.42
28:23:49:ARG:HD2	28:23:49:ARG:HA	1.92	0.42
36:b3:33:VAL:HG12	36:b3:43:ALA:HB1	2.01	0.42
42:h3:114:ASN:OD1	42:h3:114:ASN:N	2.44	0.42
43:i3:102:MET:HE3	43:i3:102:MET:HB2	1.94	0.42
45:k3:17:ARG:N	45:k3:65:ASP:O	2.47	0.42
52:s3:94:TYR:O	52:s3:106:TYR:OH	2.34	0.42
59:G6:276:ARG:NH2	84:A6:1435:G:O6	2.39	0.42
60:H6:125:HIS:ND1	60:H6:126:ILE:HG12	2.34	0.42
75:W6:114:ILE:HD13	75:W6:142:LEU:HD21	2.02	0.42
79:a6:115:TRP:HB3	79:a6:130:GLU:HA	2.01	0.42
84:A6:1231:G:H3'	84:A6:1232:A:H8	1.85	0.42
7:D:174:VAL:HB	7:D:192:HIS:CE1	2.55	0.42
2:A3:2240:C:H4'	10:K3:30:LYS:HG3	2.01	0.42
4:D3:255:ARG:HH22	4:D3:266:LEU:HD21	1.85	0.42
6:F3:133:THR:HG22	6:F3:135:ARG:H	1.84	0.42
9:J3:139:SER:HA	9:J3:142:ARG:HD2	2.01	0.42
13:N3:72:ILE:HD11	13:N3:96:TYR:CZ	2.55	0.42
15:P3:135:CYS:HB3	15:P3:140:ILE:HB	2.01	0.42
18:S3:68:ASP:O	18:S3:72:GLU:N	2.52	0.42
23:X3:21:CYS:HA	23:X3:24:LEU:HG	2.00	0.42
23:X3:132:LEU:HD23	23:X3:132:LEU:HA	1.93	0.42
24:Y3:69:ASP:O	24:Y3:74:TRP:NE1	2.42	0.42
25:Z3:137:THR:HG22	25:Z3:147:VAL:HA	2.02	0.42
26:O3:141:ILE:HG12	26:O3:175:ILE:HD13	2.01	0.42
39:e3:203:LYS:N	39:e3:237:LEU:O	2.53	0.42
52:s3:48:VAL:HB	52:s3:61:ARG:HE	1.84	0.42
52:s3:169:SER:O	52:s3:169:SER:OG	2.29	0.42
52:s3:307:ARG:HB2	52:s3:310:ARG:H	1.84	0.42
55:C6:60:HIS:CE1	84:A6:1323:A:H4'	2.55	0.42
67:O6:128:CYS:SG	67:O6:129:ALA:N	2.93	0.42
70:R6:107:THR:HG23	70:R6:110:GLN:H	1.84	0.42
73:U6:152:ARG:HA	73:U6:152:ARG:HD2	1.95	0.42
77:Y6:304:TRP:O	77:Y6:308:GLY:N	2.51	0.42
80:b6:73:ALA:HA	80:b6:113:HIS:CE1	2.55	0.42
85:24:8:U:H5'	85:24:47:A:H5'	2.01	0.42
2:A3:1862:U:H2'	2:A3:1863:A:C8	2.55	0.42
2:A3:3126:C:H2'	2:A3:3127:G:C8	2.55	0.42
7:H3:59:TRP:HB3	7:H3:60:TRP:CD1	2.55	0.42
16:Q3:116:ILE:HG12	16:Q3:136:ILE:HG22	2.02	0.42
25:Z3:104:PRO:O	48:o3:56:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:i3:97:MET:HB3	43:i3:97:MET:HE2	1.79	0.42
66:N6:31:THR:H	72:T6:65:MET:HE1	1.84	0.42
67:O6:91:ARG:NH2	84:A6:921:C:OP2	2.52	0.42
72:T6:150:PRO:HB3	72:T6:155:LEU:HG	2.02	0.42
73:U6:125:ARG:O	73:U6:129:ARG:N	2.52	0.42
74:V6:188:HIS:HA	74:V6:191:ALA:HB3	2.02	0.42
75:W6:111:ASP:OD1	75:W6:111:ASP:N	2.45	0.42
80:b6:122:HIS:HA	80:b6:125:ALA:HB3	2.02	0.42
88:n:126:LYS:HE2	88:n:126:LYS:HB2	1.89	0.42
7:D:205:THR:OG1	7:D:206:LEU:N	2.53	0.42
2:A3:2117:U:O2'	2:A3:2836:C:O2'	2.36	0.42
2:A3:2720:A:H61	2:A3:3098:U:H3	1.66	0.42
2:A3:3134:C:H3'	2:A3:3135:A:H8	1.84	0.42
10:K3:3:SER:OG	37:c3:309:GLU:N	2.45	0.42
23:X3:94:ASN:O	85:C:72:C:O2'	2.38	0.42
23:X3:220:GLU:HG3	23:X3:221:LYS:H	1.85	0.42
40:f3:187:LYS:NZ	40:f3:191:GLU:OE2	2.50	0.42
51:r3:71:PRO:HD2	51:r3:107:LEU:HD23	2.01	0.42
59:G6:118:GLU:OE2	84:A6:1311:G:O2'	2.33	0.42
59:G6:360:GLU:HA	59:G6:363:TRP:CD1	2.54	0.42
62:J6:48:LYS:HA	62:J6:48:LYS:HD3	1.93	0.42
67:O6:215:ARG:HE	79:a6:88:GLN:HA	1.85	0.42
70:R6:260:ASP:OD1	70:R6:263:ARG:NE	2.36	0.42
72:T6:59:ASN:OD1	72:T6:59:ASN:N	2.51	0.42
72:T6:141:CYS:HB2	72:T6:149:CYS:HB2	2.02	0.42
2:A3:2909:G:O5'	27:13:63:ARG:NH2	2.53	0.41
2:A3:3078:C:H2'	2:A3:3079:G:H8	1.85	0.41
9:J3:104:THR:HA	9:J3:105:GLY:HA2	1.74	0.41
13:N3:213:TRP:HZ3	13:N3:217:ARG:HH21	1.67	0.41
21:V3:129:LYS:HD3	21:V3:129:LYS:HA	1.93	0.41
23:X3:53:ASN:ND2	23:X3:54:PRO:O	2.53	0.41
26:O3:140:GLN:HA	26:O3:143:LYS:HB2	2.00	0.41
28:23:56:SER:HB2	28:23:59:LYS:HB2	2.01	0.41
28:23:78:VAL:HG22	28:23:81:ARG:HH21	1.85	0.41
39:e3:61:LYS:HD2	39:e3:62:PRO:HD2	2.02	0.41
52:s3:165:ARG:O	52:s3:307:ARG:NH2	2.53	0.41
56:D6:301:THR:O	56:D6:301:THR:OG1	2.35	0.41
58:F6:73:LEU:HD12	58:F6:73:LEU:HA	1.82	0.41
68:P6:95:HIS:CD2	68:P6:95:HIS:H	2.38	0.41
74:V6:183:LEU:HD11	74:V6:364:LEU:HD12	2.02	0.41
84:A6:926:C:H2'	84:A6:927:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:1756:A:H5''	7:H3:66:GLY:H	1.86	0.41
2:A3:2815:G:O6	85:24:73:A:N6	2.53	0.41
8:I3:40:MET:O	8:I3:45:GLN:NE2	2.53	0.41
10:K3:24:LYS:HB2	10:K3:61:ASN:ND2	2.35	0.41
17:R3:132:LEU:HD23	17:R3:132:LEU:HA	1.92	0.41
23:X3:91:TYR:CG	23:X3:96:LYS:HA	2.55	0.41
29:33:101:LYS:HA	29:33:101:LYS:HD3	1.78	0.41
39:e3:212:HIS:HE1	87:A:150:LEU:HD23	1.85	0.41
46:l3:133:SER:O	46:l3:133:SER:OG	2.36	0.41
50:q3:142:ASN:HA	50:q3:145:LYS:HD2	2.02	0.41
52:s3:246:GLN:HE21	52:s3:355:PHE:HA	1.85	0.41
57:E6:49:TYR:HB3	69:Q6:4:HIS:CE1	2.55	0.41
65:M6:93:LEU:HD21	65:M6:103:MET:HG2	2.03	0.41
66:N6:31:THR:OG1	72:T6:65:MET:SD	2.70	0.41
66:N6:64:VAL:HG23	66:N6:84:ILE:HG12	2.02	0.41
73:U6:38:LYS:HA	73:U6:38:LYS:HD3	1.93	0.41
74:V6:139:PRO:O	74:V6:143:THR:OG1	2.38	0.41
74:V6:250:ILE:O	74:V6:255:TYR:OH	2.37	0.41
83:e6:517:LYS:HD2	83:e6:517:LYS:HA	1.81	0.41
84:A6:1205:A:H2'	84:A6:1206:G:C8	2.55	0.41
85:24:9:A:H1'	85:24:43:C:H2'	2.01	0.41
2:A3:1779:A:N3	2:A3:1781:A:O2'	2.53	0.41
2:A3:1977:U:H2'	2:A3:1978:A:C8	2.54	0.41
2:A3:2862:C:H4'	22:W3:54:LYS:HG2	2.02	0.41
5:E3:112:LYS:N	5:E3:336:ASN:O	2.53	0.41
5:E3:134:SER:OG	5:E3:135:LYS:N	2.53	0.41
12:M3:269:LEU:HD23	12:M3:269:LEU:HA	1.82	0.41
18:S3:132:LYS:HE3	44:j3:48:ASP:HA	2.02	0.41
24:Y3:85:TRP:HB2	24:Y3:138:SER:HB2	2.01	0.41
24:Y3:112:LEU:HB3	24:Y3:132:LEU:HD13	2.01	0.41
33:73:134:ASP:OD2	33:73:134:ASP:N	2.52	0.41
39:e3:52:CYS:O	39:e3:54:GLN:NE2	2.53	0.41
39:e3:137:ILE:HD11	39:e3:140:ALA:HB3	2.02	0.41
40:f3:49:LYS:NZ	40:f3:50:THR:O	2.37	0.41
40:f3:179:PRO:HG2	40:f3:182:VAL:HG21	2.02	0.41
48:o3:81:LYS:HE2	48:o3:81:LYS:HB2	1.72	0.41
49:p3:103:PHE:O	49:p3:133:LEU:N	2.50	0.41
49:p3:133:LEU:HD21	49:p3:157:MET:HE1	2.01	0.41
56:D6:201:ILE:HD13	56:D6:201:ILE:HA	1.95	0.41
59:G6:88:LEU:HD13	80:b6:83:LEU:HD21	2.02	0.41
65:M6:91:LEU:HD13	65:M6:96:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:T6:29:VAL:HB	72:T6:79:TYR:HB2	2.03	0.41
74:V6:219:VAL:HA	74:V6:222:SER:HB2	2.02	0.41
76:X6:111:TYR:O	76:X6:115:THR:OG1	2.38	0.41
76:X6:136:LEU:HD23	76:X6:136:LEU:HA	1.89	0.41
76:X6:273:THR:HB	76:X6:316:LEU:HD11	2.02	0.41
76:X6:393:ARG:HH22	84:A6:1382:C:H1'	1.85	0.41
83:e6:497:LEU:HA	83:e6:500:LEU:HD13	2.02	0.41
84:A6:1006:C:H2'	84:A6:1007:A:C8	2.55	0.41
84:A6:1502:C:H2'	84:A6:1503:U:H6	1.84	0.41
85:C:9:A:H1'	85:C:43:C:H2'	2.01	0.41
88:n:1:PRO:HA	88:n:46:LYS:HD2	2.02	0.41
2:A3:2935:A:H3'	2:A3:2936:U:H2'	2.02	0.41
2:A3:2955:U:H5'	13:N3:178:GLN:NE2	2.34	0.41
2:A3:3174:U:H2'	2:A3:3175:A:C8	2.55	0.41
10:K3:58:VAL:HG22	10:K3:126:HIS:HB2	2.02	0.41
19:T3:190:LYS:HB3	19:T3:190:LYS:HE2	1.91	0.41
21:V3:52:GLU:OE1	21:V3:81:ARG:NH2	2.53	0.41
32:63:73:THR:OG1	32:63:74:TYR:N	2.53	0.41
33:73:80:VAL:O	38:d3:279:THR:OG1	2.38	0.41
36:b3:19:LEU:HD23	36:b3:19:LEU:HA	1.80	0.41
40:f3:183:ARG:HG2	87:A:174:GLU:HG3	2.01	0.41
44:j3:99:GLN:O	44:j3:103:ARG:N	2.42	0.41
54:B6:224:ASP:N	54:B6:227:CYS:SG	2.88	0.41
59:G6:389:ARG:NH2	59:G6:390:LYS:O	2.52	0.41
60:H6:74:LYS:HA	60:H6:74:LYS:HD3	1.75	0.41
65:M6:68:LEU:HD23	65:M6:70:LEU:HD23	2.02	0.41
79:a6:114:ALA:HB3	79:a6:131:ILE:HD11	2.02	0.41
83:e6:119:PHE:O	83:e6:123:SER:N	2.50	0.41
84:A6:883:U:H3	84:A6:900:A:H61	1.68	0.41
84:A6:1451:G:O2'	84:A6:1453:G:N7	2.42	0.41
2:A3:2390:A:H4'	31:53:301:PRO:HD3	2.03	0.41
6:F3:123:GLY:HA2	6:F3:141:ILE:HG23	2.03	0.41
7:H3:57:GLU:OE1	7:H3:58:ARG:N	2.54	0.41
9:J3:73:LYS:HB3	9:J3:73:LYS:HE2	1.92	0.41
10:K3:39:LEU:HD23	10:K3:39:LEU:HA	1.93	0.41
14:O3:64:LYS:NZ	14:O3:101:THR:O	2.54	0.41
14:O3:106:ARG:HD2	14:O3:135:LEU:HD11	2.03	0.41
18:S3:108:VAL:HG11	18:S3:195:ILE:HG13	2.02	0.41
31:53:122:TRP:HA	31:53:253:LEU:HD23	2.02	0.41
31:53:160:HIS:HA	31:53:164:TRP:HB2	2.02	0.41
48:o3:15:ARG:HB3	48:o3:18:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B6:231:LEU:HD23	54:B6:231:LEU:HA	1.90	0.41
56:D6:95:ALA:HA	56:D6:98:LEU:HD12	2.02	0.41
58:F6:84:SER:HA	59:G6:318:HIS:CD2	2.56	0.41
73:U6:97:LYS:HD2	73:U6:97:LYS:HA	1.74	0.41
75:W6:108:VAL:HG12	75:W6:109:GLU:H	1.84	0.41
76:X6:190:ASN:O	76:X6:193:THR:OG1	2.38	0.41
88:n:137:LEU:HA	88:n:138:PRO:HD3	1.93	0.41
2:A3:1896:U:H2'	2:A3:1897:A:H8	1.85	0.41
2:A3:2171:U:H4'	2:A3:2172:A:H3'	2.03	0.41
2:A3:2241:A:OP1	51:r3:150:TYR:OH	2.34	0.41
6:F3:97:HIS:CE1	6:F3:101:MET:HG3	2.56	0.41
12:M3:251:GLU:HG2	12:M3:252:LEU:HD22	2.02	0.41
21:V3:61:THR:OG1	21:V3:73:GLN:NE2	2.53	0.41
21:V3:194:LEU:HD13	24:Y3:146:VAL:HG23	2.02	0.41
32:63:240:ILE:HG23	32:63:245:VAL:HA	2.03	0.41
41:g3:96:VAL:HB	41:g3:158:LYS:HG3	2.03	0.41
55:C6:115:ASN:HD22	77:Y6:311:TRP:CD1	2.39	0.41
66:N6:24:LYS:HD2	84:A6:772:A:H4'	2.02	0.41
73:U6:27:ARG:NE	84:A6:704:A:N7	2.60	0.41
75:W6:84:LEU:O	75:W6:87:SER:OG	2.33	0.41
84:A6:1269:C:H2'	84:A6:1270:A:C8	2.55	0.41
84:A6:1361:A:H2'	84:A6:1362:A:H8	1.86	0.41
88:n:76:ALA:O	88:n:95:GLY:N	2.51	0.41
14:O3:16:ARG:H	14:O3:16:ARG:HG3	1.63	0.41
21:V3:208:ARG:NH2	34:93:55:GLU:OE2	2.54	0.41
24:Y3:155:LEU:HD21	24:Y3:161:GLU:HG2	2.02	0.41
26:03:104:LYS:NZ	26:03:118:GLN:HE22	2.18	0.41
37:c3:42:GLN:NE2	43:i3:36:LEU:O	2.52	0.41
38:d3:255:PRO:HB2	38:d3:256:TYR:H	1.64	0.41
44:j3:58:PRO:HA	44:j3:59:PRO:HD3	1.92	0.41
45:k3:16:VAL:HG13	45:k3:66:VAL:HG22	2.02	0.41
51:r3:56:THR:HA	51:r3:57:PRO:HD3	1.84	0.41
58:F6:144:ILE:HG13	58:F6:213:PHE:CG	2.54	0.41
58:F6:221:LYS:O	58:F6:225:ASP:N	2.48	0.41
59:G6:294:LYS:HE3	59:G6:299:ASP:HB3	2.03	0.41
61:I6:103:SER:O	61:I6:103:SER:OG	2.29	0.41
67:O6:163:LEU:HA	67:O6:163:LEU:HD23	1.88	0.41
70:R6:261:LEU:H	70:R6:261:LEU:HG	1.71	0.41
70:R6:306:VAL:HG12	70:R6:307:LEU:HD22	2.03	0.41
76:X6:366:LEU:HD22	76:X6:372:PRO:HG3	2.01	0.41
79:a6:99:ARG:HD3	84:A6:1531:A:H4'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:e6:126:LYS:HE3	83:e6:126:LYS:HB3	1.91	0.41
84:A6:1007:A:H2'	84:A6:1008:G:H8	1.85	0.41
84:A6:1142:G:H2'	84:A6:1143:A:C8	2.49	0.41
2:A3:2403:G:H5''	4:D3:103:ARG:HG3	2.02	0.41
5:E3:264:ILE:HD12	5:E3:264:ILE:HA	1.85	0.41
13:N3:204:GLU:O	13:N3:208:ASN:N	2.51	0.41
32:63:65:ALA:O	32:63:75:ARG:NH2	2.51	0.41
34:93:81:SER:OG	34:93:82:GLU:N	2.53	0.41
39:e3:178:TRP:HE1	39:e3:230:LYS:HD2	1.84	0.41
52:s3:145:VAL:HA	52:s3:148:ASP:HB2	2.01	0.41
76:X6:132:THR:H	76:X6:388:PRO:HD2	1.86	0.41
76:X6:368:HIS:HB2	76:X6:398:LEU:HB3	2.03	0.41
80:b6:143:CYS:O	80:b6:147:PHE:N	2.49	0.41
80:b6:165:ASN:HD21	80:b6:167:ARG:CZ	2.34	0.41
80:b6:211:ARG:HD2	80:b6:221:TYR:HE2	1.86	0.41
84:A6:1278:C:O2	84:A6:1305:G:N2	2.40	0.41
5:E3:274:TRP:HE1	5:E3:286:ASN:HB2	1.86	0.41
7:H3:53:THR:HG21	23:X3:130:ARG:HD3	2.03	0.41
9:J3:115:LYS:HD2	9:J3:115:LYS:HA	1.81	0.41
14:O3:45:PRO:HA	14:O3:120:MET:HA	2.02	0.41
18:S3:150:GLY:HA3	18:S3:153:LEU:HD13	2.02	0.41
18:S3:172:MET:HE3	18:S3:181:LYS:HG3	2.03	0.41
21:V3:101:THR:HG23	21:V3:102:MET:HB2	2.03	0.41
31:53:107:PHE:HB2	31:53:265:LEU:HD22	2.02	0.41
31:53:204:VAL:HA	52:s3:179:GLN:HE22	1.86	0.41
33:73:52:LYS:HD2	33:73:52:LYS:HA	1.92	0.41
33:73:67:VAL:HG13	33:73:79:PHE:HB2	2.02	0.41
37:c3:131:SER:O	37:c3:135:THR:OG1	2.32	0.41
38:d3:271:PRO:HA	38:d3:272:PRO:HD3	1.89	0.41
41:g3:97:TYR:HE2	41:g3:111:ARG:HE	1.69	0.41
45:k3:33:PHE:O	45:k3:38:SER:OG	2.34	0.41
45:k3:77:ARG:HA	45:k3:78:GLY:HA3	1.80	0.41
47:m3:63:THR:H	87:A:179:THR:HG22	1.84	0.41
48:o3:29:LEU:HD12	48:o3:29:LEU:HA	1.94	0.41
52:s3:119:PRO:HG3	52:s3:394:TRP:CD2	2.55	0.41
54:B6:125:LEU:HD13	54:B6:236:VAL:HG11	2.03	0.41
58:F6:114:THR:HG21	58:F6:205:LEU:HD23	2.02	0.41
59:G6:85:LYS:HE2	59:G6:85:LYS:HB3	1.81	0.41
60:H6:115:ILE:HG23	60:H6:137:ARG:HA	2.03	0.41
75:W6:144:LEU:HD12	75:W6:144:LEU:HA	1.88	0.41
75:W6:149:LEU:HD12	75:W6:149:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:X6:86:ARG:HG3	76:X6:393:ARG:HE	1.86	0.41
83:e6:530:GLU:HA	83:e6:533:MET:HG2	2.02	0.41
84:A6:912:C:H2'	84:A6:913:G:H8	1.86	0.41
2:A3:1810:A:H2'	2:A3:1811:A:C8	2.56	0.41
2:A3:2194:U:O2'	2:A3:2195:A:O4'	2.33	0.41
8:I3:160:LYS:HG2	8:I3:163:GLU:HB2	2.03	0.41
23:X3:238:LEU:O	23:X3:242:ALA:N	2.49	0.41
24:Y3:139:MET:HE2	24:Y3:139:MET:HB2	1.92	0.41
29:33:111:ILE:HD12	29:33:111:ILE:HA	1.93	0.41
31:53:210:SER:HB3	31:53:276:ASP:H	1.86	0.41
32:63:259:PRO:HD2	32:63:327:VAL:HG21	2.03	0.41
37:c3:228:LEU:HD12	37:c3:228:LEU:HA	1.88	0.41
39:e3:101:LYS:HD3	39:e3:101:LYS:HA	1.79	0.41
55:C6:83:ALA:HB1	63:K6:105:ARG:HG3	2.04	0.41
55:C6:141:THR:HG21	83:e6:114:GLU:HG2	2.03	0.41
58:F6:53:LYS:HA	58:F6:53:LYS:HD3	1.89	0.41
61:I6:85:ILE:HG13	61:I6:148:ARG:HE	1.84	0.41
62:J6:31:ALA:HB3	62:J6:36:MET:HE3	2.03	0.41
64:L6:130:ILE:HD13	64:L6:130:ILE:HA	1.85	0.41
64:L6:168:LYS:HB3	64:L6:168:LYS:HE3	1.77	0.41
67:O6:103:ASN:HA	67:O6:104:PRO:HD3	1.89	0.41
83:e6:452:GLN:HA	83:e6:455:ASN:HD22	1.86	0.41
84:A6:1363:U:H5'	85:24:28:A:H4'	2.02	0.41
84:A6:1578:G:H1	84:A6:1595:C:H42	1.67	0.41
88:n:200:LYS:HB3	88:n:200:LYS:HE2	1.84	0.41
14:O3:124:GLU:OE2	14:O3:128:ASN:ND2	2.55	0.40
31:53:136:VAL:HG12	31:53:420:HIS:CG	2.55	0.40
32:63:371:ASP:OD1	32:63:371:ASP:N	2.54	0.40
37:c3:166:VAL:HG13	37:c3:195:PHE:HD2	1.86	0.40
37:c3:254:GLU:HB2	37:c3:275:TYR:HB2	2.02	0.40
44:j3:87:GLY:HA3	48:o3:62:HIS:HB2	2.03	0.40
52:s3:178:ASP:HA	52:s3:239:ASN:HD21	1.86	0.40
62:J6:72:LYS:HA	62:J6:72:LYS:HD2	1.77	0.40
68:P6:80:LEU:HB2	68:P6:120:MET:HE1	2.04	0.40
68:P6:92:TYR:HB3	68:P6:96:ILE:HB	2.02	0.40
75:W6:122:CYS:HB3	75:W6:165:ALA:HB3	2.02	0.40
76:X6:188:LEU:HD21	76:X6:240:VAL:HB	2.03	0.40
83:e6:581:ILE:O	83:e6:585:ARG:N	2.54	0.40
88:n:14:VAL:HG12	88:n:16:PRO:HD3	2.02	0.40
2:A3:2373:A:H1'	2:A3:2374:A:H2'	2.03	0.40
4:D3:69:ARG:HG2	4:D3:106:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F3:290:TYR:CE1	41:g3:53:PRO:HG2	2.56	0.40
15:P3:132:ALA:HB1	15:P3:167:GLY:HA3	2.02	0.40
31:53:253:LEU:HD12	31:53:371:LYS:HE3	2.03	0.40
31:53:291:LEU:HB2	31:53:344:SER:HB3	2.04	0.40
64:L6:219:LYS:HA	64:L6:219:LYS:HD2	1.83	0.40
67:O6:215:ARG:HG3	67:O6:218:ARG:HH11	1.84	0.40
73:U6:142:LYS:HD3	73:U6:142:LYS:HA	1.81	0.40
76:X6:259:LEU:HD12	76:X6:259:LEU:HA	1.87	0.40
76:X6:380:LEU:HD23	76:X6:380:LEU:HA	1.89	0.40
84:A6:1192:A:H2	84:A6:1432:G:H2'	1.86	0.40
84:A6:1502:C:H2'	84:A6:1503:U:C6	2.56	0.40
88:n:44:HIS:HB2	88:n:213:TYR:HB2	2.04	0.40
2:A3:2043:C:H41	2:A3:2096:U:H5	1.69	0.40
4:D3:173:ALA:HB3	57:E6:84:ARG:HB3	2.03	0.40
5:E3:120:THR:HG21	5:E3:289:VAL:HG23	2.04	0.40
6:F3:244:PRO:HB2	6:F3:246:VAL:HG12	2.03	0.40
8:I3:158:GLU:HA	8:I3:159:PRO:HD3	1.92	0.40
12:M3:99:ASN:ND2	12:M3:143:GLU:OE1	2.52	0.40
15:P3:63:LYS:HA	15:P3:96:GLN:HE22	1.86	0.40
16:Q3:129:LYS:HD3	16:Q3:129:LYS:HA	1.79	0.40
16:Q3:269:MET:H	16:Q3:269:MET:HG2	1.69	0.40
26:O3:110:CYS:HB2	26:O3:117:LYS:HB2	2.02	0.40
31:53:322:LEU:HA	31:53:322:LEU:HD12	1.90	0.40
39:e3:74:LEU:HA	39:e3:77:ILE:HG22	2.02	0.40
51:r3:77:LEU:HD23	51:r3:77:LEU:HA	1.85	0.40
56:D6:425:LEU:HD23	56:D6:425:LEU:HA	1.92	0.40
57:E6:114:ALA:HB2	81:c6:7:ARG:HD2	2.04	0.40
83:e6:511:LYS:HA	83:e6:514:LYS:HE2	2.03	0.40
88:n:53[A]:ARG:HH21	88:n:56:GLN:HE21	1.69	0.40
88:n:109:ASP:OD1	88:n:109:ASP:N	2.55	0.40
7:D:197:LEU:HB2	7:D:199:VAL:HG22	2.03	0.40
2:A3:2349:G:H1	2:A3:2364:C:H42	1.70	0.40
2:A3:2499:U:OP2	2:A3:2504:A:N6	2.34	0.40
5:E3:60:PHE:O	5:E3:64:LEU:N	2.54	0.40
16:Q3:138:ILE:O	16:Q3:187:LEU:N	2.43	0.40
19:T3:206:ARG:H	19:T3:206:ARG:HG2	1.73	0.40
21:V3:73:GLN:O	38:d3:256:TYR:OH	2.28	0.40
21:V3:181:ASP:O	24:Y3:93:LYS:NZ	2.46	0.40
33:73:44:ARG:HB3	33:73:261:ILE:HD12	2.02	0.40
33:73:183:VAL:O	33:73:295:ARG:N	2.55	0.40
33:73:214:LEU:HD23	33:73:214:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h3:63:PRO:HB2	42:h3:66:LEU:HA	2.04	0.40
44:j3:69:GLU:HA	44:j3:72:THR:HG22	2.03	0.40
51:r3:187:TYR:HD1	51:r3:187:TYR:HA	1.75	0.40
52:s3:103:ASP:OD1	52:s3:325:ARG:NH1	2.55	0.40
54:B6:118:LEU:HD23	54:B6:118:LEU:HA	1.91	0.40
74:V6:253:PRO:HG3	74:V6:316:GLN:NE2	2.37	0.40
76:X6:64:GLU:HB3	76:X6:106:LEU:HD23	2.04	0.40
77:Y6:361:ASN:O	77:Y6:369:LYS:NZ	2.44	0.40
84:A6:842:U:O4	84:A6:843:A:N6	2.54	0.40
84:A6:1051:A:H4'	84:A6:1052:C:H5''	2.01	0.40
84:A6:1061:G:H4'	84:A6:1582:A:H4'	2.03	0.40
88:n:64:LEU:HD11	88:n:188:ASN:HB2	2.02	0.40
2:A3:1800:G:N1	2:A3:1803:A:OP2	2.47	0.40
2:A3:2085:A:H2'	2:A3:2086:A:H8	1.86	0.40
2:A3:2109:A:H61	2:A3:2981:A:H2	1.70	0.40
2:A3:3128:A:O2'	2:A3:3129:A:O5'	2.40	0.40
2:A3:3144:A:H61	2:A3:3167:U:H3	1.69	0.40
5:E3:61:ILE:HD13	5:E3:61:ILE:HA	1.97	0.40
6:F3:263:LEU:HA	6:F3:263:LEU:HD23	1.85	0.40
18:S3:95:LEU:HG	18:S3:138:ALA:HB2	2.03	0.40
23:X3:95:ASP:HB2	85:C:72:C:H2'	2.04	0.40
28:23:79:ILE:HG23	28:23:90:LEU:HB3	2.03	0.40
31:53:107:PHE:HD2	31:53:222:VAL:HG12	1.86	0.40
38:d3:186:VAL:HG21	38:d3:239:PRO:HB3	2.03	0.40
39:e3:205:LEU:HB3	40:f3:168:GLU:HB2	2.04	0.40
48:o3:36:ILE:HA	48:o3:39:LEU:HB2	2.04	0.40
54:B6:167:HIS:CD2	54:B6:175:MET:HE1	2.57	0.40
57:E6:15:ARG:HE	73:U6:181:LEU:HD13	1.85	0.40
58:F6:209:LEU:O	58:F6:213:PHE:N	2.53	0.40
59:G6:287:LYS:HG3	59:G6:355:PHE:CG	2.57	0.40
65:M6:10:LYS:HB3	65:M6:12:TYR:CE2	2.57	0.40
67:O6:81:HIS:CD2	67:O6:86:PRO:HB3	2.56	0.40
69:Q6:70:ARG:NH1	75:W6:152:ARG:O	2.53	0.40
70:R6:135:ARG:HG2	70:R6:186:TRP:CD1	2.57	0.40
74:V6:49:CYS:O	74:V6:78:ASN:ND2	2.54	0.40
76:X6:159:HIS:HB3	76:X6:163:LYS:HE2	2.03	0.40
76:X6:220:SER:O	76:X6:220:SER:OG	2.31	0.40
81:c6:60:GLU:HB3	81:c6:62:ARG:HE	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y2	27/29 (93%)	18 (67%)	9 (33%)	0	100	100
4	D3	234/305 (77%)	213 (91%)	21 (9%)	0	100	100
5	E3	296/348 (85%)	263 (89%)	32 (11%)	1 (0%)	36	71
6	F3	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
7	D	78/267 (29%)	66 (85%)	12 (15%)	0	100	100
7	H3	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
8	I3	154/261 (59%)	148 (96%)	6 (4%)	0	100	100
9	J3	138/192 (72%)	125 (91%)	13 (9%)	0	100	100
10	K3	175/178 (98%)	149 (85%)	24 (14%)	2 (1%)	11	45
11	L3	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
12	M3	285/296 (96%)	264 (93%)	19 (7%)	2 (1%)	18	55
13	N3	203/251 (81%)	189 (93%)	13 (6%)	1 (0%)	24	62
14	O3	150/175 (86%)	134 (89%)	15 (10%)	1 (1%)	18	55
15	P3	129/180 (72%)	118 (92%)	11 (8%)	0	100	100
16	Q3	217/292 (74%)	188 (87%)	28 (13%)	1 (0%)	24	62
17	R3	138/149 (93%)	129 (94%)	9 (6%)	0	100	100
18	S3	154/205 (75%)	138 (90%)	16 (10%)	0	100	100
19	T3	164/206 (80%)	152 (93%)	12 (7%)	0	100	100
20	U3	109/153 (71%)	97 (89%)	12 (11%)	0	100	100
21	V3	183/216 (85%)	158 (86%)	23 (13%)	2 (1%)	11	45
22	W3	109/148 (74%)	100 (92%)	9 (8%)	0	100	100
23	X3	241/256 (94%)	214 (89%)	26 (11%)	1 (0%)	30	66
24	Y3	174/250 (70%)	164 (94%)	10 (6%)	0	100	100
25	Z3	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
26	O3	106/188 (56%)	88 (83%)	17 (16%)	1 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	13	50/65 (77%)	46 (92%)	4 (8%)	0	100	100
28	23	44/92 (48%)	41 (93%)	3 (7%)	0	100	100
29	33	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
30	43	34/103 (33%)	33 (97%)	1 (3%)	0	100	100
31	53	368/423 (87%)	322 (88%)	43 (12%)	3 (1%)	16	52
32	63	313/380 (82%)	267 (85%)	46 (15%)	0	100	100
33	73	258/338 (76%)	232 (90%)	26 (10%)	0	100	100
34	93	105/137 (77%)	93 (89%)	12 (11%)	0	100	100
35	a3	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
36	b3	146/215 (68%)	130 (89%)	16 (11%)	0	100	100
37	c3	271/332 (82%)	251 (93%)	19 (7%)	1 (0%)	30	66
38	d3	156/306 (51%)	141 (90%)	14 (9%)	1 (1%)	21	58
39	e3	211/279 (76%)	193 (92%)	18 (8%)	0	100	100
40	f3	125/212 (59%)	104 (83%)	20 (16%)	1 (1%)	16	52
41	g3	127/166 (76%)	117 (92%)	10 (8%)	0	100	100
42	h3	96/158 (61%)	81 (84%)	13 (14%)	2 (2%)	5	29
43	i3	95/128 (74%)	83 (87%)	12 (13%)	0	100	100
44	j3	83/123 (68%)	75 (90%)	7 (8%)	1 (1%)	10	42
45	k3	82/112 (73%)	66 (80%)	15 (18%)	1 (1%)	10	42
46	l3	21/138 (15%)	19 (90%)	2 (10%)	0	100	100
47	m3	43/128 (34%)	38 (88%)	5 (12%)	0	100	100
48	o3	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	p3	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
50	q3	126/222 (57%)	115 (91%)	8 (6%)	3 (2%)	4	27
51	r3	140/196 (71%)	122 (87%)	18 (13%)	0	100	100
52	s3	366/467 (78%)	341 (93%)	25 (7%)	0	100	100
53	A5	26/28 (93%)	19 (73%)	7 (27%)	0	100	100
54	B6	215/296 (73%)	197 (92%)	18 (8%)	0	100	100
55	C6	130/167 (78%)	120 (92%)	10 (8%)	0	100	100
56	D6	316/430 (74%)	293 (93%)	22 (7%)	1 (0%)	36	71
57	E6	120/125 (96%)	110 (92%)	9 (8%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	F6	197/242 (81%)	187 (95%)	10 (5%)	0	100	100
59	G6	301/396 (76%)	276 (92%)	25 (8%)	0	100	100
60	H6	120/201 (60%)	104 (87%)	15 (12%)	1 (1%)	16	52
61	I6	134/194 (69%)	122 (91%)	12 (9%)	0	100	100
62	J6	106/138 (77%)	95 (90%)	11 (10%)	0	100	100
63	K6	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
64	L6	162/257 (63%)	151 (93%)	11 (7%)	0	100	100
65	M6	114/137 (83%)	106 (93%)	8 (7%)	0	100	100
66	N6	105/130 (81%)	92 (88%)	13 (12%)	0	100	100
67	O6	183/258 (71%)	164 (90%)	18 (10%)	1 (0%)	24	62
68	P6	94/142 (66%)	85 (90%)	9 (10%)	0	100	100
69	Q6	84/87 (97%)	74 (88%)	10 (12%)	0	100	100
70	R6	240/360 (67%)	207 (86%)	32 (13%)	1 (0%)	30	66
71	S6	124/190 (65%)	114 (92%)	10 (8%)	0	100	100
72	T6	160/173 (92%)	149 (93%)	11 (7%)	0	100	100
73	U6	171/205 (83%)	159 (93%)	12 (7%)	0	100	100
74	V6	320/414 (77%)	284 (89%)	35 (11%)	1 (0%)	36	71
75	W6	95/187 (51%)	82 (86%)	12 (13%)	1 (1%)	11	45
76	X6	310/398 (78%)	268 (86%)	40 (13%)	2 (1%)	21	58
77	Y6	106/395 (27%)	94 (89%)	12 (11%)	0	100	100
78	Z6	85/106 (80%)	80 (94%)	5 (6%)	0	100	100
79	a6	197/218 (90%)	176 (89%)	21 (11%)	0	100	100
80	b6	252/323 (78%)	217 (86%)	35 (14%)	0	100	100
81	c6	114/118 (97%)	100 (88%)	14 (12%)	0	100	100
82	d6	67/199 (34%)	63 (94%)	4 (6%)	0	100	100
83	e6	362/689 (52%)	334 (92%)	22 (6%)	6 (2%)	7	35
87	A	158/206 (77%)	140 (89%)	18 (11%)	0	100	100
88	n	230/229 (100%)	211 (92%)	19 (8%)	0	100	100
All	All	13175/18553 (71%)	11882 (90%)	1253 (10%)	40 (0%)	37	71

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
83	e6	68	VAL
12	M3	265	ILE
21	V3	101	THR
23	X3	52	ILE
31	53	270	ILE
50	q3	43	GLU
70	R6	266	ARG
83	e6	67	LYS
83	e6	147	PRO
16	Q3	183	LEU
44	j3	35	ALA
60	H6	126	ILE
74	V6	197	SER
75	W6	109	GLU
76	X6	97	ALA
76	X6	342	PRO
12	M3	288	GLU
21	V3	194	LEU
26	03	178	ASP
38	d3	231	LEU
42	h3	66	LEU
42	h3	138	SER
56	D6	287	ASP
83	e6	69	ALA
10	K3	4	PHE
10	K3	160	GLN
13	N3	237	HIS
31	53	269	ASN
50	q3	42	PRO
31	53	349	GLY
37	c3	313	PRO
83	e6	299	GLU
5	E3	246	GLY
45	k3	37	VAL
57	E6	15	ARG
67	O6	132	GLY
40	f3	51	LYS
50	q3	79	PRO
83	e6	146	GLU
14	O3	111	PRO

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	
4	D3	190/245 (78%)	190 (100%)	0	100	100
5	E3	255/290 (88%)	255 (100%)	0	100	100
6	F3	217/262 (83%)	213 (98%)	4 (2%)	51	67
7	D	73/228 (32%)	72 (99%)	1 (1%)	59	71
7	H3	86/228 (38%)	86 (100%)	0	100	100
8	I3	145/232 (62%)	145 (100%)	0	100	100
9	J3	113/150 (75%)	111 (98%)	2 (2%)	51	67
10	K3	155/156 (99%)	153 (99%)	2 (1%)	61	72
11	L3	98/124 (79%)	96 (98%)	2 (2%)	48	66
12	M3	245/249 (98%)	243 (99%)	2 (1%)	73	77
13	N3	172/211 (82%)	171 (99%)	1 (1%)	78	80
14	O3	133/150 (89%)	133 (100%)	0	100	100
15	P3	115/155 (74%)	115 (100%)	0	100	100
16	Q3	201/256 (78%)	200 (100%)	1 (0%)	81	81
17	R3	118/126 (94%)	118 (100%)	0	100	100
18	S3	141/180 (78%)	137 (97%)	4 (3%)	38	59
19	T3	146/176 (83%)	143 (98%)	3 (2%)	47	65
20	U3	99/135 (73%)	97 (98%)	2 (2%)	48	66
21	V3	169/191 (88%)	167 (99%)	2 (1%)	63	73
22	W3	91/119 (76%)	90 (99%)	1 (1%)	65	74
23	X3	217/227 (96%)	216 (100%)	1 (0%)	81	81
24	Y3	159/223 (71%)	159 (100%)	0	100	100
25	Z3	111/147 (76%)	111 (100%)	0	100	100
26	O3	97/164 (59%)	95 (98%)	2 (2%)	47	65
27	13	49/60 (82%)	47 (96%)	2 (4%)	27	48
28	23	40/72 (56%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	33	88/166 (53%)	88 (100%)	0	100	100
30	43	35/89 (39%)	35 (100%)	0	100	100
31	53	337/368 (92%)	336 (100%)	1 (0%)	86	84
32	63	266/332 (80%)	264 (99%)	2 (1%)	73	77
33	73	242/303 (80%)	240 (99%)	2 (1%)	73	77
34	93	91/112 (81%)	90 (99%)	1 (1%)	65	74
35	a3	78/133 (59%)	78 (100%)	0	100	100
36	b3	130/186 (70%)	127 (98%)	3 (2%)	44	63
37	c3	241/288 (84%)	241 (100%)	0	100	100
38	d3	151/274 (55%)	149 (99%)	2 (1%)	61	72
39	e3	188/236 (80%)	188 (100%)	0	100	100
40	f3	117/188 (62%)	114 (97%)	3 (3%)	40	60
41	g3	119/148 (80%)	119 (100%)	0	100	100
42	h3	95/148 (64%)	95 (100%)	0	100	100
43	i3	86/110 (78%)	83 (96%)	3 (4%)	32	53
44	j3	68/97 (70%)	68 (100%)	0	100	100
45	k3	74/90 (82%)	72 (97%)	2 (3%)	39	59
46	l3	23/116 (20%)	23 (100%)	0	100	100
47	m3	40/113 (35%)	40 (100%)	0	100	100
48	o3	80/87 (92%)	80 (100%)	0	100	100
49	p3	117/181 (65%)	117 (100%)	0	100	100
50	q3	110/178 (62%)	110 (100%)	0	100	100
51	r3	133/169 (79%)	132 (99%)	1 (1%)	73	77
52	s3	326/381 (86%)	322 (99%)	4 (1%)	63	73
54	B6	191/249 (77%)	189 (99%)	2 (1%)	68	76
55	C6	115/143 (80%)	114 (99%)	1 (1%)	70	76
56	D6	269/357 (75%)	267 (99%)	2 (1%)	76	79
57	E6	104/107 (97%)	102 (98%)	2 (2%)	50	66
58	F6	178/209 (85%)	177 (99%)	1 (1%)	78	80
59	G6	265/342 (78%)	263 (99%)	2 (1%)	73	77
60	H6	112/180 (62%)	111 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	I6	104/147 (71%)	103 (99%)	1 (1%)	68	76
62	J6	93/118 (79%)	90 (97%)	3 (3%)	34	55
63	K6	91/113 (80%)	91 (100%)	0	100	100
64	L6	152/226 (67%)	152 (100%)	0	100	100
65	M6	95/113 (84%)	94 (99%)	1 (1%)	65	74
66	N6	93/115 (81%)	89 (96%)	4 (4%)	26	47
67	O6	166/230 (72%)	166 (100%)	0	100	100
68	P6	87/123 (71%)	87 (100%)	0	100	100
69	Q6	78/79 (99%)	78 (100%)	0	100	100
70	R6	224/318 (70%)	224 (100%)	0	100	100
71	S6	109/164 (66%)	108 (99%)	1 (1%)	70	76
72	T6	150/157 (96%)	150 (100%)	0	100	100
73	U6	149/174 (86%)	149 (100%)	0	100	100
74	V6	295/364 (81%)	291 (99%)	4 (1%)	59	71
75	W6	84/158 (53%)	84 (100%)	0	100	100
76	X6	275/351 (78%)	272 (99%)	3 (1%)	65	74
77	Y6	99/357 (28%)	96 (97%)	3 (3%)	36	57
78	Z6	80/95 (84%)	80 (100%)	0	100	100
79	a6	176/190 (93%)	176 (100%)	0	100	100
80	b6	237/291 (81%)	235 (99%)	2 (1%)	73	77
81	c6	99/101 (98%)	98 (99%)	1 (1%)	68	76
82	d6	63/166 (38%)	62 (98%)	1 (2%)	55	69
83	e6	226/609 (37%)	225 (100%)	1 (0%)	84	82
87	A	151/190 (80%)	148 (98%)	3 (2%)	48	66
88	n	184/181 (102%)	182 (99%)	2 (1%)	65	74
All	All	11664/15966 (73%)	11567 (99%)	97 (1%)	70	77

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F3	193	LEU
6	F3	219	VAL
6	F3	222	THR

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Mol	Chain	Res	Type
6	F3	274	LEU
9	J3	108	VAL
9	J3	144	ILE
10	K3	81	THR
10	K3	175	ASP
11	L3	41	VAL
11	L3	105	VAL
12	M3	128	THR
12	M3	187	VAL
13	N3	83	THR
16	Q3	113	VAL
18	S3	70	VAL
18	S3	109	THR
18	S3	114	ILE
18	S3	154	VAL
19	T3	142	ILE
19	T3	166	ILE
19	T3	211	THR
20	U3	49	THR
20	U3	91	ASP
21	V3	53	ASP
21	V3	61	THR
22	W3	129	THR
23	X3	127	VAL
26	03	86	THR
26	03	105	ASN
27	13	16	ILE
27	13	54	VAL
31	53	365	ASP
32	63	171	VAL
32	63	297	THR
33	73	78	VAL
33	73	247	ASN
34	93	136	LEU
36	b3	14	VAL
36	b3	72	VAL
36	b3	123	ASN
38	d3	263	THR
38	d3	266	VAL
40	f3	50	THR
40	f3	90	VAL
40	f3	96	THR

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Mol	Chain	Res	Type
43	i3	32	ILE
43	i3	43	VAL
43	i3	44	VAL
45	k3	36	THR
45	k3	64	VAL
51	r3	152	THR
52	s3	52	THR
52	s3	206	VAL
52	s3	211	VAL
52	s3	288	THR
54	B6	71	ASP
54	B6	220	VAL
55	C6	88	GLU
56	D6	262	THR
56	D6	345	LEU
57	E6	99	THR
57	E6	111	VAL
58	F6	114	THR
59	G6	230	THR
59	G6	309	ASP
60	H6	79	LEU
61	I6	95	THR
62	J6	32	THR
62	J6	108	VAL
62	J6	121	VAL
65	M6	66	VAL
66	N6	31	THR
66	N6	77	VAL
66	N6	88	VAL
66	N6	91	VAL
71	S6	121	THR
74	V6	204	PHE
74	V6	250	ILE
74	V6	287	LEU
74	V6	390	ILE
76	X6	69	ASN
76	X6	155	ILE
76	X6	262	VAL
77	Y6	305	THR
77	Y6	324	ASP
77	Y6	353	LEU
80	b6	244	THR

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Mol	Chain	Res	Type
80	b6	296	VAL
81	c6	51	VAL
82	d6	130	VAL
83	e6	78	VAL
87	A	85	ILE
87	A	195	ILE
87	A	198	VAL
88	n	202[A]	GLU
88	n	202[B]	GLU
7	D	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (238) such sidechains are listed below:

Mol	Chain	Res	Type
4	D3	128	GLN
4	D3	165	ASN
4	D3	167	ASN
4	D3	194	ASN
4	D3	205	GLN
4	D3	233	GLN
4	D3	253	ASN
5	E3	52	HIS
5	E3	57	ASN
5	E3	115	GLN
5	E3	216	GLN
5	E3	227	GLN
5	E3	277	ASN
5	E3	280	HIS
6	F3	98	GLN
6	F3	130	GLN
6	F3	153	HIS
6	F3	184	GLN
6	F3	249	ASN
7	H3	88	HIS
8	I3	151	ASN
8	I3	189	GLN
9	J3	47	ASN
9	J3	126	GLN
10	K3	56	HIS
10	K3	61	ASN
10	K3	64	HIS
10	K3	160	GLN

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Mol	Chain	Res	Type
11	L3	113	ASN
12	M3	26	ASN
12	M3	102	GLN
12	M3	114	GLN
12	M3	120	GLN
13	N3	138	HIS
13	N3	178	GLN
14	O3	128	ASN
14	O3	158	GLN
15	P3	96	GLN
15	P3	161	GLN
16	Q3	107	HIS
16	Q3	209	GLN
16	Q3	237	ASN
16	Q3	262	GLN
17	R3	89	ASN
18	S3	75	HIS
18	S3	118	ASN
18	S3	140	ASN
19	T3	125	GLN
20	U3	4	ASN
20	U3	27	GLN
20	U3	41	GLN
20	U3	55	ASN
21	V3	73	GLN
21	V3	92	ASN
21	V3	117	HIS
22	W3	72	HIS
22	W3	80	HIS
22	W3	110	ASN
23	X3	53	ASN
23	X3	215	GLN
24	Y3	179	HIS
24	Y3	225	ASN
25	Z3	95	HIS
25	Z3	126	GLN
26	03	118	GLN
26	03	170	GLN
27	13	52	GLN
28	23	57	ASN
28	23	77	GLN
30	43	100	GLN

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Mol	Chain	Res	Type
30	43	102	GLN
31	53	65	HIS
31	53	109	HIS
31	53	156	ASN
31	53	384	GLN
31	53	420	HIS
32	63	44	ASN
32	63	243	ASN
32	63	292	GLN
32	63	308	GLN
32	63	351	HIS
33	73	55	GLN
33	73	298	GLN
34	93	123	GLN
34	93	134	ASN
35	a3	71	HIS
36	b3	24	GLN
36	b3	81	ASN
36	b3	149	GLN
37	c3	94	ASN
37	c3	172	ASN
38	d3	153	ASN
38	d3	274	GLN
39	e3	76	GLN
39	e3	199	ASN
40	f3	108	GLN
40	f3	115	ASN
40	f3	136	GLN
40	f3	153	HIS
40	f3	175	GLN
41	g3	73	GLN
41	g3	102	HIS
41	g3	104	ASN
41	g3	139	GLN
42	h3	118	HIS
42	h3	119	GLN
42	h3	135	GLN
43	i3	86	ASN
43	i3	89	GLN
44	j3	30	GLN
44	j3	63	GLN
45	k3	15	GLN

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Mol	Chain	Res	Type
45	k3	35	GLN
45	k3	57	HIS
48	o3	58	GLN
48	o3	85	HIS
48	o3	91	GLN
49	p3	53	GLN
49	p3	104	HIS
49	p3	143	GLN
50	q3	81	GLN
50	q3	137	GLN
51	r3	65	ASN
51	r3	130	ASN
52	s3	152	GLN
52	s3	179	GLN
52	s3	277	GLN
52	s3	296	HIS
52	s3	315	ASN
52	s3	420	GLN
54	B6	64	ASN
54	B6	74	ASN
54	B6	99	HIS
54	B6	120	GLN
54	B6	130	ASN
54	B6	150	GLN
54	B6	201	ASN
54	B6	226	ASN
54	B6	266	GLN
55	C6	126	GLN
56	D6	127	ASN
56	D6	155	GLN
56	D6	165	GLN
56	D6	273	ASN
56	D6	302	HIS
56	D6	415	GLN
58	F6	122	GLN
58	F6	147	GLN
58	F6	207	HIS
59	G6	242	GLN
59	G6	255	GLN
59	G6	308	GLN
59	G6	318	HIS
59	G6	366	GLN

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Mol	Chain	Res	Type
60	H6	130	HIS
60	H6	161	GLN
60	H6	163	ASN
60	H6	179	GLN
61	I6	87	HIS
61	I6	141	GLN
61	I6	146	HIS
61	I6	184	ASN
62	J6	74	ASN
64	L6	146	HIS
64	L6	169	ASN
67	O6	169	GLN
67	O6	181	HIS
67	O6	225	GLN
68	P6	71	HIS
68	P6	76	ASN
68	P6	104	GLN
69	Q6	4	HIS
69	Q6	18	ASN
69	Q6	27	ASN
69	Q6	85	GLN
70	R6	88	GLN
70	R6	221	GLN
70	R6	277	ASN
71	S6	97	GLN
72	T6	37	HIS
73	U6	43	ASN
73	U6	65	GLN
73	U6	109	ASN
73	U6	151	GLN
73	U6	172	ASN
74	V6	38	HIS
74	V6	97	HIS
74	V6	131	ASN
74	V6	141	ASN
74	V6	170	GLN
74	V6	203	ASN
74	V6	324	GLN
74	V6	338	HIS
74	V6	396	GLN
75	W6	86	HIS
75	W6	91	GLN

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Mol	Chain	Res	Type
75	W6	166	ASN
76	X6	52	ASN
76	X6	67	HIS
76	X6	81	HIS
76	X6	266	ASN
76	X6	302	HIS
76	X6	312	GLN
76	X6	368	HIS
76	X6	385	ASN
76	X6	387	ASN
77	Y6	290	ASN
77	Y6	303	GLN
77	Y6	331	HIS
78	Z6	63	GLN
78	Z6	82	GLN
79	a6	24	GLN
79	a6	66	GLN
79	a6	107	GLN
80	b6	165	ASN
80	b6	268	GLN
80	b6	301	ASN
80	b6	305	ASN
80	b6	311	GLN
81	c6	24	ASN
81	c6	31	ASN
81	c6	71	GLN
81	c6	81	GLN
81	c6	90	GLN
82	d6	129	ASN
82	d6	158	GLN
82	d6	166	GLN
83	e6	72	GLN
83	e6	79	ASN
83	e6	436	HIS
83	e6	455	ASN
87	A	127	GLN
87	A	143	GLN
88	n	56	GLN
88	n	66	HIS
88	n	71	GLN
88	n	199	HIS
7	D	185	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A3	1490/1559 (95%)	452 (30%)	29 (1%)
3	B3	52/69 (75%)	19 (36%)	1 (1%)
84	A6	921/954 (96%)	245 (26%)	16 (1%)
85	24	73/73 (100%)	40 (54%)	1 (1%)
85	C	73/73 (100%)	40 (54%)	1 (1%)
86	i4	9/10 (90%)	4 (44%)	0
All	All	2618/2738 (95%)	800 (30%)	48 (1%)

All (800) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A3	1672	C
2	A3	1674	A
2	A3	1676	A
2	A3	1678	C
2	A3	1679	U
2	A3	1680	A
2	A3	1681	G
2	A3	1689	C
2	A3	1690	C
2	A3	1693	C
2	A3	1694	U
2	A3	1699	C
2	A3	1700	U
2	A3	1701	U
2	A3	1704	U
2	A3	1705	A
2	A3	1708	A
2	A3	1709	G
2	A3	1713	A
2	A3	1714	C
2	A3	1715	C
2	A3	1716	U
2	A3	1717	U
2	A3	1724	A
2	A3	1727	A
2	A3	1728	U
2	A3	1732	C
2	A3	1748	G
2	A3	1750	G
2	A3	1751	A

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Mol	Chain	Res	Type
2	A3	1767	G
2	A3	1770	G
2	A3	1774	U
2	A3	1777	A
2	A3	1779	A
2	A3	1780	U
2	A3	1781	A
2	A3	1794	A
2	A3	1804	A
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1808	A
2	A3	1809	U
2	A3	1810	A
2	A3	1811	A
2	A3	1812	C
2	A3	1821	A
2	A3	1824	U
2	A3	1827	C
2	A3	1828	A
2	A3	1829	A
2	A3	1832	A
2	A3	1836	A
2	A3	1844	A
2	A3	1846	C
2	A3	1852	C
2	A3	1854	U
2	A3	1856	A
2	A3	1867	A
2	A3	1869	A
2	A3	1870	A
2	A3	1872	U
2	A3	1873	A
2	A3	1874	A
2	A3	1878	U
2	A3	1882	A
2	A3	1883	G
2	A3	1886	G
2	A3	1887	A
2	A3	1888	G
2	A3	1890	C

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Mol	Chain	Res	Type
2	A3	1893	A
2	A3	1901	C
2	A3	1902	C
2	A3	1903	C
2	A3	1909	A
2	A3	1918	G
2	A3	1939	G
2	A3	1940	A
2	A3	1944	C
2	A3	1956	U
2	A3	1966	G
2	A3	1968	G
2	A3	1970	G
2	A3	1974	A
2	A3	1975	U
2	A3	1985	G
2	A3	1987	G
2	A3	1992	C
2	A3	1993	A
2	A3	1994	A
2	A3	1995	A
2	A3	1998	U
2	A3	2000	C
2	A3	2001	C
2	A3	2002	G
2	A3	2010	U
2	A3	2015	G
2	A3	2021	U
2	A3	2022	G
2	A3	2029	A
2	A3	2031	A
2	A3	2032	G
2	A3	2034	A
2	A3	2036	C
2	A3	2037	U
2	A3	2039	A
2	A3	2055	U
2	A3	2060	A
2	A3	2065	A
2	A3	2074	A
2	A3	2079	C
2	A3	2083	U

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Mol	Chain	Res	Type
2	A3	2085	A
2	A3	2092	C
2	A3	2093	U
2	A3	2097	A
2	A3	2098	G
2	A3	2099	U
2	A3	2105	G
2	A3	2111	C
2	A3	2113	G
2	A3	2124	A
2	A3	2132	A
2	A3	2135	A
2	A3	2139	U
2	A3	2140	G
2	A3	2142	A
2	A3	2143	G
2	A3	2147	G
2	A3	2154	A
2	A3	2157	U
2	A3	2159	U
2	A3	2163	A
2	A3	2165	C
2	A3	2166	C
2	A3	2168	U
2	A3	2169	A
2	A3	2171	U
2	A3	2172	A
2	A3	2173	G
2	A3	2174	G
2	A3	2177	U
2	A3	2179	A
2	A3	2180	A
2	A3	2181	A
2	A3	2183	C
2	A3	2187	C
2	A3	2193	U
2	A3	2194	U
2	A3	2195	A
2	A3	2197	G
2	A3	2198	A
2	A3	2200	A
2	A3	2201	G

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Mol	Chain	Res	Type
2	A3	2202	C
2	A3	2204	U
2	A3	2207	A
2	A3	2209	G
2	A3	2210	C
2	A3	2216	A
2	A3	2217	C
2	A3	2229	A
2	A3	2230	A
2	A3	2237	A
2	A3	2239	A
2	A3	2241	A
2	A3	2243	A
2	A3	2244	U
2	A3	2245	A
2	A3	2246	A
2	A3	2262	C
2	A3	2263	C
2	A3	2283	C
2	A3	2284	C
2	A3	2285	U
2	A3	2290	A
2	A3	2294	A
2	A3	2296	U
2	A3	2297	A
2	A3	2300	G
2	A3	2309	A
2	A3	2315	A
2	A3	2322	C
2	A3	2324	U
2	A3	2331	C
2	A3	2332	C
2	A3	2342	U
2	A3	2345	G
2	A3	2349	G
2	A3	2364	C
2	A3	2369	A
2	A3	2370	A
2	A3	2371	U
2	A3	2372	U
2	A3	2373	A
2	A3	2374	A

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Mol	Chain	Res	Type
2	A3	2375	C
2	A3	2379	C
2	A3	2380	C
2	A3	2381	A
2	A3	2384	A
2	A3	2387	U
2	A3	2390	A
2	A3	2393	C
2	A3	2396	C
2	A3	2397	C
2	A3	2401	A
2	A3	2404	U
2	A3	2405	C
2	A3	2407	U
2	A3	2410	U
2	A3	2414	C
2	A3	2415	C
2	A3	2416	U
2	A3	2417	C
2	A3	2418	A
2	A3	2426	C
2	A3	2427	C
2	A3	2434	A
2	A3	2435	G
2	A3	2443	C
2	A3	2444	A
2	A3	2446	A
2	A3	2447	A
2	A3	2449	G
2	A3	2455	U
2	A3	2458	A
2	A3	2464	G
2	A3	2478	G
2	A3	2485	U
2	A3	2493	C
2	A3	2500	A
2	A3	2506	A
2	A3	2507	A
2	A3	2508	C
2	A3	2511	C
2	A3	2520	C
2	A3	2521	A

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Mol	Chain	Res	Type
2	A3	2522	U
2	A3	2523	C
2	A3	2524	A
2	A3	2526	C
2	A3	2527	A
2	A3	2530	A
2	A3	2531	U
2	A3	2532	U
2	A3	2536	G
2	A3	2539	A
2	A3	2540	C
2	A3	2544	C
2	A3	2546	G
2	A3	2556	A
2	A3	2557	C
2	A3	2558	A
2	A3	2559	U
2	A3	2560	G
2	A3	2563	U
2	A3	2569	C
2	A3	2570	C
2	A3	2581	A
2	A3	2582	A
2	A3	2586	U
2	A3	2587	G
2	A3	2588	C
2	A3	2592	G
2	A3	2593	G
2	A3	2594	U
2	A3	2596	G
2	A3	2600	A
2	A3	2601	A
2	A3	2603	C
2	A3	2607	U
2	A3	2618	U
2	A3	2626	U
2	A3	2629	A
2	A3	2632	A
2	A3	2633	A
2	A3	2634	U
2	A3	2635	G
2	A3	2644	A

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Mol	Chain	Res	Type
2	A3	2645	G
2	A3	2652	G
2	A3	2654	U
2	A3	2655	G
2	A3	2656	U
2	A3	2660	U
2	A3	2661	U
2	A3	2676	A
2	A3	2684	C
2	A3	2686	G
2	A3	2694	A
2	A3	2695	G
2	A3	2696	A
2	A3	2697	G
2	A3	2706	A
2	A3	2708	C
2	A3	2709	A
2	A3	2713	C
2	A3	2718	C
2	A3	2719	G
2	A3	2723	A
2	A3	2724	G
2	A3	2725	A
2	A3	2726	C
2	A3	2732	G
2	A3	2733	G
2	A3	2739	U
2	A3	2740	A
2	A3	2745	A
2	A3	2746	U
2	A3	2749	A
2	A3	2750	U
2	A3	2753	A
2	A3	2755	A
2	A3	2757	A
2	A3	2758	G
2	A3	2761	C
2	A3	2762	C
2	A3	2763	U
2	A3	2764	A
2	A3	2765	A
2	A3	2766	C

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Mol	Chain	Res	Type
2	A3	2767	A
2	A3	2768	A
2	A3	2769	A
2	A3	2770	C
2	A3	2773	A
2	A3	2774	C
2	A3	2775	A
2	A3	2776	G
2	A3	2777	G
2	A3	2778	U
2	A3	2779	C
2	A3	2780	C
2	A3	2781	U
2	A3	2782	A
2	A3	2784	A
2	A3	2785	C
2	A3	2786	U
2	A3	2789	C
2	A3	2790	A
2	A3	2791	A
2	A3	2792	A
2	A3	2804	A
2	A3	2810	G
2	A3	2831	G
2	A3	2832	A
2	A3	2833	A
2	A3	2842	C
2	A3	2844	G
2	A3	2847	C
2	A3	2851	A
2	A3	2854	U
2	A3	2861	A
2	A3	2864	U
2	A3	2865	C
2	A3	2869	A
2	A3	2870	G
2	A3	2871	U
2	A3	2872	C
2	A3	2879	A
2	A3	2881	C
2	A3	2892	A
2	A3	2901	A

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Mol	Chain	Res	Type
2	A3	2906	C
2	A3	2909	G
2	A3	2910	A
2	A3	2913	A
2	A3	2916	G
2	A3	2917	G
2	A3	2918	A
2	A3	2919	A
2	A3	2922	A
2	A3	2925	U
2	A3	2926	A
2	A3	2928	C
2	A3	2932	G
2	A3	2934	G
2	A3	2935	A
2	A3	2936	U
2	A3	2937	A
2	A3	2938	A
2	A3	2955	U
2	A3	2956	A
2	A3	2963	A
2	A3	2965	A
2	A3	2978	U
2	A3	2981	A
2	A3	2985	C
2	A3	2989	G
2	A3	2990	A
2	A3	2991	U
2	A3	2992	G
2	A3	2994	U
2	A3	2998	U
2	A3	3001	G
2	A3	3005	A
2	A3	3016	G
2	A3	3017	C
2	A3	3022	G
2	A3	3029	A
2	A3	3041	U
2	A3	3042	U
2	A3	3051	A
2	A3	3053	A
2	A3	3054	G

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Mol	Chain	Res	Type
2	A3	3056	C
2	A3	3059	A
2	A3	3060	C
2	A3	3069	A
2	A3	3070	G
2	A3	3071	U
2	A3	3077	C
2	A3	3084	A
2	A3	3086	U
2	A3	3089	A
2	A3	3093	C
2	A3	3095	G
2	A3	3096	U
2	A3	3100	U
2	A3	3102	U
2	A3	3109	U
2	A3	3114	U
2	A3	3123	G
2	A3	3129	A
2	A3	3135	A
2	A3	3141	A
2	A3	3147	G
2	A3	3150	U
2	A3	3155	C
2	A3	3157	C
2	A3	3158	A
2	A3	3160	A
2	A3	3162	C
2	A3	3168	C
2	A3	3169	C
2	A3	3172	C
2	A3	3180	A
2	A3	3184	C
2	A3	3189	C
2	A3	3190	A
2	A3	3202	U
2	A3	3204	C
2	A3	3206	C
2	A3	3207	A
2	A3	3217	A
2	A3	3218	A
2	A3	3221	A

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Mol	Chain	Res	Type
2	A3	3223	A
2	A3	3228	U
3	B3	1607	U
3	B3	1608	G
3	B3	1609	U
3	B3	1611	G
3	B3	1614	U
3	B3	1615	A
3	B3	1625	A
3	B3	1630	A
3	B3	1632	U
3	B3	1634	A
3	B3	1641	G
3	B3	1644	G
3	B3	1645	A
3	B3	1646	U
3	B3	1650	A
3	B3	1663	C
3	B3	1665	C
3	B3	1667	C
3	B3	1669	G
84	A6	654	U
84	A6	655	A
84	A6	662	G
84	A6	665	C
84	A6	675	U
84	A6	677	U
84	A6	678	U
84	A6	684	U
84	A6	692	A
84	A6	693	U
84	A6	694	U
84	A6	708	U
84	A6	715	U
84	A6	716	C
84	A6	722	A
84	A6	725	U
84	A6	726	C
84	A6	738	C
84	A6	745	A
84	A6	749	A
84	A6	757	A

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Mol	Chain	Res	Type
84	A6	761	A
84	A6	762	U
84	A6	765	A
84	A6	768	A
84	A6	770	G
84	A6	777	U
84	A6	781	G
84	A6	787	A
84	A6	795	G
84	A6	797	C
84	A6	798	U
84	A6	800	G
84	A6	811	A
84	A6	812	C
84	A6	817	A
84	A6	818	A
84	A6	819	C
84	A6	820	A
84	A6	821	G
84	A6	831	A
84	A6	833	C
84	A6	834	U
84	A6	836	U
84	A6	839	C
84	A6	840	A
84	A6	851	G
84	A6	857	C
84	A6	860	A
84	A6	870	A
84	A6	872	C
84	A6	874	C
84	A6	884	C
84	A6	885	A
84	A6	887	U
84	A6	890	C
84	A6	894	C
84	A6	895	C
84	A6	897	G
84	A6	901	C
84	A6	903	G
84	A6	906	G
84	A6	907	U

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Mol	Chain	Res	Type
84	A6	908	C
84	A6	909	A
84	A6	923	A
84	A6	942	A
84	A6	943	A
84	A6	945	G
84	A6	946	A
84	A6	947	G
84	A6	951	U
84	A6	952	U
84	A6	954	A
84	A6	957	U
84	A6	959	A
84	A6	970	A
84	A6	971	A
84	A6	982	A
84	A6	992	G
84	A6	996	U
84	A6	1000	A
84	A6	1005	C
84	A6	1006	C
84	A6	1014	A
84	A6	1015	C
84	A6	1018	A
84	A6	1019	A
84	A6	1025	U
84	A6	1026	A
84	A6	1032	G
84	A6	1045	A
84	A6	1046	U
84	A6	1050	A
84	A6	1052	C
84	A6	1054	C
84	A6	1069	C
84	A6	1085	U
84	A6	1086	A
84	A6	1102	C
84	A6	1106	A
84	A6	1107	A
84	A6	1109	C
84	A6	1110	C
84	A6	1113	A

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Mol	Chain	Res	Type
84	A6	1125	A
84	A6	1127	C
84	A6	1129	A
84	A6	1130	A
84	A6	1133	U
84	A6	1142	G
84	A6	1146	A
84	A6	1155	C
84	A6	1158	A
84	A6	1171	A
84	A6	1179	G
84	A6	1183	G
84	A6	1184	U
84	A6	1189	C
84	A6	1191	U
84	A6	1192	A
84	A6	1193	U
84	A6	1194	C
84	A6	1196	C
84	A6	1197	U
84	A6	1198	C
84	A6	1212	U
84	A6	1218	A
84	A6	1219	U
84	A6	1224	A
84	A6	1225	A
84	A6	1226	A
84	A6	1227	C
84	A6	1229	C
84	A6	1232	A
84	A6	1233	U
84	A6	1234	C
84	A6	1235	A
84	A6	1236	A
84	A6	1240	C
84	A6	1249	U
84	A6	1250	U
84	A6	1251	G
84	A6	1252	C
84	A6	1254	C
84	A6	1255	A
84	A6	1261	U

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Mol	Chain	Res	Type
84	A6	1265	C
84	A6	1268	C
84	A6	1269	C
84	A6	1274	U
84	A6	1275	C
84	A6	1276	A
84	A6	1280	A
84	A6	1286	G
84	A6	1287	A
84	A6	1288	U
84	A6	1289	G
84	A6	1291	A
84	A6	1294	C
84	A6	1296	A
84	A6	1297	C
84	A6	1299	A
84	A6	1300	A
84	A6	1301	G
84	A6	1304	A
84	A6	1311	G
84	A6	1330	A
84	A6	1331	G
84	A6	1332	G
84	A6	1334	C
84	A6	1336	A
84	A6	1345	C
84	A6	1346	C
84	A6	1347	A
84	A6	1348	U
84	A6	1356	C
84	A6	1357	A
84	A6	1358	A
84	A6	1359	G
84	A6	1360	A
84	A6	1371	A
84	A6	1372	U
84	A6	1373	U
84	A6	1380	C
84	A6	1381	C
84	A6	1382	C
84	A6	1385	A
84	A6	1394	A

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Mol	Chain	Res	Type
84	A6	1397	G
84	A6	1406	A
84	A6	1420	A
84	A6	1424	U
84	A6	1426	G
84	A6	1428	U
84	A6	1434	A
84	A6	1441	U
84	A6	1451	G
84	A6	1452	U
84	A6	1456	U
84	A6	1458	G
84	A6	1465	A
84	A6	1466	G
84	A6	1469	C
84	A6	1470	C
84	A6	1473	G
84	A6	1485	C
84	A6	1486	A
84	A6	1490	C
84	A6	1507	G
84	A6	1516	A
84	A6	1519	G
84	A6	1521	A
84	A6	1525	U
84	A6	1529	C
84	A6	1530	U
84	A6	1531	A
84	A6	1536	C
84	A6	1537	C
84	A6	1539	U
84	A6	1540	A
84	A6	1541	C
84	A6	1542	G
84	A6	1543	C
84	A6	1544	A
84	A6	1551	U
84	A6	1553	G
84	A6	1556	G
84	A6	1559	A
84	A6	1561	A
84	A6	1562	A

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Mol	Chain	Res	Type
84	A6	1563	G
84	A6	1566	G
84	A6	1567	U
84	A6	1568	A
84	A6	1572	U
84	A6	1575	U
84	A6	1576	A
84	A6	1586	G
84	A6	1588	A
84	A6	1589	A
84	A6	1598	G
84	A6	1599	G
84	A6	1603	A
84	A6	1604	A
85	24	2	U
85	24	3	U
85	24	7	G
85	24	8	U
85	24	9	A
85	24	12	U
85	24	13	U
85	24	14	A
85	24	16	A
85	24	17	U
85	24	18	U
85	24	19	A
85	24	20	U
85	24	21	C
85	24	22	A
85	24	27	A
85	24	28	A
85	24	29	G
85	24	31	C
85	24	32	A
85	24	33	C
85	24	38	A
85	24	40	U
85	24	41	G
85	24	45	A
85	24	46	G
85	24	47	A
85	24	50	A

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Mol	Chain	Res	Type
85	24	51	G
85	24	52	C
85	24	55	C
85	24	56	A
85	24	57	C
85	24	58	A
85	24	59	G
85	24	60	C
85	24	62	C
85	24	67	A
85	24	71	C
85	24	73	A
86	i4	17	A
86	i4	22	A
86	i4	23	A
86	i4	24	A
85	C	2	U
85	C	3	U
85	C	7	G
85	C	8	U
85	C	9	A
85	C	12	U
85	C	13	U
85	C	14	A
85	C	16	A
85	C	17	U
85	C	18	U
85	C	19	A
85	C	20	U
85	C	21	C
85	C	22	A
85	C	27	A
85	C	28	A
85	C	29	G
85	C	31	C
85	C	32	A
85	C	33	C
85	C	38	A
85	C	40	U
85	C	41	G
85	C	45	A
85	C	46	G

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Mol	Chain	Res	Type
85	C	47	A
85	C	50	A
85	C	51	G
85	C	52	C
85	C	55	C
85	C	56	A
85	C	57	C
85	C	58	A
85	C	59	G
85	C	60	C
85	C	62	C
85	C	67	A
85	C	71	C
85	C	73	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A3	1703	C
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1809	U
2	A3	1823	A
2	A3	1871	A
2	A3	1901	C
2	A3	2165	C
2	A3	2172	A
2	A3	2186	C
2	A3	2243	A
2	A3	2245	A
2	A3	2374	A
2	A3	2507	A
2	A3	2523	C
2	A3	2530	A
2	A3	2558	A
2	A3	2559	U
2	A3	2628	U
2	A3	2653	C
2	A3	2744	U
2	A3	2788	C
2	A3	2789	C

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Mol	Chain	Res	Type
2	A3	2905	A
2	A3	2989	G
2	A3	3041	U
2	A3	3092	U
2	A3	3201	A
3	B3	1607	U
84	A6	721	G
84	A6	797	C
84	A6	818	A
84	A6	886	A
84	A6	906	G
84	A6	1025	U
84	A6	1045	A
84	A6	1170	A
84	A6	1193	U
84	A6	1249	U
84	A6	1250	U
84	A6	1335	A
84	A6	1419	G
84	A6	1433	C
84	A6	1538	C
84	A6	1541	C
85	24	1	G
85	C	1	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 141 are monoatomic - leaving 5 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	$\# Z > 2$
93	MLI	n	303	-	6,6,6	1.30	0	7,7,7	1.20	0
93	MLI	n	304	-	6,6,6	1.41	0	7,7,7	1.24	0
91	GDP	X6	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.92	9 (20%)
93	MLI	n	302	-	6,6,6	1.25	0	7,7,7	1.22	0
92	SO4	n	301	-	4,4,4	0.22	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	MLI	n	303	-	-	4/4/4/4	-
93	MLI	n	302	-	-	2/4/4/4	-
93	MLI	n	304	-	-	2/4/4/4	-
91	GDP	X6	500	-	-	8/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	X6	500	GDP	C5-C4	2.97	1.46	1.38
91	X6	500	GDP	C6-N1	-2.89	1.33	1.38
91	X6	500	GDP	C5-N7	-2.10	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	X6	500	GDP	C5-C4-N3	-6.69	117.74	128.39
91	X6	500	GDP	N9-C4-N3	5.39	136.74	125.95
91	X6	500	GDP	C2-N3-C4	5.23	121.31	112.30
91	X6	500	GDP	C2'-C1'-N9	-2.82	105.41	113.25
91	X6	500	GDP	C6-C5-N7	2.59	135.01	130.29
91	X6	500	GDP	O6-C6-C5	-2.53	119.85	126.53
91	X6	500	GDP	C3'-C2'-C1'	2.45	106.11	101.46
91	X6	500	GDP	C5-C6-N1	2.24	118.95	113.25
91	X6	500	GDP	C2-N1-C6	-2.11	121.28	125.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

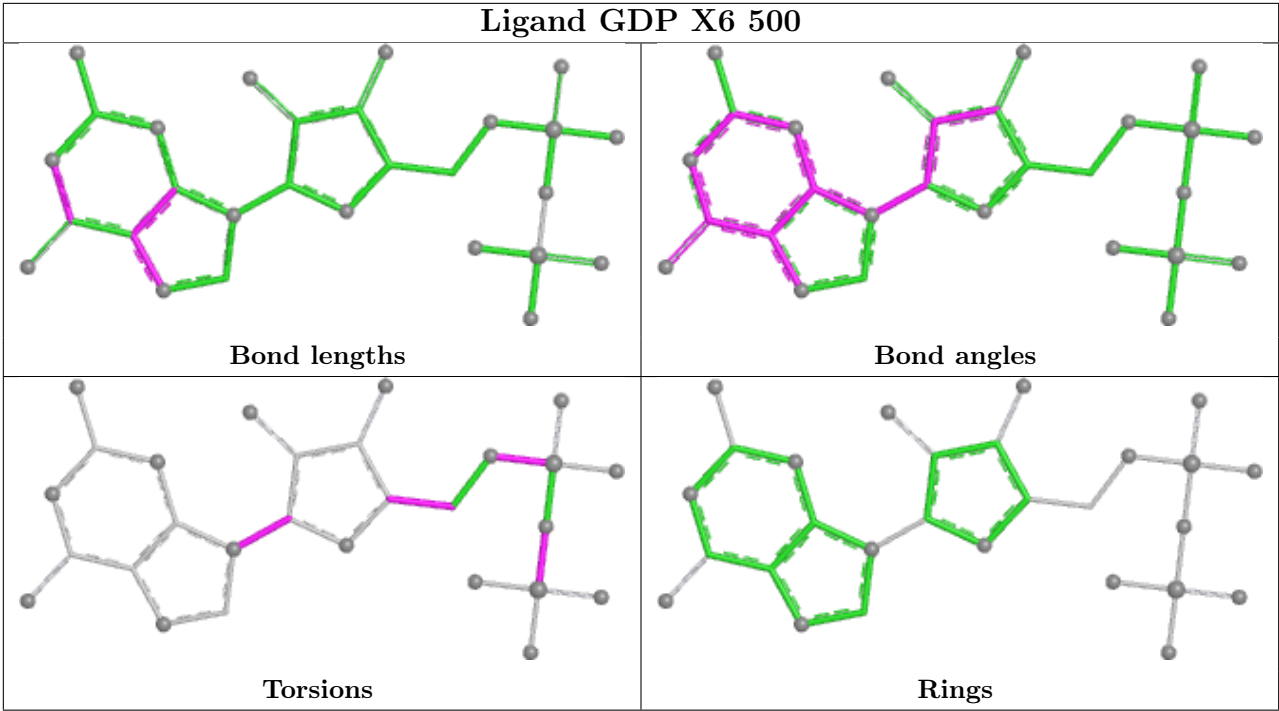
Mol	Chain	Res	Type	Atoms
91	X6	500	GDP	PA-O3A-PB-O2B
91	X6	500	GDP	PA-O3A-PB-O3B
91	X6	500	GDP	C5'-O5'-PA-O3A
91	X6	500	GDP	O4'-C1'-N9-C8
91	X6	500	GDP	O4'-C1'-N9-C4
91	X6	500	GDP	C3'-C4'-C5'-O5'
91	X6	500	GDP	O4'-C4'-C5'-O5'
93	n	302	MLI	C2-C1-C3-O8
93	n	302	MLI	C2-C1-C3-O9
93	n	304	MLI	C2-C1-C3-O8
93	n	303	MLI	C3-C1-C2-O6
93	n	304	MLI	C2-C1-C3-O9
91	X6	500	GDP	C5'-O5'-PA-O1A
93	n	303	MLI	C3-C1-C2-O7
93	n	303	MLI	C2-C1-C3-O8
93	n	303	MLI	C2-C1-C3-O9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	X6	500	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
76	X6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X6	323:TYR	C	324:LEU	N	1.19

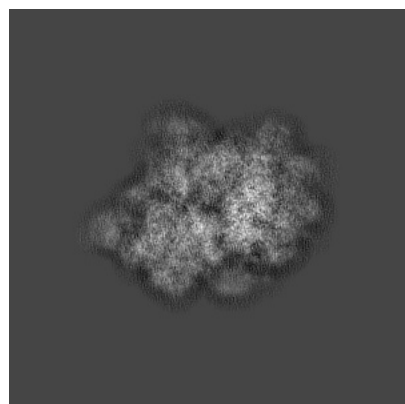
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11641. These allow visual inspection of the internal detail of the map and identification of artifacts.

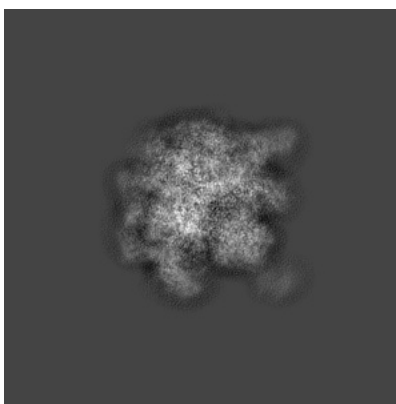
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

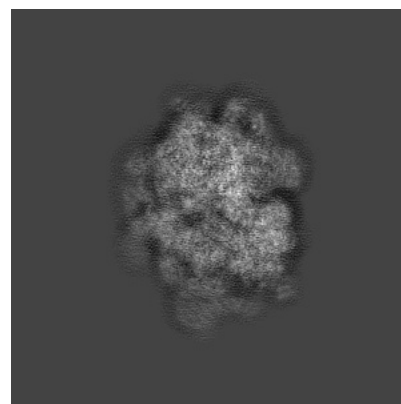
6.1.1 Primary map



X

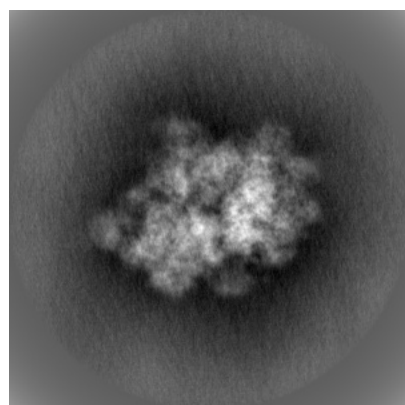


Y

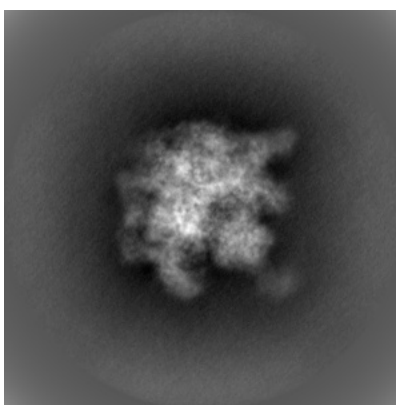


Z

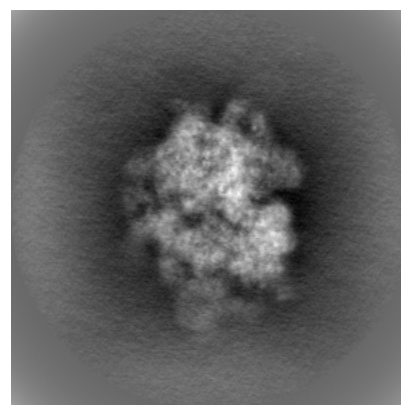
6.1.2 Raw map



X



Y

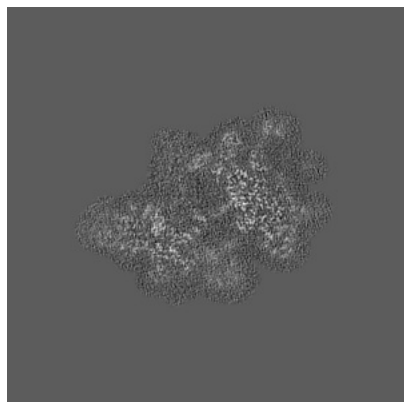


Z

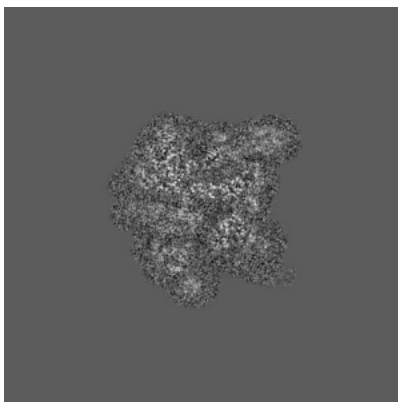
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

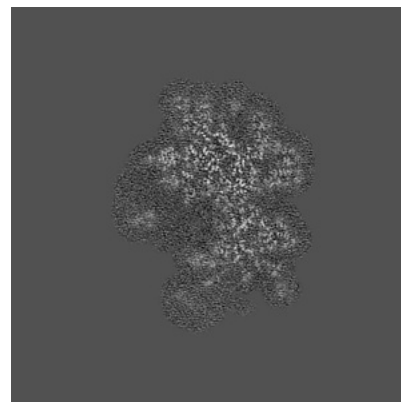
6.2.1 Primary map



X Index: 256

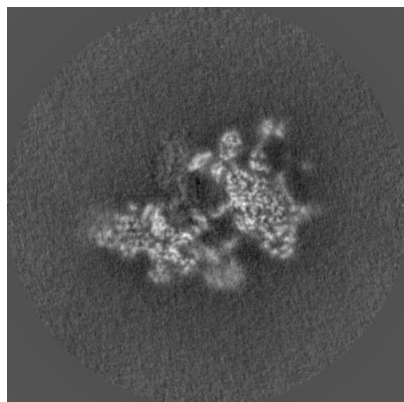


Y Index: 256

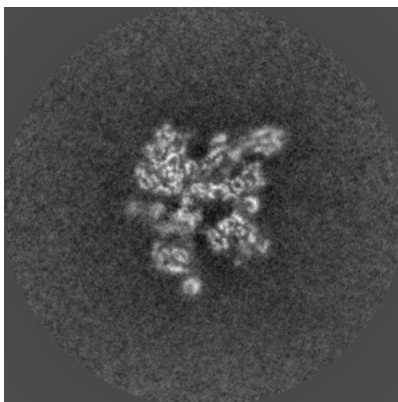


Z Index: 256

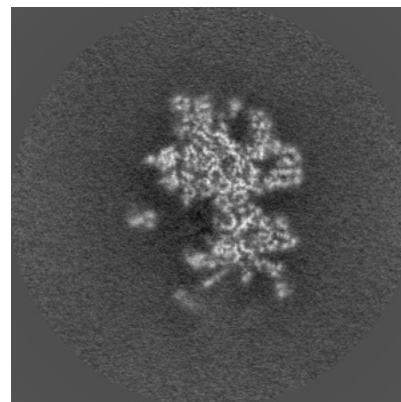
6.2.2 Raw map



X Index: 256



Y Index: 256

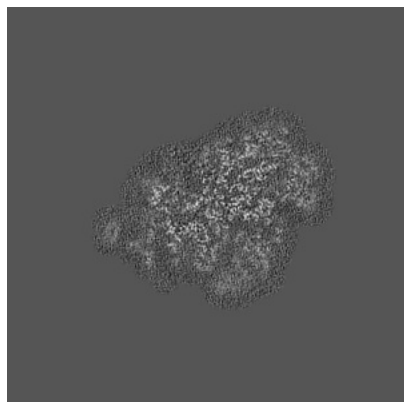


Z Index: 256

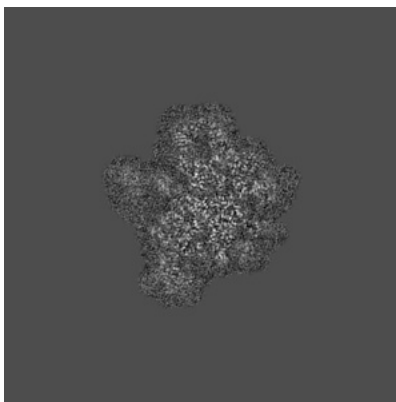
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

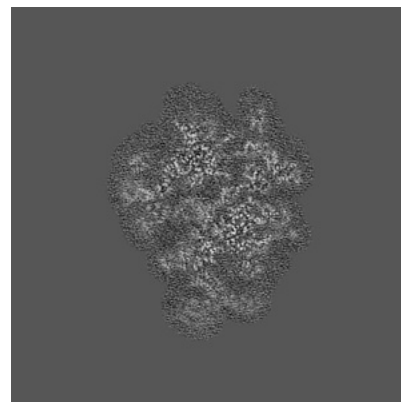
6.3.1 Primary map



X Index: 284

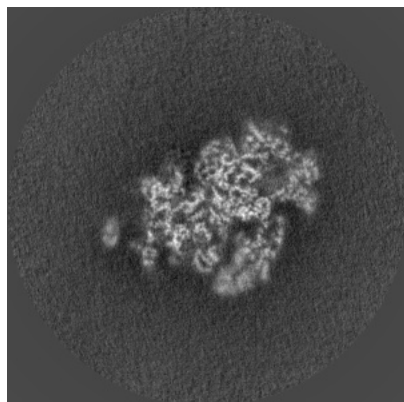


Y Index: 305

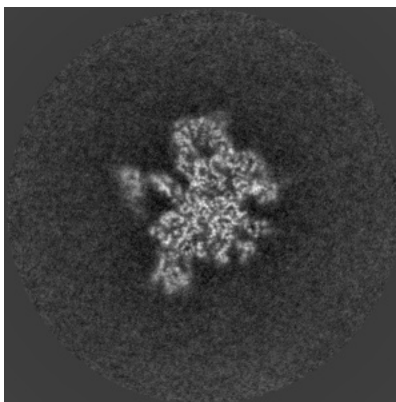


Z Index: 228

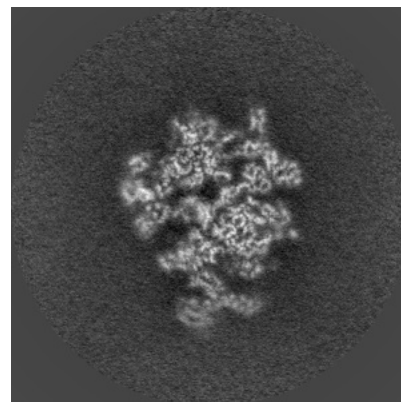
6.3.2 Raw map



X Index: 287



Y Index: 304

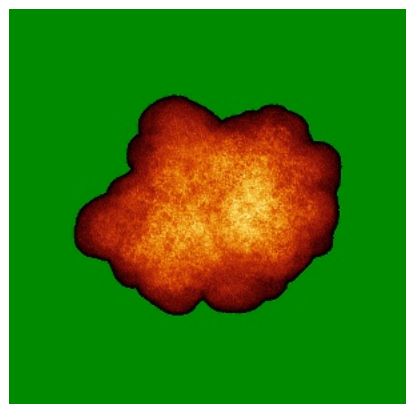


Z Index: 228

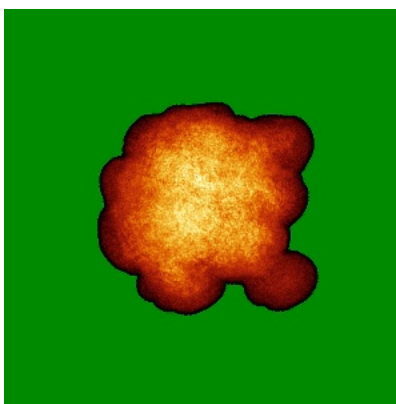
The images above show the largest variance slices of the map in three orthogonal directions.

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

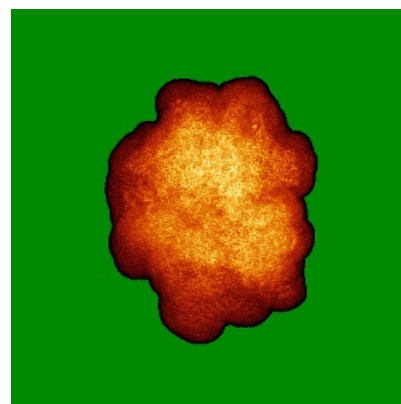
6.4.1 Primary map



X

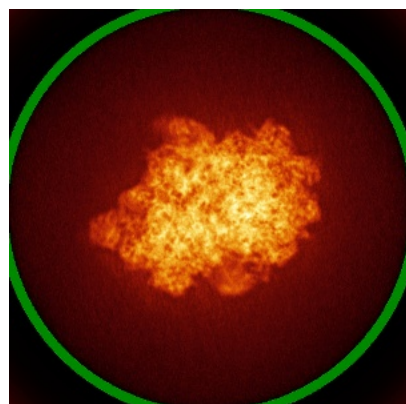


Y

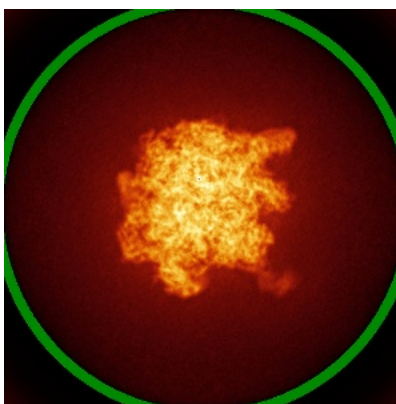


Z

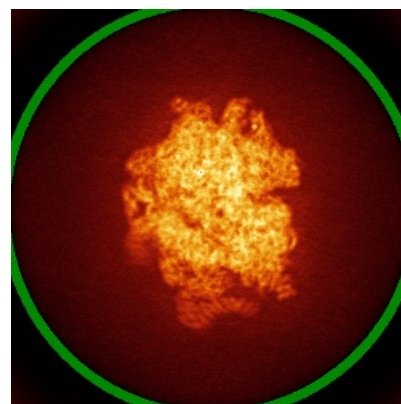
6.4.2 Raw map



X



Y

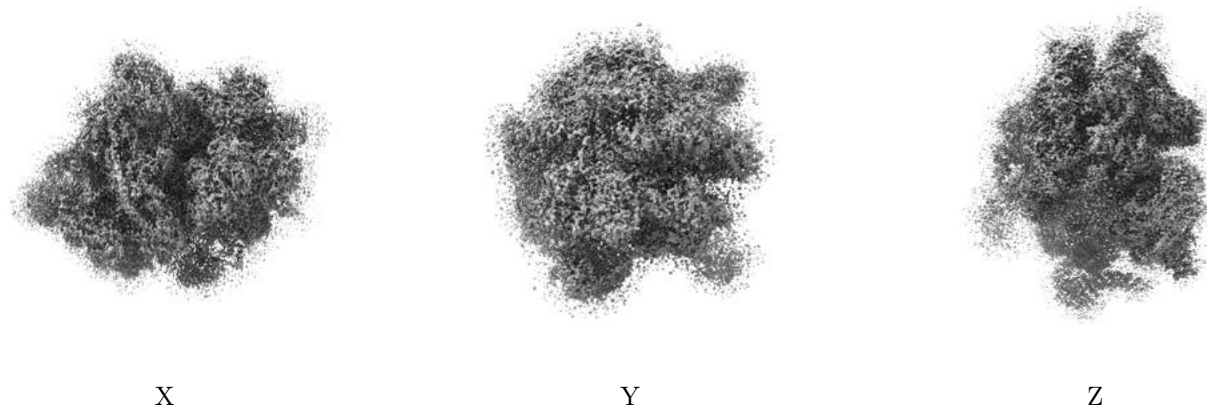


Z

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 0.05. 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.

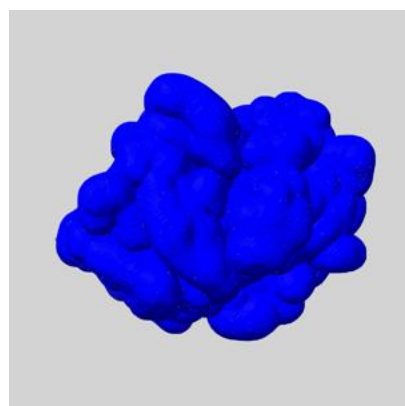
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

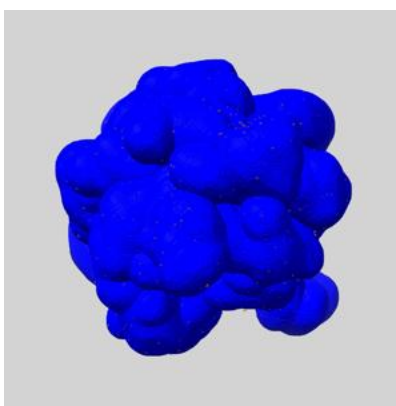
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

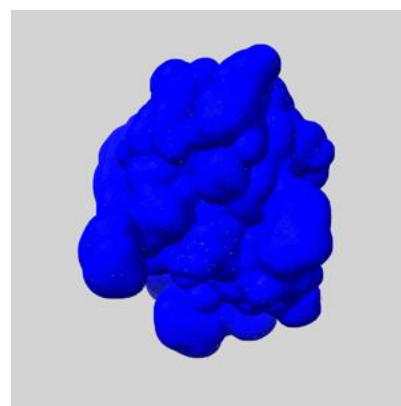
6.6.1 emd_11641_msk_1.map [i](#)



X



Y

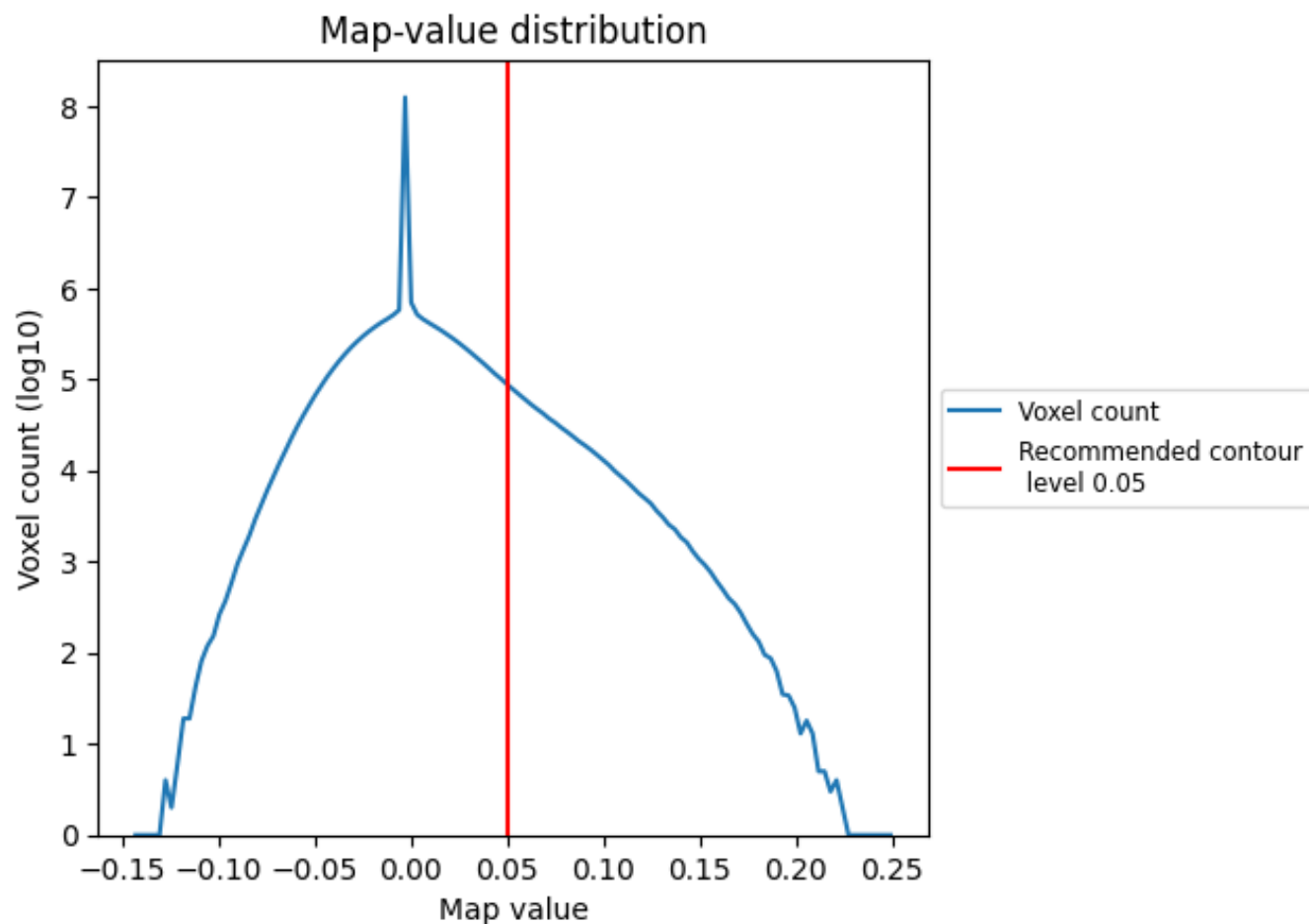


Z

7 Map analysis [i](#)

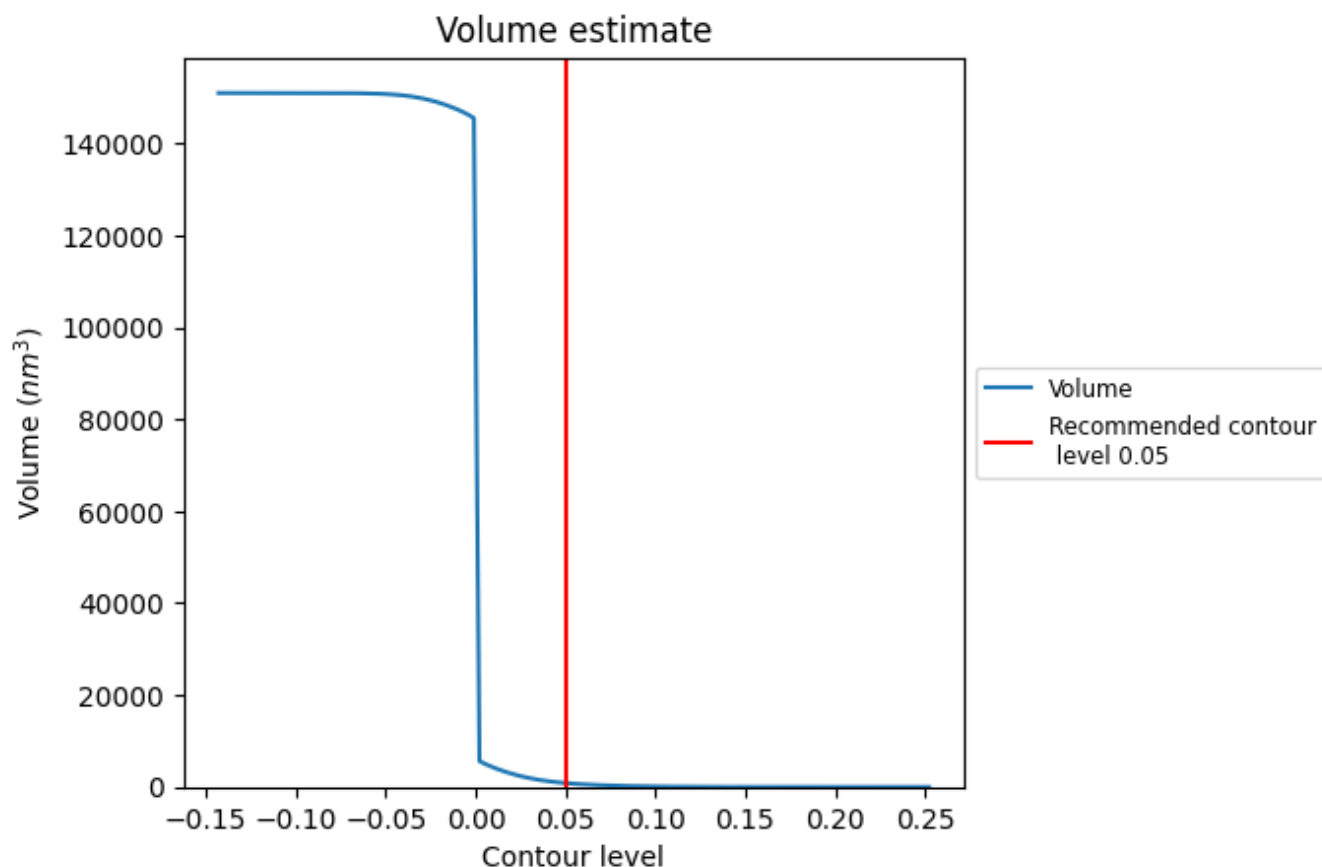
This section contains the results of statistical analysis of the map.

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.

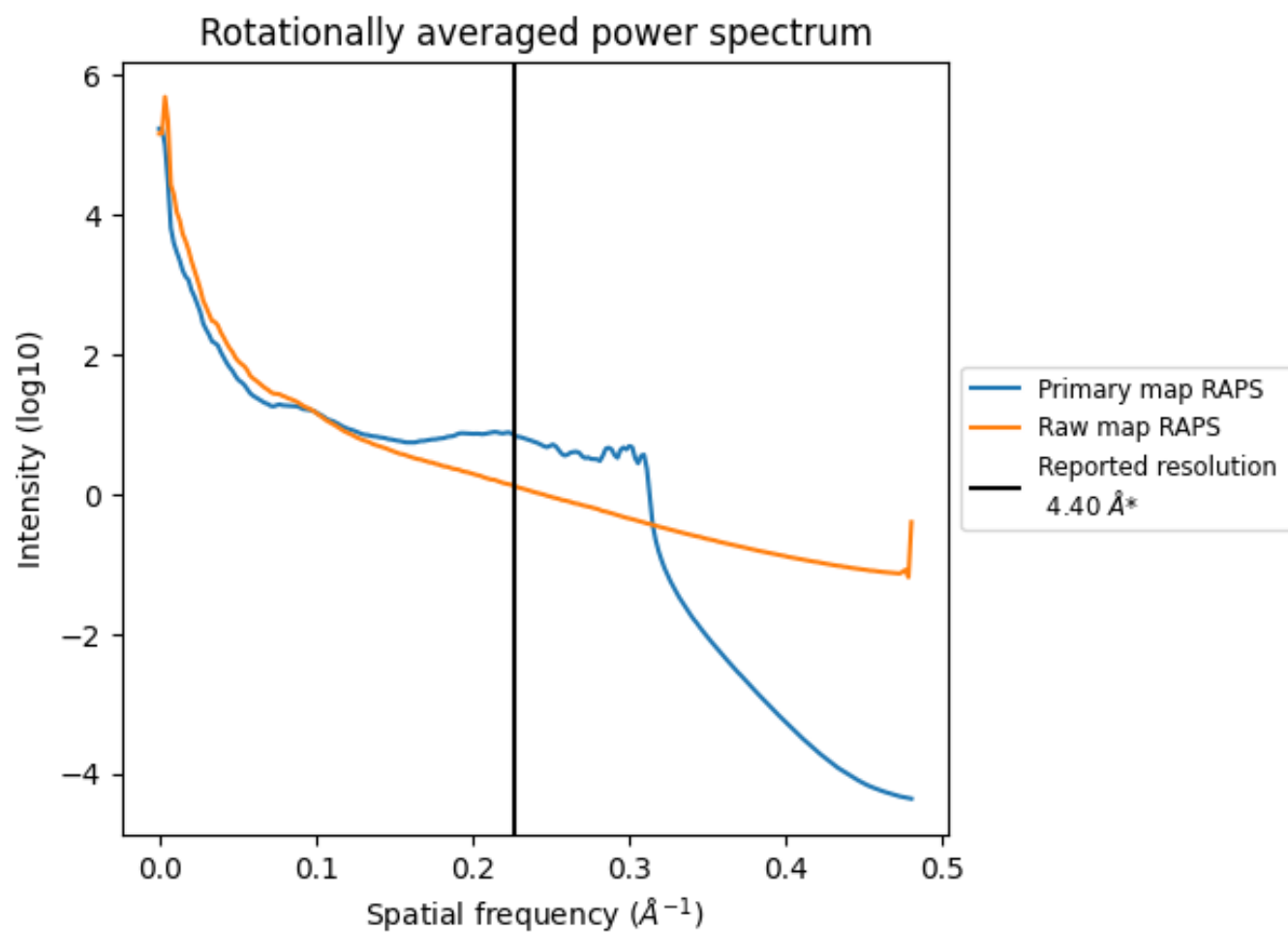
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 848 nm^3 ; this corresponds to an approximate mass of 766 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 ⓘ

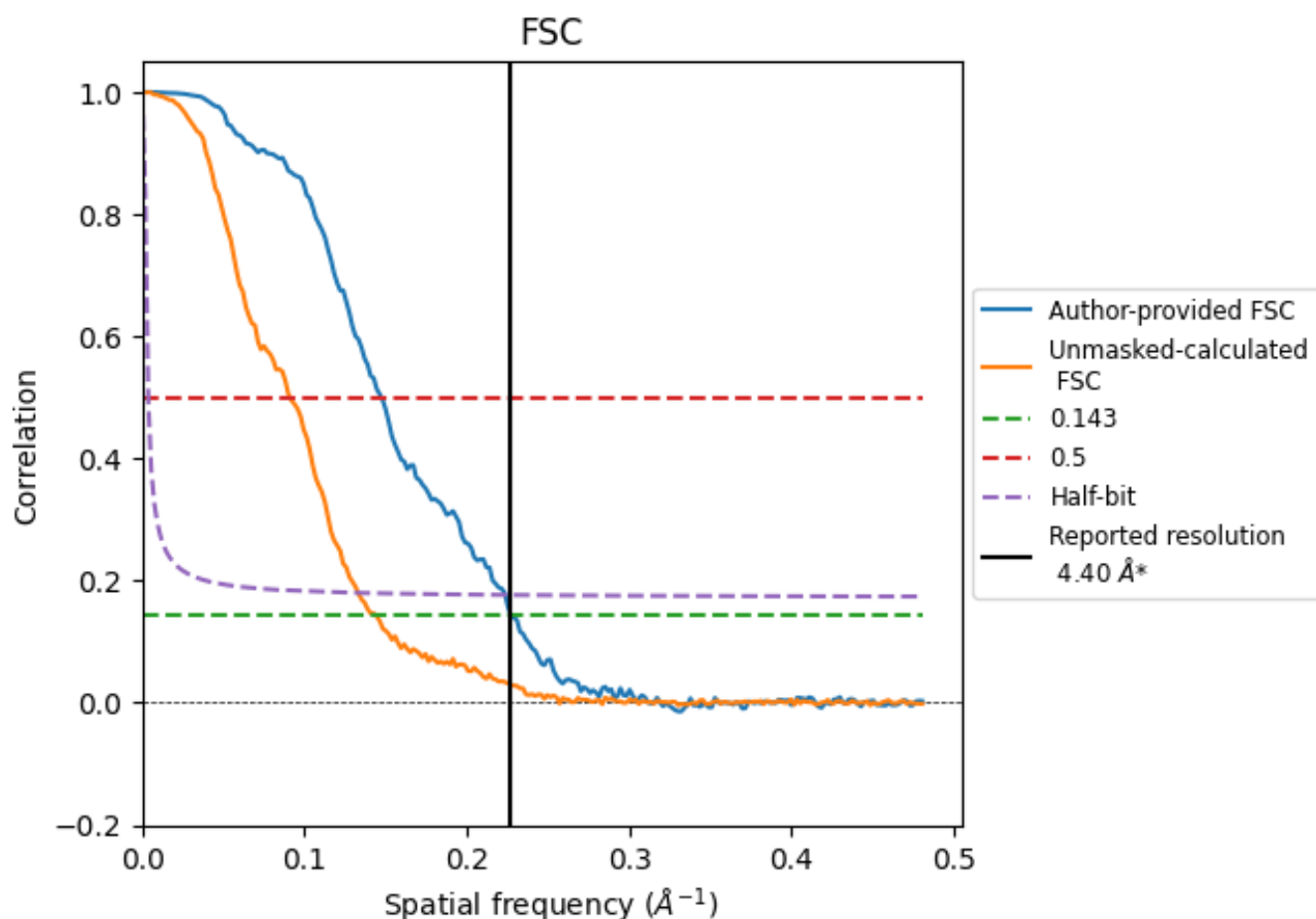


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

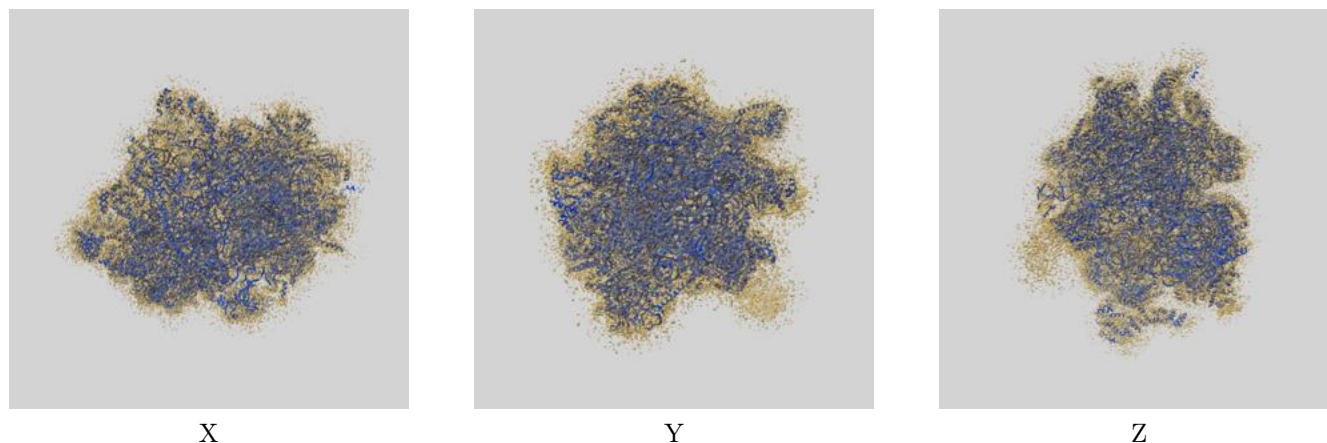
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.79	4.47
Unmasked-calculated*	6.94	10.98	7.51

*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 6.94 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

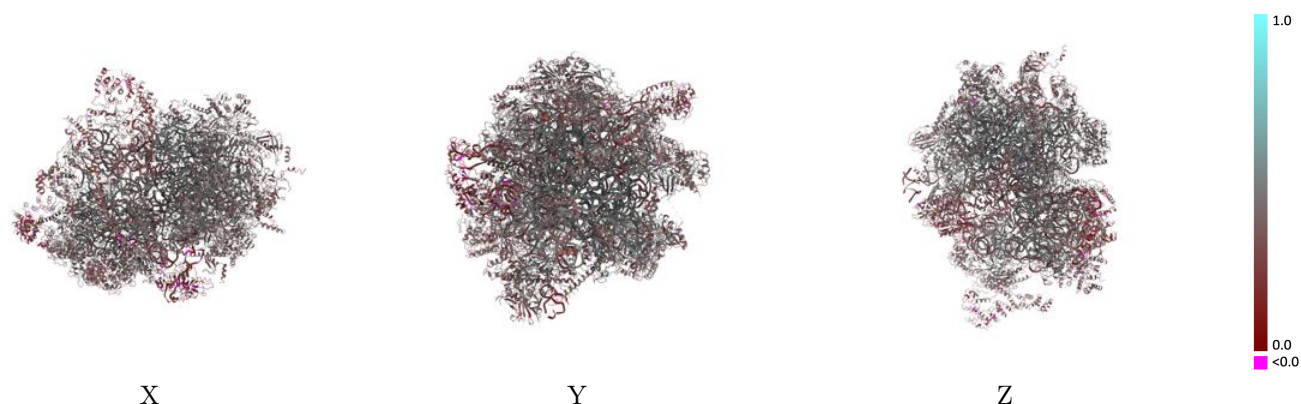
This section contains information regarding the fit between EMDB map EMD-11641 and PDB model 7A5F. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



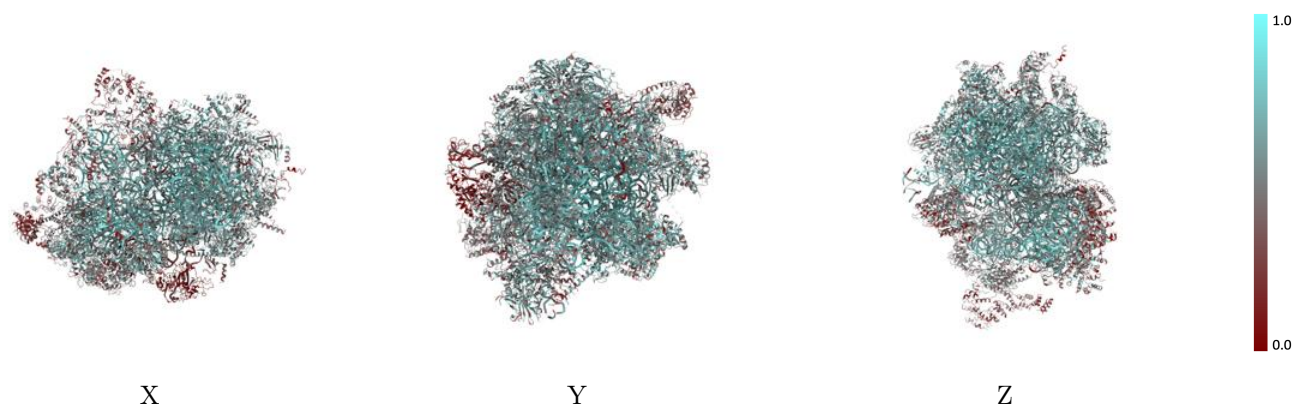
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



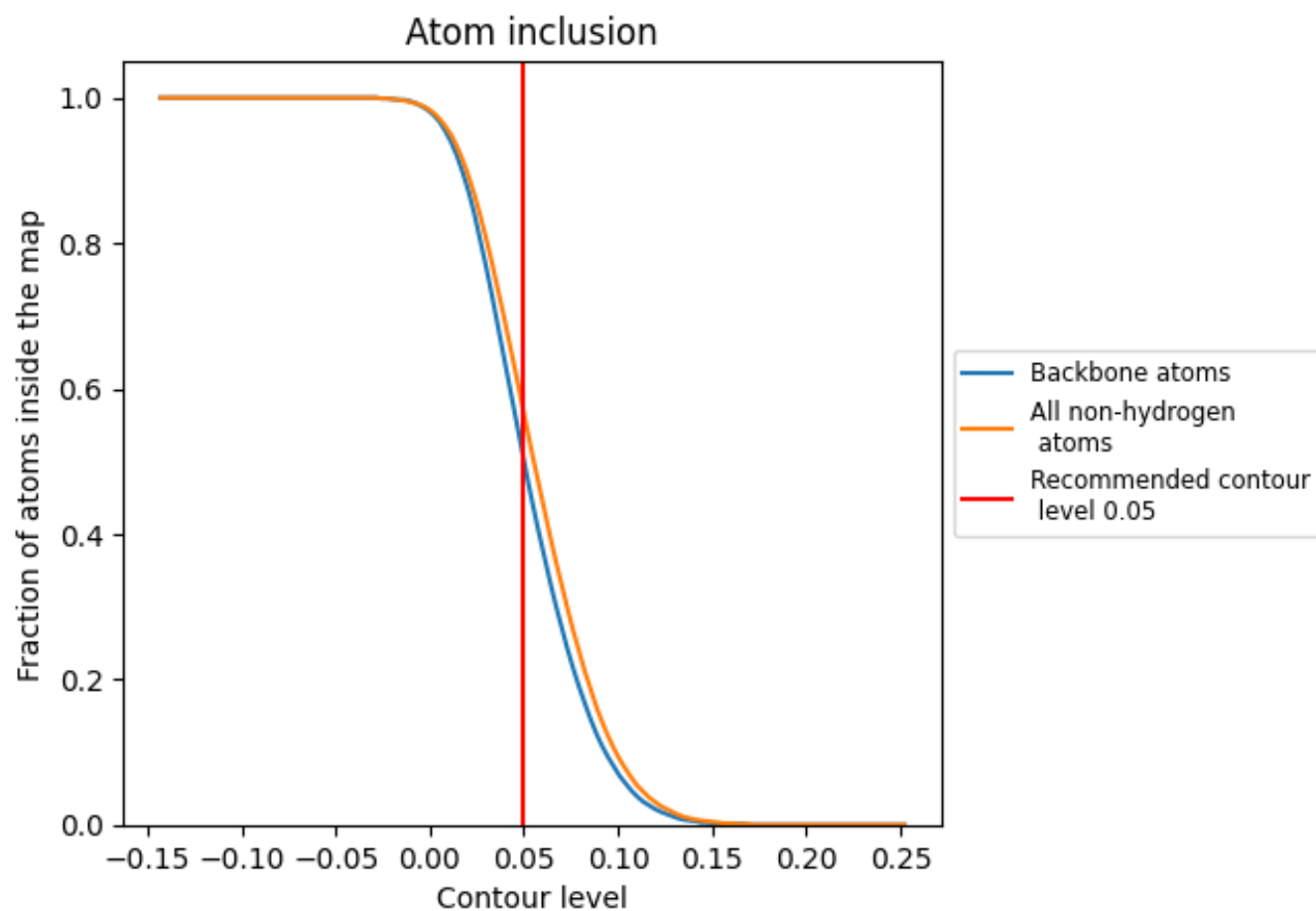
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5660	 0.3960
03	 0.5800	 0.4330
13	 0.5550	 0.4340
23	 0.6500	 0.4880
24	 0.5310	 0.2670
33	 0.6530	 0.4910
43	 0.6290	 0.4690
53	 0.5730	 0.4100
63	 0.5550	 0.3870
73	 0.5180	 0.3870
93	 0.5250	 0.4040
A	 0.3020	 0.2770
A3	 0.7460	 0.4360
A5	 0.0000	 0.1490
A6	 0.7310	 0.4150
B3	 0.6420	 0.3190
B6	 0.5830	 0.4280
C	 0.1490	 0.1190
C6	 0.4840	 0.4320
D	 0.1790	 0.1710
D3	 0.6190	 0.4630
D6	 0.4970	 0.4170
E3	 0.5970	 0.4410
E6	 0.5130	 0.4170
F3	 0.5810	 0.4360
F6	 0.4340	 0.3610
G6	 0.4810	 0.3910
H3	 0.4510	 0.3800
H6	 0.4520	 0.3750
I3	 0.3960	 0.3400
I6	 0.4950	 0.4050
J3	 0.3000	 0.2600
J6	 0.5150	 0.4290
K3	 0.6330	 0.4580
K6	 0.5160	 0.3940



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Chain	Atom inclusion	Q-score
L3	0.4920	0.4330
L6	0.5330	0.4060
M3	0.5850	0.4310
M6	0.4770	0.3710
N3	0.5810	0.4420
N6	0.5430	0.4240
O3	0.6030	0.4440
O6	0.4780	0.3580
P3	0.5770	0.4180
P6	0.5520	0.4210
Q3	0.5230	0.4270
Q6	0.5740	0.4310
R3	0.6380	0.4620
R6	0.4430	0.3440
S3	0.6110	0.4470
S6	0.4570	0.3620
T3	0.5830	0.4560
T6	0.5150	0.4150
U3	0.6380	0.4570
U6	0.4560	0.3390
V3	0.4690	0.3680
V6	0.2860	0.2600
W3	0.6290	0.4860
W6	0.4850	0.3990
X3	0.5250	0.4050
X6	0.4180	0.3240
Y2	0.2210	0.2810
Y3	0.5730	0.4160
Y6	0.3670	0.3290
Z3	0.6320	0.4610
Z6	0.4570	0.3840
a3	0.6060	0.4410
a6	0.3840	0.3250
b3	0.6060	0.4380
b6	0.3810	0.3310
c3	0.5480	0.4080
c6	0.4510	0.4040
d3	0.4930	0.3830
d6	0.5450	0.4390
e3	0.3430	0.3000
e6	0.2790	0.2730
f3	0.4370	0.3440

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Chain	Atom inclusion	Q-score
g3	 0.5690	 0.4180
h3	 0.5020	 0.3590
i3	 0.6230	 0.4580
i4	 0.4520	 0.3320
j3	 0.5600	 0.4200
k3	 0.3350	 0.2690
l3	 0.5870	 0.4110
m3	 0.4820	 0.3720
n	 0.1000	 0.2080
o3	 0.6670	 0.4720
p3	 0.4550	 0.3770
q3	 0.4930	 0.3780
r3	 0.6370	 0.4460
s3	 0.6000	 0.4270
t3	 0.2930	 0.2650